CONTENTS

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CALCULATIONS ON ELECTRONIC SPECTRA OF CATACONDENSED AND PERICONDENSED AROMATIC HYDROCARBONS

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INTRODUCTION

The tables in this volume contain certain basic results of the molecular calculations which form the background for the theoretically computed electronic spectra of 37 hydrocarbons reported in a recent paper by the present authors.[1] They follow the theoretical approach as well as the mathematical method outlined in an earlier paper.[2] In the sequel, reference 2 will be referred to as paper (I) and reference 1 will be referred to as paper (II).

The volume is ordered according to molecules. For each molecule, several calculations are reported differing in the type of approximation. Four approximations are considered, labelled TBX, IRX, TBM, IRM respectively, which are defined and discussed in papers (I) and (II). The results of any one such calculation (i. e. a given molecule in a given approximation) are collected in one section and, within each section, the information is grouped into seven subsections containing the data described below.

The first subsection is a title page. It contains the name of the molecule, the label of the approximation, a molecular skeleton printed to scale as well as indicating the numbering of the atoms, and the coordinates of the atoms. The latter are given, in units of D = 1.395 Å, in the order established by the figure, the x-coordinate being horizontal, the

*This report contains the material referred to as IS-449 and IS-450 in footnotes 6 and 12 of reference 1.

y-coordinate being vertical.

The second to the fifth subsections furnish the results of the effective one-electron approximation which is solved as a preliminary problem. The sixth and seventh subsections present the results of the many-electron problem, which are obtained by a configuration interaction calculation based on the results of the one-electron problem. All energies are given in kK (kilo Kayser = 1000 cm^{-1}). The transition moment unit is eD with e being the absolute value of the electronic charge and D = 1.395Å.

The second subsection is a list of the eigenvalues and eigenvectors of the overlap matrix as defined by Eq. (3.6) on page 1866 of paper (I) for the TBM approximation, and by Eq. (1.18) on page 1880 of paper (I) for the other three cases (TBX, IRM, IRX). For the TBM approximation, the eigenvectors are identical with those of the topological matrix [Eq. (2.2) on page 1864 and Eq. (1.5) on page 1885 of (I)]; for the other three cases they are identical with those of the augmented topological matrix [Eq. (1.2) on page 1878 of (I)]. The eigenvalues are simply related to those of the topological matrix and the augmented topological matrix respectively [See Eqs. (3.5) and (3.7) on page 1866 and Eq. (1.17) and (1.19) on page 1880 of (I). The overlap integral S has been chosen according to Eq. (1.15) on page 1911 of paper (I)]. Each column in the table corresponds to one molecular orbital. The column is headed by a counting number of the orbital and its symmetry (in the case of two symmetry planes, the first symbol corresponds to the long axis, the second symbol to the short axis). Below follows the eigenvalue

of the overlap matrix. The remaining rows contain the atomic components of the eigenvector in the order given in the skeleton on the title page, the sum of squares being normalized to unity.

The third subsection is a list of the eigenvalues and eigenvectors of the neutral framework hamiltonian matrix [see Eq. (2. 9) on page 1864 of (I) for the TBM case, and Eq. (1. 16) on page 1879 of (I) for the other cases. In all cases $\delta\alpha_P$ is set equal zero according to the discussion on page 1866 of (I)]. The eigenvectors differ from those of the previous subsection merely in the normalization, which is now chosen such that the integral of the square of the molecular orbital is unity. Hence the eigenvector components represent the expansion coefficients of the molecular orbitals given in Eq. (3. 4) and (3. 8) on page 1866 and Eq. (1. 20) on page 1880 of (I) respectively. The eigenvalues correspond to the quantities ϵ^{nf} given in Eq. (3. 10) on page 1867 and Eq. (1. 22) on page 1881 of (I) respectively, in conjunction with Eqs. (2. 10, 11) on page 1864, Eqs. (1. 10) - (1. 15) on page 1910, and Eqs. (2. 7) - (2. 10) on page 1912.

The fourth subsection gives the ground state bond orders defined by

$$p(PQ) = \sum_n g_n \; c_{Pn} \; c_{Qn} ,$$

P, Q = atomic labels ,

n = molecular orbital label ,

g_n = occupation number ,

where the c_{Pn} are the coefficients given in the second subsection. They are labelled "topological bond orders" in the TBM and TBX case, and "augmented topological bond orders" in the IRM and IRX case. The topological TBM bond orders are identical with the Coulson bond orders

[see Eq. (1. 16) on page 1886 of (I)].

The fifth subsection gives the ground state bond orders defined by

$$p(PQ) = \sum_n g_n \; c'_{Pn} \; c'_{Qn}$$

where the c'_{Pn} are the coefficients given in the second subsection. They are labelled "density bond orders" in the TBM and TBX case, and "augmented density bond orders" in the IRX and IRM case. The TBM density bond orders are related to the Mulliken bond orders [see Eqs. (1. 17), (1. 18) on page 1886 of (I)].

The sixth subsection contains the results of the configuration interaction calculation. If the molecule has symmetry, the sixth subsection contains the results for the S or SA symmetry, and the seventh subsection contains the results for the A or AS symmetry (in the case of two symmetry planes the first symbol corresponds to the long axis, the second symbol corresponds to the short axis). Within each subsection, the data are presented in two groups, the first group giving information about one-electron excitations before mixing due to configuration interaction, the second group giving explicit information about the final excited states after configuration interaction.

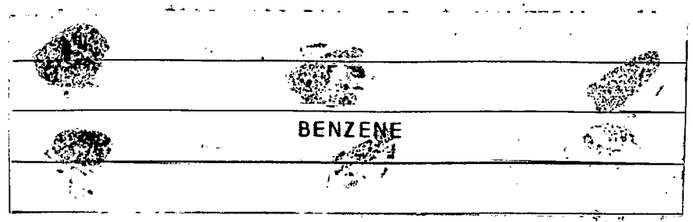
In the first group, the first row indicates the one-electron jumps selected by the program for the configuration interaction treatment [selected were the 15 lowest jumps in the absence of symmetry, and the 10 lowest jumps within one symmetry in the presence of symmetry. Excluded were moreover one-electron excitations in excess of 60, 000 wave numbers]. The labelling by orbital pairs refers to the numbering of orbitals used in subsections two and three. The next two rows give

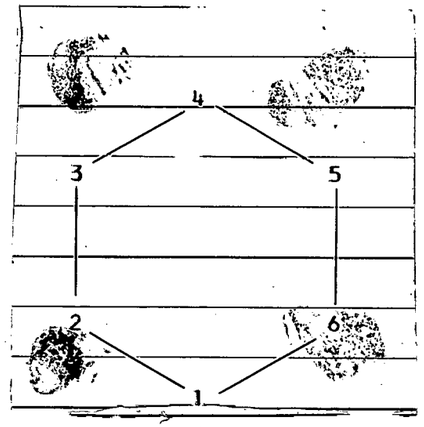
the components of the transition moment vector with respect to the x and y axes. The next row (jump energy) gives the difference in the one-electron orbital energies. The next two rows give the complete diagonal elements of the configuration interaction matrix for the singlets. Of the two, the first one is calculated with joint corrections, i. e. correctly; the second one is calculated without joint corrections in order to determine how important the joint corrections are [see Eq. (3. 9) on page 1867 of (I)]. The last two rows give the transition energies of the final states which correspond most closely to the respective one-electron jumps. Again the first one is calculated with joint corrections and the second without joint-corrections. (In some cases with very strong mixing, the final energies have been interchanged by the computer program with respect to the one-electron jumps. These cases are easy to spot by reference to the second group of data.)

In the second group, the information is given in pairs of lines, the first line giving a singlet, the second one giving a triplet. Going from left to right, the columns furnish transition energy, oscillator strength, x and y component of the transition moment, and composition of the state. The latter is given by the expansion coefficients in terms of the one-electron excitations quoted in the first group of data, assuming the same order as used there.

REFERENCES

1. Richard L. Hummel and Klaus Ruedenberg, "Electronic Spectra of Catacondensed and Pericondensed Aromatic Hydrocarbons", Phys. Chem. 66, 2334-2359 (1962).
2. Klaus Ruedenberg and E. Miller Layton, "Quantum Mechanics of Mobile Electrons in Conjugated Bond Systems. Parts I to VI", J. Chem. Phys. 34, 1861-1913 (1961).





ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	1.7320
y	0.	0.5000	1.5000	2.0000	1.5000	0.5000

BENZENE — TBX & TBM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

	1 SS	2 AS	3 SA	4 AA	5 SS	6 AS
	1.493617	1.246817	1.246800	0.753200	0.753183	0.506383
	0.408253	0.577347	0.000216	-0.000249	-0.577347	-0.408253
	0.408246	0.288866	-0.499892	-0.499875	0.288894	0.408246
	0.408246	-0.288491	-0.500108	0.500124	0.288463	-0.408246
	0.408253	-0.577347	-0.000216	-0.000249	-0.577347	0.408253
	0.408246	-0.288866	0.499892	-0.499875	0.288894	-0.408246
	0.408246	0.288491	0.500108	-0.500124	0.288463	0.408246

BENZENE — TBX & TBM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

	1 SS	2 AS	3 SA	4 AA	5 SS	6 AS
	25.81018	15.46010	15.45925	-25.59031	-25.59264	-76.12920
	0.334049	0.517054	0.000194	-0.000287	-0.665253	-0.573706
	0.334043	0.258699	-0.447690	-0.575979	0.332880	0.573697
	0.334043	-0.258363	-0.447884	0.576266	0.332384	-0.573697
	0.334049	-0.517054	-0.000194	-0.000287	-0.665253	0.573707
	0.334043	-0.258699	0.447690	-0.575979	0.332880	-0.573697
	0.334043	0.258363	0.447884	0.576266	0.332384	0.573697

BENZENE — TBX & TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6
1	1.00000	0.66667	0.00000	-0.33332	0.00000	0.66667
2	0.66667	1.00000	0.66666	0.00000	-0.33334	-0.00000
3	0.00000	0.66666	1.00000	0.66667	-0.	-0.33334
4	-0.33332	0.00000	0.66667	1.00000	0.66667	0.00000
5	0.00000	-0.33334	-0.	0.66667	1.00000	0.66666
6	0.66667	-0.00000	-0.33334	0.00000	0.66666	1.00000

BENZENE — TBX & TBM DENSITY BOND ORDERS

	1	2	3	4	5	6
1	0.75787	0.49052	-0.04418	-0.31151	-0.04418	0.49052
2	0.49052	0.75787	0.49052	-0.04418	-0.31153	-0.04418
3	-0.04418	0.49052	0.75787	0.49052	-0.04418	-0.31153
4	-0.31151	-0.04418	0.49052	0.75787	0.49052	-0.04418
5	-0.04418	-0.31153	-0.04418	0.49052	0.75787	0.49052
6	0.49052	-0.04418	-0.31153	-0.04418	0.49052	0.75787

BENZENE — IRX & IRM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

	1 SS	2 AS	3 SA	4 SS	5 AA	6 AS
	1.578467	1.196670	1.196646	0.733948	0.733935	0.560333
	0.408250	0.577346	-0.000546	0.000367	-0.577349	-0.408254
	0.408247	0.288206	-0.500273	-0.500184	0.288358	0.408245
	0.408247	-0.289152	-0.499727	0.499816	0.288995	-0.408245
	0.408250	-0.577346	-0.000546	-0.000367	-0.577349	0.408254
	0.408247	-0.288206	0.500273	-0.500184	0.288358	-0.408245
	0.408247	0.289152	0.499727	-0.499816	0.288995	0.408245

BENZENE — IRX & IRM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

	1 SS	2 AS	3 SA	4 SS	5 AA	6 AS
	28.62091	12.83523	12.83394	-28.31014	-28.31205	-61.27982
	0.324944	0.527775	0.000000	0.673916	-0.000000	-0.545391
	0.324942	0.263894	-0.457075	-0.336961	-0.583635	0.545378
	0.324942	-0.263894	-0.457075	-0.336960	0.583635	-0.545378
	0.324944	-0.527775	0.000000	0.673916	-0.000000	0.545391
	0.324942	-0.263894	0.457075	-0.336961	-0.583635	-0.545378
	0.324942	0.263894	0.457075	-0.336961	0.583635	0.545378

BENZENE — IRX & IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6
1	0.99999	0.66667	-0.00000	-0.33332	-0.00000	0.66667
2	0.66667	1.00000	0.66666	-0.00000	-0.33334	0.00000
3	-0.00000	0.66666	1.00000	0.66667	0.00000	-0.33334
4	-0.33332	-0.00000	0.66667	0.99999	0.66667	-0.00000
5	-0.00000	-0.33334	0.00000	0.66667	1.00000	0.66666
6	0.66667	0.00000	-0.33334	0.00000	0.66666	1.00000

BENZENE — IRX & IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6
1	0.76827	0.48973	-0.06738	-0.34592	-0.06738	0.48973
2	0.48973	0.76829	0.48973	-0.06738	-0.34594	-0.06738
3	-0.06738	0.48973	0.76829	0.48973	-0.06738	-0.34594
4	-0.34592	-0.06738	0.48973	0.76827	0.48973	-0.06738
5	-0.06738	-0.34594	-0.06738	0.48973	0.76829	0.48973
6	0.48973	-0.06738	-0.34594	-0.06738	0.48973	0.76829

ENERGIES FOR BENZENE , TBX APPROXIMATION 1.7
ONE ELECTRON EXCITATIONS OF any SYMMETRY
JUMP 3, 4 2, 4 3, 5 2, 5 1, 4 1, 5
XMOMNT 0.00042 0.51595 0.51595-0.00042-0.00000 0.
YMOMNT-0.51596 0.00042 0.00042 0.51595-0.00000-0.00000
JUMP E 41.0496 41.0504 41.0519 41.0527 51.4005 51.4028
DIAG E 52.3910 48.1793 48.1806 52.3941 61.7888 61.7913
DIAG E 52.3910 48.1793 48.1806 52.3941 61.7888 61.7913
CORRSP 48.6594 40.2334 56.1264 56.1257 61.7888 61.7913
CORRSP 48.6594 40.2334 56.1264 56.1257 61.7888 61.7913

FINAL EXCITED STATES

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION						SYMMETRY
48.65939	0.00000	0.00000	-0.00016	//	0.7073	0.0000	-0.0000	0.7070	-0.	-0.	AS
30.04272				//	0.7073	0.0000	-0.0000	0.7069	-0.0000	-0.0000	
40.23344	0.00000	0.00003	-0.00000	//	-0.0000	0.7071	-0.7071	-0.0000	-0.0000	0.0000	SA
35.13796				//	0.0004	0.7072	0.7070	-0.0004	-0.0000	0.0000	
56.12640	1.27076	0.72967	0.00059	//	0.0000	0.7071	0.7071	0.0000	0.	0.	SA
40.23344				//	0.0000	-0.7070	0.7072	0.0000	0.0000	0.0000	
56.12567	1.27076	-0.00059	0.72967	//	-0.7070	0.0000	-0.0000	0.7073	0.	0.	AS
35.13820				//	-0.7069	0.0004	0.0004	0.7073	0.0000	0.0000	
61.78878	0.00000	-0.00000	-0.00000	//	-0.0000	0.0000	-0.0000	-0.0000	1.0000	-0.0002	AA
50.35669				//	0.0000	0.0000	-0.0000	-0.0000	1.0000	-0.0004	
61.79131	0.00000	-0.00000	-0.00000	//	0.	0.	0.	0.	0.0002	1.0000	SS
50.35887				//	-0.0000	-0.0000	-0.0000	-0.0000	-0.0004	1.0000	

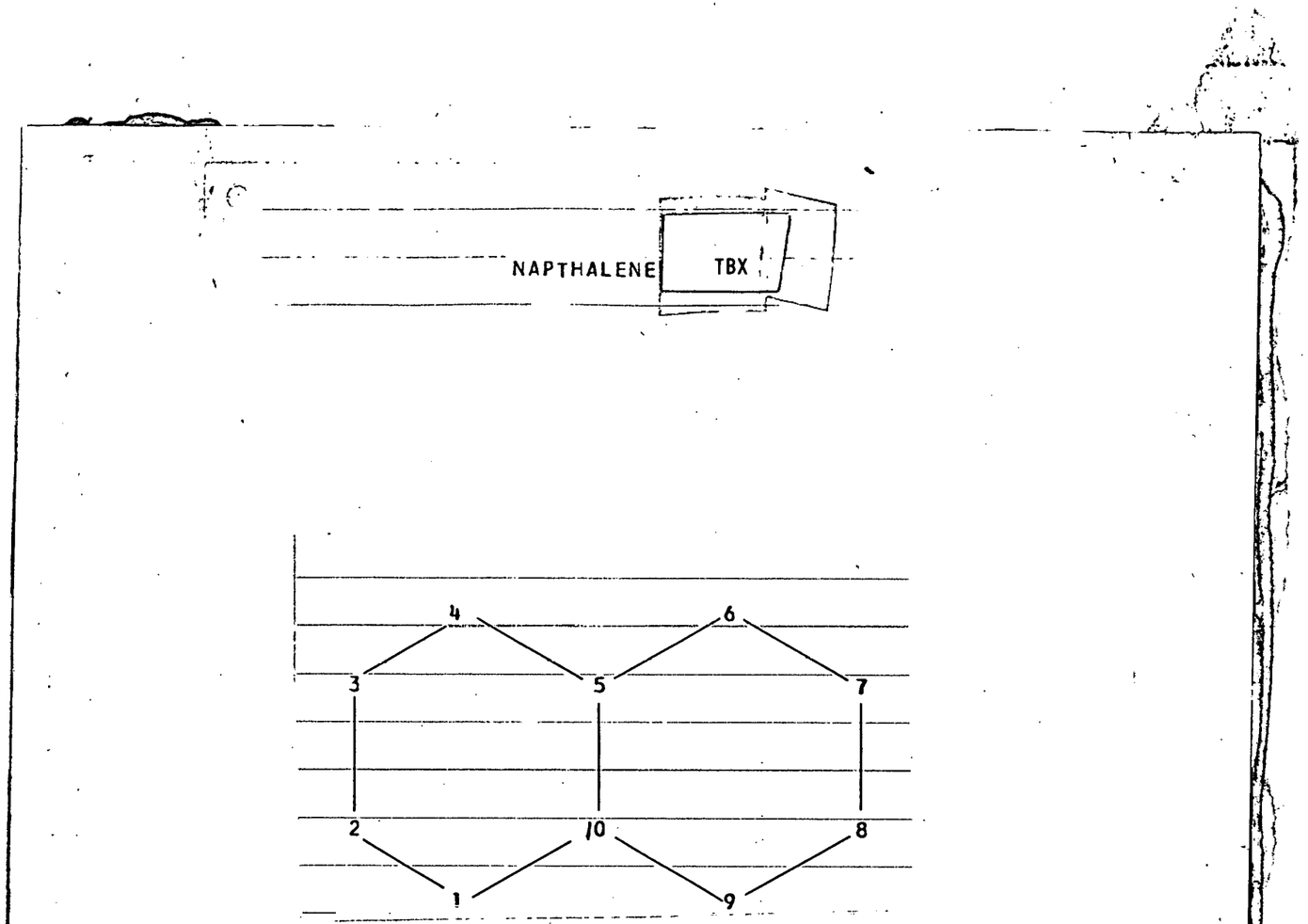
ENERGIES FOR BENZENE IRX APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF any SYMMETRY

JUMP	3, 4	2, 4	3, 5	2, 5	1, 4	1, 5
XMOMNT	-0.00081	0.51500	0.51500	0.00081	-0.00000	0.00000
YMOMNT	-0.51501	-0.00081	-0.00081	0.51500	0.00000	-0.00000
JUMP E	41.1441	41.1454	41.1460	41.1473	56.9310	56.9330
DIAG E	52.3187	48.1419	48.1420	52.3219	67.6826	67.6846
DIAG E	52.3187	48.1419	48.1420	52.3219	67.6826	67.6846
CORRSP	48.5915	40.2341	56.0498	56.0491	67.6826	67.6046
CORRSP	48.5915	40.2341	56.0498	56.0491	67.6826	67.6846

FINAL EXCITED STATES

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION						SYMMETRY
48.59154	0.00000	-0.00000	-0.00016	//	0.7073	0.0002	-0.0002	0.7070	0.0000	-0.0000	AS
30.04341				//	0.7073	0.0002	-0.0002	0.7069	0.0000	0.0000	
40.23413	0.00000	0.00001	-0.00000	//	-0.0002	0.7071	-0.7071	-0.0002	0.0000	-0.0000	SA
35.13866				//	-0.0025	0.7071	0.7071	0.0025	0.0000	0.0000	
56.04977	1.26435	0.72832	0.00017	//	-0.0013	0.7071	0.7071	0.0013	-0.0000	-0.0000	SA
40.23412				//	0.0002	-0.7071	0.7071	0.0002	0.0000	0.0000	
56.04913	1.26435	-0.00017	0.72833	//	-0.7070	-0.0013	-0.0013	0.7073	-0.0000	0.0000	AS
35.13887				//	-0.7069	-0.0025	-0.0025	0.7073	0.0000	0.0000	
67.68264	0.00000	-0.00000	0.00000	//	-0.0000	-0.0000	0.0000	0.0000	1.0000	-0.0001	AA
55.92357				//	-0.0000	-0.0000	-0.0000	-0.0000	1.0000	-0.0003	
67.68462	0.00000	0.00000	-0.00000	//	0.0000	0.0000	-0.0000	-0.0000	0.0001	1.0000	SS
55.92534				//	-0.0000	-0.0000	-0.0000	-0.0000	0.0003	1.0000	



ATOMIC COORDINATES

x	0.8446	0.	0.	0.8446	1.7376	2.6306	3.4752	3.4752	2.6306	1.7376
y	0.	0.5000	1.5160	2.0160	1.5190	2.0160	1.5160	0.5000	0.	0.4970

NAPTHALENE X TBX APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 A A	10 A S
1.553833	1.402598	1.318218	1.236433	1.164901	0.835098	0.763566	0.681781	0.597401	0.446166
0.302034	0.269525	-0.398462	0.001932	0.421136	0.421136	0.001932	0.398462	0.269525	-0.302034
0.246166	0.421137	-0.184683	-0.394074	0.269525	-0.269525	0.394074	-0.184683	-0.421137	0.246166
0.246166	0.421137	0.184683	-0.394074	-0.269525	-0.269525	-0.394074	-0.184683	0.421137	-0.246166
0.302034	0.269525	0.398462	0.001932	-0.421136	0.421136	-0.001932	0.398462	-0.269525	0.302034
0.443120	0.000000	0.337995	0.435206	0.000000	-0.000000	0.435206	-0.337995	0.000000	-0.443120
0.302034	-0.269525	0.398462	0.001932	0.421137	-0.421137	-0.001932	0.398462	0.269525	0.302034
0.246167	-0.421136	0.184683	-0.394074	0.269525	0.269526	-0.394074	-0.184683	-0.421136	-0.246167
0.246167	-0.421136	-0.184683	-0.394074	-0.269525	0.269525	0.394074	-0.184683	0.421136	0.246167
0.302034	-0.269525	-0.398462	0.001932	-0.421137	0.421137	0.001932	0.398462	-0.269525	-0.302034
0.443120	-0.000000	-0.337995	0.435206	-0.000000	0.000000	-0.435206	-0.337995	0.000000	-0.443120

NAPTHALENE X TBX APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 A A	10 A S
27.2569	21.9503	18.4603	14.6231	10.8252	-15.1005	-23.6790	-35.6930	-51.5358	-94.9261
0.242300	0.227580	-0.347051	0.001738	0.390192	0.460844	0.002211	0.482574	0.348712	-0.452176
0.197482	0.355596	-0.160855	-0.354399	0.249721	-0.294938	0.450977	-0.223669	-0.544866	0.368537
0.197482	0.355596	0.160855	-0.354399	-0.249721	-0.294938	-0.450977	-0.223668	0.544866	-0.368537
0.242300	0.227580	0.347051	0.001738	-0.390192	0.460844	-0.002211	0.482574	-0.348712	0.452176
0.355483	0.000000	0.294386	0.391390	0.000000	-0.000000	0.498048	-0.409344	0.000000	-0.663396
0.242300	-0.227579	0.347051	0.001738	0.390192	-0.460844	-0.002211	0.482574	0.348712	0.452176
0.197482	-0.355595	0.160855	-0.354399	0.249721	0.294938	-0.450977	-0.223668	-0.544866	-0.368537
0.197482	-0.355595	-0.160855	-0.354399	-0.249721	0.294938	0.450977	-0.223668	0.544866	0.368537
0.242300	-0.227580	-0.347051	0.001738	-0.390192	-0.460844	0.002211	0.482574	-0.348712	-0.452176
0.355483	-0.000000	-0.294386	0.391390	-0.000000	0.000000	-0.498048	-0.409344	0.000000	0.663396

NAPTHALENE X TBX TOPOLOGICAL BOND ORDERS BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	1.00000	0.74838	-0.00000	-0.34451	0.00000	0.07434	-0.00000	-0.15967	0.00000	0.53871
2	0.74838	1.00000	0.57299	-0.00000	-0.24969	0.00000	0.15414	0.00000	-0.15967	-0.00000
3	-0.00000	0.57299	1.00000	0.74838	-0.00000	-0.15967	0.00000	0.15414	0.00000	-0.24969
4	-0.34451	-0.00000	0.74838	1.00000	0.53871	-0.00000	-0.15967	-0.00000	0.07434	0.00000
5	0.00000	-0.24969	-0.00000	0.53871	1.00000	0.53871	0.00000	-0.24969	-0.00000	0.54304
6	0.07434	0.00000	-0.15967	-0.00000	0.53871	1.00000	0.74838	0.00000	-0.34451	-0.00000
7	-0.00000	0.15414	0.00000	-0.15967	0.00000	0.74838	1.00000	0.57299	0.00000	-0.24969
8	-0.15967	0.00000	0.15414	-0.00000	-0.24969	0.00000	0.57299	1.00000	0.74838	0.00000
9	0.00000	-0.15967	0.00000	0.07434	-0.00000	-0.34451	0.00000	0.74838	1.00000	0.53871
10	0.53871	-0.00000	-0.24969	0.00000	0.54304	-0.00000	-0.24969	0.00000	0.53871	1.00000

NAPTHALENE X TBX DENSITY BOND ORDERS BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	0.76640	0.56285	-0.05021	-0.32438	-0.03071	0.07745	0.01584	-0.15061	-0.04977	0.37796
2	0.56285	0.75856	0.40562	-0.05021	-0.23172	0.01584	0.14927	0.00333	-0.15061	-0.04231
3	-0.05021	0.40562	0.75856	0.56285	-0.04231	-0.15061	0.00333	0.14927	0.01584	-0.23172
4	-0.32438	-0.05021	0.56285	0.76640	0.37796	-0.04977	-0.15061	0.01584	0.07745	-0.03071
5	-0.03071	-0.23172	-0.04231	0.37796	0.73243	0.37796	-0.04231	-0.23172	-0.03071	0.38578
6	0.07745	0.01584	-0.15061	-0.04977	0.37796	0.76640	0.56285	-0.05021	-0.32438	-0.03071
7	0.01584	0.14927	0.00333	-0.15061	-0.04231	0.56285	0.75856	0.40562	-0.05021	-0.23172
8	-0.15061	0.00333	0.14927	0.01584	-0.23172	-0.05021	0.40562	0.75856	0.56285	-0.04231
9	-0.04977	-0.15061	0.01584	0.07745	-0.03071	-0.32438	-0.05021	0.56285	0.76640	0.37796
10	0.37796	-0.04231	-0.23172	-0.03071	0.38578	-0.03071	-0.23172	-0.04231	0.37796	0.73243

ENERGIES FOR NAPTHALENE X TBXAPPROXIMATION

CNE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	4, 6	5, 7	1, 6	2, 8
XMOMNT	-0.75544	-0.75772	0.00713	0.16728
YMOMNT	-0.00000	0.00000	-0.00000	0.00000
JUMP E	29.7236	34.5043	42.3574	57.6433
DIAG E	39.0313	43.2078	53.5654	71.6790
DIAG E	39.8021	42.3934	54.2949	71.3090
CORRSP	33.0037	47.7893	53.9980	72.6926
CORRSP	33.2873	47.7578	54.4099	72.3444

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
33.00369	0.04996	-0.18868	-0.00000	//	0.8027	-0.5741	0.1193	-0.1085
28.86427				//	0.9493	0.2605	0.0115	-0.1757
47.78926	2.00174	-0.99247	0.00000	//	0.5253	0.7938	0.3057	0.0219
34.90895				//	-0.2600	0.9552	-0.1415	0.0024
53.99798	0.32320	0.37517	-0.00000	//	-0.2550	-0.1948	0.9319	0.1691
45.28856				//	0.0115	0.1405	0.9327	0.3320
72.69259	0.03563	0.10735	0.00000	//	0.1212	-0.0477	-0.1546	0.9794
70.70167				//	0.1765	-0.0034	-0.3316	0.9268

ENERGIES FOR NAPTHALENE X TBXAPPROXIMATION

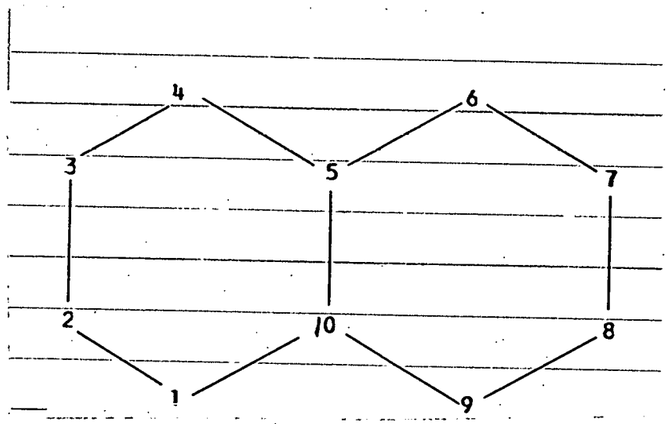
CNE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	5, 6	4, 7	1, 7	3, 8
XMOMNT	0.00000	-0.00000	-0.	0.00000
YMOMNT	-0.57536	0.52397	-0.00253	0.47901
JUMP E	25.9258	38.3021	50.9360	54.1533
DIAG E	37.5710	48.7047	62.3134	67.1633
DIAG E	37.7071	48.5250	62.0924	67.1228
CORRSP	35.9916	49.5038	62.6163	67.6408
CORRSP	36.1186	49.4538	62.2779	67.5969

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
35.99156	0.20094	0.00000	-0.36233	//	0.9448	0.3177	0.0734	0.0313
21.25297				//	0.9559	0.1407	-0.0162	-0.2573
49.50380	0.74221	-0.00000	0.59377	//	-0.3160	0.9293	0.1109	-0.1559
34.25464				//	-0.1495	0.9747	0.1632	-0.0328
62.61627	0.00251	0.00000	-0.03070	//	-0.0362	-0.1248	0.9909	0.0342
54.83419				//	-0.0427	-0.1733	0.9332	-0.3120
67.64076	1.00746	0.00000	0.59182	//	-0.0786	0.1411	-0.0192	0.9867
59.36684				//	0.2492	0.0154	0.3199	0.9140

NAPTHALENE IRX



ATOMIC COORDINATES

x	0.8446	0.	0.	0.8446	1.7376	2.6306	3.4752	3.4752	2.6306	1.7376
y	0.	0.5000	1.5160	2.0160	1.5190	2.0160	1.5160	0.5000	0.	0.4970

NAPTHALENE X — IRX APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 A A	10 A S
1.667441	1.429567	1.283046	1.169252	1.102361	0.793260	0.737084	0.679628	0.615667	0.522688
0.303511	0.274563	-0.402253	-0.018371	-0.417944	0.417870	0.007860	0.396918	0.274449	-0.296868
0.255255	0.417870	-0.184717	0.391787	-0.274450	-0.274563	-0.397994	-0.177053	-0.417944	0.239751
0.255255	0.417870	0.184717	0.391787	0.274449	-0.274563	0.397994	-0.177053	0.417944	-0.239751
0.303511	0.274562	0.402253	-0.018370	0.417944	0.417870	-0.007860	0.396917	-0.274450	0.296868
0.430641	-0.000000	0.328853	-0.438555	0.000000	-0.000000	-0.427876	-0.349596	0.000000	-0.456921
0.303511	-0.274563	0.402253	-0.018371	-0.417944	-0.417870	-0.007860	0.396918	0.274449	0.296868
0.255255	-0.417870	0.184717	0.391787	-0.274450	0.274563	0.397994	-0.177053	-0.417944	-0.239751
0.255255	-0.417870	-0.184717	0.391787	0.274449	0.274563	-0.397994	-0.177053	0.417944	0.239751
0.303511	-0.274563	-0.402253	-0.018370	0.417944	-0.417870	0.007860	0.396917	-0.274450	-0.296868
0.430641	0.000000	-0.328853	-0.438555	0.000000	-0.000000	0.427876	-0.349596	-0.000000	0.456921

NAPTHALENE X — IRX APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 A A	10 A S
30.6101	22.9789	16.8701	11.0695	7.1009	-19.9302	-27.2774	-36.0483	-47.7380	-69.8332
0.235044	0.229636	-0.355122	-0.016989	-0.398067	0.469173	0.009156	0.481465	0.349776	-0.410622
0.197674	0.349493	-0.163074	0.362323	-0.261397	-0.308272	-0.463573	-0.214767	-0.532654	0.331619
0.197674	0.349493	0.163074	0.362323	0.261397	-0.308272	0.463573	-0.214767	0.532654	-0.331619
0.235044	0.229635	0.355123	-0.016989	0.398067	0.469173	-0.009155	0.481465	-0.349776	0.410622
0.333496	-0.000000	0.290323	-0.405574	0.000000	-0.000000	-0.498379	-0.424063	0.000000	-0.632005
0.235044	-0.229636	0.355122	-0.016989	-0.398067	-0.469173	-0.009155	0.481465	0.349776	0.410622
0.197674	-0.349493	0.163074	0.362323	-0.261397	0.308272	0.463573	-0.214767	-0.532654	-0.331619
0.197674	-0.349493	-0.163074	0.362323	0.261397	0.308272	-0.463573	-0.214767	0.532654	0.331619
0.235044	-0.229635	-0.355122	-0.016988	0.398067	-0.469173	0.009155	0.481465	-0.349776	-0.410622
0.333496	0.000000	-0.290323	-0.405574	0.000000	-0.000000	0.498379	-0.424063	-0.000000	0.632005

NAPTHALENE X — IRX AUGMENTED TOPOLOGICAL BOND ORDERS — BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	1.00865	0.74803	-0.00800	-0.33729	0.01296	0.05988	-0.00811	-0.16972	0.00840	0.54209
2	0.74803	1.00542	0.56765	-0.00800	-0.24528	-0.00811	0.17048	0.00567	-0.16972	-0.00230
3	-0.00800	0.56765	1.00542	0.74803	-0.00230	-0.16972	0.00567	0.17048	-0.00811	-0.24528
4	-0.33729	-0.00800	0.74803	1.00865	0.54209	0.00840	-0.16972	-0.00811	0.05988	0.01296
5	0.01296	-0.24528	-0.00230	0.54209	0.97185	0.54209	-0.00230	-0.24528	0.01296	0.53928
6	0.05988	-0.00811	-0.16972	0.00840	0.54209	1.00865	0.74803	-0.00800	-0.33729	0.01296
7	-0.00811	0.17048	0.00567	-0.16972	-0.00230	0.74803	1.00542	0.56765	-0.00800	-0.24528
8	-0.16972	0.00567	0.17048	-0.00811	-0.24528	-0.00800	0.56765	1.00542	0.74803	-0.00230
9	0.00840	-0.16972	-0.00811	0.05988	0.01296	-0.33729	-0.00800	0.74803	1.00865	0.54209
10	0.54209	-0.00230	-0.24528	0.01296	0.53928	0.01296	-0.24528	-0.00230	0.54209	0.97185

NAPTHALENE X — IRX AUGMENTED DENSITY BOND ORDERS — DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	0.78567	0.56505	-0.08280	-0.35261	-0.03565	0.07029	0.01239	-0.17218	-0.05909	0.37675
2	0.56505	0.77484	0.39515	-0.08280	-0.25674	0.01239	0.17989	0.01294	-0.17218	-0.06736
3	-0.08280	0.39515	0.77484	0.56506	-0.06736	-0.17218	0.01294	0.17989	0.01239	-0.25674
4	-0.35261	-0.08280	0.56506	0.78567	0.37675	-0.05909	-0.17218	0.01239	0.07029	-0.03565
5	-0.03565	-0.25674	-0.06736	0.37675	0.71999	0.37675	-0.06736	-0.25674	-0.03565	0.38284
6	0.07029	0.01239	-0.17218	-0.05909	0.37675	0.78567	0.56506	-0.08280	-0.35261	-0.03565
7	0.01239	0.17989	0.01294	-0.17218	-0.06736	0.56506	0.77484	0.39515	-0.08280	-0.25674
8	-0.17218	0.01294	0.17989	0.01239	-0.25674	-0.08280	0.39515	0.77484	0.56506	-0.06736
9	-0.05909	-0.17218	0.01239	0.07029	-0.03565	-0.35261	-0.08280	0.56506	0.78567	0.37675
10	0.37675	-0.06736	-0.25674	-0.03565	0.38284	-0.03565	-0.25674	-0.06736	0.37675	0.71999

ENERGIES FOR NAPTHALENE X IRXAPPROXIMATION
ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	4, 6	5, 7	1, 6	2, 8
XMOMNT	0.78970	-0.76264	0.03646	0.13369
YMOMNT	0.00000	-0.00000	-0.00000	-0.00000
JUMP E	30.9997	34.3782	50.5402	59.0271
DIAG E	40.5041	43.0109	62.2920	72.7809
DIAG E	41.3269	42.1945	63.0036	72.3689
CORRSP	33.6853	48.8571	62.0394	74.0058
CORRSP	33.8482	48.8317	62.5673	73.6466

FINAL EXCITED STATES OF SA SYMMETRY

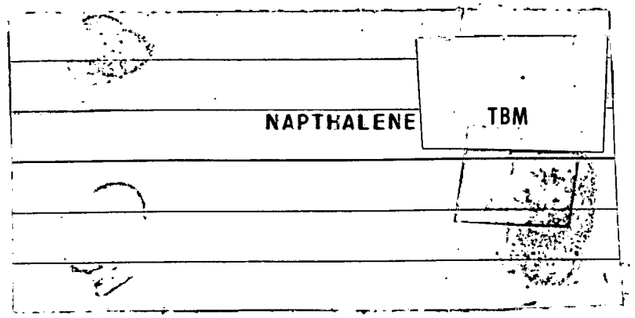
ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
33.68535	0.02853	0.14113	0.00000	//	0.7687	0.6269	-0.0648	0.1091
29.66455				//	0.9255	-0.3393	0.0157	0.1677
48.85714	2.39621	-1.07393	-0.00000	//	-0.6153	0.7739	0.1480	-0.0241
34.75362				//	0.3399	0.9364	-0.0836	0.0268
62.03942	0.13114	0.22295	0.00000	//	0.1146	-0.0845	0.9585	0.2470
52.55290				//	-0.0605	0.0896	0.8956	0.4314
74.00583	0.00474	0.03881	-0.00000	//	-0.1320	-0.0300	-0.2349	0.9625
72.80190				//	-0.1560	-0.0077	-0.4366	0.8860

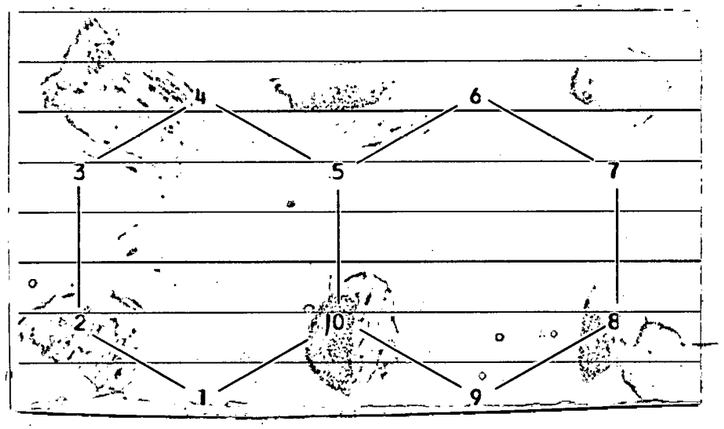
ENERGIES FOR NAPTHALENE X IRXAPPROXIMATION
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	5, 6	4, 7	3, 8	1, 7
XMOMNT	-0.00000	-0.00000	0.00000	0.00000
YMOMNT	0.55853	0.52282	0.48321	0.00921
JUMP E	27.0310	38.3469	52.9183	57.8874
DIAG E	38.0255	48.3505	65.9868	69.8624
DIAG E	38.1673	48.2151	65.8811	69.6157
CORRSP	36.5335	49.1707	66.4911	70.0299
CORRSP	36.6639	49.1063	66.3883	69.7207

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
36.53354	0.18634	-0.00000	0.34632	//	0.9450	-0.3210	-0.0293	0.0557
21.97748				//	0.9502	-0.1562	0.2690	-0.0204
49.17066	0.70999	-0.00000	0.58271	//	0.3149	0.9328	-0.1664	-0.0543
34.35509				//	0.1658	0.9813	-0.0229	-0.0948
66.49108	1.01257	-0.00000	0.59842	//	0.0818	0.1468	0.9855	-0.0234
57.38111				//	-0.2435	0.0879	0.9307	0.2586
70.02993	0.00380	0.00000	0.03572	//	-0.0337	0.0723	0.0157	0.9967
62.81580				//	0.1021	0.0699	-0.2469	0.9611





ATOMIC COORDINATES DINATES

x	0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640	3.4640	2.5980	1.7320
y	0	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	0.5000	0.	0.5000

NAPTHALENE — TBM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 A A	10 A A
1.568345	1.399341	1.321545	1.246799	1.152542	0.847457	0.753200	0.678454	0.600658	0.431654
0.300554	0.262870	-0.399584	-0.000000	-0.425323	0.425323	0.000000	-0.399584	-0.262870	-0.300554
0.230700	0.425323	-0.173525	0.408248	-0.262870	-0.262870	-0.408248	0.173525	0.425323	0.230700
0.230700	0.425323	0.173525	0.408248	0.262870	-0.262870	0.408248	0.173525	-0.425323	-0.230700
0.300554	0.262870	0.399584	0.000000	0.425323	0.425323	-0.000000	-0.399584	0.262870	0.300554
0.461399	-0.000000	0.347050	-0.408248	0.000000	-0.000000	-0.408248	0.347050	-0.000000	-0.461399
0.300554	-0.262870	0.399583	-0.000000	-0.425323	-0.425323	0.000000	-0.399584	-0.262870	0.300554
0.230700	-0.425323	0.173525	0.408248	-0.262870	0.262870	0.408248	0.173525	0.425323	-0.230700
0.230700	-0.425323	-0.173525	0.408248	0.262870	0.262870	-0.408248	0.173525	-0.425323	0.230700
0.300554	-0.262870	-0.399584	0.000000	0.425323	-0.425323	0.000000	-0.399584	0.262870	-0.300554
0.461399	0.000000	-0.347050	-0.408248	0.000000	0.000000	0.408248	0.347050	0.000000	0.461399

NAPTHALENE — TBM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 A A	10 A A
27.7123	21.8234	18.6064	15.1373	10.1212	-13.7650	-25.0575	-36.2431	-50.8417	-100.6884
0.239995	0.222218	-0.347589	-0.000000	-0.396178	0.462019	0.000000	-0.485118	-0.339178	-0.457462
0.184216	0.359548	-0.150946	0.365617	-0.244857	-0.285550	-0.470402	0.210670	0.548788	0.351139
0.184216	0.359548	0.150946	0.365617	0.244857	-0.285550	0.470402	0.210670	-0.548789	-0.351139
0.239995	0.222218	0.347589	0.000000	0.396178	0.462019	-0.000000	-0.485118	0.339178	0.457462
0.368431	-0.000000	0.301892	-0.365617	0.000000	-0.000000	-0.470402	0.421339	-0.000000	-0.702278
0.239995	-0.222218	0.347589	-0.000000	-0.396178	-0.462019	0.000000	-0.485118	-0.339178	0.457462
0.184216	-0.359548	0.150946	0.365617	-0.244857	0.285550	0.470402	0.210670	0.548788	-0.351139
0.184215	-0.359548	-0.150946	0.365617	0.244857	0.285550	-0.470402	0.210670	-0.548788	0.351139
0.239995	-0.222218	-0.347590	0.000000	0.396178	-0.462019	0.000000	-0.485118	0.339178	-0.457462
0.368431	0.000000	-0.301892	-0.365617	0.000000	0.000000	0.470402	0.421340	0.000000	0.702278

NAPTHALENE M — TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	1.00000	0.72457	-0.00000	-0.36227	0.00000	0.08493	-0.00000	-0.16987	-0.00000	0.55470
2	0.72457	1.00000	0.60315	0.00000	-0.24089	0.00000	0.15596	0.00000	-0.16987	-0.00000
3	-0.00000	0.60315	1.00000	0.72457	-0.00000	-0.16987	0.00000	0.15596	-0.00000	-0.24089
4	-0.36227	0.00000	0.72457	1.00000	0.55470	-0.00000	-0.16987	-0.00000	0.08493	0.00000
5	0.00000	-0.24089	-0.00000	0.55470	1.00000	0.55470	0.00000	-0.24089	-0.00000	0.51822
6	0.08493	0.00000	-0.16987	-0.00000	0.55470	1.00000	0.72457	-0.00000	-0.36227	-0.00000
7	-0.00000	0.15596	0.00000	-0.16987	0.00000	0.72457	1.00000	0.60315	0.00000	-0.24089
8	-0.16987	0.00000	0.15596	-0.00000	-0.24089	-0.00000	0.60315	1.00000	0.72457	-0.00000
9	-0.00000	-0.16987	-0.00000	0.08493	-0.00000	-0.36227	0.00000	0.72457	1.00000	0.55470
10	0.55470	-0.00000	-0.24089	0.00000	0.51822	-0.00000	-0.24089	-0.00000	0.55470	1.00000

NAPTHALENE M — TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	0.76951	0.54717	-0.05073	-0.34159	-0.03303	0.08871	0.01771	-0.16045	-0.05584	0.38671
2	0.54717	0.75925	0.42829	-0.05073	-0.22275	0.01771	0.15101	0.00233	-0.16045	-0.04047
3	-0.05073	0.42829	0.75925	0.54717	-0.04047	-0.16045	0.00233	0.15101	0.01771	-0.22275
4	-0.34159	-0.05073	0.54717	0.76951	0.38671	-0.05584	-0.16045	0.01771	0.08871	-0.03303
5	-0.03303	-0.22275	-0.04047	0.38671	0.72111	0.38671	-0.04047	-0.22275	-0.03303	0.35656
6	0.08871	0.01771	-0.16045	-0.05584	0.38671	0.76951	0.54717	-0.05073	-0.34159	-0.03303
7	0.01771	0.15101	0.00233	-0.16045	-0.04047	0.54717	0.75925	0.42829	-0.05073	-0.22275
8	-0.16045	0.00233	0.15101	0.01771	-0.22275	-0.05073	0.42829	0.75925	0.54717	-0.04047
9	-0.05584	-0.16045	0.01771	0.08871	-0.03303	-0.34159	-0.05073	0.54717	0.76951	0.38671
10	0.38671	-0.04047	-0.22275	-0.03303	0.35656	-0.03303	-0.22275	-0.04047	0.38671	0.72111

ENERGIES FOR NAPTHALENE TBMAPPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	4, 6	5, 7	1, 6	2, 8
XMOMNT	0.75738	-0.76037	-0.02375	-0.15723
YMOMNT	0.00000	-0.00000	-0.00000	0.00000
JUMP E	28.9023	35.1787	41.4773	58.0665
DIAG E	38.3102	43.8060	51.9655	71.7763
DIAG E	38.9983	43.1026	52.7280	71.3685
CORRSP	32.5475	48.0864	52.5436	72.6804
CORRSP	32.8898	48.0547	52.9619	72.2910

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
32.54750	0.07344	0.23035	0.00000	//	0.8219	0.5425	-0.1353	-0.1088
28.08256				//	0.9612	-0.2152	-0.0397	-0.1678
48.08636	1.96113	-0.97931	-0.00000	//	-0.4779	0.8061	0.3482	-0.0245
35.26142				//	0.2108	0.9634	-0.1652	0.0110
52.54365	0.34563	0.39330	0.00000	//	0.2854	-0.2320	0.9188	-0.1434
44.28765				//	0.0220	0.1598	0.9398	-0.3011
72.68044	0.03178	-0.10140	0.00000	//	0.1207	0.0462	0.1277	0.9834
70.56468				//	0.1764	0.0015	0.2963	0.9387

ENERGIES FOR NAPTHALENE TBMAPPROXIMATION

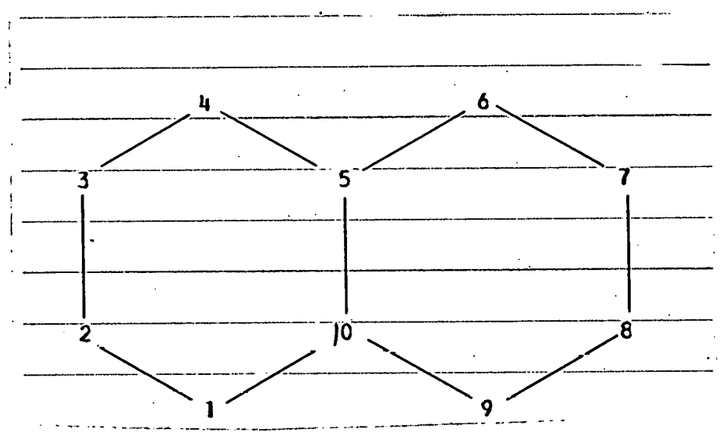
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	5, 6	4, 7	1, 7	3, 8
XMOMNT	-0.00000	-0.00000	0.00000	-0.00000
YMOMNT	0.59233	0.51596	0.00000	-0.48369
JUMP E	23.8862	40.1948	52.7698	54.8495
DIAG E	35.0580	51.0043	64.1574	67.4831
DIAG E	35.1834	50.8637	64.0911	67.4243
CORRSP	33.8269	51.2457	64.5358	68.0945
CORRSP	33.9519	51.2496	64.3355	68.0254

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
33.82686	0.26288	-0.00000	0.42749	//	0.9682	-0.2367	0.0636	0.0494
18.64285				//	0.9675	-0.0993	-0.0181	-0.2319
51.24575	0.64126	-0.00000	0.54246	//	0.2320	0.9467	-0.1424	0.1724
36.91921				//	0.1102	0.9828	-0.1399	0.0495
64.53580	0.00029	0.00000	0.01020	//	-0.0347	0.1410	0.9856	0.0868
56.45458				//	-0.0917	0.1555	0.8381	-0.5148
68.09445	1.08275	-0.00000	-0.61148	//	-0.0865	-0.1671	-0.0655	0.9799
59.60281				//	0.2084	0.0102	0.5270	0.8238

NAPTHALENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640	3.4640	2.5980	1.7320
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	0.5000	0.	0.5000

NAPTHALENE — IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 A A	10 A A
1.687686	1.425132	1.285665	1.179644	1.085318	0.802413	0.727730	0.676419	0.617729	0.512258
0.303543	0.267571	-0.404759	-0.022570	0.421390	-0.422381	0.013876	-0.396676	-0.269128	-0.293219
0.244232	0.422381	-0.173354	0.404342	0.269128	0.267571	-0.414349	0.163884	0.421390	0.219689
0.244232	0.422381	0.173354	0.404342	-0.269129	0.267571	0.414349	0.163884	-0.421390	-0.219689
0.303543	0.267571	0.404760	-0.022570	-0.421390	-0.422381	-0.013876	-0.396676	0.269129	0.293219
0.443198	-0.000000	0.335017	-0.414724	0.000000	0.000000	-0.395278	0.362739	-0.000000	-0.481164
0.303543	-0.267571	0.404759	-0.022570	0.421390	0.422381	-0.013876	-0.396676	-0.269128	0.293219
0.244232	-0.422381	0.173354	0.404342	0.269128	-0.267571	0.414349	0.163884	0.421390	-0.219689
0.244232	-0.422381	-0.173354	0.404342	-0.269129	-0.267571	-0.414349	0.163884	-0.421390	0.219689
0.303543	-0.267571	-0.404760	-0.022570	-0.421390	0.422381	0.013876	-0.396676	0.269129	-0.293219
0.443198	0.000000	-0.335017	-0.414724	0.000000	0.000000	0.395278	0.362739	-0.000000	0.481164

NAPTHALENE — IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 A A	10 A A
31.1602	22.8124	16.9915	11.6457	6.0116	-18.8306	-28.6109	-36.5821	-47.3233	-72.8121
0.233655	0.224136	-0.356971	-0.020780	0.404488	-0.471526	0.016266	-0.482312	-0.342421	-0.409682
0.188000	0.353815	-0.152886	0.372283	0.258334	0.298703	-0.485715	0.199264	0.536149	0.306948
0.188000	0.353815	0.152887	0.372283	-0.258334	0.298703	0.485715	0.199264	-0.536149	-0.306948
0.233655	0.224136	0.356971	-0.020781	-0.404488	-0.471526	-0.016266	-0.482312	0.342421	0.409682
0.341155	-0.000000	0.295463	-0.381842	0.000000	0.000000	-0.463359	0.441048	-0.000000	-0.672278
0.233655	-0.224136	0.356971	-0.020780	0.404488	0.471526	-0.016266	-0.482312	-0.342421	0.409682
0.188000	-0.353815	0.152886	0.372283	0.258334	-0.298704	0.485714	0.199264	0.536149	-0.306948
0.188000	-0.353815	-0.152887	0.372283	-0.258334	-0.298704	-0.485714	0.199264	-0.536149	0.306948
0.233655	-0.224136	-0.356971	-0.020781	-0.404488	0.471526	0.016266	-0.482312	0.342421	-0.409682
0.341155	0.000000	-0.295463	-0.381842	0.000000	0.000000	0.463359	0.441048	-0.000000	0.672278

NAPTHALENE M — IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	1.01128	0.72320	-0.01110	-0.35432	0.01658	0.06959	-0.00953	-0.18250	0.01463	0.55898
2	0.72320	1.00806	0.59813	-0.01110	-0.23505	-0.00953	0.17423	0.00472	-0.18250	-0.00274
3	-0.01110	0.59813	1.00806	0.72320	-0.00274	-0.18250	0.00472	0.17423	-0.00953	-0.23505
4	-0.35432	-0.01110	0.72320	1.01128	0.55898	0.01463	-0.18250	-0.00953	0.06959	0.01658
5	0.01658	-0.23505	-0.00274	0.55898	0.96131	0.55898	-0.00274	-0.23505	0.01658	0.51237
6	0.06959	-0.00953	-0.18250	0.01463	0.55898	1.01128	0.72320	-0.01110	-0.35432	0.01658
7	-0.00953	0.17423	0.00472	-0.18250	-0.00274	0.72320	1.00806	0.59813	-0.01110	-0.23505
8	-0.18250	0.00472	0.17423	-0.00953	-0.23505	-0.01110	0.59813	1.00806	0.72320	-0.00274
9	0.01463	-0.18250	-0.00953	0.06959	0.01658	-0.35432	-0.01110	0.72320	1.01128	0.55898
10	0.55898	-0.00274	-0.23505	0.01658	0.51237	0.01658	-0.23505	-0.00274	0.55898	0.96131

NAPTHALENE M — IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	0.79260	0.54913	-0.08715	-0.37155	-0.03565	0.08194	0.01361	-0.18606	-0.06279	0.38624
2	0.54913	0.77847	0.41803	-0.08715	-0.24638	0.01361	0.18423	0.01078	-0.18606	-0.06569
3	-0.08715	0.41803	0.77847	0.54913	-0.06569	-0.18606	0.01078	0.18423	0.01361	-0.24638
4	-0.37155	-0.08715	0.54913	0.79260	0.38624	-0.06279	-0.18606	0.01361	0.08194	-0.03565
5	-0.03565	-0.24638	-0.06569	0.38624	0.69898	0.38624	-0.06569	-0.24638	-0.03565	0.34978
6	0.08194	0.01361	-0.18606	-0.06279	0.38624	0.79260	0.54913	-0.08715	-0.37155	-0.03565
7	0.01361	0.18423	0.01078	-0.18606	-0.06569	0.54913	0.77847	0.41803	-0.08715	-0.24638
8	-0.18606	0.01078	0.18423	0.01361	-0.24638	-0.08715	0.41803	0.77847	0.54913	-0.06569
9	-0.06279	-0.18606	0.01361	0.08194	-0.03565	-0.37155	-0.08715	0.54913	0.79261	0.38624
10	0.38624	-0.06569	-0.24638	-0.03565	0.34978	-0.03565	-0.24638	-0.06569	0.38624	0.69898

ENERGIES FOR NAPTHALENE IRMAPPROXIMATION

CNE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	4, 6	5, 7	1, 6	2, 8
XMOMNT	-0.79714	0.76738	-0.00922	-0.11976
YMOMNT	0.00000	-0.00000	0.00000	0.00000
JUMP E	30.4762	34.6224	49.9908	59.3945
DIAG E	40.0697	43.2938	61.2208	72.6255
DIAG E	40.8148	42.6138	61.9503	72.1565
CORRSP	33.3537	49.0967	61.0655	73.6939
CORRSP	33.5637	49.0641	61.6400	73.2675

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
33.35368	0.03905	-0.16592	0.00000	//	0.7809	0.6114	-0.0655	0.1105
29.11185				//	0.9381	-0.3062	0.0035	0.1616
49.09666	2.46220	1.08596	-0.00000	//	-0.6008	0.7875	0.1332	-0.0327
34.73468				//	0.3066	0.9472	-0.0920	0.0171
61.06547	0.08048	-0.17604	0.00000	//	0.1085	-0.0725	0.9692	0.2087
52.06318				//	-0.0413	0.0947	0.9109	0.3995
73.69391	0.00282	-0.03001	0.00000	//	-0.1324	-0.0274	-0.1963	0.9712
72.34730				//	-0.1556	-0.0050	-0.4022	0.9022

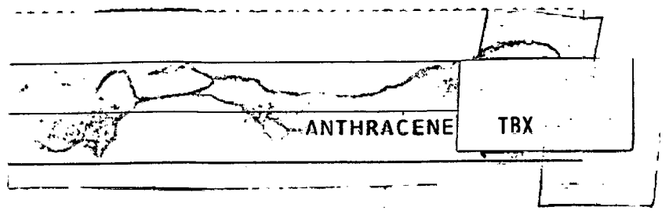
ENERGIES FOR NAPTHALENE IRMAPPROXIMATION

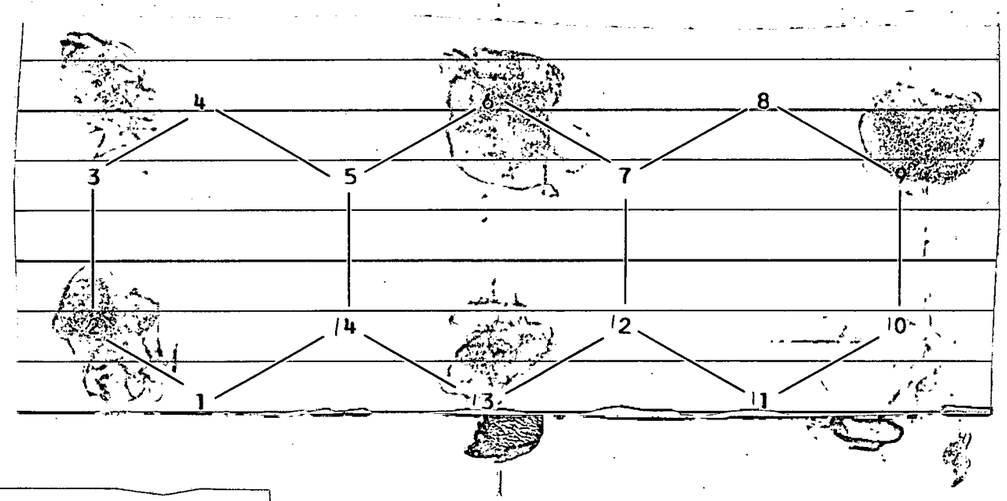
CNE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	5, 6	4, 7	3, 8	1, 7
XMOMNT	0.00000	0.00000	0.00000	-0.00000
YMOMNT	0.57441	0.51492	-0.48801	0.01129
JUMP E	24.8421	40.2565	53.5735	59.7711
DIAG E	35.2505	50.6839	66.2442	72.0110
DIAG E	35.3809	50.6186	66.0950	71.9301
CORRSP	34.1351	50.9635	66.8725	72.2184
CORRSP	34.2652	50.9645	66.7348	72.0602

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
34.13510	0.25110	0.00000	0.41591	//	0.9709	-0.2295	0.0494	0.0480
19.21311				//	0.9645	-0.1071	-0.2403	-0.0240
50.96352	0.59964	0.00000	0.52601	//	0.2198	0.9548	0.1867	-0.0716
37.01967				//	0.1188	0.9900	0.0419	-0.0632
66.87255	1.08191	-0.00000	-0.61680	//	-0.0917	-0.1672	0.9806	0.0452
57.22530				//	0.2253	-0.0783	0.9561	-0.1705
72.21845	0.01003	0.00000	0.05714	//	-0.0268	0.0873	-0.0335	0.9953
65.12724				//	0.0702	0.0474	0.1627	0.9830





ATOMIC COORDINATES

X	0.8455	0.	0.	0.8455	1.7491	2.6245	3.4999
y	0.	0.5040	1.5250	2.0290	1.5280	2.0240	1.5280

4.4035	5.2490	5.2490	4.4035	3.4999	2.6245	1.7491
2.0290	1.5250	0.5040	0.	0.5010	0.0050	0.5010

ANTHRACENE X TBX APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 AA	6 SA	7 AS	8 SS	9 AA	10SA	11SS	12AS	13AA	14 AS
1.574298	1.478985	1.347829	1.342152	1.245540	1.233054	1.113474	0.886524	0.766944	0.754459	0.657846	0.652170	0.521014	0.425701
0.215950	0.291068	0.174694	-0.278874	0.406538	-0.002398	0.308345	-0.308345	0.002398	-0.406538	0.278871	-0.174700	0.291068	-0.215950
0.162879	0.305265	0.396022	-0.123714	0.216605	0.331505	0.226566	0.226566	0.331505	0.216605	-0.123706	0.396024	-0.305265	0.162879
0.162879	0.305265	0.396026	0.123701	-0.216604	0.331505	-0.226565	0.226565	-0.331505	0.216604	-0.123708	-0.396024	0.305265	-0.162879
0.215950	0.291068	0.174704	0.278868	-0.406538	-0.002397	-0.308345	-0.308345	-0.002397	-0.406538	0.278871	0.174699	-0.291068	0.215950
0.360743	0.268500	-0.177946	0.279348	-0.194445	-0.374297	0.100818	-0.100818	0.374297	0.194445	-0.279345	0.177951	0.268500	-0.360743
0.305615	-0.000000	-0.248906	0.397228	0.000000	-0.000000	0.432267	0.432267	-0.000000	-0.000000	0.397224	-0.248913	-0.000000	0.305615
0.360743	-0.268501	-0.177946	0.279348	0.194446	0.374297	0.100818	-0.100818	-0.374297	-0.194445	-0.279345	0.177951	-0.268500	-0.360743
0.215950	-0.291068	0.174704	0.278868	0.406538	0.002397	-0.308345	-0.308345	0.002398	0.406538	0.278871	0.174699	0.291068	0.215950
0.162879	-0.305265	0.396026	0.123700	0.216604	-0.331505	-0.226566	0.226566	0.331505	-0.216604	-0.123708	-0.396024	-0.305265	-0.162879
0.162878	-0.305265	0.396022	-0.123714	-0.216605	0.331505	0.226566	-0.226565	-0.331505	-0.216605	-0.123707	0.396024	0.305265	0.162879
0.215950	-0.291068	0.174694	-0.278874	-0.406538	0.002398	0.308345	-0.308345	-0.002398	0.406538	0.278871	-0.174700	-0.291068	-0.215950
0.360743	-0.268500	-0.177955	-0.279342	-0.194445	0.374298	-0.100818	-0.100818	0.374298	-0.194445	-0.279345	-0.177950	-0.268500	0.360743
0.305615	-0.000000	-0.248919	-0.397220	-0.000000	0.000000	-0.432267	0.432267	-0.000000	-0.000000	0.397225	0.248912	-0.000000	-0.305615
0.360743	0.268500	-0.177955	-0.279342	0.194445	-0.374298	-0.100818	-0.100818	-0.374297	0.194445	-0.279346	-0.177950	-0.268500	0.360743

ANTHRACENE X TBX APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 AA	6 SA	7 AS	8 SS	9 AA	10SA	11 SS	12 AS	13 AA	14 AS
27.64242	24.54053	19.55494	19.31717	14.93793	14.32191	7.72222	-9.69923	-23.02620	-24.66126	-39.41148	-40.41405	-69.66263	102.22554
0.172112	0.239339	0.150474	-0.240717	0.364269	-0.002160	0.292211	-0.327485	0.002738	-0.468041	0.343828	-0.216328	0.403246	-0.330979
0.129814	0.251012	0.341116	-0.106787	0.194084	0.298537	0.214711	0.240629	0.378537	0.249374	-0.152521	0.490390	-0.422914	0.249639
0.129814	0.251012	0.341119	0.106775	-0.194083	0.298538	-0.214711	0.240629	-0.378537	0.249373	-0.152523	-0.490389	0.422914	-0.330979
0.172112	0.239339	0.150482	0.240712	-0.364269	-0.002159	-0.292211	-0.327485	-0.002738	-0.468041	0.343828	0.216326	-0.403246	0.552899
0.287511	0.220781	-0.153275	0.241126	-0.174228	-0.337074	0.095542	-0.107076	0.427400	0.223862	-0.344412	0.220353	0.371981	-0.468407
0.243575	-0.000000	-0.214397	0.342878	0.000000	-0.000000	0.409649	0.459099	-0.000000	-0.000000	0.489748	-0.308225	-0.000000	0.552899
0.287511	-0.220782	-0.153274	0.241126	0.174229	0.337074	0.095542	-0.107076	-0.427400	-0.223862	-0.344412	0.220353	-0.371981	-0.330979
0.172111	-0.239339	0.150482	0.240712	0.364269	0.002159	0.292211	-0.327485	0.002738	0.468041	0.343828	0.216326	0.403246	-0.249639
0.129814	-0.251012	0.341120	0.106775	0.194083	-0.298538	-0.214711	0.240629	0.378537	-0.249373	-0.152523	-0.490389	-0.422914	0.249639
0.129814	-0.251012	0.341116	-0.106787	-0.194084	-0.298537	0.214711	0.240629	-0.378537	-0.249374	-0.152521	0.490390	0.422914	-0.330979
0.172111	-0.239339	0.150474	-0.240717	-0.364269	0.002160	0.292211	-0.327485	-0.002738	0.468041	0.343828	-0.216327	-0.403246	0.552899
0.287511	-0.220782	-0.153283	-0.241121	-0.174228	0.337074	-0.095542	-0.107076	0.427401	-0.223861	-0.344413	-0.220352	0.371981	-0.468407
0.243574	-0.000000	-0.214408	-0.342871	-0.000000	0.000000	-0.409649	0.459099	-0.000000	-0.000000	0.489749	0.308223	0.000000	0.552899
0.287511	0.220781	-0.153283	-0.241122	0.174228	-0.337074	-0.095542	-0.107076	-0.427400	0.223861	-0.344413	-0.220352	-0.371981	

ANTHRACENE X

TBX TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.00000	0.76967	-0.00000	-0.35248	0.00000	0.09005	-0.00000	-0.03029	0.00000	0.06520	0.00000	-0.12894	-0.00000	0.50346
2	0.76967	1.00000	0.54579	0.00000	-0.21533	0.00000	0.12161	-0.00000	-0.07887	0.00000	0.06520	-0.00000	-0.19519	-0.00000
3	-0.00000	0.54579	1.00000	0.76967	-0.00000	-0.19519	0.00000	0.06520	-0.00000	-0.07887	-0.00000	0.12161	0.00000	-0.21533
4	-0.35248	0.00000	0.76967	1.00000	0.50346	0.00000	-0.12894	0.00000	0.06520	0.00000	-0.03029	0.00000	0.09005	0.00000
5	0.00000	-0.21533	-0.00000	0.50346	1.00000	0.61817	-0.00000	-0.12894	0.00000	0.12161	0.00000	-0.20156	-0.00000	0.49597
6	0.09005	0.00000	-0.19519	0.00000	0.61817	1.00000	0.61817	-0.00000	-0.19519	-0.00000	0.09005	0.00000	-0.37857	-0.00000
7	-0.00000	0.12161	0.00000	-0.12894	-0.00000	0.61817	1.00000	0.50346	-0.00000	-0.21533	-0.00000	0.49597	0.00000	-0.20156
8	-0.03029	-0.00000	0.06520	0.00000	-0.12894	-0.00000	0.50346	1.00000	0.76967	0.00000	-0.35248	-0.00000	0.09005	0.00000
9	0.00000	-0.07887	-0.00000	0.06520	0.00000	-0.19519	-0.00000	0.76967	1.00000	0.54579	-0.	-0.21533	-0.00000	0.12161
10	0.06520	0.00000	-0.07887	0.00000	0.12161	-0.00000	-0.21533	0.00000	0.54579	1.00000	0.76967	0.00000	-0.19519	-0.00000
11	0.00000	0.06520	-0.00000	-0.03029	0.00000	0.09005	-0.00000	-0.35248	-0.	0.76967	1.00000	0.50346	-0.	-0.12894
12	-0.12894	-0.00000	0.12161	0.00000	-0.20156	0.00000	0.49597	-0.00000	-0.21533	0.00000	0.50346	1.00000	0.61817	0.00000
13	-0.00000	-0.19519	0.00000	0.09005	-0.00000	-0.37857	0.00000	0.09005	-0.00000	-0.19519	-0.	0.61817	1.00000	0.61817
14	0.50346	-0.00000	-0.21533	0.00000	0.49597	-0.00000	-0.20156	0.00000	0.12161	-0.00000	-0.12894	0.00000	0.61817	1.00000

ANTHRACENE X

TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.77115	0.58450	-0.05208	-0.33294	-0.02720	0.09366	0.01238	-0.03132	-0.00701	0.06397	0.01123	-0.12099	-0.05502	0.34716
2	0.58450	0.76103	0.38035	-0.05208	-0.19844	0.01965	0.11766	-0.00701	-0.07751	0.00183	0.06397	0.00333	-0.18572	-0.04225
3	-0.05208	0.38035	0.76103	0.58450	-0.04225	-0.18572	0.00333	0.06397	0.00183	-0.07751	-0.00701	0.11766	0.01965	-0.19844
4	-0.33294	-0.05208	0.58450	0.77115	0.34716	-0.05502	-0.12099	0.01123	0.06397	-0.00701	-0.03132	0.01238	0.09366	-0.02720
5	-0.02720	-0.19844	-0.04225	0.34716	0.73229	0.44942	-0.03859	-0.12099	0.00333	0.11766	0.01238	-0.18624	-0.03784	0.34179
6	0.09366	0.01965	-0.18572	-0.05502	0.44942	0.78134	0.44942	-0.05502	-0.18572	0.01965	0.09366	-0.03784	-0.36016	-0.03784
7	0.01238	0.11766	0.00333	-0.12099	-0.03859	0.44942	0.73229	0.34716	-0.04225	-0.19844	-0.02720	0.34179	-0.03784	-0.18624
8	-0.03132	-0.00701	0.06397	0.01123	-0.12099	-0.05502	0.34716	0.77115	0.58450	-0.05208	-0.33294	-0.02720	0.09366	0.01238
9	-0.00701	-0.07751	0.00183	0.06397	0.00333	-0.18572	-0.04225	0.58450	0.76103	0.38035	-0.05208	-0.19844	0.01965	0.11766
10	0.06397	0.00183	-0.07751	-0.00701	0.11766	0.01965	-0.19844	-0.05208	0.38035	0.76103	0.58450	-0.04225	-0.18572	0.00333
11	0.01123	0.06397	-0.00701	-0.03132	0.01238	0.09366	-0.02720	-0.33294	-0.05208	0.58450	0.77115	0.34716	-0.05502	-0.12099
12	-0.12099	0.00333	0.11766	0.01238	-0.18624	-0.03784	0.34179	-0.02720	-0.19844	-0.04225	0.34716	0.73229	0.44942	-0.03859
13	-0.05502	-0.18572	0.01965	0.09366	-0.03784	-0.36016	-0.03784	0.09366	0.01965	-0.18572	-0.05502	0.44942	0.78134	0.44942
14	0.34716	-0.04225	-0.19844	-0.02720	0.34179	-0.03784	-0.18624	0.01238	0.11766	0.00333	-0.12099	-0.03859	0.44942	0.73229

ENERGIES FOR ANTHRACENE X TBX APPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	6, 8	7, 9	2, 8	4, 9	3,10	1,10	6,11	5,12
XMOMNT	-0.93850	-0.94201	0.00762	0.07188	-0.28558	0.00933	0.07260	-0.28843
YMOMNT	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	-0.00000	0.00000
JUMP E	24.0211	30.7484	34.2398	42.3434	44.2162	52.3037	53.7334	55.3520
DIAG E	33.9712	39.6881	49.0425	53.4009	60.9841	69.1818	64.3128	71.4657
DIAG E	34.9729	38.5278	49.6008	52.7217	61.1049	69.8388	64.6792	71.7384
CORRSP	28.3119	42.5993	46.8764	51.5261	60.1054	71.3302	67.6030	73.6946
CORRSP	28.7798	42.2290	46.9320	51.3535	60.1903	71.6985	68.1107	73.8907

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION							
28.31186	0.11604	-0.31046	0.00000	//	0.8237	-0.5103	-0.1589	-0.0338	0.1498	-0.0531	0.0202	-0.0950
25.03866				//	0.9634	0.1490	-0.0989	0.0056	0.1945	-0.0178	0.0258	0.0310
42.59929	2.98197	-1.28300	-0.00000	//	0.4797	0.8359	-0.2177	-0.0206	0.0217	-0.0847	0.0112	0.1251
30.73274				//	-0.1346	0.9149	0.2737	-0.0100	0.0854	0.0862	-0.0638	0.2259
46.87640	0.19853	-0.31558	-0.00000	//	0.1810	0.1262	0.7485	0.4746	0.3152	0.0954	-0.2022	-0.1287
37.18196				//	0.0472	-0.3211	0.7244	-0.2974	0.4113	0.1348	-0.2639	0.1564
51.52610	0.09458	0.20777	-0.00000	//	-0.1527	-0.0297	-0.5544	0.7075	0.1572	-0.1861	-0.2664	-0.1937
46.75054				//	0.0328	-0.0421	0.3400	0.8860	0.0694	0.1532	0.0241	-0.2604
60.10545	0.05823	-0.15093	0.00000	//	-0.1502	0.0266	-0.0688	-0.4706	0.7137	-0.2016	-0.4472	-0.0198
53.78026				//	-0.1407	0.0479	-0.3581	0.1565	0.5387	-0.3546	-0.6342	-0.0842
71.33023	0.01061	-0.05914	-0.00000	//	-0.0357	0.0571	-0.2304	0.0086	0.3464	0.8730	0.2069	-0.1318
68.28220				//	-0.0211	-0.0697	-0.3440	0.0647	0.0507	0.8534	-0.2605	0.2711
67.60305	0.00068	0.01538	-0.00000	//	-0.1066	0.0062	0.0288	0.1152	0.4547	-0.3613	0.7972	0.0417
66.78425				//	-0.1731	-0.0212	-0.1685	0.0154	0.6882	0.0597	0.6743	0.0951
73.69456	0.09951	-0.17820	0.00000	//	-0.0091	-0.1419	-0.0336	0.1943	0.1299	0.1137	-0.0968	0.9496
71.59062				//	-0.0137	-0.1680	-0.0051	0.3124	-0.1204	-0.3051	0.0163	0.8753

ENERGIES FOR ANTHRACENE X ITBX APPROXIMATION

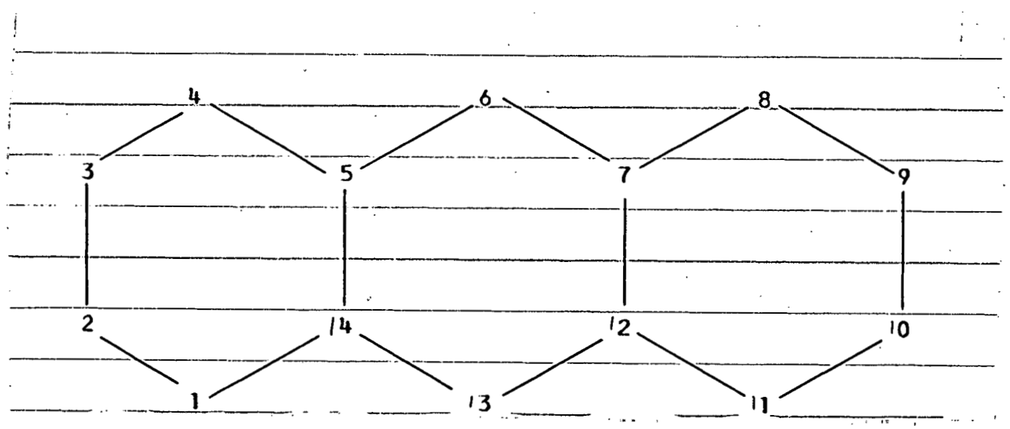
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	7, 8	4, 8	6, 9	5,10	7,11	2, 9	4,11	3,12
XMOMNT	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000
YMOMNT	0.64153	-0.00294	-0.52665	0.51292	-0.00298	-0.00322	0.47106	-0.14544
JUMP E	17.4215	29.0164	37.3481	39.5992	47.1337	47.5667	58.7286	59.9690
DIAG E	29.0277	40.2627	48.2821	56.7937	56.9117	62.3400	74.1490	79.2039
DIAG E	29.1407	40.8569	48.0104	56.9347	56.3895	61.6249	74.1079	79.4565
CORRSP	27.7283	39.3574	47.3869	53.8349	60.5822	61.6830	75.4331	80.9647
CORRSP	27.8354	39.8923	47.2570	60.3745	53.6007	61.0467	75.3995	81.1152

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION							
27.72826	0.28296	-0.00000	0.48987	//	0.9726	0.0418	0.2090	0.0209	0.0152	-0.0535	-0.0645	0.0301
12.84423				//	0.9412	0.1238	0.1018	0.2161	0.0768	0.0239	0.1544	0.1073
39.35742	0.00915	-0.00000	-0.07392	//	-0.0240	0.9751	-0.0504	-0.2074	-0.0132	-0.0205	0.0449	-0.0199
27.31360				//	-0.0262	0.8200	-0.0686	-0.4463	0.3433	-0.0422	0.0376	-0.0430
47.38690	0.38543	0.00000	-0.43734	//	-0.2064	0.0917	0.9100	0.2660	-0.0983	-0.1245	0.1134	0.1100
34.50545				//	-0.1551	0.0870	0.9496	0.0271	0.0163	-0.0948	0.0578	0.2307
53.83493	0.47377	0.00000	0.45491	//	0.0475	0.1051	-0.2458	0.5907	-0.7588	0.0220	-0.0268	-0.0190
47.12868				//	-0.1967	0.5157	-0.1043	0.6333	-0.4781	-0.0559	0.2266	-0.0177
60.58219	0.86960	0.00000	0.58098	//	0.0179	0.1332	-0.1859	0.7004	0.6150	-0.1571	0.2160	-0.0844
53.94786				//	-0.2067	-0.0429	-0.0728	0.3294	0.5688	0.5866	0.3288	0.2567
61.68298	0.00200	0.00000	0.02764	//	0.0250	0.0583	0.0695	0.1374	0.1146	0.9502	0.0329	0.2350
53.11263				//	0.0787	0.1271	0.0383	-0.2730	-0.4921	0.7095	-0.2823	0.2764
75.43311	0.68325	0.00000	0.46152	//	0.0875	-0.0825	-0.0402	-0.1645	-0.1509	0.0423	0.9590	-0.1124
72.20097				//	-0.0062	-0.1438	-0.0435	-0.4110	-0.2857	-0.0197	0.8489	0.0768
80.96472	-0.00042	-0.00000	-0.01100	//	-0.0008	-0.0017	-0.1557	-0.0151	0.0038	-0.2268	0.1133	0.9546
78.09641				//	-0.0429	-0.0023	-0.2521	-0.0169	0.0071	-0.3710	-0.1082	0.8860

ANTHRACENE IRX



ATOMIC COORDINATES

x	0.8455	0.	0.	0.8455	1.7491	2.6245	3.4999
y	0.	0.5040	1.5250	2.0290	1.5280	2.0240	1.5280

4.4035	5.2490	5.2490	4.4035	3.4999	2.6245	1.7491
2.0290	1.5250	0.5040	0.	0.5010	0.0050	0.5010

ANTHRACENE X IRX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 AA	6 SA	7 AS	8 SS	9 AA	10 SA	11 SS	12 AS	13 AA	14 AS
1.699427	1.544686	1.342764	1.314319	1.196824	1.159723	1.045507	0.835807	0.737922	0.729294	0.664107	0.652279	0.565889	0.511442
0.220197	-0.295038	0.173843	-0.284325	0.407904	0.023083	0.302318	-0.312753	0.010281	-0.403013	0.271068	0.186371	-0.288978	-0.207433
0.173206	-0.314332	0.387414	-0.124435	0.218421	-0.326335	0.232820	0.238667	-0.338401	0.211424	-0.113790	-0.395519	0.296272	0.154517
0.173206	-0.314332	0.387414	0.124435	-0.218421	-0.326335	-0.232820	0.238667	0.338400	-0.211426	-0.113789	0.395519	-0.296272	-0.154517
0.220197	-0.295038	0.173842	0.284325	-0.407904	0.023082	-0.302318	-0.312753	-0.010279	-0.403013	0.271067	-0.186372	0.288978	-0.207433
0.353906	-0.253274	-0.180948	0.271246	-0.189490	0.378117	0.104792	-0.099700	-0.367939	0.207072	-0.286476	-0.168313	-0.280561	-0.370290
0.304182	-0.000000	-0.271836	0.400251	0.000000	-0.000000	0.432244	0.412997	0.000000	-0.000000	0.403748	0.246985	-0.000000	-0.303253
0.353906	0.253274	-0.180947	0.271246	0.189490	-0.378117	-0.104792	-0.099700	0.367939	-0.207073	-0.286476	-0.168313	0.280561	-0.370290
0.220197	0.295038	0.173842	0.284325	0.407904	-0.023082	-0.302318	-0.312753	0.010279	0.403014	0.271067	-0.186372	-0.288978	0.207433
0.173206	0.314332	0.387414	0.124435	0.218421	0.326335	-0.232820	0.238667	-0.338400	-0.211426	-0.113788	0.395519	0.296272	-0.154517
0.173206	0.314332	0.387414	-0.124435	-0.218421	0.326335	0.232820	0.238667	0.338401	-0.211425	-0.113790	-0.395519	-0.296272	0.154517
0.220197	0.295038	0.173843	-0.284325	-0.407904	-0.023083	0.302318	-0.312753	-0.010281	0.403013	0.271067	0.186371	0.288979	-0.207433
0.353906	0.253274	-0.180947	-0.271247	-0.189490	-0.378117	-0.104792	-0.099700	-0.367938	-0.207074	-0.286475	0.168314	-0.280561	0.370290
0.304181	0.000000	-0.271835	-0.400252	-0.000000	-0.000000	-0.432244	0.412997	-0.000000	0.000000	0.403747	-0.246986	0.000000	-0.303253
0.353906	-0.253274	-0.180947	-0.271247	0.189490	0.378117	-0.104792	-0.099700	0.367939	0.207074	-0.286475	0.168314	0.280561	0.370290

ANTHRACENE X IRX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 AA	6 SA	7 AS	8 SS	9 AA	10 SA	11 SS	12 AS	13 AA	14 AS
31.18643	26.71972	19.34289	18.12157	12.46161	10.43613	3.29818	-14.88588	-26.91203	-28.12683	-38.32564	-40.39464	-58.12941	-72.38456
0.168912	-0.237387	0.150022	-0.248007	0.372857	0.021434	0.295666	-0.342097	0.011968	-0.471919	0.332628	0.230761	-0.384149	-0.290055
0.132866	-0.252912	0.334330	-0.108540	0.199655	-0.303030	0.227696	0.261060	-0.393937	0.247573	-0.139632	-0.489723	0.393844	0.216062
0.132866	-0.252912	0.334330	0.108541	-0.199655	-0.303031	-0.227696	0.261060	0.393936	0.247575	-0.139630	0.489723	-0.393844	-0.216062
0.168912	-0.237387	0.150022	0.248007	-0.372857	0.021434	-0.295666	-0.342097	-0.011966	-0.471920	0.332627	-0.230762	0.384149	0.290055
0.271479	-0.203784	-0.156154	0.236599	-0.173209	0.351115	0.102486	-0.109054	-0.428323	0.242477	-0.351536	-0.208401	-0.372959	-0.517778
0.233336	-0.000000	-0.234589	0.349126	0.000000	-0.000000	0.422732	0.451745	0.000000	0.000000	0.495441	0.305811	-0.000000	-0.424040
0.271479	0.203784	-0.156154	0.236599	0.173209	-0.351115	0.102486	-0.109054	0.428323	-0.242477	-0.351535	-0.208402	0.372959	-0.517778
0.168912	0.237387	0.150022	0.248007	0.372857	-0.021434	-0.295666	-0.342097	0.011966	0.471920	0.332627	-0.230762	-0.384149	0.290055
0.132866	0.252912	0.334330	0.108541	0.199655	0.303031	-0.227696	0.261060	-0.393936	-0.247575	-0.139630	0.489723	0.393845	-0.216062
0.132866	0.252911	0.334330	-0.108540	-0.199655	0.303031	0.227696	0.261060	0.393937	-0.247573	-0.139632	-0.489723	-0.393845	0.216062
0.168912	0.237387	0.150023	-0.248007	-0.372857	-0.021434	-0.295666	-0.342096	-0.011968	0.471920	0.332628	0.230761	0.384149	-0.290055
0.271479	0.203784	-0.156154	-0.236600	-0.173209	-0.351115	-0.102486	-0.109054	-0.428322	-0.242480	-0.351535	0.208403	-0.372959	0.517778
0.233336	0.000000	-0.234588	-0.349126	-0.000000	-0.000000	-0.422732	0.451745	-0.000000	0.000000	0.495440	-0.305813	0.000000	-0.424040
0.271479	-0.203784	-0.156154	-0.236599	0.173209	0.351115	-0.102486	-0.109054	0.428322	0.242479	-0.351535	0.208402	0.372959	0.517778

ANTHRACENE_X — IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.00982	0.77111	-0.00833	-0.34467	0.01438	0.07319	-0.01026	-0.02945	0.00722	0.07390	-0.00604	-0.13767	0.00570	0.50532
2	0.77111	1.00557	0.53598	-0.00833	-0.20665	-0.00359	0.13402	0.00722	-0.09438	-0.00646	0.07390	0.00589	-0.20691	-0.00368
3	-0.00833	0.53598	1.00557	0.77111	-0.00368	-0.20691	0.00589	0.07390	-0.00646	-0.09438	0.00722	0.13402	-0.00359	-0.20665
4	-0.34467	-0.00833	0.77111	1.00982	0.50532	0.00570	-0.13767	-0.00604	0.07390	0.00722	-0.02945	-0.01026	0.07319	0.01438
5	0.01438	-0.20665	-0.00368	0.50532	0.97115	0.62140	-0.00096	-0.13767	0.00589	0.13402	-0.01026	-0.19556	0.00595	0.48930
6	0.07319	-0.00359	-0.20691	0.00570	0.62140	1.02691	0.62140	0.00570	-0.20691	-0.00359	0.07319	0.00595	-0.36123	0.00595
7	-0.01026	0.13402	0.00589	-0.13767	-0.00096	0.62140	0.97115	0.50532	-0.00368	-0.20665	0.01438	0.48930	0.00595	-0.19556
8	-0.02945	0.00722	0.07390	-0.00604	-0.13767	0.00570	0.50532	1.00982	0.77111	-0.00833	-0.34467	0.01438	0.07319	-0.01026
9	0.00722	-0.09438	-0.00646	0.07390	0.00589	-0.20691	-0.00368	0.77111	1.00557	0.53598	-0.00833	-0.20665	-0.00359	0.13402
10	0.07390	-0.00646	-0.09438	0.00722	0.13402	-0.00359	-0.20665	-0.00833	0.53598	1.00557	0.77111	-0.00368	-0.20691	0.00589
11	-0.00604	0.07390	0.00722	-0.02945	-0.01026	0.07319	0.01438	-0.34467	-0.00833	0.77111	1.00982	0.50532	0.00570	-0.13767
12	-0.13767	0.00589	0.13402	-0.01026	-0.19556	0.00595	0.48930	0.01438	-0.20665	-0.00368	0.50532	0.97115	0.62140	-0.00096
13	0.00570	-0.20691	-0.00359	0.07319	0.00595	-0.36123	0.00595	0.07319	-0.00359	-0.20691	0.00570	0.62140	1.02691	0.62140
14	0.50532	-0.00368	-0.20665	0.01438	0.48930	0.00595	-0.19556	-0.01026	0.13402	0.00589	-0.13767	-0.00096	0.62140	0.97115

ANTHRACENE_X — IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.79160	0.58965	-0.08508	-0.36020	-0.02926	0.08524	0.00547	-0.03135	-0.00148	0.07771	0.00826	-0.13936	-0.06836	0.34258
2	0.58965	0.77742	0.36347	-0.08508	-0.21585	0.02187	0.14192	-0.00148	-0.10025	-0.00519	0.07771	0.01297	-0.21158	-0.06814
3	-0.08508	0.36347	0.77742	0.58965	-0.06814	-0.21158	0.01297	0.07771	-0.00519	-0.10025	-0.00148	0.14192	0.02187	-0.21585
4	-0.36020	-0.08508	0.58965	0.79160	0.34258	-0.06836	-0.13936	0.00826	0.07771	-0.00148	-0.03135	0.00547	0.08524	-0.02926
5	-0.02926	-0.21585	-0.06814	0.34258	0.71876	0.45181	-0.06049	-0.13936	0.01297	0.14192	0.00547	-0.20641	-0.05190	0.33282
6	0.08524	0.02187	-0.21158	-0.06836	0.45181	0.82014	0.45181	0.06836	-0.21158	-0.02187	0.08524	-0.05190	-0.38223	-0.05190
7	0.00547	0.14192	0.01297	-0.13936	-0.06049	0.45181	0.71876	0.34258	-0.06814	-0.21585	-0.02926	0.33282	-0.05190	-0.20641
8	-0.03135	-0.00148	0.07771	0.00826	-0.13936	-0.06836	0.34258	0.79160	0.58965	-0.08508	-0.36020	-0.02926	0.08524	0.00547
9	-0.00148	-0.10025	-0.00519	0.07771	0.01297	-0.21158	-0.06814	0.58965	0.77742	0.36347	-0.08508	-0.21585	0.02187	0.14192
10	0.07771	-0.00519	-0.10025	-0.00148	0.14192	0.02187	-0.21585	-0.08508	0.36347	0.77742	0.58965	-0.06814	-0.21158	0.01297
11	0.00826	0.07771	-0.00148	-0.03135	0.00547	0.08524	-0.02926	-0.36020	-0.08508	0.58965	0.79160	0.34258	-0.06836	-0.13936
12	-0.13936	0.01297	0.14192	0.00547	-0.20641	-0.05190	0.33282	-0.02926	-0.21585	-0.06814	0.34258	0.71876	0.45181	-0.06049
13	-0.06836	-0.21158	0.02187	0.08524	-0.05190	-0.38223	-0.05190	0.08524	0.02187	-0.21158	-0.06836	0.45181	0.82014	0.45181
14	0.34258	-0.06814	-0.21585	-0.02926	0.33282	-0.05190	-0.20641	0.00547	0.14192	0.01297	-0.13936	-0.06049	0.45181	0.71876

ENERGIES FOR ANTHRACENE X IRXAPPROXIMATION

ONE-ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	6, 8	7, 9	2, 8	4, 9	3,10	6,11	5,12	1,10
XMOMNT	1.01447	0.95430	0.04455	-0.07480	-0.24093	-0.05721	0.26607	-0.01043
YMOMNT	0.00000	0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	0.00000
JUMP E	25.3220	30.2102	41.6056	45.0336	47.4697	48.7618	52.8563	59.3133
DIAG E	35.6707	39.0808	56.7440	56.1733	63.8405	58.6824	69.2977	76.7843
DIAG E	36.7564	37.9211	57.2966	55.4908	63.9234	59.0490	69.5898	77.3527
CORRSP	29.0929	43.2986	56.5610	50.0752	66.9070	60.0601	71.8504	78.4282
CORRSP	29.3273	43.1089	56.8861	49.9377	67.2286	59.9801	72.0413	78.8696

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION							
29.09294	0.06334	0.22626	0.00000	//	0.7796	-0.5917	-0.0836	-0.0213	-0.1414	0.0330	-0.1113	-0.0338
25.92470				//	0.9476	0.2481	-0.0233	-0.0010	-0.1863	0.0425	0.0594	-0.0007
43.29861	3.55626	1.38975	0.00000	//	0.5855	0.7873	-0.1122	-0.0188	-0.0726	0.0108	0.1198	0.0683
30.14348				//	-0.2537	0.9224	0.1628	-0.0191	-0.0228	-0.0554	0.2257	-0.0584
56.56097	0.12457	0.22757	-0.00000	//	0.1148	0.0313	0.8895	-0.2654	-0.0432	0.2669	0.0918	-0.2065
53.55043				//	0.0315	-0.0874	0.5652	0.0309	0.1735	0.7300	0.1038	-0.3119
50.07523	0.01937	0.09538	0.00000	//	0.0243	0.0605	0.3480	0.6671	-0.3503	-0.4960	-0.2463	-0.0128
50.00048				//	-0.0077	0.0081	0.3106	0.8464	-0.2150	-0.2193	-0.2920	-0.0862
66.90699	0.00024	0.00922	-0.00000	//	0.1833	-0.0359	0.1183	0.0841	0.8338	-0.4429	0.1204	-0.1956
66.64501				//	0.1894	-0.0044	0.2415	-0.0201	0.8181	-0.4570	-0.0171	-0.1643
60.06014	0.04037	-0.12573	-0.00000	//	0.0435	0.0170	-0.0039	0.6415	0.3052	0.6957	-0.0934	-0.0209
40.76862				//	0.0111	0.2180	-0.5983	0.3715	0.4439	0.4406	-0.2386	0.0914
71.85039	0.04314	0.11883	0.00000	//	-0.0065	-0.1526	0.0031	0.2526	-0.1639	-0.0287	0.9378	0.0757
69.83357				//	-0.0030	-0.1795	-0.2134	0.3680	-0.0390	-0.0524	0.8778	-0.1092
78.42816	0.02045	-0.07830	0.00000	//	-0.0053	-0.0227	0.2325	-0.0352	0.1871	-0.0241	-0.0399	0.9523
75.74100				//	0.0269	-0.0139	0.3086	0.0918	0.1439	0.0920	0.1472	0.9190

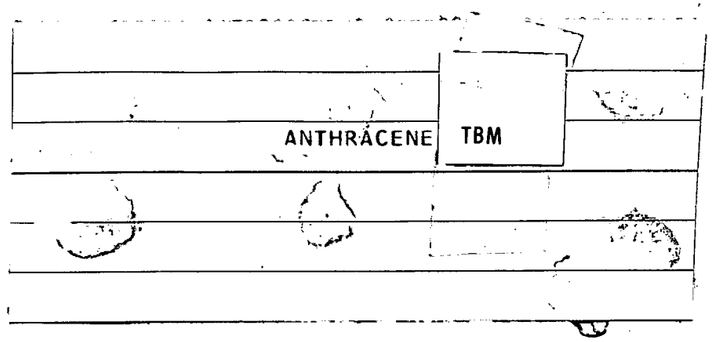
ENERGIES FOR ANTHRACENE X IRX APPROXIMATION

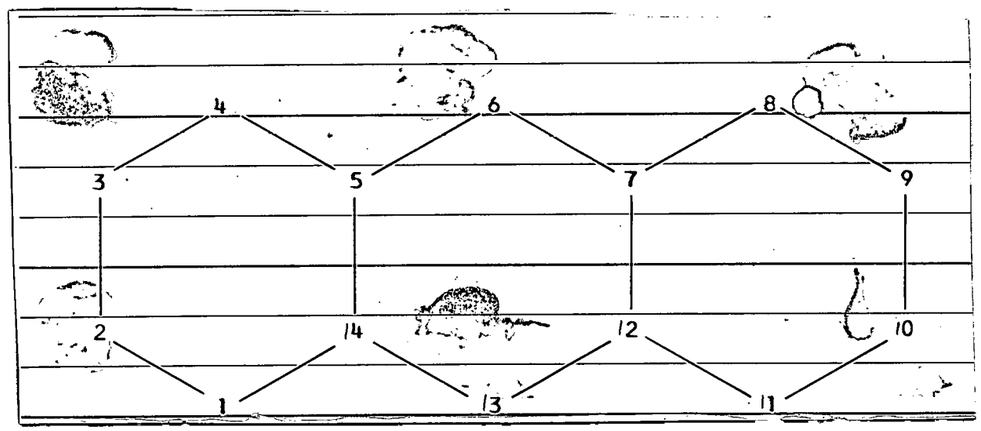
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	7, 8	4, 8	6,	5,10	7,11	2, 9	4,11	3,12
XMOMNT	-0.00000	-0.00000	0	-0.00000	0.00000	-0.00000	0.00000	-0.00000
YMOMNT	0.61300	-0.02257	-0.52537	0.50738	0.01256	-0.01442	0.47700	0.11556
JUMP E	18.1841	33.0075	37.3482	40.5884	41.6238	53.6318	56.4472	59.7375
DIAG E	28.9210	44.4571	47.6985	57.5398	50.9543	68.6021	71.9942	78.9874
DIAG E	29.0474	45.0608	47.4981	57.6158	50.3617	67.8686	71.8787	79.2865
CORRSP	27.7506	43.3107	46.8974	59.7457	49.5750	67.2874	73.3845	81.2030
CORRSP	27.8516	43.8333	46.7164	59.7350	49.1705	66.6604	73.3131	81.3371

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION							
27.75056	0.26491	-0.00000	0.47380	//	0.9755	0.0213	0.1993	0.0278	0.0307	-0.0398	-0.0651	-0.0264
13.40553				//	0.9393	0.0823	0.1114	0.2224	0.0959	0.0300	0.1608	-0.1144
43.	0.00512	0.00000	-0.05273	//	0.0141	0.9562	-0.1187	-0.2593	0.0116	-0.0151	0.0540	0.0285
29.				//	0.0064	0.7234	-0.0918	-0.4699	0.4908	-0.0413	0.0534	0.0453
46.89744	0.35535	-0.00000	-0.42211	//	-0.1828	0.1770	0.8885	0.2402	-0.2399	-0.0637	0.1141	-0.
34.40375				//	-0.1624	0.0961	0.9507	-0.0021	0.0479	-0.0391	0.0580	-0.2312
59.74571	1.13998	-0.00000	0.66984	//	0.0164	0.1905	-0.1996	0.8660	0.3426	-0.0363	0.2260	0.0624
50.99081				//	-0.2789	0.0570	-0.1072	0.6583	0.4697	-0.0616	0.4996	0.0061
49.57501	0.20054	0.00000	-0.30842	//	-0.0770	-0.0547	0.3025	-0.2907	0.8993	-0.0139	0.0743	-0.0262
46.75221				//	0.0706	-0.6456	0.0485	-0.3039	0.6848	0.0326	-0.1157	-0.0084
67.28736	0.00415	-0.00000	-0.03809	//	0.0201	0.0437	0.0158	0.0569	0.0256	0.9393	-0.0388	-0.3314
58.49049				//	-0.0826	0.0545	-0.0961	0.0064	0.0238	0.8790	0.0101	-0.4557
7	0.62393	0.00000	0.44714	//	0.0905	-0.1124	-0.0461	-0.1912	-0.1208	0.0861	0.9552	0.0783
7	2568			//	0.0038	-0.1939	-0.	-0.4508	-0.2397	-0.0144	0.8358	-0.
81.20305	0.00117	-0.00000	-0.01841	//	0.0007	0.0042	0.1521	0.0090	-0.	0.3210	-0.0966	0.
79.06557				//	0.0406	0.0108	0.2267	0.0261	0.0032	0.4671	0.0799	0.8495





ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000

4.3300	5.1960	5.1960	4.3300	3.4640	2.5980	1.7320
2.0000	1.5000	0.5000	0.	0.5000	0.	0.5000

ANTHRACENE TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 SA	6 AA	7 AS	8 SS	9 SA	10 AA	11 AS	12 SS	13 AA	14 AS
1.595849	1.493616	1.349050	1.349035	1.246816	1.246799	1.102235	0.897763	0.753200	0.753183	0.650964	0.650949	0.506383	0.404149
0.214885	-0.288678	-0.281280	0.167406	0.408245	0.000861	0.310936	-0.310936	0.000125	-0.408246	-0.168318	0.280735	0.288678	-0.214885
0.151945	-0.288673	-0.117561	0.405893	0.204872	-0.353122	0.219871	0.219871	0.353491	0.204235	0.406272	-0.116243	-0.288673	0.151945
0.151945	-0.288673	0.115028	0.406618	-0.203380	-0.353983	-0.219871	0.219871	-0.353616	0.204018	-0.406242	-0.116347	0.288673	-0.151945
0.214885	-0.288678	0.280231	0.169157	-0.408245	-0.000861	-0.310936	0.310936	0.000126	-0.408246	0.168246	0.280778	-0.288678	0.214885
0.366827	-0.288673	0.281284	-0.167401	-0.204872	0.353122	0.091074	-0.091073	0.353491	0.204235	0.168313	-0.280739	0.288673	-0.366827
0.303893	0.000000	0.397790	-0.236748	0.000000	0.000000	0.439730	0.439730	-0.000000	0.000000	-0.238037	0.397020	-0.000000	0.303893
0.366826	0.288674	0.281284	-0.167401	0.204872	-0.353122	0.091073	-0.091074	-0.353491	-0.204235	0.168313	-0.280739	-0.288673	-0.366827
0.214885	0.288679	0.280231	0.169157	0.408245	0.000861	-0.310936	-0.310936	-0.000125	0.408246	0.168246	0.280778	0.288678	0.214885
0.151944	0.288674	0.115027	0.406618	0.203380	0.353983	-0.219871	0.219871	0.353616	-0.204018	-0.406242	-0.116347	-0.288673	-0.151945
0.151944	0.288673	-0.117561	0.405893	-0.204872	0.353122	0.219871	-0.219871	-0.353491	-0.204235	0.406272	-0.116243	0.288673	0.151944
0.214885	0.288678	-0.281280	0.167406	-0.408245	-0.000861	0.310936	-0.310936	-0.000125	0.408246	-0.168318	0.280735	-0.288678	-0.214885
0.366826	0.288673	-0.280234	-0.169152	-0.203380	-0.353983	-0.091074	0.091074	0.353616	-0.204018	-0.168242	-0.280782	0.288673	0.366827
0.303893	0.000000	-0.396306	-0.239224	-0.000000	-0.000000	-0.439730	0.439730	-0.000000	-0.000000	0.237936	0.397081	0.000000	-0.303893
0.366827	-0.288673	-0.280235	-0.169152	0.203380	0.353983	-0.091074	-0.091074	-0.353616	0.204018	-0.168241	-0.280782	-0.288673	0.366826

ANTHRACENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 SA	6 AA	7 AS	8 SS	9 SA	10AA	11 AS	12 SS	13 AA	14 AS
28.29244	25.04240	19.60583	19.60522	15.00019	14.99937	7.02833	-8.62919	-24.82915	-24.83140	-40.62936	-40.63195	-73.86477	111.71760
0.170102	-0.236208	-0.144885	-0.241724	0.000000	0.365615	0.296165	-0.328163	0.470399	-0.000000	-0.208618	0.347955	0.405672	-0.338014
0.120279	-0.236204	-0.349774	-0.100127	0.316631	0.182810	0.209426	0.232053	-0.235204	0.407385	0.503545	-0.144077	-0.405665	0.239009
0.120279	-0.236204	-0.349774	0.100127	0.316631	-0.182810	-0.209426	0.232053	-0.235204	-0.407385	-0.503509	-0.144205	0.405665	-0.239009
0.170102	-0.236208	-0.144885	0.241723	-0.000000	-0.365615	-0.296165	-0.328163	0.470399	0.000000	0.208529	0.348009	-0.405672	0.338014
0.290379	-0.236204	0.144881	0.241727	-0.316631	-0.182810	0.086747	-0.096119	-0.235204	0.407385	0.208612	-0.347960	0.405665	-0.577019
0.240561	0.000000	0.204898	0.341849	-0.000000	0.000000	0.418840	0.464093	-0.000000	-0.000000	-0.295030	0.492083	-0.000000	0.478024
0.290379	0.236204	0.144881	0.241727	0.316631	0.182810	0.086747	-0.096120	0.235204	-0.407385	0.208612	-0.347960	-0.405665	-0.577019
0.170102	0.236208	-0.144885	0.241723	-0.000000	0.365615	-0.296165	-0.328163	-0.470399	0.000000	0.208529	0.348009	0.405672	0.338014
0.120279	0.236204	-0.349774	0.100126	-0.316631	0.182810	-0.209426	0.232053	0.235204	0.407385	-0.503509	-0.144205	-0.405665	-0.239009
0.120279	0.236204	-0.349774	-0.100127	0.316631	-0.182810	0.209426	0.232053	0.235204	-0.407385	0.503545	-0.144077	0.405665	0.239009
0.170102	0.236208	-0.144885	-0.241724	0.000000	-0.365615	0.296165	-0.328163	-0.470399	0.000000	-0.208618	0.347955	-0.405672	-0.338014
0.290379	0.236204	0.144881	-0.241727	0.316631	-0.182811	-0.086747	-0.096119	0.235204	0.407385	-0.208523	-0.348013	0.405665	0.577019
0.240561	0.000000	0.204899	-0.341848	0.000000	-0.000000	-0.418841	0.464093	0.000000	0.000000	0.294905	0.492159	0.000000	-0.478024
0.290379	-0.236204	0.144881	-0.241727	-0.316631	0.182810	-0.086747	-0.096119	-0.235204	-0.407385	-0.208523	-0.348013	-0.405665	0.577019

ANTHRACENE (1) — TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.00000	0.73740	-0.00000	-0.36868	0.00000	0.10101	-0.00000	-0.03536	-0.00000	0.07073	0.00000	-0.13131	-0.00000	0.53536
2	0.73740	1.00000	0.58586	0.00000	-0.21718	-0.00000	0.11616	0.00000	-0.08080	-0.00000	0.07073	0.00000	-0.20204	-0.00000
3	-0.00000	0.58586	1.00000	0.73740	-0.00000	-0.20204	0.00000	0.07073	0.00000	-0.08080	-0.00000	0.11616	0.00000	-0.21718
4	-0.36868	0.00000	0.73740	1.00000	0.53536	0.00000	-0.13131	-0.00000	0.07073	0.00000	-0.03536	0.00000	0.10101	0.00000
5	0.00000	-0.21718	-0.00000	0.53536	1.00000	0.60610	-0.00000	-0.13131	0.00000	0.11616	0.00000	-0.18181	0.00000	0.48485
6	0.10101	-0.00000	-0.20204	0.00000	0.60610	1.00000	0.60610	0.00000	-0.20204	-0.00000	0.10101	0.00000	-0.40404	-0.00000
7	-0.00000	0.11616	0.00000	-0.13131	-0.00000	0.60610	1.00000	0.53536	-0.00000	-0.21718	-0.00000	0.48485	0.00000	-0.18181
8	-0.03536	0.00000	0.07073	-0.00000	-0.13131	0.00000	0.53536	1.00000	0.73740	0.00000	-0.36868	-0.00000	0.10101	0.00000
9	-0.00000	-0.08080	0.00000	0.07073	0.00000	-0.20204	-0.00000	0.73740	1.00000	0.58586	0.00000	-0.21718	0.00000	0.11616
10	0.07073	-0.00000	-0.08080	0.00000	0.11616	-0.00000	-0.21718	0.00000	0.58586	1.00000	0.73740	0.00000	-0.20204	-0.00000
11	0.00000	0.07073	-0.00000	-0.03536	0.00000	0.10101	-0.00000	-0.36868	0.00000	0.73740	1.00000	0.53536	-0.00000	-0.13131
12	-0.13131	0.00000	0.11616	0.00000	-0.18181	0.00000	0.48485	-0.00000	-0.21718	0.00000	0.53536	1.00000	0.60610	0.00000
13	-0.00000	-0.20204	0.00000	0.10101	0.00000	-0.40404	0.00000	0.10101	0.00000	-0.20204	-0.00000	0.60610	1.00000	0.60610
14	0.53536	-0.00000	-0.21718	0.00000	0.48485	-0.00000	-0.18181	0.00000	0.11616	-0.00000	-0.13131	0.00000	0.60610	1.00000

ANTHRACENE — TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.77108	0.55999	-0.05227	-0.34819	-0.03076	0.10529	0.01342	-0.03668	-0.00809	0.06947	0.01320	-0.12298	-0.06036	0.36755
2	0.55999	0.76032	0.41110	-0.05227	-0.19934	0.02151	0.11219	-0.00809	-0.07941	0.00245	0.06947	0.00266	-0.19244	-0.04151
3	-0.05227	0.41110	0.76032	0.55999	-0.04151	-0.19244	0.00266	0.06947	0.00245	-0.07941	-0.00809	0.11219	0.02151	-0.19934
4	-0.34819	-0.05227	0.55999	0.77108	0.36755	-0.06036	-0.12298	0.01320	0.06947	-0.00809	-0.03668	0.01342	0.10529	-0.03076
5	-0.03076	-0.19934	-0.04151	0.36755	0.72147	0.43701	-0.03640	-0.12298	0.00266	0.11219	0.01342	-0.16655	-0.03886	0.32396
6	0.10529	0.02151	-0.19244	-0.06036	0.43701	0.70428	0.43701	-0.06036	-0.19244	0.02151	0.10529	-0.03885	-0.38487	-0.03886
7	0.01342	0.11219	0.00266	-0.12298	-0.03640	0.43701	0.72147	0.36755	-0.04151	-0.19934	-0.03076	0.32396	-0.03885	-0.16655
8	-0.03668	-0.00809	0.06947	0.01320	-0.12298	-0.06036	0.36755	0.77108	0.55999	-0.05227	-0.34819	-0.03076	0.10529	0.01342
9	-0.00809	-0.07941	0.00245	0.06947	0.00266	-0.19244	-0.04151	0.55999	0.76032	0.41110	-0.05227	-0.19934	0.02151	0.11219
10	0.06947	0.00245	-0.07941	-0.00809	0.11219	0.02151	-0.19934	-0.05227	0.41110	0.76032	0.55999	-0.04151	-0.19244	0.00266
11	0.01320	0.06947	-0.00809	-0.03668	0.01342	0.10529	-0.03076	-0.34819	-0.05227	0.55999	0.77108	0.36755	-0.06036	-0.12298
12	-0.12298	0.00266	0.11219	0.01342	-0.16655	-0.03885	0.32396	-0.03076	-0.19934	-0.04151	0.36755	0.72147	0.43701	-0.03640
13	-0.06036	-0.19244	0.02151	0.10529	-0.03886	-0.38487	-0.03885	0.10529	0.02151	-0.19244	-0.06036	0.43701	0.78428	0.43701
14	0.36755	-0.04151	-0.19934	-0.03076	0.32396	-0.03886	-0.16655	0.01342	0.11219	-0.00266	-0.12298	-0.03640	0.43701	0.72147

ENERGIES FOR ANTHRACENE (S) ,TDH APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	5, 8	7,10	2, 8	3, 9	4,10	1, 9	6,11	5,12
XMOMNT	-0.93180	-0.93609	-0.05508	-0.27825	0.08700	-0.02793	-0.28105	0.08788
YMOMNT	0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000
JUMP E	23.6294	31.8597	33.6716	44.4350	44.4366	53.1216	55.6287	55.6321
DIAG E	33.6964	40.7052	47.5341	60.8215	55.8237	69.4456	71.3705	66.5691
DIAG E	37.3810	36.5291	50.0805	61.0672	53.6888	72.0173	72.7481	67.5969
CORRSP	28.2830	43.1569	46.4622	60.6290	52.7474	71.7677	73.8703	69.0496
CORRSP	42.2606	29.5347	47.5443	60.7091	52.0976	73.2814	74.9278	70.7534

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION							
28.28304	0.16213	-0.36715	0.00000	//	0.8394	-0.4740	0.1832	0.1570	-0.0132	0.0545	-0.0967	0.0063
24.70044				//	0.9637	0.1175	0.1293	0.1985	-0.0035	0.0254	0.0260	0.0058
43.15688	2.81837	-1.23923	0.00000	//	0.4242	0.8414	0.2874	-0.0099	-0.0423	0.0834	0.1408	0.0272
31.47685				//	-0.0911	0.8878	-0.3355	0.1160	-0.0546	-0.0917	0.2465	-0.0740
46.46220	0.34825	0.41983	0.00000	//	-0.2540	-0.2044	0.8429	-0.2671	-0.2777	0.1143	0.0713	0.1291
37.51028				//	-0.0720	0.4010	0.7534	-0.3853	0.1984	0.1349	-0.1032	0.2231
60.62902	0.08851	-0.18529	0.00000	//	-0.1487	0.0274	0.0496	0.7409	-0.5182	0.1947	0.0303	-0.3441
54.42726				//	-0.1767	0.0474	0.3116	0.6167	0.2079	0.3401	-0.0994	-0.5660
52.74739	0.02616	0.10800	-0.00000	//	-0.1433	0.0271	0.3544	0.3012	0.7609	0.1696	-0.2446	-0.3079
48.73511				//	0.0551	0.0270	-0.2910	-0.0208	0.8876	-0.1605	-0.3006	0.0846
71.76769	0.00308	0.03178	0.00000	//	0.0510	-0.0497	-0.1942	-0.3985	-0.0423	0.7972	0.1023	-0.3882
67.84104				//	0.1344	0.0581	-0.3096	-0.5290	-0.0454	0.6418	-0.2166	-0.3769
73.87028	0.07596	-0.15550	0.00000	//	0.0099	-0.1463	0.0301	0.1111	0.2344	-0.1051	0.9428	-0.1019
72.02334				//	-0.0115	-0.1727	0.0181	-0.1066	0.3510	0.2583	0.8766	0.0059
69.04959	0.00614	-0.04574	-0.00000	//	-0.0750	-0.0128	-0.0820	0.3052	0.1289	0.5137	0.0749	0.7799
68.64216				//	-0.0730	0.0333	-0.1588	0.3561	-0.0361	0.5939	-0.1111	0.6893

ENERGIES FOR ANTHRACENE (A) , TBM APPROXIMATION 1.7

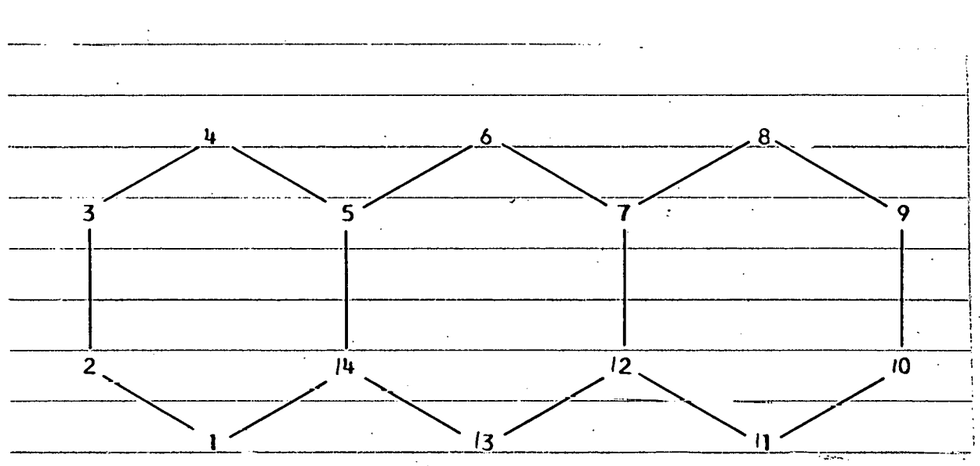
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	7, 8	4, 8	6, 9	5,10	7,12	2,10
XMOMNT	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000
YMOMNT	0.66365	-0.00000	-0.51595	-0.51596	0.00000	0.00000
JUMP E	15.6575	28.2344	39.8285	39.8316	47.6603	49.8738
DIAG E	26.8850	38.9078	56.7988	51.4717	56.6932	64.6455
DIAG E	27.3093	41.3733	57.3076	50.5559	54.4607	62.5914
CORRSP	26.0582	38.2129	61.1398	50.5129	54.2079	65.2703
CORRSP	26.4205	40.5744	60.7131	50.0473	53.0824	62.7604

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
26.05817	0.35880	-0.00000	0.56903	//	0.9832	0.0465	-0.0053	0.1671	0.0161	0.0537
11.88169				//	0.9755	0.1109	-0.1729	0.0400	0.0662	-0.0133
38.21294	0.01766	-0.00000	-0.10426	//	-0.0404	0.9810	0.1814	-0.0313	-0.0420	0.0180
26.47723				//	-0.0373	0.8362	0.4394	-0.0343	0.3230	0.0288
61.13984	0.61389	-0.00000	-0.48592	//	-0.0122	-0.1582	0.7365	0.1896	-0.6289	0.0309
47.13264				//	0.1123	-0.5250	0.5601	0.1045	0.6221	-0.0102
50.51291	0.22186	-0.00000	-0.32138	//	-0.1542	0.0841	-0.4169	0.8414	-0.2447	0.1655
40.25331				//	-0.0577	0.0772	-0.0717	0.9768	-0.0210	0.1763
54.20785	0.66958	-0.00000	-0.53895	//	-0.0856	-0.0524	0.5007	0.4337	0.7366	0.0925
57.09566				//	-0.1644	0.0608	-0.6600	-0.0866	0.6932	0.2138
65.27033	0.02312	-0.00000	0.09126	//	-0.0186	-0.0248	-0.0031	0.1977	-0.0085	0.9797
59.49349				//	0.0630	-0.0568	0.1505	-0.1573	-0.1526	0.9603

ANTHRACENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000

4.3300	5.1960	5.1960	4.3300	3.4640	2.5980	1.7320
2.0000	1.5000	0.5000	0.	0.5000	0.	0.5000

ANTHRACENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 AA	6 SA	7 AS	8 SS	9 SA	10 AA	11 SS	12 AS	13 AA	14 AS
1.731461	1.562966	1.341954	1.319912	1.193557	1.171007	1.027817	0.842955	0.724920	0.724622	0.658277	0.650193	0.553518	0.496830
0.220400	-0.293654	0.165194	-0.286668	0.410213	0.028603	-0.304297	0.316541	0.403668	0.018046	-0.271912	0.182764	-0.285308	-0.204504
0.165079	-0.303864	0.397387	-0.116501	0.206248	-0.344983	-0.228410	-0.231776	-0.196576	-0.364204	0.105413	-0.405511	0.273547	0.140774
0.165079	-0.303864	0.397387	0.116502	-0.206248	-0.344983	0.228410	-0.231776	-0.196633	0.364174	0.105414	0.405511	-0.273547	-0.140774
0.220400	-0.293654	0.165194	0.286668	-0.410213	0.028604	0.304297	0.316540	0.403671	-0.017983	-0.271913	-0.182764	0.285307	0.204504
0.358150	-0.267271	-0.173284	0.270952	-0.197956	0.360789	-0.094542	0.089553	-0.219968	-0.342131	0.289277	-0.156009	-0.306221	-0.378560
0.302988	0.000000	-0.263693	0.402079	0.000000	-0.000000	-0.438849	-0.419672	0.000000	0.000000	-0.403162	0.235879	-0.000000	0.300176
0.358150	0.267271	-0.173284	0.270952	0.197956	-0.360789	-0.094542	0.089554	0.219968	0.342131	0.289277	-0.156009	0.306221	-0.378560
0.220400	0.293654	0.165194	0.286668	0.410213	-0.028603	0.304297	0.316540	-0.403671	0.017983	-0.271913	-0.182764	-0.285308	0.204504
0.165079	0.303864	0.397387	0.116501	0.206249	0.344983	0.228410	-0.231776	0.196633	-0.364174	0.105414	0.405511	0.273547	-0.140774
0.165079	0.303864	0.397388	-0.116501	-0.206248	0.344983	-0.228410	-0.231775	0.196576	0.364204	0.105414	-0.405511	-0.273547	0.140774
0.220400	0.293654	0.165195	-0.286668	-0.410213	-0.028603	-0.304297	0.316540	-0.403668	-0.018046	-0.271913	0.182764	0.285307	-0.204504
0.358150	0.267271	-0.173283	-0.270952	-0.197957	-0.360789	0.094542	0.089554	0.220021	-0.342097	0.289278	0.156009	-0.306221	0.378560
0.302988	0.000000	-0.263692	-0.402079	-0.000000	-0.000000	0.438848	-0.419672	0.000000	0.000000	-0.403162	-0.235879	-0.000000	-0.300176
0.358150	-0.267271	-0.173283	-0.270952	0.197956	0.360788	0.094542	0.089553	-0.220021	0.342097	0.289278	0.156008	0.306221	0.378560

ANTHRACENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 AA	6 SA	7 AS	8 SS	9 SA	10 AA	11 SS	12 AS	13 AA	14 AS
32.01138	27.29344	19.30882	18.36585	12.28830	11.06574	2.05080	-14.11706	-28.75384	-28.79671	-39.33605	-40.76728	-61.12201	-76.74188
0.167497	-0.234889	0.142602	-0.249521	0.375481	0.026432	-0.300151	0.344768	0.474110	0.021199	-0.335139	0.226657	-0.383484	-0.290134
0.125455	-0.243055	0.343040	-0.101404	0.188785	-0.318800	-0.225298	-0.252444	-0.230880	-0.427848	0.129924	-0.502900	0.367677	0.199718
0.125455	-0.243055	0.343040	0.101405	-0.188786	-0.318799	0.225298	-0.252444	-0.230947	0.427812	0.129925	0.502899	-0.367677	-0.199718
0.167497	-0.234888	0.142602	0.249521	-0.375481	0.026433	0.300151	0.344768	0.474114	-0.021126	-0.335139	-0.226657	0.383484	0.290134
0.272181	-0.213785	-0.149585	0.235841	-0.181195	0.333406	-0.093254	0.097539	-0.258354	-0.401917	0.356541	-0.193476	-0.411594	-0.537070
0.230261	0.000000	-0.227630	0.349976	0.000000	-0.000000	-0.432869	-0.457096	0.000000	0.000000	-0.496907	0.292529	-0.000000	0.425865
0.272182	0.213785	-0.149585	0.235841	0.181195	-0.333406	-0.093254	0.097540	0.258353	0.401917	0.356541	-0.193477	0.411594	-0.537070
0.167497	0.234888	0.142602	0.249521	0.375481	-0.026432	0.300151	0.344768	-0.474113	0.021126	-0.335140	-0.226657	-0.383484	0.290134
0.125455	0.243055	0.343040	0.101405	0.188786	0.318800	0.225298	-0.252444	0.230947	-0.427812	0.129925	0.502900	0.367677	-0.199718
0.125455	0.243055	0.343041	-0.101404	-0.188785	0.318800	-0.225298	-0.252444	0.230880	0.427847	-0.129925	-0.502900	-0.367677	0.199718
0.167497	0.234888	0.142602	-0.249521	-0.375481	-0.026432	-0.300151	0.344768	-0.474110	-0.021199	-0.335139	0.226657	0.383484	-0.290134
0.272181	0.213785	-0.149585	-0.235841	-0.181196	-0.333406	0.093254	0.097540	0.258416	-0.401877	0.356542	0.193476	-0.411594	0.537070
0.230260	0.000000	-0.227629	-0.349977	-0.000000	-0.000000	0.432869	-0.457096	0.000000	0.000000	-0.496907	-0.292528	-0.000000	-0.425865
0.272181	-0.213785	-0.149585	-0.235842	0.181196	0.333406	0.093254	0.097539	-0.258416	0.401877	0.356542	0.193476	0.411595	0.537070

ANTHRACENE

IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.01193	0.73780	-0.01223	-0.36027	0.01801	0.08299	-0.01239	-0.03537	0.00874	0.08192	-0.00937	-0.14159	0.00988	0.53845
2	0.73780	1.00959	0.57647	-0.01223	-0.20758	-0.00275	0.12874	0.00874	-0.09877	-0.00595	0.08192	0.00532	-0.21633	-0.00438
3	-0.01223	0.57647	1.00959	0.73780	-0.00438	-0.21633	0.00532	0.08192	-0.00595	-0.09877	0.00874	0.12874	-0.00275	-0.20758
4	-0.36027	-0.01223	0.73780	1.01193	0.53845	0.00988	-0.14159	-0.00937	0.08192	0.00874	-0.03537	-0.01239	0.08299	0.01801
5	0.01801	-0.20758	-0.00438	0.53845	0.96288	0.60929	-0.00027	-0.14159	0.00532	0.12874	-0.01239	-0.17294	0.00755	0.47672
6	0.08299	-0.00275	-0.21633	0.00988	0.60929	1.03118	0.60929	0.00988	-0.21633	-0.00275	0.08299	0.00755	-0.38584	0.00755
7	-0.01239	0.12874	0.00532	-0.14159	-0.00027	0.60929	0.96288	0.53845	-0.00438	-0.20758	0.01801	0.47672	0.00755	-0.17294
8	-0.03537	0.00874	0.08192	-0.00937	-0.14159	0.00988	0.53845	1.01193	0.73780	-0.01223	-0.36027	0.01801	0.08299	-0.01239
9	0.00874	-0.09877	-0.00595	0.08192	0.00532	-0.21633	-0.00438	0.73780	1.00959	0.57646	-0.01223	-0.20758	-0.00275	0.12874
10	0.08192	-0.00595	-0.09877	0.00874	0.12874	-0.00275	-0.20758	-0.01223	0.57646	1.00959	0.73780	-0.00438	-0.21633	0.00532
11	-0.00937	0.08192	0.00874	-0.03537	-0.01239	0.08299	0.01801	-0.36027	-0.01223	0.73780	1.01193	0.53845	0.00988	-0.14159
12	-0.14159	0.00532	0.12874	-0.01239	-0.17294	0.00755	0.47672	0.01801	-0.20758	-0.00438	0.53845	0.96288	0.60929	-0.00027
13	0.00988	-0.21633	-0.00275	0.08299	0.00755	-0.38584	0.00755	0.08299	-0.00275	-0.21633	0.00988	0.60929	1.03118	0.60929
14	0.53845	-0.00438	-0.20758	0.01801	0.47672	0.00755	-0.17294	-0.01239	0.12874	0.00532	-0.14159	-0.00027	0.60929	0.96288

ANTHRACENE

IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.79520	0.56481	-0.09043	-0.37815	-0.03121	0.09741	0.00482	-0.03769	-0.00155	0.08662	0.00777	-0.14390	-0.07298	0.36436
2	0.56481	0.78161	0.39489	-0.09043	-0.21722	0.02567	0.13692	-0.00155	-0.10539	-0.00378	0.08662	0.01172	-0.22247	-0.06877
3	-0.09043	0.39489	0.78161	0.56481	-0.06877	-0.22247	0.01172	0.08662	-0.00378	-0.10539	-0.00155	0.13692	0.02567	-0.21722
4	-0.37815	-0.09043	0.56481	0.79520	0.36436	-0.07298	-0.14390	0.00777	0.08662	-0.00155	-0.03769	0.00482	0.09741	-0.03121
5	-0.03121	-0.21722	-0.06877	0.36436	0.70094	0.43926	-0.05784	-0.14390	0.01172	0.13692	0.00482	-0.18378	-0.05237	0.31235
6	0.09741	0.02567	-0.22247	-0.07298	0.43926	0.82939	0.43926	-0.07298	-0.22247	0.02567	0.09741	-0.05237	-0.41005	-0.05237
7	0.00482	0.13692	0.01172	-0.14390	-0.05784	0.43926	0.70094	0.36436	-0.06877	-0.21722	-0.03121	0.31235	-0.05237	-0.18378
8	-0.03769	-0.00155	0.08662	0.00777	-0.14390	-0.07298	0.36436	0.79520	0.56481	-0.09043	-0.37815	-0.03121	0.09741	0.00482
9	-0.00155	-0.10539	-0.00378	0.08662	0.01172	-0.22247	-0.06877	0.56481	0.78161	0.39489	-0.09043	-0.21722	0.02567	0.13692
10	0.08662	-0.00378	-0.10539	-0.00155	0.13692	0.02567	-0.21722	-0.09043	0.39489	0.78161	0.56481	-0.06877	-0.22247	0.01172
11	0.00777	0.08662	-0.00155	-0.03769	0.00482	0.09741	-0.03121	-0.37815	-0.09043	0.56481	0.79520	0.36436	-0.07298	-0.14390
12	-0.14390	0.01172	0.13692	0.00482	-0.18378	-0.05237	0.31235	-0.03121	-0.21722	-0.06877	0.36436	0.70094	0.43926	-0.05784
13	-0.07298	-0.22247	0.02567	0.09741	-0.05237	-0.41005	-0.05237	0.09741	0.02567	-0.22247	-0.07298	0.43926	0.82939	0.43926
14	0.36436	-0.06877	-0.21722	-0.03121	0.31235	-0.05237	-0.18378	0.00482	0.13692	0.01172	-0.14390	-0.05784	0.43926	0.70094

ENERGIES FOR ANTHRACENE (1) , TRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	6, 8	7,10	2, 8	4,10	3, 9	6,11	5,12
XMOMNT	-1.01919	-0.95288	-0.00524	-0.08784	0.22828	0.07320	0.25404
YMOMNT	0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000
JUMP E	25.1828	30.8475	41.4105	47.1626	48.0627	50.4018	53.0556
DIAG E	35.5427	39.8427	55.7431	58.9456	63.8204	60.3959	69.2959
DIAG E	39.6205	35.8180	58.1897	56.9473	63.8503	61.4220	70.7728
CORRSP	29.2843	43.8884	57.1621	51.5520	67.8481	61.5309	72.3203
CORRSP	43.7808	29.5550	58.8088	51.5417	68.4495	61.1827	73.3020

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION						
29.28433	0.08684	-0.26407	0.00000	//	0.7931	-0.5738	-0.0784	0.0000	-0.1479	0.0186	0.1160
25.77019				//	0.9555	0.2143	-0.0302	0.0126	-0.1909	0.0220	-0.0554
43.88839	3.63052	-1.39472	-0.00000	//	0.5755	0.7978	-0.0950	0.0347	-0.0598	0.0280	-0.1330
30.70680				//	-0.2228	0.9258	0.1608	0.0596	-0.0336	-0.0581	-0.2435
57.16207	0.03341	-0.11724	0.00000	//	0.0936	-0.0174	0.8437	0.3554	0.0459	0.3559	-0.1547
56.29748				//	0.0539	-0.0556	0.6428	-0.0941	0.2005	0.7267	-0.0603
51.55201	0.03562	0.12746	0.00000	//	-0.0216	-0.0958	-0.4982	0.5634	0.3882	0.4640	-0.2423
52.36938				//	0.0142	-0.0830	-0.2398	0.8429	0.2034	0.2277	-0.3629
67.84814	0.00017	-0.00770	0.00000	//	0.1682	-0.0418	0.1541	-0.0706	0.8206	-0.5019	-0.1261
67.27999				//	0.1831	0.0076	0.2758	0.0298	0.8140	-0.4735	0.0514
61.53091	0.05923	0.15045	-0.00000	//	0.0475	0.0279	0.0193	-0.6677	0.3451	0.6364	0.1637
42.22448				//	0.0249	0.2360	-0.6405	-0.2966	0.4597	0.4351	0.2118
72.32029	0.02714	0.09395	0.00000	//	0.0079	-0.1491	0.0245	0.3228	0.1713	-0.0017	0.9184
70.70317				//	-0.0088	0.1767	0.1274	0.4336	-0.0830	0.0526	0.8688

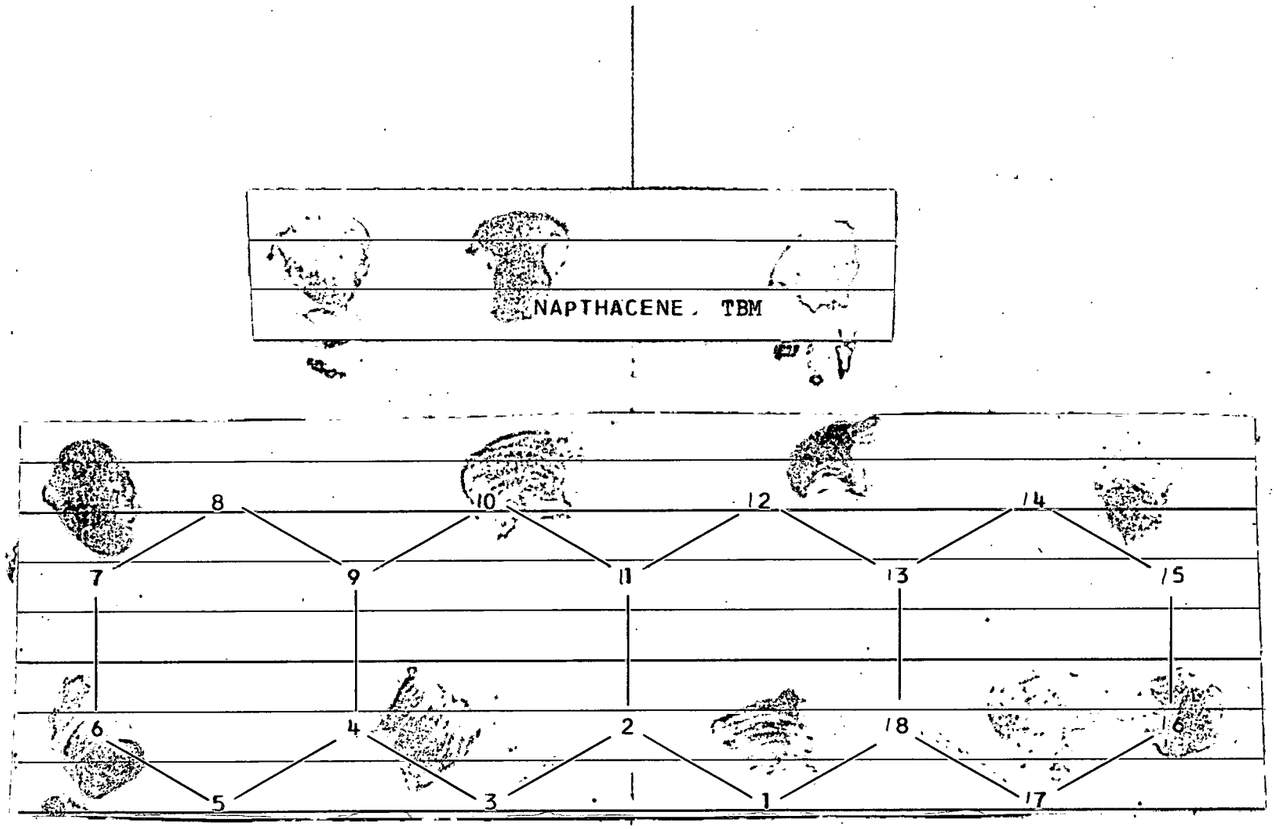
ENERGIES FOR ANTHRACENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	7, 8	4, 8	6,10	5, 9	7,11	2,10	4,11
XMOMNT	0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.00000	-0.00000
YMOMNT	0.63392	0.02052	-0.51467	-0.50960	0.01675	-0.01859	-0.48246
JUMP E	16.1679	32.4829	39.8624	41.0421	41.3868	56.0901	57.7019
DIAG E	26.3678	43.4636	50.9404	57.6934	49.7774	71.3554	72.9637
DIAG E	26.8369	45.9590	50.5246	57.8481	47.1946	69.3082	72.4072
CORRSP	25.3991	42.5180	50.5741	59.9867	48.2000	71.6110	74.2726
CORRSP	25.6943	44.7010	50.3051	59.9048	46.1395	69.3913	73.9426

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION						
25.39907	0.28984	0.00000	0.51802	//	0.9851	-0.0115	0.1467	-0.0085	0.0304	-0.0373	0.0751
11.21822				//	0.9607	-0.0831	0.0491	-0.1944	0.0994	0.0157	-0.1411
42.51805	0.01075	-0.00000	0.07711	//	-0.0005	0.9755	0.0281	-0.1969	0.0701	0.0188	0.0606
28.46389				//	0.0264	0.7352	0.0385	-0.4597	-0.4922	0.0334	0.0502
50.57415	0.35038	-0.00000	-0.40363	//	-0.1383	-0.0667	0.8981	-0.1323	0.3491	-0.0878	-0.1507
40.18913				//	-0.0863	-0.0883	0.9823	-0.0834	0.0045	-0.0768	-0.0840
59.98670	1.22692	0.00000	-0.69352	//	-0.0358	0.1807	0.2817	0.8757	-0.3055	-0.0136	0.1627
50.54252				//	0.2563	0.0869	0.1359	0.6936	-0.4415	0.0470	0.4796
48.20002	0.00218	-0.00000	-0.03264	//	0.0184	0.0230	-0.2757	0.3905	0.8774	0.0271	0.0038
45.44790				//	0.0453	0.6333	0.0900	0.2733	0.7107	0.0163	0.0929
71.61102	0.00767	-0.00000	-0.05018	//	0.0227	-0.0240	0.0965	-0.0086	0.0036	0.9947	0.0008
65.60390				//	-0.0355	-0.0559	0.0668	-0.0515	0.0378	0.9933	0.0222
74.27261	0.75329	-0.00000	-0.48836	//	-0.0918	-0.1007	0.0801	-0.1560	0.0953	-0.0106	0.9703
70.76007				//	0.0007	-0.1816	0.0146	-0.4307	0.2152	-0.0608	0.8552



ATOMIC COORDINATES

X	4.3300	3.4640	2.5980	1.7320	0.8660	0.	0.	0.8660	1.7320	
y	0.	0.5000	0.	0.5000	0.	0.5000	1.5000	2.0000	1.5000	

	2.5980	3.4640	4.3300	5.1960	6.0620	6.9280	6.9280	6.0620	5.1960	
	2.0000	1.5000	2.0000	1.5000	2.0000	1.5000	0.5000	0.	0.5000	

NAPTHACENE TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 SA	6 AA	7 SS	8 AS	9 AA	10 SA	11 SS	12 AS	13 SA	14 AA	15 SS	16 AS	17 AA	18 AS
1.608811	1.541381	1.438695	1.362011	1.319602	1.294581	1.246799	1.191896	1.072802	0.927196	0.808103	0.753199	0.705417	.680397	0.637987	0.561303	0.458618	0.391187
0.259724	0.156043	-0.145009	0.336816	0.183200	-0.211540	-0.000000	0.219251	0.383848	0.383847	0.219251	-0.000000	-0.211539	-0.183201	0.336816	-0.145008	-0.156042	-0.259724
0.354149	0.000000	-0.373012	0.273090	-0.000000	0.000000	0.316228	0.246703	0.000000	0.000000	-0.246703	-0.316228	0.000000	-0.000000	-0.273090	0.373012	-0.000000	0.354149
0.259724	-0.156043	-0.145009	0.336815	-0.183201	0.211540	-0.000000	0.219251	-0.383847	-0.383848	0.219251	0.000000	0.211539	0.183201	0.336816	-0.145008	0.156043	-0.259724
0.286513	-0.342278	0.115267	0.220934	-0.237231	0.252483	-0.316228	-0.076235	-0.113224	0.113224	0.076235	0.316227	-0.252482	-0.237231	-0.220935	-0.115267	-0.342278	0.286513
0.160519	-0.252482	0.234628	0.208164	0.113225	0.342278	-0.000000	-0.354755	0.237231	0.237231	-0.354755	0.000000	0.342278	-0.113224	0.208164	0.234628	0.252482	-0.160518
0.109438	-0.211540	0.301773	0.084390	0.383848	0.156042	0.316228	-0.199587	0.183201	-0.183201	0.199587	-0.316228	-0.156043	0.383847	-0.084389	-0.301773	-0.211540	0.109438
0.109438	-0.211540	0.301773	-0.084389	0.383847	-0.156043	0.316227	0.199587	-0.183201	-0.183201	0.199587	0.316228	-0.156042	-0.383848	-0.084389	0.301773	0.211540	-0.109438
0.160518	-0.252482	0.234628	-0.208163	0.113224	-0.342279	-0.000000	0.354755	-0.237231	0.237231	-0.354755	0.000000	0.342278	0.113225	0.208164	-0.234628	-0.252482	0.160518
0.286513	-0.342278	0.115267	-0.220935	-0.237231	-0.252482	-0.316227	0.076235	0.113225	0.113224	0.076235	-0.316228	-0.252482	0.237230	-0.220935	0.115267	0.342278	-0.286513
0.259724	-0.156042	-0.145008	-0.336816	-0.183201	-0.211539	0.000000	-0.219251	0.383847	-0.383848	0.219250	0.000000	0.211540	-0.183201	0.336816	0.145008	-0.156043	0.259724
0.354149	-0.000000	-0.373011	-0.273090	0.000001	0.000000	0.316228	-0.246703	-0.000000	0.000000	-0.246703	0.316228	-0.000000	0.000000	-0.273090	-0.373012	0.000000	-0.354149
0.259724	0.156042	-0.145008	-0.336816	0.183202	0.211539	-0.000000	-0.219250	-0.383848	0.383848	0.219251	-0.000000	-0.211540	0.183201	0.336816	0.145008	0.156042	0.259724
0.286513	0.342278	0.115267	-0.220934	0.237232	0.252481	-0.316228	0.076236	-0.113224	-0.113225	0.076235	-0.316227	0.252483	-0.237231	-0.220935	0.115267	-0.342278	-0.286513
0.160519	0.252482	0.234628	-0.208164	-0.113224	0.342278	0.000000	0.354755	0.237231	-0.237231	-0.354755	-0.000000	-0.342278	-0.113225	0.208164	-0.234628	0.252482	0.160518
0.109438	0.211540	0.301773	-0.084390	-0.383847	0.156043	0.316228	0.199587	0.183201	0.183201	0.199587	0.316228	0.156042	0.383848	-0.084390	0.301773	-0.211540	-0.109438
0.109438	0.211540	0.301773	0.084389	-0.383848	-0.156041	0.316228	-0.199587	-0.183201	0.183201	0.199587	-0.316228	-0.156043	-0.383848	-0.084389	-0.301773	0.211540	0.109438
0.160519	0.252482	0.234628	0.208164	-0.113225	-0.342278	-0.000000	-0.354755	-0.237231	-0.237231	-0.354755	-0.000000	-0.342278	0.113224	0.208164	0.234628	-0.252482	-0.160518
0.286513	0.342278	0.115267	0.220935	0.237230	-0.252483	-0.316228	-0.076235	0.113224	-0.113224	0.076235	0.316228	0.252482	0.237231	-0.220935	-0.115267	0.342278	0.286513

NAPTHACENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 SA	6 AA	7 SS	8 AS	9 AA	10 SA	11 SS	12AS	13 SA	14 AA	15 SS	16 AS	17 AA	18 AS
28.52848	26.47853	22.98769	20.03745	18.25859	17.15443	14.92270	12.13746	5.11591	-5.91947	-17.90209	-24.70230	-31.48200	-35.41201	-42.77738	-58.92084	-88.99272	117.32773
0.204767	0.125686	-0.120895	0.288604	0.159479	-0.185921	-0.000000	0.200827	0.370595	0.398633	0.243898	-0.000000	-0.251865	-0.222099	0.421684	-0.193550	-0.230419	0.415260
0.279212	0.000000	-0.310984	0.234000	-0.000000	0.000000	0.283205	0.225972	0.000000	0.000000	-0.274436	-0.364372	0.000000	-0.000000	-0.341901	0.497879	-0.000000	0.566231
0.204767	-0.125686	-0.120895	0.288603	-0.159480	0.185921	-0.000000	0.200827	-0.370594	-0.398633	0.243898	0.000000	0.251865	0.222099	0.421684	-0.193550	0.230419	-0.415260
0.225887	-0.275692	0.096099	0.189310	-0.206514	0.221905	-0.283206	-0.069829	-0.109315	0.117586	0.084805	0.364372	-0.300613	-0.287601	-0.276604	-0.153853	-0.505422	0.458091
0.126553	-0.203365	0.195612	0.178367	0.098565	0.300825	-0.000000	-0.324945	0.229040	0.246369	-0.394635	0.000000	0.407527	-0.137264	0.260615	0.313171	0.372825	-0.256645
0.086281	-0.170387	0.251591	0.072311	0.334147	0.137144	0.283205	-0.182815	0.176876	-0.190258	0.222023	-0.364372	-0.185789	0.465348	-0.105653	-0.402792	-0.312368	0.174975
0.086281	-0.170387	0.251591	-0.072309	0.334147	-0.137145	0.283205	0.182815	-0.176876	-0.190258	0.222023	0.364372	-0.185788	-0.465348	-0.105653	0.402792	0.312368	-0.174975
0.126553	-0.203365	0.195612	-0.178367	0.098563	-0.300826	-0.000000	0.324945	-0.229040	0.246369	-0.394635	0.000000	0.407527	0.137266	0.260615	-0.313171	-0.372825	0.256645
0.225887	-0.275692	0.096099	-0.189310	-0.206515	-0.221904	-0.283205	0.069829	0.109315	0.117586	0.084805	-0.364372	-0.300613	0.287600	-0.276604	0.153853	0.505422	-0.458091
0.204767	-0.125686	-0.120895	-0.288604	-0.159480	-0.185920	0.000000	-0.200827	0.370595	-0.398633	0.243897	0.000000	0.251866	-0.222099	0.421683	0.193550	-0.230419	0.415260
0.279212	-0.000000	-0.310984	-0.234000	0.000001	0.000000	0.283206	-0.225972	-0.000000	0.000000	-0.274436	0.364372	-0.000000	0.000000	-0.341901	-0.497879	0.000000	-0.566231
0.204767	0.125686	-0.120895	-0.288604	0.159481	0.185920	-0.000000	-0.200827	-0.370595	0.398633	0.243898	-0.000000	-0.251866	0.222099	0.421684	0.193550	0.230419	0.415260
0.225887	0.275692	0.096099	-0.189310	0.206515	0.221904	-0.283206	0.069829	-0.109315	-0.117586	0.084805	-0.364372	0.300613	-0.287601	-0.276604	0.153853	-0.505422	-0.458091
0.126553	0.203365	0.195612	-0.178367	0.098563	0.300826	0.000000	0.324945	0.229040	-0.246368	-0.394635	-0.000000	-0.407527	-0.137265	0.260615	-0.313171	0.372825	0.256645
0.086281	0.170387	0.251591	-0.072310	-0.334146	0.137145	0.283206	0.182815	0.176876	0.190258	0.222023	0.364372	0.185788	0.465348	-0.105653	-0.402792	0.312368	0.174975
0.086281	0.170387	0.251591	0.072310	-0.334147	-0.137144	0.283206	-0.182815	-0.176876	0.190258	0.222023	-0.364372	0.185790	-0.465348	-0.105653	-0.402792	0.312368	-0.174975
0.126553	0.203365	0.195612	0.178367	-0.098565	-0.300825	-0.000000	-0.324945	-0.229040	-0.246368	-0.394635	-0.000000	-0.407527	0.137264	0.260615	0.313171	-0.372825	-0.256645
0.225887	0.275692	0.096099	0.189310	0.206513	-0.221905	-0.283206	-0.069829	0.109315	-0.117586	0.084805	0.364372	0.300612	-0.287601	-0.276604	-0.153853	0.505422	0.458091

NAPTHACENE TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.00000	0.58428	-0.00000	-0.15669	-0.00000	0.08791	0.00000	-0.04395	0.00000	0.12229	-0.00000	-0.41442	0.00000	0.10529	-0.00000	-0.21059	0.00000	0.61828
2	0.58428	1.00000	0.58428	-0.00000	-0.12269	0.00000	0.10477	-0.00000	-0.16611	-0.00000	0.45824	0.00000	-0.16611	0.00000	0.10477	0.00000	-0.12269	-0.00000
3	-0.00000	0.58428	1.00000	0.61828	0.00000	-0.21059	-0.00000	0.10529	-0.00000	-0.41442	0.00000	0.12229	-0.00000	-0.04395	0.00000	0.08791	-0.00000	-0.15669
4	-0.15669	-0.00000	0.61828	1.00000	0.53038	-0.00000	-0.21006	0.00000	0.47524	0.00000	-0.16611	-0.00000	0.08777	0.00000	-0.06082	0.00000	0.05391	-0.00000
5	-0.00000	-0.12269	-0.00000	0.53038	1.00000	0.74097	0.00000	-0.37047	-0.00000	0.10529	0.00000	-0.04395	0.00000	0.01700	-0.00000	-0.03400	0.00000	0.05391
6	0.08791	0.00000	-0.21059	-0.00000	0.74097	1.00000	0.58053	-0.00000	-0.21006	0.00000	0.10477	-0.00000	-0.06082	-0.00000	0.04382	-0.00000	-0.03400	0.00000
7	0.00000	0.10477	-0.00000	-0.21006	0.00000	0.58053	1.00000	0.74097	0.00000	-0.21059	-0.00000	0.08791	0.00000	-0.03400	-0.00000	0.04382	-0.00000	-0.06082
8	-0.04395	0.00000	-0.10529	0.00000	-0.37047	-0.00000	0.74097	1.00000	0.53038	-0.00000	-0.12269	0.00000	0.05391	-0.00000	-0.03400	0.00000	0.01700	-0.00000
9	0.00000	-0.16611	-0.00000	0.47524	-0.00000	-0.21006	0.00000	0.53038	1.00000	0.61828	0.00000	-0.15668	-0.00000	0.05391	0.00000	-0.06082	-0.00000	0.08777
10	0.12229	-0.00000	-0.41442	0.00000	0.10529	0.00000	-0.21059	-0.00000	0.61828	1.00000	0.58428	-0.00000	-0.15669	0.00000	0.08791	0.00000	-0.04395	-0.00000
11	-0.00000	0.45824	-0.00000	-0.16611	0.00000	0.10477	-0.00000	-0.12269	0.00000	0.58428	1.00000	0.58428	0.00000	-0.12269	-0.00000	0.10477	0.00000	-0.16611
12	-0.41442	0.00000	0.12229	-0.00000	-0.04395	-0.00000	0.08791	0.00000	-0.15668	-0.00000	0.58428	1.00000	0.61828	0.00000	-0.21059	-0.00000	0.10529	0.00000
13	0.00000	-0.16611	-0.00000	0.08777	-0.00000	-0.06082	0.00000	0.05391	-0.00000	-0.15669	0.00000	0.61828	1.00000	0.53038	0.00000	-0.21006	-0.00000	0.47524
14	0.10529	-0.00000	-0.04395	0.00000	0.01700	-0.00000	-0.03400	-0.00000	0.05391	0.00000	-0.12269	0.00000	0.53038	1.00000	0.74097	-0.00000	-0.37047	-0.00000
15	0.00000	0.10477	-0.00000	-0.06082	-0.00000	0.04382	-0.00000	-0.03400	0.00000	0.08791	-0.00000	-0.21059	0.00000	0.74097	1.00000	0.58053	-0.00000	-0.21006
16	-0.21059	-0.00000	0.08791	-0.00000	-0.03400	-0.00000	0.04382	-0.00000	-0.06082	-0.00000	0.10477	-0.00000	-0.21006	0.00000	0.58053	1.00000	0.74097	-0.00000
17	-0.00000	0.12269	-0.00000	0.05391	-0.00000	-0.03400	-0.00000	0.01700	-0.00000	-0.04395	-0.00000	0.10529	-0.00000	-0.37047	-0.00000	0.74097	1.00000	0.53038
18	0.61828	-0.00000	-0.15669	0.00000	0.05391	-0.00000	-0.06082	-0.00000	0.08777	-0.00000	-0.16611	-0.00000	0.47524	-0.00000	-0.21006	-0.00000	0.53038	1.00000

NAPTHACENE

TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.78661	0.41537	-0.06594	-0.14821	0.01519	-0.08666	-0.01016	-0.04549	0.01641	0.12719	-0.03629	-0.39551	0.04032	-0.10968	0.02255	-0.20104	-0.06125	0.44920
2	0.41537	0.72139	0.41537	-0.03700	-0.11438	0.00333	0.10089	0.01239	-0.15108	-0.03629	0.29811	-0.03629	-0.15108	-0.01239	0.10089	0.00333	-0.11438	-0.03700
3	-0.06594	0.41537	0.78661	0.44920	-0.06125	-0.20104	-0.02255	-0.10968	-0.04032	-0.39551	-0.03629	-0.12719	-0.01641	-0.04549	-0.01016	-0.08666	-0.01519	-0.14821
4	-0.14821	-0.03700	0.44920	0.72205	-0.36254	-0.04203	-0.19224	-0.03016	0.31443	-0.04032	-0.15108	-0.01641	-0.08458	-0.00613	-0.05973	-0.00170	-0.05283	-0.00267
5	-0.01519	-0.11438	-0.06125	-0.36254	0.77142	-0.56358	-0.05270	-0.35001	-0.03016	-0.10968	-0.01239	-0.04549	-0.00613	-0.01752	-0.00403	-0.03384	-0.00469	-0.05283
6	-0.08666	-0.00333	-0.20104	-0.04203	-0.56358	0.76076	-0.40578	-0.05270	-0.19224	-0.02255	-0.10089	-0.01016	-0.05973	-0.00403	-0.04341	-0.00236	-0.03384	-0.00170
7	-0.01016	-0.10089	-0.02255	-0.19224	-0.05270	-0.40578	0.76076	-0.56358	-0.04203	-0.20104	-0.00333	-0.08666	-0.00170	-0.03384	-0.00236	-0.04341	-0.00403	-0.05973
8	-0.04549	-0.01239	-0.10968	-0.03016	-0.35001	-0.05270	-0.56358	0.77142	-0.36254	-0.06125	-0.11438	-0.01519	-0.05283	-0.00469	-0.03384	-0.00403	-0.01752	-0.00613
9	-0.01641	-0.15108	-0.04032	-0.31443	-0.03016	-0.19224	-0.04203	-0.36254	0.72205	-0.44920	-0.03700	-0.14821	-0.00267	-0.05283	-0.00170	-0.05973	-0.00613	-0.08458
10	-0.12719	-0.03629	-0.39551	-0.04032	-0.10968	-0.02255	-0.20104	-0.06125	-0.44920	0.78661	0.41537	-0.06594	-0.14821	-0.01519	-0.08666	-0.01016	-0.04549	-0.01641
11	-0.03629	-0.29811	-0.03629	-0.15108	-0.01239	-0.10089	-0.00333	-0.11438	-0.03700	-0.41537	0.72139	0.41537	-0.03700	-0.11438	-0.00333	-0.10089	-0.01239	-0.15108
12	-0.39551	-0.03629	-0.12719	-0.01641	-0.04549	-0.01016	-0.08666	-0.01519	-0.14821	-0.06594	-0.41537	0.78661	0.44920	-0.06125	-0.20104	-0.02255	-0.10968	-0.04032
13	-0.04032	-0.15108	-0.01641	-0.08458	-0.00613	-0.05973	-0.00170	-0.05283	-0.00267	-0.14821	-0.03700	-0.44920	0.72205	-0.36254	-0.04203	-0.19224	-0.03016	-0.31443
14	-0.10968	-0.01239	-0.04549	-0.00613	-0.01752	-0.00403	-0.03384	-0.00469	-0.05283	-0.01519	-0.11438	-0.06125	-0.36254	0.77142	-0.56358	-0.05270	-0.35001	-0.03016
15	-0.02255	-0.10089	-0.01016	-0.05973	-0.00403	-0.04341	-0.00236	-0.03384	-0.00170	-0.08666	-0.00333	-0.20104	-0.04203	-0.56358	0.76076	-0.40578	-0.05270	-0.19224
16	-0.20104	-0.00333	-0.08666	-0.00170	-0.03384	-0.00236	-0.04341	-0.00403	-0.05973	-0.01016	-0.10089	-0.02255	-0.19224	-0.05270	-0.40578	0.76076	-0.56358	-0.04203
17	-0.06125	-0.11438	-0.01519	-0.05283	-0.00469	-0.03384	-0.00403	-0.01752	-0.00613	-0.04549	-0.01239	-0.10968	-0.03016	-0.35001	-0.05270	-0.56358	0.77142	-0.36254
18	-0.44920	-0.03700	-0.14821	-0.00267	-0.05283	-0.00170	-0.05973	-0.00613	-0.08458	-0.01641	-0.15108	-0.04032	-0.31443	-0.03016	-0.19224	-0.04203	-0.36254	0.72205

ENERGIES FOR NAPTHACENE , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	7,10	3,10	9,12	1,10	5,11	6,12	2,11	7,13	8,14	3,13
XMOMNT	1.06232	-0.09794	1.06725	0.00277	-0.39111	0.13540	-0.04895	0.13591	0.39469	0.13386
YMOMNT	-0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
JUMP E	20.8422	28.9072	29.8182	34.4480	36.1607	41.8567	44.3806	46.4047	47.5495	54.4697
DIAG E	31.4242	44.1645	38.9050	47.3152	53.9152	56.4963	63.1833	61.0385	64.4083	74.1715
DIAG E	35.6366	46.6271	33.8886	51.0312	55.1436	53.1255	65.7921	63.6805	64.4166	75.0637
CORRSP	26.0412	41.6889	40.0135	46.1638	57.1979	50.1569	65.1409	62.8740	67.8628	77.8818
CORRSP	38.5284	43.3467	27.6147	49.1083	56.5735	50.1424	67.0713	65.9182	67.7017	78.4000

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
26.04123	0.31206	0.53085	-0.00000	//	0.8448	-0.2206	-0.4151	-0.0103	-0.2089	0.0150	-0.0717	-0.0098	-0.1038	0.0737
22.62891				//	0.9430	-0.1960	0.0591	-0.0028	-0.2382	-0.0005	-0.0433	-0.0207	0.0114	0.0982
41.68891	0.51191	0.53736	-0.00000	//	0.2299	0.7220	0.2615	-0.4060	-0.3292	-0.2291	-0.0062	0.1589	-0.0739	-0.0340
34.21924				//	0.0693	0.6539	-0.5244	-0.2236	-0.4147	0.0991	0.0421	0.2426	-0.0064	0.0137
40.01347	3.28470	1.38938	-0.00000	//	0.3609	-0.3133	0.8426	0.0638	0.0361	0.0687	-0.0590	-0.0507	0.2130	0.0041
30.39252				//	-0.0151	0.4287	0.8081	-0.0661	-0.2153	0.0669	0.0945	0.1288	0.2856	0.0261
46.16380	0.05723	0.17074	-0.00000	//	0.1255	0.3511	0.0551	0.8435	-0.0912	-0.0758	0.3494	0.0093	-0.0300	0.0960
40.03299				//	0.0128	0.1160	-0.0958	0.8670	-0.0712	0.1184	0.4052	0.0256	0.0534	0.1967
57.19788	0.16856	-0.26324	0.00000	//	0.1553	-0.0483	0.0158	-0.0478	0.6261	-0.7073	0.1278	0.0015	-0.2225	-0.1137
50.03335				//	0.2299	0.3561	-0.0810	-0.1554	0.5982	0.3228	0.2312	-0.4870	0.1912	-0.0224
50.15689	0.00000	-0.00060	0.00000	//	0.2289	0.3823	-0.0790	-0.1459	0.5371	0.4722	0.1862	-0.4081	0.2426	-0.0498
48.17227				//	-0.0991	-0.3155	-0.0818	-0.0172	-0.1346	0.8013	-0.1886	0.1746	0.3943	-0.0435
65.14093	0.01733	0.07910	-0.00000	//	-0.0164	-0.2066	0.0393	-0.2952	-0.0557	0.1133	0.8354	0.2472	-0.0859	0.2932
63.37510				//	0.0170	-0.2555	-0.0429	-0.3393	0.1830	-0.0644	0.7038	0.4877	0.1107	0.1858
62.87396	0.02131	0.08928	-0.00000	//	0.1032	0.0584	-0.0345	0.0888	0.2876	0.2868	-0.0932	0.8302	0.0577	-0.3328
59.87280				//	0.2062	0.1768	0.0292	0.2209	0.4783	0.0053	-0.2499	0.6132	-0.0793	-0.4506
67.86281	0.06714	0.15253	0.00000	//	0.0036	-0.0255	-0.1924	-0.0284	-0.0911	-0.3443	0.1024	0.0919	0.9031	-0.0094
66.72775				//	0.0035	-0.0294	-0.2083	0.0748	0.0225	-0.4703	-0.1327	-0.0232	0.8395	-0.0742
77.88179	0.02041	0.07850	0.00000	//	0.0004	0.1158	0.0043	0.0101	0.2526	0.0002	-0.3180	0.2161	0.0533	0.8786
77.31020				//	-0.0057	0.1136	-0.0007	-0.0019	0.2851	-0.0057	-0.3986	0.2036	0.0101	0.8399

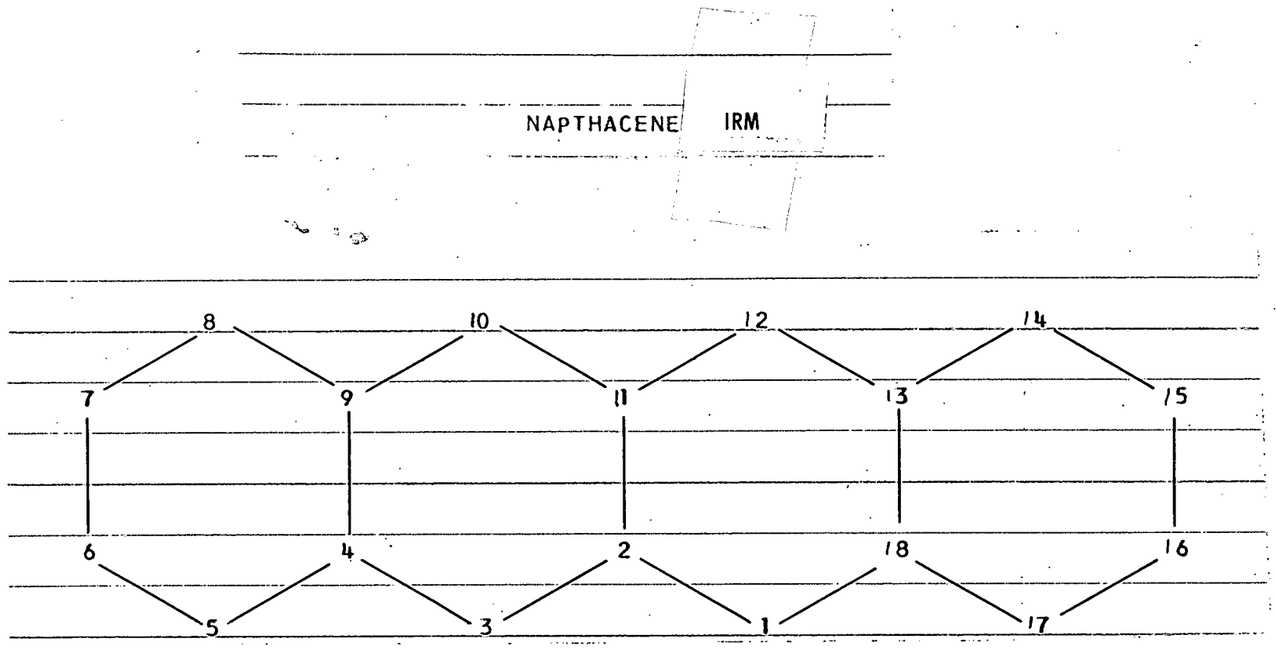
ENERGIES FOR NAPTHACENE , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	9,10	6,10	8,11	9,13	4,11	7,12	3,12	6,13	1,12	5,14
XMOMNT	0.00000	-0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000
YMOMNT	-0.72363	-0.00000	-0.55383	0.00000	0.00000	0.51596	0.00000	-0.49331	-0.00000	-0.23398
JUMP E	11.0354	23.0739	30.0396	36.5979	37.9395	39.6250	47.6900	48.6364	53.2308	53.6706
DIAG E	22.2920	35.9679	46.9056	47.9798	54.3258	52.4617	64.2297	68.1779	69.1407	73.5911
DIAG E	22.6277	37.9493	47.5159	46.7452	56.2872	51.3220	61.3402	68.5889	67.5047	74.2176
CORRSP	21.4489	33.9316	42.5224	49.5440	54.7285	53.4382	62.2162	70.5575	69.5240	77.1609
CORRSP	21.6877	35.5783	42.6126	49.2064	55.9053	53.0997	60.1240	71.2614	67.6610	76.9619

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
21.44890	0.36639	0.00000	-0.63379	//	0.9858	-0.0626	0.0213	-0.0356	-0.0148	0.1359	-0.0458	-0.0284	-0.0010	-0.0308
6.74745				//	0.9556	-0.1250	0.2102	-0.0823	0.0428	0.0465	0.0170	0.1059	-0.0025	-0.0685
33.93157	0.03614	-0.00000	-0.15825	//	0.0458	0.9349	0.3068	0.0567	-0.1467	0.0448	0.0285	-0.0284	-0.0180	-0.0330
23.25503				//	0.0115	0.7581	0.4883	0.3251	-0.2464	0.0464	0.0281	0.1239	0.0195	-0.0394
42.52236	0.07892	-0.00000	-0.20891	//	-0.0268	-0.2089	0.6373	0.6440	0.3144	0.1719	-0.0222	-0.0480	-0.0282	-0.0524
40.38571				//	-0.1186	-0.4473	0.5333	0.4948	0.2538	-0.3961	-0.0389	0.0573	0.0404	0.1705
49.54402	0.06657	-0.00000	-0.17776	//	0.1347	0.1334	-0.3597	0.5101	0.1576	-0.6838	0.1081	-0.2193	0.0053	0.1491
48.09432				//	0.2092	0.1011	-0.5015	0.7366	0.1598	0.1098	0.0175	-0.3354	0.0251	-0.0303
54.72852	0.48787	-0.00000	0.45785	//	-0.0289	0.2077	-0.2610	-0.1832	0.8273	0.2922	-0.0956	-0.2730	0.0088	-0.0298
49.87526				//	-0.0132	0.3177	0.1747	-0.2601	0.8009	0.0667	-0.1473	-0.3463	0.1025	0.0537
53.43821	0.95191	-0.00000	0.64722	//	-0.0523	0.0745	-0.5404	0.5263	-0.2721	0.5683	-0.0343	0.0368	-0.0245	-0.1497
38.49320				//	-0.1599	-0.2782	0.2578	0.1470	0.0963	0.8182	-0.0141	0.0963	-0.0231	-0.3468
62.21618	0.03005	0.00000	0.10657	//	0.0206	-0.0334	-0.0036	-0.0596	0.0651	0.0370	0.8931	-0.0270	-0.2292	-0.3721
54.50159				//	-0.0451	0.0172	0.0360	-0.0359	0.1624	-0.1823	0.8641	-0.0649	-0.1244	-0.4113
70.55754	0.72379	-0.00000	-0.49115	//	0.0543	0.1019	-0.0977	0.0734	0.2971	-0.0856	-0.0124	0.9198	-0.1693	0.0342
67.51507				//	-0.0231	0.1333	-0.2880	0.0926	0.3928	-0.0486	-0.0137	0.8446	0.1319	-0.0505
69.52396	0.00844	-0.00000	-0.05344	//	0.0133	0.0206	-0.0035	0.0305	0.0596	0.0033	0.1934	0.1588	0.9565	-0.1317
65.29263				//	-0.0045	-0.0550	0.0122	-0.0322	-0.1252	-0.0105	0.1019	-0.0834	0.9749	-0.1102
77.16094	0.02869	0.00000	-0.09350	//	0.0104	0.0025	0.0120	0.0125	-0.0073	0.2555	0.3734	0.0058	0.0452	0.8903
75.92504				//	0.0216	-0.0064	0.0113	-0.0044	0.0223	0.3423	0.4669	0.0629	0.0542	0.8104



ATOMIC COORDINATES

x	4.3300	3.4640	2.5980	1.7320	0.8660	0.	0.	0.8660	1.7320	
y	0.	0.5000	0.	0.5000	0.	0.5000	1.5000	2.0000	1.5000	
	2.5980	3.4640	4.3300	5.1960	6.0620	6.9280	6.9280	6.0620	5.1960	
	2.0000	1.5000	2.0000	1.5000	2.0000	1.5000	0.5000	0.	0.5000	

(44)

NAPTHACENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 SA	6 AA	7 SS	8 AS	9 AA	10 SA	11 SS	12 AS	13 SA	14 AA	15 SS	16 AS	17 AA	18 AS
1.752995	1.638063	1.472477	1.336392	1.292238	1.251120	1.165793	1.128192	0.994801	0.868645	0.764271	0.722761	0.690844	0.669816	0.650459	0.586009	0.525059	0.490047
0.260147	-0.153599	-0.157870	-0.342082	-0.208205	-0.212023	0.009878	0.221959	0.382322	0.367840	-0.204720	0.006245	0.218521	-0.183895	-0.339695	-0.137515	0.158297	-0.254490
0.345521	-0.000000	-0.354494	-0.262938	0.000000	0.000000	0.328580	0.243709	-0.000000	-0.000000	0.258513	0.302057	0.000000	-0.000000	0.283117	0.380974	0.000000	0.367545
0.260147	0.153599	-0.157870	-0.342081	0.208206	0.212024	0.009878	0.221959	-0.382322	-0.367840	-0.204720	0.006245	-0.218521	0.183895	-0.339695	-0.137515	-0.158297	-0.254490
0.283458	0.326641	0.088557	-0.213577	0.243083	0.244333	-0.320803	-0.071981	-0.118616	0.115944	-0.094483	-0.307590	0.266034	-0.221167	0.223535	-0.139139	0.356814	0.291945
0.166493	0.259647	0.236054	-0.213581	-0.103039	0.347247	-0.030171	-0.352880	0.229765	0.247682	0.355850	-0.019535	-0.332596	-0.132084	-0.197533	0.238632	-0.243272	-0.150105
0.120677	0.228684	-0.314134	-0.084732	-0.370060	0.157374	0.303471	-0.203301	0.192270	-0.199760	-0.197785	0.330679	0.144412	0.387068	0.074449	-0.286730	0.196072	0.099633
0.120677	0.228684	0.314134	0.084732	-0.370060	-0.157374	0.303471	0.203301	-0.192270	-0.199760	-0.197786	-0.330678	0.144413	-0.387068	0.074449	0.286730	-0.196072	-0.099633
0.166493	0.259647	0.236053	0.213581	-0.103040	-0.347247	-0.030172	0.352880	-0.229765	0.247681	0.355850	0.019534	-0.332596	0.132084	-0.197533	-0.238632	0.243272	0.150105
0.283458	0.326641	0.088556	0.213578	0.243082	-0.244334	-0.320803	0.071981	0.118616	0.115944	-0.094482	0.307591	0.266033	0.221167	0.223534	0.139139	-0.356814	-0.291945
0.260147	0.153599	-0.157870	0.342081	0.208205	-0.212024	0.009879	-0.221959	0.382322	-0.367840	-0.204720	-0.006245	-0.218521	-0.183895	-0.339695	0.137515	0.158297	0.254490
0.345521	-0.000000	-0.354494	0.262938	-0.000000	0.000000	0.328580	-0.243709	-0.000000	0.000000	0.258512	-0.302057	0.000000	0.000000	0.283117	-0.380974	-0.000000	-0.367545
0.260146	-0.153599	-0.157870	0.342081	-0.208205	0.212024	0.009878	-0.221958	-0.382322	0.367840	-0.204720	0.006245	0.218520	0.183895	-0.339695	0.137515	-0.158297	0.254490
0.283458	-0.326641	0.088557	0.213578	-0.243082	0.244334	-0.320803	0.071981	-0.118616	-0.115944	-0.094482	0.307590	-0.266033	-0.221167	0.223535	0.139139	0.356814	-0.291944
0.166493	-0.259647	0.236054	0.213581	0.103040	0.347246	-0.030171	0.352880	0.229765	-0.247681	0.355850	0.019534	0.332595	-0.132084	-0.197533	-0.238632	-0.243272	0.150105
0.120677	-0.228684	0.314134	0.084732	0.370060	0.157373	-0.303472	0.203301	0.192270	-0.199760	-0.197786	-0.330678	-0.144413	0.387068	0.074449	0.286730	0.196072	-0.099633
0.120677	-0.228684	0.314134	-0.084732	0.370060	-0.157374	0.303472	-0.203301	-0.192270	0.199760	-0.197785	0.330678	-0.144412	-0.387068	0.074449	-0.286730	-0.196072	0.099633
0.166493	-0.259647	0.236054	-0.213581	0.103039	-0.347247	-0.030171	-0.352880	-0.229765	-0.247681	0.355850	-0.019535	0.332595	0.132085	-0.197533	0.238632	0.243272	-0.150105
0.283458	-0.326641	0.088557	-0.213578	-0.243082	-0.244333	-0.320803	-0.071981	0.118616	-0.115944	-0.094483	-0.307590	-0.266033	0.221167	0.223535	-0.139139	-0.356814	0.291944

NAPTHACENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 AS	5 SA	6 AA	7 SS	8 AS	9 AA	10 SA	11 SS	12 AS	13 SA	14 AA	15 SS	16 AS	17 AA	18 AS
32.38265	29.36528	24.18985	18.97636	17.04887	15.13154	10.72126	8.56604	-0.39396	-11.39999	-23.25233	-28.91751	-33.73647	-37.16213	-40.51160	-53.25830	-68.19180	-78.45013
0.196484	-0.120012	-0.130100	-0.295912	-0.183156	-0.189555	0.009149	0.208968	0.383320	0.394673	-0.234173	0.007346	0.262907	-0.224694	-0.421191	-0.179638	0.218459	-0.363540
0.260966	-0.000000	-0.292136	-0.227451	0.000000	0.000000	0.304320	0.229446	-0.000000	-0.000000	0.295705	0.355297	0.000000	-0.000000	0.351039	0.497671	0.000000	0.525040
0.196484	0.120012	-0.130100	-0.295912	0.183156	0.189555	0.009149	0.208968	-0.383320	-0.394674	-0.234173	0.007346	-0.262907	0.224694	-0.421191	-0.179638	-0.218459	-0.363540
0.214091	0.255214	0.072979	-0.184752	0.213837	0.218440	-0.297117	-0.067768	-0.118926	0.124402	-0.108076	-0.361806	0.320071	-0.270235	0.277163	-0.181760	0.492422	0.417044
0.125749	0.202870	0.194530	-0.184755	-0.090642	0.310448	-0.027944	-0.332228	0.230364	0.265750	0.407045	-0.022978	-0.400154	-0.161389	-0.244923	0.311729	-0.335728	-0.214426
0.091145	0.178678	0.258875	-0.073296	-0.325537	0.140697	0.281065	-0.191403	0.192771	-0.214333	-0.226241	0.388964	0.173746	0.472943	0.092310	-0.374559	0.270590	0.142327
0.091145	0.178678	0.258875	0.073296	-0.325538	-0.140696	0.281065	0.191403	-0.192771	-0.214333	-0.226241	-0.388963	0.173747	-0.472943	0.092309	0.374559	-0.270590	-0.142327
0.125749	0.202870	0.194530	0.184755	-0.090643	-0.310448	-0.027944	0.332228	-0.230365	0.265749	0.407045	0.022977	-0.400154	0.161389	-0.244923	-0.311729	0.335728	0.214426
0.214091	0.255214	0.072979	0.184752	0.213836	-0.218441	-0.297117	0.067768	0.118926	0.124402	-0.108075	0.361806	0.320071	0.270236	0.277163	0.181760	-0.492422	-0.417044
0.196484	0.120012	-0.130100	0.295912	0.183155	-0.189555	0.009149	-0.208969	0.383320	-0.394674	-0.234173	-0.007346	-0.262907	-0.224694	-0.421191	0.179638	0.218459	0.363540
0.260966	-0.000000	-0.292136	0.227451	-0.000000	0.000000	0.304320	-0.229446	-0.000000	0.000000	0.295704	-0.355297	0.000000	0.000000	0.351039	-0.497671	-0.000000	-0.525040
0.196484	-0.120012	-0.130099	0.295912	-0.183156	0.189555	0.009149	-0.208968	-0.383320	0.394674	-0.234173	-0.007346	0.262907	0.224694	-0.421191	0.179638	-0.218459	0.363540
0.214091	-0.255214	0.072979	0.184752	-0.213836	0.218441	-0.297117	0.067768	-0.118926	-0.124402	-0.108075	0.361806	-0.320071	-0.270236	0.277163	0.181759	0.492422	-0.417043
0.125749	-0.202870	0.194530	0.184755	0.090643	0.310448	-0.027944	0.332228	0.230365	-0.265749	0.407046	0.022977	0.400153	-0.161388	-0.244923	-0.311729	-0.335728	0.214425
0.091145	-0.178678	0.258875	0.073296	0.325537	0.140696	0.281065	0.191403	0.192771	-0.214333	-0.226242	-0.388963	-0.173746	0.472943	0.092310	0.374559	0.270590	0.142327
0.091145	-0.178678	0.258875	-0.073296	0.325537	-0.140697	0.281065	-0.191403	-0.192771	0.214333	-0.226241	0.388963	-0.173746	-0.472943	0.092310	-0.374559	-0.270590	0.142327
0.125749	-0.202870	0.194530	-0.184755	0.090642	-0.310448	-0.027944	-0.332228	-0.230365	-0.265749	0.407045	-0.022978	0.400153	0.161389	-0.244923	0.311728	0.335728	-0.214425
0.214091	-0.255214	0.072979	-0.184752	-0.213836	-0.218440	-0.297117	-0.067768	0.118926	-0.124402	-0.108076	-0.361806	-0.320071	0.270236	0.277163	-0.181759	-0.492422	0.417043

NAPTHACENE IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	6	7	8	9	10	11	12	13	14	16	17	18
1	1.03410	0.58627	0.00183	-0.16852	-0.00745	0.10145	0.00544	-0.04327	-0.00824	0.10119	0.01011	-0.39554	0.00627	0.08732	[illegible]	-0.22681	0.00939	0.62322
2	0.58627	0.96309	0.58627	-0.00049	-0.13182	0.00557	0.11464	-0.01245	-0.15495	0.01011	0.44897	0.01011	-0.15495	-0.01245	0.11464	0.00557	-0.13182	-0.00049
3	0.00183	0.58627	1.03410	0.62322	-0.00939	-0.22681	-0.00169	0.08732	0.00627	-0.39554	0.01011	0.10119	-0.00824	-0.04327	0.00544	0.10145	-0.00745	-0.16852
4	-0.16852	-0.00049	0.62322	0.96291	0.53230	-0.00442	-0.19793	0.01787	0.46465	0.00627	-0.15495	-0.00824	0.09659	0.00917	-0.07431	-0.00597	0.06288	0.00470
5	-0.00745	-0.13182	0.00939	0.53230	1.01180	0.74252	-0.01213	-0.36226	0.01787	0.08732	-0.01245	-0.04327	0.00917	0.01910	-0.00687	-0.04281	0.00617	0.06288
6	0.10145	0.00557	-0.22681	-0.00442	0.74252	1.00965	0.56867	-0.01213	-0.19793	-0.00169	0.11464	0.00544	-0.07431	-0.00687	0.05864	0.00575	-0.04281	-0.00597
7	0.00544	0.11464	-0.00169	-0.19793	-0.01213	0.56867	1.00965	0.74252	-0.00442	-0.22681	0.00557	0.10145	-0.00597	-0.04281	0.00575	0.05864	-0.00687	-0.07431
8	-0.04327	-0.01245	0.08732	0.01787	-0.36226	-0.01213	0.74252	1.01180	0.53230	0.00939	-0.13182	-0.00745	0.06288	0.00617	-0.04281	-0.00687	0.01910	0.00917
9	-0.00824	-0.15495	0.00627	0.46465	0.01787	-0.19793	-0.00442	0.53230	0.96291	0.62322	-0.00049	-0.16852	0.00470	0.06288	-0.00597	-0.07431	0.00917	0.09659
10	0.10119	0.01011	-0.39554	0.00627	0.08732	-0.00169	-0.22681	0.00939	0.62322	1.03410	0.58627	0.00183	-0.16852	-0.00745	0.10145	0.00544	-0.04327	-0.00824
11	0.01011	0.44897	0.01011	-0.15495	-0.01245	0.11464	0.00557	-0.13182	-0.00049	0.58627	0.96309	0.58627	-0.00049	-0.13182	0.00557	0.11464	-0.01245	-0.15495
12	-0.39554	0.01011	0.10119	-0.00824	-0.04327	0.00544	0.10145	-0.00745	-0.16852	0.00183	0.58627	1.03410	0.62322	0.00939	-0.22681	-0.00169	0.08732	0.00627
13	0.00627	-0.15495	-0.00824	0.09659	0.00917	-0.07431	-0.00597	0.06288	0.00470	-0.16852	-0.00049	0.62322	0.96291	0.53230	-0.00442	-0.19793	0.01787	0.46465
14	0.08732	-0.01245	-0.04327	0.00917	0.01910	-0.00687	-0.04281	0.00617	0.06288	-0.00745	-0.13182	0.00939	0.53230	1.01180	0.74252	-0.01213	-0.36226	0.01787
15	-0.00169	0.11464	0.00544	-0.07431	-0.00687	0.05864	0.00575	-0.04281	-0.00597	0.10145	0.00557	-0.22681	-0.00442	0.74252	1.00965	0.56867	-0.01213	-0.19793
16	-0.22681	0.00557	0.10145	-0.00597	-0.04281	0.00575	0.05864	-0.00687	-0.07431	0.00544	0.11464	-0.00169	-0.19793	-0.01213	0.56867	1.00965	0.74252	-0.00442
17	0.00939	-0.13182	-0.00745	0.06288	0.00617	-0.04281	-0.00687	0.01910	0.00917	-0.04327	-0.01245	0.08732	0.01787	-0.36226	-0.01213	0.74252	1.01180	0.53230
18	0.62322	-0.00049	-0.16852	0.00470	0.06288	-0.00597	-0.07431	0.00917	0.09659	-0.00824	-0.15495	0.00627	0.46465	0.01787	-0.19793	-0.00442	0.53230	0.96291

NAPTHACENE IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.83532	0.41464	-0.08793	-0.17285	0.01220	0.10779	-0.00787	-0.04661	0.01309	0.11860	-0.04637	-0.42107	-0.05571	0.10220	0.02830	-0.23382	-0.07464	0.45430
2	0.41464	0.70087	0.41464	-0.05879	-0.13344	0.01290	0.12188	0.00338	-0.16468	-0.04637	0.28336	-0.04637	-0.16468	0.00338	0.12188	0.01290	-0.13344	-0.05879
3	-0.08793	0.41464	0.83532	0.45430	-0.07464	-0.23382	0.02830	0.10220	-0.05571	-0.42107	-0.04637	0.11860	0.01309	-0.04661	-0.00787	0.10779	0.01220	-0.17285
4	-0.17285	-0.05879	0.45430	0.70177	0.35776	-0.06959	-0.20687	-0.03051	0.29943	-0.05571	-0.16468	0.01309	0.10343	0.00160	-0.07959	-0.00478	0.06652	0.01089
5	0.01220	-0.13344	-0.07464	0.35776	0.79553	0.56988	-0.09099	-0.38029	-0.03051	0.10220	0.00338	-0.04661	0.00160	0.02000	-0.00167	-0.04549	0.00025	0.06652
6	0.10779	0.01290	-0.23382	-0.06959	0.56988	0.78237	0.38652	-0.09099	-0.20687	0.02830	0.12188	-0.00787	-0.07959	-0.00167	0.06274	0.00294	-0.04549	-0.00478
7	-0.00787	0.12188	0.02830	-0.20687	-0.09099	0.38652	0.78237	0.56988	-0.06959	-0.23382	0.01290	0.10779	-0.00478	-0.04549	0.00294	0.06274	-0.00167	-0.07959
8	-0.04661	0.00338	0.10220	-0.03051	-0.38029	-0.09099	0.56988	0.79553	0.35776	-0.07464	-0.13344	0.01220	0.06652	0.00025	-0.04549	-0.00167	0.02000	0.00160
9	0.01309	-0.16468	-0.05571	0.29943	-0.03051	-0.20687	-0.06959	0.35776	0.70177	0.45430	-0.05879	-0.17285	0.01089	0.06652	-0.00478	-0.07959	0.00160	0.10343
10	0.11860	-0.04637	-0.42107	-0.05571	0.10220	0.02830	-0.23382	-0.07464	0.45430	0.83532	0.41464	-0.08793	-0.17285	0.01220	0.10779	-0.00787	-0.04661	0.01309
11	-0.04637	0.28336	-0.04637	-0.16468	0.00338	0.12188	0.01290	-0.13344	-0.05879	0.41464	0.70087	0.41464	-0.05879	-0.13344	0.01289	0.12188	0.00338	-0.16468
12	-0.42107	-0.04637	0.11860	0.01309	-0.04661	-0.00787	0.10779	0.01220	-0.17285	-0.08793	0.41464	0.83532	0.45430	-0.07464	-0.23382	0.02830	0.10220	-0.05571
13	-0.05571	-0.16468	0.01309	0.10343	0.00160	-0.07959	-0.00478	0.06652	0.01089	-0.17285	-0.05879	0.45430	0.70177	0.35776	-0.06959	-0.20687	-0.03051	0.29943
14	0.10220	0.00338	-0.04661	0.00160	0.02000	-0.00167	-0.04549	0.00025	0.06652	0.01220	-0.13344	-0.07464	0.35776	0.79553	0.56988	-0.09099	-0.38029	-0.03051
15	0.02830	0.12188	-0.00787	-0.07959	-0.00167	0.06274	0.00294	-0.04549	-0.00478	0.10779	0.01289	-0.23382	-0.06959	0.56988	0.78237	0.38652	-0.09099	-0.20687
16	-0.23382	0.01290	0.10779	-0.00478	-0.04549	0.00294	0.06274	-0.00167	-0.07959	-0.00787	0.12188	0.02830	-0.20687	-0.09099	0.38652	0.78237	0.56988	-0.06959
17	-0.07464	-0.13344	0.01220	0.06652	0.00025	-0.04549	-0.00167	0.02000	0.00160	-0.04661	0.00338	0.10220	-0.03051	-0.38029	-0.09099	0.56988	0.79553	0.35776
18	0.45430	-0.05879	-0.17285	0.01089	0.06652	-0.00478	-0.07959	0.00160	0.10343	0.01309	-0.16468	-0.05571	0.29943	-0.03051	-0.20687	-0.06959	0.35776	0.70177

ENERGIES FOR NAPTHACENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	7,10	9,12	3,10	5,11	1,10	6,12	7,13	8,14	2,11	9,16
XMOMNT	1.20078	-1.09260	-0.01075	-0.33767	0.00985	-0.13958	-0.11666	0.36640	-0.01151	-0.10598
YMOMNT	-0.00000	0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000
JUMP E	22.1212	28.5235	35.5898	40.3012	43.7826	44.0490	44.4577	45.7282	52.6176	52.8643
DIAG E	32.8851	37.8016	51.2064	57.3712	57.4977	58.6996	58.2807	63.0768	71.9658	65.1005
DIAG E	37.5542	32.9768	53.5436	58.5055	61.1666	55.5249	60.9243	63.3512	74.1740	62.3589
CORRSP	26.8293	39.9353	46.1562	62.7317	55.9475	52.9997	60.1108	69.1202	75.1147	64.9397
CORRSP	39.3129	25.3569	54.3045	58.8967	59.9741	46.7923	65.5502	69.1722	77.0686	63.6512

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
26.82934	0.14873	0.36106	-0.00000	//	0.7941	0.5448	-0.1103	-0.1756	-0.0110	-0.0064	0.0286	-0.1210	-0.0472	0.1082
23.99214				//	0.9659	-0.0991	-0.0809	-0.2163	-0.0172	-0.0077	0.0347	0.0302	-0.0315	0.0184
39.93534	4.58567	-1.64324	0.00000	//	-0.5515	0.7997	0.0721	0.1046	0.0150	0.0164	-0.0072	-0.1562	0.0465	-0.1148
29.15591				//	0.0958	0.9388	-0.1522	0.0408	-0.0012	0.0393	0.0466	-0.2603	-0.0533	0.1020
46.15625	0.01631	0.09115	-0.00000	//	0.0171	-0.0283	0.6343	-0.4173	-0.1390	0.3932	-0.3646	-0.2746	0.0510	-0.1938
36.45114				//	-0.0303	0.1977	0.6418	-0.4666	-0.0711	-0.2447	-0.3592	0.2378	0.0934	0.2667
62.73168	0.00857	0.05667	-0.00000	//	0.1718	0.0556	0.0502	0.6431	-0.0871	-0.1664	-0.6751	0.0181	0.1233	-0.2118
52.30194				//	0.0837	0.0434	0.4639	0.3378	-0.4983	-0.0107	0.6315	0.1018	0.0227	0.0608
55.94745	0.00201	0.02908	-0.00000	//	0.0461	-0.0234	-0.0013	0.0249	0.9300	0.1615	-0.0590	-0.1060	0.2976	-0.0504
51.09583				//	0.0936	0.0280	0.4036	0.1280	0.7047	0.2214	0.2002	-0.1492	0.4355	-0.1165
52.99974	0.02200	-0.09879	-0.00000	//	-0.1537	-0.0393	-0.7129	-0.2729	-0.0249	0.3013	-0.4630	-0.2013	-0.2129	-0.0243
63.29644				//	0.1285	0.0055	0.0075	0.5478	-0.0618	0.4380	-0.4495	0.2857	0.1035	0.4396
60.11078	0.14509	-0.23824	0.00000	//	0.0953	-0.0649	-0.0580	0.5173	-0.1540	0.6945	0.3462	-0.2997	0.0044	0.0084
61.37263				//	-0.1540	-0.0471	-0.1922	-0.4780	0.0915	0.4647	0.4240	0.1679	-0.0265	0.5251
69.12019	0.00177	0.02454	0.00000	//	0.0012	0.2305	-0.0843	-0.0666	-0.0019	0.3016	0.0966	0.6452	0.0047	-0.6472
47.53253				//	0.0100	0.0641	-0.2605	0.2187	0.3322	-0.6391	0.2127	0.4608	0.1001	0.3060
75.11470	0.00610	0.04369	-0.00000	//	-0.0066	-0.0209	-0.2167	-0.1513	-0.2884	0.0075	0.0254	-0.0068	0.9186	0.0444
73.47981				//	-0.0253	-0.0003	-0.2667	-0.1280	-0.3565	-0.0549	-0.0326	-0.0739	0.8803	-0.0165
64.93965	0.04589	0.12891	0.00000	//	0.0233	0.0059	-0.1101	0.0237	0.0193	0.3567	-0.2507	0.5722	0.0114	0.6846
68.92713				//	0.0125	-0.2466	0.0646	0.1028	0.0058	-0.2650	-0.0264	-0.7173	-0.0297	0.5813

ENERGIES FOR NAPTHACENE , TRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF AS SYMMETRY

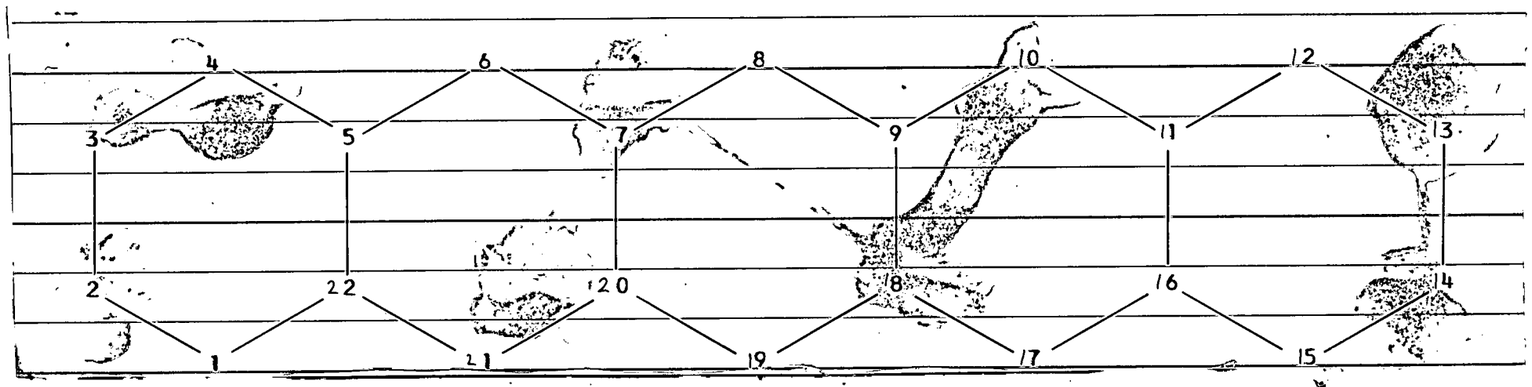
JUMP	9,10	6,10	8,11	9,13	7,12	4,11	6,13	8,15	3,12	5,14
XMOMNT	0.00000	-0.00000	-0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000
YMOMNT	-0.68742	-0.02628	0.53705	-0.02128	-0.51426	0.01869	0.49280	0.01684	-0.02533	0.19656
JUMP E	14.0060	26.5315	31.8184	33.3425	39.6388	42.2287	48.8680	49.0776	53.1074	54.2110
DIAG E	21.1119	39.2291	48.2420	44.1187	51.7672	58.7984	68.2892	63.8966	70.0260	73.9937
DIAG E	21.4643	41.2315	48.5896	42.4455	51.2591	60.4661	68.2661	62.1642	67.1861	75.0547
CORRSP	20.3870	36.7576	48.8746	40.9281	52.4649	56.6718	73.3293	64.4450	67.1466	78.4676
CORRSP	20.5144	37.9993	48.6535	40.2475	52.2073	64.1862	73.3480	57.1642	65.5149	78.2916

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	E	XMOMNT	YMOMNT	//	STATE COMPOSITION									
20.38696	0.33110	-0.00000	-0.61799	//	0.9886	-0.0344	-0.0318	0.0546	-0.1228	-0.0119	0.0239	0.0141	0.0313	0.0244
6.58142				//	0.9584	-0.0873	-0.2012	0.1107	-0.0496	0.0307	-0.1026	-0.0372	-0.0230	0.0732
36.75761	0.04341	-0.00000	-0.16664	//	0.0182	0.9055	-0.3671	-0.1308	-0.0569	-0.1074	0.0628	-0.0857	-0.0255	0.0337
39.96097				//	0.0050	0.5996	0.2145	0.6720	-0.2586	-0.1711	0.0610	-0.1744	-0.0356	0.1060
48.87464	0.03634	-0.00000	-0.13222	//	0.1305	0.1936	0.5089	-0.3747	0.6986	-0.0393	0.1385	0.1072	-0.0496	-0.1528
46.19179				//	0.2411	0.1327	0.7658	-0.4146	-0.1155	-0.2302	0.1184	0.2845	-0.0509	0.0458
40.92809	0.02988	0.00000	0.13103	//	-0.0123	0.2572	0.4006	0.8418	0.0933	-0.1977	-0.0146	-0.1233	-0.0042	-0.0359
23.99606				//	-0.0033	-0.6612	0.4892	0.4658	0.0517	0.2324	0.1418	-0.1639	0.0351	-0.0407
52.46492	0.87205	0.00000	-0.62519	//	0.0432	-0.1505	-0.5853	0.2854	0.6055	0.2880	0.1280	-0.2426	-0.0011	-0.1630
38.56259				//	0.1181	0.2534	0.1127	0.1009	0.8694	-0.0551	0.0824	-0.0336	0.0507	-0.3600
56.67180	0.66436	-0.00000	0.52505	//	-0.0148	0.1218	0.2917	-0.0211	-0.2434	0.7183	0.4540	-0.3404	0.0390	0.0272
64.07796				//	-0.0131	0.1803	0.0523	0.1874	0.0141	0.6443	-0.2282	0.6797	0.0018	0.0115
73.32931	0.51718	0.00000	0.40725	//	-0.0520	-0.0829	-0.1267	0.1099	-0.0559	-0.2647	0.8263	0.4493	0.0656	0.0143
70.94870				//	0.0210	-0.1195	-0.2679	0.1787	-0.0394	-0.2444	0.7586	0.4914	-0.0342	-0.0457
64.44498	0.06122	-0.00000	-0.14946	//	0.0005	0.1719	-0.0281	0.1881	0.0366	0.5267	-0.2591	0.7669	0.0172	-0.0070
49.56292				//	-0.0802	-0.2581	-0.0211	0.2647	0.0938	-0.6175	-0.5575	0.3917	-0.0457	0.0101
67.14657	0.02547	-0.00000	-0.09445	//	-0.0187	0.0364	0.0112	-0.0373	-0.0740	-0.0346	-0.0578	-0.0146	0.8523	-0.5100
59.06339				//	0.0449	0.0195	0.0045	0.0026	-0.2666	-0.0530	-0.0480	0.0406	0.8156	-0.5046
78.46762	0.00453	-0.00000	0.03685	//	-0.0079	0.0027	0.0112	0.0046	0.2217	-0.0096	-0.0202	-0.0293	0.5131	0.8282
77.69301				//	-0.0192	0.0077	0.0092	-0.0006	0.2780	-0.0299	0.0646	0.0268	0.5687	0.7701

54

PENTACENE TBM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640	4.3300	5.1960	6.0620	6.9280	
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	2.0000	1.5000	2.0000	1.5000	
	7.7940	8.6600	8.6600	7.7940	6.9280	6.0620	5.1960	4.3300	3.4640	2.5980	1.7320	
	2.0000	1.5000	0.5000	0.	0.5000	0.	0.5000	0.	0.5000	0.	0.5000	

PENTACENE TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 SA	5 AS	6 AA	7 SS	8 AS	9 SA	10 AA	11 AS	12 SS	13 SA
1.615913	1.568344	1.493615	1.399340	1.369113	1.321544	1.307022	1.246815	1.246798	1.152541	1.054222	0.945776	0.847457
0.124954	-0.212524	0.235705	0.185877	-0.161410	0.282548	-0.079748	0.333322	-0.002562	0.300748	0.187901	0.187901	-0.300749
0.083552	-0.163129	0.235701	0.300749	-0.064681	0.122701	-0.362997	0.168882	0.287385	0.185877	0.154062	-0.154062	0.185877
0.083552	-0.163129	0.235701	0.300749	0.064681	-0.122700	-0.362996	-0.164445	0.289947	-0.185877	-0.154062	-0.154062	0.185877
0.124954	-0.212524	0.235705	0.185877	0.161410	-0.282548	-0.079748	-0.333322	0.002562	-0.300748	-0.187901	0.187901	-0.300748
0.228268	-0.326258	0.235701	-0.000001	0.176712	-0.245402	0.265732	-0.168882	-0.287385	0.000001	0.112781	0.112782	0.000000
0.216427	-0.212524	-0.000000	-0.185877	0.279570	-0.282548	0.138128	0.000000	0.000001	0.300749	0.325454	-0.325454	0.300748
0.311820	-0.163129	-0.235701	-0.300748	0.241392	-0.122700	-0.097265	0.168883	0.287386	0.185876	-0.041281	-0.041281	-0.185877
0.249908	0.000000	-0.235705	-0.000000	0.322819	0.000000	-0.159498	0.333321	-0.002562	-0.000001	-0.375802	0.375802	0.000000
0.311820	0.163129	-0.235701	0.300748	0.241393	0.122700	-0.097265	0.164444	-0.289948	-0.185877	-0.041281	-0.041281	0.185877
0.216427	0.212524	-0.000000	0.185877	0.279570	0.282548	0.138129	0.000000	-0.000001	-0.300748	0.325454	-0.325454	-0.300748
0.228268	0.326259	0.235701	-0.000000	0.176712	0.245402	0.265733	-0.164444	0.289947	-0.000000	0.112781	0.112782	0.000000
0.124954	0.212524	0.235705	-0.185877	0.161410	0.282548	-0.079748	-0.333321	0.002562	0.300748	-0.187901	0.187901	0.300748
0.083552	0.163129	0.235701	-0.300749	0.064681	0.122701	-0.362997	-0.168883	-0.287385	0.185877	-0.154062	-0.154062	-0.185877
0.083552	0.163129	0.235701	-0.300748	-0.064681	-0.122701	-0.362997	0.164444	-0.289947	-0.185877	0.154063	-0.154062	-0.185877
0.124954	0.212524	0.235705	-0.185877	-0.161410	-0.282548	-0.079749	0.333321	-0.002562	-0.300749	0.187901	-0.187901	0.300748
0.228268	0.326259	0.235701	0.000000	-0.176712	-0.245402	0.265732	0.168883	0.287385	-0.000000	-0.112782	0.112781	-0.000000
0.216427	0.212524	-0.000000	0.185877	-0.279570	-0.282548	0.138128	0.000000	0.000000	0.300748	-0.325454	-0.325454	-0.300748
0.311820	0.163129	-0.235701	0.300749	-0.241392	-0.122701	-0.097265	-0.168883	-0.287385	0.185878	0.041281	-0.041281	0.185877
0.249908	0.000000	-0.235705	0.000001	-0.322820	0.000000	-0.159497	-0.333322	0.002562	0.000000	0.375802	0.375802	0.000000
0.311820	-0.163129	-0.235701	-0.300748	-0.241393	0.122701	-0.097265	-0.164445	0.289948	-0.185877	0.041281	-0.041281	-0.185877
0.216427	-0.212524	-0.000000	-0.185877	-0.279570	0.282548	0.138129	-0.000000	-0.000001	-0.300748	-0.325454	-0.325455	0.300748
0.228268	-0.326258	0.235701	-0.000000	-0.176712	0.245401	0.265732	0.164445	-0.289948	0.000000	-0.112782	0.112781	0.000000

OVERLAP EIGNVALUES AND EIGNVECTORS

14 SS	15 AA	16 AS	17 SA	18 SS	19 AA	20 AS	21 AA	22 AS
0.753199	0.753182	0.698976	0.678453	0.630884	0.600657	0.506383	0.431654	0.384085
-0.000654	0.333331	0.079749	-0.282548	-0.161410	-0.185877	-0.235705	-0.212524	0.124954
0.288348	-0.167234	-0.362997	0.122701	-0.064681	0.300748	0.235701	0.163129	-0.083552
-0.289001	-0.166102	0.362997	0.122701	0.064681	-0.300748	-0.235701	-0.163129	0.083552
0.000654	0.333331	-0.079749	-0.282548	-0.161409	0.185877	0.235705	0.212524	-0.124954
0.288348	-0.167235	-0.265732	0.245401	0.176712	-0.000000	-0.235701	-0.326259	0.228268
0.000000	0.000000	0.138129	-0.282548	-0.279570	-0.185877	0.000000	0.212524	-0.216427
-0.288348	0.167234	0.097265	0.122701	0.241393	0.300748	0.235701	-0.163129	0.311820
-0.000654	-0.333331	-0.159497	-0.000000	-0.322820	0.000000	-0.235705	-0.000000	-0.249908
0.289001	0.166102	0.097265	-0.122701	0.241393	-0.300748	0.235701	0.163129	0.311820
-0.000000	-0.000000	0.138128	0.282548	-0.279570	0.185877	-0.000000	-0.212524	-0.216427
-0.289001	-0.166102	-0.265732	-0.245401	0.176712	-0.000000	-0.235701	0.326259	0.228268
0.000654	0.333331	-0.079749	0.282548	-0.161410	-0.185877	0.235705	-0.212524	-0.124954
0.288347	-0.167234	0.362997	-0.122701	0.064681	0.300748	-0.235701	0.163129	0.083552
-0.289001	-0.166102	-0.362997	-0.122701	0.064681	-0.300748	0.235701	-0.163129	-0.083552
0.000654	0.333331	0.079748	0.282548	-0.161410	0.185877	-0.235705	0.212524	0.124954
0.288347	-0.167234	0.265732	-0.245401	0.176712	0.000000	0.235701	-0.326259	-0.228268
-0.000000	-0.000000	-0.138129	0.282548	-0.279570	-0.185877	0.000000	0.212524	0.216427
-0.288348	0.167234	-0.097265	-0.122701	0.241393	0.300748	-0.235701	-0.163129	-0.311820
-0.000654	-0.333330	0.159497	-0.000000	-0.322820	0.000000	0.235705	0.000000	0.249908
0.289001	0.166102	-0.097265	0.122701	0.241393	-0.300749	-0.235701	0.163129	-0.311820
0.000000	0.000000	-0.138128	-0.282548	-0.279570	0.185877	-0.000000	-0.212524	0.216427
-0.289001	-0.166102	0.265732	0.245402	0.176711	0.000000	0.235701	0.326259	-0.228268

1 0. 0. ENERGY= 28.640513 SM= 1.615913

22

2 0. 1.0 ENERGY= 27.230111 SM= 1.568344

22

3 0. 0. ENERGY= 24.832995 SM= 1.493615

PENTACENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 SA	5 AS	6 AA	7 SS	8 AS	9 SA	10 AA	11 AS	12 SS	13 SA
28.64051	27.23011	24.83300	21.44367	20.25815	18.28263	17.38572	14.87474	14.87391	9.94509	3.86476	-4.30810	-13.52551
0.098297	-0.169702	0.192863	0.157132	-0.137946	0.245783	-0.069917	0.298521	-0.000000	-0.280140	0.183005	0.193213	-0.326697
0.065728	-0.130260	0.192860	0.254239	-0.055279	0.106735	-0.318244	0.149263	0.258530	0.173140	0.150048	-0.158417	0.201914
0.065728	-0.130260	0.192860	0.254239	0.055279	-0.106734	-0.318244	-0.149263	0.258530	-0.173140	-0.150048	-0.158417	0.201914
0.098297	-0.169702	0.192863	0.157132	0.137947	-0.245783	-0.069916	-0.298521	0.000000	-0.280140	-0.183005	0.193212	-0.326697
0.179571	-0.260520	0.192860	-0.000001	0.151024	-0.213470	0.232971	-0.149263	-0.258530	0.000001	0.109843	0.115970	0.000000
0.170256	-0.169702	-0.000000	-0.157132	0.238930	-0.245783	0.121099	0.000000	0.000001	0.280140	0.316974	-0.334654	0.326696
0.245298	-0.130260	-0.192860	-0.254239	0.206302	-0.106734	-0.085274	0.149264	0.258530	0.173140	-0.040205	-0.042448	-0.201914
0.196595	0.000000	-0.192863	-0.000000	0.275892	0.000000	-0.139834	0.298521	-0.000000	-0.000000	-0.366010	0.386425	0.000000
0.245298	0.130260	-0.192860	0.254239	0.206302	0.106735	-0.085273	0.149263	-0.258531	0.173140	-0.040205	-0.042448	0.201914
0.170256	0.169702	-0.000000	-0.157132	0.238930	0.245783	0.121099	0.000000	-0.000001	-0.280140	0.316974	-0.334654	-0.326697
0.179571	0.260520	0.192860	-0.000000	-0.151024	0.213470	0.232971	-0.149262	0.258530	-0.000000	0.109843	0.115970	0.000000
0.098297	0.169702	0.192863	-0.157132	0.137946	0.245783	-0.069916	-0.298521	0.000001	0.280140	-0.183005	0.193212	0.326697
0.065728	0.130260	0.192860	-0.254239	0.055278	0.106735	-0.318245	-0.149264	-0.258529	0.173140	-0.150048	-0.158417	-0.201914
0.065728	0.130260	0.192860	-0.254239	-0.055279	-0.106735	-0.318245	0.149262	-0.258530	-0.173140	0.150048	-0.158417	-0.201914
0.098297	0.169702	0.192863	-0.157132	-0.137946	-0.245783	-0.069917	0.298521	-0.000000	-0.280140	0.183005	0.193212	0.326697
0.179571	0.260520	0.192860	0.000000	-0.151024	-0.213470	0.232971	0.149264	0.258530	-0.000000	-0.109843	0.115969	-0.000000
0.170256	0.169702	-0.000000	0.157132	-0.238930	-0.245783	0.121099	0.000000	0.000000	-0.280140	-0.316974	-0.334654	-0.326696
0.245298	0.130260	-0.192860	0.254239	-0.206302	0.106735	-0.085273	-0.149264	-0.258530	0.173141	0.040205	-0.042448	0.201914
0.196594	0.000000	-0.192863	0.000000	-0.275893	0.000000	-0.139833	-0.298521	0.000001	0.000000	0.366010	0.386425	0.000000
0.245298	-0.130260	-0.192860	-0.254238	-0.206303	0.106735	-0.085273	-0.149263	0.258530	-0.173140	0.040205	-0.042448	-0.201914
0.170256	-0.169702	-0.000000	-0.157132	-0.238930	0.245783	0.121099	-0.000000	-0.000001	-0.280140	-0.316974	-0.334654	0.326696
0.179571	-0.260520	0.192860	-0.000000	-0.151024	0.213469	0.232971	0.149263	-0.258531	0.000000	-0.109843	0.115969	0.000000

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 SS	15 AA	16 AS	17 SA	18 SS	19 AA	20 AS	21 AA	22 AS
-24.62158	-24.62383	-32.36075	-35.61263	-43.96351	-49.95726	-73.24723	-98.93665	120.49620
-0.384080	-0.000000	0.095388	-0.343030	-0.203214	-0.239835	-0.331230	-0.323474	0.201622
0.192043	0.332628	-0.434182	0.148966	0.081433	0.388052	0.331224	0.248293	-0.134816
0.192043	-0.332628	0.434182	0.148966	0.081433	-0.388052	-0.331224	-0.248293	0.134816
-0.384080	-0.000000	-0.095388	-0.343030	-0.203214	0.239835	0.331230	0.323474	-0.201622
0.192043	0.332628	-0.317843	0.297932	0.222480	-0.000000	-0.331224	-0.496586	0.368325
-0.000000	0.000000	0.165216	-0.343031	-0.351978	-0.239835	0.000000	0.323474	-0.349219
-0.192043	-0.332628	0.116338	0.148966	0.303913	0.388052	0.331224	-0.248293	0.503142
0.384079	0.000000	-0.190775	-0.000000	-0.406429	0.000000	-0.331230	-0.000000	-0.403243
-0.192043	0.332628	0.116339	-0.148966	0.303913	-0.388052	0.331224	0.248293	0.503141
0.000000	-0.000000	0.165216	0.343030	-0.351978	0.239835	-0.000000	-0.323475	-0.349219
0.192043	-0.332628	-0.317843	-0.297932	0.222480	-0.000000	-0.331224	0.496586	0.368325
-0.384080	0.000000	-0.095388	0.343030	-0.203215	-0.239835	0.331230	-0.323475	-0.201621
0.192043	0.332628	0.434182	-0.148966	0.081433	0.388052	-0.331224	0.248293	0.134816
0.192043	-0.332628	-0.434182	-0.148966	0.081433	-0.388052	0.331224	-0.248293	-0.134816
-0.384079	0.000000	0.095387	0.343030	-0.203215	0.239835	-0.331230	0.323475	0.201621
0.192043	0.332628	0.317844	-0.297932	0.222480	0.000000	0.331224	-0.496586	-0.368325
0.000000	-0.000000	-0.165216	0.343030	-0.351978	-0.239835	0.000000	0.323475	0.349219
-0.192043	-0.332628	-0.116339	-0.148966	0.303913	0.388052	-0.331224	-0.248293	-0.503141
0.384079	0.000000	0.190775	-0.000000	-0.406429	0.000000	0.331230	0.000000	0.403243
-0.192043	0.332628	-0.116339	0.148966	0.303913	-0.388052	-0.331224	0.248293	-0.503142
-0.000000	0.000000	-0.165216	-0.343031	-0.351978	0.239835	-0.000000	-0.323474	0.349219
0.192043	-0.332628	0.317843	0.297932	0.222479	0.000000	0.331224	0.496586	-0.368325

PENTACENE

TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.00000	0.74206	0.00000	-0.37101	0.00000	0.10658	0.00000	-0.04644	0.00000	0.02165	-0.00000	-0.00875	0.00000	0.01749	-0.00000
	-0.02580	0.00000	0.04959	-0.00000	-0.12028	0.00000	0.52890								
2	0.74206	1.00000	0.57879	-0.00000	-0.20778	0.00000	0.10120	-0.00000	-0.05476	0.00000	0.03311	-0.00000	-0.02437	0.00000	0.01749
	-0.00000	-0.04330	0.00000	0.09289	-0.00000	-0.21316	-0.00000								
3	0.00000	0.57879	1.00000	0.74206	0.00000	-0.21316	-0.00000	0.09289	0.00000	-0.04330	0.00000	0.01749	0.00000	-0.02437	0.00000
	0.03311	-0.00000	-0.05476	0.00000	0.10120	-0.00000	-0.20778								
4	-0.37101	-0.00000	0.74206	1.00000	0.52890	-0.00000	-0.12028	0.00000	0.04959	-0.00000	-0.02580	0.00000	0.01749	-0.00000	-0.00875
	0.00000	0.02165	-0.00000	-0.04644	-0.00000	0.10658	0.00000								
5	-0.00000	-0.20778	0.00000	0.52890	1.00000	0.62178	0.00000	-0.16357	0.00000	0.06708	-0.00000	-0.02580	0.00000	0.03311	-0.00000
	-0.04601	0.00000	0.07955	-0.00000	-0.16133	0.00000	0.47221								
6	0.10658	0.00000	-0.21316	-0.00000	0.62178	1.00000	0.57849	-0.00000	-0.14608	0.00000	0.06708	-0.00000	-0.04330	0.00000	0.02165
	-0.00000	-0.05519	0.00000	0.12822	-0.00000	-0.41745	-0.00000								
7	0.00000	0.10120	-0.00000	-0.12028	0.00000	0.57849	1.00000	0.59598	0.00000	-0.14608	0.00000	0.04959	-0.00000	-0.05476	-0.00000
	0.07955	-0.00000	-0.15259	-0.00000	0.45056	-0.00000	-0.16133								
8	-0.04644	-0.00000	0.09289	0.00000	-0.16357	-0.00000	0.59598	1.00000	0.59598	-0.00000	-0.16357	0.00000	0.09289	-0.00000	-0.04644
	0.00000	0.12822	-0.00000	-0.42620	-0.00000	0.12822	0.00000								
9	0.00000	-0.05476	0.00000	0.04959	0.00000	-0.14608	0.00000	0.59598	1.00000	0.57849	-0.00000	-0.12028	-0.00000	0.10120	0.00000
	-0.16133	-0.00000	0.45056	0.00000	-0.15259	-0.00000	0.07955								
10	0.02165	0.00000	-0.04330	-0.00000	0.06708	0.00000	-0.14608	-0.00000	0.57849	1.00000	0.62178	0.00000	-0.21316	0.00000	0.10658
	-0.00000	-0.41745	0.00000	0.12822	-0.00000	-0.05519	-0.00000								
11	-0.00000	0.03311	0.00000	-0.02580	-0.00000	0.06708	0.00000	-0.16357	-0.00000	0.62178	1.00000	0.52890	0.00000	-0.20778	-0.00000
	0.47221	0.00000	-0.16133	-0.00000	0.07955	0.00000	-0.04601								
12	-0.00875	-0.00000	0.01749	0.00000	-0.02580	-0.00000	0.04959	0.00000	-0.12028	0.00000	0.52890	1.00000	0.74206	0.00000	-0.37101
	0.00000	0.10658	-0.00000	-0.04644	-0.00000	0.02165	0.00000								
13	0.00000	-0.02437	0.00000	0.01749	0.00000	-0.04330	-0.00000	0.09289	-0.00000	-0.21316	0.00000	0.74206	1.00000	0.57879	0.00000
	-0.20778	-0.00000	0.10120	0.00000	-0.05476	-0.00000	0.03311								
14	0.01749	0.00000	-0.02437	-0.00000	0.03311	0.00000	-0.05476	-0.00000	0.10120	0.00000	-0.20778	0.00000	0.57879	1.00000	0.74206
	-0.00000	-0.21316	0.00000	0.09289	-0.00000	-0.04330	-0.00000								
15	-0.00000	0.01749	0.00000	-0.00875	0.00000	0.02165	-0.00000	-0.04644	0.00000	0.10658	-0.00000	-0.37101	0.00000	0.74206	1.00000
	0.52890	0.00000	-0.12028	-0.00000	0.04959	0.00000	-0.02580								
16	-0.02580	-0.00000	0.03311	0.00000	-0.04601	-0.00000	0.07955	0.00000	-0.16133	-0.00000	0.47221	0.00000	-0.20778	-0.00000	0.52890
	1.00000	0.62178	0.00000	-0.16357	-0.00000	0.06708	0.00000								
17	0.00000	-0.04330	-0.00000	0.02165	0.00000	-0.05519	-0.00000	0.12822	-0.00000	-0.41745	0.00000	0.10658	-0.00000	-0.21316	0.00000
	0.62178	1.00000	0.57849	0.00000	-0.14608	-0.00000	0.06708								
18	-0.04959	0.00000	-0.05476	0.00000	0.07955	0.00000	-0.15259	-0.00000	0.45056	0.00000	-0.16133	-0.00000	0.10120	0.00000	-0.12028
	0.00000	0.57849	1.00000	0.59598	0.00000	-0.14608	-0.00000								
19	-0.00000	0.09289	0.00000	-0.04644	-0.00000	0.12822	-0.00000	-0.42620	0.00000	0.12822	-0.00000	-0.04644	0.00000	0.09289	-0.00000
	-0.16357	0.00000	0.59598	1.00000	0.59598	0.00000	-0.16357								
20	-0.12028	-0.00000	0.10120	-0.00000	-0.16133	-0.00000	0.45056	-0.00000	-0.15259	-0.00000	0.07955	-0.00000	-0.05476	-0.00000	0.04959
	-0.00000	-0.14608	0.00000	0.59598	1.00000	0.57849	0.00000								
21	0.00000	-0.21316	-0.00000	0.10658	-0.00000	-0.41745	-0.00000	0.12822	-0.00000	-0.05519	0.00000	0.02165	-0.00000	-0.04330	-0.00000
	0.06708	-0.00000	-0.14608	0.00000	0.57849	1.00000	0.62178								
22	0.52890	-0.00000	-0.20778	-0.00000	0.47221	-0.00000	-0.16133	0.00000	0.07955	-0.00000	-0.04601	0.00000	0.03311	-0.00000	-0.02580
	0.00000	0.06708	-0.00000	-0.16357	0.00000	0.62178	1.00000								

PENTACENE

TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.77152	0.56468	-0.05284	-0.35057	-0.02998	0.11099	0.01209	-0.04804	-0.00561	0.02228	0.00305	-0.00898	-0.00211	0.01752	0.00201
	-0.02566	-0.00564	0.04850	0.01566	-0.11195	-0.06148	0.36105								
2	0.56468	0.76091	0.40404	-0.05284	-0.18995	0.02286	0.09732	-0.01077	-0.05369	0.00516	0.03279	-0.00211	-0.02426	0.00166	0.01752
	-0.00176	-0.04318	0.00128	0.09168	0.00361	-0.20363	-0.04223								
3	-0.05284	0.40404	0.76091	0.56468	-0.04223	-0.20363	0.00361	0.09168	0.00128	-0.04318	-0.00176	0.01752	0.00166	-0.02426	-0.00211
	0.03279	0.00516	-0.05369	-0.01077	0.09732	0.02286	-0.18995								
4	-0.35057	-0.05284	0.56468	0.77152	0.36105	-0.06148	-0.11195	0.01566	0.04050	-0.00564	-0.02566	0.00201	0.01752	-0.00211	-0.00898
	0.00305	0.02228	-0.00561	-0.04804	0.01209	0.11099	-0.02998								
5	-0.02998	-0.18995	-0.04223	0.36105	0.72229	0.45273	-0.03734	-0.15513	0.00313	0.06602	0.00118	-0.02566	-0.00176	0.03279	0.00305
	-0.04515	-0.00772	0.07643	0.01725	-0.14632	-0.04074	0.31140								
6	0.11099	0.02286	-0.20363	-0.06148	0.45273	0.78718	0.40955	-0.06712	-0.13761	0.01767	0.06602	-0.00564	-0.04318	0.00516	0.02228
	-0.00772	-0.05702	0.01514	0.13327	-0.03559	-0.39861	-0.04074								
7	0.01209	0.09732	0.00361	-0.11195	-0.03734	0.40955	0.72181	0.42707	-0.03744	-0.13761	0.00313	0.04850	0.00128	-0.05369	-0.00561
	0.07643	0.01514	-0.13778	-0.03769	0.29051	-0.03559	-0.14632								
8	-0.04804	-0.01077	0.09168	0.01566	-0.15513	-0.06712	0.42707	0.78919	0.42707	-0.06712	-0.15513	0.01566	0.09168	-0.01077	-0.04804
	0.01725	0.13327	-0.03769	-0.40759	-0.03769	0.13327	0.01725								
9	-0.00561	-0.05369	0.00128	0.04850	0.00313	-0.13761	-0.03744	0.42707	0.72181	0.40955	-0.03734	-0.11195	0.00361	0.09732	0.01209
	-0.14632	-0.03559	0.29051	-0.03769	-0.13778	0.01514	0.07643								
10	0.02228	0.00516	-0.04318	-0.00564	0.06602	0.01767	-0.13761	-0.06712	0.40955	0.78718	0.45273	-0.06148	-0.20363	0.02286	0.11099
	-0.04074	-0.39861	-0.03559	0.13327	0.01514	-0.05702	-0.00772								
11	0.00305	0.03279	-0.00176	-0.02566	0.00118	0.06602	0.00313	-0.15513	-0.03734	0.45273	0.72229	0.36105	-0.04223	-0.18995	-0.02998
	0.31140	-0.04074	-0.14632	0.01725	0.07643	-0.00772	-0.04515								
12	-0.00898	-0.00211	0.01752	0.00201	-0.02566	-0.00564	0.04850	0.01566	-0.11195	-0.06148	0.36105	0.77152	0.56468	-0.05284	-0.35057
	-0.02998	0.11099	0.01209	-0.04804	-0.00561	0.02228	0.00305								
13	-0.00211	-0.02426	0.00166	0.01752	-0.00176	-0.04318	0.00128	0.09168	0.00361	-0.20363	-0.04223	0.56468	0.76091	0.40404	-0.05284
	-0.18995	0.02286	0.09732	-0.01077	-0.05369	0.00516	0.03279								
14	0.01752	0.00166	-0.02426	-0.00211	0.03279	0.00516	-0.05369	-0.01077	0.09732	0.02286	-0.18995	-0.05284	0.40404	0.76091	0.56468
	-0.04223	-0.20363	0.00361	0.09168	0.00128	-0.04318	-0.00176								
15	0.00201	0.01752	-0.00211	-0.00898	0.00305	0.02228	-0.00561	-0.04804	0.01209	0.11099	-0.02998	-0.35057	-0.05284	0.56468	0.77152
	0.36105	-0.06148	-0.11195	0.01566	0.04850	-0.00564	-0.02566								
16	-0.02566	-0.00176	0.03279	0.00305	-0.04515	-0.00772	0.07643	0.01725	-0.14632	-0.04074	0.31140	-0.02998	-0.18995	-0.04223	0.36105
	0.72229	0.45273	-0.03734	-0.15513	0.00313	0.06602	0.00118								
17	-0.00564	-0.04318	0.00516	0.02228	-0.00772	-0.05702	0.01514	0.13327	-0.03559	-0.39861	-0.04074	0.11099	0.02286	-0.20363	-0.06148
	0.45273	0.78718	0.40955	-0.06712	-0.13761	0.01767	0.06602								
18	0.04850	0.00128	-0.05369	-0.00561	0.07643	0.01514	-0.13778	-0.03769	0.29051	-0.03559	-0.14632	0.01209	0.09732	0.00361	-0.11195
	-0.03734	0.40955	0.72181	0.42707	-0.03744	-0.13761	0.00313								
19	0.01566	0.09168	-0.01077	-0.04804	0.01725	0.13327	-0.03769	-0.40759	-0.03769	0.13327	0.01725	-0.04804	-0.01077	0.09168	0.01566
	-0.15513	-0.06712	0.42707	0.78919	0.42707	-0.06712	-0.15513								
20	-0.11195	0.00361	0.09732	0.01209	-0.14632	-0.03559	0.29051	-0.03769	-0.13778	0.01514	0.07643	-0.00561	-0.05369	0.00128	0.04850
	0.00313	-0.13761	-0.03744	0.42707	0.72181	0.40955	-0.03734								
21	-0.06148	-0.20363	0.02286	0.11099	-0.04074	-0.39861	-0.03559	0.13327	0.01514	-0.05702	-0.00772	0.02228	0.00516	-0.04318	-0.00564
	0.06602	0.01767	-0.13761	-0.06712	0.40955	0.78718	0.45273								
22	0.36105	-0.04223	-0.18995	-0.02998	0.31140	-0.04074	-0.14632	0.01725	0.07643	-0.00772	-0.04515	0.00305	0.03279	-0.00176	-0.02566
	0.00118	0.06602	0.00313	-0.15513	-0.03734	0.45273	0.72229								

ENERGIES FOR PENTACENE ,TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	9,12	4,12	11,15	7,13	2,12	3,13	9,14	8,15	1,13	10,16
XMOMNT	1.16090	-0.14631	-1.16619	0.49708	-0.00217	0.07454	-0.17198	-0.17198	0.00163	0.50114
YMOMNT	-0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000
JUMP E	19.1820	25.7518	28.4886	30.9112	31.5382	38.3585	39.4955	39.4986	42.1660	42.3058
DIAG E	30.3289	41.8940	37.9580	49.4274	48.3339	58.4914	56.0366	55.6721	61.6586	59.7163
DIAG E	34.9353	44.5135	32.3271	51.3195	51.8381	61.0942	59.5393	51.4787	64.9975	58.6301
CORRSP	25.2324	37.6510	38.7418	47.1070	45.9774	60.9363	58.9523	55.0882	65.7167	64.1139
CORRSP	36.1380	40.3347	27.0609	54.3632	48.9238	62.6013	63.3595	47.6913	68.2658	61.9345

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	E	XMOMNT	YMOMNT	//	STATE COMPOSITION									
25.23236	0.49492	0.67915	-0.00000	//	0.8515	-0.2487	0.3627	0.2425	0.0220	0.1045	-0.0024	-0.0104	0.0017	-0.1060
22.28044				//	0.9262	-0.2625	-0.0231	0.2477	0.0259	0.1015	0.0178	0.0033	0.0020	-0.0031
37.65102	2.12493	-1.15202	-0.00000	//	-0.2145	0.5424	0.6648	0.2028	0.2023	-0.0552	-0.1422	0.1650	0.0800	-0.2810
29.39295				//	0.0593	0.5915	-0.5602	0.3821	0.1987	-0.0713	-0.2381	-0.0818	0.0842	0.2678
38.74182	2.22299	-1.16160	0.00000	//	-0.3087	-0.5240	0.5996	-0.3437	-0.2883	0.0032	0.1565	-0.1801	-0.1075	-0.0290
32.20591				//	0.0489	0.4246	0.7666	0.3230	0.2143	0.0132	-0.2026	-0.0195	0.0855	-0.1742
47.10700	0.00934	0.06827	-0.00000	//	-0.2516	-0.3552	-0.0987	0.5374	-0.3210	0.1798	-0.4478	0.3431	-0.1181	-0.2111
45.85301				//	-0.2849	-0.4819	0.0208	0.4445	-0.0174	0.3739	-0.4413	-0.3389	-0.0820	0.1794
45.97743	0.02715	-0.11783	0.00000	//	-0.1881	-0.3809	0.0055	0.0213	0.7789	0.3900	-0.0476	-0.0172	0.2403	0.0033
41.11259				//	-0.0806	-0.1616	-0.1043	-0.1257	0.8125	0.3560	0.1253	0.1878	0.3049	-0.0992
60.93631	0.00808	0.05583	0.00000	//	0.0953	0.2269	0.0258	-0.3522	0.0017	0.5312	-0.4831	-0.1823	-0.5121	0.0606
58.64642				//	0.1546	0.2643	-0.0374	-0.4711	0.0398	0.4785	-0.3745	-0.0300	-0.5496	-0.0956
58.95231	0.08558	-0.18477	-0.00000	//	-0.0506	0.1094	-0.0369	0.1156	-0.0285	0.4601	0.7058	0.3316	-0.3646	-0.1313
57.64979				//	-0.1080	0.1814	-0.0139	0.3718	-0.0964	0.4532	0.6957	-0.0092	-0.3431	-0.0206
55.08824	0.19102	-0.28555	-0.00000	//	0.1492	-0.1053	-0.0729	-0.5739	0.0839	-0.1714	-0.1317	0.6834	0.0362	-0.3315
47.10473				//	-0.1037	-0.0683	-0.1784	0.3013	-0.1847	0.0490	-0.2560	0.7367	-0.0643	-0.4615
65.71673	0.00319	-0.03379	0.00000	//	0.0320	0.1537	0.0006	-0.1572	-0.3974	0.5275	0.0019	0.0215	0.7168	-0.0139
64.81372				//	0.0469	0.1803	0.0271	-0.1537	-0.4534	0.5302	-0.0364	0.0679	0.6575	0.1269
64.11388	0.04321	0.12588	-0.00000	//	0.0071	0.0057	0.2233	0.0352	-0.0013	0.0129	-0.0603	0.4600	-0.0012	0.8564
63.45240				//	-0.0034	-0.0511	0.2289	-0.0207	0.0535	0.0006	-0.0190	0.5426	-0.1723	0.7856

ENERGIES FOR PENTACENE TBM APPROXIMATION 1.7

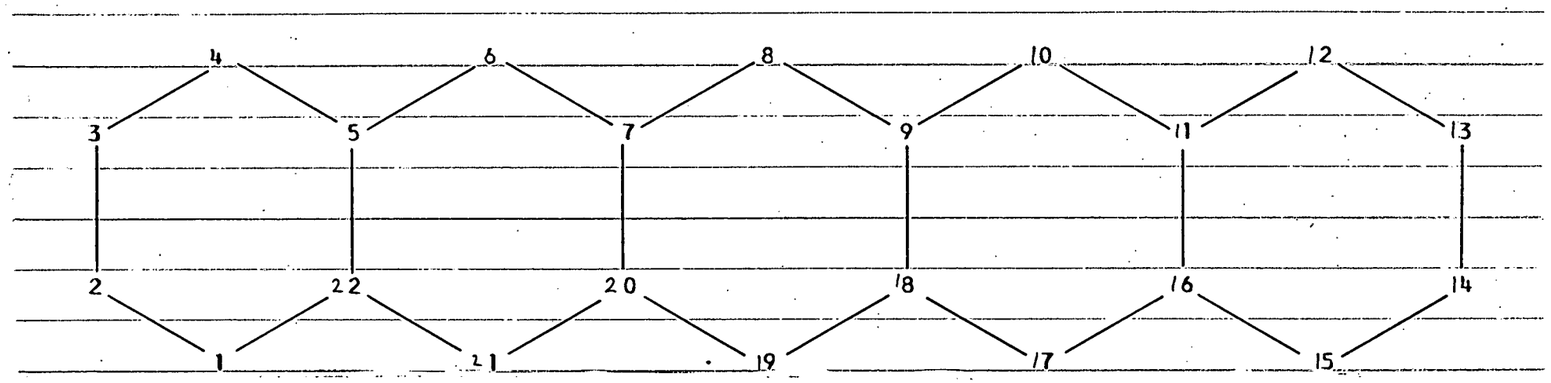
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	11,12	8,12	10,13	5,12	11,14	6,13	8,14	9,15	5,14	10,17
XMOMNT	-0.00000	0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	0.00000
YMOMNT	-0.77218	-0.00000	0.59233	0.00000	-0.00000	0.00000	0.51595	-0.51596	-0.00000	-0.00000
JUMP E	8.1729	19.1828	23.4706	24.5662	28.4863	31.8081	39.4963	39.4977	44.8797	45.5577
DIAG E	19.5192	32.9490	40.5192	37.3312	40.9424	50.3491	60.6057	53.5701	64.7916	62.9411
DIAG E	19.7898	34.6570	41.0917	39.9278	40.1093	52.1273	61.2100	52.2750	66.2846	62.1001
CORRSP	18.8346	30.0471	36.3065	35.2613	44.3742	50.5310	58.9335	54.2364	68.1184	66.8753
CORRSP	19.0025	31.4312	44.3721	37.7028	36.3410	51.3576	59.4669	53.2769	69.3612	67.2601

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
18.83457	0.41411	-0.00000	-0.71905	//	0.9884	-0.0785	-0.0349	0.0113	0.0547	-0.0078	0.0192	-0.1065	0.0258	-0.0070
4.31583				//	0.9465	-0.1548	-0.2179	-0.0052	0.1138	0.0636	-0.1095	-0.0174	-0.0398	0.0429
30.04713	0.06926	0.00000	-0.23282	//	0.0525	0.8823	-0.3822	0.2158	-0.0908	-0.1016	0.0263	-0.0398	0.0528	0.0500
18.90016				//	0.0489	0.6975	-0.5258	0.2128	-0.3833	-0.1315	-0.0691	-0.0174	0.1275	-0.0618
36.30651	0.11593	0.00000	0.27402	//	0.0068	0.2866	0.5404	-0.0953	0.7077	-0.2936	-0.0078	0.0713	0.1227	0.0974
34.56680				//	0.1668	0.5708	0.4721	0.0508	0.5542	-0.2833	0.0818	0.0316	0.1375	0.0831
35.26132	0.03816	-0.00000	0.15954	//	-0.0192	-0.1055	0.1661	0.9048	0.1483	0.3128	0.1218	0.0320	0.0723	0.0356
26.08492				//	-0.0016	-0.0339	0.0547	0.8010	0.0691	0.4634	0.2988	0.0144	0.0270	0.2110
44.37420	0.18122	-0.00000	-0.30990	//	-0.0916	-0.2244	-0.6793	-0.0137	0.6342	0.0720	-0.1352	-0.1774	-0.0001	0.1501
40.87283				//	-0.2622	0.0033	-0.5989	-0.0813	0.6753	0.1240	-0.1668	-0.0954	-0.0888	0.2231
50.53098	0.02574	0.00000	0.10944	//	0.0395	0.2060	0.0665	-0.3173	0.1392	0.7599	0.3678	0.1729	-0.2322	0.1869
45.80103				//	0.0479	0.2645	-0.0226	-0.4332	-0.0731	0.4332	0.3660	0.5549	-0.2197	0.2377
58.93347	0.53508	-0.00000	0.46207	//	-0.0474	-0.1313	-0.0410	-0.0278	-0.1279	-0.2531	0.6492	-0.2226	0.3184	0.5704
56.33436				//	0.0137	-0.2286	-0.2018	-0.0721	-0.0707	-0.4576	0.5610	-0.0327	0.3796	0.4767
54.23642	0.87830	-0.00000	-0.61710	//	0.0764	-0.1038	-0.2283	0.0363	0.0206	-0.1936	0.1103	0.9299	0.1045	0.0656
46.64368				//	-0.0469	-0.1974	-0.1011	0.2685	0.1009	-0.2966	-0.2425	0.8245	0.1440	-0.1380
68.11839	0.22580	0.00000	-0.27920	//	0.0196	0.0351	0.0782	-0.0916	-0.1344	0.3132	-0.5438	0.0577	0.6350	0.4067
64.84915				//	0.0149	-0.0265	-0.1287	-0.1414	-0.1920	0.2751	0.3307	-0.0101	0.5727	-0.6423
66.87534	0.07815	0.00000	-0.16578	//	0.0375	-0.0095	0.0856	0.1190	-0.0974	-0.1527	-0.3180	0.0455	-0.6378	0.6590
66.95033				//	-0.0175	0.0251	0.1534	-0.1379	-0.1220	0.3278	-0.4925	0.0149	0.6431	0.4217

PENTACENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640	4.3300	5.1960	6.0620	6.9280
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	2.0000	1.5000	2.0000	1.5000

7.7940	8.6600	8.6600	7.7940	6.9280	6.0620	5.1960	4.3300	3.4640	2.5980	1.7320
2.0000	1.5000	0.5000	0.	0.5000	0.	0.5000	0.	0.5000	0.	0.5000

62

PENTACENE — IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 SA	5 AS	6 AA	7 SS	8 AS	9 SA	10 AA	11 AS	12 SS	13 SA
1.765099	1.682309	1.557422	1.408341	1.345528	1.284550	1.259988	1.192504	1.162308	1.082612	0.974189	0.885921	0.794813
0.130645	0.220581	0.240809	-0.182770	-0.166138	0.288431	0.064341	-0.335415	-0.030086	0.296282	0.180499	-0.200660	0.306847
0.093021	0.179133	0.252525	-0.309461	-0.065055	0.123749	0.345500	-0.168982	0.272265	0.190546	0.162896	0.173172	-0.189297
0.093021	0.179133	0.252525	-0.309461	0.065056	-0.123750	0.345499	0.168983	0.272266	-0.190546	-0.162895	0.173172	-0.189297
0.130645	0.220581	0.240809	-0.182770	0.166138	-0.288431	0.064339	0.335416	-0.030086	-0.296282	-0.180500	-0.200660	0.306847
0.227997	0.317394	0.212344	0.029124	0.171107	-0.237593	-0.270279	0.160442	-0.289796	0.003996	0.118856	-0.119751	-0.016376
0.218073	0.210908	-0.010196	0.204854	0.284672	-0.284803	-0.156821	-0.003585	0.014883	0.303029	0.323079	0.315596	-0.282446
0.305815	0.155028	-0.231812	0.279312	0.232512	-0.118025	0.102513	-0.163926	0.301269	0.184571	-0.043688	0.043355	0.199917
0.249871	-0.000000	-0.242120	0.000000	0.327986	-0.000001	0.191513	-0.335603	-0.000000	-0.000000	-0.375418	-0.357564	-0.000000
0.305815	-0.155028	-0.231812	-0.279312	0.232512	0.118024	0.102513	-0.163925	-0.301269	-0.184571	-0.043688	0.043355	-0.199918
0.218073	-0.210909	-0.010196	-0.204854	0.284673	0.284803	-0.156820	-0.003584	-0.014883	-0.303029	0.323079	0.315596	0.282447
0.227997	-0.317394	0.212344	-0.029124	0.171108	0.237594	-0.270278	0.160441	0.289796	-0.003995	0.118856	-0.119751	0.016376
0.130644	-0.220581	0.240809	0.182770	0.166139	0.288431	0.064340	0.335415	0.030087	0.296282	-0.180500	-0.200660	-0.306847
0.093021	-0.179133	0.252525	0.309461	0.065056	0.123749	0.345500	0.168984	-0.272265	-0.190546	-0.162896	0.173172	0.189297
0.093021	-0.179133	0.252525	0.309461	-0.065056	-0.123750	0.345500	-0.168981	-0.272266	-0.190546	0.162896	0.173172	0.189298
0.130644	-0.220581	0.240809	0.182770	-0.166139	-0.288431	0.064340	-0.335415	0.030085	-0.296282	0.180500	-0.200660	-0.306847
0.227997	-0.317394	0.212344	-0.029124	-0.171108	-0.237593	-0.270278	-0.160444	0.289796	0.003995	-0.118856	-0.119750	0.016376
0.218073	-0.210909	-0.010196	-0.204854	-0.284673	-0.284803	-0.156821	0.003584	-0.014883	0.303029	-0.323079	0.315596	0.282447
0.305815	-0.155028	-0.231812	-0.279312	-0.232512	-0.118025	0.102512	0.163926	-0.301268	0.184571	0.043688	0.043355	-0.199917
0.249871	-0.000000	-0.242120	-0.000000	-0.327986	-0.000000	0.191512	0.335604	0.000001	0.000000	0.375417	-0.357564	0.000000
0.305815	0.155028	-0.231812	0.279312	-0.232512	0.118025	0.102512	0.163925	0.301269	-0.184571	0.043688	0.043355	0.199917
0.218073	0.210908	-0.010196	0.204853	-0.284673	0.284804	-0.156820	0.003584	0.014883	-0.303029	-0.323079	0.315596	-0.282446
0.227997	0.317394	0.212344	0.029124	-0.171107	0.237594	-0.270277	-0.160443	-0.289796	-0.003995	-0.118856	-0.119751	-0.016376

OVERLAP EIGNVALUES AND EIGNVECTORS

14 SS	15 AA	16 AS	17 SA	18 SS	19 AA	20 AS	21 AA	22 AS
0.722055	0.721523	0.682400	0.673365	0.646406	0.610569	0.551399	0.510192	0.486480
0.328304	-0.020052	0.100827	-0.269960	-0.150851	-0.195460	0.232007	-0.201040	-0.115415
-0.158385	0.306489	-0.369962	0.110375	0.056017	0.286818	-0.219443	0.148906	-0.075169
-0.158356	-0.306505	0.369962	0.110375	-0.056017	-0.286818	0.219443	-0.148906	0.075169
0.328302	0.020085	-0.100827	-0.269960	-0.150851	0.195460	-0.232007	0.201040	-0.115415
-0.185786	0.283176	-0.249650	0.253304	0.176141	-0.028608	0.255981	-0.335441	0.230222
0.016091	-0.009622	0.142505	-0.289058	-0.279083	-0.178440	-0.010076	0.212431	-0.210141
0.168986	-0.274528	0.088936	0.131228	0.248596	0.311241	-0.235437	-0.172517	0.322207
-0.328067	-0.000016	-0.157603	-0.000000	-0.326780	0.000000	0.232201	0.000000	-0.245154
0.168959	0.274545	0.088937	-0.131228	0.248596	-0.311241	-0.235437	0.172517	0.322207
0.016090	0.009623	0.142505	0.289058	-0.279083	0.178440	-0.010076	-0.212431	-0.210141
-0.185758	-0.283194	-0.249651	-0.253304	0.176141	0.028608	0.255981	0.335441	0.230222
0.328304	-0.020052	-0.100827	0.269960	-0.150851	-0.195460	-0.232007	-0.201040	-0.115415
-0.158386	0.306489	0.369962	-0.110375	0.056017	0.286818	0.219443	0.148906	0.075169
-0.158355	-0.306504	-0.369962	-0.110375	0.056017	-0.286818	-0.219443	-0.148906	-0.075169
0.328302	0.020085	0.100827	0.269960	-0.150851	0.195460	0.232007	0.201040	0.115415
-0.185786	0.283176	0.249651	-0.253304	0.176141	-0.028608	-0.255981	-0.335441	-0.230222
0.016091	-0.009621	-0.142505	0.289058	-0.279083	-0.178440	0.010076	0.212431	0.210141
-0.168986	-0.274529	-0.088936	-0.131228	0.248596	0.311241	0.235437	-0.172517	-0.322207
-0.328067	-0.000016	0.157603	-0.000000	-0.326780	0.000000	-0.232201	-0.000000	0.245154
0.168959	0.274545	-0.088936	0.131228	0.248596	-0.311241	0.235437	0.172517	-0.322207
0.016090	0.009623	-0.142505	-0.289059	-0.279083	0.178440	0.010076	-0.212431	0.210141
-0.185758	-0.283194	0.249650	0.253304	0.176141	0.028608	-0.255981	0.335441	-0.230222

PENTACENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 SS	4 SA	5 AS	6 AA	7 SS	8 AS	9 SA	10 AA	11 AS	13 SS	13 SA
32.57076	30.47578	26.89410	21.78685	19.29613	16.64511	15.50481	12.12998	10.49297	5.73390	-1.99088	-9.67589	-19.39830
0.098335	0.170065	0.192961	-0.154011	-0.143226	0.254488	0.057320	-0.307152	-0.027907	0.284753	0.182875	-0.213189	0.344183
0.070016	0.138109	0.202349	-0.260767	-0.056084	0.109186	0.307798	-0.154743	0.252541	0.183132	0.165040	0.183984	-0.212330
0.070016	0.138109	0.202349	-0.260767	0.056084	-0.109187	0.307797	0.154744	0.252541	-0.183132	-0.165039	0.183984	-0.212330
0.098335	0.170065	0.192961	-0.154011	0.143227	-0.254488	0.057318	0.307152	-0.027906	-0.284753	-0.182875	-0.213188	0.344183
0.171611	0.244707	0.170152	0.024542	0.147510	-0.209633	-0.240784	0.146923	-0.268801	0.003840	0.120420	-0.127227	-0.018369
0.164141	0.162608	-0.008170	0.172620	0.245414	-0.251287	-0.139708	-0.003283	0.013805	0.291238	0.327331	0.335300	-0.316813
0.230184	0.119524	-0.185752	0.235362	0.200446	-0.104135	0.091326	-0.150113	0.279443	0.177389	-0.044263	0.046062	0.224243
0.188075	-0.000000	-0.194012	0.000000	0.282754	-0.000000	0.170614	-0.307324	-0.000000	-0.000000	-0.380359	-0.379888	-0.000000
0.230183	-0.119525	-0.185752	-0.235362	0.200447	0.104135	0.091326	-0.150112	-0.279444	-0.177389	-0.044263	0.046062	-0.224243
0.164141	-0.162608	-0.008170	-0.172620	0.245414	0.251287	-0.139707	-0.003282	-0.013805	-0.291238	0.327331	0.335300	0.316814
0.171611	-0.244707	0.170152	-0.024541	0.147511	0.209633	-0.240784	0.146922	0.268801	-0.003840	0.120420	-0.127227	0.018369
0.098335	-0.170065	0.192961	0.154011	0.143227	0.254487	0.057319	0.307152	0.027907	0.284753	-0.182875	-0.213188	-0.344183
0.070016	-0.138109	0.202349	0.260767	0.056084	0.109186	0.307797	0.154744	-0.252541	0.183132	-0.165039	0.183984	0.212330
0.070016	-0.138109	0.202349	0.260767	-0.056084	-0.109187	0.307797	-0.154742	-0.252541	-0.183132	0.165040	0.183984	0.212331
0.098334	-0.170065	0.192961	0.154011	-0.143227	-0.254487	0.057319	-0.307152	0.027906	-0.284753	0.182875	-0.213188	-0.344183
0.171610	-0.244707	0.170152	-0.024541	-0.147511	-0.209632	-0.240784	0.146924	0.268801	0.003840	-0.120420	-0.127227	0.018368
0.164141	-0.162608	-0.008170	-0.172619	-0.245414	-0.251286	-0.139708	0.003282	-0.013804	0.291238	-0.327331	0.335300	0.316814
0.230183	-0.119525	-0.185752	-0.235362	-0.200447	-0.104136	0.091325	0.150113	-0.279443	0.177389	0.044263	0.046062	-0.224242
0.188075	-0.000000	-0.194012	-0.000000	-0.282754	-0.000000	0.170613	0.307325	0.000001	0.000000	0.380358	-0.379889	0.000000
0.230184	0.119524	-0.185751	0.235362	-0.200447	0.104136	0.091326	0.150112	0.279443	-0.177389	0.044263	0.046062	-0.224242
0.164141	0.162608	-0.008170	0.172619	-0.245414	0.251287	-0.139707	0.003282	0.013804	-0.291238	-0.327331	0.335301	-0.316813
0.171611	0.244706	0.170152	0.024541	-0.147510	0.209633	-0.240783	-0.146923	-0.268802	-0.003840	-0.120420	-0.127227	-0.018368

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 SS	15 AA	16 AS	17 SA	18 SS	19 AA	20 AS	21 AA	22 AS
-28.92459	-29.00138	-34.97207	-36.44945	-41.10349	-47.92646	-61.13272	-72.13922	-79.31799
0.386359	-0.023607	0.122056	-0.328984	0.187627	-0.250145	0.312441	-0.281459	0.165474
-0.186393	0.360819	-0.447855	0.134507	0.069673	0.367062	-0.295522	0.208471	-0.107771
-0.186358	-0.360838	0.447855	0.134508	0.069673	-0.367062	0.295522	-0.208471	0.107771
0.386357	0.023645	-0.122055	-0.328984	-0.187626	0.250144	-0.312441	0.281459	-0.165474
-0.218639	0.333374	-0.302213	0.308685	0.219083	-0.036611	0.344726	-0.469624	0.330076
0.018937	-0.011327	0.172508	-0.352258	-0.347121	-0.228363	-0.013569	0.297406	-0.301285
0.198868	-0.323193	0.107661	0.159920	0.309202	0.398318	-0.317060	-0.241526	0.461958
-0.386080	-0.000019	-0.190786	-0.000000	-0.406446	0.000000	0.312702	0.000000	-0.351485
0.198837	0.323213	-0.107662	-0.159920	0.309202	-0.398318	-0.317061	0.241526	0.461958
0.018936	0.011329	-0.172508	0.352258	-0.347121	0.228363	-0.013569	-0.297406	-0.301285
-0.218606	-0.333395	-0.302213	-0.308686	0.219083	0.036611	0.344726	0.469623	0.330076
0.386359	-0.023607	-0.122056	0.328984	-0.187627	-0.250144	-0.312442	-0.281459	-0.165474
-0.186393	0.360819	0.447855	-0.134507	0.069673	0.367062	0.295522	0.208471	0.107772
-0.186358	-0.360837	-0.447855	-0.134507	0.069673	-0.367062	-0.295522	-0.208471	-0.107772
0.386356	0.023645	0.122056	0.328984	-0.187627	0.250145	0.312441	0.281459	0.165475
-0.218639	0.333374	0.302213	-0.308686	0.219083	-0.036611	-0.344726	-0.469623	-0.330076
0.018937	-0.011327	-0.172508	0.352258	-0.347121	0.228363	0.013569	0.297406	0.301285
0.198868	-0.323193	-0.107661	-0.159920	0.309202	0.398318	0.317061	-0.241526	-0.461958
-0.386080	-0.000019	0.190785	-0.000000	-0.406446	0.000000	-0.312702	-0.000000	0.351485
0.198837	0.323213	-0.107661	0.159920	0.309202	-0.398318	0.317061	0.241526	-0.461958
0.018936	0.011329	-0.172508	-0.352258	-0.347121	0.228363	0.013569	-0.297406	0.301285
-0.218606	-0.333395	0.302212	0.308686	0.219083	0.036611	-0.344726	0.469623	-0.330076

64

PENTACENE

IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.01165	0.74423	-0.01193	-0.36300	0.01761	0.08887	-0.01216	-0.04605	0.00894	0.02380	-0.00664	-0.01096	0.00514	0.02410	-0.00412
	-0.03286	0.00545	0.05764	-0.00730	-0.12861	0.00944	0.53015								
2	0.74423	1.00944	0.56566	-0.01193	-0.19426	-0.00164	0.10942	0.00498	-0.06628	-0.00538	0.04453	0.00514	-0.03578	-0.00498	0.02410
	0.00550	-0.05425	-0.00585	0.10810	0.00533	-0.23049	-0.00417								
3	-0.01193	0.56566	1.00944	0.74423	-0.00417	-0.23049	0.00533	0.10810	-0.00585	-0.05425	0.00550	0.02410	-0.00498	-0.03578	0.00514
	0.04453	-0.00538	-0.06628	0.00498	0.10942	-0.00164	-0.19426								
4	-0.36300	-0.01193	0.74423	1.01165	0.53015	0.00944	-0.12861	-0.00730	0.05764	0.00545	-0.03286	-0.00412	0.02410	0.00514	-0.01096
	-0.00664	0.02380	0.00894	-0.04605	-0.01216	0.08887	0.01761								
5	0.01761	-0.19426	-0.00417	0.53015	0.96261	0.62789	-0.00020	-0.17710	0.00455	0.07800	-0.00553	-0.03286	0.00550	0.04453	-0.00664
	-0.05625	0.00738	0.08650	-0.00772	-0.14849	0.00624	0.46016								
6	0.08887	-0.00164	-0.23049	0.00944	0.62789	1.03459	0.57917	0.00041	-0.15661	-0.00385	0.07800	0.00545	-0.05425	-0.00538	0.02380
	0.00738	-0.05382	-0.00908	0.10729	0.01034	-0.39890	0.00624								
7	-0.01216	0.10942	0.00533	-0.12861	-0.00020	0.57917	0.96284	0.59970	-0.00040	-0.15661	0.00455	0.05764	-0.00585	-0.06628	0.00894
	0.08650	-0.00908	-0.13978	0.00899	0.43948	0.01034	-0.14849								
8	-0.04605	0.00498	0.10810	-0.00730	-0.17710	0.00041	0.59970	1.03776	0.59970	0.00041	-0.17710	-0.00730	0.10810	0.00498	-0.04605
	-0.00772	0.10729	0.00899	-0.40682	0.00899	0.10729	-0.00772								
9	0.00894	-0.06628	-0.00585	0.05764	0.00455	-0.15661	-0.00040	0.59970	0.96284	0.57917	-0.00020	-0.12861	0.00533	0.10942	-0.01216
	-0.14849	0.01034	0.43948	0.00899	-0.13978	-0.00908	0.08650								
10	0.02380	-0.00538	-0.05425	0.00545	0.07800	-0.00385	-0.15661	0.00041	0.57917	1.03459	0.62789	0.00944	-0.23049	-0.00164	0.08887
	0.00624	-0.39890	0.01034	0.10729	-0.00908	-0.05382	0.00738								
11	-0.00664	0.04453	0.00550	-0.03286	-0.00553	0.07800	0.00455	-0.17710	-0.00020	0.62789	0.96261	0.53015	-0.00417	-0.19426	0.01761
	0.46016	0.00624	-0.14849	-0.00772	0.08650	0.00738	-0.05625								
12	-0.01096	0.00514	0.02410	-0.00412	-0.03286	0.00545	0.05764	-0.00730	-0.12861	0.00944	0.53015	1.01165	0.74423	-0.01193	-0.36300
	0.01761	0.08887	-0.01216	-0.04605	0.00894	0.02380	-0.00664								
13	0.00514	-0.03578	-0.00498	0.02410	0.00550	-0.05425	-0.00585	0.10810	0.00533	-0.23049	-0.00417	0.74423	1.00944	0.56566	-0.01193
	-0.19426	-0.00164	0.10942	0.00498	-0.06628	-0.00538	0.04453								
14	0.02410	-0.00498	-0.03578	0.00514	0.04453	-0.00538	-0.06628	0.00498	0.10942	-0.00164	-0.19426	-0.01193	0.56566	1.00944	0.74423
	-0.00417	-0.23049	0.00533	0.10810	-0.00585	-0.05425	0.00550								
15	-0.00412	0.02410	0.00514	-0.01096	-0.00664	0.02380	-0.00894	-0.04605	-0.01216	0.08887	0.01761	-0.36300	-0.01193	0.74423	1.01165
	0.53015	0.00944	-0.12861	-0.00730	0.05764	0.00545	-0.03286								
16	-0.03286	0.00550	0.04453	-0.00664	-0.05625	0.00738	0.08650	-0.00772	-0.14849	0.00624	0.46016	0.01761	-0.19426	-0.00417	0.53015
	0.96261	0.62789	-0.00020	-0.17710	0.00455	0.07800	-0.00553								
17	0.00545	-0.05425	-0.00538	0.02380	0.00738	-0.05382	-0.00908	0.10729	0.01034	-0.39890	0.00624	0.08887	-0.00164	-0.23049	0.00944
	0.62789	1.03458	0.57917	0.00042	-0.15661	-0.00385	0.07800								
18	0.05764	-0.00585	-0.06628	0.00894	0.08650	-0.00908	-0.13978	0.00899	0.43948	0.01034	-0.14849	-0.01216	0.10942	0.00533	-0.12861
	-0.00020	0.57917	0.96284	0.59970	-0.00040	-0.15661	0.00455								
19	-0.00730	0.10810	0.00498	-0.04605	-0.00772	0.10729	0.00899	-0.40682	0.00899	0.10729	-0.00772	-0.04605	0.00498	0.10810	-0.00730
	-0.17710	0.00042	0.59970	1.03775	0.59970	0.00042	-0.17710								
20	-0.12861	0.00533	0.10942	-0.01216	-0.14849	0.01034	0.43948	0.00899	-0.13978	-0.00908	0.08650	0.00894	-0.06628	-0.00585	0.05764
	0.00455	-0.15661	-0.00040	0.59970	0.96284	0.57917	-0.00020								
21	0.00944	-0.23049	-0.00164	0.08887	0.00624	-0.39890	0.01034	0.10729	-0.00908	-0.05382	0.00738	0.02380	-0.00538	-0.05425	0.00545
	0.07800	-0.00385	-0.15661	0.00042	0.57917	1.03458	0.62789								
22	0.53015	-0.00417	-0.19426	0.01761	0.46016	-0.00624	-0.14849	-0.00772	0.08650	0.00738	-0.05625	-0.00664	0.04453	0.00550	-0.03286
	-0.00553	0.07800	0.00455	-0.17710	-0.00020	0.62789	0.96261								

PENTACENE

IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
16	17	18	19	20	21	22									
1	0.79551	0.57170	-0.09101	-0.38108	-0.03049	0.10388	0.00324	-0.04965	0.00208	0.02522	-0.00282	-0.01136	0.00232	0.02556	-0.00156
	-0.03491	-0.00173	0.06091	0.01300	-0.13001	-0.07492	0.35547								
2	0.57170	0.78245	0.38330	-0.09101	-0.20295	0.02887	0.11628	-0.00930	-0.07100	0.00155	0.04774	0.00232	-0.03827	-0.00279	0.02556
	0.00354	-0.05792	-0.00526	0.11500	0.01309	-0.23779	-0.06967								
3	-0.09101	0.38330	0.78245	0.57170	-0.06967	-0.23779	0.01309	0.11500	-0.00526	-0.05792	0.00354	0.02556	-0.00279	-0.03827	0.00232
	0.04774	0.00155	-0.07100	-0.00930	0.11628	0.02887	-0.20295								
4	-0.38108	-0.09101	0.57170	0.79551	0.35547	-0.07492	-0.13001	0.01300	0.06091	-0.00173	-0.03491	-0.00156	0.02556	0.00232	-0.01136
	-0.00282	0.02522	0.00208	-0.04965	0.00324	0.10388	-0.03049								
5	-0.03049	-0.20295	-0.06967	0.35547	0.70185	0.45933	-0.05898	-0.18213	0.01134	0.08288	-0.00495	-0.03491	0.00354	0.04774	-0.00282
	-0.06049	-0.00248	0.09265	0.01486	-0.15776	-0.05640	0.29462								
6	0.10388	0.02887	-0.23779	-0.07492	0.45933	0.83661	0.40698	-0.09097	-0.16003	0.01904	0.08288	-0.00173	-0.05792	0.00155	0.02522
	-0.00248	-0.05864	0.01051	0.12545	-0.04513	-0.42478	-0.05640								
7	0.00324	0.11628	0.01309	-0.13001	-0.05898	0.40698	0.70116	0.42911	-0.05916	-0.16003	0.01134	0.06091	-0.00526	-0.07100	0.00208
	0.09265	0.01051	-0.14860	-0.04947	0.27323	-0.04513	-0.15776								
8	-0.04965	-0.00930	0.11500	0.01300	-0.18213	-0.09097	0.42911	0.84238	0.42911	-0.09097	-0.18213	0.01300	0.11500	-0.00930	-0.04965
	0.01486	0.12545	-0.04947	-0.43390	-0.04947	0.12545	0.01486								
9	0.00208	-0.07100	-0.00526	0.06091	0.01134	-0.16003	-0.05916	0.42911	0.70116	0.40698	-0.05898	-0.13001	0.01309	0.11628	0.00324
	-0.15776	-0.04513	0.27323	-0.04947	-0.14860	0.01051	0.09265								
10	0.02522	0.00155	-0.05792	-0.00173	0.08288	0.01904	-0.16003	-0.09097	0.40698	0.83661	0.45933	-0.07492	-0.23779	0.02887	0.10388
	-0.05640	-0.42478	-0.04513	0.12545	0.01051	-0.05864	-0.00248								
11	-0.00282	0.04774	0.00354	-0.03491	-0.00495	0.08288	0.01134	-0.18213	-0.05898	0.45933	0.70185	0.35547	-0.06967	-0.20295	-0.03049
	0.29462	-0.05640	-0.15776	0.01486	0.09265	-0.00248	-0.06049								
12	-0.01136	0.00232	0.02556	-0.00156	-0.03491	-0.00173	0.06091	0.01300	-0.13001	-0.07492	0.35547	0.79551	0.57170	-0.09101	-0.38108
	-0.03049	0.10388	0.00324	-0.04965	0.00208	0.02522	-0.00282								
13	0.00232	-0.03827	-0.00279	0.02556	0.00354	-0.05792	-0.00526	0.11500	0.01309	-0.23779	-0.06967	0.57170	0.78245	0.38330	-0.09101
	-0.20295	0.02887	0.11628	-0.00930	-0.07100	0.00155	0.04774								
14	0.02556	-0.00279	-0.03827	0.00232	0.04774	0.00155	-0.07100	-0.00930	0.11628	0.02887	-0.20295	-0.09101	0.38330	0.78245	0.57170
	-0.06967	-0.23779	0.01309	0.11500	-0.00526	-0.05792	0.00354								
15	-0.00156	0.02556	0.00232	-0.01136	-0.00282	0.02522	0.00208	-0.04965	0.00324	0.10388	-0.03049	-0.38108	-0.09101	0.57170	0.79551
	0.35547	-0.07492	-0.13001	0.01300	0.06091	-0.00173	-0.03491								
16	-0.03491	0.00354	0.04774	-0.00282	-0.06049	-0.00248	0.09265	0.01486	-0.15776	-0.05640	0.29462	-0.03049	-0.20295	-0.06967	0.35547
	0.70185	0.45933	-0.05898	-0.18213	0.01134	0.08288	-0.00495								
17	-0.00173	-0.05792	0.00155	0.02522	-0.00248	-0.05864	0.01051	0.12545	-0.04513	-0.42478	-0.05640	0.10388	0.02887	-0.23779	-0.07492
	0.45933	0.83661	0.40698	-0.09097	-0.16003	0.01904	0.08288								
18	0.06091	-0.00526	-0.07100	0.00208	0.09265	0.01051	-0.14860	-0.04947	0.27323	-0.04513	-0.15776	0.00324	0.11628	0.01309	-0.13001
	-0.05898	0.40698	0.70116	0.42911	-0.05916	-0.16003	0.01134								
19	0.01300	0.11500	-0.00930	-0.04965	0.01486	0.12545	-0.04947	-0.43390	-0.04947	0.12545	0.01486	-0.04965	-0.00930	0.11500	0.01300
	-0.18213	-0.09097	0.42911	0.84238	0.42911	-0.09097	-0.18213								
20	-0.13001	0.01309	0.11628	0.00324	-0.15776	-0.04513	0.27323	-0.04947	-0.14860	0.01051	0.09265	0.00208	-0.07100	-0.00526	0.06091
	0.01134	-0.16003	-0.05916	0.42911	0.70116	0.40698	-0.05898								
21	-0.07492	-0.23779	0.02887	0.10388	-0.05640	-0.42478	-0.04513	0.12545	0.01051	-0.05864	-0.00248	0.02522	0.00155	-0.05792	-0.00173
	0.08288	0.01904	-0.16003	-0.09097	0.40698	0.83661	0.45933								
22	0.35547	-0.06967	-0.20295	-0.03049	0.29462	-0.05640	-0.15776	0.01486	0.09265	-0.00248	-0.06049	-0.00282	0.04774	0.00354	-0.03491
	-0.00495	0.08288	0.01134	-0.18213	-0.05898	0.45933	0.70185								

ENERGIES FOR PENTACENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP:	9,12	11,15	4,12	7,13	9,14	2,12	10,16	8,15	11,19	3,13
XMOMNT	-1.35105	-1.19770	-0.03450	0.44697	0.15038	-0.01413	0.47372	0.18105	0.16589	-0.02028
YMOMNT	-0.00000	0.00000	-0.00000	-0.00000	0.00003	0.00000	-0.00000	0.00003	-0.00000	-0.00000
JUMP E	20.1689	27.0105	31.4627	34.9031	39.4176	40.1517	40.7060	41.1314	45.9356	46.2924
DIAG E	31.2661	36.6801	47.8790	52.7276	55.1712	57.2625	58.5662	57.2702	59.1087	66.8723
DIAG E	36.3539	31.2661	50.3427	54.6114	58.7713	60.6591	57.8444	53.3113	56.2479	69.1112
CORRSP	25.6707	37.3799	49.8358	57.5599	59.1901	55.5424	64.8556	42.0219	60.4820	70.2654
CORRSP	36.8817	23.9605	51.4146	56.7036	62.6714	59.1786	64.0538	42.7777	58.6721	72.2050

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
25.67069	0.26751	-0.49503	-0.00000	//	0.8052	-0.5055	0.1328	-0.2046	0.0279	-0.0110	0.1279	-0.0056	0.1255	0.0597
23.00901				//	0.9596	0.0473	0.1241	-0.2376	0.0386	-0.0183	-0.0142	-0.0042	0.0169	0.0527
37.37990	5.38406	-1.84040	0.00000	//	0.5159	0.8092	0.0684	-0.1200	0.0042	-0.0101	-0.1909	-0.0191	-0.1465	0.0401
28.59835				//	-0.0384	0.9269	-0.1579	-0.0642	-0.0559	-0.0079	-0.2897	-0.0454	-0.1363	-0.0514
49.83582	0.01562	0.08586	-0.00001	//	-0.1858	0.0451	0.7066	-0.3055	-0.4676	0.0290	0.1979	0.2343	-0.0662	0.2300
33.63023				//	0.0206	0.2038	0.6393	0.4948	0.3754	0.1036	0.1939	0.1989	-0.2630	0.0810
57.55994	0.18890	0.27780	0.00002	//	0.1450	0.0717	0.0807	0.6479	0.0892	-0.3342	0.3789	0.5196	-0.1079	0.0529
48.76651				//	0.1708	-0.0489	-0.6186	0.3570	0.5603	0.1104	0.0261	0.0994	-0.0260	-0.3478
59.19011	0.06402	0.15948	0.00003	//	-0.1377	0.1177	0.0572	-0.4095	0.6939	0.1024	0.1472	0.4207	0.3151	0.0790
58.04238				//	-0.1742	0.0960	0.1457	-0.5101	0.4733	0.1308	-0.0334	0.4401	0.4931	0.0086
55.54235	0.00039	0.01291	0.00000	//	0.0914	0.0246	0.0045	0.1814	-0.0795	0.8622	0.1728	0.2020	-0.0999	-0.3575
51.61933				//	0.0179	-0.0075	0.0717	-0.0981	-0.2774	0.8691	0.0903	0.0295	-0.0929	-0.3674
64.85563	0.00274	0.03154	-0.00001	//	-0.0051	0.2531	-0.0663	0.0339	-0.0984	-0.0009	0.6994	-0.4621	0.4669	-0.0015
44.04072				//	-0.0046	0.0674	-0.2370	-0.2106	-0.2070	-0.1692	0.5317	0.6012	-0.4205	0.0498
42.02186	0.01677	-0.09688	-0.00000	//	0.0101	0.0198	-0.6230	-0.4402	-0.3550	-0.1328	0.2975	0.3555	-0.2361	-0.0578
59.48782				//	0.1289	0.0687	-0.0083	0.4823	-0.4423	-0.0687	-0.1268	0.4828	0.5382	-0.0827
60.48195	0.03845	-0.12227	-0.00000	//	0.0473	0.0590	-0.1207	0.1179	-0.3854	-0.0046	-0.3675	0.3420	0.7505	-0.0450
64.63327				//	0.0099	-0.2760	-0.0649	0.0623	-0.0080	0.0147	0.7513	-0.3945	0.4392	-0.0481
70.26538	0.00327	0.03309	-0.00000	//	0.0140	-0.0143	-0.2481	0.1455	-0.0227	-0.3403	-0.0154	-0.0068	-0.0229	0.8943
69.03307				//	0.0279	-0.0035	-0.2854	0.1284	0.0326	-0.4132	-0.0712	0.0617	0.0122	0.8488

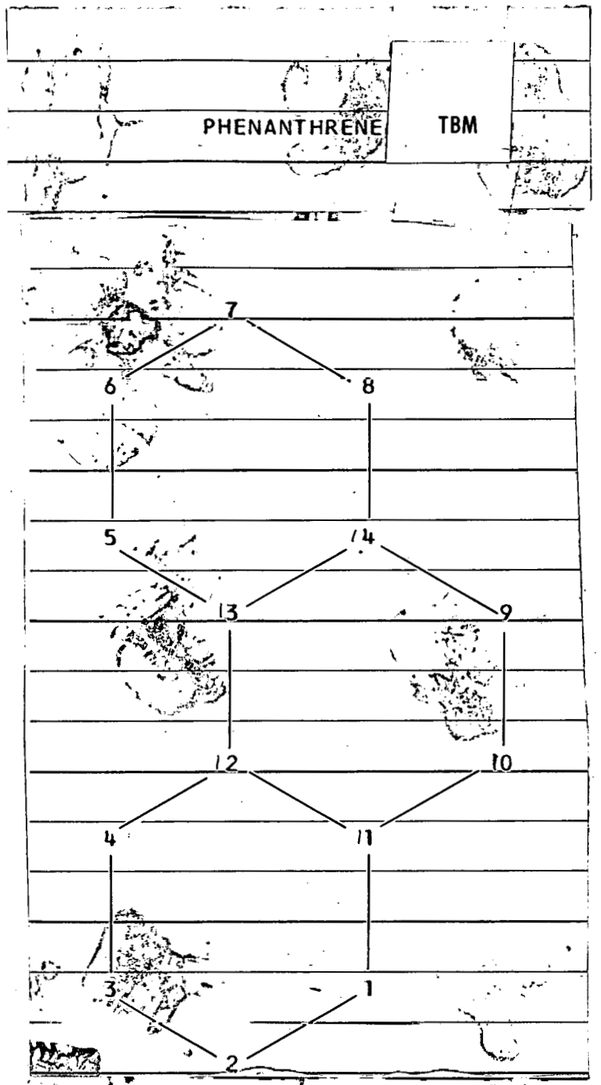
ENERGIES FOR PENTACENE IRM APPROXIMATION 5.8

ONE-ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	11,12	8,12	10,13	11,14	5,12	6,13	11,18	9,15	8,14	10,17
XMOMNT	-0.00000	0.00000	-0.00000	0.00006	-0.00000	-0.00000	-0.00000	0.00001	-0.00001	0.00000
YMOMNT	0.73335	-0.02817	-0.56690	0.02301	-0.00697	-0.02553	-0.00459	-0.51370	0.50747	-0.02266
JUMP E	7.6850	21.8059	25.1322	26.9337	28.9720	36.0434	39.1126	39.4944	41.0546	42.1833
DIAG E	17.8072	35.1388	41.5721	38.7834	41.9806	54.6073	49.1222	52.7495	61.9262	59.1537
DIAG E	18.0495	36.8363	41.9385	37.5380	44.5395	56.1611	46.5261	52.1809	62.1361	57.9066
CORRSP	17.1857	32.0856	44.4167	35.8648	39.7632	55.7271	46.2630	53.2157	67.1493	61.1698
CORRSP	17.1856	32.8698	44.3928	35.6419	41.9739	61.0658	44.2971	52.7593	67.2765	56.3498

FINAL EXCITED STATES OFAS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
17.18565	0.35655	0.00001	0.69848	//	0.9900	0.0486	-0.0500	0.0715	0.0036	-0.0047	-0.0089	0.0979	-0.0116	0.0049
3.91399				//	0.9554	0.1047	-0.2103	0.1291	0.0004	0.0396	-0.0040	0.0189	0.1057	-0.0474
32.08564	0.09885	0.00002	-0.26916	//	-0.0305	0.8227	0.4744	0.2766	-0.0971	0.0790	0.0119	-0.0492	0.0314	0.0368
35.36728				//	-0.0433	0.6713	-0.2215	-0.6528	-0.0954	0.1749	-0.1070	0.0226	0.0669	0.1271
44.41670	0.21218	-0.00003	-0.33516	//	0.1034	-0.2825	0.7707	-0.4703	0.0324	-0.0797	-0.0732	-0.2043	-0.1483	0.1334
40.86972				//	0.2872	-0.2099	0.7188	-0.4851	-0.0257	-0.1102	-0.0976	-0.1412	-0.2288	0.1636
35.86482	0.03571	0.00005	-0.15302	//	-0.0156	-0.4320	0.3293	0.8008	0.0827	-0.1588	0.1101	-0.0421	-0.0257	-0.1294
20.55463				//	-0.0171	0.6446	0.5441	0.4907	-0.1284	0.1065	0.1111	-0.0183	-0.0582	-0.0579
39.76317	0.01005	0.00000	-0.07711	//	-0.0033	0.0743	0.0061	-0.0073	0.9150	0.3568	0.1245	-0.0147	-0.1190	0.0035
26.99581				//	0.0004	0.0349	0.0202	0.0154	0.6487	0.4370	-0.3957	-0.0155	-0.3442	-0.3334
55.72706	0.42805	0.00000	-0.42500	//	-0.0139	-0.1312	0.0998	-0.0015	-0.3507	0.7018	0.3058	0.2940	-0.3894	-0.1597
60.74069				//	-0.0192	-0.1813	0.0872	0.1630	-0.1127	0.6001	-0.3197	-0.0143	0.3522	0.5774
46.26300	0.01750	-0.00001	0.09431	//	0.0083	-0.0047	0.0054	-0.0695	-0.0201	-0.1616	0.8443	0.0500	0.2521	0.4355
42.72540				//	0.0172	0.0478	0.0540	-0.0666	0.6200	0.0700	0.6709	0.0270	0.1402	0.3610
53.21570	0.68578	0.00000	-0.55049	//	-0.0770	-0.0188	0.1983	-0.0549	0.1270	-0.1728	-0.1689	0.9187	0.1734	0.0533
45.72286				//	0.0210	-0.0338	0.1304	-0.0436	0.0039	-0.0245	-0.0561	0.9877	-0.0093	0.0080
67.14929	0.42187	-0.00002	0.38437	//	0.0420	-0.0758	0.1434	-0.1265	-0.0086	0.2580	0.0916	-0.0830	-0.7641	-0.5386
53.06974				//	-0.0316	0.1738	0.0773	0.0953	0.3948	-0.5856	-0.4897	-0.0406	0.4315	0.1653
61.16982	0.10624	0.00001	0.20209	//	0.0021	-0.1596	0.0041	0.1787	-0.0769	0.4688	-0.3515	-0.0671	0.3645	0.6753
65.33937				//	0.0218	0.1048	-0.2450	-0.1972	0.0019	-0.2118	-0.1224	0.0206	-0.6929	0.5909



ATOMIC COORDINATES

x	1.7320	0.8660	0.	0.	0.	0.	0.8660
y	0.5000	0.	0.5000	1.5000	3.5000	4.5000	5.0000

1.7320	2.5980	2.5980	1.7320	0.8660	0.8660	1.7320
4.5000	3.0000	2.0000	1.5000	2.0000	3.0000	3.5000

PHENANTHRENE TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 A	9 S	10 S	11 A	12 A	13 S	14 A
1.600918	1.481431	1.374224	1.322284	1.281944	1.189816	1.149365	0.850634	0.810182	0.718054	0.677715	0.625774	0.518568	0.399081
0.207414	0.325932	0.019508	0.333369	-0.221273	-0.273024	-0.340189	-0.340189	0.273023	0.221273	-0.333369	-0.019508	0.325932	0.207414
0.149744	0.314273	-0.201752	0.405792	0.143796	0.388579	-0.042043	0.042044	-0.388579	0.143796	0.405792	-0.201752	-0.314273	-0.149744
0.157170	0.287087	-0.325411	0.196509	-0.385538	0.025822	-0.314745	-0.314745	0.025823	-0.385538	0.196509	0.325411	0.287087	0.157169
0.232932	0.245730	-0.291661	-0.149201	0.296637	-0.368738	0.232531	-0.232533	0.368738	0.296637	-0.149200	-0.291661	-0.245730	0.232932
0.232932	-0.245730	-0.291661	-0.149201	-0.296637	0.368737	-0.232533	-0.232532	-0.368738	-0.296637	0.149200	0.291661	-0.245730	0.232932
0.157170	-0.287087	-0.325411	0.196509	-0.385537	-0.025823	0.314745	-0.314745	0.025823	-0.385538	0.196510	0.325411	0.287086	-0.157169
0.149744	-0.314273	-0.201752	-0.405792	-0.143796	-0.388578	-0.042044	-0.042043	-0.388579	-0.143796	-0.405792	-0.201752	-0.314273	0.149743
0.207414	-0.325932	0.019508	0.333369	0.221273	-0.273022	-0.340190	0.340189	0.273023	0.221273	0.333369	0.019508	0.325932	-0.207414
0.247614	-0.108965	-0.448094	-0.096516	-0.185122	-0.100966	-0.415025	-0.415025	-0.100967	-0.185122	-0.096516	-0.448094	-0.108965	-0.247614
0.247614	0.108965	0.448094	-0.096516	-0.185122	-0.100968	0.415025	-0.415025	-0.100967	0.185122	-0.096516	-0.448094	0.108965	-0.247614
0.355268	0.321506	-0.231343	-0.029518	-0.396587	-0.178612	-0.163840	-0.163840	-0.178613	-0.396587	-0.029519	-0.231343	-0.321506	-0.355268
0.409962	0.192248	-0.116831	-0.391323	-0.046655	-0.309408	-0.174006	-0.174006	-0.309409	0.046655	0.391323	0.116832	0.192248	-0.409962
0.409962	-0.192248	-0.116831	-0.391323	-0.046655	-0.309409	-0.174005	-0.174006	-0.309408	-0.046655	-0.391323	-0.116832	-0.192248	-0.409962
0.355268	-0.321506	0.231343	0.029518	0.396587	0.178613	-0.163840	-0.163840	0.178613	-0.396587	-0.029518	-0.231343	-0.321506	-0.355268

PHENANTHRENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 A	9 S	10 A	11 A	12 A	13 S	14 A
28.44278	24.62511	20.63479	18.46884	16.66557	12.08870	9.84726	-13.30562	-17.75334	-29.75328	-36.03459	-45.31495	-70.34860	114.09890
0.163928	0.267785	0.016641	0.289910	-0.195431	0.250300	-0.317315	-0.368850	0.303324	0.261126	-0.404950	-0.024661	0.452610	0.328327
0.118349	0.258206	-0.172103	0.352892	0.127002	0.356237	-0.039216	0.045586	-0.431705	0.169695	0.492924	-0.255040	-0.436419	-0.237038
0.124218	0.235870	-0.277590	0.170892	0.340512	0.023673	0.293583	-0.341262	0.028689	-0.454976	0.238704	0.411361	0.398667	0.248793
0.184096	0.201891	-0.248800	-0.129750	0.261994	-0.338048	0.216897	-0.252123	0.409662	0.350064	-0.181237	-0.368697	-0.341236	-0.368721
0.184096	-0.201891	-0.248800	-0.129750	-0.261993	0.338047	-0.216898	0.252122	-0.409663	-0.350064	0.181237	0.368697	-0.341236	0.368721
0.124218	-0.235870	-0.277590	0.170892	-0.340512	-0.023674	0.293583	-0.341262	0.028689	-0.454976	0.238704	-0.411361	0.398667	-0.248793
0.118349	-0.258206	-0.172103	0.352892	-0.127002	-0.356237	-0.039217	-0.045585	-0.431705	-0.169694	-0.492924	-0.255040	-0.436419	0.237038
0.163928	-0.267785	0.016642	0.289910	0.195431	-0.250298	-0.317316	0.368849	0.303325	0.261126	0.404950	0.024661	0.452610	-0.328327
0.195700	-0.089525	0.382243	0.083934	0.163502	0.092563	0.387120	-0.449990	-0.112173	0.218464	0.117240	0.566448	0.151316	-0.391962
0.195700	0.089525	0.382243	0.083934	-0.163502	-0.092564	0.387120	0.449990	-0.112172	0.218464	-0.117240	-0.566448	0.151316	-0.391962
0.280784	0.264149	0.197346	0.025670	-0.350271	-0.163746	-0.152824	0.177643	0.198436	-0.468015	0.035857	0.292447	-0.446464	-0.562375
0.324010	0.157950	-0.099662	-0.340309	-0.041207	-0.283656	-0.162307	-0.188665	-0.343749	0.055058	0.475349	0.147690	0.266968	-0.648953
0.324010	-0.157950	-0.099662	-0.340309	0.041207	0.283656	-0.162306	-0.188666	0.343748	-0.055058	-0.475349	-0.147690	0.266968	-0.648952
0.280784	-0.264149	0.197346	0.025670	0.350270	0.163747	-0.152823	-0.177643	0.198436	-0.468015	-0.035857	-0.292447	-0.446464	-0.562375

PHENANTHRENE — TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.00000	0.70682	-0.00000	-0.34488	-0.00000	-0.06125	0.00000	0.08106	-0.19565	-0.00000	0.57511	0.00000	0.04597	0.00000
2	0.70682	1.00000	0.62279	-0.00000	0.09361	0.00000	-0.08175	-0.00000	0.00000	-0.12643	-0.00000	-0.26608	-0.00000	0.10157
3	-0.00000	0.62279	1.00000	0.70155	0.00000	0.07310	0.00000	-0.06125	0.17079	-0.00000	-0.26085	0.00000	-0.11686	0.00000
4	-0.34488	-0.00000	0.70155	1.00000	-0.13738	-0.00000	0.09361	0.00000	-0.00000	0.03637	0.00000	0.58997	0.00000	-0.10889
5	-0.00000	0.09361	0.00000	-0.13738	1.00000	0.70155	-0.00000	-0.34488	0.03637	-0.00000	-0.10889	0.00000	0.58997	0.00000
6	-0.06125	0.00000	0.07310	-0.00000	0.70155	1.00000	0.62279	0.00000	-0.00000	0.17079	0.00000	-0.11686	-0.00000	-0.26085
7	0.00000	-0.08175	0.00000	0.09361	-0.00000	0.62279	1.00000	0.70682	-0.12643	0.00000	0.10157	0.00000	-0.26608	-0.00000
8	0.08106	-0.00000	-0.06125	0.00000	-0.34488	0.00000	0.70682	1.00000	0.00000	-0.19565	-0.00000	0.04597	0.00000	0.57511
9	-0.19565	0.00000	0.17079	-0.00000	0.03637	-0.00000	-0.12643	0.00000	1.00000	0.77465	0.00000	-0.24330	-0.00000	0.50594
10	-0.00000	-0.12643	-0.00000	0.03637	-0.00000	0.17079	0.00000	-0.19565	0.77465	1.00000	0.50594	0.00000	-0.24330	0.00000
11	0.57511	-0.00000	-0.26085	0.00000	-0.10889	0.00000	0.10157	-0.00000	0.00000	0.50594	1.00000	0.54230	0.00000	-0.17020
12	0.00000	-0.26608	0.00000	0.58997	0.00000	-0.11686	0.00000	0.04597	-0.24330	0.00000	0.54230	1.00000	0.46052	0.00000
13	0.04597	-0.00000	-0.11686	0.00000	0.58997	-0.00000	-0.26608	0.00000	-0.00000	-0.24330	0.00000	0.46052	1.00000	0.54230
14	0.00000	0.10157	0.00000	-0.10889	0.00000	-0.26085	-0.00000	0.57511	0.50594	0.00000	-0.17020	0.00000	0.54230	1.00000

PHENANTHRENE — TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.76888	0.52955	-0.05066	-0.32431	0.00270	-0.06083	-0.00440	0.07867	-0.18565	-0.05461	0.40690	-0.03270	0.04990	0.01409
2	0.52955	0.75880	0.44770	-0.04942	0.09067	-0.00263	-0.08002	-0.00440	0.00487	-0.11762	-0.04059	-0.24745	0.01454	0.09786
3	-0.05066	0.44770	0.76005	0.52453	0.00921	0.07148	-0.00263	-0.06083	0.16589	0.01890	-0.24245	-0.04277	-0.10880	0.00092
4	-0.32431	-0.04942	0.52453	0.76670	-0.12801	0.00921	0.09067	0.00270	0.01494	0.04106	-0.03394	0.42076	-0.04717	-0.10160
5	0.00270	0.09067	0.00921	-0.12801	0.76670	0.52453	-0.04942	-0.32431	0.04106	0.01494	-0.10160	-0.04717	0.42076	-0.03394
6	-0.06083	-0.00263	0.07148	0.00921	0.52453	0.76005	0.44770	-0.05066	0.01890	0.16589	0.00092	-0.10880	-0.04277	-0.24245
7	-0.00440	-0.08002	-0.00263	0.09067	-0.04942	0.44770	0.75880	0.52955	-0.11762	0.00487	0.09786	0.01454	-0.24745	-0.04059
8	0.07867	-0.00440	-0.06083	0.00270	-0.32431	-0.05066	0.52955	0.76888	-0.05461	-0.18565	0.01409	0.04990	-0.03270	0.40690
9	-0.18565	0.00487	0.16589	0.01494	0.04106	0.01890	-0.11762	-0.05461	0.76926	0.59600	-0.04540	-0.22643	-0.03790	0.33890
10	-0.05461	-0.11762	0.01890	0.04106	0.01494	0.16589	0.00487	-0.18565	0.59600	0.76926	0.33890	-0.03790	-0.22643	-0.04540
11	0.40690	-0.04059	-0.24245	-0.03394	-0.10160	0.00092	0.09786	0.01409	-0.04540	0.33890	0.72215	-0.37996	-0.03045	-0.15496
12	-0.03270	-0.24745	-0.04277	0.42076	-0.04717	-0.10880	0.01454	0.04990	-0.22643	-0.03790	-0.37996	0.72835	-0.29992	-0.03045
13	0.04990	0.01454	-0.10880	-0.04717	0.42076	-0.04277	-0.24745	-0.03270	-0.03790	-0.22643	-0.03045	-0.29992	0.72835	0.37996
14	0.01409	0.09786	0.00092	-0.10160	-0.03394	-0.24245	-0.04059	0.40690	0.33890	-0.04540	-0.15496	-0.03045	0.37996	0.72215

ENERGIES FOR PHENANTHRENE .TBM APPROXIMATION. 1.7

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	7, 8	6, 8	7, 9	5, 8	4, 8	3, 8	4, 9	2, 8	3, 9	7,10
XMOMNT	-0.00000	-0.52662	-0.52725	-0.34616	-0.00000	-0.00000	0.22613	-0.00176	0.12928	0.34843
YMOMNT	-0.90114	0.00000	0.00000	-0.00000	-0.06790	0.06266	-0.00000	-0.00000	0.00000	-0.00000
JUMP E	23.1529	25.3943	27.6006	29.9712	31.7745	33.9404	36.2222	37.9307	38.3881	39.6005
DIAG E	34.8445	35.7053	37.5822	42.6547	43.2693	47.5555	50.2199	52.3297	52.2193	51.3969
DIAG E	35.2705	37.1363	36.6746	44.5043	45.0454	48.2989	50.6625	53.9410	51.6292	49.8079
CORRSP	34.7753	30.7856	39.9917	42.3265	42.5374	48.3566	48.9977	54.5663	51.6117	53.8285
CORRSP	35.2695	39.8078	31.2781	44.6054	44.5473	48.7980	53.2521	54.7380	51.7454	48.9289

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
30.78558	0.01680	-0.11328	-0.00000	//	0.0000	-0.7374	-0.5945	0.2255	-0.0000	-0.0000	-0.1025	-0.1142	0.0667	0.1550
27.09183				//	0.0000	0.8211	-0.4941	-0.1450	0.0000	-0.0000	-0.1786	-0.0391	-0.0860	0.1408
39.99165	0.39364	-0.48111	0.00000	//	-0.0000	0.6148	0.5990	-0.4894	0.0000	0.0000	-0.1209	0.0635	0.0669	0.0226
32.63946				//	-0.0000	-0.2466	0.7276	0.4448	-0.0000	-0.0000	0.1936	-0.0732	0.0364	-0.4095
42.32653	0.46559	-0.50860	-0.00000	//	0.0000	0.1593	0.5143	0.7547	-0.0000	-0.0000	0.2714	-0.2137	0.1154	0.0891
29.46121				//	0.0000	0.4289	-0.4368	0.7203	0.0000	-0.0000	-0.0309	-0.1796	0.1566	-0.2206
48.99769	0.00978	0.06849	0.00000	//	0.0000	0.1268	-0.1403	-0.1624	-0.0000	-0.0000	0.7035	0.0249	0.3437	-0.5694
40.88025				//	-0.0000	0.1511	-0.0470	-0.1017	-0.0000	0.0000	0.8939	-0.3541	-0.0267	0.1986
54.56628	0.02869	-0.11120	-0.00000	//	0.0000	0.1585	0.0024	0.1211	-0.0000	0.0000	0.3372	0.6644	-0.6332	0.0637
51.22089				//	0.0000	0.1139	-0.0731	0.1961	-0.0000	0.0000	0.2696	0.7067	-0.6080	-0.0384
51.61168	0.08339	0.19492	-0.00000	//	-0.0000	-0.0763	-0.0146	0.0947	-0.0000	0.0000	-0.0684	0.6512	0.6772	0.3124
46.24508				//	0.0000	0.2066	-0.0776	-0.3483	-0.0000	-0.0000	0.2243	0.4098	0.5468	-0.5591
53.82853	0.70134	0.55352	-0.00000	//	-0.0000	-0.0767	-0.0580	-0.3001	0.0000	-0.0000	0.5366	-0.2667	0.0032	0.7360
48.30147				//	-0.0000	-0.0501	0.1487	0.3035	0.0000	0.0000	0.0872	0.4099	0.5453	0.6405

ENERGIES FOR PHENANTHRENE , TBM APPROXIMATION 1.7

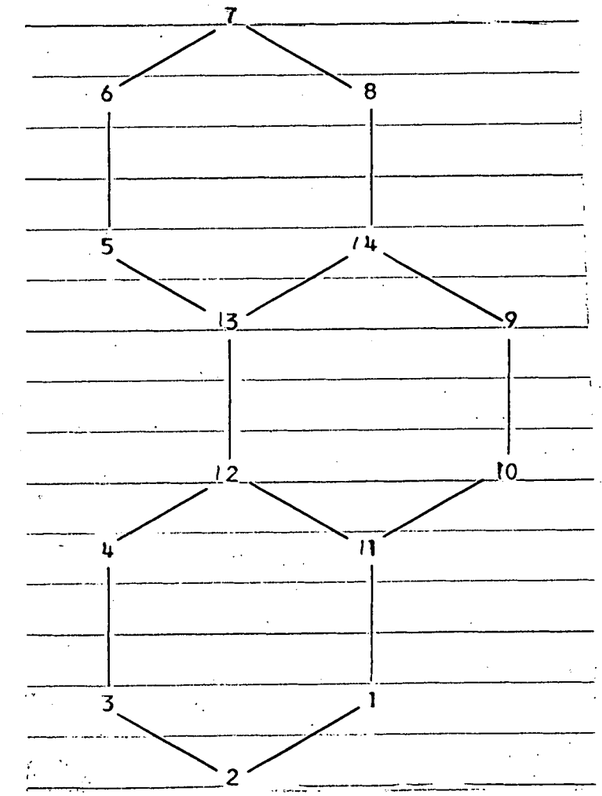
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	7, 8	6, 9	4, 8	3, 8	5, -9	1, 8	6,10	2, 9	7,11	5,10
XMOMNT	-0.00000	0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000
YMOMNT	-0.90114	0.69661	-0.06790	0.06266	0.38080	0.01405	-0.38288	-0.00062	0.06861	0.24276
JUMP E	23.1529	29.8420	31.7745	33.9404	34.4189	41.7484	41.8420	42.3785	45.8819	46.4189
DIAG E	34.8445	41.1380	43.2693	47.5555	45.1874	53.6928	52.0201	57.1272	56.1982	59.8162
DIAG E	35.2705	41.2355	45.0454	48.2989	45.7035	56.8700	51.4361	57.4049	54.7177	59.6508
CORRSP	32.5289	42.1023	43.6298	49.4079	38.8300	53.3477	54.2177	58.8605	57.5141	60.4101
CORRSP	32.9425	42.8004	45.4036	49.8692	39.0789	55.4666	53.6382	59.4935	56.1401	60.8000

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
32.52888	0.35157	-0.00000	-0.50414	//	0.8972	0.3990	0.0699	-0.0079	0.0802	-0.0804	-0.0660	-0.0721	-0.0223	-0.0887
20.27172				//	0.9451	0.2332	-0.0036	0.0761	-0.0957	0.0043	0.0797	-0.0090	0.0064	-0.1760
42.10231	1.17741	0.00000	0.81094	//	-0.3444	0.8385	-0.1043	-0.1902	-0.3049	0.0689	-0.0763	-0.1027	0.1305	-0.0075
28.95560				//	-0.2186	0.8157	-0.4157	-0.2080	-0.1304	0.0008	0.1166	-0.0325	0.1936	-0.0416
43.62975	0.61443	-0.00000	0.57547	//	-0.2014	0.2818	0.4875	0.6066	0.4928	0.0530	0.0249	-0.1469	-0.0419	0.0686
34.27576				//	-0.0640	0.4669	0.4036	0.4427	0.5402	0.0459	-0.2899	-0.1059	-0.1695	0.0334
49.40792	0.05908	0.00000	-0.16769	//	0.1308	-0.0433	-0.3674	0.7143	-0.4632	0.2800	-0.1123	0.0288	0.1056	0.1354
37.04048				//	0.0123	-0.1005	-0.5111	0.6653	0.0957	0.2106	0.3240	0.1488	0.0178	0.3241
38.82999	0.08676	-0.00000	0.22923	//	-0.0248	0.1466	-0.7091	0.0151	0.5285	0.1662	0.3432	-0.0231	-0.2229	-0.0054
39.49412				//	0.0784	-0.1298	-0.4140	-0.3693	0.7099	0.0143	0.1183	-0.0327	-0.3011	-0.2435
53.34774	0.10608	0.00000	0.21624	//	0.0174	-0.1129	-0.0136	-0.2062	0.2430	0.6601	-0.6030	-0.2557	0.1211	-0.0764
46.84141				//	-0.0700	-0.0023	0.1718	-0.0321	-0.1273	0.6264	0.3755	-0.6085	-0.1762	-0.1172
54.21767	0.54790	-0.00000	-0.48748	//	0.0979	-0.0680	0.2591	-0.1245	-0.2300	0.5046	0.6707	-0.3796	0.0135	0.0397
50.27884				//	-0.0350	0.0816	0.3150	-0.0185	0.1072	-0.5457	0.7400	-0.0465	-0.0694	0.1695
58.86048	0.00192	0.00000	-0.02773	//	0.0211	0.1249	0.1953	-0.0357	-0.0142	0.4326	0.0777	0.8260	-0.2170	-0.1474
55.54490				//	0.0092	0.1542	0.2354	-0.2442	-0.0520	0.4235	0.1587	0.6898	-0.3689	0.2050
57.51411	0.00075	-0.00000	0.01757	//	0.0404	-0.0111	-0.0469	-0.0014	0.2146	0.0059	0.1935	0.2282	0.9262	-0.0513
54.94083				//	-0.0368	-0.0691	0.2161	-0.0049	0.2955	0.2602	0.2253	0.2555	0.7533	-0.3295
60.41015	0.13414	0.00000	-0.22851	//	0.0782	0.0423	0.0341	-0.1616	0.0756	0.0488	-0.0438	0.1321	0.0110	0.9681
56.50482				//	0.2027	-0.0105	0.0296	-0.3391	0.2262	0.1273	-0.1120	-0.2258	0.3213	0.7802

PHENANTHRENE IRM



ATOMIC COORDINATES

x	1.7320	0.8660	0.	0.	0.	0.	0.8660
y	0.5000	0.	0.5000	1.5000	3.5000	4.5000	5.0000

1.7320	2.5980	2.5980	1.7320	0.8660	0.8660	1.7320
4.5000	3.0000	2.0000	1.5000	2.0000	3.0000	3.5000

PHENANTHRENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 A	9 S	10 S	11 A	12 A	13 S	14 A
1.739767	1.543349	1.378586	1.286532	1.225008	1.110802	1.078461	0.799578	0.773800	0.704445	0.670697	0.633615	0.562900	0.492450
0.214162	-0.327271	-0.013263	0.340953	-0.260237	0.245526	-0.331355	-0.328754	0.299642	0.183466	-0.344347	-0.000488	-0.323214	0.195535
0.164219	-0.326741	-0.233515	0.382734	0.111157	0.397827	-0.026220	0.040539	-0.383817	0.186218	0.392135	0.218700	0.298893	-0.139196
0.170742	-0.303638	-0.332855	0.150517	0.376426	0.032488	0.328773	0.317292	-0.001192	-0.391965	-0.191673	-0.325582	-0.275081	0.147090
0.240319	-0.251413	-0.279771	-0.202716	0.297948	-0.362160	0.215693	-0.238097	0.377567	0.274599	-0.146965	0.294331	0.241652	-0.227902
0.240319	0.251413	-0.279771	-0.202716	-0.297947	0.362160	0.215694	0.238097	0.377568	0.274599	0.146965	-0.294331	0.241652	0.227901
0.170742	0.303638	-0.332855	0.150517	-0.376426	-0.032489	0.328773	-0.317292	-0.001193	-0.391965	0.191673	0.325582	-0.275081	-0.147090
0.164219	0.326740	-0.233515	0.382734	-0.111158	-0.397827	-0.026221	-0.040538	-0.383817	0.186218	-0.392135	-0.218700	0.298893	0.139196
0.214162	0.327271	-0.013264	0.340954	0.260236	-0.245525	-0.331356	0.328753	0.299643	0.183467	0.344347	0.000488	-0.323214	-0.195535
0.253653	0.098228	0.449032	0.112412	0.194840	0.117330	0.409118	-0.421579	-0.072128	0.192197	0.111312	-0.438297	-0.108968	-0.237483
0.253653	-0.098228	0.449032	0.112412	-0.194840	-0.117331	0.409118	0.421580	-0.072127	0.192197	-0.111312	0.438297	-0.108968	0.237483
0.347630	-0.295731	0.223810	0.044850	-0.387543	-0.210574	-0.168570	0.161445	0.139374	-0.403039	-0.064145	-0.237489	0.341716	-0.362535
0.393795	-0.183367	-0.067159	-0.398582	-0.036045	-0.301873	-0.197755	-0.170645	-0.309375	0.056929	0.390914	0.105025	-0.208535	0.425425
0.393795	0.183367	-0.067159	-0.398582	0.036046	0.301874	-0.197754	0.170644	-0.309374	0.056929	-0.390914	0.105025	-0.208535	-0.425425
0.347630	0.295732	0.223809	0.044851	0.387543	0.210574	-0.168570	-0.161445	0.139373	-0.403039	-0.064145	0.237489	0.341716	0.362535

PHENANTHRENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 A	3 S	4 S	5 A	6 A	7 S	8 A	9 S	10 S	11 A	12 A	13 S	14 A
32.22032	26.67722	20.80924	16.87633	13.91824	7.55854	5.51282	-18.99378	-22.15079	-31.79188	-37.20455	-43.81655	-58.84036	-78.09841
0.162367	-0.263436	-0.011296	0.300597	-0.235125	0.232958	-0.319074	-0.367655	0.340634	0.218591	-0.420468	-0.000613	-0.430799	0.278640
0.124502	-0.263009	-0.198883	0.337433	0.100431	0.377464	-0.025248	0.045336	-0.436325	0.221869	0.478820	0.274749	0.398383	-0.198356
0.129448	-0.244413	-0.283490	0.132702	0.340103	0.030825	0.316588	0.354837	-0.001355	-0.467008	-0.234044	-0.409023	-0.366644	0.209605
0.182197	-0.202375	-0.238279	-0.178722	0.269197	-0.343623	0.207698	-0.266271	0.429220	0.327172	-0.179453	0.369762	0.322088	-0.324763
0.182197	0.202375	-0.238279	-0.178722	-0.269197	0.343623	0.207699	0.266270	0.429221	0.327172	0.179453	-0.369762	0.322088	0.324763
0.129448	0.244413	-0.283490	0.132701	-0.340103	-0.030826	0.316588	-0.354837	-0.001356	-0.467008	0.234044	0.409023	-0.366644	-0.209605
0.124502	0.263009	-0.198883	0.337433	-0.100432	-0.377464	-0.025249	-0.045335	-0.436325	0.221869	-0.478820	-0.274749	0.398383	0.198356
0.162367	0.263436	-0.011297	0.300597	0.235124	-0.232958	-0.319075	0.367654	0.340635	0.218591	0.420468	0.000613	-0.430799	-0.278640
0.192307	0.079069	0.382437	0.099107	0.176039	0.111325	0.393955	-0.471465	-0.081995	0.228993	0.135918	-0.550625	-0.145239	-0.338416
0.192307	-0.079068	0.382437	0.099106	-0.176039	-0.111326	0.393955	0.471465	-0.081994	0.228994	-0.135918	0.550625	-0.145239	0.338416
0.263555	-0.238049	0.190617	0.039542	-0.350147	-0.199795	-0.162323	0.180548	0.158440	-0.480201	0.078325	-0.298353	0.455459	-0.516617
0.298555	-0.147601	-0.057199	-0.351405	-0.032567	-0.286422	-0.190426	0.190835	-0.351698	0.067828	0.477329	-0.131940	-0.277948	0.606236
0.298555	0.147601	-0.057199	-0.351405	0.032568	0.286423	-0.190425	0.190836	-0.351698	0.067828	-0.477329	0.131940	-0.277948	-0.606236
0.263555	0.238049	0.190617	0.039543	0.350147	0.199796	-0.162322	-0.180549	0.158440	-0.480201	-0.078325	0.298353	0.455459	0.516617

PHENANTHRENE — IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.01440	0.70626	-0.01450	-0.33917	-0.00247	-0.05206	0.00354	0.07395	-0.20583	0.01035	0.57713	0.02026	0.03916	-0.00661
2	0.70626	1.01210	0.61746	-0.01451	0.10073	0.00155	-0.09742	0.00354	0.01067	-0.13429	-0.00762	-0.26240	-0.00566	0.11327
3	-0.01450	0.61746	1.01128	0.70257	-0.00434	0.07149	0.00155	-0.05206	0.18521	-0.00411	-0.25348	-0.00623	-0.13544	-0.00177
4	-0.33917	-0.01451	0.70257	1.01357	-0.11900	-0.00434	0.10073	-0.00247	-0.01670	0.01985	0.02124	0.59252	0.01376	-0.11934
5	-0.00247	0.10073	-0.00434	-0.11900	1.01357	0.70257	-0.01451	-0.33917	0.01985	-0.01670	-0.11934	0.01376	0.59252	0.02124
6	-0.05206	0.00155	0.07149	-0.00434	0.70257	1.01128	0.61746	-0.01450	-0.00411	0.18521	-0.00177	-0.13544	-0.00623	-0.25348
7	0.00354	-0.09742	0.00155	0.10073	-0.01451	0.61746	1.01210	0.70626	-0.13429	0.01067	0.11327	-0.00566	-0.26240	-0.00762
8	0.07395	0.00354	-0.05206	-0.00247	-0.33917	-0.01450	0.70626	1.01440	0.01035	-0.20583	-0.00661	0.03916	0.02026	0.57713
9	-0.20583	0.01067	0.18521	-0.01670	0.01985	-0.00411	-0.13429	0.01035	1.01472	0.76921	-0.00903	-0.23287	0.00895	0.50803
10	0.01035	-0.13429	-0.00411	0.01985	-0.01670	0.18521	0.01067	-0.20583	0.76921	1.01472	0.50803	0.00895	-0.23287	-0.00903
11	0.57713	-0.00762	-0.25348	0.02124	-0.11934	-0.00177	0.11327	-0.00661	-0.00903	0.50803	0.96671	0.53817	0.01112	-0.16125
12	0.02026	-0.26240	-0.00623	0.59252	0.01376	-0.13544	-0.00566	0.03916	-0.23287	0.00895	0.53817	0.96722	0.46302	0.01112
13	0.03916	-0.00566	-0.13544	0.01376	0.59252	-0.00623	-0.26240	0.02026	0.00895	-0.23287	0.01112	0.46302	0.96722	0.53817
14	-0.00661	0.11327	-0.00177	-0.11934	0.02124	-0.25348	-0.00762	0.57713	0.50803	-0.00903	-0.16125	0.01112	0.53817	0.96671

PHENANTHRENE — IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.79522	0.53111	-0.09061	-0.35550	0.00462	-0.05701	-0.00331	0.07941	-0.21058	-0.06544	0.40563	-0.03187	0.04887	0.01165
2	0.53111	0.78259	0.43872	-0.08984	0.10793	-0.00159	-0.10437	-0.00331	0.02057	-0.13506	-0.07126	-0.27557	0.01469	0.12063
3	-0.09061	0.43872	0.78264	0.52720	0.00550	0.07721	-0.00159	-0.05701	0.19665	0.02074	-0.26625	-0.07177	-0.13645	0.00200
4	-0.35550	-0.08984	0.52720	0.79310	-0.13289	0.00550	0.10793	0.00462	0.00231	0.02978	-0.03122	0.42161	-0.05649	-0.12151
5	0.00462	0.10793	0.00550	-0.13289	0.79310	0.52720	-0.08984	-0.35550	0.02978	0.00231	-0.12151	-0.05649	0.42161	-0.03122
6	-0.05701	-0.00159	0.07721	0.00550	0.52720	0.78264	0.43872	-0.09061	0.02074	0.19665	0.00200	-0.13645	-0.07177	-0.26625
7	-0.00331	-0.10437	-0.00159	0.10793	-0.08984	0.43872	0.78259	0.53111	-0.13506	0.02057	0.12063	0.01469	-0.27557	-0.07126
8	0.07941	-0.00331	-0.05701	0.00462	-0.35550	-0.09061	0.53111	0.79522	-0.06544	-0.21058	0.01165	0.04887	-0.03187	0.40563
9	-0.21058	0.02057	0.19665	0.00231	0.02978	0.02074	-0.13506	-0.06544	0.79580	0.59726	-0.07830	-0.24719	-0.05003	0.33251
10	-0.06544	-0.13506	0.02074	0.02978	0.00231	0.19665	0.02057	-0.21058	0.59726	0.79580	0.33252	-0.05003	-0.24719	-0.07830
11	0.40563	-0.07126	-0.26625	-0.03122	-0.12151	0.00200	0.12063	0.01165	-0.07830	0.33252	0.70579	0.37713	-0.03794	-0.17096
12	-0.03187	-0.27557	-0.07177	0.42161	-0.05649	-0.13645	0.01469	0.04887	-0.24719	-0.05003	0.37713	0.71408	0.29454	-0.03794
13	0.04887	0.01469	-0.13645	-0.05649	0.42161	-0.07177	-0.27557	-0.03187	-0.05003	-0.24719	-0.03794	0.29454	0.71408	0.37713
14	0.01165	0.12063	0.00200	-0.12151	-0.03122	-0.26625	-0.07126	0.40563	0.33251	-0.07830	-0.17096	-0.03794	0.37713	0.70579

ENERGIES FOR PHENANTHRENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF S1 SYMMETRY

JUMP	7, 8	6, 8	7, 9	5, 8	4, 8	7,10	4, 9	3, 8	7,11	3, 9
XMOMNT	-0.00000	-0.54450	-0.46154	-0.33622	-0.00000	0.41460	0.30207	-0.00000	-0.00000	0.12214
YMOMNT	-0.90682	0.00000	-0.00000	-0.00000	-0.04800	-0.00000	0.00000	0.04781	0.05650	0.00000
JUMP E	24.5066	26.5523	27.6636	32.9120	35.8701	37.3047	39.0271	39.8030	42.7174	42.9600
DIAG E	35.7238	36.2091	37.0815	45.4980	46.8338	48.8288	53.0585	53.6814	52.7692	57.2092
DIAG E	36.3710	37.8841	36.5281	47.3957	48.8447	47.1660	53.8689	54.4234	51.2921	56.7506
CORRSP	35.6714	31.4525	40.1959	44.7210	45.9703	48.7225	55.0943	54.4705	52.8961	57.6989
CORRSP	36.0703	40.4105	31.7405	46.2300	47.7047	48.3421	55.6664	54.7372	52.4190	57.2038

FINAL EXCITED STATES OF S1 SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
31.45254	0.01151	-0.09275	-0.00000	//	0.0000	0.7307	-0.6262	0.1471	0.0000	0.1985	-0.0856	-0.0000	-0.0000	0.0751
27.60609				//	0.0000	0.7510	0.5853	-0.1911	0.0000	0.1286	-0.1880	0.0000	0.0000	-0.0710
40.19585	0.60265	-0.59377	0.00000	//	-0.0000	0.6340	0.7448	-0.1644	-0.0000	0.0943	-0.0298	-0.0000	0.0000	0.0804
30.32303				//	-0.0000	-0.5874	0.5510	-0.5392	-0.0000	0.1754	0.0921	0.0000	0.0000	-0.1462
44.72104	0.07146	-0.19384	-0.00000	//	-0.0000	-0.0469	0.2125	0.9096	-0.0000	0.2523	0.2421	-0.0000	-0.0000	0.0556
33.38241				//	-0.0000	-0.1506	0.5531	0.5446	-0.0000	-0.5934	0.1395	-0.0000	0.0000	0.0569
48.72254	0.23603	0.33751	-0.00000	//	-0.0000	-0.2132	0.0399	-0.1252	0.0000	0.8444	-0.4616	0.0000	0.0000	-0.1056
46.31547				//	-0.0000	-0.2107	0.1885	-0.5745	0.0000	0.6663	-0.3822	0.0000	0.0000	-0.0027
55.09428	0.87847	0.61233	0.00000	//	-0.0000	-0.0383	-0.0800	-0.3291	-0.0000	0.4176	0.8219	-0.0000	0.0000	0.1842
44.30963				//	-0.0000	0.1527	0.0609	0.1770	-0.0000	0.3884	0.8892	0.0000	-0.0000	-0.0106
57.69886	0.03189	0.11401	0.00000	//	-0.0000	-0.1224	-0.0060	-0.0010	0.0000	-0.0250	-0.2112	-0.0000	-0.0000	0.9694
53.84514				//	-0.0000	-0.0232	0.0932	-0.1218	-0.0000	0.0756	0.0006	-0.0000	-0.0000	0.9850

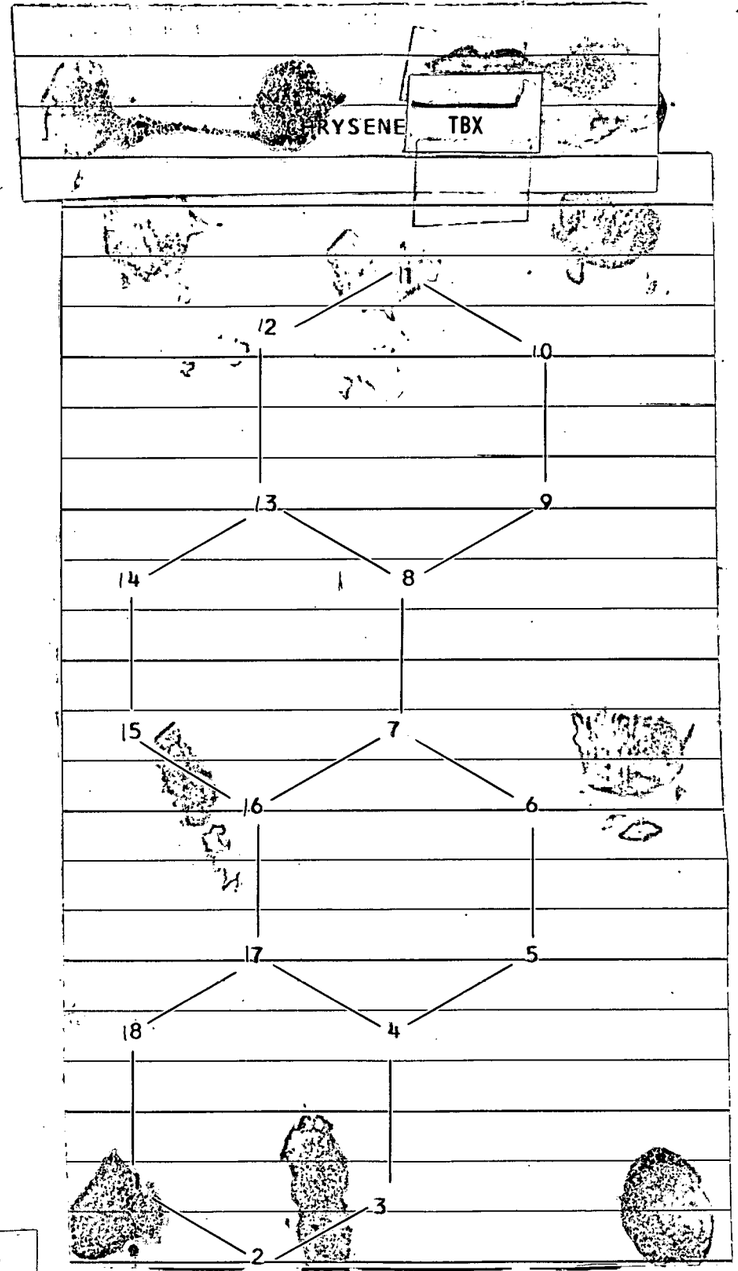
ENERGIES FOR PHENANTHRENE , TRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	7, 8	6, 9	4, 8	5, 9	6,10	3, 8	7,11	5,10	2, 9	7,12
XMOMNT	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	0.00000
YMOMNT	-0.90682	0.71112	-0.04800	0.39506	-0.44198	0.04781	0.05650	0.25043	-0.02943	0.05082
JUMP E	24.5066	29.7093	35.8701	36.0690	39.3504	39.8030	42.7174	45.7101	48.8280	49.3294
DIAG E	35.7238	40.8139	46.8338	46.8385	49.2174	53.6814	52.7692	58.7259	63.8898	61.5773
DIAG E	36.3710	41.2883	48.8447	47.5356	48.5823	54.4234	51.2921	58.3136	64.2429	62.3772
CORRSP	33.2731	42.6064	47.1372	40.3291	51.5230	54.6023	54.0030	58.4784	64.7605	63.3579
CORRSP	33.6563	43.4420	48.7052	40.0217	53.2322	54.5995	50.7177	59.5504	63.8841	65.4618

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
33.27305	0.26790	-0.00000	-0.43513	//	0.8771	0.4545	0.0087	0.0661	-0.0865	-0.0130	-0.0328	-0.0906	0.0521	-0.0035
20.99982				//	0.9407	0.2415	-0.0140	-0.1145	0.0506	0.0870	-0.0120	-0.1679	0.0012	0.0701
42.60639	1.41146	0.00000	0.88262	//	-0.4105	0.8269	0.0440	-0.3091	-0.0856	-0.0535	0.1850	0.0166	0.0713	-0.0235
28.77828				//	-0.2276	0.8380	-0.3331	-0.1495	0.0872	-0.1734	0.2187	-0.0790	0.0202	-0.1434
47.13721	0.40311	-0.00000	0.44844	//	-0.1188	0.1315	0.7081	0.5427	-0.0822	0.3866	-0.0686	0.0635	0.0764	0.0438
40.71270				//	-0.0417	0.0618	0.4778	-0.6336	-0.4416	0.0478	0.3587	0.1608	0.0159	0.1123
40.32915	0.19693	-0.00000	0.33886	//	-0.1487	0.2821	-0.5133	0.5492	0.4828	0.0900	-0.2982	-0.0438	-0.0098	-0.0319
37.96466				//	0.0296	0.0615	0.3437	0.2440	-0.4123	-0.5264	-0.1652	-0.4638	0.1328	-0.3324
51.52301	0.70889	-0.00000	-0.56881	//	0.1235	-0.0371	0.2859	-0.1933	0.7991	0.0613	0.3935	0.0061	0.0250	-0.2580
48.00623				//	-0.0700	0.1667	0.6077	-0.0996	0.6713	0.0013	-0.1972	0.0426	0.2949	-0.0984
54.60227	0.03832	0.00000	-0.12846	//	0.0753	0.0058	-0.1451	-0.4114	0.0647	0.7525	-0.2777	0.3672	-0.0024	0.1466
34.34352				//	-0.0679	0.4378	0.2820	0.4857	-0.3318	0.4495	-0.2388	0.1694	-0.0113	0.3004
54.00304	0.13258	-0.00000	0.24027	//	0.0148	-0.0436	-0.3471	0.2535	-0.2707	0.4088	0.7268	-0.0162	-0.0633	-0.2005
51.45217				//	0.0470	-0.0591	0.1969	0.4102	0.1326	0.2530	0.7656	-0.1296	-0.0970	-0.3055
58.47836	0.11520	-0.00000	0.21523	//	0.0660	0.0211	-0.0417	0.1791	0.0683	-0.2994	0.2460	0.8019	0.0982	0.3922
55.82504				//	0.1888	0.0466	0.0755	0.2787	0.0376	-0.5982	0.1825	0.6790	-0.0519	0.1499
64.76047	0.00003	0.00000	-0.00314	//	-0.0081	-0.0724	-0.0670	0.0032	-0.1081	-0.0363	-0.1278	0.1920	0.8046	-0.5260
59.49913				//	0.0065	-0.0821	-0.1880	-0.0926	-0.0869	0.0113	0.2172	-0.0468	0.9057	0.2682
63.35791	0.06733	0.00000	-0.15809	//	-0.0189	-0.0624	-0.0601	-0.0312	0.1140	0.1064	-0.1843	-0.4129	0.5698	0.6617
61.21343				//	-0.1148	-0.0019	0.1174	-0.0558	0.1937	-0.2429	0.1833	-0.4626	-0.2493	0.7508



ATOMIC COORDINATES

X	0.	0.8646	1.7184	1.7399	2.6286	2.6577	1.7956	1.8342	2.7024
Y	0.5050	0.	0.4790	1.5050	2.0060	2.9880	3.5380	4.5910	5.1090

2.7024	1.8378	0.9840	0.9625	0.0738	0.0447	0.9068	0.8682	0.
6.1010	6.6060	6.1270	5.1010	4.6000	3.6180	3.0680	2.0150	1.4970

CHRYSENEX TBX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 A	8 S	9 S	10 A	11 A	12 S	13 S	14 A	15 S	16 A	17 S	18 A
-1.592050	-1.523731	-1.419901	-1.375200	-1.307574	-1.293192	-1.217847	-1.199527	-1.134603	-0.865395	-0.800470	-0.782151	-0.706806	-0.692424	-0.624798	-0.580097	-0.476267	-0.407948
-0.131544	-0.235781	-0.315367	-0.214541	-0.231231	-0.260957	-0.269020	-0.169392	-0.242872	-0.242872	-0.169392	-0.269020	-0.260957	-0.231231	-0.214541	0.315367	0.235781	-0.131544
0.126809	-0.245567	0.349006	-0.102719	0.035326	-0.394010	-0.121986	0.330972	0.101707	0.101707	0.330973	0.121986	0.394010	-0.035325	-0.102719	-0.349006	-0.245567	-0.126809
0.164795	-0.272391	-0.266037	-0.054985	-0.261463	-0.197977	-0.357955	-0.093983	-0.283415	-0.283415	-0.093984	-0.357955	-0.197978	0.261462	0.054985	0.266037	0.272390	-0.164795
0.278866	-0.340562	0.091625	0.203655	0.307148	0.189937	-0.199832	-0.288876	0.050814	0.050814	-0.288876	0.199832	-0.189936	-0.307148	-0.203655	-0.091625	-0.340562	-0.278868
0.211805	-0.182389	-0.092098	-0.391638	-0.311817	-0.050767	-0.129015	-0.004897	-0.378860	-0.378860	-0.004897	-0.129015	-0.050767	0.311817	0.391638	-0.092098	0.182389	-0.211805
0.232455	-0.059778	-0.234286	0.385097	0.091860	-0.115976	0.292241	0.268238	-0.244860	-0.244861	0.268238	-0.292241	0.115976	-0.091860	-0.385096	-0.234286	-0.059778	-0.232455
0.355395	-0.066601	-0.319198	-0.187145	-0.221850	-0.201078	-0.130303	-0.223325	-0.275400	-0.275399	-0.223325	-0.130303	-0.201078	-0.221850	0.187145	-0.319198	-0.066601	-0.355395
0.319421	0.299593	-0.006537	0.118284	-0.164156	-0.371912	-0.037969	-0.334267	0.125454	0.125454	-0.334267	0.037969	0.371911	-0.164157	-0.118285	-0.006537	-0.299593	-0.319420
-0.185633	-0.250788	-0.185109	-0.219607	-0.317408	-0.081291	-0.352439	-0.189463	-0.229538	-0.229537	-0.189464	-0.352439	-0.081290	-0.317408	0.219607	0.185109	-0.250788	-0.185633
0.131544	0.235781	0.315367	0.214542	-0.231232	0.260956	-0.269019	0.169393	-0.242872	-0.242872	0.169392	0.269020	-0.260956	-0.231232	-0.214542	-0.315367	-0.235781	-0.131544
-0.126810	-0.245567	-0.349006	-0.102719	-0.035324	-0.394010	-0.121987	-0.330972	-0.101707	-0.101707	-0.330972	-0.121987	-0.394011	0.035324	0.102719	0.349006	-0.245567	-0.126809
0.164795	0.272390	0.266037	-0.054985	0.261462	0.197979	0.357955	0.093982	0.283415	0.283415	0.093983	-0.357955	-0.197979	-0.261462	-0.054985	-0.266037	-0.272390	-0.164795
-0.278867	-0.340561	-0.091625	-0.203655	-0.307149	-0.189935	-0.199831	-0.288877	-0.050814	-0.050814	-0.288876	-0.199832	-0.189936	0.307149	-0.203655	0.091626	-0.340562	-0.278866
0.211805	-0.182388	-0.092098	-0.391638	0.311817	-0.050766	-0.129015	0.004898	-0.378860	-0.378860	0.004897	0.129015	0.050766	-0.311817	-0.391638	-0.092098	-0.182389	-0.211805
-0.232455	-0.059778	-0.234286	-0.385096	-0.091859	-0.115976	-0.292240	-0.268239	-0.244860	-0.244861	-0.268238	-0.292241	-0.115976	0.091859	-0.385097	-0.234286	-0.059778	-0.232455
0.355395	-0.066601	-0.319198	-0.187145	-0.221851	0.201077	-0.130302	0.223325	-0.275400	0.275400	0.223325	0.130303	-0.201078	-0.221850	-0.187145	-0.319198	-0.066601	-0.355395
0.319420	-0.299593	-0.006538	-0.118285	-0.164158	-0.371911	-0.037968	-0.334267	-0.125454	-0.125454	-0.334267	-0.037968	-0.371911	-0.164157	-0.118285	-0.006537	0.299593	-0.319420
0.185632	-0.250788	0.185109	-0.219607	-0.317408	0.081290	0.352438	-0.189464	-0.229537	-0.229538	-0.189464	-0.352438	-0.081290	-0.317408	-0.219607	-0.185109	-0.250788	-0.185633

CHRYSENE TBX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 A	8 S	9 S	10 A	11 A	12 S	13 S	14 A	15 S	16 A	17 S	18 A
28.03514	25.91202	22.29410	20.56827	17.73309	17.09188	13.48526	12.53989	8.94359	11.72596	18.79157	20.99738	31.27200	33.48738	45.27164	54.56944	82.90131	109.40968
0.104254	-0.191009	-0.264660	-0.182948	-0.202215	-0.229476	-0.243775	-0.154663	-0.228011	-0.261078	-0.189331	-0.304186	-0.310398	-0.277882	-0.271420	0.414063	0.341652	-0.205953
0.100502	-0.198937	0.292889	-0.087593	0.030893	-0.346478	-0.110539	0.302194	0.095483	0.109331	0.369930	0.137932	0.468660	-0.042452	-0.129951	-0.458228	0.355832	-0.198540
-0.130607	-0.220667	-0.223261	-0.046888	-0.228653	-0.174094	-0.324363	-0.085812	-0.266073	-0.304660	-0.105046	-0.404746	-0.235487	0.314212	0.069563	0.349295	0.394699	-0.258013
0.221013	-0.275894	0.076893	0.173665	0.268605	0.167024	-0.181079	-0.263759	0.047705	0.054623	-0.322879	0.225954	-0.225921	-0.369115	-0.257647	-0.120300	-0.493481	-0.436610
-0.167864	-0.147756	-0.077290	-0.333966	-0.272688	-0.044643	-0.116908	-0.004472	-0.355677	-0.407259	-0.005474	-0.145880	-0.060385	0.374726	0.495467	-0.120920	0.264285	-0.331614
0.184230	-0.048427	-0.196615	0.328388	0.080333	-0.101985	0.264816	0.244915	-0.229877	-0.263216	0.299811	-0.330442	0.137949	-0.110392	-0.487191	-0.307606	-0.086620	-0.363946
0.281665	-0.053954	-0.267874	-0.159586	-0.194011	-0.176821	-0.118075	-0.203907	-0.258548	-0.296044	-0.249612	-0.147336	-0.239174	-0.266608	0.236760	-0.419092	-0.096506	-0.556428
0.253154	0.242704	-0.005486	0.100866	-0.143557	-0.327046	-0.034406	-0.305203	0.117777	0.134858	-0.373612	0.042932	0.442374	-0.197275	-0.149644	-0.008583	-0.434117	-0.500104
-0.147122	-0.203166	-0.155346	-0.187268	-0.277578	-0.071484	-0.319365	-0.172990	-0.215492	-0.246744	-0.211765	-0.398509	-0.096692	-0.381445	0.277828	0.243040	-0.363397	-0.290638
0.104254	0.191009	0.264660	0.182948	-0.202216	0.229475	-0.243774	0.154664	-0.228011	-0.261078	0.189331	0.304185	-0.310397	0.277883	-0.271420	-0.414063	-0.341652	-0.205954
0.100502	-0.198937	-0.292889	-0.087593	-0.030891	-0.346479	-0.110540	-0.302194	-0.095484	-0.109331	-0.369929	-0.137933	-0.468660	0.042451	0.129952	0.458229	-0.355832	-0.198540
0.130607	0.220667	0.223261	-0.046888	0.228652	0.174095	0.324364	0.085811	0.266073	0.304660	0.105045	-0.404746	-0.235488	-0.314212	-0.069563	-0.349295	-0.394699	-0.258013
-0.221013	-0.275893	-0.076893	-0.173665	-0.268606	-0.167022	-0.181079	-0.263759	-0.047705	-0.054623	-0.322879	-0.225953	-0.225921	0.369116	-0.257647	0.120300	-0.493481	-0.436610
0.167864	0.147755	-0.077289	-0.333966	0.272689	-0.044641	-0.116908	-0.004472	-0.355677	-0.407259	0.005474	0.145880	0.060384	-0.374726	-0.495467	-0.120920	-0.264285	-0.331614
-0.184230	-0.048427	-0.196615	-0.328388	-0.080332	-0.101985	-0.264816	-0.244916	-0.229878	-0.263216	-0.299811	-0.330442	-0.137949	0.110392	-0.487192	-0.307606	-0.086620	-0.363946
0.281665	-0.053954	-0.267874	-0.159587	-0.194012	0.176820	-0.118075	-0.203907	0.258548	0.296044	0.249612	0.147336	-0.239174	-0.266609	0.236761	-0.419092	-0.096506	-0.556428
0.253153	-0.242704	-0.005486	-0.100866	-0.143559	-0.327045	-0.034405	-0.305203	-0.117777	-0.134858	-0.373612	-0.042932	-0.442373	-0.197276	-0.149644	-0.008583	0.434117	-0.500104
0.147121	-0.203167	0.155345	-0.187268	-0.277578	0.071483	-0.319365	-0.172991	-0.215492	-0.246744	-0.211765	-0.398509	-0.096691	-0.381445	-0.277828	-0.243040	-0.363397	-0.290638

CHRYSENE

TBX TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	8	9	10	11	12	13	14	15	16	17	18	
1	1.00000	0.59976	0.00000	0.26687	0.00000	0.16143	0.00000	0.03671	0.00000	0.03164	0.00000	0.03118	0.00000	0.07824	0.00000	0.12669	0.00000	0.71938	1
2	0.59976	1.00000	0.73165	0.00000	0.12472	0.00000	0.11101	0.00000	0.03648	0.00000	0.03608	0.00000	0.04901	0.00000	0.05932	0.00000	0.26179	0.00000	2
3	0.00000	0.73165	1.00000	0.55157	0.00000	0.17676	0.00000	0.04848	0.00000	0.03118	0.00000	0.02181	0.00000	0.05993	0.00000	0.05874	0.00000	0.34406	3
4	0.26687	0.00000	0.55157	1.00000	0.50294	0.00000	0.19520	0.00000	0.05722	0.00000	0.04901	0.00000	0.06613	0.00000	0.07343	0.00000	0.56397	0.00000	4
5	0.00000	0.12472	0.00000	0.50294	1.00000	0.77415	0.00000	0.12839	0.00000	0.07824	0.00000	0.05993	0.00000	0.17653	0.00000	0.27100	0.00000	0.03732	5
6	0.16143	0.00000	0.17676	0.00000	0.77415	1.00000	0.51795	0.00000	0.09596	0.00000	0.05932	0.00000	0.07343	0.00000	0.00291	0.00000	0.23871	0.00000	6
7	0.00000	0.11101	0.00000	0.19520	0.00000	0.51795	1.00000	0.44770	0.00000	0.12669	0.00000	0.05874	0.00000	0.27100	0.00000	0.61252	0.00000	0.11289	7
8	0.03671	0.00000	0.04848	0.00000	0.12839	0.00000	0.44770	1.00000	0.57890	0.00000	0.26179	0.00000	0.56397	0.00000	0.23871	0.00000	0.02597	0.00000	8
9	0.00000	0.03648	0.00000	0.05722	0.00000	0.09596	0.00000	0.57890	1.00000	0.71938	0.00000	0.34406	0.00000	0.03732	0.00000	0.11289	0.00000	0.03223	9
10	0.03164	0.00000	0.03118	0.00000	0.07824	0.00000	0.12669	0.00000	0.71938	1.00000	0.59976	0.00000	0.26687	0.00000	0.16143	0.00000	0.03671	0.00000	10
11	0.00000	0.03608	0.00000	0.04901	0.00000	0.05932	0.00000	0.26179	0.00000	0.59976	1.00000	0.73165	0.00000	0.12472	0.00000	0.11101	0.00000	0.03648	11
12	0.03118	0.00000	0.02181	0.00000	0.05993	0.00000	0.05874	0.00000	0.34406	0.00000	0.73165	1.00000	0.55157	0.00000	0.17676	0.00000	0.04848	0.00000	12
13	0.00000	0.04901	0.00000	0.06613	0.00000	0.07343	0.00000	0.56397	0.00000	0.26687	0.00000	0.55157	1.00000	0.50294	0.00000	0.19520	0.00000	0.05722	13
14	0.07824	0.00000	0.05993	0.00000	0.17653	0.00000	0.27100	0.00000	0.03732	0.00000	0.12472	0.00000	0.50294	1.00000	0.77415	0.00000	0.12839	0.00000	14
15	0.00000	0.05932	0.00000	0.07343	0.00000	0.00291	0.00000	0.23871	0.00000	0.16143	0.00000	0.17676	0.00000	0.77415	1.00000	0.51795	0.00000	0.09596	15
16	0.12669	0.00000	0.05874	0.00000	0.27100	0.00000	0.61252	0.00000	0.11289	0.00000	0.11101	0.00000	0.19520	0.00000	0.51795	1.00000	0.44770	0.00000	16
17	0.00000	0.26179	0.00000	0.56397	0.00000	0.23871	0.00000	0.02597	0.00000	0.03671	0.00000	0.04848	0.00000	0.12839	0.00000	0.44770	1.00000	0.57890	17
18	0.71938	0.00000	0.34406	0.00000	0.03732	0.00000	0.11289	0.00000	0.03223	0.00000	0.03648	0.00000	0.05722	0.00000	0.09596	0.00000	0.57890	1.00000	18

CHRYSENE

TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.75951	0.42660	0.05296	0.24828	0.01814	0.15670	0.00029	0.03648	0.00089	0.03135	0.00026	0.03076	0.00210	0.07663	0.00818	0.11914	0.04388	0.53896
2	0.42660	0.75358	0.54577	0.04060	0.11640	0.00481	0.10733	0.00317	0.03579	0.00026	0.03553	0.00190	0.04788	0.00341	0.05708	0.01333	0.24317	0.04878
3	0.05296	0.54577	0.76751	0.39238	0.04932	0.16734	0.01394	0.04686	0.00354	0.03076	0.00190	0.02186	0.00234	0.05961	0.00089	0.06170	0.03022	0.32347
4	0.24828	0.04060	0.39238	0.73143	0.34261	0.04597	0.17998	0.01050	0.05522	0.00210	0.04788	0.00234	0.06358	0.00241	0.06758	0.02764	0.40185	0.03422
5	0.01814	0.11640	0.04932	0.34261	0.76813	0.58823	0.04947	0.12056	0.00973	0.07663	0.00341	0.05961	0.00241	0.17202	0.01531	0.25440	0.03737	0.04175
6	0.15670	0.00481	0.16734	0.04597	0.58823	0.76518	0.35715	0.04005	0.08839	0.00818	0.05708	0.00089	0.06758	0.01531	0.00233	0.03923	0.22250	0.01411
7	0.00029	0.10733	0.01394	0.17998	0.04947	0.35715	0.74149	0.30360	0.04306	0.11914	0.01333	0.06170	0.02764	0.25440	0.03923	0.44714	0.02823	0.10618
8	0.03648	0.00317	0.04686	0.01050	0.12056	0.04005	0.30360	0.73794	0.41244	0.04388	0.24317	0.03022	0.40185	0.03737	0.22250	0.02823	0.02905	0.00219
9	0.00089	0.03579	0.00354	0.05522	0.00973	0.08839	0.04306	0.41244	0.76528	0.53896	0.04878	0.32347	0.03422	0.04175	0.01411	0.10618	0.00219	0.03148
10	0.03135	0.00026	0.03076	0.00210	0.07663	0.00818	0.11914	0.04388	0.53896	0.75951	0.42660	0.05296	0.24828	0.01814	0.15670	0.00029	0.03648	0.00089
11	0.00026	0.03553	0.00190	0.04788	0.00341	0.05708	0.01333	0.24317	0.04878	0.42660	0.75358	0.54577	0.04060	0.11640	0.00481	0.10733	0.00317	0.03579
12	0.03076	0.00190	0.02186	0.00234	0.05961	0.00089	0.06170	0.03022	0.32347	0.05296	0.54577	0.76751	0.39238	0.04932	0.16734	0.01394	0.04686	0.00354
13	0.00210	0.04788	0.00234	0.06358	0.00241	0.06758	0.02764	0.40185	0.03422	0.24828	0.04060	0.39238	0.73143	0.34261	0.04597	0.17998	0.01050	0.05522
14	0.07663	0.00341	0.05961	0.00241	0.17202	0.01531	0.25440	0.03737	0.04175	0.01814	0.11640	0.04932	0.34261	0.76812	0.58823	0.04947	0.12056	0.00973
15	0.00818	0.05708	0.00089	0.06758	0.01531	0.00233	0.03923	0.22250	0.01411	0.15670	0.00481	0.16734	0.04597	0.58823	0.76518	0.35715	0.04005	0.08839
16	0.11914	0.01333	0.06170	0.02764	0.25440	0.03923	0.44714	0.02823	0.10618	0.00029	0.10733	0.01394	0.17998	0.04947	0.35715	0.74149	0.30360	0.04306
17	0.04388	0.24317	0.03022	0.40185	0.03737	0.22250	0.02823	0.02905	0.00219	0.03648	0.00317	0.04686	0.01050	0.12056	0.04005	0.30360	0.73794	0.41244
18	0.53896	0.04878	0.32347	0.03422	0.04175	0.01411	0.10618	0.00219	0.03148	0.00089	0.03579	0.00354	0.05522	0.00973	0.08839	0.04306	0.41244	0.76528

ENERGIES FOR CHRYSENE , TBX APPROXIMATION 1.7

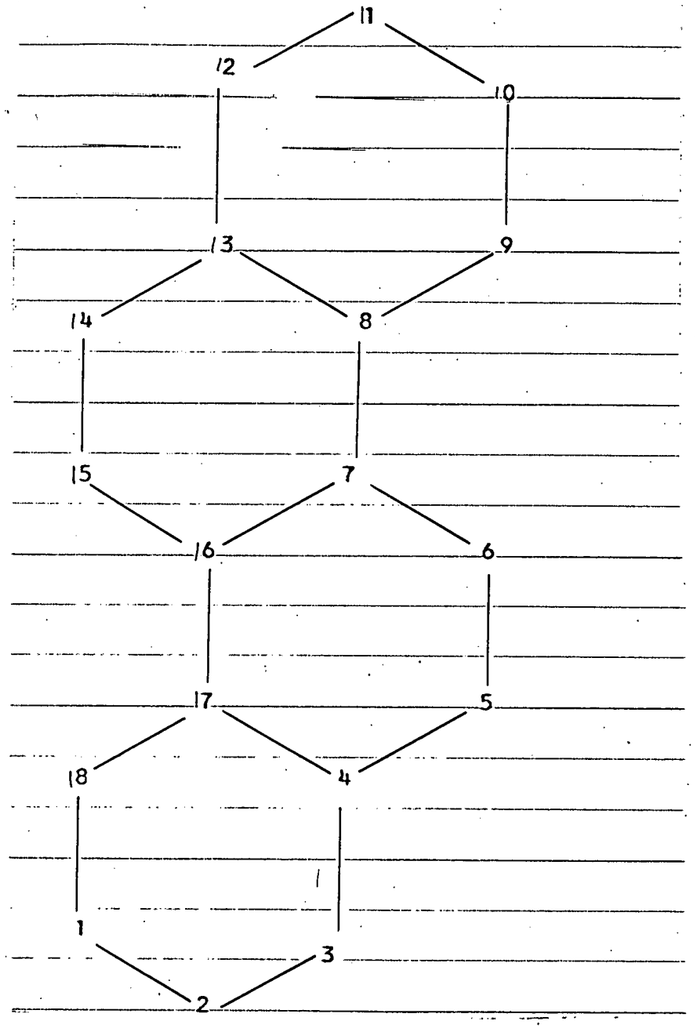
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	9,10	8,10	9,11	5,10	8,11	3,10	7,12	5,11	6,12	1,10
XMOMNT	-0.31514	-0.56190	-0.56295	0.19053	0.18764	-0.04161	0.05194	0.21557	0.47857	0.00102
YMOMNT	0.86314	-0.51358	-0.51455	0.07474	-0.73866	-0.00717	-0.43364	0.10023	-0.19611	-0.01289
JUMP E	20.6696	24.2658	27.7352	29.4591	31.3315	34.0201	34.4826	36.5247	38.0893	39.7611
DIAG E	32.3690	35.4784	38.4117	43.1740	42.7550	50.9204	51.3395	50.1727	54.3566	53.9247
DIAG E	32.4488	36.0769	37.7622	43.5220	42.6242	51.0974	51.5383	49.7914	55.0619	54.6124
CORRSP	30.7644	30.3878	42.4357	40.9693	43.4232	46.9071	53.0102	51.8122	58.0816	55.1103
CORRSP	30.9810	30.5914	41.0142	42.7716	43.3467	46.8720	53.1039	51.7935	58.4818	55.5793

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
30.76443	0.40508	-0.28816	0.47603	//	0.7539	0.4482	-0.3763	-0.1008	0.2192	-0.1059	-0.1091	-0.0175	-0.0732	0.0463
20.37060				//	0.9485	0.0006	-0.0165	-0.0749	0.1020	-0.0132	-0.2868	0.0342	-0.0036	0.0224
30.38777	0.41132	-0.04826	-0.56212	//	-0.5692	0.6401	-0.4463	-0.0232	-0.1328	-0.0315	0.0963	0.0632	-0.1723	-0.0707
26.93859				//	0.0018	0.9373	0.1785	-0.1007	-0.0249	-0.1090	0.0233	-0.0053	-0.2573	0.0103
42.43570	1.20521	-0.62054	-0.53178	//	0.0129	0.3951	0.6026	-0.6334	-0.0939	-0.1740	0.1475	-0.0906	0.1016	0.0041
32.16227				//	-0.0220	-0.1185	0.9004	0.3424	0.0855	0.0445	-0.1955	-0.0955	0.0168	0.0241
40.96929	0.89003	-0.41924	-0.57888	//	-0.0098	0.4199	0.5069	0.5962	0.2634	0.1795	-0.2252	-0.1265	-0.1504	-0.1423
33.38192				//	-0.1223	0.1397	-0.3535	0.6446	0.4642	0.1652	-0.3886	0.0794	-0.1437	-0.0663
43.42317	1.46236	0.25486	-0.85263	//	-0.2468	-0.1305	-0.0673	-0.2978	0.8945	0.0678	0.0676	-0.0543	-0.1204	-0.0458
35.68965				//	-0.0668	-0.0501	0.0980	-0.4282	0.8632	-0.0381	0.1810	-0.1369	0.0061	0.0431
46.90709	0.02479	-0.08665	0.07015	//	0.1154	-0.0658	-0.0732	-0.1602	-0.1940	0.5747	0.2295	-0.5895	-0.3685	-0.2178
41.90512				//	0.0196	-0.0751	0.0898	-0.2111	-0.0479	0.7665	0.0668	0.1967	-0.4590	-0.3125
53.01018	0.22383	-0.17818	-0.25989	//	0.1766	0.0209	0.0913	0.1926	0.0600	0.0285	0.8090	0.4453	-0.1085	-0.2325
50.09496				//	0.1927	-0.0751	0.0114	0.3533	0.0638	-0.0178	0.6393	0.2337	-0.3280	0.5069
51.81225	0.35217	-0.30184	0.26216	//	0.0402	0.0177	0.0371	-0.2767	-0.0707	0.5383	-0.3920	0.6105	-0.0369	-0.3126
46.03272				//	-0.1226	-0.0232	0.1097	-0.1762	0.0684	-0.1878	-0.2195	0.9163	0.0965	0.0652
58.08165	0.36753	0.37920	-0.07079	//	-0.0183	0.1819	-0.0940	0.0663	0.0976	0.4738	0.1905	-0.0989	0.7942	0.2063
56.77035				//	0.0501	0.2655	0.0046	0.0612	0.0358	0.5454	0.1558	0.0770	0.7341	0.2352
55.11025	0.29519	-0.31318	-0.16696	//	-0.0063	0.0413	0.1040	-0.0157	-0.0132	0.2745	-0.0685	0.2009	-0.3713	0.8537
51.58491				//	-0.1595	-0.0548	-0.0483	-0.2529	0.0930	0.1913	-0.4578	0.1606	-0.2151	0.7605

CHRYSENE IRX



ATOMIC COORDINATES

x	0.	0.8646	1.7184	1.7399	2.6286	2.6577	1.7956	1.8342	2.7024
y	0.5050	0.	0.4790	1.5050	2.0060	2.9880	3.5380	4.5910	5.1090

2.7024	1.8378	0.9840	0.9625	0.0738	0.0447	0.9068	0.8682	0.
6.1010	6.6060	6.1270	5.1010	4.6000	3.6180	3.0680	2.0150	1.4970

CHRYSENE — IRX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 A	8 S	9 S	10 A	11 A	12 S	13 S	14 A	15 S	16 A	17 S	18 A
1.729199	1.613248	1.448926	1.377182	1.262789	1.245473	1.155493	1.120425	1.064021	0.812305	0.763867	0.755133	0.691474	0.686301	0.633223	0.602461	0.538487	0.499974
-0.140316	-0.248521	-0.319559	-0.214339	-0.217099	0.228478	-0.292047	0.179654	0.239981	-0.243098	0.166553	0.280843	-0.251102	0.238847	0.216004	-0.307957	0.229371	-0.126810
0.136264	-0.256507	-0.345241	-0.115756	0.062605	0.387834	0.098992	0.330034	-0.108710	-0.112970	-0.339206	0.106198	0.395772	-0.008117	-0.116622	-0.343447	-0.236784	-0.121428
-0.170510	-0.277217	-0.259818	-0.042313	0.285054	0.212022	0.355522	0.065979	-0.272976	-0.279681	-0.109392	-0.349475	-0.221174	-0.245951	-0.044461	-0.273385	0.265083	-0.156816
0.277318	-0.326608	-0.070847	0.206275	0.292621	-0.175584	0.212285	-0.304570	-0.038272	-0.045315	0.272309	0.208392	-0.160477	-0.327418	-0.217789	-0.109274	-0.348722	-0.282020
-0.216249	-0.178156	-0.117987	-0.399823	-0.306372	-0.053486	-0.114333	-0.000701	-0.381134	-0.374512	-0.035786	-0.127745	-0.041605	-0.317804	-0.388149	-0.087423	-0.177423	-0.205640
0.236215	-0.061761	-0.242800	-0.391331	-0.074032	-0.116923	-0.294101	-0.271096	-0.233126	-0.247197	-0.267770	-0.300417	-0.115713	-0.081868	-0.380900	-0.227062	-0.056606	-0.227624
-0.346001	-0.059496	-0.310426	-0.170421	-0.219029	-0.206034	-0.135004	-0.218652	-0.295444	-0.276039	-0.208332	-0.135070	-0.209045	-0.218344	-0.184861	-0.327938	-0.068785	-0.363213
0.311693	-0.289608	-0.006942	-0.090822	-0.173676	-0.383414	-0.010022	-0.326197	-0.128604	-0.114268	-0.344576	-0.032465	-0.372978	-0.152487	-0.105808	-0.002433	-0.313576	-0.325151
-0.190615	-0.256814	-0.192046	-0.214544	-0.323392	-0.124946	-0.339934	-0.184332	-0.226216	-0.239260	-0.189642	-0.344125	-0.087794	-0.310748	-0.221853	-0.183784	-0.248396	-0.182484
0.140316	-0.248521	-0.319558	-0.214339	-0.217101	-0.228476	-0.292046	-0.179655	-0.239981	-0.243099	-0.166552	-0.280843	-0.251102	-0.238847	-0.216005	-0.307957	-0.229372	-0.126810
-0.136264	-0.256507	-0.345241	-0.115756	-0.062603	-0.387835	-0.098993	-0.330034	-0.108710	-0.112970	-0.339206	-0.106197	-0.395772	-0.008118	-0.116623	-0.343447	-0.236784	-0.121428
0.170510	-0.277216	-0.259818	-0.042313	0.285053	-0.212024	-0.355522	-0.065978	-0.272976	-0.279681	-0.109393	-0.349474	-0.221174	-0.245951	-0.044461	-0.273385	0.265083	-0.156816
-0.277318	-0.326607	-0.070847	-0.206275	-0.292622	-0.175582	-0.212284	-0.304571	-0.038272	-0.045315	-0.272309	-0.208392	-0.160478	-0.327417	-0.217789	-0.109274	-0.348723	-0.282020
0.216249	-0.178155	-0.117986	-0.399823	-0.306372	-0.053484	-0.114333	-0.000701	-0.381134	-0.374512	-0.035785	-0.127745	-0.041606	-0.317803	-0.388149	-0.087423	-0.177423	-0.205640
-0.236215	-0.061761	-0.242799	-0.391331	-0.074031	-0.116923	-0.294100	-0.271097	-0.233126	-0.247198	-0.267769	-0.300417	-0.115713	-0.081868	-0.380900	-0.227062	-0.056606	-0.227624
0.346001	-0.059496	-0.310425	-0.170422	-0.219030	-0.206033	-0.135004	-0.218652	-0.295444	-0.276039	-0.208332	-0.135070	-0.209046	-0.218344	-0.184861	-0.327937	-0.068784	-0.363213
-0.311692	-0.289608	-0.006942	-0.090823	-0.173678	-0.383414	-0.010021	-0.326197	-0.128604	-0.114268	-0.344576	-0.032466	-0.372978	-0.152486	-0.105808	-0.002433	-0.313576	-0.325151
-0.190614	-0.256814	-0.192047	-0.214544	-0.323393	-0.124945	-0.339934	-0.184333	-0.226215	-0.239260	-0.189642	-0.344126	-0.087794	-0.310748	-0.221853	-0.183784	-0.248396	-0.182484

CHRYSENE — IRX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 A	8 S	9 S	10 A	11 A	12 S	13 S	14 A	15 S	16 A	17 S	18 A
31.79086	28.65737	23.35769	20.64717	15.68835	14.85836	10.14480	8.10277	4.53599	-17.41944	-23.30451	-24.44597	-33.63695	-34.45878	-43.66622	-49.74520	-64.61150	-75.39566
-0.106705	-0.195664	-0.265477	-0.182644	-0.193194	0.204728	-0.271687	0.169725	0.232649	-0.269726	0.190565	0.323185	-0.301969	0.288312	0.271446	-0.396758	0.312573	-0.179341
0.103623	-0.201952	-0.286813	-0.098639	0.055712	0.347519	0.092091	0.311793	-0.105389	-0.125344	-0.388110	0.122209	0.475946	-0.009798	-0.146556	-0.442482	-0.322674	-0.171729
-0.129666	-0.218257	-0.215847	-0.036056	-0.253666	-0.189983	-0.330737	-0.062332	-0.264636	-0.310315	-0.125164	-0.402165	-0.265978	-0.296887	-0.055873	-0.352217	0.361239	-0.221777
0.210890	-0.257144	-0.058857	0.175772	0.260399	-0.157332	0.197485	-0.287737	-0.037103	-0.050278	0.311568	0.239811	-0.192986	-0.395225	-0.273689	-0.140784	-0.475217	-0.398847
-0.164449	-0.140265	-0.098019	-0.340700	-0.272636	-0.047926	-0.106362	-0.000662	-0.369490	-0.415533	-0.040945	-0.147005	-0.050033	-0.383620	-0.487775	-0.112632	-0.241781	-0.290827
0.179633	-0.048625	-0.201709	-0.333463	-0.065880	-0.104769	-0.273598	-0.256113	-0.226003	-0.274274	-0.306375	-0.345711	-0.139154	-0.098823	-0.478666	-0.292537	-0.077139	-0.321917
-0.263121	-0.046842	-0.257890	-0.145220	-0.194911	-0.184617	-0.125592	-0.206567	-0.286418	-0.306275	-0.238368	-0.155434	-0.251392	-0.263563	-0.232309	-0.422500	-0.093735	-0.513674
0.237031	-0.228013	-0.005767	-0.077392	-0.154552	-0.343559	-0.009323	-0.308169	-0.124675	-0.126784	-0.394254	-0.037360	-0.448533	-0.184067	-0.132966	-0.003134	-0.427323	-0.459845
-0.144955	-0.202194	-0.159545	-0.182819	-0.287782	-0.111958	-0.316236	-0.174145	-0.219304	-0.265467	-0.216983	-0.396008	-0.105579	-0.375103	-0.278796	-0.236779	-0.338499	-0.258078
0.106705	-0.195664	-0.265477	-0.182644	-0.193195	-0.204726	-0.271687	-0.169726	-0.232649	-0.269726	-0.190564	-0.323185	-0.301969	-0.288311	-0.271447	-0.396758	-0.312573	-0.179341
-0.103624	-0.201952	-0.286813	-0.098639	-0.055710	-0.347520	-0.092091	-0.311793	-0.105389	-0.125344	-0.388110	-0.122208	-0.475946	-0.009799	-0.146556	-0.442482	-0.322674	-0.171729
0.129666	-0.218257	-0.215847	-0.036056	-0.253665	-0.189985	-0.330737	-0.062332	-0.264636	-0.310315	-0.125164	-0.402164	-0.265978	-0.296888	-0.055873	-0.352217	-0.361239	-0.221777
-0.210890	-0.257143	-0.058857	-0.175772	-0.260400	-0.157330	-0.197485	-0.287738	-0.037103	-0.050279	-0.311568	-0.239811	-0.192987	-0.395225	-0.273689	-0.140784	-0.475218	-0.398846
0.164449	-0.140265	-0.098018	-0.340700	-0.272636	-0.047924	-0.106362	-0.000662	-0.369490	-0.415533	-0.040945	-0.147005	-0.050034	-0.383620	-0.487775	-0.112632	-0.241781	-0.290827
-0.179632	-0.048625	-0.201708	-0.333464	-0.065879	-0.104769	-0.273597	-0.256114	-0.226004	-0.274274	-0.306374	-0.345711	-0.139153	-0.098823	-0.478666	-0.292537	-0.077139	-0.321917
0.263121	-0.046842	-0.257890	-0.145221	-0.194912	-0.184616	-0.125592	-0.206568	-0.286418	-0.306274	-0.238368	-0.155435	-0.251393	-0.263562	-0.232310	-0.422500	-0.093735	-0.513674
-0.237030	-0.228013	-0.005767	-0.077392	-0.154554	-0.343558	-0.009322	-0.308169	-0.124675	-0.126784	-0.394254	-0.037361	-0.448534	-0.184066	-0.132966	-0.003135	-0.427322	-0.459845
0.144955	-0.202194	-0.159545	-0.182818	-0.287783	-0.111957	-0.316236	-0.174146	-0.219304	-0.265467	-0.216982	-0.396009	-0.105579	-0.375103	-0.278796	-0.236780	-0.338499	-0.258079

CHRYSENE— IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.00800	0.59463	0.00830	0.26207	0.00507	0.17642	0.00094	0.03402	0.00208	0.02722	0.00160	0.02605	0.00144	0.07594	0.00011	0.13981	0.00695	0.72007
2	0.59463	1.00366	0.73173	0.00595	0.13187	0.00780	0.12420	0.00084	0.04400	0.00160	0.04602	0.00281	0.05722	0.00129	0.06070	0.00202	0.25873	0.00959
3	0.00830	0.73173	1.01338	0.55394	0.00775	0.18709	0.00522	0.04767	0.00306	0.02605	0.00281	0.01343	0.00389	0.04952	0.00273	0.04916	0.01401	0.33786
4	0.26207	0.00595	0.55394	0.97379	0.50448	0.00718	0.18907	0.00330	0.05984	0.00144	0.05722	0.00389	0.07333	0.00136	0.07890	0.00739	0.56089	0.01744
5	0.00507	0.13187	0.00775	0.50448	1.01468	0.77258	0.01230	0.14233	0.00010	0.07594	0.00129	0.04952	0.00136	0.18456	0.00677	0.26012	0.00541	0.02219
6	0.17642	0.00780	0.18709	0.00718	0.77258	1.01038	0.51620	0.00716	0.08010	0.00011	0.06070	0.00273	0.07890	0.00677	0.18110	0.00895	0.23099	0.01102
7	0.00094	0.12420	0.00522	0.18907	0.01230	0.51620	0.98482	0.45013	0.00345	0.13981	0.00202	0.04916	0.00739	0.26012	0.00895	0.61178	0.00872	0.12332
8	0.03402	0.00084	0.04767	0.00330	0.14233	0.00716	0.45013	0.97907	0.58091	0.00695	0.25873	0.01401	0.56089	0.00541	0.23099	0.00872	0.02216	0.00022
9	0.00208	0.04400	0.00306	0.05984	0.00010	0.08010	0.00345	0.58091	1.01220	0.72007	0.00959	0.33786	0.01744	0.02219	0.01102	0.12332	0.00022	0.03960
10	0.02722	0.00160	0.02605	0.00144	0.07594	0.00011	0.13981	0.00695	0.72007	1.00800	0.59463	0.00830	0.26207	0.00507	0.17642	0.00094	0.03402	0.00208
11	0.00160	0.04602	0.00281	0.05722	0.00129	0.06070	0.00202	0.25873	0.00959	0.59463	1.00366	0.73173	0.00595	0.13187	0.00780	0.12420	0.00084	0.04400
12	0.02605	0.00281	0.01343	0.00389	0.04952	0.00273	0.04916	0.01401	0.33786	0.00830	0.73173	1.01338	0.55394	0.00775	0.18709	0.00522	0.04767	0.00306
13	0.00144	0.05722	0.00389	0.07333	0.00136	0.07890	0.00739	0.56089	0.01744	0.26207	0.00595	0.55394	0.97379	0.50448	0.00718	0.18907	0.00330	0.05984
14	0.07594	0.00129	0.04952	0.00136	0.18456	0.00677	0.26012	0.00541	0.02219	0.00507	0.13187	0.00775	0.50448	1.01468	0.77258	0.01230	0.14233	0.00010
15	0.00011	0.06070	0.00273	0.07890	0.00677	0.18110	0.00895	0.23099	0.01102	0.17642	0.00780	0.18709	0.00718	0.77258	1.01038	0.51620	0.00716	0.08010
16	0.13981	0.00202	0.04916	0.00739	0.26012	0.00895	0.61178	0.00872	0.12332	0.00094	0.12420	0.00522	0.18907	0.01230	0.51620	0.98482	0.45013	0.00345
17	0.00695	0.25873	0.01401	0.56089	0.00541	0.23099	0.00872	0.02216	0.00022	0.03402	0.00084	0.04767	0.00330	0.14233	0.00716	0.45013	0.97907	0.58091
18	0.72007	0.00959	0.33786	0.01744	0.02219	0.01102	0.12332	0.00022	0.03960	0.00208	0.04400	0.00306	0.05984	0.00010	0.08010	0.00345	0.58091	1.01220

CHRYSENE IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.77898	0.41699	-0.08740	-0.27460	-0.01846	-0.18666	-0.00384	-0.03727	-0.00213	-0.02950	-0.00236	-0.02803	-0.00399	-0.08125	-0.00910	-0.14107	-0.07349	0.54167
2	0.41699	0.76838	-0.54760	-0.06892	-0.13269	-0.01722	-0.13168	-0.00416	-0.04700	-0.00236	-0.04932	-0.00040	-0.06133	-0.00578	-0.06465	-0.01645	-0.27044	-0.08365
3	-0.08740	-0.54760	0.79217	-0.39175	-0.05960	-0.19065	-0.01246	-0.05090	-0.00067	-0.02803	-0.00040	-0.01450	-0.00020	-0.05406	-0.00114	-0.05827	-0.03462	0.35396
4	-0.27460	-0.06892	-0.39175	0.72138	-0.33699	-0.07662	-0.19924	-0.01092	-0.06394	-0.00399	-0.06133	-0.00020	-0.07829	-0.00704	-0.07903	-0.03777	-0.39988	0.03597
5	-0.01846	-0.13269	-0.05960	-0.33699	0.79373	-0.59092	-0.08573	-0.14387	-0.01116	-0.08125	-0.00578	-0.05406	-0.00704	-0.19629	-0.01288	-0.27540	-0.05158	0.03146
6	-0.18666	-0.01722	-0.19065	-0.07662	-0.59092	0.78672	-0.34894	-0.05076	-0.08760	-0.00910	-0.06465	-0.00114	-0.07903	-0.01288	-0.01086	-0.05047	-0.24341	0.00704
7	-0.00384	-0.13168	-0.01246	-0.19924	-0.08573	-0.34894	0.74315	-0.30041	-0.05745	-0.14107	-0.01645	-0.05827	-0.03777	-0.27540	-0.05047	-0.45059	-0.03629	0.12534
8	-0.03727	-0.00416	-0.05090	-0.01092	-0.14387	-0.05076	-0.30041	0.73343	-0.41181	-0.07349	-0.27044	-0.03462	0.39988	-0.05158	-0.24341	-0.03629	0.02903	-0.00515
9	-0.00213	-0.04700	-0.00067	-0.06394	-0.01116	-0.08760	-0.05745	-0.41181	0.78910	-0.54167	-0.08365	-0.35396	-0.03597	-0.03146	-0.00704	-0.12534	-0.00515	0.04172
10	-0.02950	-0.00236	-0.02803	-0.00399	-0.08125	-0.00910	-0.14107	-0.07349	-0.54167	0.77898	-0.41699	-0.08740	-0.27460	-0.01846	0.18666	-0.00384	-0.03727	-0.00213
11	-0.00236	-0.04932	-0.00040	-0.06133	-0.00578	-0.06465	-0.01645	-0.27044	-0.08365	-0.41699	0.76838	-0.54760	-0.06892	-0.13269	-0.01722	-0.13168	-0.00416	-0.04700
12	-0.02803	-0.00040	-0.01450	-0.00020	-0.05406	-0.00114	-0.05827	-0.03462	-0.35396	-0.08740	-0.54760	0.79217	-0.39175	-0.05960	-0.19065	-0.01246	-0.05090	-0.00067
13	-0.00399	-0.06133	-0.00020	-0.07829	-0.00704	-0.07903	-0.03777	-0.39988	-0.03597	-0.27460	-0.06892	-0.39175	0.72138	-0.33699	-0.07662	-0.19924	-0.01092	-0.06394
14	-0.08125	-0.00578	-0.05406	-0.00704	-0.19629	-0.01288	-0.27540	-0.05158	-0.03146	-0.01846	-0.13269	-0.05960	-0.33699	-0.79373	-0.59092	-0.08573	-0.14387	-0.01116
15	-0.00910	-0.06465	-0.00114	-0.07903	-0.01288	-0.01086	-0.05047	-0.24341	-0.00704	-0.18666	-0.01722	-0.19065	-0.07662	-0.59092	0.78672	-0.34894	-0.05076	-0.08760
16	-0.14107	-0.01645	-0.05827	-0.03777	-0.27540	-0.05047	-0.45059	-0.03629	-0.12534	-0.00384	-0.13168	-0.01246	-0.19924	-0.08573	-0.34894	0.74315	0.30041	-0.05745
17	-0.07349	-0.27044	-0.03462	-0.39988	-0.05158	-0.24341	-0.03629	-0.02903	-0.00515	-0.03727	-0.00416	-0.05090	-0.01092	-0.14387	-0.05076	-0.30041	0.73343	-0.41181
18	-0.54167	-0.08365	-0.35396	-0.03597	-0.03146	-0.00704	-0.12534	-0.00515	-0.04172	-0.00213	-0.04700	-0.00067	-0.06394	-0.01116	-0.08760	-0.05745	-0.41181	0.78910

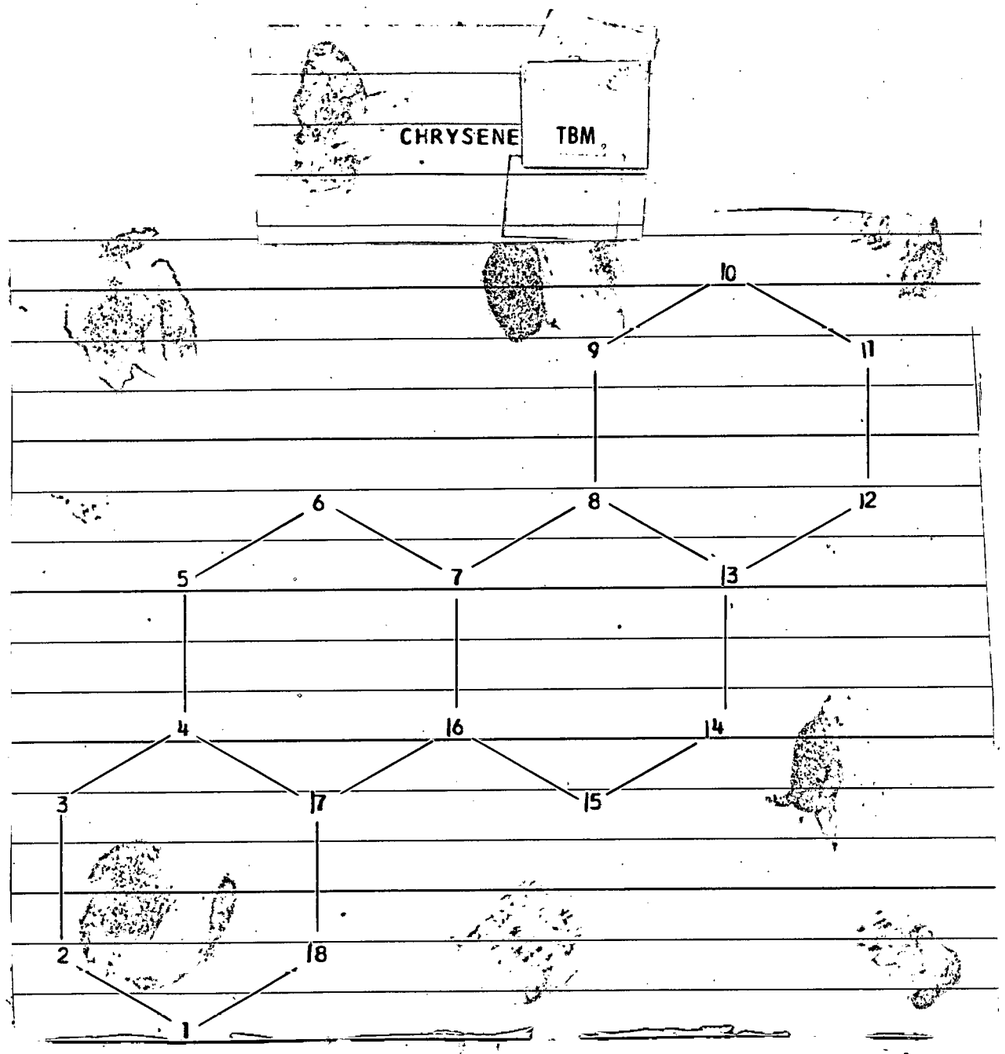
ENERGIES FOR CHRYSENE X , TDX-APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	9,10	8,10	9,11	8,11	5,10	7,12	5,11	6,12	3,10	4,12
XMOMNT	-0.33065	0.56914	-0.52274	-0.19790	-0.16215	0.01646	0.25464	-0.50028	-0.05758	-0.16280
YMOMNT	-0.81566	-0.58649	-0.56286	-0.74687	-0.06446	-0.49514	-0.09293	-0.15615	-0.01301	-0.04215
JUMP E	21.9554	25.5222	27.8405	31.4073	33.1078	34.5908	38.9929	39.3043	40.7771	45.0931
DIAG E	33.0006	36.5786	38.0777	42.5835	46.6800	51.0636	52.5925	55.3897	57.6487	63.8225
DIAG E	33.1414	37.2386	37.4804	42.5053	47.0431	51.2574	52.2175	56.1149	57.8403	64.1219
CORRSP	31.4097	31.1562	41.9338	43.0389	44.7990	53.2977	49.9593	56.2467	60.4098	65.1863
CORRSP	31.5923	31.3034	41.8843	43.0753	45.1343	53.3150	50.0127	56.3705	60.8117	65.4613

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	E	XMOMNT	YMOMNT	//	STATE COMPOSITION								
31.40965	0.55109	-0.25255	0.59060	//	0.9050	-0.2001	-0.1964	-0.2688	0.0494	0.1455	0.0447	0.0218	-0.0464	-0.0440
21.22300				//	0.9428	0.0173	-0.0480	-0.1132	0.0498	0.2985	-0.0457	0.0150	0.0052	-0.0431
31.15621	0.15267	0.11784	0.31834	//	0.2689	0.7239	0.5973	-0.0671	-0.0451	0.0650	0.0349	-0.1746	0.0400	0.0531
27.89356				//	-0.0382	0.9330	-0.2175	-0.0409	-0.0552	0.0384	0.0057	-0.2657	0.0631	0.0017
41.93377	1.99643	-0.70513	-0.78889	//	-0.0161	-0.6233	0.7506	-0.0523	-0.0884	0.1347	0.0984	0.0533	0.0240	-0.0781
31.64475				//	-0.0056	0.1704	0.8900	-0.0704	-0.3239	0.2097	0.0612	-0.0198	-0.0045	0.1442
43.03891	1.20465	-0.28229	0.76059	//	0.2653	-0.0748	0.0640	0.8971	0.2484	-0.1121	-0.0035	-0.1730	-0.0811	-0.0661
34.33809				//	0.1773	0.1056	0.2533	0.8039	0.3825	-0.2810	0.0186	-0.1215	-0.0659	-0.0471
44.79900	0.62285	-0.03962	-0.57041	//	-0.0765	-0.0180	0.1101	-0.3028	0.8643	-0.3220	0.0444	-0.0969	-0.0789	-0.1477
36.07972				//	0.0264	0.0735	0.2820	-0.5624	0.6431	-0.3682	0.1094	-0.0739	0.0074	-0.1773
53.29769	0.40655	0.16512	0.39001	//	-0.1366	0.0907	-0.1037	0.0917	0.3164	0.7998	0.3648	0.0694	0.2280	-0.1556
50.67087				//	-0.2018	-0.0530	-0.0058	0.1158	0.3229	0.6597	0.4818	-0.0652	0.2873	-0.2910
49.95925	0.07781	-0.05213	-0.18414	//	0.0798	0.0684	-0.0049	0.0696	-0.0831	-0.4264	0.6955	0.4393	0.3441	-0.0156
48.53382				//	0.1704	0.0731	-0.0578	0.0250	-0.2726	-0.4089	0.6961	0.3642	0.3190	0.0360
56.24668	0.71924	-0.54419	0.06750	//	0.0827	0.0579	0.0879	0.0806	0.1634	0.0175	-0.6041	0.5769	0.4975	-0.0579
57.55993				//	-0.0744	0.2111	-0.0396	0.0124	0.3115	0.2184	0.0892	0.6467	-0.4508	0.4172
60.40980	0.22720	0.29550	-0.03345	//	0.0082	-0.1109	-0.0804	-0.0646	-0.0967	-0.1238	0.0401	-0.6228	0.7222	-0.2034
46.37634				//	-0.0451	0.1386	0.0885	0.0563	0.0915	0.0124	-0.5071	0.5303	0.6205	-0.1894
65.18631	0.13234	-0.21821	0.01113	//	0.0179	-0.1138	0.0120	0.0096	0.1898	0.0551	0.0408	-0.0920	0.2086	0.9454
63.45929				//	0.0151	-0.1084	-0.0428	-0.0227	0.2138	0.0274	-0.0107	-0.2688	0.4680	0.8048



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	2.5980	3.4640	3.4640
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	3.5000	4.5000

4.3300	5.1960	5.1960	4.3300	4.3000	3.4640	2.5980	1.7320	1.7320
5.0000	4.5000	3.5000	3.0000	2.0000	1.5000	2.0000	1.5000	0.5000

CHRYSENE TBM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1.618252	1.534958	1.420200	1.384538	1.318198	1.299987	1.217357	1.195843	1.130967	0.869031	0.804155	0.782641	0.700011	0.681800	0.615459	0.579798	0.465040	0.381746
0.111689	-0.218867	0.301957	-0.198432	-0.264185	0.311339	0.223098	0.192829	0.235345	0.235345	-0.192830	-0.223098	0.311340	-0.264185	-0.198432	0.301957	-0.218867	-0.111689
0.104239	-0.225507	0.342746	-0.089925	-0.013699	0.403615	-0.158129	0.327217	-0.132478	0.132478	0.327217	-0.158129	-0.403615	0.013699	0.089926	-0.342746	0.225507	0.104239
0.149433	-0.269927	0.281587	0.058329	0.246536	0.179244	-0.362374	0.066819	-0.305658	-0.305658	-0.066819	0.362374	0.179244	0.246537	0.058329	0.281587	-0.269927	-0.149432
0.270087	-0.359564	0.136676	0.180799	0.331542	-0.185732	-0.161009	-0.274180	-0.029723	0.029723	-0.274180	-0.161008	0.185732	-0.331541	-0.180799	-0.136677	0.359564	0.270087
0.199093	-0.188835	-0.038646	0.366529	0.338186	-0.063012	0.131396	0.046703	0.388690	0.388690	-0.046703	-0.131396	-0.063013	0.338186	0.366529	-0.038646	-0.188835	-0.199093
0.228645	-0.049749	-0.202464	0.390272	0.104476	0.109134	0.276716	0.311224	0.235976	-0.235976	0.311224	0.276715	-0.109134	-0.104476	-0.390272	0.202464	0.049749	0.228645
0.373652	0.081005	-0.306052	0.241523	-0.203492	0.195659	0.112297	0.200252	-0.263472	-0.263472	-0.200252	-0.112297	0.195660	-0.203492	0.241524	-0.306052	0.081005	-0.373652
0.331247	0.311763	0.006847	0.170624	-0.159416	0.333405	-0.062798	-0.337985	-0.095755	0.095755	-0.337985	-0.062798	-0.333406	0.159416	-0.170624	-0.006847	-0.311763	0.331247
0.177525	0.242334	0.192358	0.226097	-0.301159	0.008773	-0.363640	-0.198947	0.243002	0.243002	0.198948	0.363640	0.008774	-0.301159	0.226097	0.192358	0.242333	-0.177525
0.113463	0.213504	0.320645	0.181650	-0.228856	-0.322725	-0.257449	0.180105	0.224696	-0.224696	0.180104	-0.257449	0.322724	0.228857	-0.181650	-0.320645	-0.213504	0.113463
0.106693	0.220430	0.353544	0.056917	0.006110	-0.401029	0.136915	0.341859	-0.123769	-0.123769	-0.341859	-0.136914	-0.401029	0.006109	0.056917	0.353544	0.220430	-0.106693
0.153806	0.264285	0.281283	-0.092976	0.236745	-0.164715	0.378044	0.091163	-0.290388	0.290388	0.091164	0.378044	0.164716	-0.236745	0.092976	-0.281283	0.264285	0.153806
0.278588	0.352412	0.125362	-0.201773	0.299110	0.200806	0.196020	-0.269504	-0.030329	-0.030329	0.269504	-0.196021	0.200805	0.299111	-0.201773	0.125362	0.352412	-0.278589
0.213033	0.188002	-0.074783	-0.392448	0.308635	0.075462	-0.142776	0.033009	0.370458	-0.370458	0.033008	-0.142775	-0.075462	-0.308635	0.392448	-0.074783	-0.188002	0.213033
0.240459	0.052230	-0.237809	-0.385981	0.093340	-0.102512	-0.302783	0.278166	0.213639	0.213640	-0.278165	0.302783	-0.102513	-0.093339	-0.385981	-0.237810	0.052230	-0.240459
0.376108	0.086442	-0.325457	-0.184606	-0.207419	-0.204736	-0.115028	0.185669	-0.280044	0.280043	-0.185669	-0.115028	0.204736	-0.207419	0.184606	-0.325457	0.086442	0.376108
0.328040	-0.320592	-0.010250	-0.143151	-0.157270	-0.341984	0.089191	-0.331079	-0.098783	-0.098784	0.331079	-0.089191	-0.341983	-0.157271	-0.143150	-0.010249	-0.320592	-0.328040
0.175537	-0.248881	0.171340	-0.219236	-0.326897	-0.025198	0.354602	-0.174208	0.257361	-0.257361	-0.174208	0.354602	0.025197	0.326897	0.219236	-0.171340	0.248881	0.175537

CHRYSENE TBM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
28.80186	26.27388	22.30529	20.93803	18.19776	17.39662	13.46037	12.34626	8.72999	-11.36149	-18.36007	-20.93708	-32.30740	-35.1839	-47.1025	-54.6365	-86.7225	-122.0938
0.087799	-0.176657	0.253379	-0.168639	-0.230101	0.273064	0.202203	0.176334	0.221299	0.252457	-0.215032	-0.252182	0.372119	-0.319948	-0.252937	0.396558	-0.320948	-0.180769
0.081942	-0.182017	0.287606	-0.076424	-0.011932	0.353996	-0.143318	0.299225	-0.124572	0.142111	0.364893	-0.178743	-0.482409	0.016590	-0.114626	-0.450126	0.330685	-0.168711
0.117469	-0.217870	0.236286	0.049571	0.214729	0.157208	-0.328434	0.061103	-0.287416	-0.327883	-0.074512	0.409615	0.214236	0.298575	-0.074350	0.369806	-0.395823	-0.241856
0.212315	-0.290220	0.114688	0.153654	0.288767	-0.162898	-0.145929	-0.250725	-0.027949	0.031884	-0.305749	-0.181998	0.221991	-0.401522	-0.230460	-0.179496	0.527267	0.437136
0.156507	-0.152417	-0.032429	0.311498	0.294554	-0.055265	0.119089	0.042708	0.365492	0.416951	-0.052081	-0.148525	-0.075314	0.409569	-0.467206	-0.050753	-0.276909	-0.322232
0.179738	-0.040155	-0.169892	0.331676	0.090997	0.095718	0.250798	0.284601	0.221892	-0.253134	0.347059	0.312789	-0.130439	-0.126529	-0.497471	0.265895	0.072952	0.370063
0.293727	0.065383	-0.256815	0.205261	-0.177238	0.171606	0.101779	0.183121	-0.247747	-0.282629	-0.223309	-0.126936	0.233856	-0.246444	0.307865	-0.401936	0.118787	-0.604756
0.260393	0.251638	0.005746	0.145006	-0.138849	0.292417	-0.056916	-0.309073	-0.090040	0.102717	-0.376902	-0.070984	-0.398493	0.193064	-0.217490	-0.008993	-0.457172	0.536123
0.139552	0.195598	0.161412	0.192151	-0.262304	0.007695	-0.329581	-0.181929	0.228499	0.260670	0.221855	0.411046	0.010487	-0.364726	0.288201	0.252623	0.355360	-0.287325
0.089193	0.172329	0.269060	0.154377	-0.199330	-0.283050	-0.233336	0.164698	0.211286	-0.241034	0.200842	-0.291011	0.385726	0.277163	-0.231545	-0.421101	0.313083	0.183639
0.083871	0.177919	0.296667	0.048372	0.005322	-0.351728	0.124091	0.312615	-0.116382	-0.132768	-0.381222	-0.154763	-0.479318	0.007398	0.072551	0.464307	0.323240	-0.172682
0.120906	0.213316	0.236031	-0.079017	0.206201	-0.144465	0.342636	0.003365	-0.273057	0.311502	0.101661	0.427327	0.196871	-0.286716	0.118514	-0.369407	-0.387549	0.248935
0.218998	0.284447	0.105194	-0.171479	0.260520	0.176119	0.177661	-0.246450	-0.028519	-0.032534	0.300535	-0.221575	0.240006	0.362246	-0.257195	0.164636	0.516779	-0.450896
0.167465	0.151745	-0.062752	-0.333526	0.268816	0.066185	-0.129403	0.030185	0.348349	-0.397394	0.036809	-0.161388	-0.090193	-0.373781	0.500245	0.098212	-0.275687	0.344794
0.189025	0.042157	-0.199551	-0.328030	0.081297	-0.089910	-0.274424	0.254370	-0.200889	0.229173	-0.310194	0.342255	-0.122525	0.113041	-0.492001	-0.312314	0.076590	-0.389184
0.295658	-0.069771	-0.273098	-0.156889	-0.180658	-0.179566	-0.104255	0.169786	-0.263330	0.300405	0.207047	-0.130024	0.244704	0.251201	0.235313	0.427421	0.126759	0.608731
0.257871	-0.258764	-0.008601	-0.121658	-0.136979	-0.299941	0.080837	-0.302758	-0.092888	-0.105966	0.369200	-0.100819	-0.408745	-0.190467	-0.182471	-0.013461	-0.470118	-0.530932
0.137990	-0.200883	0.143775	-0.186320	-0.284722	-0.022100	0.321390	-0.159306	0.242002	-0.276074	-0.194266	0.400830	0.030116	0.395898	0.279455	-0.225019	0.364961	0.284107

CHRYSENE | TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.00000	0.61652	-0.00000	-0.25389	0.00000	0.16302	-0.00000	-0.03766	-0.00000	0.03375	-0.00000	-0.03506	0.00000	0.08319	-0.00000	-0.13086	0.00000	0.70784
2	0.61652	1.00000	0.71268	-0.00000	-0.13985	0.00000	0.11699	-0.00000	-0.04534	-0.00000	0.04427	-0.00000	-0.05507	0.00000	0.06886	0.00000	-0.25875	-0.00000
3	-0.00000	0.71268	1.00000	0.56801	0.00000	-0.18588	0.00000	0.05425	-0.00000	-0.03482	-0.00000	0.02426	0.00000	-0.06507	0.00000	0.05795	0.00000	-0.35009
4	-0.25389	-0.00000	0.56801	1.00000	0.52194	0.00000	-0.19066	-0.00000	0.06476	-0.00000	-0.05483	-0.00000	0.06857	0.00000	-0.08001	0.00000	0.53463	0.00000
5	0.00000	-0.13985	0.00000	0.52194	1.00000	0.75372	-0.00000	-0.13365	0.00000	0.08264	-0.00000	-0.06546	0.00000	0.18471	-0.00000	-0.27284	0.00000	0.04899
6	0.16302	0.00000	-0.18588	0.00000	0.75372	1.00000	0.53789	0.00000	-0.11576	-0.00000	0.07202	0.00000	-0.08318	0.00000	0.00331	0.00000	-0.23652	-0.00000
7	-0.00000	0.11699	0.00000	-0.19066	-0.00000	0.53789	1.00000	0.47262	0.00000	-0.12638	0.00000	0.05430	-0.00000	-0.26427	-0.00000	0.57750	-0.00000	-0.12248
8	-0.03766	-0.00000	0.05425	-0.00000	-0.13365	0.00000	0.47262	1.00000	0.58399	-0.00000	-0.26155	0.00000	0.53906	-0.00000	-0.23214	-0.00000	0.02206	0.00000
9	-0.00000	-0.04534	-0.00000	0.06476	0.00000	-0.11576	0.00000	0.58399	1.00000	0.70622	-0.00000	-0.34896	-0.00000	0.04670	0.00000	-0.12203	-0.00000	0.04143
10	0.03375	-0.00000	-0.03482	-0.00000	0.08264	-0.00000	-0.12638	-0.00000	0.70622	1.00000	0.61881	-0.00000	-0.25736	0.00000	0.15969	-0.00000	-0.03789	-0.00000
11	-0.00000	0.04427	-0.00000	-0.05483	-0.00000	0.07202	0.00000	-0.26155	-0.00000	0.61881	1.00000	0.71038	0.00000	-0.13420	-0.00000	0.11745	-0.00000	-0.04557
12	-0.03506	-0.00000	0.02426	-0.00000	-0.06546	0.00000	0.05430	0.00000	-0.34896	-0.00000	0.71038	1.00000	0.57217	0.00000	-0.18476	-0.00000	0.05494	0.00000
13	0.00000	-0.05507	0.00000	0.06857	0.00000	-0.08318	-0.00000	0.53906	-0.00000	-0.25736	0.00000	0.57217	1.00000	0.50953	0.00000	-0.19296	-0.00000	0.06545
14	0.08319	-0.00000	-0.06507	0.00000	0.18471	0.00000	-0.26427	-0.00000	0.04670	0.00000	-0.13420	0.00000	0.50953	1.00000	0.76587	-0.00000	-0.13609	-0.00000
15	-0.00000	0.06886	0.00000	-0.08001	-0.00000	0.00331	-0.00000	-0.23214	0.00000	0.15969	-0.00000	-0.18476	0.00000	0.76587	1.00000	0.52570	0.00000	-0.11138
16	-0.13086	0.00000	0.05795	0.00000	-0.27284	0.00000	0.57750	-0.00000	-0.12203	0.00000	0.11745	-0.00000	-0.19296	0.00000	0.52570	1.00000	0.47885	0.00000
17	0.00000	-0.25875	0.00000	0.53463	0.00000	-0.23652	-0.00000	0.02206	-0.00000	-0.03789	0.00000	0.05494	-0.00000	-0.13609	0.00000	0.47885	1.00000	0.58182
18	0.70784	-0.00000	-0.35009	0.00000	0.04899	-0.00000	-0.12248	0.00000	0.04143	-0.00000	-0.04557	0.00000	0.06545	-0.00000	-0.11138	0.00000	0.58182	1.00000

CHRYSENE | TBM DENSITY | BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.76004	-0.44147	-0.05082	-0.23555	0.01909	0.15819	0.00048	-0.03745	0.00099	0.03344	-0.00027	-0.03456	-0.00230	0.08141	0.00894	-0.12267	-0.04258	-0.53077
2	0.44147	0.75890	0.53539	-0.04055	-0.13092	0.00440	0.11310	-0.00366	-0.04448	0.00022	0.04359	0.00251	-0.05377	-0.00410	0.06623	0.01502	-0.24019	-0.04968
3	-0.05082	0.53539	0.76918	0.39985	-0.05524	-0.17602	0.01528	0.05230	-0.00443	-0.03434	0.00246	0.02438	-0.00295	-0.06480	0.00173	0.06181	-0.03262	-0.32949
4	-0.23555	-0.04055	0.39985	0.72186	0.35473	-0.04436	-0.17501	0.01156	0.06245	-0.00220	-0.05355	-0.00301	0.06573	0.00299	-0.07323	-0.03064	0.37236	-0.03376
5	0.01909	-0.13092	-0.05524	0.35473	0.77043	0.57542	-0.04805	-0.12513	0.01091	0.08091	-0.00389	-0.06514	0.00261	0.17989	0.01594	-0.25561	-0.03769	0.05358
6	0.15819	0.00440	-0.17602	-0.04436	0.57542	0.76673	0.36969	-0.04609	-0.10666	0.00922	0.06932	0.00173	-0.07631	0.01655	0.00864	-0.03916	-0.21965	0.01517
7	0.00048	0.11310	0.01528	-0.17501	-0.04805	0.36969	0.72954	0.31186	-0.04778	-0.11825	0.01483	0.05815	-0.03045	-0.24693	-0.03753	0.41428	-0.03066	-0.11503
8	-0.03745	-0.00366	0.05230	0.01156	-0.12513	-0.04609	0.31186	0.72769	0.41487	-0.04244	-0.24293	-0.03299	0.37659	-0.03647	-0.21510	-0.03029	0.02598	0.00283
9	0.00099	-0.04448	-0.00443	0.06245	0.01091	-0.10666	-0.04778	0.41487	0.76701	0.52915	-0.04956	-0.32835	-0.03397	0.05117	0.01488	-0.11462	0.00289	0.04048
10	0.03344	-0.00022	-0.03434	-0.00220	0.08091	0.00922	-0.11825	-0.04244	0.52915	0.75988	0.44374	-0.05054	-0.23893	0.01833	0.15482	-0.00027	-0.03767	0.00104
11	0.00027	-0.04359	-0.00246	-0.05355	-0.00389	0.06932	0.01483	-0.24293	-0.04956	0.44374	0.75891	0.53312	-0.04070	-0.12544	0.00486	-0.11352	-0.00377	-0.04471
12	-0.03456	0.00251	0.02438	-0.00301	-0.06514	0.00173	0.05815	-0.03299	-0.32835	-0.05054	0.53312	0.76875	0.40385	-0.05382	-0.17451	0.01565	0.05294	-0.00454
13	-0.00230	-0.05377	-0.00295	0.06573	0.00261	-0.07631	-0.03045	0.37659	-0.03397	-0.23893	-0.04070	0.40385	0.72269	0.34351	-0.04636	-0.17694	-0.01188	0.06309
14	0.08141	-0.00410	-0.06480	0.00299	0.17989	0.01655	-0.24693	-0.03647	0.05117	0.01833	-0.12544	-0.05382	0.34351	0.76379	0.57811	-0.05035	-0.12719	0.01130
15	0.00894	0.06623	0.00173	-0.07323	0.01594	0.00864	-0.03753	-0.21510	0.01488	0.15482	0.00486	-0.17451	-0.04636	0.57811	0.75999	0.35853	-0.04513	-0.10244
16	-0.12267	0.01502	0.06181	-0.03064	-0.25561	-0.03916	0.41428	-0.03029	-0.11462	0.00027	0.11352	0.01565	-0.17694	-0.05035	0.35853	0.73080	0.31793	-0.04819
17	-0.04258	-0.24019	-0.03262	0.37236	-0.03769	-0.21965	-0.03066	0.02598	0.00289	-0.03767	-0.00377	0.05294	0.01188	-0.12719	-0.04513	0.31793	0.72777	0.41272
18	0.53077	-0.04968	-0.32949	-0.03376	0.05358	0.01517	-0.11503	0.00283	0.04048	0.00104	-0.04471	-0.00454	0.06309	0.01130	-0.10244	-0.04819	0.41272	0.76714

ENERGIES FOR CHRYSENE TBMAPPROXIMATION

ONE ELECTRON EXCITATIONS OF A SYMMETRY

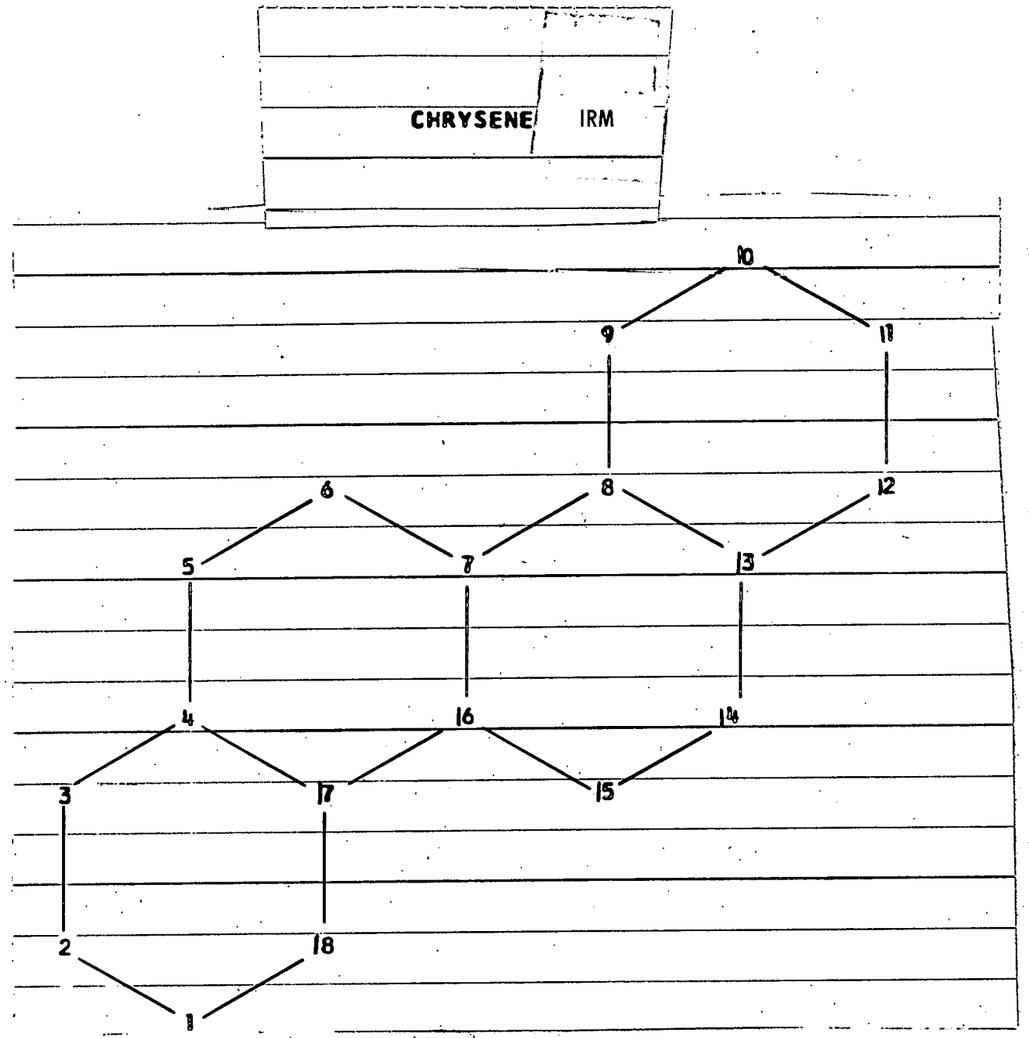
JUMP	9,10	8,10	7,10	9,11	6,10	5,10	9,12	8,11	7,11	4,10	8,12	3,10	7,12	6,11	5,11
XMOMNT	-0.87963	-0.29913	0.02243	-0.29967	-0.00142	-0.00557	-0.02249	-0.70973	0.03403	0.01024	0.03407	0.00910	0.40379	0.00679	0.23410
YMOMNT	-0.02764	-0.76198	0.02858	0.76334	-0.01294	0.21404	-0.02866	-0.11793	-0.01300	-0.00224	-0.01302	-0.02870	0.07903	0.01413	-0.14889
JUMP E	20.0915	23.7078	24.8219	27.0901	28.7581	29.5592	29.6671	30.7063	31.8204	32.2995	33.2833	33.6668	34.3975	35.7567	36.5578
DIAG E	31.6466	34.5294	38.4758	37.3637	42.5453	42.9410	42.8659	41.8659	44.7532	45.7871	46.3047	50.0791	51.1136	50.6277	50.0099
DIAG E	31.7347	35.0993	38.4751	36.7896	43.0026	43.3224	43.1665	41.7736	44.0903	45.9967	47.0871	50.3194	51.3253	50.4229	49.7291
CORRSP	30.0819	30.3100	37.2496	40.5377	38.4251	42.1547	42.4096	42.7524	47.4843	44.8275	48.9988	51.5848	53.3235	52.0502	48.7185
CORRSP	30.2077	30.5272	37.3203	40.4662	38.6632	42.7229	42.5845	42.4701	47.4235	44.9532	49.4815	51.6197	53.3808	51.8373	48.6762

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
30.08189	0.55206	-0.65691	0.00430	//	0.9238	-0.1495	0.0087	-0.1435	-0.0032	0.0644	0.0012	-0.2717	0.0078	-0.0075
					0.0059	0.0762	-0.1293	-0.0039	0.0536					
19.16129				//	0.9452	0.0073	0.0330	-0.0199	0.0047	0.0560	-0.0270	-0.1117	-0.0106	0.0122
					-0.0102	0.0103	-0.2923	-0.0020	-0.0519					
30.30995	0.08396	-0.19257	-0.16751	//	0.2038	0.7679	-0.0170	0.5818	0.0161	-0.0791	-0.0152	-0.0571	-0.0042	0.0060
					0.0054	-0.1160	-0.0365	-0.0062	0.0722					
27.49725				//	-0.0092	0.9340	-0.1004	-0.2613	0.0460	-0.0573	0.0649	-0.0710	-0.0154	0.0157
					-0.0242	-0.1810	0.0107	-0.0069	-0.0242					
37.24956	0.00005	0.00163	0.00535	//	0.0036	0.0163	0.8190	-0.0058	-0.3172	-0.0256	-0.2774	0.0293	-0.1638	-0.0478
					0.2905	-0.0114	0.0077	-0.1900	0.0064					
25.92801				//	-0.0275	0.1057	0.7840	-0.0569	0.0192	-0.0004	-0.5893	0.0072	0.0409	0.1175
					0.0466	-0.0099	0.0589	-0.0352	0.0037					
40.53769	1.45852	0.38875	0.83363	//	-0.0184	-0.5700	0.0173	0.6583	-0.0052	-0.4209	0.0069	-0.0989	-0.0022	-0.0001
					-0.0174	-0.0613	-0.2096	0.0181	0.0759					
30.90636				//	-0.0389	0.1979	0.0228	0.8600	-0.0258	-0.3713	-0.0376	-0.1193	-0.0055	-0.0091
					0.0161	-0.1114	-0.2168	-0.0011	0.0723					
38.42507	0.00042	-0.00903	-0.01326	//	0.0055	0.0056	0.4507	-0.0079	0.6732	-0.0127	-0.0436	0.0252	0.4207	0.1654
					-0.3623	0.0162	0.0081	-0.0702	0.0039					
31.75480				//	-0.0140	-0.0434	0.0343	0.0460	0.7225	0.0030	0.0311	-0.0607	-0.2564	0.2060
					-0.5947	0.0271	0.0260	0.0679	0.0013					
42.15474	0.74217	0.10912	0.63412	//	0.0523	-0.2166	-0.0029	0.4297	0.0147	0.7885	-0.0624	0.2163	-0.0032	0.0068
					0.0223	0.1727	0.2289	-0.0117	0.1007					
33.07462				//	0.1584	0.1985	-0.0257	0.3617	0.0284	0.4967	-0.0028	0.6581	-0.0035	-0.0078
					-0.0043	0.1124	0.3286	-0.0059	0.0519					
42.40963	0.04842	0.15875	0.04060	//	-0.0528	0.0074	0.2425	0.0268	0.1277	0.0913	0.8240	-0.1763	-0.3636	0.2411
					0.1104	0.0201	0.0021	0.0088	0.0010					
41.98012				//	0.0138	0.0163	0.5505	0.0096	0.1791	-0.0167	0.7453	-0.0023	0.1615	-0.1454
					0.1496	0.0339	0.0099	-0.1783	0.0772					

CHRYSENE TBM APPROXIMATION (cont.)

42.75245 1.47430-0.88068-0.18793 //	0.2778	-0.0152	0.0062	-0.0321	0.0193	-0.2403	0.1747	0.9033	-0.0984	0.0544
	0.0072	-0.0416	0.0091	0.0033	0.0493					
35.09965 //	0.0300	-0.0543	0.0167	-0.2037	0.0251	-0.5934	0.0087	0.7158	-0.0354	-0.0035
	-0.0585	-0.0675	-0.2535	-0.0131	-0.1243					
47.48435 0.00306 0.03321-0.02030 //	-0.0029	-0.0009	0.0094	-0.0094	-0.3571	0.0239	0.0922	0.0121	0.5832	0.6269
	0.2523	-0.0789	-0.0248	0.2319	0.0750					
39.65077 //	0.0176	0.0052	-0.1018	-0.0096	0.2904	-0.0397	-0.1733	0.0024	0.7976	-0.4066
	-0.1209	0.0181	0.0076	0.2340	0.0454					
44.82755 0.00011-0.00776-0.00000 //	-0.0014	-0.0135	-0.1909	-0.0155	0.2524	-0.0318	-0.3904	-0.0219	-0.4416	0.6749
	0.1265	0.0253	-0.0276	-0.2740	-0.0500					
41.00751 //	-0.0190	-0.0147	-0.0908	0.0185	0.0721	0.0200	0.0882	0.0292	0.4513	0.8555
	0.1851	-0.0059	-0.0667	-0.0025	-0.0472					
48.99881 0.09633 0.19319-0.09439 //	-0.0199	-0.0460	-0.0905	-0.0801	0.3861	0.0073	-0.0111	-0.0276	0.0980	-0.2027
	0.6279	-0.3645	0.0841	-0.0570	0.4948					
47.80698 //	0.0058	-0.0468	-0.1004	-0.0121	0.5418	0.0124	-0.1096	0.0229	-0.2286	-0.0845
	0.7328	-0.1823	-0.0148	0.2247	0.0312					
51.58476 0.35526 0.38397-0.12046 //	0.0064	0.0331	-0.0333	0.0026	-0.0770	-0.3141	0.0383	-0.0889	0.0471	0.0362
	-0.0399	0.5892	0.5659	-0.1478	0.4352					
46.70957 //	-0.0432	0.1497	-0.0049	0.0464	0.0671	-0.1113	-0.0041	-0.0703	-0.0465	-0.0279
	0.1397	0.8299	-0.0236	0.1068	-0.4780					
53.32354 0.21139 0.16874 0.25446 //	0.1456	-0.1021	-0.0025	0.0760	0.0049	-0.1161	0.0113	-0.0794	0.0124	0.0171
	0.0148	-0.4371	0.7354	0.0080	-0.4583					
50.90423 //	0.2392	-0.0757	-0.0196	0.0526	-0.0161	-0.3755	0.0333	-0.1097	0.0293	0.0333
	0.0154	-0.2071	0.7857	-0.0176	-0.3417					
52.05018 0.00672 0.05345-0.01331 //	0.0066	0.0186	0.1313	-0.0095	0.1768	-0.0580	-0.2078	-0.0136	-0.2606	0.0311
	0.0652	0.1318	0.0947	0.8958	0.0477					
43.73647 //	-0.0062	0.0039	0.1916	0.0067	-0.2296	0.0410	0.1963	0.0199	-0.0831	0.0806
	-0.0966	-0.1059	-0.0118	0.9128	-0.0502					
48.71845 0.06774 0.16851-0.06558 //	-0.0144	-0.0383	0.0598	-0.0924	-0.2268	0.0815	-0.0411	-0.0453	-0.1978	0.1305
	-0.5397	-0.4993	0.0832	0.0428	0.5647					
45.14428 //	0.1341	0.0465	-0.0515	-0.0919	-0.0275	-0.3152	-0.0210	-0.0170	-0.0526	0.0966
	0.0488	0.3988	0.2612	0.1090	0.7838					



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	2.5980	3.4640	3.4640
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	3.5000	4.5000

4.3300	5.1960	5.1960	4.3300	4.3000	3.4640	2.5980	1.7320	1.7320
5.0000	4.5000	3.5000	3.0000	2.0000	1.5000	2.0000	1.5000	0.5000

CHRYSENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1.768810	1.625858	1.445962	1.387598	1.273321	1.251866	1.152170	1.109651	1.055510	0.811057	0.764385	0.755360	0.684524	0.677506	0.624370	0.600512	0.529105	0.482417
0.123393	0.237599	0.313183	-0.214270	-0.241460	0.272855	-0.257385	0.198926	0.227760	0.229719	0.213709	0.221083	0.303095	0.284562	0.191744	-0.290043	0.206043	-0.101841
0.116886	0.243657	0.345305	-0.111809	0.021640	0.397925	0.125933	0.323766	-0.149551	0.154328	-0.322479	0.159468	-0.407420	-0.061261	-0.095077	0.329462	-0.209410	0.094592
0.157042	0.277297	0.272068	0.050157	0.276719	0.192417	0.360931	0.030662	-0.290485	-0.307386	0.058709	-0.358024	0.214772	-0.218114	-0.051347	-0.290569	0.258767	-0.137384
0.269529	0.341270	0.103358	0.196469	0.316120	-0.174136	0.178381	-0.288772	-0.004984	0.023523	0.261182	0.154054	0.143645	0.355790	0.190909	0.167959	-0.372020	0.270810
0.207263	0.185432	-0.073589	0.385639	0.323066	-0.065174	-0.120986	0.053991	0.391763	0.378457	0.098757	0.120422	-0.051810	-0.350306	-0.354566	0.026481	0.183576	-0.189400
0.235723	0.052638	-0.212217	0.398608	0.067586	0.116298	-0.286581	0.317916	0.208846	-0.240591	-0.333083	-0.262036	-0.100929	0.097602	0.383231	-0.192901	-0.044999	0.222542
0.361296	-0.071946	-0.292520	0.211366	-0.210684	0.207042	-0.121011	0.182365	-0.296440	-0.259274	0.188572	0.109030	0.197680	0.195259	-0.247444	0.318866	-0.085207	-0.385974
0.321734	-0.297901	0.000186	0.128591	-0.168401	0.356816	0.036944	-0.330354	-0.094043	0.074577	0.354743	0.035258	-0.326062	-0.156168	0.170289	0.022208	0.329915	0.338376
0.185499	-0.250422	0.198389	0.222108	-0.313380	0.069193	0.352262	-0.189221	0.241864	0.260054	-0.211729	-0.344505	-0.000218	0.291449	-0.234115	-0.192271	-0.236346	-0.170532
0.125001	-0.232688	0.332320	0.187848	-0.217587	-0.282316	0.283752	0.191740	0.214455	-0.216408	-0.166972	0.285488	0.325853	-0.231409	0.180915	0.307855	0.199722	0.104165
0.118845	-0.238617	0.357848	0.078181	0.039046	-0.394110	-0.116560	0.332725	-0.141723	-0.143896	0.354294	0.093712	-0.408311	0.021965	-0.066452	-0.340192	-0.203919	-0.097995
0.160164	-0.271471	0.273442	-0.075809	0.273744	-0.178252	-0.379040	0.043908	-0.274135	0.288933	-0.130772	-0.363546	0.192121	0.214865	-0.088305	0.290387	0.252992	0.143946
0.276095	-0.334834	0.092036	-0.203044	0.296622	0.187162	-0.202286	-0.288357	-0.002343	-0.025512	-0.234147	0.223237	0.173423	-0.308332	0.218917	-0.156158	-0.363227	-0.283148
0.219823	-0.183556	-0.111226	-0.391146	0.307734	0.075989	0.133958	0.048313	0.374456	-0.358023	-0.062784	0.147840	-0.079251	0.311439	-0.392773	-0.059896	0.184354	0.206272
0.244771	-0.054038	-0.247045	-0.384807	0.073507	-0.111800	0.301925	0.295018	0.192754	0.210959	0.254292	-0.332655	-0.090572	-0.082820	0.386967	0.226833	-0.048077	-0.237508
0.362978	0.074961	-0.309361	-0.168158	-0.204148	-0.215933	0.115616	0.172254	-0.308507	0.282111	-0.153184	0.130462	0.214260	-0.196552	-0.183675	-0.337766	-0.094598	0.388259
0.318495	0.304148	-0.013216	-0.111633	-0.159499	-0.365068	-0.052272	-0.326539	-0.099005	-0.075690	-0.338151	0.110004	-0.340611	0.141279	0.135145	-0.005334	0.343405	-0.333421
0.183753	0.255734	0.177722	-0.228338	-0.325301	-0.084310	-0.339181	-0.175718	0.255846	-0.277801	0.141405	-0.353378	0.028705	-0.322025	-0.220472	0.171085	-0.245073	0.168214

CHRYSENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
32.76716	29.01981	23.25103	21.05810	16.18215	15.16745	9.95664	7.44948	3.96466	-17.56223	-23.23761	-24.41594	-34.74395	-35.8848	-45.3543	-50.1514	-67.0940	-80.8832
0.092779	0.186339	0.260448	-0.181898	-0.213982	0.243867	-0.239787	0.188842	0.221691	0.255077	0.244437	0.254377	0.366340	0.345716	0.242661	-0.374284	0.283262	-0.146626
0.087886	0.191090	0.287161	-0.094918	0.019177	0.355650	0.117322	0.307354	-0.145565	0.171364	-0.368847	0.183484	-0.492435	-0.074426	-0.120325	0.425152	-0.287890	0.136189
0.118080	0.217472	0.226255	0.042579	0.245228	0.171975	0.336253	0.029108	-0.282744	-0.341318	0.067150	-0.411940	0.259587	-0.264988	-0.064982	-0.374963	0.355744	-0.197799
0.202659	0.267644	0.085954	0.166787	0.280145	-0.155636	0.166184	-0.274133	-0.004851	0.026120	0.298736	0.177253	0.173618	0.432252	0.241605	0.216742	-0.511441	0.389900
0.155841	0.145426	-0.061198	0.327378	0.286301	-0.058250	-0.112713	0.051254	0.381322	0.420234	0.112957	0.138557	-0.062621	-0.425589	-0.448721	0.034172	0.252374	-0.272690
0.177240	0.041282	-0.176482	0.338387	0.059894	0.103942	-0.266987	0.301800	0.203280	-0.267149	-0.380975	-0.301497	-0.121990	0.118577	0.484997	-0.248928	-0.061863	0.320406
0.271658	-0.056424	-0.243263	0.179433	-0.186708	0.185046	-0.112737	0.173120	-0.288539	-0.287895	0.215685	0.125449	0.238929	0.237222	-0.313152	0.411479	-0.117140	-0.555708
0.241912	-0.233631	0.000155	0.109164	-0.149237	0.318908	0.034418	-0.313607	-0.091537	0.082809	0.405749	0.040568	-0.394100	-0.189730	0.215510	0.028658	0.453557	0.487178
0.139476	-0.196395	0.164983	0.188553	-0.277717	0.061842	0.328177	-0.179629	0.235419	0.288761	-0.242173	-0.396386	-0.000264	0.354083	-0.296284	-0.248115	-0.324920	-0.245524
0.093988	-0.182487	0.276362	0.159469	-0.192825	-0.252323	0.264351	0.182020	0.208740	-0.240297	-0.190980	0.328481	0.393847	-0.281141	0.228957	0.397269	0.274571	0.149972
0.089359	-0.187137	0.297591	0.066370	0.034603	-0.352240	-0.108591	0.315858	-0.137946	-0.159780	0.405235	0.107825	-0.493511	0.026686	-0.084098	-0.438998	-0.280341	-0.141089
0.120427	-0.212903	0.227398	-0.064356	0.242592	-0.159315	-0.353123	0.041682	-0.266829	0.320827	-0.149575	-0.418295	0.232209	0.261041	-0.111755	0.374729	0.347805	0.207247
0.207595	-0.262596	0.076538	-0.172368	0.262866	0.167278	-0.188455	-0.273739	-0.002280	-0.028329	-0.267813	0.256855	0.209610	-0.374595	0.277051	-0.201513	-0.499352	-0.407663
0.165285	-0.143955	-0.092497	-0.332053	0.272713	0.067916	0.124799	0.045864	0.364477	-0.397544	-0.071811	0.170104	-0.095788	0.378370	-0.497074	-0.077293	0.253444	0.296981
0.184043	-0.042380	-0.205446	-0.326671	0.065142	-0.099923	0.281282	0.280063	0.187617	0.234246	0.290855	-0.382752	-0.109471	-0.100619	0.489726	0.292715	-0.066095	-0.341953
0.272923	0.058789	-0.257268	-0.142753	-0.180915	-0.192992	0.107711	0.163522	-0.300285	0.313252	-0.175210	0.150109	0.258969	-0.238792	-0.232449	-0.435868	-0.130050	0.558998
0.239476	0.238530	-0.010990	-0.094768	-0.141348	-0.326284	-0.048698	-0.309986	-0.096366	-0.084045	-0.386772	0.126571	-0.411684	0.371642	0.171033	-0.006883	0.472102	-0.480045
0.138163	0.200562	0.147796	-0.193841	-0.288282	-0.075353	-0.315990	-0.166810	0.249027	-0.308467	0.161737	-0.406596	0.034695	-0.391231	-0.279018	0.220776	-0.336918	0.242187

CHRYSENE IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.01224	0.61140	-0.01510	-0.24744	-0.00145	0.17941	-0.00429	-0.03440	-0.00148	0.02685	0.00047	-0.02747	0.00092	0.07867	-0.00186	-0.14728	-0.00761	0.70836
2	0.61140	1.01326	0.71128	-0.00872	-0.14882	0.01176	0.13205	0.00162	-0.05597	0.00071	0.05767	-0.00411	-0.06484	-0.00059	0.06996	-0.00241	-0.25393	-0.01553
3	-0.01510	0.71128	1.01457	0.57176	0.00867	-0.19881	-0.00526	0.05400	0.00497	-0.02719	-0.00391	0.01218	0.00458	-0.05085	-0.00440	0.04755	0.02132	-0.34339
4	-0.24744	-0.00872	0.57176	0.96777	0.52332	-0.00995	-0.18261	-0.00516	0.06767	0.00018	-0.06450	0.00508	0.07628	0.00078	-0.08639	0.00778	-0.52991	0.02224
5	-0.00145	-0.14882	0.00867	0.52332	1.02225	0.75173	-0.01725	-0.15158	-0.00154	0.07778	-0.00191	-0.05122	0.00336	0.19287	-0.00712	-0.26076	0.00501	0.03310
6	0.17941	0.01176	-0.19881	-0.00995	0.75173	1.01434	0.53659	0.01248	-0.09350	-0.00308	0.07413	-0.00336	-0.09077	-0.01069	-0.01324	0.01284	-0.22670	-0.01795
7	-0.00429	0.13205	-0.00526	-0.18261	-0.01725	0.53659	0.97797	0.47464	0.01093	-0.14231	-0.00215	0.04390	0.00570	-0.25003	0.00949	0.57576	0.01521	-0.13605
8	-0.03440	0.00162	0.05400	-0.00516	-0.15158	0.01248	0.47464	0.96763	0.58624	-0.00674	-0.25731	0.02055	0.53464	0.00830	-0.22277	0.01296	0.01872	-0.00047
9	-0.00148	-0.05597	0.00497	0.06767	-0.00154	-0.09350	0.01093	0.58624	1.01439	0.70661	-0.01529	-0.34230	0.02192	0.03047	-0.01832	-0.13522	-0.00070	0.05269
10	0.02685	0.00071	-0.02719	0.00018	0.07778	-0.00308	-0.14231	-0.00674	0.70661	1.01162	0.61416	-0.01469	-0.25141	-0.00217	0.17586	-0.00282	-0.03445	0.00171
11	0.00047	0.05767	-0.00391	-0.06450	-0.00191	0.07413	-0.00215	-0.25731	-0.01529	0.61416	1.01291	0.70863	-0.00889	-0.14200	0.01215	0.13218	0.00189	-0.05621
12	-0.02747	-0.00411	0.01218	0.00508	-0.05122	-0.00336	0.04390	0.02055	-0.34230	-0.01469	0.70863	1.01465	0.57634	0.00733	-0.19757	-0.00628	0.05464	0.00521
13	0.00092	-0.06484	0.00458	0.07628	0.00336	-0.09077	0.00570	0.53464	0.02192	-0.25141	-0.00889	0.57634	0.97026	0.50986	-0.00930	-0.18503	-0.00625	-0.06847
14	-0.07867	-0.00059	-0.05085	0.00078	0.19287	-0.01069	-0.25003	0.00830	0.03047	-0.00217	-0.14200	0.00733	0.50986	1.01670	0.76544	-0.00946	-0.15471	-0.00327
15	-0.00186	0.06996	-0.00440	-0.08639	-0.00712	-0.01324	0.00949	-0.22277	-0.01832	0.17586	0.01215	-0.19757	-0.00930	0.76544	1.01038	-0.52265	0.01127	-0.08860
16	-0.14728	-0.00241	0.04755	0.00778	-0.26076	0.01284	0.57576	0.01296	-0.13522	-0.00282	0.13218	-0.00628	-0.18503	-0.00946	0.52265	0.97574	0.48182	0.01097
17	-0.00761	-0.25393	0.02132	0.52991	0.00501	-0.22670	0.01521	0.01872	-0.00070	-0.03445	0.00189	0.05464	-0.00625	-0.15471	0.01127	0.48182	0.96892	0.58378
18	0.70836	-0.01553	-0.34339	0.02224	0.03310	-0.01795	-0.13605	-0.00047	0.05269	-0.00171	-0.05621	0.00521	0.06847	-0.00327	-0.08860	0.01097	0.58378	1.01439

CHRYSENE — IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.78363	-0.43217	-0.09138	-0.25974	0.02368	0.19046	-0.00094	-0.03794	-0.00180	0.02935	0.00131	-0.02987	-0.00170	0.08513	0.00763	-0.14926	-0.07301	0.53346
2	0.43217	-0.78397	0.53657	-0.07245	-0.15073	0.02126	0.14084	-0.00434	-0.06020	0.00150	0.06212	-0.00095	-0.06995	-0.00592	0.07514	0.01878	-0.26650	-0.09122
3	-0.09138	0.53657	0.79562	0.39978	-0.06783	-0.20304	0.01432	0.05803	0.00041	-0.02956	-0.00079	0.01328	-0.00016	-0.05611	0.00120	0.05810	-0.03059	-0.36011
4	-0.25974	-0.07245	0.39978	0.70681	0.34897	-0.07850	-0.19386	0.01082	0.07309	-0.00234	-0.06955	0.00035	0.08192	0.00773	-0.08665	-0.04199	0.36832	-0.02995
5	0.02368	-0.15073	-0.06783	0.34897	0.80491	0.57875	-0.08984	-0.15342	0.01054	0.08405	-0.00704	-0.05651	0.00981	0.20633	0.01362	-0.27745	-0.05390	0.04415
6	0.19046	-0.02126	-0.20304	-0.07850	0.57875	0.79370	0.36243	-0.05618	-0.10576	0.00665	0.07958	0.00247	-0.09103	0.01064	-0.00467	-0.04689	-0.24072	0.00127
7	-0.00094	0.14084	0.01432	-0.19386	-0.08984	0.36243	0.72678	0.30713	-0.06012	-0.14399	0.01887	0.05421	-0.04389	-0.26740	-0.04853	0.41734	-0.03418	-0.13949
8	-0.03794	-0.00434	0.05803	0.01082	-0.15342	-0.05618	0.30713	0.71382	0.41496	-0.07192	-0.27007	-0.03186	0.37290	-0.05027	-0.23636	-0.03594	0.02651	0.00612
9	-0.00180	-0.06020	0.00041	0.07309	0.01054	-0.10576	-0.06012	0.41496	0.79427	0.53152	-0.09083	-0.35884	-0.03043	0.04088	0.00081	-0.13850	0.00593	0.05601
10	-0.02935	0.00150	-0.02956	-0.00234	0.08405	0.00665	-0.14399	-0.07192	0.53152	0.78275	0.43515	-0.09057	-0.26384	0.02197	0.18662	0.00039	-0.03800	-0.00199
11	0.00131	-0.06212	-0.00079	-0.06955	-0.00704	0.07958	0.01887	-0.27007	-0.09083	0.43515	0.78366	0.53367	-0.07296	-0.14337	0.02208	0.14089	-0.00418	-0.06046
12	-0.02987	-0.00095	0.01328	0.00035	-0.05651	0.00247	0.05421	-0.03186	-0.35884	-0.09057	0.53367	0.79509	0.40454	-0.06637	-0.20100	0.01360	0.05867	0.00055
13	-0.00170	-0.06995	-0.00016	0.08192	0.00981	-0.09103	-0.04389	0.37290	-0.03043	-0.26384	-0.07296	0.40454	0.71031	0.33683	-0.07955	-0.19616	0.01018	0.07400
14	0.08513	-0.00592	-0.05611	0.00773	0.20633	0.01064	-0.26740	-0.05027	0.04088	0.02197	-0.14337	-0.06637	0.33683	0.79273	0.58261	-0.08621	-0.15679	0.00921
15	0.00763	0.07514	0.00120	-0.08665	0.01362	-0.00467	-0.04853	-0.23636	0.00081	0.18662	0.02208	-0.20100	-0.07955	0.58261	0.78315	0.34896	-0.05603	-0.10048
16	-0.14926	-0.01878	0.05810	-0.04199	-0.27745	-0.04689	0.41734	-0.03594	-0.13850	0.00039	0.14089	0.01360	-0.19616	-0.08621	0.34896	0.72599	0.31456	-0.06050
17	-0.07301	-0.26650	-0.03059	0.36832	-0.05390	-0.24072	-0.03418	0.02651	0.00593	-0.03800	-0.00418	0.05867	0.01018	-0.15679	-0.05603	0.31456	0.71507	0.41221
18	0.53346	-0.09122	-0.36011	-0.02995	0.04415	0.00127	-0.13949	0.00612	0.05601	-0.00199	-0.06046	0.00055	0.07400	0.00921	-0.10048	-0.06050	0.41221	0.79441

ENERGIES FOR CHRYSENE IRMAPPROXIMATION

ONE-ELECTRON EXCITATIONS OF A SYMMETRY

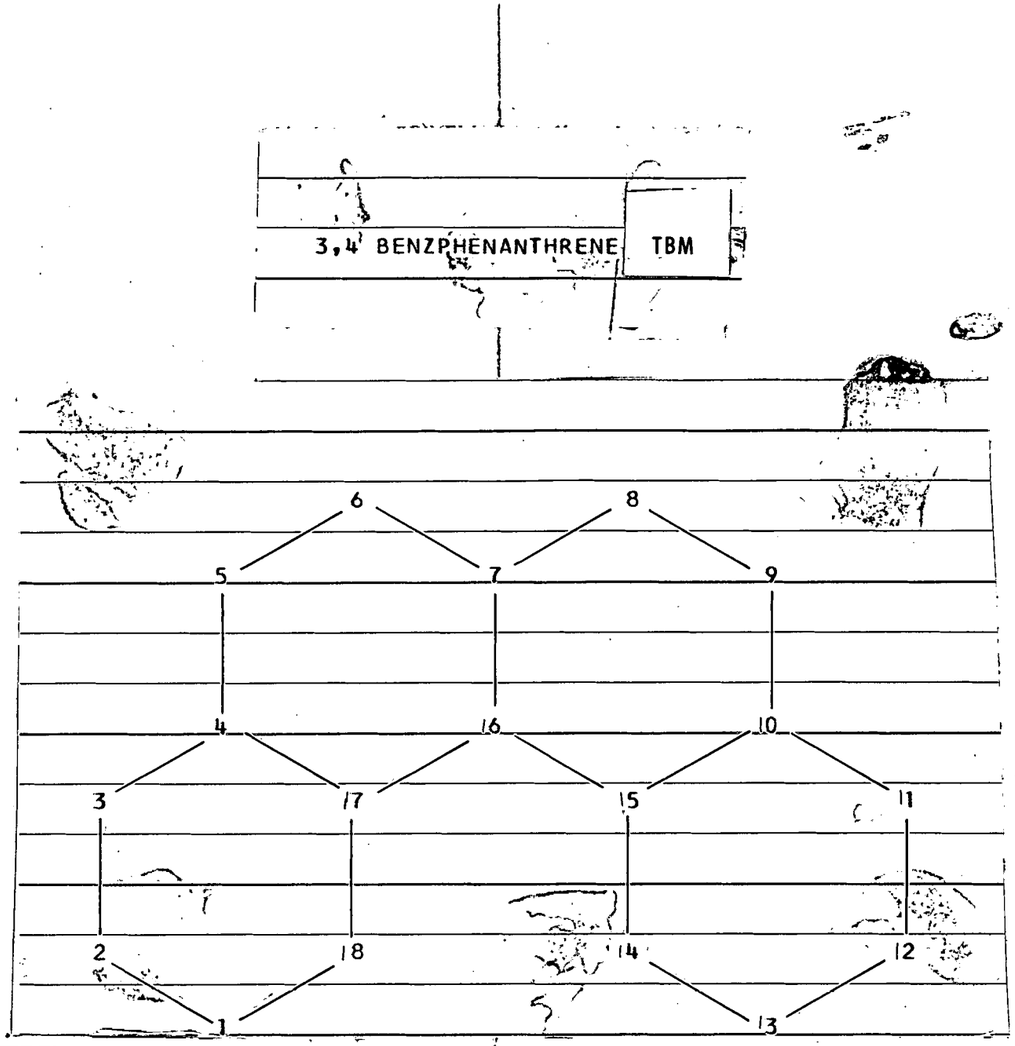
JUMP	9,10	8,10	9,11	7,10	9,12	8,11	8,12	6,10	7,11	5,10	7,12	6,11	4,10	9,13	5,11
XMOMNT	-0.80523	-0.40045	-0.40453	-0.01591	0.05324	0.68959	-0.07144	-0.00167	0.05074	0.01323	0.43999	-0.00242	0.00928	-0.00202	-0.25378
YMOMNT	0.05785	-0.80749	-0.74452	-0.00998	0.07616	0.07942	0.01502	-0.01785	-0.00306	0.17160	0.18637	-0.04966	0.00163	-0.00733	0.19967
JUMP E	21.5269	25.0117	27.2023	27.5189	28.3806	30.6871	31.8654	32.7297	33.1942	33.7444	34.3726	38.4051	38.6203	38.7086	39.4198
DIAG E	32.3164	35.7823	37.1335	40.7422	40.9299	41.4527	44.5686	45.9320	45.3660	46.9842	50.6077	52.6923	52.5689	51.7236	52.9114
DIAG E	32.4967	36.4153	36.6499	40.7748	41.2575	41.4216	45.3488	46.4942	44.7347	47.4060	50.7876	52.5905	52.7803	51.4010	52.6692
CORRSP	30.7698	31.2012	41.2728	38.9752	41.7666	42.3010	48.1697	47.1886	37.2861	45.6482	52.0745	54.5436	53.1163	53.5667	53.8310
CORRSP	30.9187	31.3539	41.3031	39.0740	41.9450	42.2566	48.8219	47.1668	37.4994	46.0526	53.6965	54.4096	53.3889	53.1815	52.1593

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
30.76975	0.50059	-0.61850	-0.00561	//	0.9348	0.0994	-0.0527	-0.0100	0.0036	0.2910	-0.0308	-0.0030	-0.0116	0.0021
					-0.1519	0.0084	-0.0002	0.0012	-0.0667					
20.23693				//	0.9351	0.0410	0.0495	-0.0352	0.0235	0.1278	-0.0006	0.0013	-0.0374	0.0005
					-0.3132	-0.0010	0.0162	0.0052	0.0594					
31.20121	0.02454	0.05268	-0.12536	//	-0.1116	0.7391	-0.6575	-0.0031	0.0618	-0.0189	0.0009	0.0268	0.0006	-0.0559
					-0.0024	0.0204	0.0031	-0.0167	-0.0173					
28.76192				//	-0.0619	0.8886	0.4146	0.0726	-0.1092	0.0835	0.0335	0.0701	-0.0394	0.0036
					0.0240	0.0291	0.0128	0.0308	0.0168					
41.27283	2.09438	-0.43897	-1.00030	//	-0.0140	0.6517	0.7217	0.0691	-0.0053	0.0563	0.0024	0.0124	0.0435	0.1141
					0.1693	0.0099	-0.0015	0.0023	0.0503					
30.98143				//	0.0510	-0.3966	0.8465	0.0151	-0.0826	-0.1621	0.0291	0.0055	-0.0021	0.2360
					0.1716	-0.0171	0.0089	0.0355	0.0516					
38.97518	0.00178	0.02974	0.01381	//	-0.0166	0.0011	-0.0688	0.7498	-0.5702	0.0625	-0.0478	-0.0567	-0.1974	0.0157
					-0.0072	-0.1761	-0.0030	0.1672	0.0094					
26.83312				//	0.0286	-0.0899	-0.1095	0.7154	-0.6720	0.0066	0.0153	0.0276	-0.0410	-0.0041
					-0.0660	-0.0453	-0.0752	0.0184	0.0227					
41.76662	0.02915	0.06127	0.11251	//	0.0008	-0.0617	-0.0079	0.6119	0.7313	0.0396	0.1471	-0.0233	0.2388	0.0077
					-0.0406	-0.0435	-0.0452	-0.0017	0.0241					
41.65092				//	-0.0063	0.0098	0.0581	0.6434	0.6935	0.0125	0.1675	-0.0073	0.1630	-0.0089
					-0.0338	-0.1864	-0.0550	0.0697	0.0546					
42.30105	1.35125	0.86277	0.08245	//	-0.3037	-0.0366	-0.0120	-0.0766	0.0209	0.9378	-0.0791	-0.0145	-0.0068	-0.0445
					-0.0946	-0.0044	-0.0060	-0.0135	0.0531					
33.60107				//	-0.1793	-0.1687	0.1856	-0.0101	-0.0069	0.9150	-0.1290	-0.0563	0.0193	-0.1459
					-0.1595	-0.0154	0.0005	-0.0179	-0.0137					
48.16969	0.00173	0.01454	0.02512	//	0.0049	0.0249	-0.0170	-0.1239	-0.0722	0.0447	0.6267	-0.6710	0.0091	0.0390
					0.0488	-0.1890	-0.2959	0.0466	-0.0639					
31.85551				//	-0.0174	-0.0772	-0.0565	-0.0840	-0.0082	0.1383	0.6411	-0.5600	-0.4060	-0.0049
					0.0520	-0.0685	0.0689	0.2505	0.0015					
47.18861	0.00194	-0.02587	0.01731	//	0.0031	-0.0090	0.0179	-0.0230	0.1554	0.0471	0.4863	0.2924	-0.7337	0.0298
					0.0497	0.2840	0.1378	0.0875	0.0409					
47.27134				//	0.0570	-0.0265	0.0240	0.0312	0.0550	-0.0450	-0.5525	0.6439	0.1535	-0.1369
					0.0796	0.0187	-0.2212	0.3098	-0.2751					

CHRYSENE IRM APPRXIMATION (cont.)

37.28606	0.00001	0.00188	0.00242	//	0.0024	-0.0175	-0.0176	0.0353	-0.2844	0.0578	0.5529	0.5297	0.4621	-0.0109
					-0.0476	-0.0527	0.0216	-0.3290	-0.0104					
37.92814				//	0.0341	0.0107	-0.0264	-0.0874	-0.1238	0.0771	0.3092	0.3366	0.7263	0.1328
					0.0301	-0.0559	-0.0133	-0.4578	-0.0374					
45.64822	0.57187	0.35971	0.40645	//	0.0294	-0.0792	-0.1674	-0.0117	0.0079	0.0886	-0.0479	0.0411	0.0554	0.8776
					0.4137	0.0102	0.0230	-0.0019	-0.0877					
37.04182				//	0.1426	0.0753	-0.2225	0.0559	0.0366	0.2760	-0.1200	-0.0549	-0.0566	0.7434
					0.5051	0.0024	0.0174	0.0944	-0.0790					
52.07454	0.52444	0.48653	-0.01038	//	0.0365	-0.0505	-0.0150	0.0272	0.0202	0.0905	-0.0378	0.1363	0.0236	-0.3802
					0.6331	0.0435	-0.2206	0.1126	-0.5978					
51.69063				//	0.1981	-0.0069	-0.0292	0.0174	-0.0257	0.0888	-0.0069	-0.0197	0.0712	-0.4993
					0.6962	0.0349	0.0111	-0.0126	0.4582					
54.54362	0.00389	0.01913	-0.03622	//	-0.0100	-0.0147	0.0019	0.1817	-0.0945	-0.0044	-0.1033	-0.2495	-0.0638	0.0057
					-0.0055	0.6194	-0.1978	-0.6734	-0.0660					
45.30084				//	-0.0228	-0.0470	0.0045	0.1893	0.1218	0.0050	-0.0445	0.1785	-0.0602	0.0433
					-0.0505	0.8681	0.3385	-0.1779	0.0691					
53.11630	0.05092	0.14664	0.03223	//	0.0215	-0.0123	-0.0094	0.0285	0.0067	0.0341	0.0667	-0.2853	0.0209	-0.1294
					0.2221	-0.1254	0.8644	-0.2605	-0.1189					
46.47941				//	-0.0744	0.0047	-0.0342	0.0115	-0.0129	-0.0425	-0.2957	0.2298	-0.0079	0.1077
					-0.1343	-0.3965	0.7216	-0.0336	0.3770					
53.56672	0.00184	0.01705	0.02270	//	0.0088	-0.0178	-0.0314	0.0291	-0.1269	0.0253	0.1211	-0.1220	0.3766	-0.0365
					0.0341	0.6649	0.2055	0.5555	0.1196					
52.47789				//	-0.0125	0.0007	-0.0283	-0.0670	-0.1126	0.0096	0.1812	-0.2109	0.4894	-0.0011
					-0.0692	0.1692	0.2479	0.7548	0.0214					
53.83098	0.28549	0.02808	0.35203	//	0.1344	-0.0596	-0.0949	-0.0042	-0.0042	0.0380	-0.0200	0.0019	0.0014	-0.2148
					0.5550	-0.0620	-0.1144	-0.1044	0.7652					
48.68642				//	-0.1249	0.0081	-0.0500	-0.0884	0.0081	-0.0027	-0.0679	0.1303	0.0336	0.2665
					-0.2565	0.1142	-0.4896	0.1114	0.7411					



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	2.5980	3.4640	4.3300
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	3.5000	3.0000

4.3300	5.1960	5.1960	4.3300	3.4640	3.4640	2.5980	1.7320	1.7320
2.0000	1.5000	0.5000	0.	0.5000	1.5000	2.0000	1.5000	0.5000

3,4 BENZPHENANTHRENE — TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 S	7 A	8 A	9 S	10 S	11 A	12 A	13 S	14 S	15 A	16 S	17 A	18 S
1.618746	1.527126	1.436707	1.349040	1.349035	1.277266	1.246799	1.163432	1.140079	0.859919	0.836566	0.753199	0.722732	0.650963	0.650958	0.563292	0.472873	0.381252
0.116964	-0.217585	0.275991	-0.353557	-0.000728	-0.363166	0.000001	0.278663	-0.168104	0.168104	0.278664	-0.000000	0.363166	-0.002630	-0.353548	0.275991	0.217585	-0.116964
0.107943	-0.232353	0.279127	-0.250437	0.203607	-0.255225	-0.353553	0.092262	0.231565	0.231565	-0.092262	0.353553	-0.255225	0.205976	0.248492	-0.279127	-0.232352	0.107943
0.153651	-0.278673	0.217904	-0.000609	0.288679	0.076452	-0.353553	-0.217581	0.299546	-0.299546	-0.217581	0.353553	-0.076452	-0.288672	0.002132	0.217904	0.278673	-0.153651
0.277259	-0.362831	0.106445	0.249562	0.204647	0.341097	-0.000000	-0.236334	-0.061544	-0.061543	0.236334	0.000000	0.341097	0.202268	-0.251494	-0.106445	-0.362831	0.277259
0.193891	-0.217577	-0.123753	0.352929	0.289422	0.115165	0.000000	0.278682	-0.317018	0.317018	0.278682	-0.000000	-0.115166	-0.286057	0.355662	-0.123753	0.217577	-0.193891
0.208830	-0.101874	-0.325407	0.249562	0.204658	-0.211704	0.000001	0.420858	-0.118385	-0.118386	-0.420858	0.000000	-0.211704	0.202278	-0.251494	0.325407	-0.101874	0.208830
0.329638	0.000000	-0.452019	-0.000000	0.000000	-0.352992	0.000001	-0.000000	0.249828	-0.249828	0.000000	-0.000000	0.352992	-0.000000	0.000000	-0.452020	0.000000	-0.329637
0.208831	0.101874	-0.325407	-0.250437	0.203586	-0.211704	0.000000	-0.420858	-0.118387	-0.118386	0.420858	0.000000	-0.211704	0.205955	0.248492	0.325407	0.101874	0.208830
0.193891	0.217577	-0.123753	-0.354167	0.287907	0.115166	-0.000000	-0.278681	-0.317019	0.317019	-0.278682	0.000000	-0.115166	-0.291257	-0.351416	-0.123753	-0.217577	-0.193891
0.277259	0.362831	0.106446	-0.250437	0.203575	0.341098	-0.000001	0.236334	-0.061543	-0.061543	-0.236334	-0.000000	0.341098	0.205945	0.248492	-0.106445	0.362831	0.277259
0.153651	0.278673	0.217904	-0.000628	0.288679	0.076453	0.353553	0.217581	0.299546	-0.299546	0.217581	0.353553	-0.076452	-0.288672	0.002114	0.217904	-0.278673	-0.153651
0.107942	0.232352	0.279127	0.249562	0.204679	-0.255224	0.353554	-0.092262	0.231565	0.231565	0.092262	-0.353553	-0.255225	0.202299	-0.251494	-0.279127	0.232352	0.107942
0.116964	0.217585	0.275991	0.353557	0.000788	-0.363166	0.000001	-0.278663	-0.168104	0.168104	-0.278663	-0.000000	0.363166	0.002570	0.353548	0.275991	-0.217585	-0.116964
0.185280	0.232352	0.209209	0.250437	-0.203565	-0.152754	-0.353553	-0.092262	0.326974	-0.326974	0.092262	0.353553	-0.152753	-0.205934	-0.248492	-0.209209	0.232353	0.185281
0.347544	0.278673	0.094186	0.000610	-0.288679	0.191574	-0.353554	0.217581	-0.017473	0.017473	0.217581	-0.353553	-0.191574	0.288672	-0.002132	0.094186	-0.278673	-0.347544
0.408746	0.000000	-0.148992	0.000875	-0.408265	0.026861	-0.000000	-0.000000	0.378583	0.378583	0.000000	-0.000000	0.026861	-0.408255	0.003002	0.148992	0.000000	-0.408746
0.347544	-0.278672	0.094186	0.000628	-0.288680	0.191575	0.353553	-0.217581	-0.017474	0.017474	-0.217581	0.353553	-0.191574	0.288672	-0.002114	0.094186	0.278673	-0.347544
0.185281	-0.232352	0.209209	-0.249562	-0.204637	-0.152752	0.353554	0.092262	-0.326974	-0.326974	-0.092262	-0.353553	-0.152753	-0.202257	0.251494	-0.209209	-0.232353	0.185281

3,4 BENZPHENANTHRENE — TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 S	7 A	8 A	9 S	10 S	11 A	12 A	13 S	14 S	15 A	16 S	17 A	18 S
28.81609	26.02198	22.91515	19.50524	19.50505	16.36501	14.92270	10.59003	9.26274	-12.28071	-14.72799	-24.70229	-28.92169	-40.42193	-40.42272	-58.44662	-84.03730	122.34985
0.091931	-0.176073	0.230256	-0.304402	-0.000627	-0.321339	0.000001	0.258351	-0.157438	0.181280	0.304670	-0.000000	0.427185	-0.003259	-0.438200	0.367729	0.316415	-0.189429
0.084841	-0.188023	0.232872	-0.215618	0.175300	-0.225831	-0.316633	0.085536	0.216873	0.249715	-0.100873	0.407380	-0.300216	0.255293	0.307989	-0.371907	-0.337890	0.174818
0.120766	-0.225506	0.181795	-0.000525	0.248545	0.067647	-0.316633	-0.201721	0.280541	-0.323024	-0.237887	-0.407380	-0.089929	-0.357789	0.002642	0.290335	0.405249	-0.248845
0.217920	-0.293607	0.088806	0.214865	0.176195	0.301813	-0.000000	-0.219107	-0.057639	-0.066367	0.258390	0.000000	0.401227	0.250697	-0.311710	-0.141828	-0.527633	0.449034
0.152394	-0.176066	-0.103246	0.303861	0.249184	0.101902	0.000000	0.258368	-0.296904	0.341866	0.304690	-0.000000	-0.135467	-0.354548	0.440820	-0.164888	0.316403	-0.314016
0.164136	-0.082438	-0.271484	0.214865	0.176204	-0.187322	0.000001	0.390180	-0.110874	-0.127665	-0.460135	0.000000	-0.249023	0.250710	-0.311711	0.433571	-0.148147	0.338211
0.259088	0.000000	-0.377114	-0.000000	0.000000	-0.312337	0.000000	-0.000000	0.233977	-0.269409	0.000000	-0.000000	0.415218	-0.000000	0.000000	-0.602269	0.000000	-0.533864
0.164136	0.082438	-0.271483	-0.215619	0.175282	-0.187321	0.000000	-0.390180	-0.110875	-0.127665	0.460135	0.000000	-0.249023	0.255267	0.307990	0.433572	0.148147	-0.338211
0.152394	0.176066	-0.103246	-0.304926	0.247879	0.101902	-0.000000	-0.258367	-0.296905	0.341866	-0.304690	0.000000	-0.135467	-0.360993	-0.435557	-0.164888	-0.316403	-0.314016
0.217919	0.293607	0.088806	-0.215618	0.175272	0.301813	-0.000001	0.219107	-0.057638	-0.066367	-0.258390	-0.000000	0.401227	0.255254	0.307990	-0.141827	0.527633	0.449034
0.120766	0.225505	0.181795	-0.000541	0.248544	0.067648	0.316633	0.201720	0.280541	-0.323024	0.237887	0.407380	-0.089929	-0.357789	0.002620	0.290335	-0.405249	-0.248845
0.084840	0.188023	0.232872	0.214865	0.176222	-0.225830	0.316634	-0.005537	0.216873	0.249715	0.100873	-0.407380	-0.300216	0.250736	-0.311711	-0.371907	0.337890	0.174818
0.091931	0.176073	0.230256	0.304402	0.000678	-0.321340	0.000001	-0.258350	-0.157439	0.181280	-0.304670	-0.000000	0.427185	0.003186	0.438200	0.367729	-0.316415	-0.189429
0.145626	0.188023	0.174540	0.215618	-0.175263	-0.135161	-0.316633	-0.085536	-0.306229	0.352602	0.100872	0.407380	-0.179680	-0.255241	-0.307990	-0.278749	0.337890	0.300071
0.273162	0.225505	0.078578	0.000525	-0.248544	0.169510	-0.316634	0.201721	-0.016365	0.018843	0.237887	-0.407380	-0.225346	0.357789	-0.002643	0.125493	-0.405249	-0.562864
0.321266	0.000000	-0.124302	0.000753	-0.351504	0.023767	-0.000000	-0.000000	0.354563	0.408256	0.000000	-0.000000	0.031596	-0.506003	0.003721	0.198516	0.000000	-0.661985
0.273162	-0.225505	0.078578	0.000541	-0.248545	0.169511	0.316633	-0.201721	-0.016365	0.018843	-0.237887	0.407380	-0.225345	0.357789	-0.002620	0.125493	0.405249	-0.562864
0.145626	-0.188022	0.174540	-0.214865	-0.176186	-0.135159	0.316634	0.005537	-0.306228	-0.352602	-0.100873	-0.407380	-0.179681	-0.250684	0.311710	-0.278749	-0.337890	0.300071

ENERGIES FOR 3,4 BENZPHENANTHRENE TBMAPPROXIMATION

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	9,10	9,11	8,11	6,10	7,11	6,11	5,10	9,12	5,11	4,11
XMOMNT	-0.00000	0.83310	-0.00000	0.00000	0.00000	-0.18641	0.00018	-0.06603	-0.01458	0.00003
YMOMNT	-0.50488	-0.00000	-0.74021	0.53797	-0.00000	0.00000	-0.14356	-0.00000	0.00030	0.14105
JUMP E	21.5435	23.9907	25.3180	28.6457	29.6507	31.0930	31.7858	33.9650	34.2330	34.2332
DIAG E	33.3706	34.4607	38.1275	41.3363	43.4167	44.3302	44.7050	44.9473	46.8409	50.3556
DIAG E	33.4390	34.5550	38.2130	41.7691	43.5871	44.7888	45.1076	44.6592	47.2694	50.3502
CORRSP	31.2848	33.9859	39.9687	38.8701	42.1360	43.6302	47.7349	45.4245	47.2385	51.3169
CORRSP	31.4359	34.0676	38.9277	40.3689	42.4383	43.9395	47.9441	45.6754	47.5898	51.3508

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
31.28481	0.02174	0.00004	-0.12783	//	0.8682	0.0001	-0.4759	-0.0927	0.0695	-0.0000	-0.0771	-0.0000	-0.0001	-0.0210
21.36674				//	0.8436	0.0001	-0.5074	0.0331	-0.0865	-0.0000	-0.0959	-0.0000	-0.0003	-0.1146
39.96875	1.27450	0.00003	-0.86594	//	0.3444	0.0000	0.6153	-0.4169	-0.5688	0.0000	0.0727	-0.0000	-0.0000	-0.0133
27.53779				//	0.4820	-0.0018	0.7930	-0.2984	-0.2060	-0.0002	0.0713	0.0001	0.0005	0.0469
38.87007	0.05218	-0.00007	-0.17768	//	0.3424	-0.0001	0.5516	0.6793	0.2849	-0.0000	-0.1428	0.0000	0.0003	0.1245
34.70067				//	0.0845	0.0004	0.0767	0.7342	-0.3307	0.0006	0.4544	-0.0001	0.0009	0.3635
42.13601	0.16934	-0.00022	-0.30741	//	-0.0359	-0.0002	0.2091	-0.4312	0.4370	-0.0004	-0.7053	0.0001	-0.0005	-0.2840
42.87167				//	0.1662	0.0008	-0.0181	-0.1343	0.7609	-0.0004	0.5754	-0.0006	0.0038	0.2094
47.73491	0.48639	0.00024	-0.48950	//	0.0922	0.0001	0.2167	-0.3281	0.6181	-0.0004	0.6708	-0.0003	-0.0004	-0.0689
37.32688				//	-0.1456	0.0006	-0.2926	-0.5277	-0.5069	0.0028	0.5964	-0.0000	0.0000	-0.0452
51.31695	0.00190	-0.00004	0.02947	//	-0.0250	-0.0000	0.0041	-0.2502	0.1320	0.0000	-0.1445	-0.0000	0.0020	0.9479
46.64431				//	-0.0022	-0.0001	-0.1477	-0.2726	-0.0694	0.0003	-0.3040	-0.0001	0.0024	0.8981

ENERGIES FOR 3,4 BENZPHENANTHRENE TBMAPPROXIMATION

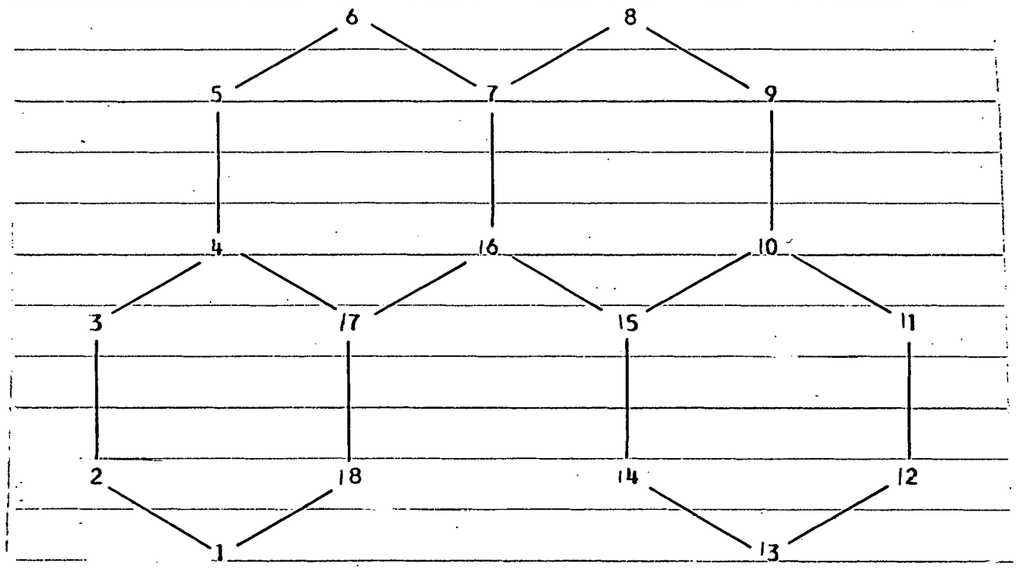
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	8,10	9,11	7,10	6,11	4,10	9,12	5,11	3,11	2,10	8,13
XMOMNT	-0.83264	0.83310	0.06576	-0.18641	0.08350	-0.06603	-0.01458	-0.02301	-0.01034	0.18750
YMOMNT	0.00000	-0.00000	-0.00000	0.00000	0.00031	-0.00000	0.00030	-0.00000	0.00000	-0.00000
JUMP E	22.8707	23.9907	27.2034	31.0930	31.7859	33.9650	34.2330	37.6431	38.3027	39.5117
DIAG E	33.4894	34.4607	38.5557	44.3302	46.7142	44.6473	46.8409	52.8828	53.2008	51.9306
DIAG E	33.5491	34.5550	38.7003	44.7888	46.6830	44.6592	47.2694	53.0945	53.5915	51.4393
CORRSP	28.6005	35.7065	37.8521	43.9645	46.6205	44.9483	47.3133	56.2339	53.4031	52.4098
CORRSP	28.8322	35.7422	38.1403	44.4603	46.6233	45.1051	47.6057	53.4007	56.2928	52.1274

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
28.60050	0.00542	-0.06678	-0.00004	//	0.6944	0.6060	-0.2129	-0.2095	-0.0644	-0.1357	-0.0569	-0.0942	0.1019	-0.1282
23.65645				//	0.7023	-0.6140	0.2297	-0.1292	0.0180	-0.1902	0.1118	-0.0769	-0.0011	0.0731
35.70647	1.39160	0.95733	0.00000	//	-0.6099	0.6461	-0.3672	0.2016	0.0411	0.1367	-0.0361	0.0051	0.0083	-0.1158
28.13104				//	0.5909	0.5875	-0.4052	-0.3143	-0.1006	0.0201	-0.0246	-0.1206	0.1258	-0.0356
37.85213	0.40762	-0.50322	-0.00011	//	-0.1482	-0.3789	0.8406	-0.0397	-0.1062	-0.1946	-0.2373	-0.0479	-0.1284	-0.0448
29.40673				//	0.0098	0.3854	0.7005	-0.1019	-0.1617	-0.4787	-0.3044	-0.0421	-0.0029	-0.0226
43.96449	0.33552	-0.42363	-0.00016	//	0.2884	-0.0039	0.0403	0.7863	-0.2081	0.2082	-0.3220	0.3259	0.0107	-0.0119
34.35342				//	0.2941	0.1426	-0.0234	0.7398	0.2779	-0.1412	-0.0251	0.1666	-0.0077	-0.4689
46.62048	0.00211	-0.03264	0.00018	//	0.1288	0.0245	0.1077	0.0655	0.8542	0.3370	-0.2714	-0.2219	-0.0262	0.0049
39.34756				//	-0.1259	0.1534	0.0503	-0.1647	-0.6761	-0.2695	0.4809	-0.4041	-0.0790	0.0192
44.94832	0.00291	-0.03904	-0.00017	//	-0.0039	-0.0175	0.0877	-0.3688	-0.3704	0.8116	-0.1803	-0.0587	0.1105	-0.1094
44.41263				//	0.1641	0.1300	0.4716	-0.0294	0.1909	0.7947	-0.0512	-0.1835	-0.1250	-0.1141
47.31329	0.00005	-0.00509	0.00026	//	0.1496	0.1887	0.2145	0.2090	0.0403	0.3221	0.8066	-0.0314	-0.3009	0.0692
44.83311				//	0.0563	0.1856	0.1437	0.0957	-0.4379	0.0156	0.7154	-0.2236	-0.4223	0.0194
56.23389	0.03318	0.11779	0.00014	//	-0.0289	0.0865	0.1797	-0.1361	-0.2361	0.0306	0.2159	0.6547	0.6379	-0.0447
53.92032				//	0.0065	0.0730	0.1947	-0.1867	0.2191	0.0785	0.2670	0.6375	0.6237	0.0301
53.40314	0.10805	-0.21813	0.00003	//	-0.0273	-0.1196	0.1127	0.2840	-0.0695	-0.0600	0.1790	-0.5423	0.5316	-0.5238
49.93953				//	0.0370	0.0898	0.0842	0.4843	-0.2045	0.0612	0.1737	-0.4133	0.4957	0.5066
52.40982	0.12494	0.23676	-0.00003	//	-0.0143	0.1163	0.0361	0.1116	-0.1023	0.0328	0.0041	-0.3259	0.4241	0.8215
49.26335				//	0.1538	0.1440	-0.0350	0.1426	0.3331	-0.0003	-0.2156	0.3546	-0.3862	0.7083

3,4 BENZPHENANTHRENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	2.5980	3.4640	4.3300
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	3.5000	3.0000

4.3300	5.1960	5.1960	4.3300	3.4640	3.4640	2.5980	1.7320	1.7320
2.0000	1.5000	0.5000	0.	0.5000	1.5000	2.0000	1.5000	0.5000

3,4 BENZPHENANTHRENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 S	7 A	8 A	9 S	10S	11 A	12 A	13 S	14 S	15A	16 S	17 A	18 S
1.772895	1.609463	1.475087	1.336338	1.323920	1.214855	1.171506	1.089052	1.067052	0.815449	0.785680	0.724299	0.706547	0.653054	0.647280	0.591931	0.532266	0.483308
0.132168	-0.231673	0.288092	0.340021	0.007578	0.350283	0.076498	-0.288096	0.145843	0.203774	-0.275728	0.006137	0.366108	0.011942	-0.347167	0.263493	-0.212776	0.101874
0.121708	-0.250253	0.279123	0.263808	0.225391	0.227485	-0.319474	-0.138866	-0.241025	0.218902	0.109400	-0.357655	-0.278916	-0.185676	0.244389	-0.277522	0.216381	-0.097088
0.160466	-0.289357	0.202392	0.024107	0.310736	-0.111890	-0.369847	0.192830	-0.266548	-0.318153	0.186448	0.369753	-0.051579	0.270833	-0.003941	0.235998	-0.265001	0.142255
0.273708	-0.350360	0.065554	-0.236394	0.198448	-0.339936	-0.019674	0.251823	0.082385	-0.035572	-0.229965	-0.030371	0.341970	-0.207037	-0.256555	-0.137991	0.371398	-0.280974
0.199294	-0.217183	-0.152075	-0.372135	0.266646	-0.104398	0.006858	-0.255266	0.336261	0.300745	-0.289804	-0.003570	-0.149150	0.290883	0.350224	-0.099450	-0.206109	0.186787
0.211168	-0.108380	-0.328469	-0.270670	0.174772	0.247152	0.029767	-0.406755	0.111620	-0.139748	0.422565	0.029530	-0.183861	-0.231508	-0.244031	0.309739	0.098338	-0.201395
0.318040	0.000000	-0.426796	0.000000	-0.016878	0.353391	0.000000	0.000000	-0.276325	-0.223857	0.000000	0.000000	0.357484	0.057194	-0.000000	-0.467031	0.000000	0.340401
0.211168	0.108381	-0.328468	0.270674	0.174768	0.247153	-0.029766	0.406754	0.111621	-0.139748	-0.422565	-0.029530	-0.183861	-0.231507	0.244031	0.309739	-0.098338	-0.201395
0.199294	0.217183	-0.152074	0.372140	0.266640	-0.104398	-0.006858	0.255265	0.336262	0.300745	0.289803	0.003569	-0.149150	0.290882	-0.350225	-0.099450	0.206109	0.186787
0.273708	0.350360	0.065554	0.236397	0.198444	-0.339937	0.019674	-0.251823	0.082385	-0.035572	0.229965	0.030372	0.341970	-0.207036	0.256556	-0.137991	-0.371398	-0.280974
0.160466	0.289357	0.202393	-0.024102	0.310736	-0.111890	0.369847	-0.192829	-0.266548	-0.318153	-0.186448	-0.369753	-0.051578	0.270833	0.003940	0.235998	0.265001	0.142255
0.121708	0.250253	0.279123	-0.263805	0.225396	0.227485	0.319475	0.138866	-0.241025	0.218902	-0.109401	0.357654	-0.278916	-0.185677	-0.244388	-0.277522	-0.216381	-0.097088
0.132168	0.231672	0.288092	-0.340020	0.007584	0.350283	-0.076498	0.288096	0.145843	-0.203775	0.275728	-0.006136	0.366108	0.011943	0.347167	0.263493	0.212776	0.101874
0.204821	0.222318	0.231566	-0.214417	-0.231479	0.142904	-0.379192	0.043686	0.314198	-0.328527	-0.085382	-0.347874	-0.147519	0.185992	-0.267740	-0.197262	-0.242724	-0.168827
0.339041	0.262453	0.080391	0.024588	-0.285022	-0.202373	-0.331949	-0.254165	-0.008779	0.029952	-0.233497	0.335418	-0.163654	-0.300310	-0.004415	0.103815	0.297787	0.357317
0.387989	0.000000	-0.152655	-0.000003	-0.391398	-0.057852	0.000000	0.000000	-0.400737	0.358359	-0.000000	-0.000000	-0.012173	0.411202	-0.000001	0.168751	0.000000	-0.427664
0.339041	-0.262453	0.080390	-0.024593	-0.285022	-0.202373	0.331949	0.254166	-0.008779	0.029953	0.233497	-0.335418	-0.163653	-0.300310	0.004416	0.103815	-0.297787	0.357318
0.204821	-0.222318	0.231566	0.214413	-0.231483	0.142904	0.379192	-0.043687	0.314198	-0.328527	0.085383	0.347873	-0.147520	0.185993	-0.267740	-0.197262	0.242724	-0.168827

3,4 BENZPHENANTHRENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 S	7 A	8 A	9 S	10S	11A	12A	12 S	14 S	15 A	16 S	17 A	18 S
32.86538	28.54747	24.28045	18.97408	18.44492	13.33284	11.03663	6.16446	4.73725	-17.06159	-20.56449	-28.69603	-31.31109	-40.05107	-41.08087	-51.97139	-66.24784	-80.59506
0.099262	-0.182614	0.237204	0.294135	0.006586	0.317802	0.070677	-0.276066	0.141186	0.225658	-0.311070	0.007211	0.435550	0.014777	-0.431512	0.342479	-0.291647	0.146538
0.091406	-0.197260	0.229819	0.228208	0.195887	0.206391	-0.295164	-0.133068	-0.233330	0.242411	0.123423	-0.420247	-0.331820	-0.229764	0.303763	-0.360713	0.296589	-0.139655
0.120515	-0.228084	0.166642	0.020854	0.270060	-0.101515	-0.341703	0.184778	-0.258037	-0.352320	0.210347	0.434463	-0.061363	0.335141	-0.004899	0.306742	-0.363231	0.204623
0.205564	-0.276168	0.053975	-0.204493	0.172471	-0.308415	-0.018177	0.241307	0.079755	-0.039392	-0.259441	-0.035686	0.406835	-0.256197	-0.318885	-0.179356	0.509067	-0.404160
0.149676	-0.171193	-0.125213	-0.321916	0.231742	-0.094718	0.006336	-0.244607	0.325525	0.333043	-0.326950	-0.004195	-0.177440	0.359951	0.435312	-0.129261	-0.282509	0.268680
0.158594	-0.085430	-0.270449	-0.234144	0.151895	0.224235	0.027501	-0.389770	0.108056	-0.154755	0.476728	0.034697	-0.218736	-0.286478	-0.303318	0.402587	0.134790	-0.289692
0.238858	0.000000	-0.351408	0.000000	-0.014668	0.320622	0.000000	0.000000	-0.267502	-0.247897	0.000000	0.000001	0.425291	0.070774	-0.000000	-0.607030	-0.000000	0.489642
0.158594	0.085430	-0.270449	0.234147	0.151891	0.224235	-0.027501	0.389770	0.108057	-0.154756	-0.476728	-0.034698	-0.218735	-0.286477	0.303319	0.402587	-0.134790	-0.289692
0.149676	0.171193	-0.125212	0.321920	0.231736	-0.094718	-0.006336	0.244606	0.325525	0.333043	0.326949	0.004194	-0.177440	0.359950	-0.435313	-0.129262	0.282509	0.268680
0.205564	0.276168	0.053975	0.204495	0.172468	-0.308415	0.018177	-0.241307	0.079754	-0.039392	0.259442	0.035687	0.406834	-0.256196	0.318886	-0.179356	-0.509067	-0.404160
0.120515	0.228083	0.166643	-0.020849	0.270060	-0.101515	0.341704	-0.184777	-0.258037	-0.352320	-0.210346	-0.434463	-0.061361	0.335141	0.004898	0.306742	0.363231	0.204623
0.091406	0.197260	0.229819	-0.228204	0.195891	0.206391	0.295165	0.133068	-0.233329	0.242410	-0.123423	0.420246	-0.331821	-0.229764	-0.303762	-0.360713	-0.296589	-0.139655
0.099262	0.182614	0.237204	-0.294135	0.006591	0.317802	-0.070677	0.276066	0.141186	0.225659	0.311070	-0.007210	0.435550	0.014778	0.431512	0.342479	0.291647	0.146538
0.153827	0.175240	0.190663	-0.185482	-0.201178	0.129653	-0.350338	0.041862	0.304166	-0.363808	-0.096326	-0.408754	-0.175500	0.230154	-0.332788	-0.256394	-0.332696	-0.242846
0.254631	0.206876	0.066191	0.021270	-0.247712	-0.183607	-0.306690	-0.243552	-0.008499	0.033169	-0.263426	0.394119	-0.194695	-0.371617	-0.005488	0.134935	0.408170	0.513975
0.291392	0.000000	-0.125691	-0.000003	-0.340164	-0.052487	0.000000	0.000000	-0.387942	0.396844	-0.000000	-0.000000	-0.014483	0.508839	-0.000001	0.219337	0.000000	-0.615163
0.254631	-0.206876	0.066190	-0.021274	-0.247712	-0.183607	0.306690	0.243553	-0.008498	0.033169	0.263426	-0.394119	-0.194694	-0.371617	0.005489	0.134936	-0.408171	0.513975
0.153827	-0.175240	0.190663	0.185478	-0.201181	0.129653	0.350337	-0.041863	0.304166	-0.363808	0.096327	0.408754	-0.175502	0.230156	0.332787	-0.256394	0.332696	-0.242846

3,4 BENZPHENANTHRENE IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.00526	0.61197	-0.00962	-0.24752	-0.01026	0.17999	0.00487	-0.03016	-0.00165	0.04554	0.02484	-0.04101	-0.02729	0.04381	-0.02194	-0.14875	-0.00349	0.70782
2	0.61197	1.01387	0.71000	-0.00843	-0.14691	0.01084	0.12554	0.00008	-0.10465	0.00504	0.02940	-0.00040	-0.04101	-0.00591	0.07538	-0.00036	-0.25322	-0.01742
3	-0.00962	0.71000	1.01023	0.57289	0.01644	-0.20060	-0.01295	0.05783	0.00799	-0.03317	-0.02289	0.02940	0.02484	-0.02553	0.01100	0.04606	0.01736	-0.34221
4	-0.24752	-0.00843	0.57289	0.96675	0.52067	-0.00986	-0.17435	-0.00563	0.12208	-0.00300	-0.03317	0.00504	0.04554	-0.01226	-0.09132	0.01034	0.52963	0.02271
5	-0.01026	-0.14691	0.01644	0.52067	1.01755	0.75734	-0.01205	-0.15586	0.01410	0.12208	0.00799	-0.10465	-0.00165	0.10474	-0.01206	-0.26507	0.00214	0.03372
6	0.17999	0.01084	-0.20060	-0.00986	0.75734	1.01583	0.52179	0.01045	-0.15586	-0.00563	0.05783	0.00008	-0.03016	0.00402	0.00556	0.00928	-0.22805	-0.01552
7	0.00487	0.12554	-0.01295	-0.17435	-0.01205	0.52179	0.96966	0.52179	-0.01205	-0.17435	-0.01295	0.12554	0.00487	-0.13221	0.01848	0.57089	0.01848	-0.13221
8	-0.03016	0.00008	0.05783	-0.00563	-0.15586	0.01045	0.52179	1.01583	0.75734	-0.00986	-0.20060	0.01084	0.17999	-0.01552	-0.22805	0.00928	0.00556	0.00402
9	-0.00165	-0.10465	0.00799	0.12208	0.01410	-0.15586	-0.01205	0.75734	1.01755	0.52067	0.01644	-0.14691	-0.01026	0.03372	0.00214	-0.26507	-0.01206	0.10474
10	0.04554	0.00504	-0.03317	-0.00300	0.12208	-0.00563	-0.17435	-0.00986	0.52067	0.96675	0.57289	-0.00843	-0.24752	0.02271	0.52963	0.01034	-0.09132	-0.01226
11	0.02484	0.02940	-0.02289	-0.03317	0.00799	0.05783	-0.01295	-0.20060	0.01644	0.57289	1.01023	0.71000	-0.00962	-0.34221	0.01736	0.04606	0.01100	-0.02553
12	-0.04101	-0.00040	0.02940	0.00504	-0.10465	0.00008	0.12554	0.01084	-0.14691	-0.00843	0.71000	1.01387	0.61197	-0.01742	-0.25322	-0.00036	0.07538	-0.00591
13	-0.02729	-0.04101	0.02484	0.04554	-0.00165	-0.03016	0.00487	0.17999	-0.01026	-0.24752	-0.00962	0.61197	1.00526	0.70782	-0.00349	-0.14875	-0.02194	0.04381
14	0.04381	-0.00591	-0.02553	-0.01226	0.10474	0.00402	-0.13221	-0.01552	0.03372	0.02271	-0.34221	-0.01742	0.70782	1.01879	0.58040	0.00108	-0.09097	0.05441
15	-0.02194	0.07538	0.01100	-0.09132	-0.01206	0.00556	0.01848	-0.22805	0.00214	0.52963	0.01736	-0.25322	-0.00349	0.58040	0.97591	0.49211	-0.00119	-0.09097
16	-0.14875	-0.00036	0.04606	0.01034	-0.26507	0.00928	0.57089	0.00928	-0.26507	0.01034	0.04606	-0.00036	-0.14875	0.00108	0.49211	0.98194	0.49211	0.00108
17	-0.00349	-0.25322	0.01736	0.52963	0.00214	-0.22805	0.01848	0.00556	-0.01206	-0.09132	0.01100	0.07538	-0.02194	-0.09097	-0.00119	0.49211	0.97591	0.58040
18	0.70782	-0.01742	-0.34221	0.02271	0.03372	-0.01552	-0.13221	0.00402	0.10474	-0.01226	-0.02553	-0.00591	0.04381	0.05441	-0.09097	0.00108	0.58040	1.01879

3,4 BENZPHENANTHRENE IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.77633	0.43309	-0.08560	-0.26006	0.01418	0.19077	0.00877	-0.03433	-0.00402	0.05042	0.02391	-0.04299	0.02795	0.04089	-0.01234	-0.14917	-0.06849	0.53239
2	0.43309	0.78481	0.53498	-0.07244	-0.14844	0.02066	0.13358	-0.00801	-0.11238	0.00330	0.03090	0.00153	-0.04299	-0.00960	0.08206	0.02160	-0.26586	-0.09337
3	-0.08560	0.53498	0.79095	0.40120	-0.05931	-0.20479	0.00549	0.06247	0.00081	-0.03690	-0.02249	0.03090	0.02391	-0.02412	0.01741	0.05548	-0.03480	-0.35855
4	-0.26006	-0.07244	0.40120	0.70608	0.34624	-0.07884	-0.18523	0.01348	0.13037	-0.00050	-0.03690	0.00330	0.05042	-0.00502	-0.09107	-0.04061	0.36764	-0.02903
5	0.01418	-0.14844	-0.05931	0.34624	0.79907	0.58450	-0.08219	-0.15756	0.02782	0.13037	0.00081	-0.11238	-0.00402	0.11303	0.00482	-0.28158	-0.05665	0.04403
6	0.19077	0.02066	-0.20479	-0.07884	0.58450	0.79625	0.34736	-0.06295	-0.15756	0.01348	0.06247	-0.00801	-0.03433	0.01344	0.01321	-0.05030	-0.24215	0.00341
7	0.00877	0.13358	0.00549	-0.18523	-0.08219	0.34736	0.71022	0.34736	-0.08219	-0.18523	0.00549	0.13358	0.00877	-0.13420	-0.03080	0.41141	-0.03080	-0.13420
8	-0.03433	-0.00801	0.06247	0.01348	-0.15756	-0.06295	0.34736	0.79625	0.58450	-0.07884	-0.20479	0.02066	0.19077	0.00341	-0.24215	-0.05030	0.01321	0.01344
9	-0.00402	-0.11238	0.00081	0.13037	0.02782	-0.15756	-0.08219	0.58450	0.79907	0.34624	-0.05931	-0.14844	0.01418	0.04403	-0.05665	-0.28158	0.00482	0.11303
10	0.05042	0.00330	-0.03690	-0.00050	0.13037	0.01348	-0.18523	-0.07884	0.34624	0.70608	0.40120	-0.07244	-0.26006	-0.02903	0.36764	-0.04061	-0.09107	-0.00502
11	0.02391	0.03090	-0.02249	-0.03690	0.00081	0.06247	0.00549	-0.20479	-0.05931	0.40120	0.79095	0.53498	-0.08560	-0.35855	-0.03480	0.05548	0.01741	-0.02412
12	-0.04299	0.00153	0.03090	0.00330	-0.11238	-0.00801	0.13358	0.02066	-0.14844	-0.07244	0.53498	0.78481	0.43309	-0.09337	-0.26586	0.02160	0.08206	-0.00960
13	-0.02795	-0.04299	0.02391	0.05042	-0.00402	-0.03433	0.00877	0.19077	0.01418	-0.26006	-0.08560	0.43309	0.77633	0.53239	-0.06849	-0.14917	-0.01234	0.04089
14	0.04089	-0.00960	-0.02412	-0.00502	0.11303	0.01344	-0.13420	0.00341	0.04403	-0.02903	-0.35855	-0.09337	0.53239	0.79883	0.40958	-0.07102	-0.10865	0.04043
15	-0.01234	0.08206	0.01741	-0.09107	0.00482	0.01321	-0.03080	-0.24215	-0.05665	0.36764	-0.03480	-0.26586	-0.06849	0.40958	0.72198	0.32615	-0.06453	-0.10865
16	-0.14917	0.02160	0.05548	-0.04061	-0.28158	-0.05030	0.41141	-0.05030	-0.28158	-0.04061	0.05548	0.02160	-0.14917	-0.07102	0.32615	0.73935	0.32615	-0.07102
17	-0.06849	-0.26586	-0.03480	0.36764	-0.05665	-0.24215	-0.03080	0.01321	0.00482	-0.09107	0.01741	0.08206	-0.01234	-0.10865	-0.06453	0.32615	0.72198	0.40958
18	0.53239	-0.09337	-0.35855	-0.02903	0.04403	0.00341	-0.13420	0.01344	0.11303	-0.00502	-0.02412	-0.00960	0.04089	0.04043	-0.10865	-0.07102	0.40958	0.79883

ENERGIES FOR 3,4 BENZPHENANTHRENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	9,10	9,11	8,11	6,10	7,11	9,12	6,11	8,12	5,10	9,13
XMOMNT	0.00000	0.82266	-0.00000	0.00000	-0.00000	-0.12858	-0.18647	-0.00000	0.00000	-0.00000
YMOMNT	0.48622	-0.00000	-0.73363	-0.58046	0.11965	-0.00000	-0.00000	-0.11903	-0.18948	-0.56381
JUMP E	21.7988	25.3017	26.7289	30.3944	31.6011	33.4333	33.8973	34.8605	35.5065	36.0483
DIAG E	32.9661	34.9001	38.6684	43.2411	44.9211	44.3913	46.5138	47.8538	48.9068	47.6305
DIAG E	33.8366	35.4968	39.3178	45.4638	45.3691	44.9567	48.4626	48.4719	50.7841	46.0642
CORRSP	31.1612	34.7849	39.6331	37.4417	45.0839	44.2842	46.7360	48.5938	49.2830	52.9988
CORRSP	31.6634	34.8725	40.6816	37.5865	46.2382	45.3591	48.6845	50.6205	53.6300	48.8874

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
31.16118	0.03755	0.00000	0.16832	//	0.8909	0.0000	0.4430	-0.0480	0.0146	-0.0000	0.0000	-0.0484	0.0428	-0.0583
22.00594				//	0.8873	0.0000	0.4155	0.1123	-0.1338	-0.0000	0.0000	0.0962	0.0162	0.0043
39.63311	0.79096	-0.00000	-0.68505	//	-0.4486	0.0000	0.8644	-0.1084	0.0970	-0.0000	-0.0000	-0.1108	-0.0550	-0.1226
27.73807				//	-0.4202	0.0000	0.8280	0.3268	-0.0600	0.0000	0.0000	-0.0119	0.0383	0.1609
37.44173	-0.03272	0.00000	-0.14335	//	0.0005	0.0000	0.0166	0.6354	0.4982	-0.0000	-0.0000	-0.3549	0.1583	-0.4436
34.57609				//	-0.0455	-0.0000	-0.2922	0.6326	-0.4203	0.0000	0.0000	0.3869	-0.2571	0.3462
45.08386	0.11164	-0.00000	0.24131	//	-0.0083	-0.0000	-0.0670	-0.5756	0.6176	0.0000	-0.0000	0.1847	0.4649	-0.1803
37.13870				//	0.0444	0.0000	-0.1374	0.5006	0.5434	0.0000	0.0000	0.3163	0.3524	-0.4571
48.59385	0.29796	0.00000	0.37972	//	-0.0235	0.0000	-0.0071	-0.3745	-0.4644	0.0000	0.0000	0.5489	0.1527	-0.5647
47.38139				//	0.0129	-0.0000	0.0750	-0.3743	0.4577	0.0000	0.0000	0.6630	-0.2829	0.3536
49.28300	0.01118	0.00000	0.07304	//	-0.0446	0.0000	-0.0699	0.0888	-0.1776	0.0000	-0.0000	-0.6078	0.6976	-0.3124
44.55188				//	0.0589	0.0000	-0.1248	-0.0213	0.0578	0.0000	-0.0000	-0.0544	0.7564	0.6340
52.99884	1.73067	-0.00000	-0.87630	//	-0.0493	0.0000	0.2165	0.3206	-0.3370	0.0000	-0.0000	0.3931	0.4939	0.5795
46.21151				//	0.1685	-0.0000	-0.1279	0.2986	0.5419	-0.0000	0.0000	-0.5462	-0.3947	0.3438

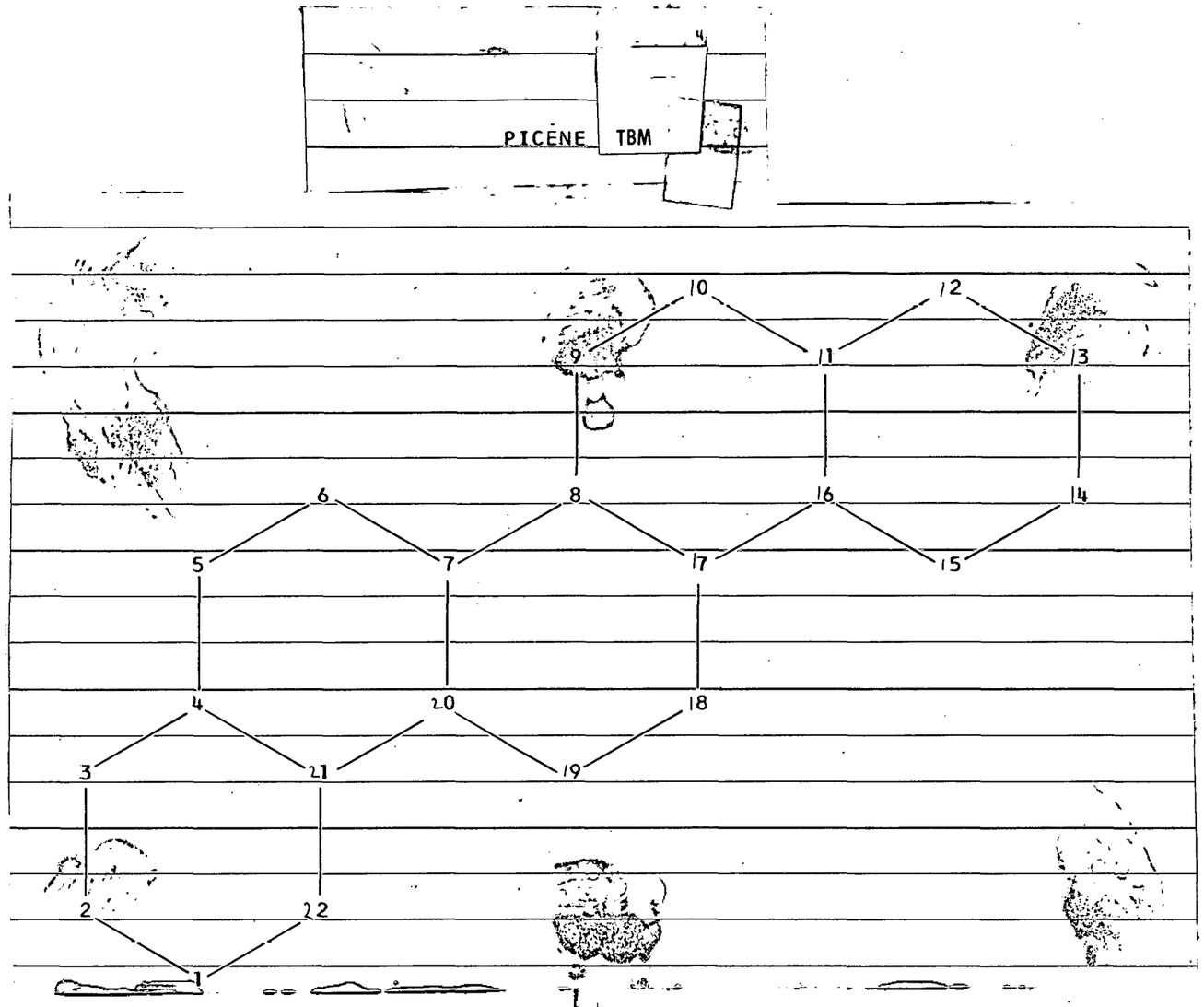
ENERGIES FOR 3,4 BENZPHENANTHRENE ,IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	8,10	9,11	7,10	9,12	6,11	4,10	8,13	5,11	6,12	7,13
XMOMNT	0.84935	0.82266	-0.10759	-0.12858	-0.18647	-0.08647	-0.28970	0.02630	0.38958	-0.44570
YMOMNT	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	-0.00000	0.00000
JUMP E	23.2261	25.3017	28.0982	33.4333	33.8973	36.0357	37.4755	39.0094	42.0289	42.3477
DIAG E	33.5362	34.9001	38.7886	44.3913	46.5138	50.9186	49.6479	52.0261	55.3379	54.7967
DIAG E	34.4594	35.4968	39.5104	44.9567	48.4626	51.0782	48.1264	53.6296	57.2555	53.0738
CORRSP	28.6541	36.4208	38.2073	44.9088	46.7994	52.5868	49.9845	48.1037	58.1759	57.0157
CORRSP	29.0895	36.7193	39.1989	45.4417	47.8257	52.2523	49.4088	57.2192	60.1188	48.7753

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
28.65412	0.01938	0.12611	-0.00000	//	0.7327	-0.5859	0.1549	0.1354	0.1371	-0.0828	-0.1405	0.0009	0.1324	0.1212
23.86787				//	0.7577	0.5393	-0.2528	0.1668	0.1300	-0.0247	0.0197	0.0445	0.1335	-0.0752
36.42076	1.43838	0.96369	-0.00000	//	0.5700	0.6721	-0.3657	0.1945	0.1740	0.0020	0.1433	0.0160	-0.0038	0.0279
28.22396				//	-0.5650	0.6535	-0.4029	0.0708	-0.1991	0.1416	0.0580	-0.0019	-0.1235	-0.0902
38.20733	0.28359	0.41778	-0.00000	//	0.1785	0.3789	0.8608	-0.2135	-0.0455	0.0571	0.0393	0.1715	0.0393	-0.0172
29.99643				//	0.0278	0.4482	0.6977	-0.4975	-0.0887	0.0961	0.0051	0.2077	-0.0235	-0.0567
44.90876	0.34893	-0.42745	-0.00000	//	-0.1848	-0.0247	0.2252	0.9056	-0.0018	0.1836	0.1622	0.1638	-0.0523	0.0694
45.67114				//	-0.1399	0.1432	0.4543	0.6455	-0.1441	-0.3969	0.1619	-0.1695	0.2702	-0.1752
46.79945	0.26187	-0.36274	-0.00000	//	-0.1640	-0.0204	0.0723	-0.0677	0.9432	0.1074	-0.1256	0.0541	-0.2029	-0.0421
35.49636				//	-0.1584	0.0660	-0.0204	-0.1345	0.7212	-0.2386	0.6063	0.0177	-0.0835	-0.0065
52.58682	0.01499	0.08188	-0.00000	//	0.0218	0.0269	-0.1719	-0.1032	-0.1324	0.5600	-0.4769	0.5638	0.0200	0.2862
40.51933				//	0.0129	-0.0136	0.1990	0.5089	0.1252	0.5248	0.1340	0.4463	-0.2797	0.3384
49.98454	0.40843	-0.43835	0.00000	//	0.1041	-0.2278	-0.0628	-0.2417	0.0011	0.4375	0.7798	0.1432	-0.2248	0.0660
48.70206				//	0.2089	-0.1270	0.0040	-0.0727	-0.4357	0.3138	0.6791	-0.3560	-0.1707	-0.1720
48.10368	0.09960	-0.22066	0.00000	//	-0.1499	-0.0064	-0.0632	-0.0618	0.1317	-0.5445	0.2606	0.5345	0.3348	0.4360
47.39979				//	0.0170	-0.0402	-0.1751	-0.1275	-0.4099	-0.3869	0.3342	0.5125	0.2506	0.4430
58.17589	0.45974	0.43109	-0.00000	//	-0.0331	-0.0354	-0.0629	0.0062	0.1149	0.2297	0.1029	0.1360	0.7536	-0.5751
56.18625				//	-0.0932	0.1015	0.0418	-0.0649	0.1311	0.3563	0.0406	-0.3999	0.6351	0.5159
57.01565	0.08912	-0.19172	-0.00000	//	-0.1028	0.0812	0.0631	-0.0250	0.1052	0.3008	0.0455	-0.5459	0.4539	-0.6087
55.66825				//	0.0921	0.1677	0.0901	0.0138	-0.0631	-0.3243	-0.0991	-0.4211	-0.5594	-0.5881



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	2.5980	3.4640	3.4640	4.3300	5.1960	6.0620	6.9280	6.9280
	6.0620	5.1960	4.3300	4.3300	3.4640	2.5980	1.7320	1.7320						
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	3.5000	4.5000	5.0000	4.5000	5.0000	4.5000	3.5000
	3.0000	3.5000	3.0000	2.0000	1.5000	2.0000	1.5000	0.5000						

PICENE

TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 S	9 A	10A	11S	12A	13 S
1.625609	1.566668	1.477902	1.385299	1.378715	1.337039	1.296571	1.246806	1.212125	1.167898	1.123882	0.876115	0.832099
0.087399	-0.169128	0.243565	-0.123959	0.334862	-0.098602	0.351138	0.000039	0.294060	-0.091189	0.221646	0.221646	0.091188
0.080917	-0.167965	0.265415	-0.024441	0.340582	0.112420	0.254025	0.316252	0.163139	0.269600	-0.041472	0.041473	0.269600
0.117711	-0.216524	0.270373	0.085809	0.187746	0.252132	-0.045902	0.316223	-0.153857	0.274604	-0.242475	-0.242475	-0.274604
0.217457	-0.329171	0.258121	0.158396	-0.052482	0.231890	-0.309168	-0.000019	-0.295364	-0.082781	-0.080236	0.080236	-0.082781
0.164447	-0.202456	0.073724	0.301467	-0.199244	0.303345	-0.176218	0.000019	0.117077	-0.196509	0.347215	0.347216	0.196508
0.199388	-0.135676	-0.115356	0.312234	-0.253247	0.182361	0.097407	0.000039	0.395972	-0.050902	0.254512	-0.254512	-0.050902
0.340954	-0.109050	-0.297087	0.185962	-0.189345	-0.054318	0.293263	0.000019	0.223246	0.161881	-0.219467	-0.219467	-0.161881
0.340955	0.109045	-0.297087	0.185930	0.189387	0.054380	0.293214	0.000020	-0.223311	-0.161913	-0.219419	0.219419	-0.161913
0.199383	0.135675	-0.115341	0.312199	0.253282	-0.182341	0.097376	-0.000026	-0.395978	0.050969	0.254534	0.254535	-0.050970
0.164450	0.202464	0.073737	0.301455	0.199266	-0.303377	-0.176192	-0.000045	-0.117028	0.196578	0.347167	-0.347167	0.196578
0.217458	0.329173	0.258118	0.158404	0.052477	-0.231942	-0.309089	-0.000019	0.295397	0.082757	-0.080279	-0.080279	-0.082756
0.117714	0.216530	0.270374	0.085835	-0.187760	-0.252161	-0.045804	0.316223	0.153807	-0.274631	-0.242435	0.242435	-0.274632
0.080919	0.167970	0.265408	-0.024406	-0.340581	-0.112402	0.254051	0.316236	-0.163206	-0.269581	-0.041408	-0.041407	0.269581
0.087401	0.169130	0.243547	-0.123942	-0.334854	0.098674	0.351092	0.000006	-0.294091	0.091248	0.221663	-0.221663	0.091248
0.140627	0.220353	0.206186	-0.169082	-0.173246	0.247142	0.167837	-0.316213	-0.089563	0.331640	0.152666	0.152665	-0.331640
0.269053	0.336790	0.155690	-0.140013	0.069020	0.238817	-0.149417	-0.316213	0.217115	0.134358	-0.145034	0.145035	0.134357
0.323912	0.223745	-0.162827	-0.207889	0.226678	0.310910	-0.038305	0.000026	-0.019216	-0.322993	-0.145188	-0.145188	0.322993
0.211042	0.067876	-0.173895	-0.370473	0.089418	0.131379	-0.189834	0.316236	-0.010320	-0.192178	0.291593	-0.291594	-0.192177
0.211046	-0.067892	-0.173894	-0.370469	-0.089460	-0.131486	-0.189804	0.316204	0.010345	0.192243	0.291542	0.291541	-0.192244
0.323910	-0.223754	-0.162815	-0.207868	-0.226689	-0.310933	-0.038236	-0.000039	0.019212	0.322955	-0.145258	0.145259	0.322955
0.269050	-0.336792	0.155706	-0.139988	-0.069042	-0.238800	-0.149389	-0.316262	-0.217068	-0.134419	-0.144996	-0.144996	0.134419
0.140619	-0.220346	0.206199	-0.169072	0.173240	-0.247068	0.167906	-0.316214	0.089595	-0.331633	0.152724	-0.152725	-0.331633

OVERLAP EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 A	17 S	18 S	19 A	20 A	21 S	22 A
0.787873	0.753192	0.703427	0.662959	0.621283	0.614699	0.522096	0.433329	0.374389
0.294061	0.000039	-0.351138	-0.098601	0.334863	0.123958	0.243565	-0.169129	-0.087399
-0.163139	-0.316252	0.254025	-0.112420	-0.340582	-0.024439	-0.265415	0.167965	0.080916
-0.153856	0.316223	0.045902	0.252132	0.187746	-0.085809	0.270373	-0.216524	-0.117711
0.295365	0.000019	-0.309168	-0.231890	0.052482	0.158396	-0.258121	0.329171	0.217456
0.117076	0.000020	0.176218	0.303345	-0.199246	-0.301466	0.073724	-0.202457	-0.164447
-0.395972	-0.000039	0.097407	-0.182361	0.253248	0.312233	0.115355	0.135676	0.199388
0.223247	0.000019	-0.293263	-0.054318	-0.189346	-0.185962	-0.297087	-0.109050	-0.340954
0.223311	-0.000020	0.293214	-0.054381	-0.189387	0.185931	0.297087	-0.109045	0.340955
-0.395978	-0.000026	-0.097376	-0.182341	0.253281	-0.312200	-0.115341	0.135675	-0.199383
0.117028	0.000046	-0.176191	0.303377	-0.199265	0.301456	-0.073737	-0.202464	0.164450
0.295397	-0.000020	0.309089	-0.231942	0.052477	-0.158404	0.258118	0.329173	-0.217458
-0.153806	-0.316223	-0.045804	0.252162	0.187760	0.085835	-0.270374	-0.216530	0.117714
-0.163206	0.316236	-0.254051	-0.112402	-0.340580	0.024407	0.265408	0.167970	-0.080920
0.294091	-0.000007	0.351092	-0.098673	0.334854	-0.123943	-0.243547	-0.169130	0.087402
-0.089562	-0.316213	-0.167837	0.247142	-0.173246	0.169082	0.206186	0.220352	-0.140627
-0.217115	0.316213	-0.149417	-0.238817	-0.069020	-0.140013	-0.155690	-0.336790	0.269054
-0.019217	0.000026	0.038305	0.310910	0.226678	0.207888	-0.162827	0.223745	-0.323912
0.010321	-0.316236	-0.189834	-0.131379	-0.089419	-0.370473	0.173895	-0.067876	0.211043
0.010346	0.316203	0.189804	-0.131487	-0.089459	0.370469	-0.173894	-0.067893	-0.211046
-0.019212	0.000039	-0.038236	0.310933	0.226688	-0.207869	0.162815	0.223755	0.323909
-0.217069	-0.316262	0.149388	-0.238799	-0.069041	0.139988	0.155706	-0.336793	-0.269050
-0.089595	0.316213	0.167906	0.247068	-0.173241	-0.169071	-0.206199	0.220346	0.140619

112

PICENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 S	9 A	10A	11 S	12 A	13 S
28.91786	27.17887	24.29810	20.89938	20.64035	18.94153	17.18745	14.87428	13.14993	10.80239	8.28263	-10.62518	-15.16200
0.068549	-0.135123	0.200351	-0.105319	0.285187	-0.085273	0.308375	0.000035	0.267093	-0.084380	0.209074	0.236799	0.099966
0.063464	-0.134193	0.218325	-0.020765	0.290058	0.097224	0.223089	0.283227	0.148178	0.249469	-0.039120	0.044308	0.295551
0.092323	-0.172988	0.222403	0.072906	0.159895	0.218050	-0.040312	0.283201	-0.139747	0.254100	-0.228721	-0.259052	-0.301036
0.170555	-0.262986	0.212325	0.134578	-0.044696	0.200544	-0.271516	-0.000017	-0.268278	-0.076600	-0.075685	0.085721	-0.090749
0.128979	-0.161749	0.060644	0.256135	-0.169687	0.262341	-0.154757	0.000017	0.106340	-0.181836	0.327521	0.370953	0.215423
0.156384	-0.108396	-0.094889	0.265282	-0.215679	0.157711	0.085545	0.000035	0.359659	-0.047102	0.240075	-0.271911	-0.055802
0.267416	-0.087124	-0.244377	0.157999	-0.161257	-0.046976	0.257548	0.000017	0.202773	0.149794	-0.207019	-0.234471	-0.177463
0.267417	0.087120	-0.244377	0.157971	0.161292	0.047029	0.257506	0.000017	-0.202832	-0.149824	-0.206973	0.234419	-0.177498
0.156379	0.108396	-0.094877	0.265253	0.215709	-0.157693	0.085517	-0.000023	-0.359664	0.047163	0.240097	0.271936	-0.055877
0.128981	0.161756	0.060655	0.256124	0.169706	-0.262368	-0.154734	-0.000041	-0.106296	0.181900	0.327475	-0.370901	0.215500
0.170556	0.262988	0.212322	0.134584	0.044692	-0.200589	-0.271447	-0.000017	0.268307	0.076578	-0.075726	-0.085768	-0.090722
0.092325	0.172994	0.222404	0.072928	-0.159906	-0.218075	-0.040226	0.283201	0.139702	-0.254125	-0.228684	0.259009	-0.301067
0.063466	0.134197	0.218319	-0.020736	-0.290057	-0.097208	0.223112	0.283212	-0.148239	-0.249452	-0.039059	-0.044238	0.295530
0.068551	0.135124	0.200336	-0.105304	-0.285180	0.085336	0.308335	0.000006	-0.267121	0.084434	0.209089	-0.236817	0.100032
0.110296	0.176047	0.169604	-0.143656	-0.147546	0.213735	0.147398	-0.283192	-0.081349	0.306877	0.144006	0.163102	-0.363563
0.211023	0.269073	0.128067	-0.118959	0.058781	0.206535	-0.131220	-0.283192	0.197204	0.124325	-0.136808	0.154950	0.147290
0.254050	0.178758	-0.133938	-0.176628	0.193051	0.268882	-0.033640	0.000023	-0.017454	-0.298876	-0.136953	-0.155113	0.354083
0.165524	0.054229	-0.143042	-0.314764	0.076153	0.113620	-0.166716	0.283212	-0.009374	-0.177828	0.275054	-0.311528	-0.210675
0.165527	-0.054242	-0.143041	-0.314761	-0.076189	-0.113712	-0.166689	0.283183	0.009397	0.177889	0.275005	0.311472	-0.210749
0.254048	-0.178765	-0.133928	-0.176610	-0.193060	-0.268902	-0.033579	-0.000035	0.017450	0.298841	-0.137019	0.155190	0.354042
0.211021	-0.269075	0.128080	-0.118937	-0.058800	-0.206520	-0.131196	-0.283235	-0.197162	-0.124382	-0.136772	-0.154908	0.147358
0.110290	-0.176042	0.169615	-0.143648	0.147540	-0.213671	0.147458	-0.283192	0.081378	-0.306870	0.144061	-0.163166	-0.363555

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 A	17 S	18 S	19 A	20 A	21 S	22 A
-20.23108	-24.62259	-31.68052	-38.20107	-45.80415	-47.09960	-68.78115	-98.26356	125.56280
0.331290	0.000045	-0.418666	-0.121099	0.424837	0.158104	0.337085	-0.256926	-0.142838
-0.183794	-0.364402	0.302877	-0.138071	-0.432093	-0.031172	-0.367325	0.255159	0.132244
-0.173336	0.364369	0.054729	0.309660	0.238191	-0.109447	0.374186	-0.328925	-0.192378
0.332760	0.000022	-0.368625	-0.284800	0.066584	0.202028	-0.357230	0.500050	0.355394
0.131899	0.000023	0.210107	0.372558	-0.252781	-0.384510	0.102032	-0.307555	-0.268759
-0.446104	-0.000045	0.116140	-0.223970	0.321294	0.398242	0.159648	0.206108	0.325865
0.251511	0.000022	-0.349661	-0.066711	-0.240221	-0.237188	-0.411158	-0.165660	-0.557229
0.251584	-0.000023	0.349603	-0.066788	-0.240273	0.237149	0.411158	-0.165652	0.557231
-0.446111	-0.000030	-0.116102	-0.223944	0.321335	-0.398201	-0.159628	0.206106	-0.325856
0.131844	0.000052	-0.210076	0.372597	-0.252806	0.384497	-0.102050	-0.307566	0.268765
0.332795	-0.000023	0.368531	-0.284864	0.066577	-0.202039	0.357226	0.500052	-0.355397
-0.173279	-0.364368	-0.054612	0.309696	0.238209	0.109480	-0.374188	-0.328934	0.192384
-0.183869	0.364384	-0.302908	-0.138048	-0.432091	0.031130	0.367315	0.255166	-0.132249
-0.331324	-0.000008	0.418611	-0.121187	0.424825	-0.158085	-0.337060	-0.256927	0.142843
-0.100901	-0.364357	-0.200115	0.303531	-0.219796	0.215659	0.285354	0.334741	-0.229830
-0.244603	0.364357	-0.178152	-0.293306	-0.087565	-0.178581	-0.215470	-0.511623	0.439721
-0.021650	0.000030	0.045671	0.381848	0.287584	0.265154	-0.225347	0.339894	-0.529378
0.011627	-0.364384	-0.226342	-0.161355	-0.113445	-0.472525	0.240664	-0.103112	0.344912
0.011656	0.364346	0.226306	-0.161487	-0.113496	0.472521	-0.240663	-0.103137	-0.344919
-0.021645	0.000045	-0.045589	0.381877	-0.287597	0.265129	0.225330	0.339909	-0.529373
-0.244551	-0.364413	0.178118	-0.293285	-0.087591	0.178549	0.215492	-0.511627	-0.439715
-0.100938	0.364357	0.200197	0.303440	-0.219789	-0.215645	-0.285372	0.334731	0.229817

PICENE

TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.00000	0.61905	-0.00000	-0.25636	0.00000	0.16497	-0.00000	-0.04514	-0.00000	0.04021	0.00000	-0.01733	-0.00000	0.01894	0.00000
	-0.02327	0.00000	0.07999	-0.00000	-0.12482	0.00000	0.70499								
2	0.61905	1.00000	0.71036	0.00000	-0.13456	0.00000	0.11116	-0.00000	-0.03164	0.00000	0.02810	-0.00000	-0.02460	0.00000	0.02621
	0.00000	-0.06253	0.00000	0.07868	-0.00000	-0.26175	-0.00000								
3	-0.00000	0.71036	1.00000	0.57043	-0.00000	-0.18838	0.00000	0.06214	0.00000	-0.04375	-0.00000	0.02083	0.00000	-0.01733	-0.00000
	0.01504	0.00000	-0.06384	-0.00000	0.05291	0.00000	-0.34770								
4	-0.25636	0.00000	0.57043	1.00000	0.51658	0.00000	-0.18449	0.00000	0.05002	-0.00000	-0.03598	0.00000	0.02810	0.00000	-0.02849
	0.00000	0.07587	0.00000	-0.08961	-0.00000	0.53740	0.00000								
5	0.00000	-0.13456	-0.00000	0.51658	1.00000	0.75845	-0.00000	-0.15056	-0.00000	0.09979	-0.00000	-0.04376	-0.00000	0.04021	0.00000
	-0.04199	0.00000	0.17951	0.00000	-0.26034	-0.		0.04319							
6	0.16497	0.00000	-0.18838	0.00000	0.75845	1.00000	0.53205	0.00000	-0.10078	-0.00000	0.05002	0.00000	-0.03164	-0.00000	0.02671
	0.00000	-0.08892	-0.00000	0.00878	0.00000	-0.23794	-0.00000								
7	-0.00000	0.11116	0.00000	-0.18449	-0.00000	0.53205	1.00000	0.49292	-0.00000	-0.15055	-0.00000	0.06214	0.00000	-0.04514	-0.00000
	0.02980	-0.00000	-0.25964	-0.00000	0.56320	-0.00000	-0.11615								
8	-0.04514	-0.00000	0.06214	0.00000	-0.15056	0.00000	0.49292	1.00000	0.53203	-0.00000	-0.18449	0.00000	0.11116	-0.00000	-0.11615
	-0.00000	0.56322	0.00000	-0.25963	-0.00000	0.02981	0.00000								
9	-0.00000	-0.03164	0.00000	0.05002	-0.00000	-0.10078	-0.00000	0.53203	1.00000	0.75845	-0.00000	-0.18839	0.00000	0.16499	0.00000
	-0.23796	-0.00000	0.00879	0.00000	-0.08891	0.00000	0.02671								
10	0.04021	0.00000	-0.04375	-0.00000	0.09979	-0.00000	-0.15055	-0.00000	0.75845	1.00000	0.51660	-0.00000	-0.13457	0.00000	0.04318
	0.00000	-0.26032	0.	0.17949	0.00000	-0.04199	-0.00000								
11	0.00000	0.02810	-0.00000	-0.03598	-0.00000	0.05002	-0.00000	-0.18449	-0.00000	0.51660	1.00000	0.57043	0.00000	-0.25637	-0.00000
	0.53739	0.00000	-0.08961	-0.00000	0.07587	0.00000	-0.02849								
12	-0.01733	-0.00000	0.02083	0.00000	-0.04376	0.00000	0.06214	0.00000	-0.18839	-0.00000	0.57043	1.00000	0.71038	0.00000	-0.34767
	-0.00000	0.05291	0.00000	-0.06384	-0.00000	0.01504	0.00000								
13	-0.00000	-0.02460	0.00000	0.02810	-0.00000	-0.03164	0.00000	0.11116	0.00000	-0.13457	0.00000	0.71038	1.00000	0.61903	0.00000
	-0.26175	-0.00000	0.07868	0.00000	-0.06253	-0.00000	0.02621								
14	0.01894	0.00000	-0.01733	0.00000	0.04021	-0.00000	-0.04514	-0.00000	0.16499	0.00000	-0.25637	0.00000	0.61903	1.00000	0.70499
	-0.00000	-0.12483	-0.00000	0.07999	0.00000	-0.02327	-0.00000								
15	0.00000	0.02621	-0.00000	-0.02849	0.00000	0.02671	-0.00000	-0.11615	0.00000	0.04318	-0.00000	-0.34767	0.00000	0.70499	1.00000
	0.58554	0.00000	-0.12351	-0.00000	0.07411	0.00000	-0.03054								
16	-0.02327	0.00000	0.01504	0.00000	-0.04199	0.00000	0.02980	-0.00000	-0.23796	0.00000	0.53739	-0.00000	-0.26175	-0.00000	0.58554
	1.00000	0.47072	-0.00000	-0.12940	0.00000	0.03835	-0.00000								
17	0.00000	-0.06253	0.00000	0.07587	0.00000	-0.08892	-0.00000	0.56322	-0.00000	-0.26032	0.00000	0.05291	-0.00000	-0.12483	0.00000
	0.47072	1.00000	0.55442	0.00000	-0.21121	-0.00000	0.07411								
18	0.07999	0.00000	-0.06384	0.00000	0.17951	-0.00000	-0.25964	0.00000	0.00879	0.	-0.08961	0.00000	0.07868	-0.00000	-0.12351
	-0.00000	0.55442	1.00000	0.73226	0.00000	-0.12941	-0.00000								
19	-0.00000	0.07868	-0.00000	-0.08961	0.00000	0.00878	-0.00000	-0.25963	0.00000	0.17949	-0.00000	-0.06384	0.00000	0.07999	-0.00000
	-0.12940	0.00000	0.73226	1.00000	0.55443	0.00000	-0.12351								
20	-0.12482	-0.00000	0.05291	-0.00000	-0.26034	0.00000	0.56320	-0.00000	-0.08891	0.00000	0.07587	-0.00000	-0.06253	0.00000	0.07411
	0.00000	-0.21121	0.00000	0.55443	1.00000	0.47072	0.00000								
21	0.00000	-0.26175	0.00000	0.53740	-0.	-0.23794	0.00000	0.02981	0.00000	-0.04199	0.00000	0.01504	-0.00000	-0.02327	0.00000
	-0.03835	-0.00000	-0.12941	0.00000	0.47072	1.00000	0.58553								
22	-0.70499	-0.00000	-0.34770	0.00000	0.04319	-0.00000	-0.11615	0.00000	0.02671	-0.00000	-0.02849	0.00000	0.02621	-0.00000	-0.03054
	-0.00000	0.07411	-0.00000	-0.12351	0.00000	0.58553	1.00000								

PICENE

TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.76012	0.44399	-0.05084	-0.23800	0.01921	0.16014	0.00036	-0.04490	0.00124	0.03989	0.00007	-0.01725	-0.00038	0.01878	0.00102
	-0.02290	-0.00259	0.07829	0.00948	-0.11670	-0.04275	0.52793								
2	0.44399	0.75885	0.53308	-0.04054	-0.12568	0.00453	0.10733	-0.00376	-0.03091	0.00081	0.02763	-0.00082	-0.02430	-0.00038	0.02583
	0.00190	-0.06118	-0.00364	0.07593	0.01479	-0.24317	-0.04957								
3	-0.05084	0.53308	0.76915	0.40227	-0.05522	-0.17850	0.01520	0.06014	-0.00419	-0.04317	0.00183	0.02058	-0.00082	-0.01725	0.00051
	0.01518	-0.00291	-0.06354	0.00167	0.05679	-0.03257	-0.32711								
4	-0.23800	-0.04054	0.40227	0.72190	0.34942	-0.04455	-0.16890	0.01186	0.04787	-0.00317	-0.03503	0.00183	0.02763	0.00007	-0.02790
	-0.00248	0.07296	0.00240	-0.08268	-0.03049	0.37511	-0.03384								
5	0.01921	-0.12568	-0.05522	0.34942	0.77058	0.58014	-0.04813	-0.14191	0.01086	0.09790	-0.00317	-0.04317	0.00081	0.03989	0.00049
	-0.04188	0.00222	0.17479	0.01690	-0.24325	-0.03801	0.04783								
6	0.16014	0.00453	-0.17850	-0.04455	0.58014	0.76700	0.36389	-0.04691	-0.09188	0.01086	0.04788	-0.00419	-0.03091	0.00124	0.02590
	0.00202	-0.08197	0.01672	0.01422	-0.03875	-0.22110	0.01504								
7	0.00036	0.10733	0.01520	-0.16890	-0.04813	0.36389	0.72948	0.33196	-0.04690	-0.14190	0.01186	0.06014	-0.00376	-0.04490	0.00277
	0.03370	-0.03039	-0.24253	-0.03892	0.40024	-0.03025	-0.10877								
8	-0.04490	-0.00376	0.06014	0.01186	-0.14191	-0.04691	0.33196	0.72948	0.36388	-0.04812	-0.16890	0.01520	0.10733	0.00036	-0.10877
	-0.03026	0.40025	-0.03892	-0.24252	-0.03039	0.03370	0.00276								
9	0.00124	-0.03091	-0.00419	0.04787	0.01086	-0.09188	-0.04690	0.36388	0.76701	0.58014	-0.04456	-0.17851	0.00453	0.16016	0.01504
	-0.22111	-0.03875	0.01422	0.01672	-0.08196	0.00202	0.02591								
10	0.03989	0.00081	-0.04317	-0.00317	0.09790	0.01086	-0.14190	-0.04812	0.58014	0.77057	0.34943	-0.05522	-0.12568	0.01921	0.04782
	-0.03801	-0.24324	0.01690	0.17477	0.00222	-0.04188	0.00049								
11	0.00007	0.02763	0.00183	-0.03503	-0.00317	0.04788	0.01186	-0.16890	-0.04456	0.34943	0.72190	0.40226	-0.04054	-0.23801	-0.03384
	0.37510	-0.03049	-0.08268	0.00240	0.07296	-0.00248	-0.02790								
12	-0.01725	-0.00082	0.02058	0.00183	-0.04317	-0.00419	0.06014	0.01520	-0.17851	-0.05522	0.40226	0.76915	0.53309	-0.05084	-0.32709
	-0.03256	0.05679	0.00167	-0.06354	-0.00291	0.01519	0.00051								
13	-0.00038	-0.02430	-0.00082	0.02763	0.00081	-0.03091	-0.00376	0.10733	0.00453	-0.12568	-0.04054	0.53309	0.75885	0.44398	-0.04956
	-0.24316	0.01479	0.07593	-0.00364	-0.06118	0.00190	0.02583								
14	0.01878	-0.00038	-0.01725	0.00007	0.03989	0.00124	-0.04490	0.00036	0.16016	0.01921	-0.23801	-0.05084	0.44398	0.76012	0.52794
	-0.04276	-0.11671	0.00948	0.07829	-0.00259	-0.02290	0.00102								
15	0.00102	0.02583	0.00051	-0.02790	0.00049	0.02590	0.00277	-0.10877	0.01504	0.04782	-0.03384	-0.32709	-0.04956	0.52794	0.76693
	0.41638	-0.04770	-0.11433	0.01053	0.07167	-0.00341	-0.02995								
16	-0.02290	0.00190	0.01518	-0.00248	-0.04188	0.00202	0.03370	-0.03026	-0.22111	-0.03801	0.37510	-0.03256	-0.24316	-0.04276	0.41638
	0.72815	0.30999	-0.04665	-0.12096	0.01247	0.03673	-0.00341								
17	-0.00259	-0.06118	-0.00291	0.07296	0.00222	-0.08197	-0.03039	0.40025	-0.03875	-0.24324	-0.03049	0.05679	0.01479	-0.11671	-0.04770
	0.30999	0.72944	0.38602	-0.04711	-0.19516	0.01247	0.07167								
18	0.07829	-0.00364	-0.06354	0.00240	0.17479	0.01672	-0.24253	-0.03892	0.01422	0.01690	-0.08268	0.00167	0.07593	0.00948	-0.11433
	-0.04665	0.38602	0.76791	0.55436	-0.04711	-0.12097	0.01053								
19	0.00948	0.07593	0.00167	-0.08268	0.01690	0.01422	-0.03892	-0.24252	0.01672	0.17477	0.00240	-0.06354	-0.00364	0.07829	0.01053
	-0.12096	-0.04711	0.55436	0.76790	0.38603	-0.04665	-0.11434								
20	-0.11670	0.01479	0.05679	-0.03049	-0.24325	-0.03875	0.40024	-0.03039	-0.08196	0.00222	0.07296	-0.00291	-0.06118	-0.00259	0.07167
	0.01247	-0.19516	-0.04711	0.38603	0.72944	0.30999	-0.04770								
21	-0.04275	-0.24317	-0.03257	0.37511	-0.03801	-0.22110	-0.03025	0.03370	0.00202	-0.04188	-0.00248	0.01519	0.00190	-0.02290	-0.00341
	0.03673	0.01247	-0.12097	-0.04665	0.30999	0.72815	0.41638								
22	0.52793	-0.04957	-0.32711	-0.03384	0.04783	0.01504	-0.10877	0.00276	0.02591	0.00049	-0.02790	0.00051	0.02583	0.00102	-0.02995
	-0.00341	0.07167	0.01053	-0.11434	-0.04770	0.41638	0.76694								

ENERGIES FOR PICENE , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	11,12	10,12	11,13	9,12	8,12	7,12	6,12	8,13	5,12	4,12
XMOMNT	-0.97805	0.26736	-0.26761	0.18436	-0.07494	-0.10253	-0.09711	0.11570	0.03491	0.01928
YMOMNT	-0.56450	-0.46349	0.46393	-0.31953	-0.04327	-0.05924	0.16821	-0.20044	-0.06048	0.01112
JUMP E	18.9078	21.4276	23.4446	23.7751	25.4995	27.8126	29.5667	30.0363	31.2655	31.5246
DIAG E	30.3609	34.2098	35.9036	37.1062	40.5087	42.8125	43.8130	46.0786	48.9124	45.7357
DIAG E	30.4468	34.5090	35.7270	37.5052	40.6352	43.2751	44.2888	45.9425	49.0488	45.9537
CORRSP	30.2446	30.2877	35.8900	39.0268	40.4158	41.9682	42.4238	48.7561	49.6392	46.7891
CORRSP	30.3615	30.7430	35.8298	39.2637	40.6491	42.3290	42.8315	48.6905	49.6628	46.9711

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
30.28766	0.10509	0.14465	-0.24631	//	-0.0019	0.7091	-0.5398	0.3775	-0.0002	0.0001	-0.1089	0.1888	-0.1259	-0.0000
24.30108				//	0.0001	0.7651	-0.5782	-0.1767	0.0000	-0.0000	-0.1825	0.1240	-0.0212	0.0000
35.89003	0.29602	-0.22007	0.38148	//	0.0000	-0.6258	0.4952	0.5710	-0.0001	0.0000	0.0354	-0.1894	-0.0039	-0.0000
34.23764				//	-0.0000	0.3052	0.6367	-0.5679	0.0000	-0.0001	0.0604	0.3909	0.1498	-0.0000
39.02678	0.69617	0.32365	-0.56101	//	-0.0000	0.1608	-0.6658	0.7027	0.0001	0.0001	0.0753	-0.1369	-0.1124	0.0000
27.56178				//	-0.0000	0.4475	0.4063	0.7580	0.0000	-0.0001	-0.0135	0.1624	-0.1833	0.0000
42.42380	0.00411	-0.02392	0.04129	//	0.0000	-0.0216	0.0283	0.0602	-0.0004	0.0005	0.8572	0.4832	0.1636	0.0003
36.51182				//	0.0003	-0.0965	-0.2855	0.1331	-0.0014	0.0011	0.7422	-0.5687	0.1314	0.0010
48.75612	0.20751	0.15817	-0.27398	//	-0.0000	-0.2066	-0.1341	0.1709	0.0000	-0.0000	-0.4961	0.7476	0.3241	0.0001
44.30867				//	-0.0000	-0.1995	-0.0844	0.2133	-0.0000	-0.0001	-0.5491	0.4426	-0.6404	0.0002
49.63923	0.01696	0.04481	-0.07763	//	-0.0000	0.1913	0.0370	0.0693	-0.0000	-0.0001	0.0168	-0.3424	0.9164	0.0000
47.69269				//	-0.0000	0.2686	0.0813	0.0921	-0.0000	-0.0001	0.3323	-0.5350	0.7184	-0.0000

ENERGIES FOR PICENE TBM APPROXIMATION 1.7

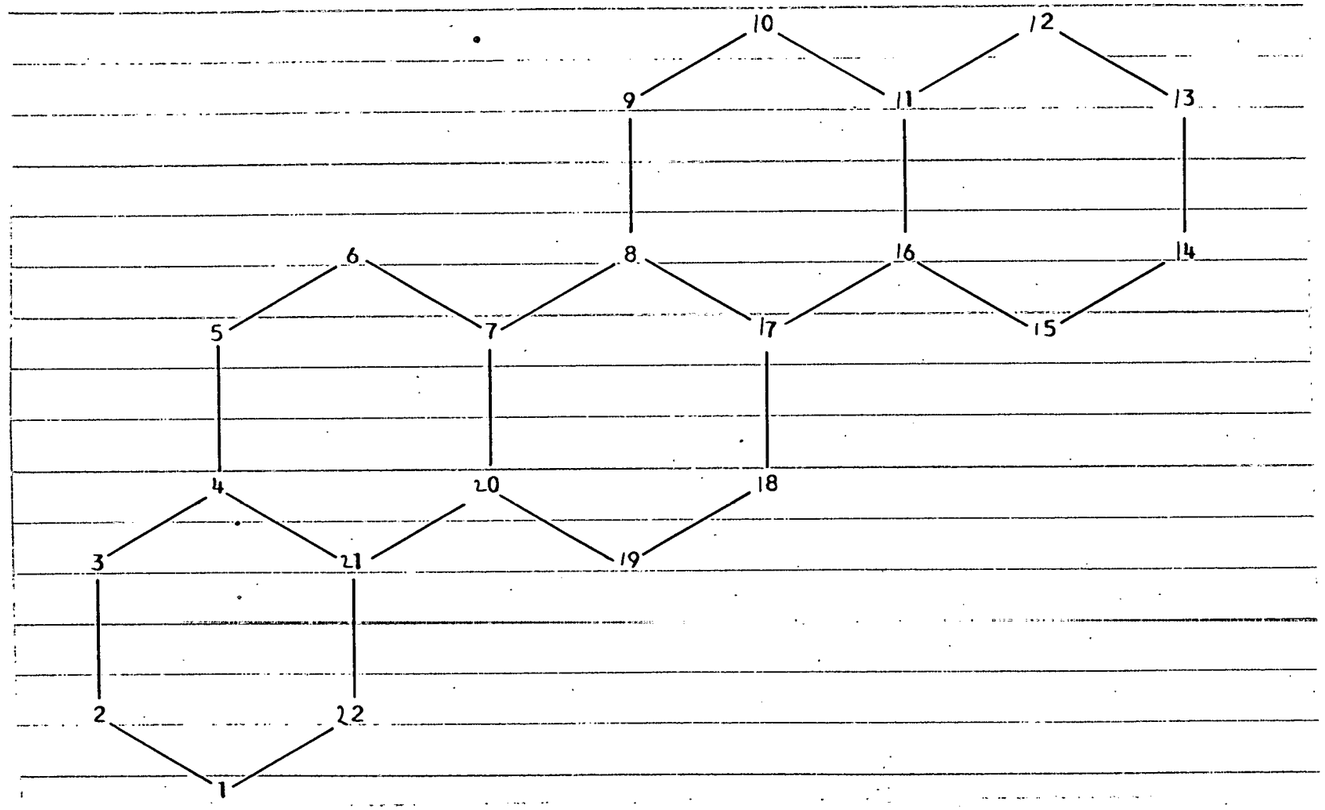
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	11,12	8,12	10,13	7,12	9,13	10,14	4,12	9,14	6,13	3,12
XMOMNT	-0.97805	-0.07494	-0.44222	-0.10253	-0.63320	0.63425	0.01928	-0.05372	0.05943	0.00791
YMOMNT	-0.56450	-0.04327	-0.25523	-0.05924	-0.36546	0.36607	0.01112	-0.03095	0.03426	0.00457
JUMP E	18.9078	25.4995	25.9644	27.8126	28.3119	31.0335	31.5246	33.3810	34.1035	34.9233
DIAG E	30.3609	40.5087	39.9750	42.8125	41.5975	44.0142	45.7357	47.9915	50.2180	52.0026
DIAG E	30.4468	40.6352	40.0116	43.2751	41.7339	43.9094	45.9537	47.9865	50.4311	52.4572
CORRSP	28.6257	39.6929	40.3000	43.2192	35.2848	46.8329	44.8591	49.9543	52.9329	53.5146
CORRSP	28.7340	40.3899	39.6776	43.3044	35.7431	47.1917	44.9969	50.1063	53.0065	53.6898

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
28.62569	0.96795	-0.77231	-0.44575	//	0.9357	0.0641	-0.2872	-0.0112	-0.0114	0.0275	0.0111	0.1785	0.0676	0.0196
19.04519				//	0.9354	0.0320	-0.2373	-0.0530	0.1194	-0.1115	0.0519	0.1820	0.0471	-0.0158
39.69291	0.24360	-0.32903	-0.18989	//	0.1577	0.5050	0.6007	-0.5138	-0.1967	-0.0980	-0.0459	-0.1255	0.1146	0.1261
34.36437				//	-0.1202	0.3971	-0.5137	0.1790	-0.2369	0.5412	0.1257	0.3320	0.2208	-0.0905
40.30002	2.13756	-0.96727	-0.55828	//	0.2619	-0.4253	0.6157	0.2730	0.3281	-0.3485	-0.0302	-0.0371	-0.2552	-0.0201
29.52577				//	0.1262	0.5944	0.6839	0.2292	0.2271	0.1390	0.0162	0.1403	0.0316	-0.1366
43.21917	0.06400	0.16163	0.09326	//	-0.0080	0.0910	0.1803	0.4232	-0.5971	-0.1480	0.5565	0.2645	0.0686	-0.1316
31.90632				//	-0.0868	-0.3704	-0.0951	0.7184	0.3586	-0.1010	0.1609	0.3178	-0.1907	-0.1676
35.28481	0.10524	-0.22935	-0.13241	//	0.0080	0.5582	0.1723	0.4249	0.5089	0.4111	0.1242	0.0293	0.0363	-0.1803
38.89546				//	-0.0523	0.1869	-0.3230	-0.0215	0.7236	0.1897	-0.1087	-0.5306	0.0572	-0.0368
46.83288	0.30512	0.33899	0.19568	//	0.0315	-0.4178	0.2450	-0.2788	0.0257	0.6857	0.3616	0.2012	0.0294	0.2090
45.31594				//	0.0840	-0.4368	0.2561	-0.2619	0.2060	0.7092	0.1413	0.1689	-0.1104	0.2487
44.85911	0.23036	-0.30096	-0.17373	//	-0.0124	-0.0444	-0.1516	-0.1568	0.3811	-0.3379	0.6175	-0.3158	0.4430	0.1165
38.72766				//	-0.0587	-0.0218	0.0672	-0.0388	0.0683	-0.1703	0.8364	-0.1385	0.4702	0.1283
49.95431	0.14371	-0.22529	-0.12998	//	-0.1711	0.0900	-0.0085	-0.1910	0.2896	-0.2923	-0.0319	0.8587	0.0920	0.1000
46.92426				//	-0.2445	0.0574	-0.0585	-0.3147	0.4002	-0.2806	-0.2391	0.6051	0.3296	0.2523
52.93292	0.00897	-0.05468	0.03152	//	-0.0028	-0.1372	0.1512	0.3414	-0.0907	0.0737	-0.3871	0.0136	0.7570	0.3241
49.83374				//	0.1103	-0.1452	0.1043	0.4636	-0.1366	-0.0939	0.3621	-0.2013	0.5295	0.5113
53.51456	0.00014	-0.00685	-0.00396	//	-0.0225	-0.1916	-0.0971	0.2152	-0.0052	-0.0449	-0.0937	-0.0503	-0.3641	0.8724
51.68855				//	-0.0448	0.3165	-0.1198	0.1094	0.0045	-0.0979	-0.1888	0.0083	-0.5349	0.7349

PICENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	2.5980	3.4640	3.4640	4.3300	5.1960	6.0620	6.9280	6.9280
	6.0620	5.1960	4.3300	4.3300	3.4640	2.5980	1.7320	1.7320						
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	3.5000	4.5000	5.0000	4.5000	5.0000	4.5000	3.5000
	3.0000	3.5000	3.0000	2.0000	1.5000	2.0000	1.5000	0.5000						

PICENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 S	9 A	10 A	11 S	12 A	13 S
1.781779	1.677703	1.531158	1.390336	1.383517	1.299204	1.241426	1.186781	1.134703	1.080903	1.049824	0.814585	0.789118
0.097273	-0.186411	-0.262361	0.129062	0.331612	-0.071938	0.334422	-0.018500	-0.311591	0.051504	0.221876	0.220004	-0.122385
0.091554	-0.185790	-0.281427	0.036286	0.325780	0.151535	-0.234644	0.316363	-0.117359	-0.290921	-0.029281	0.042780	-0.261947
0.124612	-0.226276	-0.272818	-0.080088	0.164992	0.278029	-0.071268	0.324531	0.214005	-0.219946	-0.225007	-0.232293	0.299650
0.218991	-0.320639	-0.228628	-0.164981	-0.083809	0.208612	-0.312539	-0.002136	0.278622	0.146422	-0.081256	0.082074	0.047121
0.172196	-0.205759	-0.053466	-0.307746	-0.246079	0.273627	-0.180401	-0.007776	-0.145406	0.182150	0.343942	0.345234	-0.198813
0.205906	-0.139279	0.120982	-0.316439	-0.275110	0.148067	0.127161	-0.007588	-0.393758	-0.026389	0.247670	-0.267800	0.098458
0.329250	-0.105936	0.283559	-0.162122	-0.180435	-0.062920	0.312510	0.020809	-0.176783	-0.203660	-0.233163	-0.213188	0.134405
0.329251	0.105931	0.283556	-0.162093	0.180477	0.062998	0.312457	0.020810	0.176867	0.203743	-0.233068	0.213107	0.134478
0.205902	0.139281	0.120963	-0.316404	0.275152	-0.148038	0.127114	-0.007657	0.393775	0.026277	0.247721	0.267808	0.098576
0.172197	0.205766	-0.053484	-0.307727	0.246100	-0.273668	-0.180378	-0.007844	0.145341	-0.182284	0.343859	-0.345155	-0.198951
0.218993	0.320641	-0.228628	-0.164983	0.083804	-0.208677	-0.312449	-0.002135	-0.278667	-0.146383	-0.081342	-0.082131	0.047085
0.124616	0.226281	-0.272817	-0.080112	-0.165008	-0.278074	-0.071144	0.324524	-0.213952	0.220019	-0.224945	0.232192	0.299712
0.091558	0.185795	-0.281416	0.036252	-0.325786	-0.151520	-0.234680	0.316340	0.117436	-0.290911	-0.029162	-0.042649	-0.261928
0.097277	0.186414	-0.262341	0.129046	-0.331615	0.072023	0.334365	-0.018538	0.311629	-0.051604	0.221895	-0.219999	-0.122486
0.148343	0.228751	-0.211040	-0.173104	-0.180464	0.255524	0.144478	-0.331698	0.127974	-0.309424	0.133480	0.160661	0.338731
0.263162	0.323180	-0.138469	0.116099	0.063253	0.252182	-0.160128	-0.313968	-0.197717	-0.143353	-0.162214	0.140494	-0.122655
0.315256	0.206609	0.168150	0.198780	-0.197966	0.315396	-0.040273	-0.008928	-0.044265	0.334349	-0.155959	-0.139685	-0.311164
0.218108	0.065551	0.188109	0.379926	0.071169	0.147935	-0.189489	0.291574	-0.028501	0.198507	0.300458	-0.296174	0.174432
0.218110	-0.065571	0.188106	0.379921	-0.071205	-0.148060	-0.189455	0.291528	0.028469	-0.198631	0.300366	0.296092	0.174571
0.315253	-0.206621	0.168140	0.198760	-0.197974	-0.315417	-0.040203	-0.009006	0.044268	-0.334281	-0.156091	0.139820	-0.311099
0.263157	-0.323183	-0.138484	0.116074	-0.063274	-0.252164	-0.160093	-0.314027	0.197660	0.143441	-0.162148	-0.140423	-0.122752
0.148335	-0.228746	-0.211059	0.173094	0.180453	-0.255438	0.144571	-0.331707	-0.128016	0.309394	0.133588	-0.160792	0.338696

OVERLAP EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 A	17 S	18 S	19 A	20 A	21 S	22 A
0.753619	0.730706	0.689512	0.662075	0.627811	0.623677	0.562456	0.510586	0.478495
0.289295	0.052412	0.354720	-0.135557	0.319676	0.117278	0.230999	0.156218	-0.079207
-0.206557	0.267128	-0.312322	-0.055660	-0.342318	0.025707	0.247465	-0.153417	0.073122
-0.101273	-0.325930	0.027980	0.226822	0.223324	0.087218	-0.264437	0.203065	-0.107656
0.287515	0.064843	0.286070	-0.267052	0.003682	-0.175651	0.277046	-0.334754	0.217215
0.114591	-0.035257	-0.171405	0.324683	-0.160118	0.296975	-0.075571	0.195371	-0.155554
-0.385655	-0.028438	-0.091209	-0.192094	0.228950	-0.310002	-0.113848	-0.132371	0.193244
0.240685	0.041608	0.284011	-0.034142	-0.203932	0.184998	0.307840	0.117080	-0.350269
0.240747	-0.041602	-0.283977	-0.034177	-0.203967	-0.184963	-0.307842	0.117074	0.350270
-0.385635	0.028492	0.091171	-0.192078	0.228982	0.309968	0.113841	-0.132366	-0.193240
0.114535	0.035196	0.171407	0.324703	-0.160147	-0.296970	-0.075575	0.195376	0.155559
0.287530	-0.064835	-0.286018	-0.267076	0.003692	0.175663	-0.277039	-0.334756	-0.217217
-0.101215	0.325935	-0.028040	-0.226837	0.223330	-0.087248	0.264440	0.203071	-0.107659
-0.206617	-0.267123	0.312326	-0.055658	-0.342316	-0.025666	-0.247461	-0.153419	-0.073123
0.289306	-0.052441	-0.354678	-0.135586	0.319669	0.117247	0.230988	0.156217	0.079206
-0.052598	0.324095	0.129065	0.256622	-0.160875	-0.170835	-0.207472	-0.213376	-0.134024
-0.237293	-0.295385	0.189559	-0.216913	-0.074748	0.135122	0.182048	0.351525	0.272019
-0.039684	-0.008146	-0.056951	0.287449	0.265329	-0.216618	0.155349	-0.235318	-0.333199
0.016500	0.345434	0.140898	-0.129336	-0.095913	0.366423	-0.158001	0.069910	0.205910
0.016530	-0.345406	-0.140888	-0.129400	-0.095968	-0.366422	0.158002	0.069916	-0.205914
-0.039673	0.008084	0.056926	-0.287465	0.265348	0.216595	-0.155341	-0.235322	0.333198
-0.237263	0.295420	-0.189561	0.216891	-0.074765	-0.135100	-0.182058	0.351526	-0.272018
-0.052633	0.324083	-0.129101	0.256578	-0.160863	0.170836	0.207475	-0.213369	0.134019

PICENE IRM APPROXIMATION 5.80

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 S	9 A	10 A	11 S	12 A	13 S
32.96928	30.35314	26.06651	21.09590	20.82953	17.30492	14.61310	11.82612	8.92023	5.62417	3.56619	-17.10364	-20.08056
0.072872	-0.143918	-0.212026	0.109456	0.281928	-0.063114	0.300147	-0.016981	-0.292512	0.049539	0.216547	0.243760	-0.137771
0.068588	-0.143439	-0.227434	0.030774	0.276970	0.132946	0.210595	0.290403	-0.110173	-0.279822	-0.028577	0.047399	-0.294878
0.093354	-0.174695	-0.220477	-0.067922	0.140272	0.243922	-0.063964	0.297901	0.200901	-0.211554	-0.219603	-0.257376	0.337321
0.164059	-0.247548	-0.184765	-0.139918	-0.071253	0.183021	-0.280507	-0.001961	0.261562	0.140836	-0.079304	0.090936	0.053044
0.129002	-0.158855	-0.043208	-0.260995	-0.209210	0.240060	-0.161912	-0.007138	-0.136503	0.175201	0.335681	0.382512	-0.223807
0.154256	-0.107530	0.097771	-0.268367	-0.233891	0.129903	0.114128	-0.006965	-0.369648	-0.025382	0.241721	-0.296717	0.110836
0.246660	-0.081787	0.229157	-0.137494	-0.153401	-0.055201	0.280481	0.019102	-0.165959	-0.195890	-0.227563	-0.236208	0.151302
0.246661	0.081783	0.229155	-0.137469	0.153437	0.055270	0.280434	0.019103	0.166038	0.195970	-0.227470	0.236118	0.151384
0.154253	0.107531	0.097756	-0.268338	0.233927	-0.129877	0.114086	-0.007029	0.369664	0.025275	0.241771	0.296726	0.110968
0.129003	0.158861	-0.043223	-0.260979	0.209228	-0.240096	-0.161891	-0.007201	0.136442	-0.175330	0.335600	-0.382425	-0.223962
0.164061	0.247549	-0.184765	-0.139920	0.071248	-0.183078	-0.280426	-0.001960	-0.261604	-0.140798	-0.079389	-0.090999	0.053004
0.093357	0.174699	-0.220476	-0.067942	-0.140286	-0.243962	-0.063853	0.297894	-0.200851	0.211625	-0.219542	0.257264	0.337390
0.068591	0.143442	-0.227425	0.030745	-0.276975	-0.132933	0.210628	0.290381	0.110246	0.279812	-0.028462	-0.047254	-0.294857
0.072876	0.143920	-0.212010	0.109442	-0.281930	0.063188	0.300096	-0.017017	0.292548	-0.049635	0.216566	-0.243754	-0.137884
0.111133	0.176606	-0.170551	0.146807	-0.153426	0.224178	0.129670	-0.304479	0.120138	-0.297619	0.130274	0.178009	0.381315
0.197149	0.249509	-0.111903	0.098462	0.053776	0.221246	-0.143717	-0.288204	-0.185611	-0.137883	-0.158318	0.155665	-0.138075
0.236176	0.159511	0.135890	0.168583	0.168306	0.276705	-0.036146	-0.008196	-0.041554	0.321593	-0.152213	-0.154769	-0.350282
0.163398	0.050608	0.152020	0.322210	0.060506	0.129787	-0.170069	0.267648	-0.026756	0.190934	0.293242	-0.328155	0.196361
0.163399	-0.050624	0.152017	0.322206	-0.060536	-0.129897	-0.170038	0.267606	0.026726	-0.191053	0.293152	0.328064	0.196517
0.236174	-0.159521	0.135882	0.168565	-0.168312	-0.276724	-0.036083	-0.008267	0.041557	-0.321527	-0.152342	0.154918	-0.350209
0.197146	-0.249512	-0.111915	0.098441	-0.053794	-0.221230	-0.143685	-0.288258	0.185557	0.137968	-0.158254	-0.155585	-0.138184
0.111126	-0.176602	-0.170566	0.146799	0.153416	-0.224103	0.129754	-0.304487	-0.120177	0.297591	0.130379	-0.178154	0.381275

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 A	17 S	18 S	19 A	20 A	21 S	22 A
-24.56596	-27.69264	-33.83631	-38.35238	-44.54658	-45.33993	-58.45366	-72.02572	-81.89559
0.333246	0.061314	0.427183	-0.166597	0.403455	-0.148503	-0.308011	0.218623	-0.114504
-0.237938	0.312498	-0.376125	-0.068406	-0.432031	0.032552	0.329966	-0.214703	0.105709
-0.116659	-0.381289	0.033696	0.278761	0.281852	0.110439	-0.352597	0.284185	-0.155632
0.331196	0.075856	0.344510	-0.328203	0.004647	-0.222419	0.369408	-0.468481	0.314016
0.132001	-0.041245	-0.206421	0.399030	-0.202081	0.376045	-0.100766	0.273418	-0.224876
-0.444245	-0.033269	-0.109842	-0.236080	0.288952	-0.392541	-0.151803	-0.185250	0.279362
0.277251	0.048674	0.342030	-0.041960	-0.257378	0.234254	0.410469	0.163851	-0.506365
0.277322	-0.048667	-0.341989	-0.042003	-0.257422	-0.234210	-0.410472	0.163842	0.506366
-0.444222	0.033331	0.109796	-0.236061	0.288993	0.392498	0.151794	-0.185243	-0.279357
0.131936	0.041174	0.206422	0.399055	-0.202118	-0.376038	0.100771	0.273425	0.224883
0.331213	-0.075847	-0.344447	-0.328233	0.004660	0.222434	-0.369400	-0.468483	-0.314019
-0.116592	0.381294	-0.033768	0.278780	0.281860	-0.110478	0.352601	0.284194	0.155637
-0.238007	-0.312492	0.376129	-0.068403	-0.432029	-0.032500	-0.329961	-0.214706	-0.105710
0.333258	-0.061348	-0.427133	-0.166634	0.403447	0.148465	0.307996	0.218622	0.114503
-0.060589	0.379141	0.155431	0.315384	-0.203036	-0.216320	-0.276641	-0.298615	-0.193750
-0.273344	-0.345555	0.228283	-0.266583	-0.094337	0.171099	0.242740	0.491952	0.393242
-0.045714	-0.009529	-0.068586	0.353271	0.334865	-0.274293	0.207141	-0.329323	-0.481687
0.019006	0.404104	0.169681	-0.158952	-0.121050	0.463983	-0.210676	0.097837	0.297672
0.019041	-0.404071	-0.169670	-0.159031	-0.121118	-0.463982	0.210677	-0.097846	-0.297678
-0.045700	0.009457	0.068555	0.353290	0.334889	0.274264	-0.207129	0.329328	0.481686
-0.273309	0.345596	-0.228286	-0.266555	-0.094360	-0.171070	-0.242754	0.491952	-0.393241
-0.060629	-0.379127	-0.155474	0.315330	-0.203022	0.216321	0.276644	-0.298605	0.193744

PICENE

IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.01199	0.61379	-0.01503	-0.24964	-0.00211	0.18096	-0.00373	-0.03988	-0.00068	0.03089	-0.00037	-0.01049	0.00040	0.01337	-0.00094
	-0.02002	-0.00049	0.07728	-0.00210	-0.14232	-0.00719	0.70589								
2	0.61379	1.01384	0.70922	-0.00929	-0.14324	0.01217	0.12512	-0.00036	-0.03810	0.00245	0.03639	0.00201	-0.03427	0.00040	0.03348
	-0.00238	-0.07425	-0.00236	0.08158	-0.00161	-0.25719	-0.01615								
3	-0.01503	0.70922	1.01460	0.57377	0.00898	-0.20085	-0.00547	0.05988	0.00385	-0.03443	-0.00286	0.01492	0.00201	-0.01049	-0.00166
	0.00786	0.00629	-0.05153	-0.00467	0.04390	-0.02118	-0.34148								
4	-0.24964	-0.00929	0.57377	0.96831	0.51799	-0.01037	-0.17572	-0.00316	0.04951	-0.00146	-0.04146	-0.00286	0.03639	-0.00037	-0.03537
	0.00327	0.08532	0.00253	-0.09757	0.00701	0.53284	0.02284								
5	-0.00211	-0.14324	0.00898	0.51799	1.02041	0.75599	-0.01543	-0.16570	-0.00131	0.09193	-0.00146	-0.03443	0.00245	0.03090	-0.00346
	-0.03579	0.00045	0.19123	-0.00804	-0.24927	0.00601	0.02748								
6	0.18096	0.01217	-0.20085	-0.01037	0.75599	1.01497	0.53060	0.01029	-0.07606	-0.00131	0.04951	0.00385	-0.03810	-0.00068	0.03516
	-0.00180	-0.09852	-0.01054	-0.00727	0.01317	-0.22793	-0.01829								
7	-0.00373	0.12512	-0.00547	-0.17572	-0.01543	0.53060	0.97605	0.49400	0.01029	-0.16568	-0.00316	0.05988	-0.00036	-0.03988	0.00141
	0.02488	0.01025	-0.24826	0.00983	0.56121	0.01433	-0.12915								
8	-0.03988	-0.00036	0.05988	-0.00316	-0.16570	0.01029	0.49400	0.97605	0.53058	-0.01543	-0.17573	-0.00547	0.12512	-0.00373	-0.12915
	0.01433	0.56123	0.00983	-0.24825	0.01024	0.02488	0.00142								
9	-0.00068	-0.03810	0.00385	0.04951	-0.00131	-0.07606	0.01029	0.53058	1.01499	0.75599	-0.01036	-0.20087	0.01216	0.18098	-0.01829
	-0.22794	0.01317	-0.00726	-0.01054	-0.09851	-0.00179	0.03516								
10	0.03089	0.00245	-0.03443	-0.00146	0.09193	-0.00131	-0.16568	-0.01543	0.75599	1.02039	0.51801	0.00898	-0.14324	-0.00212	0.02747
	0.00602	-0.24926	-0.00804	0.19121	0.00046	-0.03579	-0.00346								
11	-0.00037	0.03639	-0.00286	-0.04146	-0.00146	0.04951	-0.00316	-0.17573	-0.01036	0.51801	0.96831	0.57377	-0.00928	-0.24965	0.02284
	0.53283	0.00700	-0.09757	0.00253	0.08532	0.00327	-0.03537								
12	-0.01049	0.00201	0.01492	-0.00286	-0.03443	0.00385	0.05988	-0.00547	-0.20087	0.00898	0.57377	1.01459	0.70923	-0.01503	-0.34146
	0.02118	0.04391	-0.00467	-0.05153	0.00629	0.00786	-0.00166								
13	0.00040	-0.03427	0.00201	0.03639	0.00245	-0.03810	-0.00036	0.12512	0.01216	-0.14324	-0.00928	0.70923	1.01385	0.61377	-0.01616
	-0.25719	-0.00161	0.08158	-0.00237	-0.07425	-0.00238	0.03348								
14	0.01337	0.00040	-0.01049	-0.00037	0.03090	-0.00068	-0.03988	-0.00373	0.18098	-0.00212	-0.24965	-0.01503	0.61377	1.01200	0.70589
	-0.00718	-0.14233	-0.00210	0.07728	-0.00049	-0.02002	-0.00094								
15	-0.00094	0.03348	-0.00166	-0.03537	-0.00346	0.03516	0.00141	-0.12915	-0.01829	0.02747	0.02284	-0.34146	-0.01616	0.70589	1.01506
	-0.58744	0.01004	-0.10136	-0.00087	0.07799	0.00342	-0.03405								
16	-0.02002	-0.00238	0.00786	0.00327	-0.03579	-0.00180	0.02488	0.01433	-0.22794	0.00602	0.53283	0.02118	-0.25719	-0.00718	0.58744
	0.96824	0.47392	0.01138	-0.14929	-0.00466	0.04151	0.00342								
17	-0.00049	-0.07425	0.00629	0.08532	0.00045	-0.09852	0.01025	0.56123	0.01317	-0.24926	0.00700	0.04391	-0.00161	-0.14233	0.01004
	0.47392	0.97660	0.55201	-0.01584	-0.20376	-0.00466	0.07799								
18	0.07728	-0.00236	-0.05153	0.00253	0.19123	-0.01054	-0.24826	0.00983	-0.00726	-0.00804	-0.09757	-0.00467	0.08158	-0.00210	-0.10136
	0.01138	0.55201	1.01992	0.73388	-0.01584	-0.14930	-0.00087								
19	-0.00210	0.08158	-0.00467	-0.09757	-0.00804	-0.00727	0.00983	-0.24825	-0.01054	0.19121	0.00253	-0.05153	-0.00237	0.07728	-0.00087
	-0.14929	-0.01584	0.73388	1.01991	0.55202	0.01139	-0.10136								
20	-0.14232	-0.00161	0.04390	0.00701	-0.24927	0.01317	0.56121	0.01024	-0.09851	0.00046	0.08532	0.00629	-0.07425	-0.00049	0.07799
	-0.00466	-0.20376	-0.01584	0.55202	0.97660	0.47392	0.01004								
21	-0.00719	-0.25719	0.02118	0.53284	0.00601	-0.22793	0.01433	0.02488	-0.00179	-0.03579	0.00327	0.00786	-0.00238	-0.02002	0.00342
	0.04151	-0.00466	-0.14930	0.01139	0.47392	0.96824	0.58742								
22	0.70589	-0.01615	-0.34148	0.02284	0.02748	-0.01829	-0.12915	0.00142	0.03516	-0.00346	-0.03537	-0.00166	0.03348	-0.00094	-0.03405
	0.00342	0.07799	-0.00087	-0.10136	0.01004	0.58742	1.01507								

PICENE

IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	-0.78342	0.43476	-0.09130	-0.26213	0.02309	0.19212	-0.00046	-0.04386	-0.00069	0.03377	0.00010	-0.01142	-0.00004	0.01457	-0.00015
	-0.02181	-0.00341	0.08344	0.00796	-0.14388	-0.07274	0.53078								
2	0.43476	0.78456	0.53435	-0.07306	-0.14470	0.02186	0.13338	-0.00668	-0.04107	0.00429	0.03944	0.00071	-0.03706	-0.00004	0.03623
	0.00023	-0.08010	-0.00730	0.08763	0.01940	-0.27003	-0.09179								
3	-0.09130	0.53435	0.79562	0.40195	-0.06743	-0.20523	0.01394	0.06433	-0.00029	-0.03731	-0.00067	0.01631	0.00071	-0.01142	-0.00039
	0.00859	0.00158	-0.05680	0.00105	0.05414	-0.03073	-0.35804								
4	-0.26213	-0.07306	0.40195	0.70742	0.34323	-0.07916	-0.18645	0.01333	0.05364	-0.00541	-0.04505	-0.00067	0.03943	0.00010	-0.03831
	-0.00079	0.09173	0.00874	-0.09857	-0.04261	0.37149	-0.02937								
5	0.02309	-0.14470	-0.06743	0.34323	0.80307	0.58328	-0.08793	-0.16851	0.01043	0.09911	-0.00541	-0.03731	0.00429	0.03377	-0.00477
	-0.03969	0.00661	0.20408	0.01369	-0.26504	-0.05320	0.03805								
6	0.19212	0.02186	-0.20523	-0.07916	0.58328	0.79461	0.35609	-0.05924	-0.08712	0.01043	0.05364	-0.00029	-0.04107	-0.00069	0.03728
	0.00365	-0.09952	0.01103	0.00178	-0.04607	-0.24203	0.00076								
7	0.00046	0.13338	0.01394	-0.18645	-0.08793	0.35609	0.72452	0.32764	-0.05924	-0.16850	0.01333	0.06432	-0.00668	-0.04386	0.00826
	0.03321	-0.03936	-0.26406	-0.04973	0.40167	-0.03460	-0.13205								
8	-0.04386	-0.00668	0.06433	0.01333	-0.16851	-0.05924	0.32764	0.72452	0.35608	-0.08793	-0.18645	0.01394	0.13338	-0.00046	-0.13204
	-0.03460	0.40167	-0.04973	-0.26404	-0.03936	0.03321	0.00827								
9	-0.00069	-0.04107	-0.00029	0.05364	0.01043	-0.08712	-0.05924	0.35608	0.79463	0.58328	-0.07917	-0.20525	0.02186	0.19215	0.00076
	-0.24204	-0.04607	0.00179	0.01104	-0.09952	0.00365	0.03728								
10	0.03377	0.00429	-0.03731	-0.00541	0.09911	0.01043	-0.16850	-0.08793	0.58328	0.80305	0.34324	-0.06743	-0.14470	0.02309	0.03804
	-0.05320	-0.26502	0.01369	0.20405	0.00661	-0.03969	-0.00477								
11	0.00010	0.03944	-0.00067	-0.04505	-0.00541	0.05364	0.01333	-0.18645	-0.07917	0.34324	0.70742	0.40195	-0.07306	-0.26214	-0.02937
	0.37148	-0.04260	-0.09857	0.00873	0.09173	-0.00079	-0.03831								
12	-0.01142	0.00071	0.01631	-0.00067	-0.03731	-0.00029	0.06432	0.01394	-0.20525	-0.06743	0.40195	0.79560	0.53435	-0.09130	-0.35802
	-0.03073	0.05414	0.00105	-0.05680	0.00158	0.00859	-0.00039								
13	-0.00004	-0.03706	0.00071	0.03943	0.00429	-0.04107	-0.00668	0.13338	0.02186	-0.14470	-0.07306	0.53435	0.78456	0.43476	-0.09179
	-0.27003	0.01940	0.08763	-0.00730	-0.08010	0.00023	0.03623								
14	0.01457	-0.00004	-0.01142	0.00010	0.03377	-0.00069	-0.04386	-0.00046	0.19215	0.02309	-0.26214	-0.09130	0.43476	0.78345	0.53078
	-0.07274	-0.14390	0.00796	0.08344	-0.00341	-0.02181	-0.00015								
15	-0.00015	0.03623	-0.00039	-0.03831	-0.00477	0.03728	0.00826	-0.13204	0.00076	0.03804	-0.02937	-0.35802	-0.09179	0.53078	0.79496
	0.41618	-0.06105	-0.11420	0.01099	0.08422	-0.00042	-0.03692								
16	-0.02181	0.00023	0.00859	-0.00079	-0.03969	0.00365	0.03321	-0.03460	-0.24204	-0.05320	0.37148	-0.03073	-0.27003	-0.07274	0.41618
	0.71485	0.30610	-0.05792	-0.15083	0.01237	0.04461	-0.00041								
17	-0.00341	-0.08010	0.00158	0.09173	0.00661	-0.09952	-0.03936	0.40167	-0.04607	-0.26502	-0.04260	0.05414	0.01940	-0.14390	-0.06105
	0.30610	0.72539	0.37914	-0.08772	-0.21650	0.01236	0.08422								
18	0.08344	-0.00730	-0.05680	0.00874	0.20408	0.01103	-0.26406	-0.04973	0.00179	0.01369	-0.09857	0.00105	0.08763	0.00796	-0.11420
	-0.05792	0.37914	0.80083	0.55971	-0.08773	-0.15084	0.01099								
19	0.00796	0.08763	0.00105	-0.09857	0.01369	0.00178	-0.04973	-0.26404	0.01104	0.20405	0.00873	-0.05680	-0.00730	0.08344	0.01099
	-0.15083	-0.08772	0.55971	0.80081	0.37915	-0.05791	-0.11420								
20	-0.14388	0.01940	0.05414	-0.04261	-0.26504	-0.04607	0.40167	-0.03936	-0.09952	0.00661	0.09173	0.00158	-0.08010	-0.00341	0.08422
	0.01237	-0.21650	-0.08773	0.37915	0.72539	0.30610	-0.06105								
21	-0.07274	-0.27003	-0.03073	0.37149	-0.05320	-0.24203	-0.03460	0.03321	0.00365	-0.03969	-0.00079	0.00859	0.00023	-0.02181	-0.00042
	-0.04461	0.01236	-0.15084	-0.05791	0.30610	0.71485	0.41618								
22	0.53078	-0.09179	-0.35804	-0.02937	0.03805	0.00076	-0.13205	0.00827	0.03728	-0.00477	-0.03831	-0.00039	0.03623	-0.00015	-0.03692
	-0.00041	0.08422	0.01099	-0.11420	-0.06105	0.41618	0.79498								

ENERGIES FOR PICENE IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	11,12	10,12	11,13	9,12	8,12	7,12	8,13	6,12	5,12	4,12
XMOMNT	-0.94742	-0.30021	0.22807	-0.14116	-0.05886	-0.09320	-0.14211	-0.08380	0.04673	-0.01480
YMOMNT	-0.54669	0.52080	-0.39578	0.24485	-0.03402	-0.05388	0.24619	0.14517	-0.08098	-0.00851
JUMP E	20.6698	22.7278	23.6467	26.0239	28.9298	31.7167	31.9067	34.4086	37.9332	38.1995
DIAG E	31.4274	34.3506	35.9952	39.5527	43.3781	46.0363	47.8312	48.6774	55.1890	52.7991
DIAG E	31.6043	34.8458	35.9793	39.8853	43.5438	46.6133	47.8041	49.2116	55.3470	53.0269
CORRSP	31.3990	31.5665	36.6951	40.2155	43.2039	45.8476	45.8497	51.8391	55.4304	53.1900
CORRSP	31.5900	32.0665	36.7047	40.5667	43.4732	46.3274	46.2081	51.9839	55.5432	53.3975

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
31.56652	0.14900	-0.16621	0.28874	//	-0.0002	0.7800	0.5519	0.2224	-0.0000	-0.0000	0.1734	0.0600	0.0621	-0.0000
24.83243				//	-0.0004	0.7202	-0.6021	-0.2785	-0.0001	0.0001	0.1710	0.1085	-0.0119	0.0000
36.69508	0.53215	0.29164	-0.50593	//	-0.0000	-0.5711	0.6910	0.4124	0.0001	0.0000	-0.1609	0.0174	-0.0130	-0.0000
28.52153				//	0.0000	0.5942	0.4681	0.6220	-0.0000	-0.0001	0.1664	-0.0002	0.1148	0.0000
40.21548	0.36362	-0.23030	0.39948	//	0.0001	0.1163	-0.4579	0.8600	-0.0000	-0.0001	-0.1822	-0.0222	0.0590	-0.0000
36.17991				//	0.0001	-0.1671	-0.6042	0.6861	0.0001	-0.0002	-0.3446	0.0726	0.1110	0.0000
45.84968	0.00660	0.00579	0.05790	//	-0.0048	-0.1100	-0.0091	0.1302	0.0989	-0.3411	0.6198	-0.6686	-0.0886	0.0757
39.15748				//	0.0003	-0.1839	-0.2251	-0.1780	-0.0025	0.0005	0.6771	-0.6476	-0.0774	-0.0003
51.83907	0.18222	-0.14371	0.24901	//	0.0000	-0.1768	-0.0902	0.1404	-0.0001	-0.0002	0.6782	0.6921	-0.0435	-0.0006
48.78339				//	-0.0002	-0.1929	-0.0380	0.1700	-0.0004	-0.0009	0.4893	0.6831	-0.4758	0.0032
55.43044	0.04164	0.06644	-0.11511	//	-0.0000	-0.0824	-0.0031	-0.0402	-0.0000	-0.0001	0.0915	-0.0407	0.9907	-0.0002
52.46761				//	-0.0000	-0.1708	-0.0340	-0.0652	-0.0001	-0.0001	0.3556	0.3113	0.8614	-0.0001

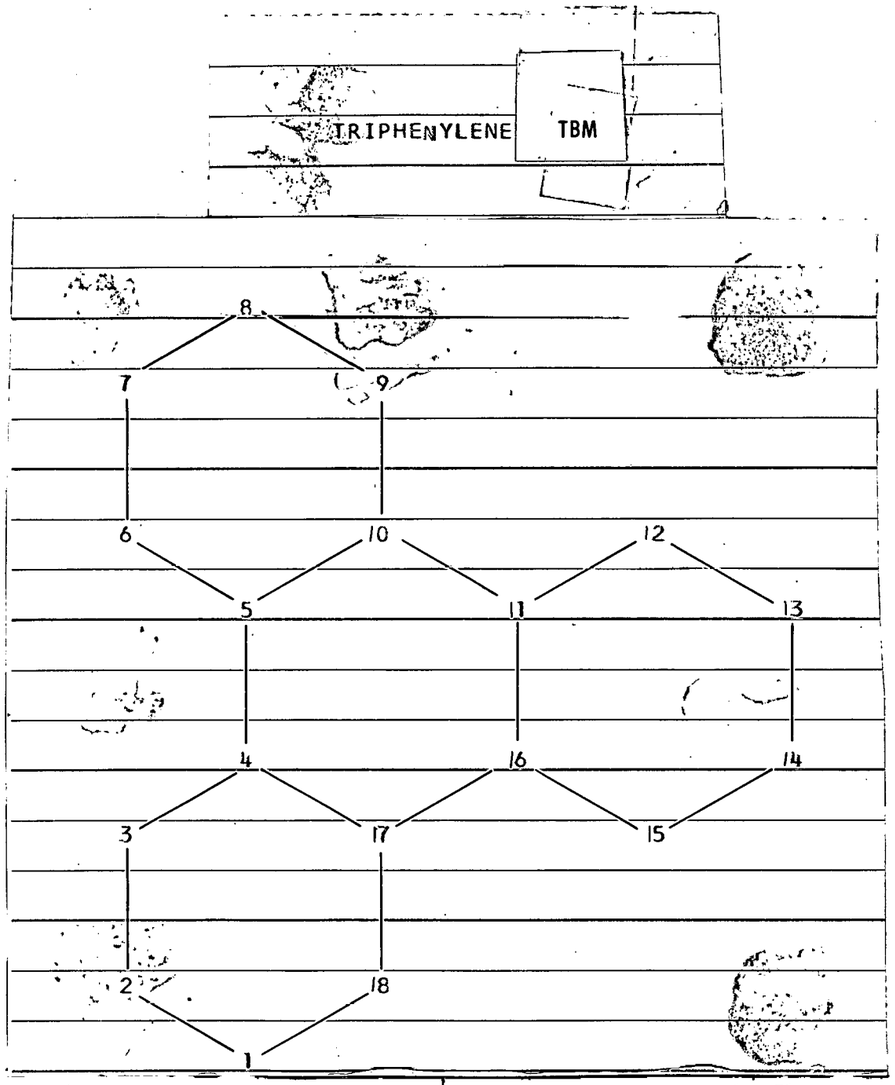
ENERGIES FOR PICENE , IRM APPROXIMATION 5.8

ONE-ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	11,12	10,13	8,12	9,13	10,14	7,12	9,14	6,13	4,12	5,13
XMOMNT	-0.94742	-0.51553	-0.05886	-0.62113	-0.71482	-0.09320	0.13315	-0.03677	-0.01480	0.06821
YMOMNT	-0.54669	-0.29744	-0.03402	-0.35845	-0.41254	-0.05388	0.07682	-0.02115	-0.00851	0.03937
JUMP E	20.6698	25.7047	28.9298	29.0008	30.1901	31.7167	33.4862	37.3855	38.1995	40.9101
DIAG E	31.4274	39.1228	43.3781	42.9084	42.0273	46.0363	47.5732	53.9387	52.7991	60.0478
DIAG E	31.6043	39.4253	43.5438	43.0483	41.9884	46.6133	47.3717	54.2801	53.0269	60.0131
CORRSP	29.5263	40.1517	42.3716	36.4407	46.6448	45.0642	49.9228	57.2409	50.8377	61.0581
CORRSP	29.7008	40.0292	42.4717	36.8312	45.1743	47.0302	50.1741	57.5386	50.9467	61.0182

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
29.52635	0.79433	-0.68891	-0.39753	//	0.9186	-0.3270	0.0259	0.0607	-0.1073	0.0160	-0.1722	-0.0494	-0.0044	-0.0317
20.33660				//	0.9249	-0.2433	-0.0090	0.1919	0.0631	-0.0262	-0.2018	-0.0297	-0.0450	0.0139
40.15173	2.24395	-0.99295	-0.57294	//	0.3568	0.7893	-0.0305	-0.1130	0.4688	-0.1030	0.0360	0.0523	0.0032	0.0400
30.11512				//	0.1817	0.8390	0.4585	0.1342	-0.0113	0.1519	-0.0854	-0.0647	-0.0031	-0.0111
42.37158	0.64863	0.51966	0.29989	//	-0.0040	0.0188	0.6115	-0.6169	-0.1960	-0.4003	-0.0287	-0.2057	-0.0333	-0.0477
34.53256				//	0.0238	-0.2511	0.5436	-0.3350	-0.6613	-0.1816	-0.0905	-0.2193	0.0265	-0.0363
36.44067	0.11672	-0.23770	-0.13719	//	0.0491	0.4067	0.4900	0.4788	-0.5070	0.2986	0.0984	-0.0333	-0.0327	-0.0689
39.56176				//	-0.0213	-0.1619	0.2297	0.6617	-0.1352	-0.0313	0.6657	-0.0747	0.0763	-0.0947
46.64484	0.10834	-0.20237	-0.11690	//	-0.0701	-0.1303	0.3539	-0.1667	0.4457	0.6756	-0.2990	-0.0986	-0.2567	-0.0699
43.16178				//	-0.1372	-0.2121	0.3057	0.0008	0.4501	0.1643	-0.0642	-0.5451	-0.5578	-0.0271
45.06418	0.40540	0.39834	0.22994	//	-0.0158	0.2619	-0.3444	-0.4074	-0.4842	0.2551	-0.5312	0.2516	0.0029	0.0405
48.29188				//	0.2477	0.0471	-0.1223	-0.4728	-0.1299	0.5560	0.5545	0.0806	-0.2261	-0.0826
49.92285	0.23072	0.28554	0.16476	//	0.1403	-0.0415	-0.0974	-0.4169	-0.1225	0.4082	0.7465	0.1892	0.0727	-0.1240
34.25011				//	0.1669	0.1479	0.0791	-0.3787	0.3602	-0.6797	0.4297	-0.0877	0.0669	0.1093
57.24088	0.00228	-0.02651	-0.01526	//	0.0161	-0.0972	0.2084	0.0576	0.0366	-0.1791	0.0363	0.7853	-0.5075	0.1861
53.52482				//	-0.0481	-0.1439	0.3915	0.0278	0.0938	-0.0216	0.0003	0.7080	-0.3620	0.4259
50.83770	0.05982	-0.14408	-0.08312	//	-0.0276	-0.0788	0.2739	0.0313	0.1542	0.0192	-0.1587	0.4705	0.7801	-0.1943
45.48100				//	-0.0123	-0.2344	0.4165	-0.1647	0.4261	0.2751	-0.0319	0.1769	0.5916	-0.3238
61.05814	0.02267	0.08093	0.04669	//	0.0241	-0.0371	0.1120	-0.0438	0.0082	0.1381	0.0572	-0.0677	0.2460	0.9466
58.82177				//	0.0036	-0.0537	0.0053	-0.0163	0.0269	0.2606	0.0583	-0.3122	0.3790	-0.8269



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	0.	0.	0.8660	1.7320
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	4.5000	5.0000	4.5000

1.7320	2.5980	3.4640	4.3300	4.3300	3.4640	2.5980	1.7320	1.7320	1
3.5000	3.0000	3.5000	3.0000	2.0000	1.5000	2.0000	1.5000	0.5000	

TRIPHENYLENE — TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 S	3 A	4 S	5 S	6 A	7 A	8 S	9 A	10 A	11 S	12 S	13 S	14 A	15 A	16 S	17 A	18 Z
1.624939	1.486117	1.486115	1.332523	1.317292	1.317287	1.217038	1.168835	1.168817	0.831182	0.831163	0.782960	0.682711	0.682706	0.667475	0.513883	0.513881	0.375059
0.119669	0.294981	-0.155241	0.344666	0.190893	-0.273159	0.183343	0.331923	-0.030455	0.029070	-0.332047	0.183342	0.273313	-0.190672	-0.344666	0.139738	0.302633	-0.119669
0.119667	0.263539	-0.204099	0.344581	0.332019	-0.029323	-0.183362	0.142161	0.301507	0.302098	0.140902	0.183362	-0.029592	0.331994	0.344582	-0.190161	-0.273767	0.119667
0.183343	0.224094	-0.246762	0.119585	0.235950	0.235475	-0.344603	-0.234688	0.236696	-0.235714	0.235673	-0.344603	-0.235284	-0.238139	-0.119585	0.234811	0.236587	-0.183343
0.344571	0.177847	-0.281927	-0.183450	-0.028673	0.332035	-0.119681	-0.302696	-0.139594	-0.140856	-0.302110	0.119681	0.332058	-0.028404	-0.183450	-0.272327	-0.192225	0.344571
0.344572	-0.204103	-0.263542	-0.183450	0.029446	0.331967	0.119681	0.301502	-0.142153	0.140893	-0.302093	0.119681	-0.331943	-0.029715	0.183450	0.273770	-0.190165	-0.344571
0.183343	-0.246759	-0.224097	0.119585	-0.235400	0.236024	0.344603	0.236684	0.234700	0.235685	0.235703	-0.344603	0.236214	-0.235209	0.119585	-0.236589	0.234808	-0.183343
0.119667	-0.281925	-0.177843	0.344582	-0.332084	-0.028549	0.183362	-0.139602	0.302701	-0.302116	0.140864	0.183362	0.028281	0.332108	-0.344581	0.192221	-0.272324	-0.119667
0.119669	-0.308528	-0.126190	0.344667	-0.191528	-0.272713	-0.183342	-0.332169	-0.027643	-0.029029	-0.332051	0.183342	-0.272559	-0.191749	0.344666	-0.142017	0.301570	-0.119669
0.183340	-0.325748	-0.070698	0.119778	0.085863	-0.322035	-0.344587	-0.087623	-0.321608	0.321971	0.086280	-0.344588	0.322105	-0.085602	-0.119778	0.087493	-0.321644	-0.183340
0.344574	-0.333077	-0.013056	-0.183302	0.301926	-0.141284	-0.119684	0.272243	-0.192344	-0.191207	0.273044	0.119684	-0.141528	0.301812	-0.183301	-0.030308	0.331953	0.344574
0.344575	-0.126190	0.308521	-0.183280	0.272840	-0.191575	0.119642	-0.027652	0.332182	-0.332063	0.029038	0.119642	-0.191795	-0.272686	0.183280	-0.301564	-0.142017	-0.344575
0.183349	-0.070698	0.325754	0.119643	0.322100	0.085935	0.344530	-0.321622	0.087636	0.086293	-0.321985	-0.344530	0.085675	0.322169	0.119644	0.321650	0.087493	0.183349
0.119672	-0.013055	0.333076	0.344472	0.141240	0.302048	0.183327	-0.192359	-0.272240	0.273040	0.191221	0.183327	-0.301934	-0.141483	-0.344473	0.331951	-0.030307	-0.119672
0.119672	0.044987	0.330282	0.344473	-0.140534	0.302377	-0.183327	0.190046	-0.273859	-0.273064	0.191187	0.183327	0.302490	-0.140291	0.344473	0.332170	-0.027801	0.119672
0.183348	0.101659	0.317457	0.119645	-0.321898	0.086685	-0.344530	0.322353	0.084908	-0.086252	-0.321995	-0.344530	-0.086945	0.321829	-0.119644	-0.322301	0.085063	-0.183349
0.344575	0.155240	0.294974	-0.183279	-0.273287	-0.190939	-0.119642	0.030464	0.331936	0.332060	0.029079	0.119642	-0.190718	-0.273440	0.183280	0.302627	-0.139737	0.344575
0.344574	0.330284	-0.044988	-0.183301	-0.302255	-0.140580	0.119684	-0.273863	-0.190031	0.191173	0.273067	0.119684	0.140336	0.302368	0.183302	0.027803	0.332172	-0.344574
0.183340	0.317451	-0.101659	0.119779	-0.086613	-0.321834	0.344588	0.084896	-0.322338	-0.321981	0.086240	-0.344588	-0.321764	-0.086873	0.119778	-0.085063	-0.322295	0.183340

TRIPHENYLENE — TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 S	3 A	4 S	5 S	6 A	7 A	8 S	9 A	10 A	11 S	12 S	13 S	14 A	15 A	16 S	17 A	18 A
28.99357	24.65978	24.65970	18.81256	18.15843	18.15820	13.44415	10.88955	10.88855	-15.31177	-15.31374	-20.89787	-35.03636	-35.03718	-37.55691	-71.31449	-71.31511	125.61482
0.093878	0.115563	0.247816	0.298580	0.237805	0.166599	0.166192	0.026869	0.307135	0.031886	-0.364214	0.207202	0.231416	0.330328	-0.421873	-0.421429	0.196523	-0.195403
0.093876	0.156835	0.223981	0.298506	0.025212	0.289312	-0.166210	-0.279437	0.130312	0.331360	0.154552	0.207224	-0.401871	-0.035021	0.421769	0.380896	-0.266710	0.195400
0.143829	0.193347	0.193344	0.103595	-0.205404	0.205340	-0.312368	-0.218013	-0.218004	-0.258546	0.258504	-0.389448	0.285229	-0.285321	-0.146373	-0.328796	0.328800	-0.299374
0.270309	0.223984	0.156839	-0.158921	-0.289267	-0.025319	-0.108486	0.130303	-0.279434	-0.154499	-0.331377	0.135256	0.035170	0.401812	-0.224543	0.266715	-0.380901	0.562639
0.270309	0.223983	-0.156839	-0.158921	-0.289267	0.025319	0.108486	0.130303	0.279435	0.154540	-0.331358	0.135256	0.035170	-0.401812	0.224543	0.266715	0.380900	-0.562639
0.143829	0.193346	-0.193345	0.103595	-0.205405	-0.205339	0.312368	-0.218013	0.218004	0.258514	0.258536	-0.389448	0.285230	0.285321	0.146372	-0.328796	-0.328800	0.299374
0.093876	0.156835	-0.223982	0.298508	0.025211	-0.289311	0.166210	-0.279437	-0.130312	-0.331379	0.154510	0.207224	-0.401872	0.035021	-0.421768	0.380896	0.266710	-0.195400
0.093878	0.115563	-0.247817	0.298581	0.237804	-0.166598	-0.166192	0.026870	-0.307135	-0.031840	-0.364218	0.207202	0.231417	-0.330327	0.421872	-0.421429	-0.196523	0.195403
0.143826	0.070774	-0.264114	0.103763	0.280497	0.075138	-0.312354	0.297815	-0.079788	0.353158	0.094639	-0.389430	0.104371	0.389629	-0.146609	0.449144	0.120357	-0.299369
0.270311	0.023834	-0.272393	-0.158793	0.122792	0.263206	-0.108488	0.176843	0.252567	-0.209728	0.299494	0.135259	-0.365611	-0.170566	-0.224361	-0.463224	-0.040532	0.562643
0.270312	-0.247811	-0.115562	-0.158774	0.166639	-0.237916	0.108451	-0.307144	-0.026878	-0.364228	0.031851	0.135212	0.330481	0.231473	0.224335	0.196523	-0.421420	-0.562645
0.143833	-0.264119	-0.070774	0.103646	-0.075200	0.280553	0.312302	-0.079799	-0.297830	0.094651	-0.353177	-0.389365	-0.389706	0.104459	0.146445	-0.120357	0.449154	0.299383
0.093880	-0.272392	-0.023833	0.298413	-0.263312	0.122754	0.166178	0.252562	-0.176857	0.299487	0.209745	0.207184	0.170511	-0.365759	-0.421636	0.040530	-0.463222	-0.195408
0.093880	-0.272392	0.023834	0.298413	-0.263313	-0.122752	-0.166178	0.252562	0.176858	-0.299513	0.209708	0.207184	0.170512	0.365759	0.421636	0.040531	0.463222	0.195408
0.143833	-0.264119	0.070775	0.103647	-0.075201	-0.280553	-0.312302	-0.079799	0.297831	-0.094607	-0.353188	-0.389365	-0.389706	-0.104459	-0.146444	-0.120357	-0.449154	-0.299383
0.270312	-0.247811	0.115563	-0.158773	0.166639	-0.237917	-0.108451	-0.307144	0.026878	0.364224	0.031896	0.135212	0.330480	-0.231473	-0.224335	0.196522	0.421420	0.562645
0.270311	0.023835	0.272393	-0.158792	0.122791	-0.263207	-0.108489	0.176843	-0.252568	0.209690	0.299521	0.135259	-0.365611	0.170566	0.224362	-0.463223	0.040532	-0.562643
0.143826	0.070775	0.264114	0.103763	0.280496	-0.075138	0.312355	0.297815	0.079788	-0.353169	0.094594	-0.389431	0.104371	-0.389629	0.146609	0.449144	-0.120357	0.299369

TRIPHENYLENE

TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.00000	0.63657	-0.00000	-0.28020	0.00000	0.10068	-0.00000	-0.08680	0.00000	0.10468	-0.00000	-0.03298	0.00000	0.04686	0.00000	-0.08776	-0.00000	0.69040
2	0.63657	1.00000	0.69038	-0.00000	-0.08776	-0.00000	0.04687	-0.00000	-0.03299	0.00000	0.10469	-0.00000	-0.08682	0.00000	0.10070	-0.00000	-0.28022	-0.00000
3	-0.00000	0.69038	1.00000	0.60264	-0.00000	-0.14159	0.00000	0.10068	0.00000	-0.12074	-0.00000	0.05086	0.00000	-0.03298	-0.00000	0.01292	0.00000	-0.33405
4	-0.28020	-0.00000	0.60264	1.00000	0.42804	0.00000	-0.08776	-0.00000	0.01294	0.00000	-0.16164	-0.00000	0.10469	0.00000	-0.12075	-0.00000	0.56174	0.00000
5	0.00000	-0.08776	-0.00000	0.42804	1.00000	0.60264	-0.00000	-0.28020	-0.00000	0.56174	-0.00000	-0.12075	-0.00000	0.10469	0.00000	-0.16164	-0.00000	0.01294
6	0.10068	-0.00000	-0.14159	0.00000	0.60264	1.00000	0.69038	0.00000	-0.33405	-0.00000	0.01292	0.00000	-0.03298	0.00000	0.05086	0.00000	-0.12074	-0.00000
7	-0.00000	0.04687	0.00000	-0.08776	-0.00000	0.69038	1.00000	0.63657	0.00000	-0.28022	0.00000	0.10070	0.00000	-0.08682	-0.00000	0.10469	-0.00000	-0.03299
8	-0.08680	-0.00000	0.10068	-0.00000	-0.28020	0.00000	0.63657	1.00000	0.69040	0.00000	-0.08776	-0.00000	0.04686	0.00000	-0.03298	-0.00000	0.10468	-0.00000
9	0.00000	-0.03299	0.00000	0.01294	-0.00000	-0.33405	0.00000	0.69040	1.00000	0.60262	-0.00000	-0.14159	-0.00000	0.10070	0.00000	-0.12075	-0.00000	0.05086
10	0.10468	0.00000	-0.12074	0.00000	0.56174	-0.00000	-0.28022	0.00000	0.60262	1.00000	0.42807	0.00000	-0.08777	-0.00000	0.01293	0.00000	-0.16164	-0.00000
11	-0.00000	-0.10469	-0.00000	-0.16164	-0.00000	0.01292	0.00000	-0.08776	-0.00000	0.42807	1.00000	0.60263	0.00000	-0.28022	-0.00000	0.56172	0.00000	-0.12075
12	-0.03298	-0.00000	0.05086	-0.00000	-0.12075	0.00000	0.10070	-0.00000	-0.14159	0.00000	0.60263	1.00000	0.69040	0.00000	-0.33403	-0.00000	0.01293	0.00000
13	0.00000	-0.08682	0.00000	0.10469	-0.00000	-0.03298	0.00000	0.04686	-0.00000	-0.08777	0.00000	0.69040	1.00000	0.63655	0.00000	-0.28022	-0.00000	0.10070
14	0.04686	-0.00000	-0.03298	0.00000	0.10469	0.00000	-0.08682	0.00000	0.10070	-0.00000	-0.28022	0.00000	0.63655	1.00000	0.69040	0.00000	-0.08777	-0.00000
15	0.00000	0.10070	-0.00000	-0.12075	0.00000	0.05086	-0.00000	-0.03298	0.00000	0.01293	-0.00000	-0.33403	0.00000	0.69040	1.00000	0.60263	-0.00000	-0.14159
16	-0.08776	-0.00000	0.01292	-0.00000	-0.16164	0.00000	0.10469	-0.00000	-0.12075	0.00000	0.56172	-0.00000	-0.28022	0.00000	0.60263	1.00000	0.42807	-0.00000
17	-0.00000	-0.28022	0.00000	0.56174	-0.00000	-0.12074	-0.00000	0.10468	-0.00000	-0.16164	0.00000	0.01293	0.00000	-0.08777	-0.00000	0.42807	1.00000	0.60262
18	0.69040	-0.00000	-0.33405	0.00000	0.01294	-0.00000	-0.03299	0.00000	0.05086	-0.00000	-0.12075	0.00000	0.10070	-0.00000	-0.14159	0.00000	0.60262	1.00000

TRIPHENYLENE

TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.75942	0.46132	-0.04935	-0.26137	0.01545	0.09764	-0.00311	-0.08506	-0.00396	0.10112	0.00295	-0.03294	-0.00311	0.04552	0.00854	-0.08012	-0.04244	0.51344
2	0.46132	0.75943	0.51343	-0.04244	-0.08012	0.00854	0.04552	-0.00311	-0.03295	0.00295	0.10113	-0.00396	-0.08507	-0.00310	0.09765	0.01545	-0.26138	-0.04935
3	-0.04935	0.51343	0.76634	0.43332	-0.04640	-0.13225	0.00854	0.09764	0.00381	-0.11306	0.01149	0.04900	-0.00396	-0.03294	0.00380	0.01751	-0.03390	-0.31350
4	-0.26137	-0.04244	0.43332	0.72848	0.26811	-0.04640	-0.08012	0.01545	0.01753	-0.03406	-0.14767	0.01149	0.10113	0.00295	-0.11307	-0.03405	-0.39872	-0.03390
5	0.01545	-0.08012	-0.04640	0.26811	0.72848	0.43332	-0.04244	-0.26137	-0.03390	0.39872	-0.03405	-0.11307	0.00295	0.10113	0.01149	-0.14767	-0.03406	0.01753
6	0.09764	0.00854	-0.13225	-0.04640	0.43332	0.76634	0.51343	-0.04935	-0.31350	-0.03390	0.01751	0.00380	-0.03294	-0.00396	0.04900	0.01149	-0.11306	0.00381
7	-0.00311	0.04552	0.00854	-0.08012	-0.04244	0.51343	0.75943	0.46132	-0.04935	-0.26138	0.01545	0.09765	-0.00310	-0.08507	-0.00396	0.10113	0.00295	-0.03295
8	-0.08506	-0.00311	0.09764	0.01545	-0.26137	-0.04935	0.46132	0.75942	0.51344	-0.04244	-0.08012	0.00854	0.04552	-0.00311	-0.03294	0.00295	0.10112	-0.00396
9	-0.00396	-0.03295	0.00381	0.01753	-0.03390	-0.31350	-0.04935	0.51344	0.76633	0.43330	-0.04640	-0.13225	0.00854	0.09765	0.00381	-0.11307	-0.01148	-0.04900
10	0.10112	0.00295	-0.11306	-0.03406	0.39872	-0.03390	-0.26138	-0.04244	0.43330	0.72848	0.26813	-0.04640	-0.08013	0.01545	0.01752	-0.03405	-0.14767	-0.01148
11	0.00295	0.10113	-0.01149	-0.14767	-0.03405	0.01751	0.01545	-0.08012	-0.04640	0.26813	0.72847	0.43331	-0.04244	-0.26138	-0.03390	0.39870	-0.03405	-0.11307
12	-0.03294	-0.00396	0.04900	0.01149	-0.11307	0.00380	0.09765	0.00854	-0.13225	-0.04640	0.43331	0.76633	0.51344	-0.04935	-0.31348	-0.03390	0.01752	0.00381
13	-0.00311	-0.08507	-0.00396	0.10113	0.00295	-0.03294	-0.00310	0.04552	0.00854	-0.08013	-0.04244	0.51344	0.75942	0.46130	-0.04935	-0.26138	0.01545	0.09765
14	0.04552	-0.00310	-0.03294	0.00295	0.10113	-0.00396	-0.08507	-0.00311	0.09765	0.01545	-0.26138	-0.04935	0.46130	0.75942	0.51344	-0.04244	-0.08013	-0.00854
15	0.00854	0.09765	0.00380	-0.11307	0.01149	0.04900	-0.00396	-0.03294	0.00381	0.01752	-0.03390	-0.31348	-0.04935	0.51344	0.76633	0.43331	-0.04640	-0.13225
16	-0.08012	0.01545	0.01751	-0.03405	-0.14767	0.01149	0.10113	0.00295	-0.11307	-0.03405	0.39870	-0.03390	-0.26138	-0.04244	0.43331	0.72847	0.26813	-0.04640
17	-0.04244	-0.26138	-0.03390	0.39872	-0.03406	-0.11306	0.00295	0.10112	0.01148	-0.14767	-0.03405	0.01752	0.01545	-0.08013	-0.04640	0.26813	0.72848	0.43330
18	0.51344	-0.04935	-0.31350	-0.03390	0.01753	0.00381	-0.03295	-0.00396	0.04900	0.01148	-0.11307	0.00381	0.09765	0.00854	-0.13225	-0.04640	0.43330	0.76633

ENERGIES FOR TRIPHENYLENE ,TBM APPROXIMATION 1.7

ONE-ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	2,10	8,10	8,11	7,10	6,10	5,10	5,11	4,10	4,11	3,10
XMOMNT	-0.79245	-0.00005	0.79245	0.16939	-0.03358	0.00000	-0.03362	-0.00000	0.03701	-0.04987
YMOMNT	-0.00005	0.79247	0.00005	-0.00001	-0.00000	-0.03357	-0.00000	-0.03702	-0.00000	-0.00000
JUMP E	26.2003	26.2013	26.2033	28.7559	33.4700	33.4702	33.4722	34.1243	34.1263	39.9715
DIAG E	36.4305	37.5438	36.4334	41.4146	47.5570	45.6796	47.5593	49.2741	49.2765	55.4789
DIAG E	36.4305	37.5438	36.4334	41.0067	47.5570	45.6796	47.5593	49.0759	49.0782	55.4789
CORRSP	31.4334	37.4802	41.1914	40.4575	44.9139	45.7137	49.6953	49.3036	49.9520	56.5067
CORRSP	31.4797	37.5086	41.2714	40.0794	44.9377	45.6835	49.9547	49.1071	49.5905	56.2308

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
31.43340	0.00006	-0.00643	-0.00001	//	0.7112	-0.0000	0.6995	0.0005	0.0245	-0.0000	-0.0133	0.0000	-0.0025	-0.0641
29.51043				//	0.7454	-0.0000	-0.6480	-0.0751	0.0708	0.0000	0.0432	-0.0000	0.0641	-0.0889
41.19140	1.78035	1.00815	0.00007	//	-0.6471	0.0000	0.6707	-0.2627	-0.1247	0.0000	-0.0953	-0.0000	0.1648	0.1030
31.40695				//	0.6473	-0.0001	0.7564	0.0052	0.0453	0.0000	-0.0344	-0.0000	-0.0037	-0.0740
40.45755	0.42754	0.49850	0.00002	//	-0.2315	0.0000	-0.2310	0.8909	0.1784	-0.0000	0.1778	-0.0000	-0.1896	-0.0023
35.94273				//	0.0553	0.0000	-0.0536	0.9969	-0.0113	0.0000	-0.0093	-0.0000	0.0060	0.0034
44.91392	0.00016	0.00912	0.00001	//	-0.0697	0.0000	0.0457	-0.2801	0.7003	0.0000	0.6311	0.0000	0.0769	-0.1416
40.44872				//	-0.1126	0.0000	0.0126	0.0165	0.9461	0.0000	-0.1075	-0.0000	0.1595	-0.2342
49.69528	0.01329	-0.07931	-0.00001	//	0.0948	0.0000	-0.0446	-0.1455	-0.4577	-0.0000	0.5674	0.0000	0.6120	0.2488
41.10125				//	-0.0251	-0.0000	0.0635	0.0131	0.0681	-0.0001	0.9662	-0.0000	0.2386	0.0107
49.95199	0.00005	0.00508	-0.00001	//	0.0239	0.0000	-0.0568	0.1927	0.4048	0.0000	-0.4763	-0.0000	0.7429	-0.1285
44.53740				//	-0.0215	-0.0000	0.0288	-0.0073	-0.1761	0.0000	-0.2265	-0.0001	0.9557	0.0548
56.50668	0.04671	-0.13942	-0.00001	//	0.0864	0.0000	-0.0142	-0.0234	0.2971	0.0000	-0.1100	0.0000	-0.0674	0.9417
52.27411				//	0.0924	0.0000	-0.0008	-0.0058	0.2493	0.0000	-0.0226	0.0000	-0.0126	0.9637

ENERGIES FOR TRIPHENYLENE ,TBM APPROXIMATION 1.7

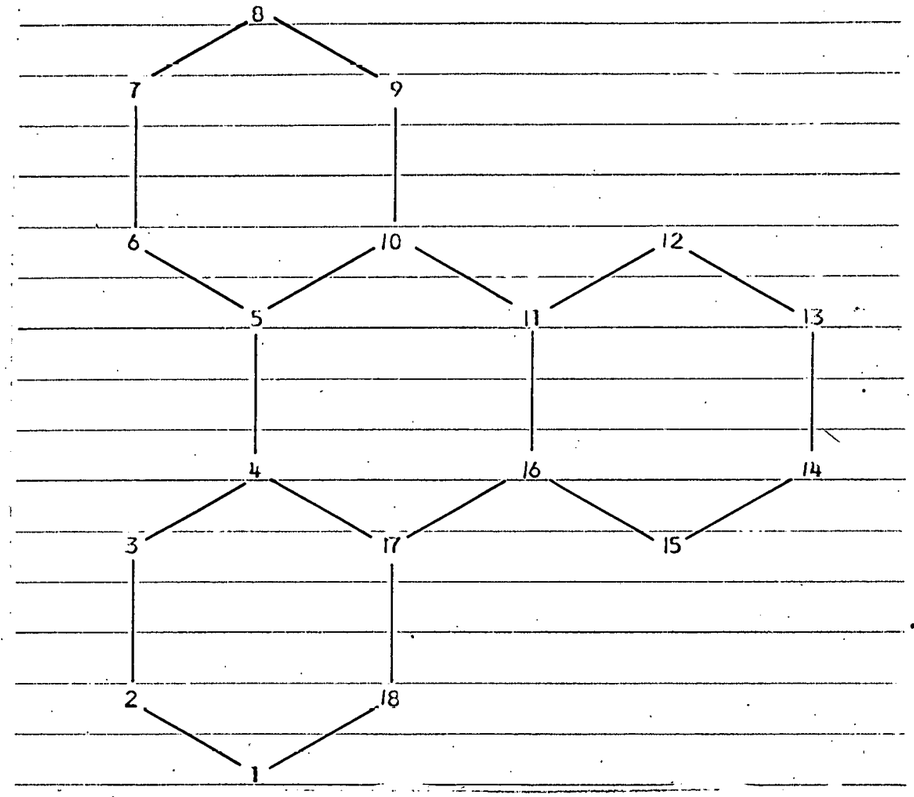
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	8,10	9,11	7,11	9,12	5,10	6,11	4,10	7,12	6,12	2,10
XMOMNT	-0.00005	-0.00005	0.00001	-0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000	0.00000
YMOMNT	0.79247	0.79240	0.16944	-0.16976	-0.03357	0.03358	-0.03702	0.00007	-0.47860	-0.04986
JUMP E	26.2013	26.2023	28.7579	31.7864	33.4702	33.4719	34.1243	34.3420	39.0561	39.9715
DIAG E	37.5438	37.5447	41.4164	44.2975	45.6796	45.6816	49.2741	49.7018	55.0626	54.8964
DIAG E	37.5438	37.5447	41.0084	44.9316	45.6796	45.6816	49.0759	49.9280	55.6967	54.8964
CORRSP	32.9371	40.8398	39.1593	42.8874	46.5929	45.0516	49.6975	51.5000	57.7951	54.6377
CORRSP	33.0273	41.0082	39.0301	42.9042	46.9254	45.1846	49.5951	51.6461	58.0742	54.5913

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
32.93712	0.00021	-0.00000	0.01212	//	0.7020	-0.6803	0.0001	-0.0089	-0.0532	-0.0315	-0.0039	0.1760	0.0057	0.0968
				//										
28.96081				//	0.6773	0.7046	0.0370	-0.0952	-0.0638	-0.0459	-0.0001	-0.0146	-0.1562	0.0597
				//										
40.83983	2.08542	-0.00006	1.09580	//	0.6266	0.6694	0.2282	-0.2497	-0.1374	0.0835	-0.0632	-0.0177	0.0338	0.1164
				//										
24.98874				//	-0.6616	0.6335	-0.0100	0.0105	-0.0512	-0.0675	-0.0017	-0.3865	-0.0077	-0.0644
				//										
39.15931	0.00763	0.00001	-0.06767	//	0.0094	-0.0085	0.7575	0.3962	0.2726	-0.2600	0.2816	0.0049	0.2154	-0.0379
				//										
30.38789				//	-0.0655	-0.0448	0.7220	-0.5979	-0.1886	0.1650	-0.0744	-0.0157	0.2034	0.0710
				//										
42.88741	0.09812	-0.00003	0.23195	//	0.2750	0.2568	-0.5153	0.5731	0.3824	-0.3258	-0.0819	0.0176	-0.0264	-0.0661
				//										
47.75029				//	-0.0102	-0.0050	0.2920	0.5880	-0.3333	0.3351	-0.5764	0.0039	-0.1123	0.0245
				//										
46.59290	0.02742	0.00001	0.11765	//	-0.0265	-0.0579	0.0976	-0.5589	0.4391	-0.5812	-0.3054	-0.0636	-0.1904	-0.0994
				//										
40.11348				//	0.0397	-0.0335	0.1984	-0.1078	0.4491	-0.5689	-0.5535	-0.0527	-0.2811	-0.1812
				//										
45.05157	0.01308	-0.00000	0.08264	//	0.0128	0.0286	0.0396	-0.1092	0.6431	0.5964	-0.0238	0.4381	-0.0371	-0.1497
				//										
37.14494				//	-0.1834	0.2025	0.0370	-0.0313	0.6095	0.5367	-0.0463	0.4924	-0.0412	-0.1308
				//										
49.69754	0.00976	-0.00001	-0.06794	//	0.0496	0.0414	-0.2930	-0.3430	0.1303	-0.1368	0.8383	-0.0131	0.2300	-0.0285
				//										
38.65663				//	0.0702	0.0746	0.5476	0.5243	0.2720	-0.2630	0.4491	0.0038	0.2642	0.0065
				//										
51.49995	0.00706	0.00000	-0.05678	//	-0.1555	0.1241	-0.0138	-0.0122	-0.2582	-0.3226	-0.0126	0.8720	0.0456	0.1636
				//										
50.88701				//	-0.1843	0.1515	0.0556	-0.0046	-0.4388	-0.3524	0.1046	0.7243	-0.1816	-0.2341
				//										
57.79507	0.21830	-0.00000	-0.29803	//	-0.0359	-0.0199	-0.0676	-0.0805	-0.1136	-0.0245	-0.2674	0.0326	0.7424	-0.5916
				//										
55.82042				//	0.1334	0.0925	-0.1691	-0.0015	-0.0503	-0.0407	-0.2546	0.0209	0.7495	-0.5603
				//										
54.63767	0.39958	0.00001	-0.41470	//	-0.1000	-0.0371	-0.0834	-0.0594	0.2342	0.0372	-0.2044	-0.1043	0.5549	0.7493
				//										
49.85580				//	-0.0846	0.1451	-0.1404	0.0073	0.0670	-0.2169	-0.2761	0.2827	0.4199	0.7536
				//										

TRIPHENYLENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	0.	0.	0.8660	1.7320
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	4.5000	5.0000	4.5000

1.7320	2.5980	3.4640	4.3300	4.3300	3.4640	2.5980	1.7320	1.7320
3.5000	3.0000	3.5000	3.0000	2.0000	1.5000	2.0000	1.5000	0.5000

TRIPHENYLENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 S	3 A	4 S	5 S	6 A	7 A	8 S	9 A	10A	11 S	12 S	13 S	14 A	15 A	16 S	17 A	18 A
1.779158	1.549493	1.549488	1.312312	1.277403	1.277394	1.144550	1.088127	1.088103	0.781394	0.781378	0.764702	0.675490	0.675487	0.659838	0.558716	0.558716	0.478234
0.132889	-0.318228	-0.152984	0.337730	-0.162249	-0.268706	0.191464	-0.338701	0.023646	-0.027882	0.335220	0.187059	-0.269260	-0.209489	0.343358	0.127822	0.286748	-0.110257
0.132889	-0.293369	-0.196483	0.337662	-0.313891	-0.005578	-0.191462	-0.149864	-0.304703	-0.304150	-0.143716	0.187073	0.043551	0.338385	-0.343308	-0.175302	-0.260437	0.110255
0.191606	-0.244236	-0.235088	0.113967	-0.228666	0.272597	-0.343253	0.233470	-0.210621	0.247129	-0.219609	-0.341997	0.222930	-0.242402	0.135192	0.234518	0.231334	-0.174874
0.335100	-0.182997	-0.245471	-0.199195	0.019080	0.328292	-0.110556	0.299556	0.171519	0.131475	0.305917	0.121366	-0.329151	-0.010184	0.174756	-0.287220	-0.209198	0.352033
0.335100	0.180788	-0.247103	-0.199195	-0.018627	0.328318	0.110556	-0.299014	0.172463	-0.131717	0.305812	0.121367	0.329231	-0.007129	-0.174756	0.294448	-0.198894	-0.352033
0.191606	0.242117	-0.237269	0.113967	0.229043	0.272281	0.343252	-0.234132	-0.209885	-0.246955	-0.219804	-0.341997	-0.220671	-0.244460	-0.135193	-0.242564	0.222884	0.174874
0.132889	0.291595	-0.199107	0.337661	0.313884	-0.006012	0.191461	0.148903	-0.305174	0.304264	-0.143475	0.187073	-0.046690	0.337966	0.343309	0.184415	-0.254065	-0.110255
0.132889	0.316843	-0.155832	0.337730	0.161879	-0.268930	-0.191464	0.338773	0.022579	0.027617	0.335242	0.187059	0.271193	-0.206981	-0.343358	-0.137897	0.282041	0.110257
0.191603	0.325708	-0.093980	0.114131	-0.121660	-0.334305	-0.343234	0.065635	0.307532	-0.313765	-0.104202	-0.341982	-0.321362	-0.071804	0.135300	0.083087	-0.318765	-0.174873
0.335102	0.304082	-0.035745	-0.199079	-0.293881	-0.147705	-0.110533	-0.298327	0.173664	0.199191	-0.266825	0.121365	0.155804	0.290166	0.174678	-0.037562	0.353334	0.352036
0.335104	0.123611	0.280110	-0.199066	-0.275082	-0.180366	0.110505	0.000162	-0.345185	0.330695	-0.038837	0.121334	-0.170841	-0.281601	-0.174670	-0.319464	-0.155556	-0.352036
0.191612	0.084427	0.328316	0.114030	-0.350330	0.062283	0.343155	0.298876	-0.097844	-0.066889	0.323786	-0.341948	-0.101430	0.313337	-0.135222	0.314313	0.098627	0.174878
0.132895	0.026634	0.352082	0.337591	-0.151683	0.274976	0.191427	0.189864	0.281520	-0.276376	-0.191769	0.187052	0.316137	-0.128510	0.343241	-0.312236	-0.032678	-0.110256
0.132895	-0.023475	0.352307	0.337591	0.152063	0.274766	-0.191427	-0.188975	0.282117	0.276528	-0.191550	0.187052	-0.314931	-0.131437	-0.343241	0.313197	-0.021599	0.110256
0.191612	-0.081479	0.329060	0.114028	0.350417	0.061799	-0.343155	-0.299183	-0.096900	0.066632	0.323838	-0.341949	0.098518	0.314264	0.135223	-0.317609	0.087433	-0.174878
0.335104	-0.121093	0.281207	-0.199067	0.274833	-0.180746	-0.110505	-0.001250	-0.345182	-0.330664	-0.039099	0.121335	0.173447	-0.280004	0.174670	0.324773	-0.144145	0.352036
0.335102	-0.304391	-0.033016	-0.199080	0.293676	-0.148111	0.110533	0.298874	0.172723	-0.198980	-0.266983	0.121366	-0.158490	-0.288708	-0.174677	0.025025	0.354443	-0.352036
0.191603	-0.326538	-0.091054	0.114131	0.121198	-0.334473	0.343235	-0.064665	0.307736	0.313847	-0.103954	-0.341983	0.322015	-0.068819	-0.135300	-0.071745	-0.321508	0.174873

TRIPHENYLENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 S	3 A	4 S	5 S	6 A	7 A	8 S	9 A	10A	11S	12 S	13 S	14 A	15 A	16 S	17 A	18 A
33.01507	26.73461	26.73444	17.94124	16.37133	16.37092	9.52106	6.10565	6.10409	-21.09076	-21.09280	-23.19669	-36.21684	-36.21733	-38.86411	-59.54264	-59.54276	-82.25010
0.099628	0.124045	-0.255096	0.294816	0.237845	-0.143391	0.178966	-0.022157	-0.324734	-0.379235	-0.031392	0.213910	0.253366	-0.328794	0.422696	-0.380535	0.177773	-0.159436
0.099628	0.158901	-0.234968	0.294756	0.005127	-0.277722	-0.178964	0.292330	-0.143209	0.162445	-0.344142	0.213927	-0.411469	0.054900	-0.422635	0.344215	-0.240660	0.159432
0.143649	0.189736	-0.195359	0.099486	-0.241049	-0.202487	-0.320846	0.201559	0.224136	0.248546	0.279473	-0.391090	0.296191	0.269873	0.166430	-0.303883	0.319180	-0.252874
0.251227	0.197857	-0.146125	-0.173884	-0.290478	0.016681	-0.103339	-0.164880	0.286913	-0.346015	0.148871	0.138788	0.010533	-0.400538	0.215136	0.273024	-0.389151	0.509054
0.251227	0.197857	0.146125	-0.173884	-0.290478	-0.016681	0.103339	-0.164879	-0.286913	-0.346014	-0.148871	0.138788	0.010532	0.400538	-0.215136	0.273024	0.389151	-0.509054
0.143649	0.189736	0.195359	0.099486	-0.241049	0.202488	0.320845	0.201560	-0.224136	0.248547	-0.279473	-0.391089	0.296191	-0.269873	-0.166431	-0.303884	-0.319180	0.252874
0.099628	0.158901	0.234968	0.294756	0.005128	0.277723	0.178963	0.292330	0.143209	0.162445	0.344143	0.213926	-0.411469	-0.054900	0.422636	0.344215	0.240660	-0.159432
0.099628	0.124045	0.255095	0.294816	0.237845	0.143392	-0.178966	-0.022157	0.324734	-0.379235	0.031392	0.213910	0.253366	0.328794	-0.422697	-0.380535	-0.177773	0.159436
0.143647	0.074324	0.261994	0.099629	0.295861	-0.107439	-0.320829	-0.294914	0.062457	0.117740	-0.355002	-0.391072	0.085550	-0.391410	0.166563	0.428359	0.103586	-0.252873
0.251229	0.027620	0.244411	-0.173783	0.130866	-0.259931	-0.103317	-0.166032	-0.286257	0.301939	0.225221	0.138787	-0.352167	0.191206	0.215040	-0.473521	0.041872	0.509058
0.251231	-0.225470	0.098293	-0.173771	0.159752	-0.243279	0.103291	0.330911	0.000677	0.044083	0.374091	0.138751	0.341661	-0.209454	-0.215031	0.200507	-0.431012	-0.509058
0.143653	-0.264054	0.066641	0.099540	-0.054893	-0.310005	0.320755	0.093346	0.286669	-0.366318	-0.075525	-0.391034	-0.381812	-0.121642	0.166468	-0.124479	0.422772	0.252881
0.099632	-0.282938	0.020128	0.294695	-0.243201	-0.134375	0.178931	-0.270165	0.181589	0.216818	-0.312744	0.213903	0.158143	0.383921	0.422552	0.036312	-0.418430	-0.159435
0.099632	-0.282938	-0.020128	0.294695	-0.243200	0.134376	-0.178931	-0.270166	-0.181589	0.216818	0.312744	0.213902	0.158142	-0.383921	-0.422552	0.036313	0.418430	0.159435
0.143653	-0.264054	-0.066641	0.099539	-0.054892	0.310005	-0.320755	0.093345	-0.286669	-0.366318	0.075524	-0.391034	-0.381812	0.121642	0.166468	-0.124479	-0.422772	-0.252881
0.251231	-0.225469	-0.098293	-0.173772	0.159753	0.243278	-0.103292	0.330911	-0.000677	0.044084	-0.374091	0.138752	0.341661	0.209454	0.215030	0.200507	0.431012	0.509058
0.251229	0.027620	-0.244411	-0.173784	0.130866	0.259931	0.103318	-0.166032	0.286257	0.301940	-0.225221	0.138787	-0.352167	-0.191206	-0.215039	-0.473521	0.041872	-0.509058
0.143647	0.074324	-0.261994	0.099628	0.295861	0.107438	0.320829	-0.294914	-0.062457	0.117740	0.355001	-0.391073	0.085550	0.391410	-0.166563	0.428359	-0.103587	0.252873

TRIPHENYLENE IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.01372	0.62888	-0.01657	-0.27367	-0.00230	0.10587	-0.00188	-0.10027	0.00726	0.11471	0.00230	-0.02171	-0.00188	0.04154	-0.00112	-0.10421	-0.00924	0.69392
2	0.62888	1.01373	0.69390	-0.00924	-0.10421	-0.00112	0.04155	-0.00188	-0.02172	0.00230	0.11473	0.00726	-0.10029	-0.00188	0.10588	-0.00230	-0.27369	-0.01657
3	-0.01657	-0.69390	1.01582	0.60159	0.01023	-0.12017	-0.00112	0.10587	-0.00536	-0.13139	-0.01195	0.04318	0.00726	-0.02171	-0.00537	0.00643	0.02311	-0.33148
4	-0.27367	-0.00924	0.60159	0.97046	0.42952	0.01023	-0.10421	-0.00230	0.00644	0.00724	-0.15054	-0.01195	0.11472	0.00230	-0.13140	0.00724	0.55934	0.02310
5	-0.00230	-0.10421	0.01023	0.42952	0.97046	0.60159	-0.00924	-0.27367	0.02310	0.55934	0.00724	-0.13140	0.00230	0.11472	-0.01195	-0.15054	0.00724	0.00644
6	0.10587	-0.00112	-0.12017	0.01023	0.60159	1.01582	0.69390	-0.01657	-0.33148	0.02311	0.00643	-0.00537	-0.02171	0.00726	0.04318	-0.01195	-0.13139	-0.00536
7	-0.00188	0.04155	-0.00112	-0.10421	0.00924	0.69390	1.01373	0.62888	-0.01657	-0.27369	-0.00230	0.10588	-0.00188	-0.10029	0.00726	0.11473	0.00230	-0.02172
8	-0.10027	-0.00188	0.10587	-0.00230	-0.27367	-0.01657	0.62888	1.01372	0.69392	-0.00924	-0.10421	-0.00112	0.04154	-0.00188	-0.02171	0.00230	0.11471	0.00726
9	0.00726	-0.02172	-0.00536	0.00644	0.02310	-0.33148	-0.01657	0.69392	1.01582	0.60157	0.01023	-0.12017	-0.00112	0.10588	-0.00536	-0.13140	-0.01195	0.04319
10	0.11471	-0.00230	-0.13139	0.00724	0.55934	0.02311	-0.27369	-0.00924	0.60157	0.97046	0.42955	0.01023	-0.10422	-0.00230	0.00644	0.00724	-0.15053	-0.01195
11	0.00230	-0.11473	-0.01195	-0.15054	0.00724	0.00643	-0.00230	-0.10421	0.01023	0.42955	0.97046	0.60158	-0.00924	-0.27368	0.02310	-0.55932	0.00724	-0.13140
12	-0.02171	0.00726	0.04318	-0.01195	-0.13140	-0.00537	0.10588	-0.00112	-0.12017	0.01023	0.60158	1.01581	0.69392	-0.01657	-0.33146	0.02310	0.00644	-0.00536
13	-0.00188	-0.10029	0.00726	0.11472	-0.00230	-0.02171	-0.00188	0.04154	-0.00112	-0.10422	-0.00924	0.69392	1.01373	0.62886	-0.01657	-0.27368	-0.00230	0.10588
14	0.04154	-0.00188	-0.02171	0.00230	0.11472	0.00726	-0.10029	-0.00188	0.10588	-0.00230	-0.27368	-0.01657	0.62886	1.01373	0.69392	-0.00924	-0.10422	-0.00112
15	-0.00112	0.10588	-0.00537	-0.13140	-0.01195	0.04318	0.00726	-0.02171	-0.00536	0.00644	0.02310	-0.33146	-0.01657	0.69392	1.01581	-0.60158	0.01023	-0.12017
16	-0.10421	-0.00230	0.00643	0.00724	-0.15054	-0.01195	0.11473	0.00230	-0.13140	0.00724	0.55932	0.02310	-0.27368	-0.00924	0.60158	0.97046	0.42955	-0.01023
17	-0.00924	-0.27369	0.02311	0.55934	0.00724	-0.13139	0.00230	0.11471	-0.01195	-0.15053	0.00724	0.00644	-0.00230	-0.10422	0.01023	0.42955	0.97046	0.60157
18	0.69392	-0.01657	-0.33148	0.02310	0.00644	-0.00536	-0.02172	0.00726	0.04319	-0.01195	-0.13140	-0.00536	0.10588	-0.00112	-0.12017	0.01023	0.60157	1.01582

TRIPHENYLENE

IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.78481	-0.45103	-0.09191	-0.28782	0.01931	0.11343	-0.00592	-0.10765	0.00136	0.12283	0.00914	-0.02491	-0.00592	0.04533	0.00803	-0.10316	-0.07473	0.51787
2	0.45103	0.78483	0.51786	-0.07473	-0.10316	0.00802	0.04533	-0.00592	-0.02492	0.00915	0.12284	0.00136	-0.10766	-0.00591	0.11344	0.01930	-0.28783	-0.09192
3	-0.09191	0.51786	0.79522	0.43150	-0.05903	-0.13416	0.00802	0.11343	0.00279	-0.13419	0.00256	0.04715	0.00137	-0.02491	0.00278	-0.01428	-0.02969	-0.34724
4	-0.28782	-0.07473	0.43150	0.71738	0.25886	-0.05903	-0.10316	0.01931	0.01430	-0.04669	-0.16229	0.00257	0.12285	0.00914	-0.13421	-0.04669	0.39933	-0.02969
5	0.01931	-0.10316	-0.05903	0.25886	0.71738	0.43150	-0.07473	-0.28782	-0.02969	0.39933	-0.04669	-0.13421	0.00914	0.12285	0.00257	-0.16229	-0.04669	0.01430
6	0.11343	0.00802	-0.13416	-0.05903	0.43150	0.79522	0.51786	-0.09191	-0.34724	-0.02969	0.01428	0.00278	-0.02491	0.00137	0.04716	0.00256	-0.13419	0.00279
7	-0.00592	-0.04533	0.00802	-0.10316	-0.07473	0.51786	0.78483	0.45103	-0.09192	-0.28783	0.01930	0.11344	-0.00591	-0.10766	0.00136	0.12284	0.00915	-0.02492
8	-0.10765	-0.00592	0.11343	0.01931	-0.28782	-0.09191	0.45103	0.78481	0.51787	-0.07473	-0.10316	0.00803	0.04533	-0.00592	-0.02491	0.00914	0.12283	0.00136
9	0.00136	-0.02492	0.00279	0.01430	-0.02969	-0.34724	-0.09192	0.51787	0.79522	0.43148	-0.05903	-0.13416	0.00802	0.11344	0.00279	-0.13420	-0.00256	-0.04715
10	-0.12283	-0.00915	-0.13419	-0.04669	0.39933	-0.02969	-0.28783	-0.07473	0.43148	0.71738	0.25889	-0.05903	-0.10318	0.01930	0.01430	-0.04668	-0.16229	0.00256
11	0.00914	-0.12284	0.00256	-0.16229	-0.04669	0.01428	0.01930	-0.10316	-0.05903	0.25889	0.71738	0.43148	-0.07473	-0.28782	-0.02969	0.39931	-0.04668	-0.13420
12	-0.02491	0.00136	-0.04715	0.00257	-0.13421	0.00278	0.11344	0.00803	-0.13416	-0.05903	0.43148	0.79521	0.51787	-0.09192	-0.34722	-0.02969	0.01430	0.00279
13	-0.00592	-0.10766	0.00137	0.12285	0.00914	-0.02491	-0.00591	0.04533	0.00802	-0.10318	-0.07473	0.51787	0.78483	0.45102	-0.09192	-0.28782	0.01930	-0.11344
14	0.04533	-0.00591	-0.02491	0.00914	0.12285	0.00137	-0.10766	-0.00592	0.11344	0.01930	-0.28782	-0.09192	0.45102	0.78483	0.51787	-0.07473	-0.10318	0.00802
15	0.00803	0.11344	0.00278	-0.13421	0.00257	0.04716	0.00136	-0.02491	0.00279	0.01430	-0.02969	-0.34722	-0.09192	0.51787	0.79521	0.43148	-0.05903	-0.13416
16	-0.10316	0.01930	0.01428	-0.04669	-0.16229	0.00256	0.12284	0.00914	-0.13420	-0.04668	0.39931	-0.02969	-0.28782	-0.07473	0.43148	0.71738	0.25889	-0.05903
17	-0.07473	-0.28783	-0.02969	0.39933	-0.04669	-0.13419	0.00915	0.12283	0.00256	-0.16229	-0.04668	0.01430	0.01930	-0.10318	-0.05903	0.25889	0.71738	0.43148
18	0.51787	-0.09192	-0.34724	-0.02969	0.01430	0.00279	-0.02492	0.00136	0.04715	0.00256	-0.13420	0.00279	0.11344	0.00802	-0.13416	-0.05903	0.43148	0.79522

ENERGIES FOR TRIPHENYLENE ,IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	8,10	9,11	8,11	7,11	5,10	6,11	5,11	4,10	4,11	2,10
XMOMNT	-0.79356	-0.79358	-0.00000	-0.16767	-0.00550	-0.00546	-0.00000	-0.03177	-0.00000	-0.06249
YMOMNT	-0.00000	-0.00000	0.79360	-0.00000	-0.00000	0.00000	0.00546	-0.00000	0.03177	0.00000
JUMP E	27.1964	27.1969	27.1985	30.6139	37.4621	37.4637	37.4641	39.0320	39.0340	47.8254
DIAG E	37.0362	37.0366	38.0835	42.6631	51.3077	51.3092	49.4454	53.3671	53.3686	63.6488
DIAG E	37.0825	37.0830	38.1299	42.2091	51.2957	51.2972	49.4335	53.2230	53.2245	63.5832
CORRSP	32.1372	41.7399	38.0315	42.0510	48.7696	53.9580	49.4606	53.7802	53.4054	63.9327
CORRSP	32.1824	41.9655	38.0983	41.4690	48.7564	53.9969	49.4262	53.6438	53.2635	63.7595

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
32.13725	0.00000	-0.00065	-0.00000	//	0.7082	-0.7055	-0.0000	0.0001	-0.0081	0.0100	-0.0000	-0.0007	-0.0000	-0.0242
				//										
30.20297				//	0.7200	0.6869	-0.0000	0.0575	0.0380	0.0318	0.0000	0.0488	0.0000	-0.0388
				//										
41.73989	2.04591	-1.07361	-0.00000	//	0.6293	0.6326	-0.0000	0.4461	-0.0410	-0.0454	-0.0000	0.0100	-0.0000	-0.0294
				//										
31.99794				//	-0.6879	0.7236	-0.0000	0.0015	-0.0296	0.0268	0.0000	0.0008	0.0000	0.0399
				//										
42.05100	0.22999	0.35863	-0.00000	//	-0.3107	-0.3131	-0.0000	-0.8520	-0.1426	-0.1391	-0.0000	0.1982	0.0000	0.0225
				//										
37.21156				//	-0.0423	-0.0421	-0.0000	0.9975	0.0276	0.0275	-0.0000	-0.0006	0.0000	-0.0005
				//										
48.76963	0.00004	0.00463	0.00000	//	-0.0282	-0.0247	0.0000	0.2040	0.7000	0.6804	0.0000	0.0272	-0.0000	-0.0571
				//										
44.59722				//	-0.0564	-0.0015	-0.0000	-0.0240	0.9612	-0.1822	-0.0000	0.1632	-0.0000	-0.1118
				//										
53.95795	0.00001	-0.00217	0.00000	//	-0.0249	-0.0113	0.0000	0.0742	-0.6372	0.6554	0.0000	-0.3856	-0.0000	0.0975
				//										
44.79138				//	-0.0103	-0.0472	0.0000	-0.0329	0.1388	0.9591	-0.0000	0.2392	0.0000	-0.0037
				//										
53.78020	0.00337	-0.03837	0.00000	//	0.0544	-0.0574	-0.0000	-0.1663	-0.2552	0.2887	0.0000	0.8993	-0.0000	0.0945
				//										
48.55761				//	-0.0222	-0.0236	0.0000	0.0100	-0.2011	-0.2104	0.0000	0.9559	0.0000	0.0184
				//										
63.93271	0.02678	-0.09925	0.00000	//	0.0388	0.0029	0.0000	0.0142	0.1296	-0.0509	-0.0000	-0.0506	0.0000	0.9881
				//										
59.64472				//	0.0498	-0.0022	-0.0000	-0.0003	0.1153	-0.0129	-0.0000	0.0035	0.0000	0.9920
				//										

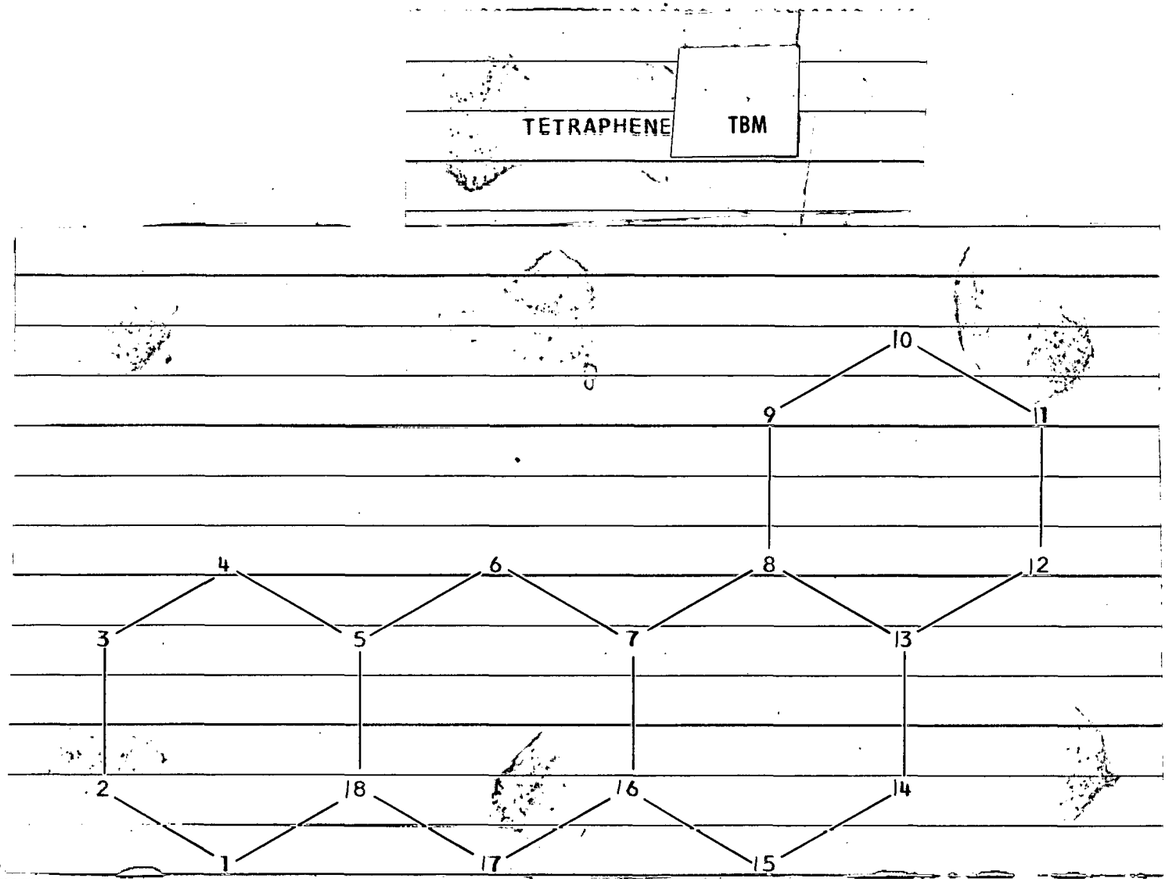
ENERGIES FOR TRIPHENYLENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	9,10	8,11	9,12	7,10	7,12	6,10	5,11	4,11	6,12	3,10
XMOMNT	0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000	-0.00000	-0.00000	0.00000	0.00000
YMOMNT	-0.79352	0.79360	0.22506	0.16778	0.00005	-0.00547	0.00546	0.03177	0.51683	-0.06249
JUMP E	27.1948	27.1985	29.3008	30.6118	32.7178	37.4617	37.4641	39.0340	39.5676	47.8252
DIAG E	38.0799	38.0835	41.4370	42.6608	47.5655	49.4435	49.4454	53.3686	55.9031	63.0432
DIAG E	38.1263	38.1299	42.1244	42.2067	47.7524	49.4315	49.4335	53.2245	56.5321	62.9776
CORRSP	41.5301	33.5073	39.4790	42.7265	46.3569	49.1997	52.1364	52.8364	57.5494	63.7086
CORRSP	41.5692	33.5955	42.7084	39.7907	46.5464	49.2938	52.1431	52.7905	57.9017	63.5994

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
41.53013	1.90847	0.00000	-1.03953	//	0.6155	-0.6267	-0.1932	-0.4201	-0.0039	0.0157	-0.0071	0.0063	0.1110	-0.0441
29.41548				//	0.6383	-0.6451	-0.3366	-0.1981	-0.0044	0.0773	-0.0729	-0.0354	-0.1017	-0.0299
33.50730	0.00001	-0.00000	-0.00207	//	0.6942	0.6867	-0.0038	-0.0008	0.2086	0.0182	0.0131	-0.0014	0.0033	-0.0507
25.42705				//	0.6383	0.6321	-0.0036	-0.0031	0.4254	-0.0731	-0.0770	0.0004	0.0033	-0.0253
39.47902	0.12855	0.00000	0.27671	//	-0.0530	0.0594	0.7758	-0.4885	0.0015	-0.2056	0.2027	0.2021	0.1691	0.0188
30.29359				//	0.2620	-0.2576	0.6361	0.5984	0.0034	-0.1424	0.1384	0.0808	-0.2359	0.0269
42.72647	0.18672	0.00000	-0.32057	//	0.3265	-0.3259	0.5215	0.7033	0.0003	-0.0281	0.0273	-0.1210	-0.0668	0.0034
39.29484				//	-0.0768	0.1056	-0.5725	0.6590	-0.0300	0.1138	-0.0697	-0.3379	-0.2947	0.0341
46.35694	0.00038	0.00000	-0.01394	//	-0.1070	-0.1162	-0.0056	-0.0021	0.8075	-0.4073	-0.3946	-0.0005	-0.0056	0.0353
38.59474				//	-0.2707	-0.2635	-0.0308	0.0206	0.6330	-0.4786	-0.4719	-0.0221	-0.0247	0.0488
49.19970	0.04914	0.00000	0.15325	//	-0.0229	0.0079	0.2333	-0.0639	0.0204	0.6718	-0.6590	0.1535	0.1654	-0.0633
51.50582				//	-0.1538	-0.1589	0.0044	0.0066	0.6452	0.5071	0.5226	-0.0305	0.0244	-0.0548
52.13644	0.00159	-0.00000	0.02677	//	-0.1044	-0.0943	-0.0066	0.0117	0.5503	0.5572	0.5991	0.0030	0.0244	-0.0853
49.94632				//	0.0101	-0.0152	-0.3890	0.2156	0.0058	-0.3944	0.3993	0.6610	0.2208	-0.0324
52.83640	0.11743	0.00000	0.22861	//	0.0265	-0.0240	-0.1810	0.2852	-0.0120	-0.1185	0.0898	0.8110	0.4521	-0.0153
43.42370				//	0.0132	-0.0345	0.0309	0.2757	0.0160	0.5326	-0.5484	0.4584	0.3352	-0.1202
57.54938	0.66733	0.00000	-0.52219	//	-0.0679	0.0523	-0.0322	0.0685	-0.0166	-0.0780	0.0168	-0.5015	0.8178	-0.2449
53.95823				//	0.0856	-0.0947	0.0313	0.1982	-0.0271	-0.1682	0.0881	-0.4673	0.7343	-0.3860
63.70862	0.00288	0.00000	0.03258	//	0.0410	0.0168	-0.0222	0.0066	0.0269	-0.0927	0.0263	-0.1079	0.2313	0.9604
60.44256				//	0.0776	-0.0407	-0.0031	0.0786	0.0085	0.0417	0.0300	-0.1058	0.3815	0.9092



ATOMIC COORDINATES

x	0.8660	0.	0.	-0.8660	1.7320	2.5980	3.4640	4.3300	4.3300
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	2.0000	3.0000

	5.1960	6.0620	6.0620	5.1960	5.1960	4.3300	3.4640	2.5980	1.7320
	3.5000	3.0000	2.0000	1.5000	0.5000	0.	0.5000	0.	0.5000

TETRAPHENE TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1.613232	1.536936	1.433052	1.365246	1.326543	1.287682	1.246811	1.176455	1.111639	0.888359	0.823543	0.753187	0.712316	0.673455	0.634752	0.566946	0.463062	0.386766
0.151287	-0.276117	0.183190	-0.246103	-0.176850	0.241909	0.316221	-0.110635	-0.323597	-0.323597	-0.110635	0.316221	0.241909	-0.176849	-0.246103	-0.183190	-0.276117	-0.151286
0.102459	-0.232517	0.267139	0.248822	0.112887	0.441600	-0.000000	-0.238406	-0.193832	0.193832	0.238406	0.000000	-0.441600	-0.112887	0.248821	0.267139	0.232517	0.102459
0.103289	-0.229732	0.285543	0.122123	0.326221	0.272831	-0.316238	-0.059814	0.235934	0.235934	-0.059814	-0.316237	0.272832	0.326221	-0.122123	-0.285542	-0.229732	-0.103289
0.154180	-0.267274	0.233883	0.068084	0.318724	-0.123567	-0.316237	0.195630	0.300541	-0.300541	-0.195630	0.316237	0.123567	-0.318724	-0.068084	0.233883	0.267274	0.154180
0.279788	-0.351720	0.124825	-0.222878	0.095466	-0.416860	0.000001	0.199678	-0.099991	-0.099991	0.199678	-0.000000	-0.416860	0.095466	0.222877	-0.124825	-0.351720	-0.279787
0.267569	-0.129735	-0.069140	-0.377112	0.154431	-0.202697	0.000033	-0.212173	-0.393228	0.393228	0.212172	-0.000032	0.202698	-0.154431	-0.377112	-0.069147	0.129735	0.267569
0.385016	0.069483	-0.246150	-0.335193	0.108853	0.180598	0.000033	-0.351369	-0.077876	-0.077877	-0.351369	0.000032	0.180597	0.108853	0.335194	0.246150	0.069483	-0.385017
0.345551	0.289375	0.064829	-0.221827	0.142205	0.266557	0.316204	0.102490	0.204163	-0.204163	-0.102490	-0.316205	-0.266556	-0.142205	-0.221827	0.064829	-0.289375	0.345551
0.187884	0.223543	0.215242	-0.245362	-0.172758	0.300527	-0.000066	0.433618	0.003104	0.003104	0.433618	-0.000065	0.300527	-0.172758	0.245362	-0.215242	0.223543	-0.187884
0.121286	0.196955	0.312835	-0.141285	-0.370764	0.083749	-0.316254	0.207526	-0.202749	0.202748	-0.207527	0.316254	-0.083750	0.370765	-0.141285	0.312835	-0.196955	0.121286
0.113466	0.204930	0.333653	0.036281	-0.317781	-0.202909	-0.316188	-0.285249	-0.094812	-0.094813	-0.285248	-0.316189	-0.202909	-0.317781	-0.036281	-0.333653	0.204930	-0.113466
0.160640	0.248881	0.272602	0.194985	-0.049677	-0.320275	0.000066	-0.411484	0.159871	-0.159870	0.411484	-0.000065	0.320275	0.049677	0.194986	0.272602	-0.248881	0.160640
0.285668	0.336517	0.144667	0.252271	0.252040	-0.170412	0.316238	-0.008952	0.167121	0.167121	-0.008953	0.316237	-0.170412	0.252040	-0.252271	-0.144667	0.336517	-0.285668
0.203594	0.193844	-0.083604	0.400187	0.240944	-0.144920	-0.000032	0.302609	-0.288455	0.288454	-0.302609	0.000033	0.144920	-0.240944	0.400187	-0.083604	-0.193844	0.203594
0.220199	0.085205	-0.291350	0.339961	0.066754	0.001485	-0.316254	0.225300	-0.297589	-0.297588	0.225300	-0.316254	0.001486	0.066754	-0.339961	0.291351	0.085205	-0.220199
0.343515	-0.008481	-0.427595	0.102906	-0.152626	0.146652	-0.316222	-0.141533	0.153847	-0.153847	0.141533	0.316221	-0.146652	0.152626	0.102906	-0.427595	0.008481	0.343515
0.248306	-0.173135	-0.212763	0.147502	-0.377533	-0.011137	-0.000001	0.024864	0.445050	-0.445050	0.024863	0.000000	-0.011137	-0.377533	-0.147502	0.212763	-0.173135	-0.248306
0.273429	-0.368172	0.054283	0.115375	-0.346867	-0.159633	0.316221	0.159309	0.047461	-0.047461	-0.159308	-0.316221	0.159633	0.346867	0.115375	0.054284	0.368172	0.273429

TETRAPHENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
28.65690	26.33711	22.78134	20.16858	18.55754	16.84244	14.92332	11.30734	7.57098	-9.47403	-16.15304	-24.70400	-30.44695	-36.55408	-43.37948	-57.58402	-87.41513	119.53060
0.119111	-0.222723	0.153028	0.210626	-0.153548	0.213180	0.283198	-0.102001	-0.306918	-0.343329	-0.121913	0.364367	0.286625	-0.215501	-0.308898	-0.243294	-0.405764	-0.243263
0.080668	-0.187554	0.223155	0.212953	0.098013	0.389157	-0.000000	-0.219801	-0.183841	0.205651	0.262709	0.000000	-0.523230	-0.137559	0.312310	0.354786	0.341692	0.164750
0.081322	-0.185308	0.238528	0.104519	0.283238	0.240430	-0.283213	-0.055146	0.223773	0.250320	-0.065912	-0.364386	0.323265	0.397519	-0.153284	-0.379227	-0.337600	-0.166085
0.121389	-0.215590	0.195374	-0.058269	0.276729	-0.108893	-0.283213	0.180363	0.285050	-0.318867	-0.215572	0.364386	0.146408	-0.388383	-0.085456	0.310619	0.392770	0.247915
0.220282	-0.283706	0.104272	-0.190749	0.082887	-0.367355	0.000001	0.184095	-0.094837	-0.106088	0.220033	-0.000000	-0.493917	0.116331	0.279746	-0.165780	-0.516866	-0.449888
0.210662	-0.104648	-0.057763	0.322749	0.134083	-0.178626	0.000030	-0.195615	-0.372960	0.417206	0.233800	-0.000037	0.240167	-0.188183	-0.473334	-0.091834	0.190651	0.430240
0.303131	0.056047	-0.205622	-0.286873	0.094511	0.159150	0.000029	-0.323948	-0.073863	-0.082626	-0.387187	0.000037	0.213980	0.132644	0.420721	0.326911	0.102107	-0.619092
0.272059	0.233417	0.054155	-0.189849	0.123468	0.234901	0.283183	0.094492	0.193640	-0.216612	-0.112937	-0.364349	-0.315829	-0.173285	-0.278428	0.086099	-0.425247	0.555632
0.147925	0.180316	0.179802	-0.209992	-0.149995	0.264837	-0.000059	0.399779	0.002944	0.003293	0.477820	-0.000075	0.356079	-0.210515	0.307968	-0.285862	0.328505	-0.302111
0.095491	0.158869	0.261327	-0.120918	-0.321912	0.073803	-0.283228	0.191331	-0.192299	0.215111	-0.228682	0.364405	-0.099231	0.451798	-0.177334	0.415474	-0.289432	0.195024
0.089334	0.165302	0.278717	0.031051	-0.275910	-0.178812	-0.283169	-0.262988	-0.089925	-0.100594	-0.314326	-0.364330	-0.240417	-0.387234	-0.045539	-0.443123	0.301152	-0.182448
0.126475	0.200754	0.227718	0.166877	-0.043132	-0.282240	0.000059	-0.379372	0.151631	-0.169618	0.453430	-0.000075	0.379478	0.060534	0.244737	0.362041	-0.365739	0.258303
0.224912	0.271444	0.120848	0.215905	0.218831	-0.150175	0.283213	-0.008254	0.158508	0.177312	-0.009866	0.364386	-0.201913	0.307125	-0.316640	-0.192132	0.494525	-0.459343
0.160294	0.156359	-0.069839	0.342498	0.209197	-0.127710	-0.000029	0.278993	-0.273587	0.306043	-0.333456	0.000038	0.171708	-0.293604	0.502297	-0.111035	-0.284861	0.327372
0.173367	0.068728	-0.243380	0.290954	0.057958	0.001309	-0.283227	0.207717	-0.282250	-0.315734	0.248267	-0.364405	0.001761	0.081343	-0.426704	0.386941	0.125212	-0.354072
0.270457	0.006841	-0.357192	0.088072	-0.132516	0.129236	-0.283199	-0.130488	0.145918	-0.163229	0.155960	0.364367	-0.173761	0.185984	0.129163	-0.567887	0.012464	0.552360
0.195497	-0.139655	-0.177732	0.126238	-0.327789	-0.009815	-0.000001	0.022924	0.422112	0.472188	0.027397	0.000000	-0.013196	-0.460045	-0.185138	0.282570	-0.254429	-0.399267
0.215277	-0.296977	0.045346	0.098743	-0.301164	-0.140675	0.203198	0.146877	0.045014	-0.050355	-0.175548	-0.364368	0.189142	0.422677	0.144814	-0.072094	0.541043	0.439664

TETRAPHENE

TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.00000	0.73168	-0.00000	-0.36389	0.00000	0.09042	-0.00000	-0.01684	-0.00000	0.02995	-0.00000	-0.04275	0.00000	0.08527	-0.00000	-0.14070	0.00000	0.54220
2	0.73168	1.00000	0.59301	-0.00000	-0.22639	0.00000	0.13007	-0.00000	-0.05409	0.00000	0.04608	0.00000	-0.04924	0.00000	0.04334	0.00000	-0.18833	-0.00000
3	-0.00000	0.59301	1.00000	0.73054	-0.00000	-0.18675	0.00000	0.04358	-0.00000	-0.03797	0.00000	0.03958	-0.00000	-0.09117	0.00000	0.12577	0.00000	-0.22525
4	-0.36389	-0.00000	0.73054	1.00000	0.54492	0.00000	-0.14747	-0.00000	0.05970	-0.00000	-0.04446	-0.00000	0.04124	0.00000	-0.00874	-0.00000	0.08884	0.00000
5	0.00000	-0.22639	-0.00000	0.54492	1.00000	0.58421	0.00000	-0.09011	0.00000	0.05321	-0.00000	-0.04281	0.00000	0.12367	-0.00000	-0.19313	0.00000	0.49511
6	0.09042	0.00000	-0.18675	0.00000	0.58421	1.00000	0.64562	-0.00000	-0.16380	0.00000	0.11374	-0.00000	-0.12540	0.00000	0.03804	-0.00000	-0.37668	-0.00000
7	-0.00000	0.13007	0.00000	-0.14747	0.00000	0.64562	1.00000	0.44653	0.00000	-0.10328	0.00000	0.03113	0.00000	-0.21103	0.00000	0.50008	0.00000	-0.19718
8	-0.01684	-0.00000	0.04358	-0.00000	-0.09011	-0.00000	0.44653	1.00000	0.59718	-0.00000	-0.27151	0.00000	0.54625	-0.00000	-0.24266	-0.00000	0.05189	0.00000
9	-0.00000	-0.05409	-0.00000	0.05970	0.00000	-0.16380	0.00000	0.59718	1.00000	0.69483	-0.00000	-0.33790	0.00000	0.02109	-0.00000	-0.09015	0.00000	0.06720
10	0.02995	0.00000	-0.03797	-0.00000	0.05321	0.00000	-0.10328	-0.00000	0.69483	1.00000	0.62845	0.00000	-0.26586	0.00000	0.17359	-0.00000	-0.07483	-0.00000
11	-0.00000	0.04608	0.00000	-0.04446	-0.00000	0.11374	0.00000	-0.27151	-0.00000	0.62845	1.00000	0.70046	0.00000	-0.11334	-0.00000	0.08564	0.00000	-0.05887
12	-0.04275	-0.00000	0.03958	-0.00000	-0.04281	-0.00000	0.03113	0.00000	-0.33790	0.00000	0.70046	1.00000	0.58150	0.00000	-0.20130	0.00000	0.10160	0.00000
13	0.00000	-0.04924	-0.00000	0.04124	0.00000	-0.12540	0.00000	0.54625	0.00000	-0.26586	0.00000	0.58150	1.00000	0.49350	0.00000	-0.15421	-0.00000	0.07492
14	0.08527	0.00000	-0.09117	0.00000	0.12367	0.00000	-0.21103	-0.00000	0.02109	0.00000	-0.11334	0.00000	0.49350	1.00000	0.78330	0.00000	-0.23279	-0.00000
15	-0.00000	0.04334	0.00000	-0.00874	-0.00000	0.03804	0.00000	-0.24266	-0.00000	0.17359	-0.00000	-0.20130	0.00000	0.78330	1.00000	0.49370	0.00000	-0.09877
16	-0.14070	0.00000	0.12577	-0.00000	-0.19313	0.00000	0.50008	-0.00000	-0.09015	-0.00000	0.08564	0.00000	-0.15421	0.00000	0.49370	1.00000	0.62772	0.00000
17	0.00000	-0.18833	0.00000	0.08884	0.00000	-0.37668	0.00000	0.05189	0.00000	-0.07483	0.00000	0.10160	-0.00000	-0.23279	0.00000	0.62772	1.00000	0.58984
18	0.54220	-0.00000	-0.22525	0.00000	0.49511	-0.00000	-0.19718	0.00000	0.06720	-0.00000	-0.05887	0.00000	0.07492	-0.00000	-0.09877	0.00000	0.58984	1.00000

TETRAPHENE

TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.77080	0.55428	-0.05204	-0.34339	-0.03101	0.09469	0.01374	-0.01807	-0.00293	0.02994	0.00299	-0.04205	-0.00583	0.08375	0.01198	-0.13230	-0.05974	0.37436
2	0.55428	0.75998	0.41822	-0.05177	-0.20847	0.02038	0.12589	-0.00606	-0.05306	0.00188	0.04544	0.00070	-0.04828	0.00147	0.04233	0.00261	-0.17881	-0.04122
3	-0.05204	0.41822	0.76026	0.55317	-0.04160	-0.17727	0.00319	0.04262	-0.00125	-0.03756	-0.00041	0.03920	0.00194	-0.08970	-0.00790	0.12172	-0.02114	-0.20736
4	-0.34339	-0.05177	0.55317	0.77042	0.37700	-0.05879	-0.13882	0.00994	0.05812	-0.00354	-0.04380	0.00084	0.04041	-0.00743	-0.01031	0.01382	0.09315	-0.03128
5	-0.03101	-0.20847	-0.04160	0.37700	0.72195	0.41545	-0.03822	-0.08292	0.00766	0.05189	-0.00229	-0.04259	0.00141	0.11980	0.01429	-0.17769	-0.03861	0.33411
6	0.09469	0.02038	-0.17727	-0.05879	0.41545	0.78017	0.47524	-0.05014	-0.15408	0.01072	0.11064	0.00183	-0.11803	0.01844	0.04329	-0.03972	-0.35758	-0.03765
7	0.01374	0.12589	0.00319	-0.13882	-0.03822	0.47524	0.72853	0.28606	-0.04707	-0.09532	0.01484	0.03519	-0.03128	-0.19453	-0.03556	0.33862	-0.03876	-0.18157
8	-0.01807	-0.00606	0.04262	0.00994	-0.08292	-0.05014	0.28606	0.72903	0.42791	-0.04320	-0.25287	-0.03235	0.38392	-0.03898	-0.22596	-0.02871	0.05625	0.01104
9	-0.00293	-0.05306	-0.00125	0.05812	0.00766	-0.15408	-0.04707	0.42791	0.76658	0.51785	-0.04948	-0.31737	-0.03368	0.02591	0.01412	-0.08312	0.00449	0.06493
10	0.02994	0.00188	-0.03756	-0.00354	0.05189	0.01072	-0.09532	-0.04320	0.51785	0.76030	0.45334	-0.05081	-0.24745	0.01943	0.16873	0.00025	-0.07444	-0.00182
11	0.00299	0.04544	-0.00041	-0.04380	-0.00229	0.11064	0.01484	-0.25287	-0.04948	0.45334	0.75897	0.52324	-0.04091	-0.10462	0.00556	0.08210	-0.00606	-0.05755
12	-0.04205	0.00070	0.03920	0.00084	-0.04259	0.00183	0.03519	-0.03235	-0.31737	-0.05081	0.52324	0.76887	0.41323	-0.05478	-0.19126	0.01409	0.09900	-0.00355
13	-0.00583	-0.04828	0.00194	0.04041	0.00141	-0.11803	-0.03128	0.38392	-0.03368	-0.24745	-0.04091	0.41323	0.72266	0.32657	-0.04625	-0.13917	0.01660	0.07191
14	0.08375	0.00147	-0.08970	-0.00743	0.11980	0.01844	-0.19453	-0.03898	0.02591	0.01943	-0.10462	-0.05478	0.32657	0.77017	0.60464	-0.04630	-0.22252	0.00468
15	0.01198	0.04233	-0.00790	-0.01031	0.01429	0.04329	-0.03556	-0.22596	0.01412	0.16873	0.00556	-0.19126	-0.04625	0.60464	0.77012	0.32677	-0.05822	-0.09088
16	-0.13230	0.00261	0.12172	0.01382	-0.17769	-0.03972	0.33862	-0.02871	-0.08312	0.00025	0.08210	0.01409	-0.13917	-0.04630	0.32677	0.72264	0.45841	-0.03663
17	-0.05974	-0.17881	0.02114	0.09315	-0.03861	-0.35758	-0.03876	0.05625	0.00449	-0.07444	-0.00606	0.09900	0.01660	-0.22252	-0.05822	0.45841	0.78299	0.42087
18	0.37436	-0.04122	-0.20736	-0.03128	0.33411	-0.03765	-0.18157	0.01104	0.06493	-0.00182	-0.05755	-0.00355	0.07191	0.00468	-0.09088	-0.03663	0.42087	0.72127

ENERGIES FOR TETRAPHENE , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF No SYMMETRY

JUMP	9,10	8,10	9,11	7,10	6,10	8,11	5,10	4,10	7,11	3,10	6,11	2,10	1,10
XMOMNT	-0.32249	0.77424	0.77530	0.39286	-0.38718	0.00163	-0.04290	-0.01400	0.20970	0.03526	-0.22333	-0.04169	-0.00683
YMOMNT	-0.66931	0.05356	0.05363	-0.09062	0.14042	0.28933	-0.07077	-0.09215	0.54729	0.01367	0.00338	0.00721	0.00882
JUMP E	17.0450	20.7814	23.7240	24.3974	26.3165	27.4604	28.0316	29.6426	31.0764	32.2554	32.9955	35.8111	38.1309
DIAG E	28.5210	32.9651	35.4191	36.2746	39.5233	39.7031	42.6392	43.1148	44.8471	48.0264	48.4075	51.2067	51.6601
DIAG E	28.6216	33.2715	35.2967	36.8828	40.0556	39.7864	43.0114	43.5649	45.2322	48.4625	48.7167	51.8744	52.5179
CORRSP	27.8223	29.4569	34.4866	37.0882	38.6719	40.2764	39.7736	43.7094	47.2912	48.1453	49.7801	50.6848	55.1211
CORRSP	27.9583	30.0080	34.7647	37.5961	39.0147	40.3156	40.3446	44.2876	47.7213	48.5459	50.0503	51.1284	55.5589

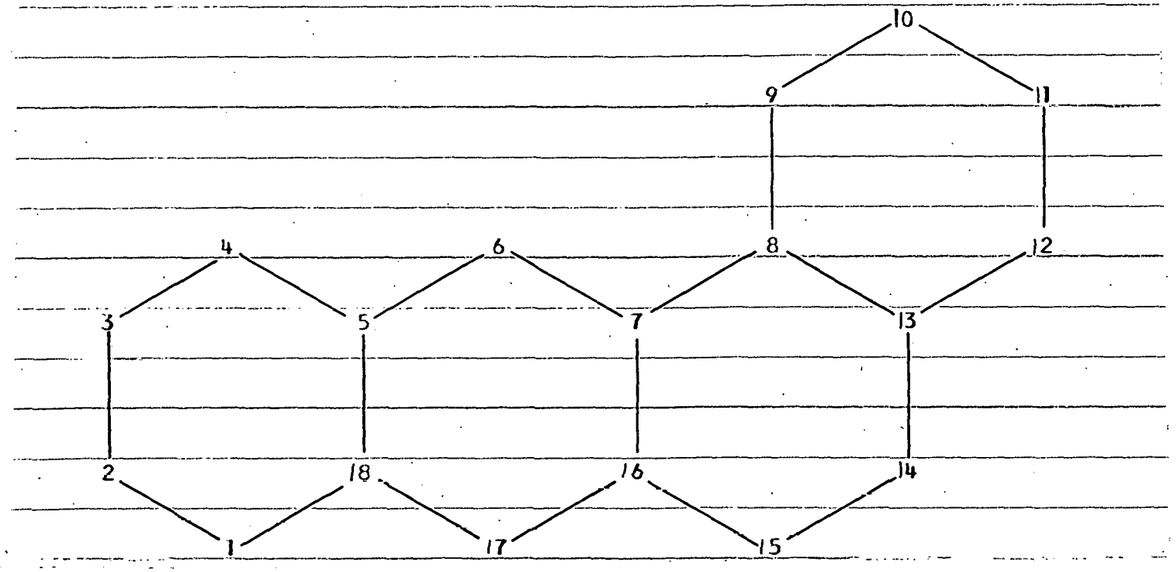
FINAL EXCITED STATES OF No SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
27.82230	0.42270	-0.23536	-0.54943	//	0.9733	0.0345	0.0551	0.0036	0.0381	0.1945	-0.0310	0.0351	0.0670	-0.0021
				//	-0.0348	0.0323	0.0168							
15.53879				//	0.9655	0.0530	0.0395	-0.0447	0.0284	0.1806	-0.1333	0.0700	-0.0665	-0.0240
				//	0.0141	-0.0090	0.0088							
29.45693	0.19851	0.38553	-0.09921	//	0.0159	0.7428	-0.5183	0.2798	-0.2294	-0.0182	-0.0582	0.0259	-0.0743	0.1523
				//	-0.1035	-0.0674	-0.0075							
23.34589				//	-0.0126	0.7430	0.5211	-0.1344	-0.1689	-0.2894	0.0082	0.1718	0.0937	0.0152
				//	-0.0822	-0.0199	-0.0111							
34.48659	0.47485	0.56522	0.06570	//	-0.0100	0.5075	0.4434	-0.6873	-0.1866	-0.1368	0.0012	0.0595	0.0349	-0.0682
				//	-0.0651	-0.0661	-0.0414							
26.84078				//	0.0267	-0.4247	0.4129	-0.5888	0.3861	-0.2659	0.0926	0.0620	0.0938	-0.2189
				//	0.0604	0.0951	0.0124							
37.08821	1.46497	0.93818	0.22061	//	-0.0611	0.0839	0.5577	0.5272	-0.3191	0.0182	-0.3255	0.0767	0.3946	0.0958
				//	0.0716	-0.1273	0.0095							
31.44476				//	-0.0530	-0.1378	0.2918	0.5616	0.3148	-0.0307	-0.4781	0.3339	0.3269	-0.0285
				//	0.1716	-0.0059	0.0195							
38.67193	0.10640	0.14487	-0.20908	//	0.0642	0.2441	0.2375	0.2420	0.6774	-0.5408	-0.1253	0.0438	-0.2083	0.0002
				//	-0.0089	0.0934	-0.0157							
34.92458				//	0.0769	0.3242	-0.2713	-0.1235	0.5516	0.2151	0.2348	0.4400	-0.1683	0.1905
				//	0.3007	0.1614	-0.1407							
40.27641	0.28416	0.21260	0.34743	//	-0.1822	0.2739	0.1814	0.0464	0.4032	0.7493	0.1125	0.2369	-0.0737	0.0628
				//	0.1898	0.1285	-0.0445							
29.37041				//	-0.1547	-0.0346	0.3274	-0.2362	-0.2525	0.8037	-0.0175	0.0201	0.2457	0.0225
				//	0.1971	-0.0319	-0.0260							
39.77362	0.25844	0.35992	-0.15249	//	0.0379	0.0912	0.2979	0.2149	-0.1428	-0.0118	0.6707	-0.5330	-0.2020	0.2260
				//	-0.0238	0.0893	0.0199							
34.39485				//	0.1014	-0.1632	0.4558	0.4243	0.0249	-0.0074	0.5937	-0.1951	-0.1893	0.3145
				//	0.1500	0.1441	-0.0777							
43.70941	0.28707	-0.07234	-0.38627	//	0.0734	-0.1065	0.0375	0.0642	-0.2601	-0.2332	0.3352	0.7073	-0.2515	0.2174
				//	0.3134	0.0593	-0.1757							
39.20799				//	0.0099	-0.2821	-0.0318	-0.0461	-0.5504	-0.2053	0.0530	0.6466	-0.2336	0.0443
				//	0.2971	-0.0754	-0.0269							

cont.

TETRAPHENE	TBM APPROXIMATION (cont.)										
47.29116	0.31145	-0.02125	0.39296	//	-0.0286	0.0066	-0.1381	-0.0898	-0.2345	-0.1131	-0.2905	0.0867	0.7284	0.3573
				//	-0.2107	0.1319	-0.3038							
43.16288				//	-0.1476	-0.0286	-0.2664	0.0058	-0.1151	-0.1334	0.3913	0.1229	0.8222	0.1069
				//	-0.0442	0.1252	-0.0456							
48.14529	0.09057	-0.19827	-0.07018	//	0.0217	-0.1188	0.0152	-0.1735	0.0477	0.0665	-0.3642	-0.2059	-0.2598	0.7290
				//	0.0975	-0.2684	-0.3047							
44.08302				//	0.0165	-0.0810	0.0054	-0.2224	0.0509	-0.1474	-0.2660	-0.1559	-0.0809	0.7531
				//	0.0925	-0.3919	-0.2975							
49.78005	0.12077	-0.21707	0.09964	//	0.0444	0.1144	-0.1360	-0.0824	-0.0101	-0.1170	-0.0709	-0.2940	0.2257	-0.0869
				//	0.8556	0.2391	-0.0822							
45.70238				//	0.0346	0.1449	-0.0907	-0.0271	-0.0049	-0.1523	0.0181	-0.3058	0.0897	-0.0893
				//	0.7493	-0.1938	0.4866							
50.68484	0.04922	0.12714	-0.08167	//	-0.0174	-0.0187	0.0575	0.0601	-0.1899	0.0505	-0.2190	-0.0761	-0.1769	-0.1566
				//	-0.2310	0.6530	-0.6037							
46.75037				//	0.0118	0.0511	-0.0482	-0.0343	-0.1757	-0.1218	-0.2599	-0.2548	0.0098	-0.0999
				//	0.3587	0.6172	-0.5440							
55.12111	0.00283	-0.00257	0.03467	//	-0.0311	-0.0241	0.0108	-0.1084	-0.0799	-0.0287	-0.1706	0.0641	0.0050	0.4117
				//	-0.0676	0.6034	0.6388							
53.36058				//	-0.0226	-0.0473	0.0118	-0.1150	-0.0648	0.0034	-0.2064	0.0476	-0.0356	0.4650
				//	-0.1389	0.5910	0.5906							

TETRAPHENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640	4.3300	4.3300
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	2.0000	3.0000

5.1960	6.0620	6.0620	5.1960	5.1960	4.3300	3.4640	2.5980	1.7320
3.5000	3.0000	2.0000	1.5000	0.5000	0.	0.5000	0.	0.5000

TETRAPHENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1.760478	1.630040	1.464516	1.352458	1.295040	1.234165	1.179839	1.099079	1.034762	0.832273	0.781307	0.722979	0.697006	0.669039	0.641427	0.591191	0.528135	0.486248
0.158052	-0.282646	0.187188	-0.227696	0.219439	0.252057	-0.320539	-0.049087	0.313237	-0.334418	-0.089960	0.296184	0.290733	0.146921	0.222611	-0.194010	-0.271251	-0.136929
0.113887	-0.250614	0.276583	-0.277672	-0.085415	0.404106	-0.006482	-0.253479	0.204240	0.212601	0.219553	0.025518	-0.441430	0.151970	-0.242362	0.257838	0.220804	0.089629
0.114529	-0.248520	0.290168	-0.179843	-0.319572	0.200012	0.315787	-0.119477	-0.241257	0.246881	-0.073042	-0.321901	0.242581	-0.338523	0.151890	-0.267465	-0.219522	-0.089996
0.160608	-0.275224	0.227634	0.024601	-0.335383	-0.185285	0.303494	0.168106	-0.293000	-0.318039	-0.158572	0.316315	0.157987	0.316412	0.025225	0.226138	0.265404	0.139158
0.278136	-0.334591	0.094083	0.220767	-0.108065	-0.403621	-0.025482	0.222462	0.103406	-0.087560	0.181979	-0.009441	-0.436388	-0.087418	-0.206627	-0.131526	-0.375328	-0.279045
0.269967	-0.125055	-0.083517	0.382445	-0.191524	-0.195087	-0.050964	-0.185120	0.403741	0.388213	0.191812	0.007122	0.213413	0.158566	0.364333	-0.074743	0.132138	0.263815
0.370781	0.061088	-0.239854	0.301303	-0.153863	0.182750	-0.024845	-0.359887	0.084869	-0.101419	-0.339919	0.002161	0.174480	-0.154810	-0.316544	0.263903	0.069205	-0.401480
0.333617	0.276941	0.051631	0.180686	-0.187013	0.296034	-0.281056	0.082604	-0.228123	-0.215886	-0.106842	-0.306614	-0.246436	0.187783	0.205056	0.080906	-0.299738	0.360222
0.195914	0.228689	0.225357	0.264120	0.089781	0.336470	0.051145	0.412579	-0.043371	0.027882	0.446277	-0.016918	0.285836	0.111894	-0.266369	-0.220530	0.209349	-0.186868
0.133119	0.213548	0.330754	0.178286	0.307859	0.087001	0.340436	0.207135	0.200298	0.188368	-0.234577	0.326992	-0.111300	-0.340299	0.175722	0.304559	-0.177855	0.115471
0.126141	0.221252	0.345267	0.007079	0.305201	-0.235921	0.269820	-0.287668	0.134186	-0.118681	-0.281856	-0.328998	-0.142393	0.347712	-0.011095	-0.324052	0.184195	-0.107239
0.167436	0.256382	0.268827	-0.178738	0.084160	-0.354805	-0.085397	-0.388673	-0.135116	-0.120899	0.434062	0.021062	-0.290593	-0.126827	-0.175451	0.282897	-0.233002	0.152739
0.282304	0.322819	0.109029	-0.269552	-0.199808	-0.155680	-0.341680	0.020301	-0.184300	0.161964	-0.041104	0.304327	-0.207952	-0.189409	0.287760	-0.176080	0.341586	-0.293453
0.210394	0.192998	-0.115193	-0.425185	-0.194743	-0.141935	-0.013482	0.318377	0.268300	0.291604	-0.295888	-0.005592	0.184956	0.186475	-0.417025	-0.062950	-0.186840	0.196099
0.225153	0.091923	-0.299264	-0.346247	-0.031295	0.000724	0.339234	0.200636	0.287193	-0.284905	0.261244	-0.303014	-0.015061	-0.037818	0.350410	0.274095	0.084659	-0.211278
0.335502	-0.006114	-0.402533	-0.074911	0.159224	0.121679	0.324877	-0.196067	-0.137685	-0.153053	0.123109	0.319971	-0.150668	-0.154428	-0.118359	-0.436866	0.010984	0.352364
0.249971	-0.167416	-0.215837	-0.072072	0.423434	-0.009899	0.034918	0.005732	-0.440295	0.427177	0.011052	-0.012972	0.030812	0.393325	0.124577	0.202028	-0.177719	-0.238446
0.272700	-0.348156	0.037794	-0.044647	0.369310	-0.123350	-0.291798	0.207967	-0.060494	-0.047895	-0.146786	-0.332993	-0.097545	-0.364207	-0.092451	0.077044	0.389788	-0.272092

TETRAPHENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
32.56546	29.13875	23.91154	19.64646	17.17509	14.30373	11.49111	6.79603	2.53261	-15.19283	-21.10155	-28.88603	-32.77161	-37.29292	-42.14361	-52.13081	-67.35568	-79.65206
0.119120	-0.221383	0.154679	-0.195791	0.192829	0.226888	-0.295100	-0.046822	0.307930	-0.366570	-0.101774	0.348336	0.348238	0.179621	0.277955	-0.252325	-0.373250	-0.196365
0.085834	-0.196294	0.228549	-0.238765	-0.075057	0.363754	-0.005968	-0.241784	0.200780	0.233041	0.248387	0.030012	-0.528742	0.185794	-0.302615	0.335338	0.303833	0.128535
0.086318	-0.194654	0.239774	-0.154643	-0.280819	0.180040	0.290725	-0.113965	-0.237170	0.270617	-0.082635	-0.378582	0.290562	-0.413868	0.189651	-0.347859	-0.302069	-0.129061
0.121046	-0.215569	0.188101	0.021154	-0.294713	-0.166784	0.279408	0.160350	-0.288037	-0.348616	-0.179397	0.372012	0.189236	-0.386836	0.031496	0.294110	0.365204	0.199563
0.209624	-0.262069	0.077744	0.189833	-0.094961	-0.363318	-0.023460	0.212198	0.101654	-0.095978	0.205878	-0.011103	-0.522702	-0.106875	-0.257996	-0.171060	-0.516463	-0.400170
0.203468	-0.097950	-0.069013	0.328857	-0.168299	-0.175607	-0.046919	-0.176579	0.396902	0.425537	0.217003	0.008376	0.255625	0.193858	0.454910	-0.097210	-0.181826	0.378330
0.279448	0.047848	-0.198198	0.259085	-0.135205	0.164501	-0.022873	-0.343282	0.083431	-0.111169	-0.384561	0.002541	0.208990	-0.189266	-0.395240	0.343226	0.095227	-0.575752
0.251439	0.216914	0.042664	0.155368	-0.164335	0.266474	-0.258751	0.078793	-0.224259	-0.236642	-0.120874	-0.360603	-0.295179	0.229578	0.256035	0.105224	-0.412448	0.516585
0.147656	0.179121	0.186219	0.227111	0.078894	0.302873	0.047086	-0.393544	-0.042637	0.030562	0.504886	-0.019897	0.342372	0.136798	-0.332591	-0.286816	0.288071	-0.267982
0.100329	0.167262	0.273312	0.153305	0.270526	0.078313	0.313418	0.197578	0.196905	0.206479	-0.265384	0.384569	-0.133314	-0.416040	0.219408	0.396102	-0.244733	0.165594
0.095069	0.173296	0.285304	0.006087	0.268191	-0.212363	0.248406	-0.274396	0.131913	-0.130091	-0.318872	-0.386928	-0.170557	0.425103	-0.013854	-0.421454	0.253458	-0.153788
0.126192	0.200812	0.222140	-0.153693	0.073954	-0.319377	-0.078620	-0.370740	-0.132827	-0.132522	0.491067	0.024771	0.348070	-0.155055	-0.219070	0.367930	-0.320618	0.219038
0.212766	0.252848	0.090094	-0.231783	-0.175579	-0.140135	-0.314564	0.019364	-0.181177	0.177536	-0.046502	0.357913	-0.249083	-0.231566	0.359300	-0.229005	0.470032	-0.420833
0.158569	0.151166	-0.095188	-0.365609	-0.171128	-0.127762	-0.012412	0.303687	0.263755	0.319639	-0.334747	-0.006576	0.221539	0.227979	-0.520702	-0.081871	-0.257097	0.281220
0.169692	0.071998	-0.247291	-0.297731	-0.027500	0.000652	0.312312	0.191379	0.282328	-0.312296	0.295553	-0.356369	-0.018040	-0.046235	0.437525	-0.356482	0.116493	-0.302988
0.252860	-0.004789	-0.332625	-0.064414	0.139916	0.109529	0.299094	-0.187021	-0.135352	-0.167768	0.139277	0.376312	-0.180469	-0.188799	-0.147784	-0.568178	0.015114	0.505315
0.188397	-0.131129	-0.178352	-0.061973	0.372087	-0.008911	0.032147	0.005467	-0.432836	0.468247	0.012503	0.015256	-0.036907	0.480868	0.155548	-0.262753	-0.244547	-0.341949
0.205527	-0.272693	0.031230	-0.038391	0.324526	-0.111033	-0.268640	0.198372	-0.059469	-0.052500	-0.166064	-0.391626	0.116839	-0.445270	-0.115435	-0.100202	0.536360	-0.390200

TETRAPHENE

IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.01342	0.73089	-0.01406	-0.35485	0.02013	0.07198	-0.01531	-0.01773	0.00530	0.02987	-0.00482	-0.04364	0.00574	0.09636	-0.00577	-0.15113	0.00774	0.54614
2	0.73089	1.01197	0.58521	-0.01451	-0.21746	0.00006	0.14525	0.00518	-0.06296	-0.00264	0.05923	-0.00058	-0.06033	-0.00949	0.04909	0.00850	-0.20207	-0.00682
3	-0.01406	0.58521	1.01150	0.72997	-0.00633	-0.20042	0.00780	0.05451	-0.00116	-0.04092	0.00171	0.03963	-0.00185	-0.10801	0.00478	0.13861	-0.00033	-0.21668
4	-0.35485	-0.01451	0.72997	1.01399	0.54800	0.00734	-0.15923	-0.00629	0.06291	0.00473	-0.05260	-0.00205	0.04851	0.01284	-0.00576	-0.01575	0.07142	0.02049
5	0.02013	-0.21746	-0.00633	0.54800	0.96464	0.58961	-0.00229	-0.10490	-0.00406	0.05157	0.00070	-0.03506	-0.00030	0.13297	-0.00791	-0.18300	0.00483	0.48672
6	0.07198	0.00006	-0.20042	0.00734	0.58961	1.03275	0.64739	0.01043	-0.14570	-0.00194	0.12301	-0.00564	-0.13693	-0.01053	0.01847	-0.01245	-0.36178	-0.00441
7	-0.01531	0.14525	-0.00780	-0.15923	-0.00229	0.64739	0.96787	0.44688	0.01276	-0.12137	-0.00451	0.02431	0.00972	-0.19626	0.01048	0.49309	0.01051	-0.18954
8	-0.01773	0.00518	0.05451	-0.00629	-0.10490	0.01043	0.44688	0.96755	0.60094	-0.00648	-0.26933	0.02078	0.54308	0.00831	-0.23132	0.01213	0.04369	-0.00830
9	0.00530	-0.06296	-0.00116	0.06291	-0.00406	-0.14570	0.01276	0.60094	1.01444	0.69528	-0.01539	-0.33176	0.02216	0.00177	-0.01731	-0.09847	0.00189	0.07138
10	0.02987	-0.00264	-0.04092	0.00473	0.05157	-0.00194	-0.12137	-0.00648	0.69528	1.01155	0.62416	-0.01503	-0.25913	-0.00378	0.18777	-0.00225	-0.06467	0.00216
11	-0.00482	0.05923	0.00171	-0.05260	0.00070	0.12301	-0.00451	-0.26933	-0.01539	0.62416	1.01298	0.69885	-0.00849	-0.11743	0.01119	0.09386	-0.00056	-0.06952
12	-0.04364	-0.00058	0.03963	-0.00205	-0.03506	-0.00564	0.02431	0.02078	-0.33176	-0.01503	0.69885	1.01513	0.58426	0.00973	-0.21189	-0.00584	0.09444	0.00329
13	0.00574	-0.06033	-0.00185	0.04851	-0.00030	-0.13693	0.00972	0.54308	0.02216	-0.25913	-0.00849	0.58426	0.96747	0.49276	-0.00937	-0.14264	-0.00263	0.08246
14	0.09636	-0.00949	-0.10801	0.01284	0.13297	-0.01053	-0.19626	0.00831	0.00177	-0.00378	-0.11743	0.00973	0.49276	1.01433	0.77831	-0.00879	-0.24409	0.00863
15	-0.00577	0.04909	0.00478	-0.00576	-0.00791	0.01847	0.01048	-0.23132	-0.01731	0.18777	0.01119	-0.21189	-0.00937	0.77831	1.01477	0.49563	0.00745	-0.10548
16	-0.15113	0.00850	0.13861	-0.01575	-0.18300	0.01245	0.49309	0.01213	-0.09847	-0.00225	0.09386	-0.00584	-0.14264	-0.00879	0.49563	0.96669	0.62846	-0.00340
17	0.00774	-0.20207	-0.00033	0.07142	0.00483	-0.36178	0.01051	0.04369	0.00189	-0.06467	-0.00056	0.09444	-0.00263	-0.24409	0.00745	0.62846	1.03360	0.59350
18	0.54614	-0.00682	-0.21668	0.02049	0.48672	0.00441	-0.18954	-0.00830	0.07138	0.00216	-0.06952	0.00329	0.08246	0.00863	-0.10548	-0.00340	0.59350	0.96532

TETRAPHENE | IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.79644	0.55749	-0.09210	-0.37246	-0.02922	0.08579	0.00216	-0.01901	0.00151	0.03202	-0.00081	-0.04703	-0.00167	0.10192	-0.00995	-0.15402	-0.07456	0.37252
2	0.55749	0.78380	0.40422	-0.09235	-0.22782	0.02763	0.15462	-0.00322	-0.06779	-0.00057	0.06373	0.00119	-0.06483	-0.00910	0.05171	0.01520	-0.20729	-0.07115
3	-0.09210	0.40422	0.78356	0.55649	-0.07093	-0.20556	0.01498	0.05758	-0.00253	-0.04408	0.00119	0.04293	-0.00004	-0.11548	-0.00551	0.14753	0.02778	-0.22696
4	-0.37246	-0.09235	0.55649	0.79674	0.37456	-0.07428	-0.16269	0.00782	0.06774	0.00098	-0.05653	-0.00233	0.05162	0.00394	-0.00634	0.00155	0.08514	-0.02904
5	-0.02922	-0.22782	-0.07093	0.37456	0.70326	0.41829	-0.06188	-0.10509	0.00428	0.05599	-0.00221	-0.03879	0.00400	0.14207	-0.01063	-0.19474	-0.05493	0.32312
6	0.08579	0.02763	-0.20556	-0.07428	0.41829	0.82796	0.47945	-0.06371	-0.16151	0.00972	0.13198	0.00041	-0.14066	0.01334	0.02951	-0.04764	-0.38444	-0.05480
7	0.00216	0.15462	0.01498	-0.16269	-0.06188	0.47945	0.71491	0.27731	-0.05762	-0.12134	0.01643	0.03295	-0.04047	-0.20831	-0.04544	0.32967	-0.04966	-0.20161
8	-0.01901	-0.00322	0.05758	0.00782	-0.10509	-0.06371	0.27731	0.71540	0.43068	-0.07258	-0.28306	-0.03091	0.38248	-0.05227	-0.24575	-0.03448	0.05470	0.00691
9	0.00151	-0.06779	-0.00253	0.06774	0.00428	-0.16151	-0.05762	0.43068	0.79402	0.51933	-0.09097	-0.34755	-0.02984	0.01044	0.00059	-0.09925	0.01164	0.07706
10	0.03202	-0.00057	-0.04408	0.00098	0.05599	0.00972	-0.12134	-0.07258	0.51933	0.78320	0.44594	-0.09130	-0.27237	0.02175	0.19947	0.00070	-0.07078	0.00009
11	-0.00081	0.06373	0.00119	-0.05653	-0.00221	0.13198	0.01643	-0.28306	-0.09097	0.44594	0.78386	0.52315	-0.07269	-0.11699	0.02208	0.09988	-0.01001	-0.07487
12	-0.04703	0.00119	0.04293	-0.00233	-0.03879	0.00041	0.03295	-0.03091	-0.34755	-0.09130	0.52315	0.79592	0.41330	-0.06617	-0.21710	0.01225	0.10130	-0.00210
13	-0.00167	-0.06483	-0.00004	0.05162	0.00400	-0.14066	-0.04047	0.38248	-0.02984	-0.27237	-0.07269	0.41330	0.70732	0.31615	-0.07982	-0.15109	0.01911	0.08838
14	0.10192	-0.00910	-0.11548	0.00394	0.14207	0.01334	-0.20831	-0.05227	0.01044	0.02175	-0.11699	-0.06617	0.31615	0.79656	0.60703	-0.07912	-0.25150	0.01795
15	0.00995	-0.05171	-0.00551	-0.00634	0.01063	0.02951	-0.04544	-0.24575	0.00059	0.19947	0.02208	-0.21710	-0.07982	0.60703	0.79681	0.31925	-0.07254	-0.10554
16	-0.15402	0.01520	0.14753	0.00155	-0.19474	-0.04764	0.32967	-0.03448	-0.09925	0.00070	0.09988	0.01225	-0.15109	-0.07912	0.31925	0.70615	0.45969	-0.06159
17	-0.07456	-0.20729	0.02778	0.08514	-0.05493	-0.38444	-0.04966	0.05470	0.01164	-0.07078	-0.01001	0.10130	0.01911	-0.25150	-0.07254	0.45969	0.83055	0.42244
18	0.37252	-0.07115	-0.22696	-0.02904	0.32312	-0.05480	-0.20161	0.00691	0.07706	0.00009	-0.07487	-0.00210	0.08838	0.01795	-0.10554	-0.06159	0.42244	0.70351

ENERGIES FOR TETRAPHENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF No SYMMETRY

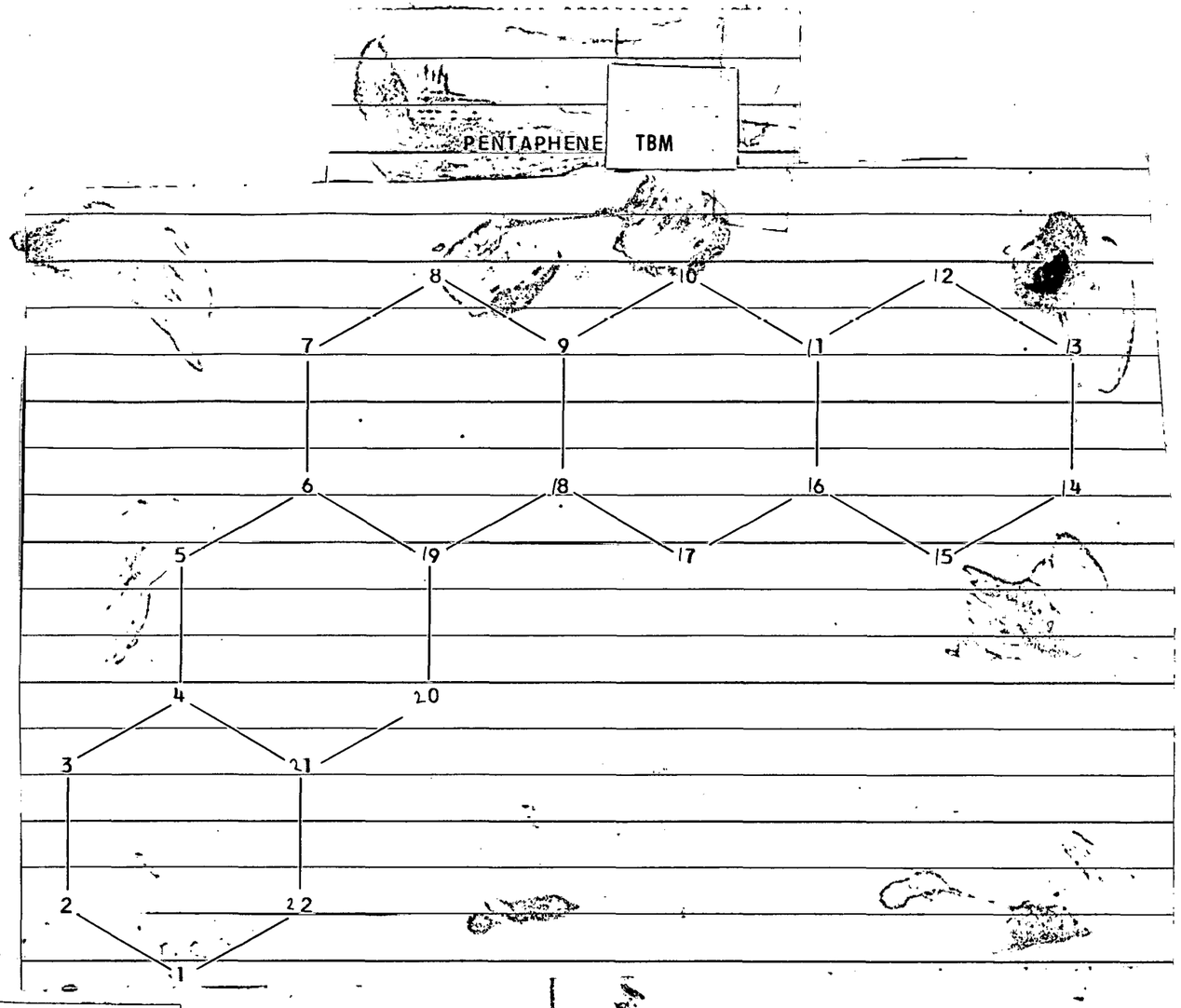
JUMP	9,10	8,10	9,11	7,10	8,11	6,10	5,10	7,11	4,10	6,11	3,10	2,10	1,10
XMOMNT	0.24619	0.89465	-0.76929	-0.40077	-0.04610	-0.36205	0.04311	-0.20581	-0.01189	-0.22769	-0.01742	-0.01216	-0.00645
YMOMNT	0.62757	0.09780	-0.15682	0.06353	0.30434	0.17455	0.04000	-0.54557	0.09471	0.05892	0.01834	0.00940	0.01156
JUMP E	17.7254	21.9889	23.6342	26.6839	27.8976	29.4966	32.3679	32.5927	34.8393	35.4053	39.1044	44.3316	47.7583
DIAG E	28.1639	33.6597	35.0252	38.3462	39.2746	42.6173	45.7815	46.3499	49.2195	50.1269	55.0706	60.0316	62.3080
DIAG E	28.2856	34.0631	34.9705	38.9614	39.5016	43.1480	46.2092	46.7888	49.6222	50.4812	55.4715	60.6584	63.1265
CORRSP	27.6099	30.2993	35.9729	38.4293	39.4839	42.0046	43.7044	50.2809	47.5678	51.9991	55.0550	59.1498	64.4176
CORRSP	27.7390	36.1943	30.7410	39.0196	39.7402	42.2889	44.2613	50.6227	48.1689	52.3402	55.4107	59.7296	65.0313

FINAL EXCITED STATES OF No SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
27.60993	0.34884	0.15961	0.52119	//	0.9782	-0.0451	0.0543	-0.0182	-0.1850	-0.0000	-0.0172	0.0447	0.0193	0.0225
				//	-0.0068	-0.0165	-0.0095							
16.15877				//	0.9719	-0.0260	0.0230	-0.0875	-0.1697	0.0031	-0.0994	-0.0806	0.0321	-0.0147
				//	0.0100	0.0074	-0.0019							
30.29925	0.14346	0.31344	-0.11444	//	-0.0091	0.7390	0.6155	-0.1892	-0.0237	-0.1288	0.0463	0.0769	0.0135	-0.0848
				//	0.0725	-0.0346	0.0039							
24.18275				//	-0.0224	0.7057	-0.5562	0.1324	-0.3244	-0.1575	0.0019	-0.1534	-0.1106	-0.0932
				//	-0.0027	-0.0077	0.0010							
35.97292	1.20308	-0.87840	-0.12197	//	-0.0236	-0.5689	0.5837	-0.4767	0.2521	0.1841	-0.0166	0.0759	0.0010	0.0449
				//	0.0086	0.0447	0.0193							
27.49486				//	0.0413	0.5674	0.4362	-0.4780	0.3466	-0.2976	0.0943	0.1379	0.0682	-0.0046
				//	0.1159	-0.0545	-0.0061							
38.42932	1.42192	-0.89453	-0.26443	//	-0.0572	-0.1796	0.4453	0.7721	-0.1340	0.1007	-0.2141	0.2729	-0.0152	-0.1180
				//	-0.0749	0.0402	-0.0143							
33.41038				//	0.0605	0.1441	0.3051	0.7465	0.1294	-0.3105	-0.3697	0.2058	0.1370	-0.1181
				//	-0.0131	-0.0043	-0.0131							
39.48390	0.31158	0.06754	0.42545	//	0.1805	0.0803	-0.0007	0.2582	0.8940	-0.2598	-0.0578	-0.1151	-0.0482	0.0911
				//	-0.0142	-0.0073	0.0063							
29.38949				//	0.1520	-0.0506	-0.4619	0.1215	0.7922	-0.1044	0.0364	-0.1878	-0.0232	0.2650
				//	0.0122	-0.0006	-0.0144							
42.00456	0.01443	0.00175	0.08986	//	0.0512	0.2716	-0.1805	-0.0300	0.2383	0.8111	-0.0582	0.3698	-0.1284	0.0939
				//	0.0350	0.0932	-0.0130							
37.20123				//	0.0920	0.2855	0.3341	0.3549	0.1074	0.5429	0.4384	-0.1861	-0.3530	0.0948
				//	-0.0757	0.0001	-0.0052							
43.70440	0.16446	-0.18117	0.23594	//	0.0276	-0.0271	0.1494	0.2049	-0.0091	0.2333	0.7881	-0.3607	-0.3258	-0.0096
				//	-0.1387	-0.0535	-0.0089							
38.22361				//	0.0096	-0.1695	0.0932	0.1098	-0.0448	-0.4552	0.5607	-0.4276	0.2420	-0.3141
				//	-0.2596	-0.1172	0.0757							
50.28086	0.09626	0.02020	-0.21121	//	0.0008	-0.0456	-0.0950	-0.0002	0.1169	-0.1233	0.5052	0.5448	0.5741	-0.1862
				//	-0.1711	-0.0666	0.1006							
45.11328				//	0.1077	0.0642	-0.2577	0.0572	0.1089	0.2648	0.3723	0.6572	0.4001	-0.2898
				//	-0.1328	-0.0186	0.0105							

TETRAPHENE IRM APPROXIMATION (cont.)

47.56785	0.36699	0.09852	0.41439	//	0.0403	0.0420	0.0319	0.0363	0.0816	0.3448	-0.1529	-0.5329	0.5228	-0.5354
				//	-0.0179	0.0092	0.0314							
42.42537				//	-0.0717	0.1416	0.0369	-0.0772	0.1724	0.4420	-0.3407	-0.4633	0.4862	-0.4140
				//	0.0419	0.0463	0.0023							
51.99914	0.24001	-0.27077	0.18767	//	-0.0334	0.0639	0.1186	0.1204	-0.0802	0.1214	0.0211	-0.2230	0.5031	0.7952
				//	-0.0681	0.0673	0.0145							
48.09128				//	-0.0329	0.1256	0.0640	0.0778	-0.2026	0.0464	0.0871	-0.0821	0.6042	0.7330
				//	-0.0720	0.0453	0.0773							
55.05502	0.05712	-0.15404	0.02586	//	0.0007	-0.0838	0.0063	0.1160	0.0143	0.0303	0.1608	0.0252	0.1126	0.0189
				//	0.9281	-0.2389	-0.1428							
50.80971				//	0.0063	-0.0722	-0.0310	0.1344	-0.0669	0.0078	0.1958	-0.0359	0.1152	-0.0188
				//	0.8577	-0.4126	-0.1093							
59.14981	0.00824	0.05714	-0.00319	//	0.0119	0.0040	-0.0086	-0.0039	0.0040	-0.0894	0.1215	0.0121	0.0583	-0.0694
				//	0.0931	0.7946	-0.5732							
55.02462				//	0.0001	-0.0192	0.0142	0.0332	-0.0258	-0.0866	0.1605	-0.0350	0.0675	-0.0354
				//	0.1920	0.6908	-0.6658							
64.41757	0.00249	0.00688	0.02936	//	0.0185	0.0007	-0.0062	0.0401	-0.0249	-0.0431	0.0623	-0.0243	-0.0455	-0.0181
				//	0.2532	0.5346	0.7993							
62.22811				//	0.0099	-0.0180	-0.0013	0.0441	0.0120	-0.0467	0.1019	0.0076	-0.0173	-0.0708
				//	0.3405	0.5755	0.7297							



ATOMIC COORDINATES

x	0.8660	0.	0.	-0.8660	-0.8660	-1.7320	-1.7320	-2.5980	-3.4640	-4.3300	-5.1960	
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	4.5000	5.0000	4.5000	5.0000	4.5000	
	6.0620	6.9280	6.9280	6.0620	5.1960	4.3300	3.4640	2.5980	2.5980	1.7320	1.7320	0.
	5.0000	4.5000	3.5000	3.0000	3.5000	3.0000	3.5000	3.0000	2.0000	1.5000	0.5000	0.

PENTAPHENE — TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 S	8 S	9 A	10 A	11 S	12 A	13 S
1.620616	1.563657	1.493615	1.394158	1.371083	1.318133	1.304910	1.246812	1.246802	1.128549	1.107897	0.892100	0.871448
0.081016	0.170346	0.235706	-0.302552	0.026896	0.031834	0.384180	0.235261	-0.236126	-0.107415	0.212957	-0.212958	-0.107413
0.080062	0.171997	0.235701	-0.268799	0.146208	0.265386	0.262708	0.322136	0.085681	0.238939	-0.084689	-0.084690	-0.238938
0.120309	0.222462	0.235700	-0.126727	0.192940	0.310258	-0.059634	0.086880	0.321821	0.231877	-0.249994	0.249995	0.231875
0.222462	0.336061	0.235702	0.066403	0.143885	0.134542	-0.336366	-0.235239	0.236132	-0.118155	-0.024605	-0.024604	0.118155
0.209159	0.219710	-0.000007	0.272594	0.209336	0.184208	-0.233528	0.000032	-0.000033	-0.247252	0.374498	-0.374499	-0.247250
0.303485	0.165720	-0.235704	0.368933	0.170860	0.102905	0.047848	0.235259	-0.236152	-0.010631	0.188322	0.188323	0.010630
0.200376	0.050466	-0.235703	0.142014	0.339274	0.045042	0.203283	-0.086902	-0.321785	-0.007070	-0.334621	0.334621	-0.007072
0.200383	-0.050460	-0.235706	-0.142119	0.339250	-0.044841	0.203289	-0.322149	-0.085633	0.006948	-0.334599	-0.334599	-0.006946
0.303492	-0.165704	-0.235701	-0.368977	0.170791	-0.102841	0.047860	-0.235248	0.236155	0.010689	0.188345	-0.188345	0.010690
0.209172	-0.219705	-0.000001	-0.272642	0.209305	-0.184276	-0.233452	-0.000006	-0.000022	0.247350	0.374426	0.374424	-0.247352
0.222477	-0.336049	0.235700	-0.066432	0.143901	-0.134686	-0.336266	0.235242	-0.236177	0.118142	-0.024658	0.024658	0.118142
0.120320	-0.222460	0.235704	0.126692	0.193040	-0.310263	-0.059437	0.322133	0.085650	-0.231933	-0.249938	-0.249936	0.231935
0.080070	-0.171994	0.235700	0.268758	0.146337	-0.265234	0.262838	0.086891	0.321824	-0.238943	-0.084607	0.084606	-0.238944
0.081023	-0.170341	0.235700	-0.302530	0.026980	-0.031619	0.384166	-0.235253	0.236175	0.107486	0.212961	0.212960	-0.107487
0.123669	-0.217031	0.235704	0.214396	-0.105765	0.224464	0.211774	-0.322141	-0.085641	0.294915	0.177703	-0.177701	0.294916
0.229945	-0.325303	0.235700	0.039860	-0.185999	0.320948	-0.122541	-0.086888	-0.321813	0.046119	-0.135275	-0.135275	-0.046118
0.232070	-0.189850	0.000000	-0.084311	-0.317779	0.323909	-0.026912	0.000022	0.000006	-0.389030	0.212184	-0.212182	-0.389031
0.353602	-0.108267	-0.235699	-0.174504	-0.291784	0.096563	0.089294	0.086911	0.321818	-0.248744	0.042514	-0.042515	0.248743
0.353597	0.108290	-0.235702	0.174585	-0.291703	-0.096607	0.089368	0.322125	0.085658	0.248785	0.042435	-0.042433	0.248785
0.232055	0.189864	0.000007	0.084388	-0.317670	-0.324008	-0.026739	-0.000044	-0.000011	0.388973	-0.212296	-0.212299	-0.388972
0.229930	0.325318	0.235704	-0.039808	-0.185932	-0.321036	-0.122396	-0.322152	-0.085665	-0.046177	-0.135242	0.135241	-0.046178
0.123655	0.217032	0.235703	-0.214376	-0.105770	-0.224353	0.211907	-0.086874	-0.321798	-0.294885	0.177787	0.177789	0.294884

OVERLAP EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 A	17 S	18 A	19 S	20 A	21 S	22 A
0.753196	0.753186	0.695087	0.681864	0.628915	0.605840	0.506383	0.436341	0.379382
-0.235339	-0.236049	-0.384180	0.031834	0.026894	-0.302552	-0.235706	0.170347	0.081016
-0.086757	0.321848	0.262708	-0.265386	-0.146207	0.268800	0.235700	-0.171997	-0.080062
0.322109	-0.085805	0.059634	0.310258	0.192939	-0.126727	-0.235699	0.222463	0.120309
-0.235345	-0.236027	-0.336366	-0.134542	-0.143886	-0.066402	0.235702	-0.336061	-0.222461
-0.000032	-0.000032	0.233528	0.184208	0.209337	0.272593	0.000007	0.219711	0.209158
0.235365	0.236047	0.047848	-0.102905	-0.170861	-0.368932	-0.235704	-0.165720	-0.303485
-0.322074	0.005026	-0.203283	0.045042	0.339274	0.142012	0.235703	0.050466	0.200376
0.086709	-0.321861	0.203289	0.044841	-0.339249	0.142120	-0.235706	0.050460	-0.200383
0.235368	0.236036	-0.047861	-0.102841	0.170790	-0.368978	0.235701	-0.165704	0.303492
0.000022	-0.000006	-0.233452	0.184277	-0.209304	0.272643	-0.000000	0.219705	-0.209172
-0.235390	-0.236030	0.336266	-0.134687	0.143901	-0.066432	-0.235700	-0.336048	0.222477
-0.086725	0.321845	-0.059436	0.310263	-0.193041	-0.126691	0.235704	0.222459	-0.120320
0.322112	-0.085815	-0.262839	-0.265235	0.146338	0.268758	-0.235700	-0.171994	0.080070
-0.235387	-0.236041	0.384167	0.031619	-0.026981	-0.302530	0.235700	0.170340	-0.081023
0.086717	0.321853	-0.211774	0.224465	-0.105765	0.214397	-0.235704	-0.217030	0.123669
0.322101	-0.085813	-0.122541	-0.320948	0.185999	-0.039861	0.235700	0.325303	-0.229946
0.000006	-0.000022	0.026913	0.323909	-0.317779	-0.084309	-0.000001	-0.189850	0.232071
-0.322107	0.085835	0.089294	-0.096563	0.291785	0.174503	-0.235699	0.108267	-0.353603
0.086733	-0.321837	-0.089368	-0.096607	-0.291702	0.174586	0.235702	0.108290	0.353597
0.000012	-0.000044	-0.026739	0.324008	0.317670	-0.084389	0.000007	-0.189865	-0.232055
-0.086741	0.321864	0.122396	-0.321036	-0.185932	-0.039808	-0.235704	0.325319	0.229930
0.322087	-0.085799	0.211908	0.224353	0.105771	0.214375	0.235703	-0.217033	-0.123655

PENTAPHENE | TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 S	8 S	9 A	10 A	11 S	12 A	13 S
28.77545	27.08650	24.83300	21.24407	20.33699	18.13549	17.55783	14.87456	14.87410	8.55912	7.31797	-9.08837	-11.08452
0.063640	0.136227	0.192864	-0.256238	0.022969	0.027728	0.336314	-0.000016	0.298514	-0.101112	0.202322	-0.225469	-0.115063
0.062891	0.137546	0.192860	-0.227652	0.124865	0.231153	0.229977	-0.258538	0.149251	0.224919	-0.080459	-0.089666	-0.255956
0.094506	0.177904	0.192859	-0.107328	0.164774	0.270236	-0.052204	-0.258534	-0.149269	0.218271	-0.237508	0.264682	0.248389
0.174749	0.268749	0.192861	0.056238	0.122881	0.117187	-0.294457	-0.000001	-0.298504	-0.111222	-0.023376	-0.026050	0.126570
0.164299	0.175703	-0.000006	0.230866	0.178777	0.160446	-0.204432	0.000000	0.000041	-0.232745	0.355795	-0.396501	-0.264859
0.238395	0.132527	-0.192862	0.312458	0.145918	0.089631	0.041887	0.000002	0.298530	-0.010007	0.178917	0.199387	0.011387
0.157401	0.040358	-0.192862	0.120275	0.289747	0.039232	0.177955	0.258525	0.149232	-0.006655	-0.317910	0.354280	-0.007576
0.157406	-0.040353	-0.192864	-0.120363	0.289726	-0.039057	0.177960	0.258516	-0.149289	0.006541	-0.317888	-0.354256	-0.007441
0.238400	-0.132514	-0.192860	-0.312495	0.145859	-0.089575	0.041897	-0.000011	-0.298524	0.010062	0.178939	-0.199410	0.011451
0.164310	-0.175699	-0.000001	-0.230907	0.178751	-0.160505	-0.204365	0.000018	0.000010	0.232837	0.355726	0.396421	-0.264969
0.174761	-0.268739	0.192859	-0.056263	0.122894	-0.117312	-0.294370	0.000028	0.298535	0.111210	-0.023426	0.026107	0.126556
0.094514	-0.177902	0.192862	0.107298	0.164860	-0.270240	-0.052031	-0.258516	0.149269	-0.218324	-0.237455	-0.264620	0.248453
0.062897	-0.137544	0.192859	0.227618	0.124975	-0.231020	0.230090	-0.258543	-0.149264	-0.224923	-0.080382	0.089577	-0.255962
0.063646	0.136222	0.192859	0.256220	0.023041	-0.027541	0.336302	-0.000019	-0.298540	0.101179	0.202325	0.225471	-0.115143
0.097145	-0.173560	0.192863	0.181577	-0.090326	0.195509	0.185388	0.258516	-0.149279	0.277611	0.168828	-0.188141	0.315920
0.180628	-0.260146	0.192859	0.033759	-0.158847	0.279547	-0.107273	0.258534	0.149258	0.043413	-0.128519	-0.143222	-0.049403
0.182297	-0.151824	0.000000	-0.071405	-0.271389	0.282126	-0.023559	-0.000018	0.000010	-0.366204	-0.201588	0.224648	-0.416739
0.277763	-0.086582	-0.192859	-0.147792	-0.249189	0.084106	0.078169	-0.258552	-0.149248	-0.234149	0.040391	0.045013	0.266459
0.277759	0.086600	-0.192861	0.147860	-0.249120	-0.084145	0.078233	-0.258516	0.149258	-0.234188	-0.040315	-0.044926	0.266504
0.182285	0.151835	0.000006	0.071470	-0.271297	-0.282212	-0.023407	0.000035	-0.000021	0.366150	-0.201694	-0.224771	-0.416675
0.180616	0.260158	0.192862	-0.033714	-0.158789	-0.279624	-0.107147	0.258538	-0.149271	-0.043468	-0.128487	0.143187	-0.049467
0.097134	0.173562	0.192862	-0.181560	-0.090330	-0.195413	0.185505	0.258516	0.149258	-0.277583	0.168908	0.188234	0.315886

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 A	17 S	18 A	19 S	20 A	21 S	22 A
-24.62207	-24.62335	-32.96217	-35.05859	-44.33653	-48.88712	-73.24721	-97.06669	122.92125
0.384069	0.000044	-0.460803	0.038552	0.033913	-0.388706	-0.331231	0.257882	0.131532
-0.192007	-0.332651	0.315104	-0.321388	-0.184362	0.345342	0.331223	-0.260380	-0.129983
-0.192069	0.332623	0.071527	0.375728	0.243290	-0.162814	-0.331222	0.336778	0.195325
0.384056	0.000021	-0.403453	-0.162933	-0.181435	-0.085311	0.331226	-0.508751	-0.361174
0.000053	-0.000000	0.280104	0.223080	0.263967	0.350216	0.000010	0.332612	0.339576
-0.384089	-0.000021	0.057391	-0.124620	-0.215451	-0.473989	-0.331229	-0.250878	-0.492718
0.192023	-0.332611	-0.243826	0.054547	0.427814	0.182451	0.331227	0.076399	0.325318
0.192056	0.332623	0.243834	0.054303	-0.427783	0.182589	-0.331231	0.076390	-0.325328
-0.384083	-0.000009	-0.057406	-0.124543	0.215360	-0.474047	0.331224	-0.250853	0.492730
-0.000013	0.000023	-0.280012	0.223163	-0.263926	0.350280	-0.000001	0.332604	-0.339598
0.384096	-0.000013	0.403333	-0.163108	0.181454	-0.085350	-0.331223	-0.508732	0.361200
-0.192030	-0.332623	-0.071291	0.375734	-0.243418	-0.162767	0.331228	0.336774	-0.195343
-0.192063	0.332634	-0.315261	-0.321204	0.184527	0.345288	-0.331223	-0.260375	0.129997
0.384103	-0.000002	0.460787	0.038291	-0.034022	-0.388678	0.331223	0.257872	-0.131544
-0.192043	-0.332623	-0.254011	0.271831	-0.133366	0.275448	-0.331229	-0.328555	0.200781
-0.192056	0.332623	-0.146982	-0.388675	0.234538	-0.051212	0.331223	0.492465	-0.373325
0.000013	0.000023	0.032280	0.392261	-0.400709	-0.108317	-0.000001	-0.287407	0.376775
0.192043	-0.332645	0.107103	-0.116939	0.367931	0.224195	-0.331222	0.163902	-0.574086
0.192017	0.332623	-0.107192	-0.116993	-0.367827	0.224301	0.331226	0.163937	0.574077
0.000026	0.000046	-0.032072	0.392379	0.400572	-0.108420	0.000010	-0.287429	-0.376749
-0.192033	-0.332651	0.146808	-0.388781	-0.234454	-0.051143	-0.331228	0.492489	0.373299
-0.192056	0.332600	0.254171	0.271695	0.133374	0.275420	0.331227	-0.328558	-0.200758

PENTAPHENE

TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.00000	0.59566	-0.00000	-0.22797	0.00000	0.12850	-0.00000	-0.09339	0.00000	0.05051	-0.00000	-0.02239	0.00000	0.02315	-0.00000
	-0.02673	0.00000	0.03441	-0.00000	-0.18103	0.00000	0.72782								
2	0.59566	1.00000	0.72906	0.00000	-0.18277	-0.00000	0.03408	-0.00000	-0.03854	-0.00000	0.03248	0.00000	-0.02833	0.00000	0.02909
	0.00000	-0.06792	-0.00000	0.13320	0.00000	-0.22923	0.00000								
3	-0.00000	0.72906	1.00000	0.54507	0.00000	-0.14399	-0.00000	0.08894	0.00000	-0.05657	0.00000	0.02654	0.00000	-0.02239	0.00000
	0.02039	-0.00000	-0.00767	0.00000	0.08500	0.00000	-0.36140								
4	-0.22797	0.00000	0.54507	1.00000	0.58381	-0.00000	-0.08913	-0.00000	0.06324	-0.00000	-0.04213	0.00000	0.03248	-0.00000	-0.03109
	-0.00000	0.08064	0.00000	-0.19986	-0.00000	0.49791	0.00000								
5	0.00000	-0.18277	0.00000	0.58381	1.00000	0.63435	0.00000	-0.23933	0.00000	0.12922	-0.00000	-0.05657	-0.00000	0.05052	-0.00000
	-0.05153	0.00000	0.03175	-0.00000	-0.36473	0.00000	0.08331								
6	0.12850	-0.00000	-0.14399	-0.00000	0.63435	1.00000	0.48412	-0.00000	-0.14159	0.00000	0.06324	-0.00000	-0.03854	0.00000	0.03007
	-0.00000	-0.10042	-0.00000	0.50124	0.00000	-0.19550	-0.00000								
7	-0.00000	0.03408	-0.00000	-0.08913	0.00000	0.48412	1.00000	0.78970	0.00000	-0.23934	0.00000	0.08895	-0.00000	-0.09341	-0.00000
	0.12450	-0.00000	-0.20781	-0.00000	0.01710	0.00000	0.00102								
8	-0.09339	-0.00000	0.08894	-0.00000	-0.23933	-0.00000	0.78970	1.00000	0.48414	-0.00000	-0.08913	0.00000	0.03408	-0.00000	0.00102
	0.00000	0.01710	0.00000	-0.20781	0.00000	0.12449	0.00000								
9	0.00000	-0.03854	0.00000	0.06324	0.00000	-0.14159	0.00000	0.48414	1.00000	0.63435	0.00000	-0.14400	-0.00000	0.12851	0.00000
	-0.19551	0.00000	0.50122	0.00000	-0.10041	-0.00000	0.03007								
10	0.05051	-0.00000	-0.05657	-0.00000	0.12922	0.00000	-0.23934	-0.00000	0.63435	1.00000	0.58383	0.00000	-0.18277	0.00000	0.08329
	-0.00000	-0.36470	-0.00000	0.03176	-0.00000	-0.05153	0.00000								
11	-0.00000	0.03248	0.00000	-0.04213	-0.00000	0.06324	0.00000	-0.08913	0.00000	0.58383	1.00000	0.54506	0.00000	-0.22798	0.00000
	0.49789	0.00000	-0.19985	-0.00000	0.08064	0.00000	-0.03109								
12	-0.02239	0.00000	0.02654	0.00000	-0.05657	-0.00000	0.08895	0.00000	-0.14400	0.00000	0.54506	1.00000	0.72908	0.00000	-0.36138
	0.00000	0.08501	0.00000	-0.00767	0.00000	0.02039	-0.00000								
13	0.00000	-0.02833	0.00000	0.03248	-0.00000	-0.03854	-0.00000	0.03408	-0.00000	-0.18277	0.00000	0.72908	1.00000	0.59564	0.00000
	-0.22923	-0.00000	0.13320	0.00000	-0.06792	-0.00000	0.02909								
14	0.02315	0.00000	-0.02239	-0.00000	0.05052	0.00000	-0.09341	-0.00000	0.12851	0.00000	-0.22798	0.00000	0.59564	1.00000	0.72783
	-0.00000	-0.18105	0.00000	0.03442	-0.		-0.02674	0.00000							
15	-0.00000	0.02909	0.00000	-0.03109	-0.00000	0.03007	-0.00000	0.00102	0.00000	0.08329	0.00000	-0.36138	0.00000	0.72783	1.00000
	0.54803	0.00000	-0.15132	-0.00000	0.07559	-0.00000	-0.03268								
16	-0.02673	0.00000	0.02039	-0.00000	-0.05153	-0.00000	0.12450	0.00000	-0.19551	-0.00000	0.49789	0.00000	-0.22923	-0.00000	0.54803
	1.00000	0.57776	-0.00000	-0.08007	0.00000	0.03857	0.00000								
17	0.00000	-0.06792	-0.00000	0.08064	0.00000	-0.10042	-0.00000	0.01710	0.00000	-0.36470	0.00000	0.08501	-0.00000	-0.18105	0.00000
	0.57776	1.00000	0.65335	0.00000	-0.19773	-0.00000	0.07560								
18	0.03441	-0.00000	-0.00767	0.00000	0.03175	-0.00000	-0.20781	0.00000	0.50122	-0.00000	-0.19985	0.00000	0.13320	0.00000	-0.15132
	-0.00000	0.65335	1.00000	0.43529	0.00000	-0.08007	-0.00000								
19	-0.00000	0.13320	0.00000	-0.19986	-0.00000	0.50124	-0.00000	-0.20781	0.00000	0.03176	-0.00000	-0.00767	0.00000	0.03442	-0.00000
	-0.08007	0.00000	0.43529	1.00000	0.65334	0.00000	-0.15132								
20	-0.18103	0.00000	0.08500	-0.00000	-0.36473	0.00000	0.01710	0.00000	-0.10041	-0.00000	0.08064	0.00000	-0.06792	-0.	0.07559
	0.00000	-0.19773	0.00000	0.65334	1.00000	0.57777	0.00000								
21	0.00000	-0.22923	0.00000	0.49791	0.00000	-0.19550	0.00000	0.12449	-0.00000	-0.05153	-0.00000	0.02039	-0.00000	-0.02674	-0.00000
	0.03857	-0.00000	-0.08007	0.00000	0.57777	1.00000	0.54802								
22	0.72782	0.00000	-0.36140	0.00000	0.08331	-0.00000	0.00102	0.00000	0.03007	0.00000	-0.03109	-0.00000	0.02909	0.00000	-0.03268
	0.00000	0.07560	-0.00000	-0.15132	0.00000	0.54802	1.00000								

PENTAPHENE | TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.76027	0.42085	-0.05202	-0.21006	0.02113	0.12443	-0.00802	-0.09192	0.00205	0.05009	-0.00035	-0.02225	-0.00018	0.02298	0.00085
	-0.02643	-0.00175	0.03351	0.00337	-0.17158	-0.04166	0.55046								
2	0.42085	0.75997	0.55168	-0.04125	-0.17326	0.00275	0.03313	0.00112	-0.03766	0.00139	0.03201	-0.00098	-0.02805	-0.00018	0.02877
	0.00148	-0.06679	-0.00606	0.12900	0.02031	-0.21130	-0.05172								
3	-0.05202	0.55168	0.77074	0.37721	-0.05964	-0.13557	0.01189	0.08738	-0.00560	-0.05574	0.00225	0.02622	-0.00098	-0.02226	0.00045
	0.02042	-0.00283	-0.00895	0.01363	0.08929	-0.03100	-0.34091								
4	-0.21006	-0.04125	0.37721	0.72136	0.41488	-0.03686	-0.08131	0.00517	0.06035	-0.00475	-0.04111	0.00224	0.03201	-0.00035	-0.03060
	-0.00161	0.07825	0.01126	-0.18424	-0.03768	0.33689	-0.03130								
5	0.02113	-0.17326	-0.05964	0.41488	0.78284	0.46499	-0.05824	-0.22900	0.01639	0.12635	-0.00475	-0.05575	0.00140	0.05010	0.00031
	-0.05136	0.00373	0.03626	-0.03840	-0.34570	-0.03870	0.08764								
6	0.12443	0.00275	-0.13557	-0.03686	0.46499	0.72307	0.31727	-0.04703	-0.12674	0.01638	0.06035	-0.00560	-0.03766	0.00205	0.02934
	0.00090	-0.09335	-0.02955	0.33980	-0.03942	-0.18006	0.01373								
7	-0.00802	0.03313	0.01189	-0.08131	-0.05824	0.31727	0.77088	0.61104	-0.04703	-0.22901	0.00517	0.08740	0.00112	-0.09193	-0.00709
	0.12066	0.01748	-0.19149	-0.03660	0.02252	0.01466	-0.00062								
8	-0.09192	0.00112	0.08738	0.00517	-0.22900	-0.04703	0.61104	0.77088	0.31728	-0.05824	-0.08131	0.01189	0.03313	-0.00802	-0.00061
	0.01466	0.02251	-0.03660	-0.19148	0.01748	0.12065	-0.00709								
9	0.00205	-0.03766	-0.00560	0.06035	0.01639	-0.12674	-0.04703	0.31728	0.72307	0.46498	-0.03686	-0.13558	0.00275	0.12445	0.01373
	0.18007	-0.03942	0.33979	-0.02955	-0.09334	0.00090	0.02934								
10	0.05009	0.00139	-0.05574	-0.00475	0.12635	0.01638	-0.22901	-0.05824	0.46498	0.78284	0.41489	-0.05964	-0.17326	0.02113	0.08763
	-0.03870	-0.34568	-0.03839	0.03627	0.00372	-0.05136	0.00031								
11	-0.00035	0.03201	0.00225	-0.04111	-0.00475	0.06035	0.00517	-0.08131	-0.03686	0.41489	0.72136	0.37720	-0.04125	-0.21007	-0.03130
	0.33688	-0.03767	-0.18424	0.01126	0.07825	-0.00162	-0.03060								
12	-0.02225	-0.00098	0.02622	0.00224	-0.05575	-0.00560	0.08740	0.01189	-0.13558	-0.05964	0.37720	0.77074	0.55169	-0.05202	-0.34089
	-0.03099	0.08929	0.01363	-0.00896	-0.00283	0.02042	0.00045								
13	-0.00018	-0.02805	-0.00098	0.03201	0.00140	-0.03766	0.00112	0.03313	0.00275	-0.17326	-0.04125	0.55169	0.75997	0.42084	-0.05172
	-0.21130	0.02031	0.12900	-0.00606	-0.06679	0.00148	0.02877								
14	0.02298	-0.00018	-0.02226	-0.00035	0.05010	0.00205	-0.09193	-0.00802	0.12445	0.02113	-0.21007	-0.05202	0.42084	0.76028	0.55047
	-0.04166	-0.17160	0.00337	0.03351	-0.00175	-0.02643	0.00085								
15	0.00085	0.02877	0.00045	-0.03060	0.00031	0.02934	-0.00709	-0.00061	0.01373	0.08763	-0.03130	-0.34089	-0.05172	0.55047	0.77033
	0.38009	-0.05861	-0.14264	0.00973	0.07386	-0.00273	-0.03222								
16	-0.02643	0.00148	0.02042	-0.00161	-0.05136	0.00090	0.12066	0.01466	-0.18007	-0.03870	0.33688	-0.03099	-0.21130	-0.04166	0.38009
	0.72209	0.40905	-0.03851	-0.07295	0.00875	0.03748	-0.00273								
17	-0.00175	-0.06679	-0.00283	0.07825	0.00373	-0.09335	0.01748	0.02251	-0.03942	-0.34568	-0.03767	0.08929	0.02031	-0.17160	-0.05861
	0.40905	0.77985	0.48291	-0.04985	-0.18759	0.00875	0.07387								
18	0.03351	-0.00606	-0.00895	0.01126	0.03626	-0.02955	-0.19149	-0.03660	0.33979	-0.03839	-0.18424	0.01363	0.12900	0.00337	-0.14264
	-0.03851	0.48291	0.72909	0.27494	-0.04985	-0.07295	0.00973								
19	0.00337	0.12900	0.01363	-0.18424	-0.03840	0.33980	-0.03660	-0.19148	-0.02955	0.03627	0.01126	-0.00896	-0.00606	0.03351	0.00973
	-0.07295	-0.04985	0.27494	0.72909	0.48290	-0.03851	-0.14264								
20	-0.17158	0.02031	0.08929	-0.03768	-0.34570	-0.03942	0.02252	0.01748	-0.09334	0.00372	0.07825	-0.00283	-0.06679	-0.00175	0.07386
	0.00875	-0.18759	-0.04985	0.48290	0.77986	0.40906	-0.05861								
21	-0.04166	-0.21130	-0.03100	0.33689	-0.03870	-0.18006	0.01466	0.12065	0.00090	-0.05136	-0.00162	0.02042	0.00148	-0.02643	-0.00273
	0.03748	0.00875	-0.07295	-0.03851	0.40906	0.72209	0.38009								
22	0.55046	-0.05172	-0.34091	-0.03130	0.08764	0.01373	-0.00062	-0.00709	0.02934	0.00031	-0.03060	0.00045	0.02877	0.00085	-0.03222
	-0.00273	0.07387	0.00973	-0.14264	-0.05861	0.38009	0.77033								

ENERGIES FOR PENTAPHENE , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	11,12	10,12	11,13	9,12	8,12	8,13	7,12	6,12	5,12	4,12
XMOMNT	0.97861	-0.22124	0.22130	-0.25779	0.18614	0.20241	0.21868	-0.06246	0.00202	-0.00920
YMOMNT	0.56479	0.38379	-0.38390	0.44677	-0.10749	-0.35045	0.12625	0.10838	0.00113	0.01595
JUMP E	16.4063	17.6475	18.4025	23.9625	23.9629	25.9591	26.6462	27.2239	29.4254	30.3324
DIAG E	29.5049	30.0075	30.6216	37.9285	37.4055	41.4756	43.8780	43.2397	43.1155	47.2883
DIAG E	29.6150	30.2038	30.6442	38.8026	37.9220	41.9046	44.3096	43.6808	43.6449	47.8270
CORRSP	29.1863	28.3104	30.1723	36.6241	36.6697	40.2088	43.6822	46.6488	44.3656	48.5968
CORRSP	29.3790	28.7033	30.2098	37.4376	37.2422	40.8225	44.1453	46.9891	44.7250	48.9007

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
28.31036	0.12296	-0.15973	0.27681	//	-0.0000	0.7614	0.5388	0.2849	-0.0000	-0.1944	0.0000	-0.0502	0.0000	0.0927
18.63943				//	0.0015	0.7211	-0.6611	-0.1032	-0.0004	-0.1443	-0.0002	-0.0748	-0.0001	-0.0773
30.17230	0.37314	0.26885	-0.46748	//	-0.0004	-0.5988	0.7735	0.1846	0.0002	0.0786	-0.0000	0.0365	-0.0000	0.0396
26.47738				//	-0.0000	0.5340	0.5206	0.5679	-0.0000	-0.2721	0.0000	0.0787	0.0000	0.2028
36.62414	0.11538	-0.13587	0.23585	//	-0.0002	-0.0167	-0.2513	0.7657	-0.0010	0.5156	0.0003	-0.1786	-0.0004	0.2292
32.50522				//	-0.0001	-0.0869	-0.3136	0.6240	-0.0002	0.6020	0.0002	-0.3103	-0.0002	0.2146
40.20876	0.46524	0.26079	-0.45175	//	-0.0000	0.1279	0.1819	-0.3812	0.0002	0.5183	0.0002	-0.6967	-0.0002	-0.2264
33.84559				//	-0.0001	0.3481	0.4323	-0.3616	0.0002	0.4300	0.0001	-0.5750	-0.0001	-0.2138
46.64878	0.16030	0.14219	-0.24615	//	0.0000	0.2066	0.1232	-0.2821	0.0002	0.6427	-0.0001	0.6523	-0.0003	0.1550
46.16418				//	-0.0000	0.1639	0.0602	0.1359	0.0001	0.4490	-0.0003	0.6195	-0.0003	-0.6047
48.59681	0.03820	0.06798	-0.11775	//	0.0000	-0.0496	-0.0010	-0.2712	-0.0000	-0.0922	0.0002	-0.2312	0.0002	0.9285
43.40230				//	0.0000	0.1984	0.0560	-0.3582	-0.0002	0.3953	0.0002	0.4213	-0.0003	0.7039

ENERGIES FOR PENTAPHENE TBM APPROXIMATION 1.7

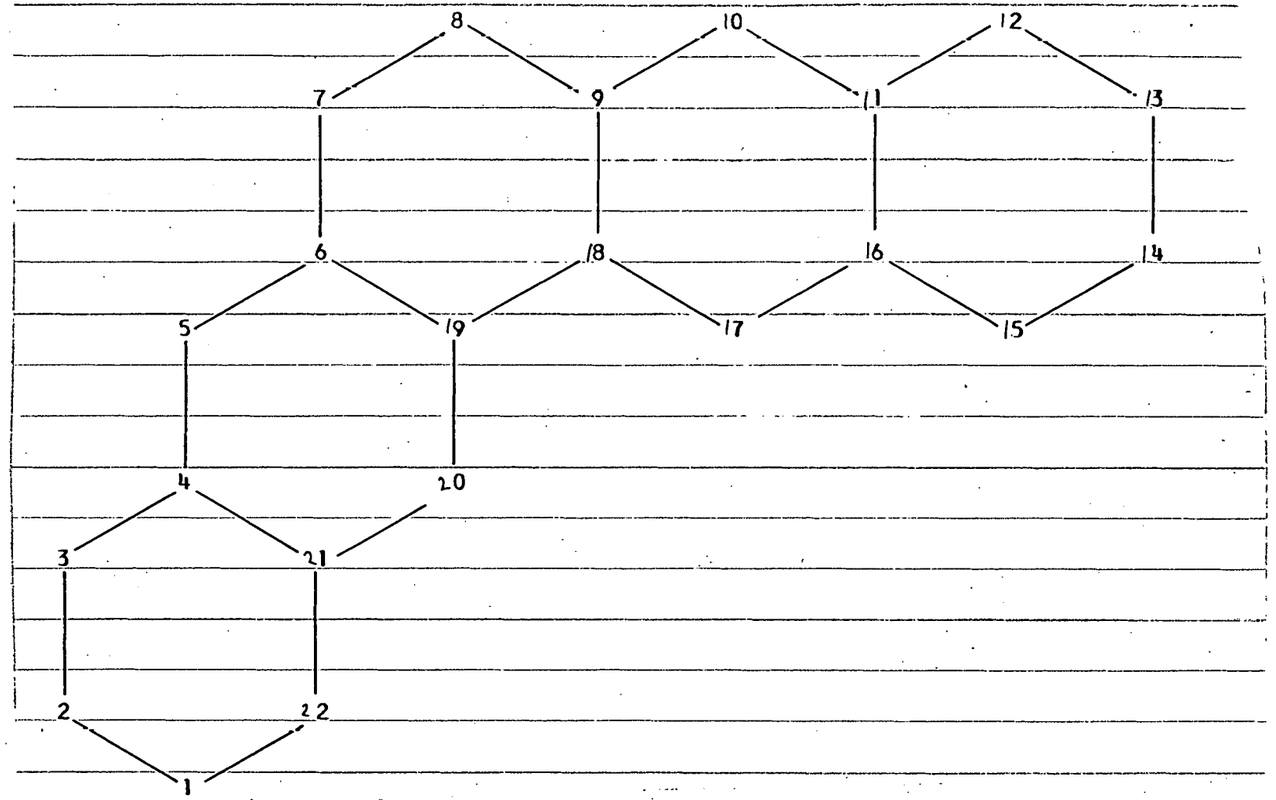
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	11,12	10,13	8,12	9,13	7,12	6,13	5,12	4,13	10,14	3,12
XMOMNT	0.97861	0.42958	-0.18614	0.62731	0.21868	0.15202	0.00202	0.01680	0.63006	-0.04633
YMOMNT	0.56479	0.24792	-0.10749	0.36206	0.12625	0.08774	0.00113	0.00972	0.36362	-0.02676
JUMP E	16.4063	19.6436	23.9629	25.9586	26.6462	29.2200	29.4254	32.3286	33.1812	33.9214
DIAG E	29.5049	32.8255	37.4055	38.8566	43.8780	45.2389	43.1155	50.0731	45.0623	51.3564
DIAG E	29.6150	32.9343	37.9220	39.6432	44.3096	45.5926	43.6449	50.5243	44.1822	52.0302
CORRSP	27.2937	35.0884	36.5393	32.2453	45.0330	50.0779	40.2180	48.4022	46.2305	56.1885
CORRSP	27.4618	35.0582	33.0404	37.0231	45.6190	50.4151	40.8055	48.8338	45.7161	56.4254

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
27.29370	0.53907	0.59025	0.34066	//	0.8466	-0.5095	-0.0856	-0.0306	0.0416	0.0601	0.0438	-0.0408	-0.0577	-0.0559
14.81869				//	0.8499	-0.4946	-0.0221	0.0666	-0.0996	0.0943	0.0655	0.0322	0.0633	0.0049
35.08841	0.31552	0.39829	0.22983	//	0.4089	0.5989	0.1389	-0.4736	-0.3412	-0.1673	0.0278	-0.0270	0.2688	0.1111
23.52666				//	0.4159	0.7459	-0.4255	0.2263	0.0340	-0.0387	-0.1393	0.0919	0.0694	-0.0560
36.53927	0.62391	0.54883	0.31672	//	0.2020	0.1691	0.6693	0.5280	0.2833	-0.3190	0.0497	0.0977	0.0863	-0.0490
29.80145				//	0.0771	0.0435	0.5661	0.5290	0.4276	-0.3731	-0.0488	-0.0142	0.2395	-0.0997
32.24528	1.25853	0.82972	0.47892	//	0.2561	0.5497	-0.5828	0.4112	0.2336	0.0988	-0.1069	0.0513	-0.1539	-0.1463
32.04670				//	-0.1626	-0.2230	-0.4010	0.4694	0.4916	0.4385	0.1917	-0.0945	-0.2130	-0.1333
45.03298	0.02440	-0.09776	-0.05642	//	-0.0359	0.0923	-0.0104	-0.3835	0.7098	-0.0643	0.3770	-0.4320	-0.0099	-0.0791
40.97612				//	0.1433	0.1204	-0.0206	-0.4765	0.4878	0.0547	0.1692	-0.5901	0.3106	0.1527
50.07793	0.01650	0.07624	0.04400	//	0.0721	0.1312	0.3552	-0.1538	0.2494	0.7256	-0.4732	0.0232	-0.0762	0.0943
49.08982				//	0.0958	0.1325	0.3967	-0.1870	0.2100	0.6373	-0.5251	0.2030	-0.0887	-0.0768
40.21800	0.07757	0.18446	0.10643	//	0.0142	0.0991	0.0967	0.1440	-0.1805	0.5315	0.7779	0.1974	0.0131	-0.0253
35.23807				//	0.0293	0.2794	0.3169	0.0258	-0.1700	0.3757	0.7584	0.2099	0.1601	-0.0707
48.40215	0.27390	-0.31595	-0.18233	//	-0.0253	0.0088	0.0621	-0.3378	0.1121	-0.1061	-0.0209	0.6111	-0.1922	-0.6684
42.97924				//	0.1661	0.0723	0.0793	-0.3371	0.2913	-0.3004	0.2104	0.1471	-0.6340	-0.4519
46.23047	1.03243	0.62764	0.36225	//	-0.0419	-0.1189	-0.1674	0.0638	0.1743	0.1263	-0.0770	0.1370	0.9219	-0.1760
45.42603				//	-0.1192	-0.1712	-0.2471	-0.2200	0.1345	-0.0504	-0.0510	0.3817	0.5970	-0.5672
56.18849	0.00279	-0.02958	-0.01706	//	0.0229	-0.0350	-0.1354	-0.1313	0.3249	-0.1286	0.0772	0.6059	-0.0158	0.6835
55.24098				//	-0.0002	-0.0533	-0.1079	-0.1396	0.3879	-0.1229	0.1035	0.6169	0.0129	0.6395

PENTAPHENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	1.7320	2.5980	3.4640	4.3300	5.1960
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	4.5000	5.0000	4.5000	5.0000	4.5000

6.0620	6.9280	6.9280	6.0620	5.1960	4.3300	3.4640	2.5980	2.5980	1.7320	1.7320
5.0000	4.5000	3.5000	3.0000	3.5000	3.0000	3.5000	3.0000	2.0000	1.5000	0.5000

PENTAPHENE — IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 S	8 S	9 A	10 A	11 S	12 A	13 S
1.773168	1.673949	1.557515	1.399122	1.356325	1.277391	1.267535	1.184144	1.170625	1.046276	1.033375	0.832707	0.821955
0.090592	0.187255	-0.251481	-0.310481	0.059995	-0.005723	0.360681	0.020584	-0.326473	-0.089638	-0.232952	0.226494	-0.112872
0.089850	0.188561	-0.251166	-0.285611	0.168377	0.241211	-0.209065	0.309063	-0.146225	0.257267	0.068510	0.087373	-0.245150
0.126716	0.230419	-0.239198	-0.134794	0.192378	0.312369	-0.112675	0.274829	0.191223	0.201883	0.249693	-0.255931	0.235347
0.224063	0.325261	-0.210644	0.084085	0.107874	0.142777	-0.346106	-0.042097	0.313983	-0.147600	0.038191	0.033763	0.112640
0.211831	0.216972	0.012327	0.281575	0.181443	0.197768	-0.273855	-0.039798	-0.039975	-0.246316	-0.366862	0.356981	-0.242003
0.297738	0.157349	0.234389	0.339849	0.164083	0.104194	0.032403	0.005880	-0.349753	0.019202	-0.195248	-0.191043	0.026128
0.205661	0.046632	0.250351	0.131790	0.353362	0.052224	0.218755	-0.248845	-0.187766	0.001306	0.331507	-0.344683	-0.028184
0.205666	-0.046628	0.250351	-0.131895	0.353345	-0.051845	0.218801	-0.249062	0.187532	-0.001494	0.331463	0.344695	-0.027826
0.297746	-0.157334	0.234381	-0.339889	0.164033	-0.104113	0.032494	0.005467	0.349744	-0.019100	-0.195300	0.191037	0.026310
0.211844	-0.216964	0.012316	-0.281606	0.181421	-0.198074	-0.273623	-0.039863	0.039854	0.246489	-0.366737	-0.356752	-0.242330
0.224080	-0.325246	-0.210646	-0.084095	0.107889	-0.143202	-0.345898	-0.041745	-0.314061	0.147572	0.038291	-0.033889	0.112606
0.126728	-0.230412	-0.239202	0.134767	0.192479	-0.312483	-0.112232	0.275041	-0.190883	-0.201997	0.249609	0.255719	0.235575
0.089860	-0.188556	-0.251166	0.285570	0.168498	-0.240918	0.209378	0.308891	-0.146608	-0.257280	0.068368	-0.087122	-0.245214
0.090602	-0.187249	-0.251478	0.310453	0.060065	0.006215	0.360655	0.020189	0.326511	0.089768	-0.232952	-0.226420	-0.113096
0.129712	-0.225586	-0.240229	0.203106	-0.088679	0.256970	0.230820	-0.288764	0.151094	0.286644	-0.158701	0.188905	0.292269
0.230511	-0.315916	-0.212343	-0.002174	-0.191376	0.311630	-0.084044	-0.292332	-0.181187	0.047047	0.151813	0.126974	-0.040195
0.235817	-0.186103	0.007621	-0.118021	-0.338679	0.316676	-0.001369	0.013688	-0.038266	-0.391185	0.206674	-0.196219	-0.381540
0.340691	-0.105622	0.226853	-0.171522	-0.274863	0.087437	0.097610	0.306742	0.143739	-0.254455	-0.060925	-0.037899	0.257614
0.340685	0.105645	0.226857	0.171589	-0.274790	-0.087398	0.097745	0.306881	-0.143377	0.254513	-0.060789	0.037645	0.257683
0.235801	0.186122	0.007616	0.118097	-0.338563	-0.316774	-0.000954	0.013584	0.038306	0.391093	0.206863	0.196587	-0.381350
0.230492	0.315934	-0.212345	0.002223	-0.191297	-0.311766	-0.083658	-0.292557	0.180855	-0.047143	0.151764	-0.126919	-0.040334
0.129696	0.225592	-0.240230	-0.203097	-0.088664	-0.256665	0.231167	-0.288578	-0.151434	-0.286590	-0.158842	-0.189182	0.292106

OVERLAP EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 A	17 S	18 A	19 S	20 A	21 S	22 A
0.721933	0.721645	0.680494	0.679161	0.639127	0.616074	0.551357	0.513616	0.482480
-0.003712	0.344692	0.382512	0.024753	0.051266	0.288089	-0.220347	-0.158354	0.070755
0.283058	-0.194777	-0.270811	-0.248457	-0.144605	-0.270281	0.220486	0.159067	-0.070353
-0.298760	-0.138130	-0.040891	0.307901	0.179262	0.154174	-0.233395	-0.212008	0.109357
0.031418	0.337916	0.333025	-0.151018	-0.132493	0.032586	0.258024	0.345966	-0.222590
-0.010938	-0.016856	-0.250000	0.196691	0.204234	-0.255951	-0.012514	-0.218430	0.201146
-0.019398	-0.321452	-0.030694	-0.116244	-0.194273	0.377761	-0.232075	0.172977	-0.311300
0.290629	0.154652	0.181643	0.053752	0.347489	-0.139327	0.223095	-0.048148	0.191945
-0.286632	0.161991	-0.181800	0.053111	-0.347493	-0.139361	-0.223101	-0.048142	-0.191950
0.011275	-0.321833	0.031027	-0.116119	0.194266	0.377769	0.232080	0.172965	0.311304
0.010481	-0.017177	0.249405	0.197433	-0.204242	-0.255963	0.012512	-0.218431	-0.201155
-0.022839	0.338628	-0.332531	-0.152035	0.132516	0.032593	-0.258017	0.345964	0.222595
0.295149	-0.145623	0.039908	0.308031	-0.179313	0.154174	0.233398	-0.212012	-0.109361
-0.287882	-0.187584	0.271570	-0.247627	0.144656	-0.270268	-0.220485	0.159068	0.070355
0.012417	0.344506	-0.382555	0.023559	-0.051290	0.288071	0.220339	-0.158352	-0.070755
0.276123	-0.180126	0.224940	0.229393	-0.078601	-0.207923	-0.232790	0.208454	0.111865
-0.300915	-0.153321	0.099121	-0.328517	0.183913	0.045219	0.256618	-0.336453	-0.230545
0.018635	-0.001134	-0.011975	0.310608	-0.323190	0.098905	-0.008124	0.186926	0.230440
0.282369	0.155781	-0.103793	-0.089116	0.286588	-0.190858	-0.240595	-0.115910	-0.368185
-0.278305	0.162869	0.104085	-0.088866	-0.286547	-0.190888	0.240594	-0.115925	0.368182
-0.018728	-0.000653	0.011009	0.310692	0.323128	0.098923	0.008131	0.186929	-0.230431
0.296968	-0.160886	-0.098124	-0.328816	-0.183873	0.045205	-0.256625	-0.336456	0.230540
-0.280590	-0.173078	-0.225661	0.228672	0.078588	-0.207921	0.232788	0.208448	-0.111859

PENTAPHENE — IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 S	8 S	9 A	10A	11S	12A	13 S
32.76449	30.25270	26.89698	21.43529	19.74068	16.31731	15.85988	11.68512	10.95225	3.32344	2.42682	-15.09608	-16.27651
0.068032	0.144731	-0.201507	-0.262487	0.051515	-0.005064	0.320364	0.018916	-0.301744	-0.087633	-0.229159	0.248205	-0.124498
0.067475	0.145741	-0.201254	-0.241461	0.144577	0.213420	0.185696	0.284017	-0.135149	0.251513	0.067394	0.095748	-0.270400
0.095160	0.178093	-0.191664	-0.113957	0.165186	0.276379	-0.100080	0.252557	0.176739	0.197368	0.245628	-0.280463	0.259588
0.168265	0.251398	-0.168785	0.071087	0.092627	0.126327	-0.307418	-0.038686	0.290200	-0.144299	0.037569	0.036999	-0.124242
0.159079	0.167700	0.009877	0.238049	0.155797	0.174982	-0.243243	-0.036573	-0.036947	-0.240807	-0.360889	0.391200	-0.266929
0.223594	0.121617	0.187811	0.287315	0.140891	0.092189	0.028781	0.005403	-0.323260	0.018772	-0.192069	-0.209356	0.028819
0.154446	0.036043	0.200601	0.111418	0.303416	0.046207	0.194302	-0.228679	-0.173543	0.001277	0.326110	-0.377724	-0.031087
0.154450	-0.036039	0.200601	-0.111507	0.303401	-0.045872	0.194343	-0.228878	0.173327	-0.001460	0.326067	0.377737	-0.030692
0.223600	-0.121605	0.187805	-0.287349	0.140847	-0.092118	0.028862	0.005024	0.323252	-0.018673	-0.192120	0.209349	0.029020
0.159089	-0.167694	0.009868	-0.238075	0.155778	-0.175253	-0.243037	-0.036633	0.036835	0.240976	-0.360766	-0.390949	-0.267291
0.168279	-0.251386	-0.168786	-0.071096	0.092639	-0.126703	-0.307233	-0.038362	-0.290272	0.144272	0.037668	-0.037137	0.124204
0.095169	-0.178088	-0.191667	0.113935	0.165273	-0.276481	-0.099687	0.252752	-0.176424	-0.197479	0.245545	0.280231	-0.259839
0.067483	-0.145737	-0.201254	0.241426	0.144682	-0.213161	0.185974	0.283859	0.135503	-0.251526	0.067255	-0.095474	-0.270471
0.068040	-0.144726	-0.201504	0.262463	0.051575	0.005499	0.320341	0.018553	0.301779	0.087760	-0.229159	-0.248123	-0.124745
0.097410	-0.174357	-0.192491	0.171710	-0.076144	0.227364	0.205018	-0.265363	0.139650	0.280233	-0.156117	0.207012	0.322373
0.173108	-0.244175	-0.170146	-0.001838	-0.164326	0.275726	-0.074650	-0.268642	-0.167463	0.045995	0.149342	0.139145	-0.044336
0.177093	-0.143841	0.006107	-0.099777	-0.290808	0.280190	-0.001216	0.012579	-0.035367	-0.382436	0.203309	-0.215028	-0.420839
0.255850	-0.081636	0.181773	-0.145008	-0.236012	0.077363	0.086699	0.281884	0.132851	-0.248765	-0.059933	0.041531	0.284149
0.255846	0.081654	0.181776	0.145064	-0.235950	-0.077328	0.086819	0.282012	-0.132517	-0.248820	0.059800	0.041253	0.284224
0.177081	0.143855	0.006103	0.099841	-0.290708	-0.280277	-0.000847	0.012483	0.035404	0.382346	0.203495	0.215432	-0.420630
0.173094	0.244189	-0.170148	0.001879	-0.164258	-0.275846	-0.074307	-0.268849	0.167156	-0.046089	0.149293	-0.139085	-0.044488
0.097399	0.174362	-0.192491	-0.171702	-0.076132	-0.227093	0.205327	0.265192	-0.139964	-0.280180	-0.156256	0.207316	0.322193

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 A	17 S	18 A	19 S	20 A	21 S	22 A
-28.94223	-28.98376	-35.28041	-35.49710	-42.42737	-46.82684	-61.14316	-71.15753	-80.59857
-0.405592	-0.009494	0.463696	0.030036	0.064127	0.367038	-0.296750	-0.220959	0.101863
0.225014	0.336075	-0.328287	-0.301484	-0.180880	-0.344350	0.296938	0.221953	-0.101284
0.166998	-0.349609	-0.049569	0.373615	0.224230	0.196424	-0.314322	-0.295824	0.157437
-0.398140	0.031958	0.403705	-0.183250	-0.165730	0.041516	0.347491	0.482742	-0.320454
0.019999	-0.012624	-0.303059	0.238670	0.255467	-0.326092	-0.016853	-0.304785	0.289582
0.378586	-0.018054	-0.037208	-0.141053	-0.243007	0.481283	-0.312544	0.241362	-0.448167
-0.106320	0.339792	0.220194	0.065224	0.434658	-0.177508	0.300450	0.067183	0.276335
-0.186377	-0.339795	-0.220385	0.064447	-0.434663	-0.177552	-0.300459	-0.067175	-0.276344
0.378577	0.018055	0.037612	-0.140901	0.242998	0.481293	0.312551	0.241345	0.448172
0.020058	0.012592	0.302339	0.239570	-0.255477	-0.326108	0.016851	-0.304787	-0.289595
-0.398171	-0.031918	-0.403107	-0.184483	0.165758	0.041524	-0.347481	0.482739	0.320462
0.166988	0.349577	0.048378	0.373773	-0.224295	0.196424	0.314326	-0.295829	-0.157443
0.225035	-0.336069	0.329207	-0.300477	0.180943	-0.344333	-0.296935	0.221954	0.101287
-0.405613	0.009494	-0.463748	0.028587	-0.064156	0.367014	0.296740	-0.220956	-0.101863
0.207876	0.327695	0.272681	0.278351	-0.098319	-0.264903	-0.313507	0.290865	0.161047
0.184907	-0.351920	0.120158	-0.398631	0.230049	0.057611	0.345598	-0.469467	-0.331907
0.001058	0.021952	-0.014517	0.376900	-0.404263	0.126010	-0.010940	0.260826	0.331756
-0.187526	0.330054	-0.125822	-0.108136	0.358479	-0.243161	-0.324018	-0.161734	-0.530061
-0.107534	-0.330007	0.126176	-0.107832	-0.358429	-0.243200	0.324017	-0.161755	0.530058
0.001047	-0.022035	0.013346	-0.377002	0.404186	0.126032	0.010951	0.260831	-0.331745
0.184923	0.351945	-0.118949	0.398994	-0.229999	0.057592	-0.345607	-0.469471	0.331900
0.207855	-0.327702	-0.273555	0.277477	0.098303	-0.264900	0.313505	0.290857	-0.161039

PENTAPHENE

IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	1.01189	0.58899	-0.01458	-0.22029	0.00009	0.14196	0.00425	-0.11025	-0.00121	0.05146	0.00108	-0.02512	-0.00006	0.02737	-0.00135	-0.02845	-0.00338	0.04379	0.00812	-0.19337	-0.00662	0.72636
2	0.58899	1.01262	0.72723	-0.00736	-0.19506	0.00909	0.03635	-0.00972	-0.04631	0.00233	0.04130	0.00230	-0.03880	-0.00006	0.03657	-0.00176	-0.07938	0.00414	0.14951	0.00082	-0.22103	-0.01526
3	-0.01458	0.72723	1.01403	0.54990	0.00712	-0.15514	-0.00491	0.10043	0.00472	-0.05884	-0.00401	0.02943	0.00230	-0.02512	-0.00096	-0.01983	-0.00816	-0.00733	-0.01586	0.06543	0.02059	-0.35162
4	-0.22029	-0.00736	0.54990	0.96571	0.58635	-0.00380	-0.09311	0.00865	0.06823	0.00084	-0.04909	-0.00401	0.04130	0.00107	-0.03633	0.00129	0.08594	-0.00745	-0.19287	0.00382	0.48997	0.02116
5	0.00009	-0.19506	0.00712	0.58635	1.03371	0.63589	0.00777	-0.25096	-0.00291	0.12231	0.00084	-0.05884	0.00232	0.05147	-0.00530	-0.04206	0.00098	0.02303	0.01084	-0.34886	0.00455	0.06504
6	0.14196	0.00909	-0.15514	-0.00380	0.63589	0.96705	0.48411	-0.00876	-0.12818	-0.00291	0.06823	0.00472	-0.04631	-0.00121	0.03498	-0.00066	-0.10883	0.01082	0.49445	0.01325	-0.18554	-0.01648
7	0.00425	0.03635	-0.00491	-0.09311	0.00777	0.48411	1.01408	0.78415	-0.00877	-0.25098	0.00864	0.10044	-0.00972	-0.11027	0.01322	0.13329	-0.01096	-0.19146	0.00971	-0.00646	-0.00764	0.00667
8	-0.11025	-0.00972	0.10043	0.00865	-0.25096	-0.00876	0.78415	1.01406	0.48414	0.00778	-0.09311	-0.00491	0.03635	0.00425	0.00667	-0.00764	-0.00647	0.00971	-0.19145	0.01097	0.13328	0.01322
9	-0.00121	-0.04631	0.00472	0.06823	-0.00291	-0.12818	-0.00877	0.48414	0.96705	0.63588	-0.00379	-0.15515	0.00909	0.14197	-0.01648	-0.18555	0.01325	0.49443	0.01082	-0.10883	-0.00066	0.03499
10	0.05146	0.00233	-0.05884	0.00084	0.12231	-0.00291	-0.25098	0.00778	0.63588	1.03370	0.58637	0.00712	-0.19506	0.00009	0.06502	0.00455	-0.34884	0.01083	0.02304	-0.00097	-0.04286	-0.00531
11	0.00108	0.04130	-0.00401	-0.04909	0.00084	0.06823	0.00864	-0.09311	-0.00379	0.58637	0.96571	0.54989	-0.00736	-0.22030	0.02116	0.48995	0.00382	-0.19287	-0.00745	0.08594	0.00129	-0.03633
12	-0.02512	0.00230	0.02943	-0.00401	-0.05884	0.00472	0.10044	-0.00491	-0.15515	0.00712	0.54989	1.01402	0.72724	-0.01458	-0.35160	0.02059	0.06544	-0.01586	-0.00734	0.00816	0.01983	-0.00096
13	-0.00006	-0.03880	0.00230	0.04130	0.00232	-0.04631	-0.00972	0.03635	0.00909	-0.19506	-0.00736	0.72724	1.01262	0.58898	-0.01527	-0.22103	0.00082	0.14951	0.00414	-0.07938	-0.00176	0.03657
14	0.02737	-0.00006	-0.02512	0.00107	0.05147	-0.00121	-0.11027	0.00425	0.14197	0.00009	-0.22030	-0.01458	0.58898	1.01191	0.72636	-0.00662	-0.19338	0.00812	0.04380	-0.00337	-0.02845	-0.00135
15	-0.00135	0.03657	-0.00096	-0.03633	-0.00530	0.03498	0.01322	0.00667	-0.01648	0.06502	0.02116	-0.35160	-0.01527	0.72636	1.01483	0.55164	0.00640	-0.16414	-0.00499	0.08060	0.00367	-0.03767
16	-0.02845	-0.00176	0.01983	0.00129	-0.04286	-0.00066	0.13329	-0.00764	-0.18555	0.00455	0.48995	0.02059	-0.22103	-0.00662	0.55164	0.96476	0.58262	-0.00237	-0.09448	-0.00254	0.03694	0.00368
17	-0.00338	-0.07938	0.00816	0.08594	-0.00098	-0.10883	-0.01096	-0.00647	0.01325	-0.34884	0.00382	0.06544	0.00082	-0.19338	0.00640	0.58262	1.03322	0.65652	0.00995	-0.18015	-0.00253	0.08060
18	0.04379	0.00414	-0.00733	-0.00745	0.02303	0.01082	-0.19146	0.00971	0.49443	0.01083	-0.19287	-0.01586	0.14951	0.00812	-0.16414	-0.00237	0.65652	0.96808	0.43367	0.00994	-0.09447	-0.00499
19	0.00812	0.14951	-0.01586	-0.19287	0.01084	0.49445	0.00971	-0.19145	0.01082	0.02304	-0.00745	-0.00734	0.00414	0.04380	-0.00499	-0.09448	0.00995	0.43367	0.96808	0.65651	-0.00237	-0.16414
20	-0.19337	0.00082	0.06543	0.00382	-0.34886	0.01325	-0.00646	-0.01097	-0.10883	-0.00097	0.08594	0.00816	-0.07938	-0.00337	0.08060	-0.00254	-0.18015	0.00994	0.65651	1.03323	0.58263	0.00639
21	-0.00662	-0.22103	0.02059	0.48997	0.00455	-0.18554	-0.00764	0.13328	-0.00066	-0.04286	0.00129	0.01983	-0.00176	-0.02845	-0.00367	-0.03694	-0.00253	-0.09447	-0.00237	0.58263	0.96476	0.55162
22	0.72636	-0.01526	-0.35162	0.02116	0.06504	-0.01648	0.00667	0.01322	0.03499	-0.00531	-0.03633	-0.00096	0.03657	-0.00135	-0.03767	0.00368	0.08060	-0.00499	-0.16414	0.00639	0.55162	1.01484

PENTAPHENE

IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.78399	0.40829	-0.09261	-0.23086	0.02819	0.15115	-0.00621	-0.11792	0.00076	0.05571	0.00063	-0.02711	-0.00019	0.02953	-0.00045
	-0.03075	-0.00553	0.04606	0.01557	-0.19797	-0.07131	0.55261								
2	0.40829	0.78453	0.55357	-0.07181	-0.19975	0.01606	0.03803	-0.00987	-0.04978	0.00539	0.04463	0.00083	-0.04188	-0.00019	0.03949
	-0.00005	-0.08551	-0.00443	0.15923	0.02843	-0.23168	-0.09313								
3	-0.09261	0.55357	0.79698	0.37656	-0.07503	-0.15834	0.01069	0.10632	-0.00237	-0.06333	-0.00107	0.03189	0.00083	-0.02711	-0.00018
	0.02131	0.00468	-0.00787	0.00141	0.07876	-0.02872	-0.36900								
4	-0.23086	-0.07181	0.37656	0.70409	0.41476	-0.06235	-0.09226	0.01864	0.07311	-0.00639	-0.05316	-0.00107	0.04463	0.00062	-0.03923
	-0.00068	0.09284	0.00818	-0.20524	-0.05556	0.32663	-0.02831								
5	0.02819	-0.19975	-0.07503	0.41476	0.83037	0.46767	-0.07202	-0.25885	0.01827	0.13095	-0.00639	-0.06333	0.00539	0.05572	-0.00663
	-0.04737	0.00789	0.03256	-0.04889	-0.37057	-0.05531	0.07830								
6	0.15115	0.01606	-0.15834	-0.06235	0.46767	0.70711	0.30691	-0.08004	-0.13563	0.01827	0.07311	-0.00237	-0.04978	0.00076	0.03712
	0.00301	-0.11064	-0.03690	0.33120	-0.04637	-0.19751	0.00062								
7	-0.00621	0.03803	0.01069	-0.09226	-0.07202	0.30691	0.79704	0.61332	-0.08005	-0.25886	0.01864	0.10633	-0.00987	-0.11795	0.00482
	0.14246	0.01165	-0.20338	-0.04777	0.00283	0.01138	0.00701								
8	-0.11792	-0.00987	0.10632	0.01864	-0.25885	-0.08004	0.61332	0.79701	0.30692	-0.07201	-0.09226	0.01068	0.03803	-0.00620	0.00701
	0.01137	0.00282	-0.04777	-0.20337	0.01164	0.14244	0.00482								
9	0.00076	-0.04978	-0.00237	0.07311	0.01827	-0.13563	-0.08005	0.30692	0.70711	0.46767	-0.06235	-0.15835	0.01605	0.15117	0.00062
	-0.19752	-0.04637	0.33119	-0.03690	-0.11064	0.00301	0.03712								
10	0.05571	0.00539	-0.06333	-0.00639	0.13095	0.01827	-0.25886	-0.07201	0.46767	0.83035	0.41477	-0.07503	-0.19975	0.02819	0.07828
	-0.05531	-0.37054	-0.04888	0.03257	0.00789	-0.04737	-0.00663								
11	0.00063	0.04463	-0.00107	-0.05316	-0.00639	0.07311	0.01864	-0.09226	-0.06235	0.41477	0.70409	0.37655	-0.07181	-0.23087	-0.02830
	0.32663	-0.05555	-0.20524	0.00818	0.09284	-0.00068	-0.03923								
12	-0.02711	0.00083	0.03189	-0.00107	-0.06333	-0.00237	0.10633	0.01068	-0.15835	-0.07503	0.37655	0.79697	0.55358	-0.09261	-0.36897
	-0.02871	0.07877	0.00141	-0.00788	0.00468	0.02131	-0.00018								
13	-0.00019	-0.04188	0.00083	0.04463	0.00539	-0.04978	-0.00987	0.03803	0.01605	-0.19975	-0.07181	0.55358	0.78453	0.40828	-0.09313
	-0.23168	0.02843	0.15923	-0.00443	-0.08551	-0.00005	0.03949								
14	0.02953	-0.00019	-0.02711	0.00062	0.05572	0.00076	-0.11795	-0.00620	0.15117	0.02819	-0.23087	-0.09261	0.40828	0.78401	0.55261
	-0.07132	-0.19798	0.01557	0.04607	-0.00553	-0.03075	-0.00045								
15	-0.00045	0.03949	-0.00018	-0.03923	-0.00663	0.03712	0.00482	0.00701	0.00062	0.07828	-0.02830	-0.36897	-0.09313	0.55261	0.79755
	0.37849	-0.07513	-0.16800	0.00902	0.08676	0.00076	-0.04076								
16	-0.03075	-0.00005	0.02131	-0.00068	-0.04737	0.00301	0.14246	0.01137	-0.19752	-0.05531	0.32663	-0.02871	-0.23168	-0.07132	0.37849
	0.70354	0.41075	-0.06232	-0.09386	0.00711	0.04035	0.00076								
17	-0.00553	-0.08551	0.00468	0.09284	0.00789	-0.11064	0.01165	0.00282	-0.04637	-0.37054	-0.05555	0.07877	0.02843	-0.19798	-0.07513
	0.41075	0.82825	0.48927	-0.06408	-0.19839	0.00711	0.08677								
18	0.04606	-0.00443	-0.00787	0.00818	0.03256	-0.03690	-0.20338	-0.04777	0.33119	-0.04888	-0.20524	0.00141	0.15923	0.01557	-0.16800
	-0.06232	0.48927	0.71596	0.26321	-0.06408	-0.09385	0.00902								
19	0.01557	0.15923	0.00141	-0.20524	-0.04889	0.33120	-0.04777	-0.20337	-0.03690	0.03257	0.00818	-0.00788	-0.00443	0.04607	0.00902
	-0.09386	-0.06408	0.26321	0.71596	0.48926	-0.06232	-0.16800								
20	-0.19797	0.02843	0.07876	-0.05556	-0.37057	-0.04637	0.00283	0.01164	-0.11064	0.00789	0.09284	0.00468	-0.08551	-0.00553	0.08676
	0.00711	-0.19839	-0.06408	0.48926	0.82827	0.41075	-0.07514								
21	-0.07131	-0.23168	-0.02872	0.32663	-0.05531	-0.19751	0.01138	0.14244	0.00301	-0.04737	-0.00068	0.02131	-0.00005	-0.03075	0.00076
	0.04035	0.00711	-0.09385	-0.06232	0.41075	0.70354	0.37849								
22	0.55261	-0.09313	-0.36900	-0.02831	0.07830	0.00062	0.00701	0.00482	0.03712	-0.00663	-0.03923	-0.00018	0.03949	-0.00045	-0.04076
	0.00076	0.08677	0.00902	-0.16800	-0.07514	0.37849	0.79757								

ENERGIES FOR PENTAPHENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	11,12	10,12	11,13	9,12	8,12	8,13	7,12	6,12	5,12	4,12
XMOMNT	1.02230	0.23090	-0.17982	-0.26409	-0.18762	-0.23412	-0.18550	0.06884	0.00132	-0.00940
YMOMNT	0.58982	-0.40123	0.31298	0.45797	-0.10892	0.40616	-0.10705	-0.11969	0.00087	0.01630
JUMP E	17.5229	18.4195	18.7033	26.0483	26.7812	27.9616	30.9560	31.4134	34.8368	36.5314
DIAG E	30.0229	29.7153	29.9554	40.0699	39.7008	43.2719	47.4880	47.0547	49.0773	53.6569
DIAG E	30.1848	29.9701	29.9973	40.9973	40.3099	43.7610	47.9575	47.5214	49.5956	54.1817
CORRSP	29.8430	28.5785	29.7557	38.7111	39.4354	43.3092	47.4817	49.2850	49.5289	54.0845
CORRSP	30.0732	28.9412	29.8002	39.5791	40.0667	43.9246	47.9422	49.6797	49.9656	54.5041

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
28.57853	0.13718	0.16826	-0.29079	//	0.0005	0.7906	0.5571	-0.1849	0.0002	-0.1671	0.0001	-0.0313	0.0000	0.0380
26.42630				//	-0.0001	0.5986	0.5739	-0.4633	0.0005	-0.2920	0.0002	-0.0704	0.0000	0.0864
29.75565	0.34792	-0.28307	0.44139	//	-0.0210	-0.5770	0.7999	-0.1375	0.0025	0.0889	0.0004	0.0081	0.0004	0.0057
19.03527				//	-0.0432	-0.6947	0.6807	-0.1437	0.0052	0.1656	-0.0050	0.0310	-0.0008	0.0556
38.71105	0.08541	-0.11375	0.19734	//	0.0001	-0.0339	0.1721	0.8014	0.0006	-0.5335	-0.0002	0.1518	-0.0002	-0.1393
34.60403				//	-0.0001	0.0658	0.3501	0.7872	0.0000	-0.4456	-0.0003	0.1450	-0.0000	-0.1839
43.30921	0.68107	-0.30366	0.52687	//	-0.0001	0.1398	0.1225	0.4902	-0.0004	0.6203	0.0000	-0.5793	-0.0004	-0.0693
35.94465				//	0.0005	0.3467	0.2857	0.3014	0.0045	0.6546	-0.0000	-0.5262	-0.0017	-0.0431
47.48174	0.06467	-0.15480	-0.08979	//	-0.0006	-0.0003	-0.0001	-0.0003	-0.1384	-0.0012	0.9712	-0.0013	-0.1938	-0.0006
42.29689				//	-0.1140	-0.0002	-0.0000	0.0001	0.0256	-0.0003	0.9903	-0.0004	0.0745	-0.0010
49.28497	0.09885	-0.10901	0.18703	//	0.0004	0.1413	0.0703	0.2141	0.0007	-0.5377	0.0036	0.7948	0.0080	0.0914
46.54192				//	-0.0003	0.1697	0.0357	0.1828	-0.0022	0.4371	0.0014	0.7437	-0.0069	0.4385
54.08454	0.01625	-0.04206	0.07279	//	-0.0000	-0.0353	0.0004	0.1362	-0.0000	-0.0759	0.0004	-0.0921	0.0002	0.9828
50.53099				//	0.0000	-0.0692	-0.0304	0.1440	0.0002	-0.2629	0.0006	-0.3782	0.0006	0.8726

ENERGIES FOR PENTAPHENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	11,12	10,13	8,12	9,13	7,12	11,15	6,13	5,12	4,13	8,15
XMOMNT	1.02230	0.51329	-0.18762	-0.65678	-0.18550	-0.46268	0.14751	0.00132	-0.02633	-0.02021
YMOMNT	0.58982	0.29605	-0.10892	-0.37854	-0.10705	-0.09399	0.08511	0.00087	-0.01517	-0.01141
JUMP E	17.5229	19.5999	26.7812	27.2288	30.9560	31.4106	32.5938	34.8368	37.7118	40.6689
DIAG E	30.0229	31.9922	39.7008	39.6470	47.4880	43.5179	48.0753	49.0773	55.4502	59.1372
DIAG E	30.1848	32.1271	40.3099	40.4545	47.9575	43.1409	48.4220	49.5956	55.8551	59.2075
CORRSP	27.3035	33.1442	39.0018	36.0865	49.3239	45.3355	53.2493	43.7130	56.4200	60.5309
CORRSP	27.4651	33.3573	39.4871	36.6650	49.7683	45.2955	53.6299	44.1858	56.7269	60.6740

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
27.30352	0.36227	0.48379	0.27921	//	0.7917	-0.6047	0.0019	0.0410	-0.0111	-0.0441	0.0172	-0.0304	-0.0396	0.0332
15.01611				//	0.8072	-0.5564	0.0238	-0.0910	0.0932	-0.0293	0.0325	-0.0068	0.0197	0.1381
33.14418	2.31763	1.11067	0.64091	//	0.5613	0.7354	-0.3202	-0.0968	-0.0281	-0.1589	0.0207	0.0181	-0.0053	-0.0736
22.07245				//	0.4814	0.7130	-0.3841	-0.0816	0.0673	-0.2966	0.0427	0.0764	0.0541	-0.0510
39.00184	0.21477	0.31200	0.17929	//	0.1707	0.1888	0.8210	-0.3380	-0.1495	0.0264	-0.3373	-0.0432	0.0750	-0.0505
37.68939				//	0.1594	0.2411	0.6340	0.0444	0.2639	0.0523	0.2573	-0.5044	0.1460	-0.3135
36.08653	0.44801	-0.46806	-0.26993	//	0.0454	0.1322	0.3122	0.7774	0.3383	-0.3912	-0.1010	-0.0046	-0.0129	-0.0266
30.51314				//	-0.1013	-0.1524	-0.1650	0.7319	0.4836	-0.3781	0.1468	0.0295	0.0507	0.0421
49.32391	0.01155	0.06430	0.03705	//	0.0087	-0.0664	-0.0317	-0.3374	0.7121	-0.0918	-0.0958	0.5218	0.2893	-0.0089
43.04524				//	-0.0315	0.0641	-0.1990	-0.1365	0.5912	0.6379	0.0083	0.1962	0.3682	0.0782
45.33547	0.11328	-0.20999	-0.12110	//	0.1377	0.1210	-0.0207	0.3466	0.0704	0.8505	-0.2517	0.2311	0.0225	0.0150
44.63956				//	0.2499	0.1343	-0.1248	0.6007	-0.3416	0.5877	-0.0508	-0.1066	-0.2359	-0.1068
53.24933	0.02455	0.09023	0.05197	//	0.0359	0.0358	0.2514	0.1138	-0.3244	-0.0010	0.6392	0.6146	0.0639	-0.1598
34.25749				//	-0.1194	-0.1921	-0.5040	-0.1977	-0.0626	0.0629	0.6788	-0.3526	-0.1104	-0.2250
43.71301	0.01440	-0.07638	-0.04375	//	-0.0685	-0.0782	-0.1923	0.0643	-0.4207	-0.2892	-0.5815	0.5289	-0.1582	0.2111
51.34884				//	0.0568	0.0017	0.2647	0.0189	-0.0316	0.0298	0.4427	0.7472	-0.1748	-0.3737
56.41998	0.00793	-0.04987	-0.02860	//	0.0113	-0.0125	-0.0805	0.1328	-0.2404	-0.0447	-0.0398	-0.1163	0.9235	0.2187
54.52848				//	0.0035	0.0059	0.0538	0.1683	-0.4564	-0.0329	0.2968	0.0800	0.7826	0.2286
60.53085	0.03477	0.10062	0.05816	//	0.0435	0.1177	0.1334	-0.0401	0.1012	0.0405	0.2332	-0.0142	-0.1626	0.9338
57.42760				//	-0.0127	0.2042	0.2013	-0.0122	0.0619	0.0850	0.4023	-0.0005	-0.3554	0.7863

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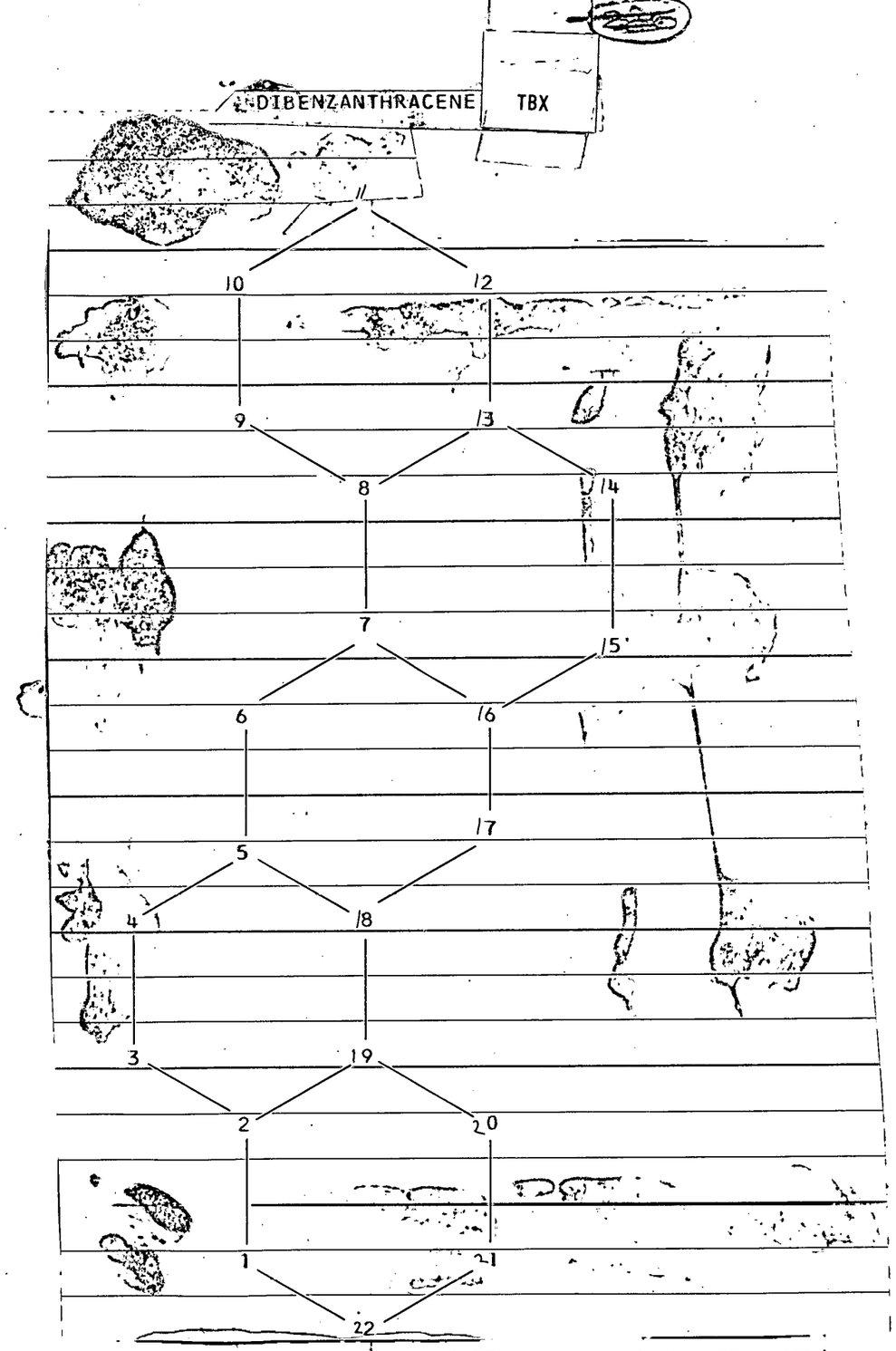

ATOMIC COORDINATES													
x	0.8779	0.8858	0.	0.	0.9096	0.9002	1.7340	1.7535	0.8851	0.8937	1.7721	2.6621	2.6542	3.5400
	3.5400	2.6304	2.6398	1.8060	1.7865	2.6549	2.6463	1.7679						
y	0.5320	1.5710	2.0600	3.0760	3.5940	4.5140	5.1350	6.1510	6.6570	7.6970	8.2060	7.6740	6.6350	6.1460
	5.1300	4.6120	3.6920	3.0710	2.0550	1.5490	0.5090	0.						

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DIBENZANTHRACENE x TBX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 A	8 S	9 S	10A	11 A	12 S	13 S
1.603947	1.538141	1.458388	1.403236	1.333015	1.327763	1.289930	1.258611	1.175346	1.145711	1.124526	0.875471	0.854287
0.098505	0.202563	0.262462	-0.092071	0.088728	0.263901	0.181340	-0.215106	0.336588	0.251080	0.197225	-0.197226	0.251079
0.197092	0.327224	0.282319	0.002908	0.263979	0.033701	0.319948	0.142283	0.178320	-0.101394	0.197118	0.197118	0.101394
0.148907	0.215361	0.116083	0.195875	0.386240	0.050477	0.276688	-0.006474	-0.213666	-0.175126	-0.273778	0.273779	-0.175125
0.179303	0.157107	-0.061257	0.329352	0.274532	0.035568	0.014370	-0.150738	-0.337709	-0.004956	-0.342504	-0.342505	0.004955
0.329922	0.150965	-0.251971	0.390360	-0.001739	-0.001541	-0.278807	-0.169471	-0.038149	0.185134	0.101495	-0.101495	0.185134
0.285558	-0.006501	-0.233851	0.290698	-0.097883	0.241042	-0.194191	-0.109636	0.119720	-0.180222	0.339112	0.339111	0.180223
0.332279	-0.214676	-0.144664	0.006753	-0.142754	0.353585	0.117191	0.097352	0.143727	-0.361028	0.054046	-0.054045	-0.361028
0.261108	-0.336672	0.181465	0.107343	-0.105852	0.258321	0.061818	0.370666	0.029076	0.124932	-0.196009	-0.196009	-0.124933
0.133730	-0.219683	0.211037	0.173690	-0.258820	0.035054	0.266392	0.161649	-0.290253	0.329034	0.036453	-0.036453	0.329034
0.076094	-0.160829	0.233739	0.195341	-0.268904	-0.229429	0.276848	-0.216445	-0.258266	0.077830	0.233134	0.233134	-0.077829
0.066900	-0.156320	0.250954	0.167012	-0.132020	-0.348832	0.085900	-0.387467	0.083491	-0.262602	0.087543	-0.087543	-0.262603
0.098505	-0.202563	0.262461	0.092071	0.088723	-0.263903	-0.181340	-0.215106	0.336588	-0.251078	-0.197226	-0.197225	0.251078
0.197092	-0.327224	0.282319	-0.002908	0.263978	-0.033707	-0.319948	0.142284	0.178320	0.101394	-0.197119	0.197118	0.101395
0.148907	-0.215361	0.116083	-0.195875	0.386239	-0.050484	-0.276688	-0.006474	-0.213665	0.175125	0.273779	0.273778	-0.175125
0.179303	-0.157107	-0.061257	-0.329352	0.274531	-0.035573	-0.014370	-0.150738	-0.337708	0.004955	0.342504	-0.342503	0.004954
0.329922	-0.150965	-0.251970	-0.390360	-0.001739	0.001540	-0.278807	-0.169471	-0.038149	-0.185134	-0.101495	-0.101495	0.185134
0.285558	0.006501	-0.233851	-0.290698	-0.097888	-0.241040	0.194191	-0.109636	0.119719	0.180223	-0.339112	0.339111	0.180223
0.332278	0.214676	-0.144664	-0.006753	-0.142761	-0.353582	-0.117191	0.097352	0.143726	0.361028	-0.054046	-0.054045	-0.361028
0.261108	0.336672	0.181465	-0.107343	-0.105857	-0.258319	-0.061818	0.370666	0.029077	-0.124933	0.196009	-0.196009	-0.124933
0.133730	0.219682	0.211037	-0.173690	-0.258820	-0.035049	-0.266392	0.161649	-0.290253	-0.329034	-0.036453	-0.036454	0.329034
0.076094	0.160829	0.233740	-0.195341	-0.268900	0.229435	-0.276848	-0.216445	-0.258266	-0.077830	-0.233134	0.233135	-0.077830
0.066900	0.156320	0.250955	-0.167012	-0.132013	0.348834	-0.085900	-0.387467	0.083490	-0.262603	-0.087543	-0.087543	-0.262603

OVERLAP EIGNVALUES AND EIGNVECTORS

14 A	15 A	16 S	17 S	18 A	19 S	20 A	21 S	22 A
0.824651	0.741386	0.710068	0.672235	0.666982	0.596761	0.541610	0.461857	0.396051
-0.336588	0.215106	-0.181340	-0.263902	-0.088725	-0.092071	-0.262461	-0.202563	-0.098505
0.178320	0.142284	0.319948	0.033705	-0.263979	-0.002908	0.282319	0.327224	0.197092
-0.213665	0.006474	-0.276688	-0.050482	-0.386239	0.195874	-0.116083	-0.215361	-0.148907
-0.337708	-0.150738	0.014370	0.035572	0.274532	-0.329352	-0.061257	0.157107	0.179303
0.038150	0.169471	0.278807	0.001540	0.001738	0.390360	0.251971	-0.150965	-0.329922
0.119719	-0.109636	-0.194191	0.241041	-0.097886	-0.290698	-0.233851	-0.006501	0.285558
-0.143727	-0.097352	-0.117191	-0.353583	0.142759	0.006753	0.144664	0.214676	-0.332279
0.029076	0.370666	0.061818	0.258319	-0.105856	-0.107343	0.181465	-0.336672	0.261108
0.290253	-0.161649	-0.266392	-0.035051	0.258820	0.173690	-0.211037	0.219683	-0.133730
-0.258267	-0.216446	0.276848	-0.229433	-0.268901	-0.195341	0.233739	-0.160829	0.076094
-0.083490	0.387467	-0.085900	0.348834	0.132015	0.167012	-0.250954	0.156320	-0.066900
0.336589	-0.215105	-0.181340	-0.263902	0.088727	-0.092071	0.262461	-0.202563	0.098505
-0.178320	-0.142284	0.319948	0.033703	-0.263979	-0.002908	-0.282319	0.327224	-0.197092
-0.213666	-0.006474	-0.276688	-0.050479	0.386240	0.195875	0.116083	-0.215361	0.148907
0.337709	0.150738	0.014370	0.035569	-0.274532	-0.329353	0.061257	0.157107	-0.179303
-0.038149	-0.169471	0.278806	0.001541	-0.001739	0.390361	-0.251970	-0.150965	0.329922
-0.119720	0.109636	-0.194191	0.241042	0.097885	-0.290698	0.233851	-0.006501	-0.285558
0.143727	0.097352	-0.117191	-0.353584	-0.142756	0.006753	-0.144664	0.214676	0.332279
-0.029076	-0.370666	0.061818	0.258320	0.105854	-0.107343	-0.181465	-0.336672	-0.261108
-0.290252	0.161649	-0.266392	-0.035053	-0.258820	0.173690	0.211037	0.219683	0.133730
0.258266	0.216446	0.276848	-0.229431	0.268903	-0.195341	-0.233740	-0.160829	-0.076094
0.083490	-0.387467	-0.085900	0.348833	-0.132018	0.167012	0.250955	0.156320	-0.066900

DIBENZANTHRACENE X **TBX APPROXIMATION**

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 A	8 S	9 S	10 A	11 A	12 S	13 S
28.29360	26.28931	23.61781	21.59276	18.77190	18.54891	16.88908	15.43958	11.21011	9.55644	8.32092	-10.68827	-12.81666
0.077779	0.163329	0.217335	-0.077724	0.076850	0.229024	0.159665	-0.191737	0.310468	0.234571	0.185985	-0.210787	0.271649
0.155623	0.263844	0.233778	0.002455	0.228640	0.029247	0.281706	0.126826	0.164482	-0.094727	0.185884	0.210672	0.109701
0.117577	0.173648	0.096124	0.165353	0.334534	0.043806	0.243617	-0.005771	-0.197084	-0.163611	-0.258175	0.292603	-0.189473
0.141577	0.126677	-0.050725	0.278032	0.237780	0.030867	0.012653	-0.134362	-0.311501	-0.004630	-0.322983	-0.366054	0.005361
0.260505	0.121725	-0.208648	0.329534	-0.001506	-0.001337	-0.245482	-0.151060	-0.035189	0.172961	0.095710	-0.108473	0.200301
0.225476	-0.005242	-0.193644	0.245401	-0.084779	0.209186	-0.170980	-0.097725	0.110429	-0.168372	0.319785	0.362428	0.194988
0.262366	-0.173096	-0.119791	0.005700	-0.123643	0.306855	0.103184	0.086775	0.132573	-0.337290	0.050965	-0.057761	-0.390606
0.206170	-0.271462	0.150264	0.090617	-0.091682	0.224181	0.054429	0.330398	0.026820	0.116718	-0.184838	-0.209486	-0.135168
0.105593	-0.177132	0.174752	0.146626	-0.224171	0.030421	0.234551	0.144088	-0.267728	0.307399	0.034376	-0.038960	0.355990
0.060083	-0.129678	0.193551	0.164903	-0.232906	-0.199108	0.243757	-0.192931	-0.238223	0.072712	0.219847	0.249163	-0.084205
0.052824	-0.126042	0.207806	0.140988	-0.114346	-0.302731	0.075632	-0.345373	0.077011	-0.245336	0.082554	-0.093562	-0.284117
0.077779	-0.163329	0.217334	0.077725	0.076846	-0.229026	-0.159665	-0.191737	0.310467	-0.234570	-0.185985	-0.210786	0.271648
0.155623	-0.263844	0.233778	-0.002455	0.228639	-0.029252	-0.281706	0.126826	0.164481	0.094727	-0.185884	0.210671	0.109702
0.117577	-0.173648	0.096124	-0.165353	0.334533	-0.043812	-0.243616	-0.005771	-0.197084	0.163611	0.258175	0.292603	-0.189472
0.141577	-0.126677	-0.050724	-0.278032	0.237779	-0.030872	-0.012653	-0.134362	-0.311500	0.004630	0.322984	-0.366053	0.005360
0.260505	-0.121725	-0.208647	-0.329534	-0.001506	0.001337	0.245482	-0.151060	-0.035189	-0.172961	-0.095710	-0.108474	0.200301
0.225476	0.005242	-0.193643	0.245401	-0.084783	-0.209185	0.170980	-0.097725	0.110428	0.168373	-0.319785	0.362427	0.194988
0.262366	0.173096	-0.119791	0.005701	-0.123649	-0.306853	-0.103184	0.086776	0.132573	0.337290	-0.050966	-0.057761	-0.390606
0.206170	0.271462	0.150265	-0.090617	-0.091686	-0.224179	-0.054429	0.330398	0.026820	-0.116718	0.184838	-0.209486	-0.135168
0.105593	0.177132	0.174752	-0.146625	-0.224172	-0.030417	-0.234551	0.144088	-0.267728	-0.307400	-0.034375	-0.038961	0.355991
0.060083	0.129678	0.193551	-0.164903	-0.232902	0.199113	-0.243758	-0.192931	-0.238224	-0.072713	-0.219847	0.249164	-0.084206
0.052824	0.126042	0.207806	-0.140988	-0.114341	0.302733	-0.075633	-0.345373	0.077011	0.245336	-0.082554	-0.093562	-0.284117

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 A	15 A	16 S	17 S	18 A	19 S	20 A	21 S	22 A
-15.97762	-26.21118	-30.68144	-36.63711	-37.51736	-50.77391	-63.59584	-87.55276	14.58535
-0.370649	-0.249821	-0.215200	-0.321872	-0.108639	-0.119185	-0.356634	-0.298063	-0.156524
0.196365	0.165247	0.379690	0.041109	0.323230	-0.003765	0.383616	0.481494	-0.313180
0.235287	0.007519	-0.328352	-0.061571	-0.472933	0.253558	-0.157734	-0.316894	-0.236614
-0.371883	-0.175066	0.017054	0.043385	0.336152	-0.426344	-0.083236	0.231175	0.284913
0.042010	0.196822	0.330867	0.001879	0.002129	0.505319	0.342379	-0.222138	-0.524247
0.131834	-0.127330	-0.230451	0.293989	-0.119857	-0.376307	-0.317758	-0.009566	0.453753
-0.158272	-0.113063	-0.139073	-0.431251	0.174802	0.008741	0.196570	0.315886	-0.527992
0.032019	0.430487	0.073360	0.315062	-0.129616	-0.138955	0.246576	-0.495397	0.414901
0.319626	-0.187737	-0.316134	-0.042750	0.316914	0.224840	-0.286758	0.323253	-0.212498
-0.284402	-0.251378	0.328542	-0.279831	-0.329257	-0.252868	0.317606	-0.236653	0.120913
-0.091939	0.450000	-0.101939	0.425459	0.161646	0.216196	-0.340998	0.230018	-0.106304
0.370651	-0.249821	-0.215200	-0.321871	0.108642	-0.119186	0.356634	-0.298063	0.156524
-0.196366	-0.165247	0.379690	0.041106	-0.323230	-0.003764	-0.383616	0.481495	-0.313180
-0.235288	-0.007519	-0.328352	-0.061568	0.472933	0.253558	0.157734	-0.316894	0.236614
0.371884	0.175066	0.017054	0.043383	-0.336152	-0.426345	0.083236	0.231175	-0.284913
-0.042009	-0.196822	0.330867	0.001879	-0.002129	0.505319	-0.342379	-0.222138	0.524247
-0.131835	0.127330	-0.230451	0.293989	0.119855	-0.376307	0.317757	-0.009566	-0.453753
0.158271	0.113063	-0.139073	-0.431253	-0.174798	0.008741	-0.196570	0.315886	0.527992
-0.032019	-0.430487	0.073360	0.315063	0.129613	-0.138955	-0.246576	-0.495397	-0.414901
-0.319625	0.187737	-0.316134	-0.042752	-0.316914	0.224840	0.286758	0.323253	0.212498
0.284401	0.251378	0.328542	-0.279828	0.329259	-0.252867	-0.317606	-0.236653	-0.120913
0.091939	-0.450000	-0.101939	0.425458	-0.161650	0.216196	0.340998	0.230018	0.106304

DIBENZANTHRACENE X TBX TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.00000	0.58539	-0.00000	-0.22121	0.00000	0.08779	-0.00000	-0.02396	0.00000	0.01846	0.00000	-0.01590	0.00000	0.03552	0.00000
	-0.04070	0.00000	0.03813	-0.00000	-0.34748	-0.00000	0.68876								
2	0.58539	1.00000	0.50023	-0.00000	-0.14994	0.00000	0.10578	0.00000	-0.04458	0.00000	0.03577	-0.00000	-0.03889	0.00000	0.03539
	-0.00000	-0.11932	-0.00000	0.53070	0.00000	-0.26739	-0.00000								
3	-0.00000	0.50023	1.00000	0.79502	-0.00000	-0.18921	0.00000	0.04179	-0.00000	-0.03525	0.00000	0.03552	0.00000	-0.07790	-0.00000
	0.11382	-0.00000	-0.21517	0.00000	0.02166	0.00000	-0.10891								
4	-0.22121	-0.00000	0.79502	1.00000	0.45017	-0.00000	-0.13585	-0.00000	0.05460	-0.00000	-0.03764	0.00000	0.03539	0.00000	-0.00784
	0.00000	0.05900	0.00000	-0.23621	-0.00000	0.18140	0.00000								
5	0.00000	-0.14994	-0.00000	0.45017	1.00000	0.66927	-0.00000	-0.09328	0.00000	0.05284	0.00000	-0.04070	-0.00000	0.11382	-0.00000
	-0.18993	0.00000	0.49738	-0.00000	-0.09971	-0.00000	0.08619								
6	0.08779	0.00000	-0.18921	-0.00000	0.66927	1.00000	0.59689	-0.00000	-0.15320	0.00000	0.10326	-0.00000	-0.11932	-0.00000	0.05900
	-0.00000	-0.31134	-0.00000	0.02132	-0.00000	-0.05519	-0.00000								
7	-0.00000	0.10578	0.00000	-0.13585	-0.00000	0.59689	1.00000	0.46354	-0.00000	-0.11333	-0.00000	0.03813	0.00000	-0.21517	-0.00000
	0.49738	-0.00000	-0.27259	-0.00000	0.09950	0.00000	-0.08380								
8	-0.02396	0.00000	0.04179	-0.00000	-0.09328	-0.00000	0.46354	1.00000	0.60836	0.00000	-0.25684	-0.00000	0.53070	0.00000	-0.23621
	-0.00000	0.02132	0.00000	0.00220	-0.00000	0.01204	-0.00000								
9	0.00000	-0.04458	-0.00000	0.05460	0.00000	-0.15320	-0.00000	0.60836	1.00000	0.67630	-0.00000	-0.34748	-0.00000	0.02166	-0.00000
	-0.09971	0.00000	0.09950	0.00000	-0.04086	-0.00000	0.03684								
10	0.01846	0.00000	-0.03525	-0.00000	0.05284	0.00000	-0.11333	0.00000	0.67630	1.00000	0.64620	0.00000	-0.26739	-0.00000	0.18140
	0.00000	-0.05519	-0.00000	0.01204	0.00000	-0.01487	-0.00000								
11	0.00000	0.03577	0.00000	-0.03764	0.00000	0.10326	-0.00000	-0.25684	-0.00000	0.64620	1.00000	0.68876	-0.00000	-0.10891	-0.00000
	0.08619	0.00000	-0.08380	-0.00000	0.03684	0.00000	-0.03207								
12	-0.01590	-0.00000	0.03552	0.00000	-0.04070	-0.00000	0.03813	-0.00000	-0.34748	0.00000	0.68876	1.00000	0.58539	0.00000	-0.22121
	-0.00000	0.08779	0.00000	-0.02396	-0.00000	0.01846	0.00000								
13	0.00000	-0.03889	0.00000	0.03539	-0.00000	-0.11932	0.00000	0.53070	-0.00000	-0.26739	-0.00000	0.58539	1.00000	0.50023	0.00000
	-0.14994	-0.00000	0.10578	0.00000	-0.04458	-0.00000	0.03577								
14	0.03552	0.00000	-0.07790	-0.00000	0.11382	-0.00000	-0.21517	0.00000	0.02166	-0.00000	-0.10891	0.00000	0.50023	1.00000	0.79502
	0.00000	-0.18921	-0.00000	0.04179	0.00000	-0.03525	-0.00000								
15	0.00000	0.03539	-0.00000	-0.00784	-0.00000	0.05900	-0.00000	-0.23621	-0.00000	0.18140	-0.00000	-0.22121	0.00000	0.79502	1.00000
	0.45017	0.00000	-0.13585	-0.00000	0.05460	-0.00000	-0.03764								
16	-0.04070	-0.00000	0.11382	0.00000	-0.18993	-0.00000	0.49738	-0.00000	-0.09971	0.00000	0.08619	-0.00000	-0.14994	0.00000	0.45017
	1.00000	0.66927	0.00000	-0.09328	0.00000	0.05284	0.00000								
17	0.00000	-0.11932	-0.00000	0.05900	0.00000	-0.31134	-0.00000	0.02132	0.00000	-0.05519	0.00000	0.08779	-0.00000	-0.18921	0.00000
	0.66927	1.00000	0.59689	0.00000	-0.15320	-0.00000	0.10326								
18	0.03813	-0.00000	-0.21517	0.00000	0.49738	-0.00000	-0.27259	0.00000	0.09950	-0.00000	-0.08380	0.00000	0.10578	-0.00000	-0.13585
	0.00000	0.59689	1.00000	0.46354	0.00000	-0.11333	-0.00000								
19	-0.00000	0.53070	0.00000	-0.23621	-0.00000	0.02132	-0.00000	0.00220	0.00000	0.01204	-0.00000	-0.02396	0.00000	0.04179	-0.00000
	-0.09328	0.00000	0.46354	1.00000	0.60836	0.00000	-0.25684								
20	-0.34748	0.00000	0.02166	-0.00000	-0.09971	-0.00000	0.09950	-0.00000	-0.04086	0.00000	0.03684	-0.00000	-0.04458	0.00000	0.05460
	0.00000	-0.15320	0.00000	0.60836	1.00000	0.67630	0.00000								
21	-0.00000	-0.26739	0.00000	0.18140	-0.00000	-0.05519	0.00000	0.01204	-0.00000	-0.01487	0.00000	0.01846	-0.00000	-0.03525	-0.00000
	0.05284	-0.00000	-0.11333	0.00000	0.67630	1.00000	0.64620								
22	0.68876	-0.00000	-0.10891	0.00000	0.08619	-0.00000	-0.08380	-0.00000	0.03684	-0.00000	-0.03207	0.00000	0.03577	-0.00000	-0.03764
	0.00000	0.10326	-0.00000	-0.25684	0.00000	0.64620	1.00000								

DIBENZANTHRACENE X — TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.78524	0.42833	-0.05258	-0.21135	0.01196	0.08524	-0.00442	-0.02344	0.00161	0.01827	-0.00076	-0.01587	0.00060	0.03523	0.00060
	-0.04060	0.00260	0.04199	-0.03006	-0.32874	-0.05079	0.52322								
2	0.42833	0.73529	0.33549	-0.04953	-0.13678	0.01754	0.10235	-0.00472	-0.04374	0.00142	0.03530	0.00060	-0.03815	0.00094	0.03458
	0.00267	-0.11272	-0.03289	0.37498	-0.03518	-0.25063	-0.03721								
3	-0.05258	0.33549	0.77208	0.62006	-0.03873	-0.17900	0.00566	0.04074	-0.00211	-0.03485	0.00033	0.03523	0.00094	-0.07667	-0.00613
	0.11024	0.01234	-0.20030	-0.03746	0.02673	0.01813	-0.10133								
4	-0.21135	-0.04953	0.62006	0.78609	0.30109	-0.06066	-0.12720	0.00919	0.05306	-0.00309	-0.03704	0.00060	0.03458	-0.00613	-0.00912
	0.01237	0.06193	-0.02934	-0.22111	0.01422	0.17685	0.00570								
5	0.01196	-0.13678	-0.03873	0.30109	0.71641	0.46711	-0.04527	-0.08541	0.00927	0.05150	-0.00308	-0.04060	0.00267	0.11024	0.01237
	-0.17458	-0.02653	0.34829	-0.02803	-0.09312	0.00109	0.08323								
6	0.08524	0.01754	-0.17900	-0.06066	0.46711	0.76225	0.44188	-0.04335	-0.14453	0.00848	0.10066	0.00260	-0.11272	0.01234	0.06193
	-0.02653	-0.29317	-0.04589	0.02669	0.00585	-0.05504	-0.00618								
7	-0.00442	0.10235	0.00566	-0.12720	-0.04527	0.44188	0.74948	0.30556	-0.05080	-0.10566	0.01566	0.04199	-0.03289	-0.20030	-0.02934
	0.34829	-0.04589	-0.25517	0.01306	0.09679	-0.00214	-0.08229								
8	-0.02344	-0.00472	0.04074	0.00919	-0.08541	-0.04335	0.30556	0.73257	0.43898	-0.04136	-0.24019	-0.03006	0.37498	-0.03746	-0.22111
	-0.02803	0.02669	0.01306	0.00093	-0.00295	0.01213	0.00241								
9	0.00161	-0.04374	-0.00211	0.05306	0.00927	-0.14453	-0.05080	0.43898	0.77774	0.51307	-0.04781	-0.32874	-0.03518	0.02673	0.01422
	-0.09312	0.00585	0.09679	-0.00295	-0.04022	0.00037	0.03638								
10	0.01827	0.00142	-0.03485	-0.00309	0.05150	0.00848	-0.10566	-0.04136	0.51307	0.77196	0.47386	-0.05079	-0.25063	0.01813	0.17685
	0.00109	-0.05504	-0.00214	0.01213	0.00037	-0.01481	-0.00061								
11	-0.00076	0.03530	0.00033	-0.03704	-0.00308	0.10066	0.01566	-0.24019	-0.04781	0.47386	0.76879	0.52322	-0.03721	-0.10133	0.00570
	0.08323	-0.00618	-0.08229	0.00241	0.03638	-0.00061	-0.03175								
12	-0.01587	0.00060	0.03523	0.00060	-0.04060	0.00260	0.04199	-0.03006	-0.32874	-0.05079	0.52322	0.78524	0.42833	-0.05258	-0.21135
	0.01196	0.08524	-0.00442	-0.02344	0.00161	0.01828	-0.00076								
13	0.00060	-0.03815	0.00094	0.03458	0.00267	-0.11272	-0.03289	0.37498	-0.03518	-0.25063	-0.03721	0.42833	0.73529	0.33549	-0.04953
	-0.13678	0.01754	0.10235	-0.00472	-0.04374	0.00142	0.03530								
14	0.03523	0.00094	-0.07667	-0.00613	0.11024	0.01234	-0.20030	-0.03746	0.02673	0.01813	-0.10133	-0.05258	0.33549	0.77208	0.62006
	-0.03873	-0.17900	0.00566	0.04074	-0.00211	-0.03485	0.00033								
15	0.00060	0.03458	-0.00613	-0.00912	0.01237	0.06193	-0.02934	-0.22111	0.01422	0.17685	0.00570	-0.21135	-0.04953	0.62006	0.78609
	0.30109	-0.06066	-0.12720	0.00919	0.05306	-0.00309	-0.03704								
16	-0.04060	0.00267	0.11024	0.01237	-0.17458	-0.02653	0.34829	-0.02803	-0.09312	0.00109	0.08323	0.01196	-0.13678	-0.03873	0.30109
	0.71641	0.46711	-0.04527	-0.08541	0.00927	0.05150	-0.00308								
17	0.00260	-0.11272	0.01234	0.06193	-0.02653	-0.29317	-0.04589	0.02669	0.00585	-0.05504	-0.00618	0.08524	0.01754	-0.17900	-0.06066
	0.46711	0.76225	0.44188	-0.04335	-0.14453	0.00848	0.10066								
18	0.04199	-0.03289	-0.20030	-0.02934	0.34829	-0.04589	-0.25517	0.01306	0.09679	-0.00214	-0.08229	-0.00442	0.10235	0.00566	-0.12720
	-0.04527	0.44188	0.74948	0.30556	-0.05080	-0.10566	0.01566								
19	-0.03006	0.37498	-0.03746	-0.22111	-0.02803	0.02669	0.01306	0.00093	-0.00295	0.01213	0.00241	-0.02344	-0.00472	0.04074	0.00919
	-0.08541	-0.04335	0.30556	0.73257	0.43898	-0.04136	-0.24019								
20	-0.32874	-0.03518	0.02673	0.01422	-0.09312	0.00585	0.09679	-0.00295	-0.04022	0.00037	0.03638	0.00161	-0.04374	-0.00211	0.05306
	0.00927	-0.14453	-0.05080	0.43898	0.77774	0.51307	-0.04781								
21	-0.05079	-0.25063	0.01813	0.17685	0.00109	-0.05504	-0.00214	0.01213	0.00037	-0.01481	-0.00061	0.01828	0.00142	-0.03485	-0.00309
	0.05150	0.00848	-0.10566	-0.04136	0.51307	0.77196	0.47386								
22	0.52322	-0.03721	-0.10133	0.00570	0.08323	-0.00618	-0.08229	0.00241	0.03638	-0.00061	-0.03175	-0.00076	0.03530	0.00033	-0.03704
	-0.00308	0.10066	0.01566	-0.24019	-0.04781	0.47386	0.76879								

ENERGIES FOR DIBENZANTHRACENE X , TBX APPROXIMATION 1.7

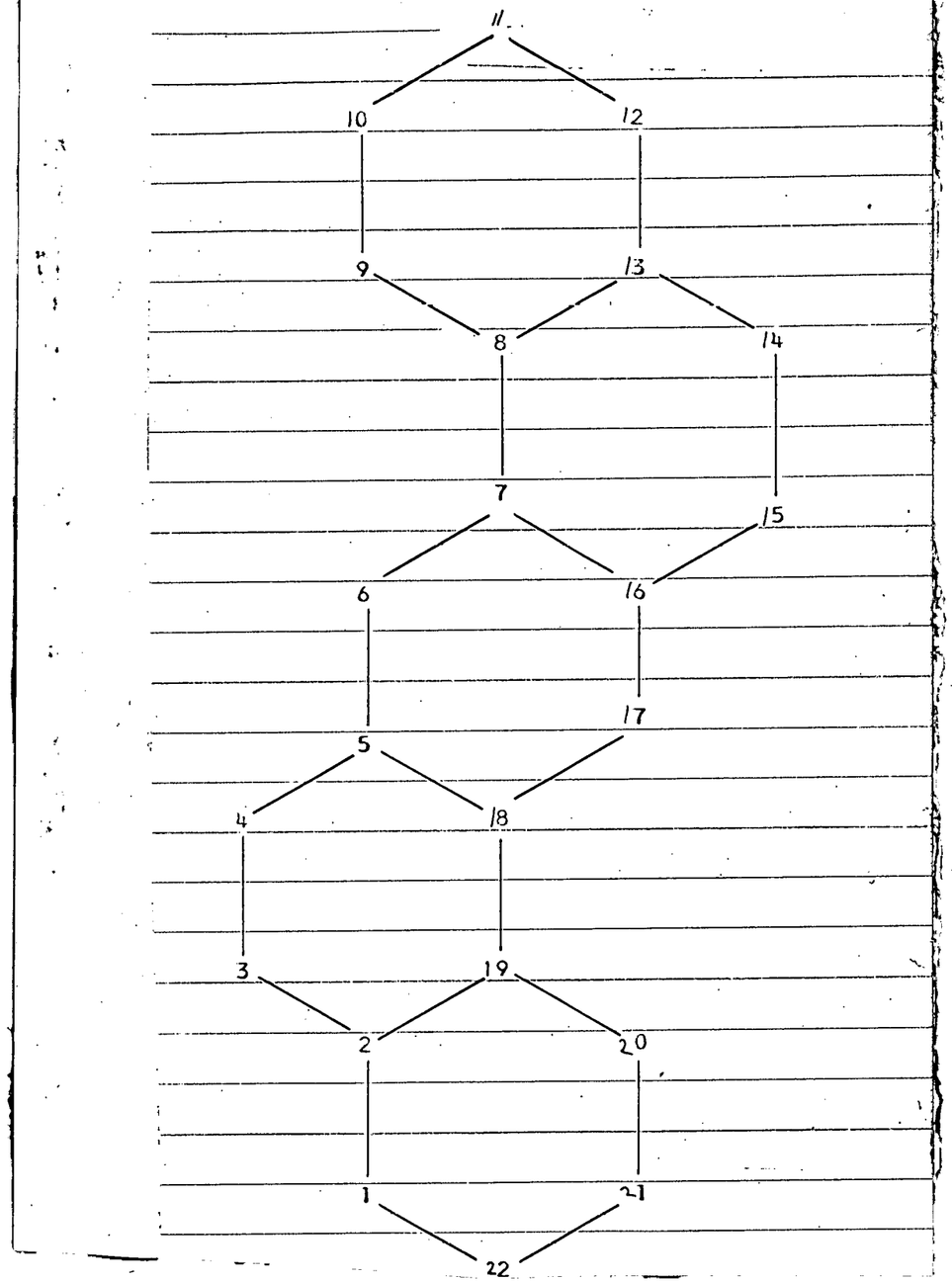
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	11,12	10,12	11,13	10,13	9,14	7,12	6,12	7,13	6,13	4,12
XMOMNT	-0.42890	0.41875	-0.41892	-0.39908	-0.08635	-0.33387	0.03273	0.06867	-0.21486	0.00495
YMOMNT	0.72939	0.82134	-0.82166	0.70292	0.57531	-0.15932	-0.01387	-0.28501	0.12757	0.09195
JUMP E	19.0092	20.2447	21.1376	22.3731	27.1877	27.5774	29.2372	29.7057	31.3656	32.2810
DIAG E	31.5300	31.4207	32.1166	35.2951	45.4060	43.3070	45.0175	43.9931	48.2093	47.5865
DIAG E	31.6227	31.8697	31.7499	35.2847	45.5905	43.7749	45.4696	44.0016	48.2020	47.9540
CORRSP	28.6058	27.7051	33.7874	36.6344	48.4296	41.3837	44.4343	42.9084	49.5654	50.4285
CORRSP	28.7121	33.8400	27.9136	36.7542	48.6021	41.6868	44.9289	43.0936	49.5093	50.4789

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
28.60581	0.09019	-0.25386	0.09850	//	0.8139	-0.1187	0.1486	-0.5118	0.1547	-0.0594	0.0394	0.0818	0.0497	0.0356
				//										
18.18623				//	0.8007	-0.0072	-0.0135	-0.4000	0.4265	-0.0119	0.0798	-0.0735	0.0580	-0.0389
				//										
27.70514	0.03667	0.08783	0.15300	//	-0.0024	0.7432	0.6310	0.0149	0.0057	-0.1589	-0.1207	-0.0521	-0.0022	0.0814
				//										
22.96050				//	0.0063	0.7197	-0.5279	0.2683	0.2671	-0.0457	-0.1676	-0.0755	-0.1456	-0.0534
				//										
33.78740	2.53800	-0.49071	-1.23516	//	-0.0983	-0.5924	0.7024	0.1009	-0.3339	-0.0761	0.1291	-0.0279	0.0315	-0.0087
				//										
27.66032				//	-0.1076	0.6105	0.6726	-0.3071	-0.0407	-0.2105	-0.0810	0.0006	0.0491	0.1190
				//										
36.63443	1.97274	-0.49235	1.01187	//	0.5540	0.0271	-0.0604	0.8154	-0.0853	-0.0264	0.0126	-0.0691	-0.1033	0.0138
				//										
26.05755				//	0.4860	0.0012	0.3402	0.7477	-0.1926	-0.1744	-0.0259	-0.0724	-0.0911	0.0861
				//										
48.42965	0.04787	0.13792	0.06498	//	-0.1233	-0.1285	0.0928	0.1257	0.5989	-0.4948	0.1410	0.3916	-0.3870	-0.1319
				//										
48.96992				//	-0.1763	-0.2064	0.1235	0.1753	0.6501	-0.1181	-0.2757	0.3851	0.0228	0.4679
				//										
41.38365	0.29907	-0.29373	-0.28925	//	0.0217	0.0425	0.2154	0.0394	0.1585	0.7821	-0.0117	0.3072	-0.2761	-0.3773
				//										
35.56556				//	-0.1090	0.0063	0.3564	0.1569	0.3540	0.6928	-0.0887	-0.2163	-0.1932	-0.3730
				//										
44.43427	0.08214	-0.05235	0.20182	//	-0.0426	0.0668	0.0472	0.0071	0.2492	0.2351	0.7750	-0.3174	-0.0873	0.4063
				//										
40.88339				//	0.0191	0.2320	-0.0213	0.1535	0.0098	0.4192	0.6319	0.2002	0.4402	0.3359
				//										
42.90637	0.08670	0.15836	-0.14980	//	0.0110	0.1718	-0.0931	0.0246	-0.3848	-0.0401	0.3827	0.7633	0.2382	0.1601
				//										
38.61825				//	0.2025	0.1069	-0.0079	-0.0289	-0.2400	0.2198	-0.3007	0.8048	0.0480	-0.3166
				//										
49.56542	0.38910	-0.28597	0.32066	//	-0.0174	0.0016	0.0753	0.1554	0.3632	-0.0038	0.1671	-0.0545	0.7912	-0.4255
				//										
43.85241				//	-0.0421	-0.0311	0.0009	0.1285	0.0805	-0.0977	-0.3350	-0.2149	0.8543	-0.2766
				//										
50.42948	0.20737	-0.30798	0.04298	//	-0.0548	-0.1719	0.1053	0.1435	0.3625	0.2267	-0.4148	0.2258	0.2636	0.6786
				//										
45.81804				//	0.1582	0.0203	-0.1015	-0.1360	-0.3096	0.4422	-0.5220	-0.2336	0.0304	0.5713
				//										

DIBENZANTHRACENE IRX



ATOMIC COORDINATES

x	0.8779	0.8858	0.	0.	0.9096	0.9002	1.7340	1.7535	0.8851	0.8937	1.7721	2.6621	2.6542	3.5400
	3.5400	2.6304	2.6398	1.8060	1.7865	2.6549	2.6463	1.7679						
y	0.5320	1.5710	2.0600	3.0760	3.5940	4.5140	5.1350	6.1510	6.6570	7.6970	8.2060	7.6740	6.6350	6.1460
	5.1300	4.6120	3.6920	3.0710	2.0550	1.5490	0.5090	0.						

DIBENZANTHRACENE X IRX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 A	8 S	9 S	10A	11A	12S	13S
1.744613	1.636852	1.508504	1.412650	1.321522	1.299809	1.239193	1.208327	1.117318	1.069358	1.049300	0.822972	0.811691
0.108417	0.214720	0.267790	0.109688	0.091143	0.256357	0.210602	0.219909	0.334826	0.282405	0.104147	0.180347	0.269328
0.202572	0.320586	0.252062	-0.035914	0.264741	0.024230	0.309239	-0.139667	0.190932	-0.041880	0.226581	-0.204856	0.081622
0.157718	0.218138	0.094453	-0.228069	0.396650	0.062862	0.248702	-0.006771	-0.197106	-0.274752	-0.184627	-0.282667	-0.159231
0.186076	0.163364	-0.069642	-0.339044	0.277608	0.069352	-0.041230	0.136250	-0.343962	-0.119209	-0.304127	0.354338	0.022681
0.321633	0.144732	-0.248494	-0.342421	-0.017138	0.036729	-0.303779	0.169082	-0.039586	0.229577	0.039867	0.086989	0.159628
0.284438	-0.005417	-0.241389	-0.234467	-0.125761	0.268592	-0.232211	0.126770	0.107826	-0.032717	0.382947	-0.311911	0.183779
0.323587	-0.200848	-0.149644	0.027291	-0.146404	0.350910	0.092595	-0.099220	0.146008	-0.331250	0.182304	0.051229	-0.350293
0.254988	-0.321961	0.164074	-0.073196	-0.086910	0.281719	0.048220	-0.374316	0.052074	0.020094	-0.222549	0.204492	-0.133630
0.141490	-0.224572	0.213853	-0.194128	-0.245911	0.090100	0.256353	-0.201268	-0.273798	0.307033	-0.098283	0.036738	0.336745
0.086441	-0.176870	0.252915	-0.241329	-0.255434	-0.188645	0.264240	0.185254	-0.280363	0.162791	0.188875	-0.241341	-0.084120
0.078355	-0.173655	0.268236	-0.213207	-0.128032	-0.324398	0.061827	0.379576	0.059017	-0.210040	0.186814	0.105646	-0.273201
0.108417	-0.214720	0.267790	-0.109688	0.091142	-0.256357	-0.210602	0.219909	0.334826	-0.282405	-0.104148	0.180346	0.269328
0.202572	-0.320586	0.252062	0.035915	0.264741	-0.024231	-0.309239	-0.139666	0.190932	0.041880	-0.226581	-0.204855	0.081622
0.157717	-0.218138	0.094453	0.228069	0.396649	-0.062863	-0.248702	-0.006771	-0.197106	0.274752	0.184627	-0.282666	-0.159230
0.186076	-0.163364	-0.069642	0.339045	0.277607	-0.069353	0.041230	0.136250	-0.343962	0.119209	0.304127	0.354337	0.022680
0.321633	-0.144733	-0.248494	0.342421	-0.017138	-0.036729	0.303779	0.169082	-0.039586	-0.229577	-0.039867	0.086989	0.159628
0.284438	0.005417	-0.241388	0.234467	-0.125762	-0.268592	0.232211	0.126769	0.107826	0.032717	-0.382947	-0.311911	0.183779
0.323587	0.200848	-0.149644	-0.027291	-0.146406	-0.350909	-0.092595	-0.099221	0.146008	0.331250	-0.182304	0.051228	-0.350294
0.254988	0.321961	0.164074	0.073196	-0.086911	-0.281718	-0.048221	-0.374317	0.052074	-0.020094	0.222549	0.204492	-0.133630
0.141490	0.224572	0.213853	0.194127	-0.245911	-0.090098	-0.256354	-0.201268	-0.273798	-0.307033	0.098283	0.036739	0.336746
0.086441	0.176870	0.252915	0.241329	-0.255434	0.188645	-0.264240	0.185255	-0.280364	-0.162791	-0.188874	-0.241342	-0.084120
0.078355	0.173655	0.268236	0.213206	-0.128031	0.324397	-0.061826	0.379576	0.059016	0.210040	-0.186815	0.105645	-0.273201

OVERLAP EIGNVALUES AND EIGNVECTORS

14 A	15 A	16 S	17 S	18 A	19 S	20 A	21 S	22 A
0.787223	0.719777	0.700552	0.668225	0.668110	0.612650	0.578267	0.531213	0.491845
-0.337724	-0.229781	0.166250	-0.268423	-0.059878	-0.088918	-0.252242	-0.187371	0.084350
0.189719	-0.108911	-0.326312	0.053658	0.263087	0.007757	0.306132	0.333677	-0.189291
0.197508	-0.027826	0.302439	-0.030677	-0.388294	0.168377	-0.127480	-0.209681	0.134933
-0.334784	0.155708	-0.037723	0.015561	0.281028	-0.308925	-0.047297	0.153030	-0.166148
0.044267	-0.174918	-0.266433	-0.012325	-0.015090	0.419877	0.250248	-0.154501	0.344189
0.119273	0.097752	0.158285	0.255332	-0.102406	-0.309472	-0.227910	-0.014665	-0.291573
-0.133233	0.117856	0.147084	-0.350314	0.134096	-0.000313	0.132811	0.224927	0.342060
0.008478	-0.369219	-0.082354	0.231739	-0.099427	-0.113095	0.212820	-0.353159	-0.260384
0.299448	0.140589	0.262090	0.000087	0.251813	0.172271	-0.214124	0.212567	0.124194
-0.260984	0.225938	-0.266279	-0.247997	-0.267373	-0.176337	0.218948	-0.146976	-0.065358
-0.084072	-0.386189	0.094535	0.347348	0.154705	0.150384	-0.229963	0.141356	0.057092
0.337725	0.229780	0.166250	-0.268392	0.060016	-0.088918	0.252242	-0.187371	-0.084350
-0.189720	0.108911	-0.326311	0.053522	-0.263115	0.007756	-0.306132	0.333677	0.189291
-0.197509	0.027825	0.302439	-0.030477	0.388309	0.168377	0.127480	-0.209681	-0.134933
0.334785	-0.155708	-0.037723	0.015416	-0.281036	-0.308925	0.047297	0.153030	0.166148
-0.044266	0.174918	-0.266433	-0.012317	0.015096	0.419876	-0.250249	-0.154501	-0.344189
-0.119273	-0.097752	0.158285	0.255385	0.102275	-0.309472	0.227911	-0.014665	0.291573
0.133232	-0.117856	0.147084	-0.350383	-0.133916	-0.000314	-0.132811	0.224927	-0.342060
-0.008478	0.369219	-0.082354	0.231790	0.099308	-0.113095	-0.212820	-0.353159	0.260384
-0.299447	-0.140590	0.262090	-0.000043	-0.251813	0.172272	0.214123	0.212567	-0.124194
0.260983	-0.225937	-0.266279	-0.247860	0.267501	-0.176338	-0.218948	-0.146976	0.065358
0.084072	0.386189	0.094536	0.347268	-0.154884	0.150384	0.229963	0.141356	-0.057092

DIBENZANTHRACENE X IRX APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 A	8 S	9 S	10 A	11 A	12 S	13 S
32.07089	29.23538	25.32954	21.94961	18.28168	17.33181	14.50405	12.95510	7.88981	4.87365	3.53044	-16.16354	-17.43251
0.082082	0.167830	0.218033	0.092287	0.079284	0.224857	0.189188	0.200055	0.316760	0.273094	0.101671	0.198800	0.298942
0.153367	0.250576	0.205227	-0.030217	0.230295	0.021253	0.277795	-0.127058	0.180630	-0.040499	0.221194	-0.225816	0.090597
0.119407	0.170501	0.076903	-0.191888	0.345040	0.055137	0.223413	-0.006160	-0.186471	-0.265693	-0.180237	-0.311589	-0.176739
0.140877	0.127689	-0.056702	-0.285259	0.241487	0.060830	-0.037038	0.123950	-0.325404	-0.115278	-0.296896	0.390594	0.025174
0.243507	0.113126	-0.202322	-0.288100	-0.014908	0.032216	-0.272890	0.153818	-0.037450	0.222007	0.038919	0.095890	0.177180
0.215347	-0.004234	-0.196537	-0.197272	-0.109398	0.235588	-0.208599	0.115325	0.102009	-0.031638	0.373843	-0.343826	0.203986
0.244986	-0.156987	-0.121839	0.022962	-0.127355	0.307791	0.083180	-0.090263	0.138130	-0.320327	0.177970	0.056471	-0.388809
0.193050	-0.251651	0.133588	-0.061585	-0.075602	0.247102	0.043317	-0.340523	0.049264	0.019432	-0.217258	0.225416	-0.148323
0.107121	-0.175530	0.174118	-0.163332	-0.213914	0.079028	-0.230287	-0.183098	-0.259025	0.296909	-0.095946	0.040497	0.373772
0.065444	-0.138245	0.205922	-0.203045	-0.222198	-0.165465	0.237372	0.168529	-0.265236	0.157423	0.184384	-0.266035	-0.093369
0.059322	-0.135732	0.218396	-0.179384	-0.111373	-0.284536	0.055540	0.345308	0.055833	-0.203114	0.182373	0.116455	-0.303240
0.082082	-0.167830	0.218033	-0.092287	0.079283	-0.224857	-0.189188	0.200055	0.316760	-0.273093	-0.101672	0.198799	0.298941
0.153366	-0.250576	0.205227	0.030217	0.230295	-0.021253	-0.277795	-0.127057	0.180630	0.040499	-0.221194	-0.225816	0.090597
0.119407	-0.170501	0.076903	0.191888	0.345040	-0.055139	-0.223414	-0.006160	-0.186471	0.265693	0.180238	-0.311588	-0.176738
0.140877	-0.127689	-0.056702	0.285259	0.241487	-0.060832	0.037038	0.123950	-0.325403	0.115278	0.296897	0.390592	0.025174
0.243507	-0.113126	-0.202322	0.288100	-0.014908	-0.032216	0.272890	0.153817	-0.037450	-0.222007	-0.038920	0.095890	0.177180
0.215347	0.004234	-0.196536	0.197272	-0.109398	-0.235588	0.208600	0.115325	0.102008	0.031638	-0.373843	-0.343825	0.203987
0.244986	0.156987	-0.121839	-0.022962	-0.127356	-0.307790	-0.083180	-0.090263	0.138130	0.320327	-0.177970	0.056470	-0.388810
0.193050	0.251651	0.133588	0.061585	-0.075603	-0.247101	-0.043318	-0.340523	0.049264	-0.019432	0.217258	0.225416	-0.148323
0.107121	0.175530	0.174118	0.163331	-0.213915	-0.079027	-0.230287	-0.183097	-0.259025	-0.296909	0.095946	0.040498	0.373772
0.065444	0.138245	0.205922	0.203045	-0.222198	0.165465	-0.237371	0.168530	-0.265237	-0.157423	-0.184384	-0.266036	-0.093369
0.059322	0.135732	0.218396	0.179384	-0.111373	0.284536	-0.055539	0.345308	0.055832	0.203114	-0.182373	0.116455	-0.303240

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 A	15 A	16 S	17 S	18 A	19 S	20 A	21 S	22 A
-20.30988	-29.25403	-32.11885	-37.30778	-37.32718	-47.50846	-54.80090	-66.31107	-77.63311
-0.380639	-0.270841	0.198628	0.328366	-0.073256	-0.113602	-0.331705	-0.257080	0.120274
0.213827	-0.128373	-0.389863	0.065640	0.321867	0.009910	0.402573	0.457816	-0.269908
0.222605	-0.032798	0.361341	-0.037528	-0.475047	0.215118	-0.167640	-0.287690	0.192400
-0.377325	0.183532	-0.045070	0.019036	0.343816	-0.394682	-0.062196	0.209963	-0.236909
0.049892	-0.206175	-0.318323	-0.015078	-0.018462	0.536433	0.329083	-0.211981	0.490775
0.134429	0.115219	0.189112	0.312351	-0.125286	-0.395381	-0.299709	-0.020120	-0.415751
-0.150163	0.138917	0.175730	-0.428545	0.164056	-0.000400	0.174650	0.308608	0.487740
0.009556	-0.435196	-0.098393	0.283489	-0.121642	-0.144489	0.279864	-0.484547	-0.371278
0.337499	0.165712	0.313134	0.000107	0.308074	0.220094	-0.281579	0.291650	0.177087
-0.294148	0.266312	-0.318139	-0.303379	-0.327110	-0.225288	0.287924	-0.201657	-0.093193
-0.094755	-0.455198	0.112947	0.424916	0.189269	0.192130	-0.302409	0.193945	0.081407
0.380640	0.270841	0.198628	-0.328328	0.073425	-0.113601	0.331705	-0.257080	-0.120274
-0.213828	0.128373	-0.389863	0.065474	-0.321900	0.009910	-0.402573	0.457816	0.269908
-0.222606	0.032797	0.361341	-0.037283	0.475066	0.215118	0.167639	-0.287690	-0.192400
0.377327	-0.183532	-0.045070	0.018859	-0.343825	-0.394682	0.062197	0.209963	0.236909
-0.049891	0.206175	-0.318322	-0.015068	0.018469	0.536432	-0.329084	-0.211981	-0.490776
-0.134430	-0.115219	0.189112	0.312416	0.125125	-0.395380	0.299709	-0.020120	0.415751
0.150162	-0.138917	0.175729	-0.428630	-0.163835	-0.000401	-0.174650	0.308608	-0.487740
-0.009555	0.435196	-0.098392	0.283552	0.121495	-0.144490	-0.279864	-0.484547	0.371279
-0.337499	-0.165712	0.313134	-0.000052	-0.308074	0.220094	0.281579	0.291650	-0.177087
0.294146	-0.266311	-0.318139	-0.303211	0.327267	-0.225288	-0.287923	-0.201657	0.093193
0.094755	0.455198	0.112947	0.424819	-0.189488	0.192131	0.302409	0.193945	-0.081407

DIBENZANTHRACENE X

IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.02210	0.58962	0.00911	-0.23347	-0.00273	0.08486	0.00700	-0.02701	-0.00339	0.01834	0.00243	-0.01313	-0.00240	0.03513	-0.00005
	-0.03450	-0.01000	0.02793	0.02214	-0.33957	-0.01560	0.68513								
2	0.58962	0.96799	0.50061	-0.00301	-0.13625	-0.00823	0.11551	0.00421	-0.05079	-0.00136	0.04443	-0.00240	-0.04551	-0.00430	0.03874
	0.00349	-0.12632	0.00772	0.52468	0.02398	-0.26170	-0.01305								
3	0.00911	0.50061	1.01001	0.79145	-0.01379	-0.20044	0.00625	0.05049	-0.00240	-0.03814	0.00331	0.03513	-0.00430	-0.08991	0.00757
	0.12226	0.00071	-0.20336	0.00356	0.00362	-0.00101	-0.11248								
4	-0.23347	-0.00301	0.79145	1.01653	0.44874	0.01851	-0.14250	-0.00392	0.05604	0.00267	-0.04226	-0.00005	0.03874	0.00757	-0.00288
	-0.01254	0.04153	0.00750	-0.22415	-0.01636	0.19427	0.00936								
5	0.00273	-0.13625	-0.01379	0.44874	0.96354	0.67691	-0.00244	-0.10543	-0.00127	0.05299	-0.00202	-0.03450	0.00349	0.12226	-0.01254
	-0.18096	0.00625	0.48730	0.01495	-0.10517	-0.00597	0.09236								
6	0.08486	-0.00823	-0.20044	0.01851	0.67691	1.02295	0.59566	-0.00098	-0.14353	0.00286	0.11195	-0.01000	-0.12632	0.00071	0.04153
	0.00625	-0.29220	0.00330	0.00904	0.00158	-0.04721	0.00053								
7	0.00700	0.11551	0.00625	-0.14250	-0.00244	0.59566	0.99091	0.46838	0.01063	-0.12816	-0.00101	0.02793	0.00772	-0.20336	0.00750
	0.48730	0.00330	-0.27212	-0.00667	0.10848	0.00098	-0.09934								
8	-0.02701	0.00421	0.05049	-0.00392	-0.10543	-0.00098	0.46838	0.96591	0.61184	-0.00552	-0.25316	0.02214	0.52468	0.00356	-0.22415
	0.01495	0.00904	-0.00667	0.00336	0.00264	0.01270	-0.00241								
9	-0.00339	-0.05079	-0.00240	0.05604	-0.00127	-0.14353	0.01063	0.61184	1.01516	0.67468	-0.01692	-0.33957	0.02398	0.00362	-0.01636
	-0.10517	0.00158	0.10848	0.00264	-0.04837	-0.00024	0.04644								
10	0.01834	-0.00136	-0.03814	0.00267	0.05299	0.00286	-0.12816	-0.00552	0.67468	1.01343	0.64376	-0.01560	-0.26170	-0.00101	0.19427
	-0.00597	-0.04721	0.00098	0.01270	-0.00024	-0.01500	0.00059								
11	0.00243	0.04443	0.00331	-0.04226	-0.00202	0.11195	-0.00101	-0.25316	-0.01692	0.64376	1.01146	0.68513	-0.01305	-0.11248	0.00936
	0.09236	0.00053	-0.09934	-0.00241	0.04644	0.00059	-0.04329								
12	-0.01313	-0.00240	0.03513	-0.00005	-0.03450	-0.01000	0.02793	0.02214	-0.33957	-0.01560	0.68513	1.02210	0.58962	0.00911	-0.23347
	-0.00273	0.08486	0.00700	-0.02701	-0.00339	0.01834	0.00243								
13	-0.00240	-0.04551	-0.00430	0.03874	0.00349	-0.12632	0.00772	0.52468	0.02398	-0.26170	-0.01305	0.58962	0.96799	0.50061	-0.00301
	-0.13625	-0.00823	0.11551	0.00421	-0.05079	-0.00136	0.04443								
14	0.03513	-0.00430	-0.08991	0.00757	0.12226	0.00071	-0.20336	0.00356	0.00362	-0.00101	-0.11248	0.00911	0.50061	1.01001	0.79145
	-0.01379	-0.20044	0.00625	0.05049	-0.00240	-0.03814	0.00331								
15	-0.00005	0.03874	0.00757	-0.00288	-0.01254	0.04153	0.00750	-0.22415	-0.01636	0.19427	0.00936	-0.23347	-0.00301	0.79145	1.01653
	0.44874	0.01851	-0.14250	-0.00392	0.05604	0.00268	-0.04226								
16	-0.03450	0.00349	0.12226	-0.01254	-0.18096	0.00625	0.48730	0.01495	-0.10517	-0.00597	0.09236	-0.00273	-0.13625	-0.01379	0.44874
	0.96354	0.67691	-0.00244	-0.10543	-0.00127	0.05299	-0.00202								
17	-0.00019	-0.12632	0.00071	0.04153	0.00625	-0.29220	0.00330	0.00904	0.00158	-0.04721	0.00053	0.08486	-0.00823	-0.20044	0.01851
	0.67691	1.02295	0.59566	-0.00098	-0.14353	0.00286	0.11195								
18	0.02793	0.00772	-0.20336	0.00750	0.48730	0.00330	-0.27212	-0.00667	0.10848	0.00098	-0.09934	0.00700	0.11551	0.00625	-0.14250
	-0.00244	0.59566	0.99091	0.46838	0.01063	-0.12816	-0.00101								
19	0.02214	0.52468	0.00356	-0.22415	0.01495	0.00904	-0.00667	0.00336	0.00264	0.01270	-0.00241	-0.02701	0.00421	0.05049	-0.00392
	-0.10543	-0.00098	0.46838	0.96591	0.61184	-0.00552	-0.25316								
20	-0.33957	0.02398	0.00362	-0.01636	-0.10517	0.00158	0.10848	0.00264	-0.04837	-0.00024	0.04644	-0.00339	-0.05079	-0.00240	0.05604
	-0.00127	-0.14353	0.01063	0.61184	1.01516	0.67468	-0.01692								
21	-0.01560	-0.26170	-0.00101	0.19427	-0.00597	-0.04721	0.00098	0.01270	-0.00024	-0.01500	0.00059	0.01834	-0.00136	-0.03814	0.00268
	0.05299	0.00286	-0.12816	-0.00552	0.67468	1.01343	0.64376								
22	0.68513	-0.01305	-0.11248	0.00936	0.09236	0.00053	-0.09934	-0.00241	0.04644	0.00059	-0.04329	0.00243	0.04443	0.00331	-0.04226
	-0.00202	0.11195	-0.00101	-0.25316	-0.01692	0.64376	1.01146								

DIBENZANTHRACENE X | IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.81775	0.43084	-0.06337	-0.23965	0.01240	0.09099	0.00095	-0.02897	-0.00150	0.01970	0.00138	-0.01407	-0.00128	0.03788	-0.00008
	-0.03800	-0.00485	0.03562	-0.02520	-0.35403	-0.09030	0.52031								
2	0.43084	0.71867	0.32661	-0.07666	-0.14474	0.01441	0.12323	-0.00196	-0.05454	0.00026	0.04767	-0.00128	-0.04889	-0.00399	0.04088
	0.00907	-0.12932	-0.04460	0.36906	-0.02796	-0.27305	-0.06975								
3	-0.06337	0.32661	0.79192	0.62285	-0.07242	-0.20467	0.01631	0.05272	-0.00515	-0.04071	0.00401	0.03788	-0.00399	-0.09578	-0.00006
	0.13006	0.01715	-0.21335	-0.05212	0.01235	0.02233	-0.11236								
4	-0.23965	-0.07666	0.62285	0.81363	0.28995	-0.06678	-0.14467	0.00850	0.05974	-0.00079	-0.04509	-0.00008	0.04088	-0.00006	-0.00311
	0.00376	0.05144	-0.03721	-0.23600	0.00088	0.20513	0.01994								
5	0.01240	-0.14474	-0.07242	0.28995	0.69524	0.47229	-0.06840	-0.10369	0.00933	0.05664	-0.00610	-0.03800	0.00907	0.13006	0.00376
	-0.19319	-0.04129	0.33699	-0.02877	-0.10700	-0.00287	0.09787								
6	0.09099	0.01441	-0.20467	-0.06678	0.47229	0.79877	0.44456	-0.06020	-0.15401	0.01281	0.11900	-0.00485	-0.12932	0.01715	0.05144
	-0.04129	-0.31607	-0.06729	0.01757	0.01286	-0.05157	-0.00879								
7	0.00095	0.12323	0.01631	-0.14467	-0.06840	0.44456	0.75884	0.30210	-0.06376	-0.12873	0.02081	0.03562	-0.04460	-0.21335	-0.03721
	0.33699	-0.06729	-0.28560	0.01066	0.11584	-0.00170	-0.10620								
8	-0.02897	-0.00196	0.05272	0.00850	-0.10369	-0.06020	0.30210	0.71370	0.44010	-0.06765	-0.26411	-0.02520	0.36906	-0.05212	-0.23600
	-0.02877	0.01757	0.01066	0.00316	-0.00130	0.01359	0.00096								
9	-0.00150	-0.05454	-0.00515	0.05974	0.00933	-0.15401	-0.06376	0.44010	0.80459	0.51262	-0.08772	-0.35403	-0.02796	0.01235	0.00088
	-0.10700	0.01286	0.11584	-0.00130	-0.05191	0.00035	0.04979								
10	0.01970	0.00026	-0.04071	-0.00079	0.05664	0.01281	-0.12873	-0.06765	0.51262	0.79531	0.46818	-0.09030	-0.27305	0.02233	0.20513
	-0.00287	-0.05157	-0.00170	0.01359	0.00035	-0.01606	-0.00023								
11	0.00138	0.04767	0.00401	-0.04509	-0.00610	0.11900	0.02081	-0.26411	-0.08772	0.46818	0.79027	0.52031	-0.06975	-0.11236	0.01994
	-0.09787	-0.00879	-0.10620	0.00096	0.04979	-0.00023	-0.04638								
12	-0.01407	-0.00128	0.03788	-0.00008	-0.03800	-0.00485	0.03562	-0.02520	-0.35403	-0.09030	0.52031	0.81775	0.43084	-0.06337	-0.23965
	0.01240	0.09099	0.00095	-0.02897	-0.00150	0.01970	0.00138								
13	-0.00128	-0.04889	-0.00399	0.04088	0.00907	-0.12932	-0.04460	0.36906	-0.02796	-0.27305	-0.06975	0.43084	0.71867	0.32661	-0.07666
	-0.14474	0.01441	0.12323	-0.00196	-0.05454	0.00026	0.04767								
14	0.03788	-0.00399	-0.09578	-0.00006	0.13006	0.01715	-0.21335	-0.05212	0.01235	0.02233	-0.11236	-0.06337	0.32661	0.79192	0.62285
	-0.07242	-0.20467	0.01631	0.05272	-0.00515	-0.04071	0.00401								
15	-0.00008	0.04088	-0.00006	-0.00311	0.00376	0.05144	-0.03721	-0.23600	0.00088	0.20513	0.01994	-0.23965	-0.07666	0.62285	0.81363
	0.28995	-0.06678	-0.14467	0.00850	0.05974	-0.00079	-0.04509								
16	-0.03800	0.00907	0.13006	0.00376	-0.19319	-0.04129	0.33699	-0.02877	-0.10700	-0.00287	0.09787	0.01240	-0.14474	-0.07242	0.28995
	0.69524	0.47229	-0.06840	-0.10369	0.00933	0.05664	-0.00610								
17	-0.00485	-0.12932	0.01715	0.05144	-0.04129	-0.31607	-0.06729	0.01757	0.01286	-0.05157	-0.00879	0.09099	0.01441	-0.20467	-0.06678
	0.47229	0.79877	0.44456	-0.06020	-0.15401	0.01281	0.11900								
18	0.03562	-0.04460	-0.21335	-0.03721	0.33699	-0.06729	-0.28560	0.01066	0.11584	-0.00170	-0.10620	0.00095	0.12323	0.01631	-0.14467
	-0.06840	0.44456	0.75884	0.30210	-0.06376	-0.12873	0.02081								
19	-0.02520	0.36906	-0.05212	-0.23600	-0.02877	0.01757	0.01066	0.00316	-0.00130	0.01359	0.00096	-0.02897	-0.00196	0.05272	0.00850
	-0.10369	-0.06020	0.30210	0.71370	0.44010	-0.06765	-0.26411								
20	-0.35403	-0.02796	0.01235	0.00088	-0.10700	0.01286	0.11584	-0.00130	-0.05191	0.00035	0.04979	-0.00150	-0.05454	-0.00515	0.05974
	0.00933	-0.15401	-0.06376	0.44010	0.80459	0.51262	-0.08772								
21	-0.09030	-0.27305	0.02233	0.20513	-0.00287	-0.05157	-0.00170	0.01359	0.00035	-0.01606	-0.00023	0.01970	0.00026	-0.04071	-0.00079
	0.05664	0.01281	-0.12873	-0.06765	0.51262	0.79531	0.46818								
22	0.52031	-0.06975	-0.11236	0.01994	0.09787	-0.00879	-0.10620	0.00096	0.04979	-0.00023	-0.04638	0.00138	0.04767	0.00401	-0.04509
	-0.00610	0.11900	0.02081	-0.26411	-0.08772	0.46818	0.79027								

ENERGIES FOR DIBENZANTHRACENE X , IRX APPROXIMATION 5.8

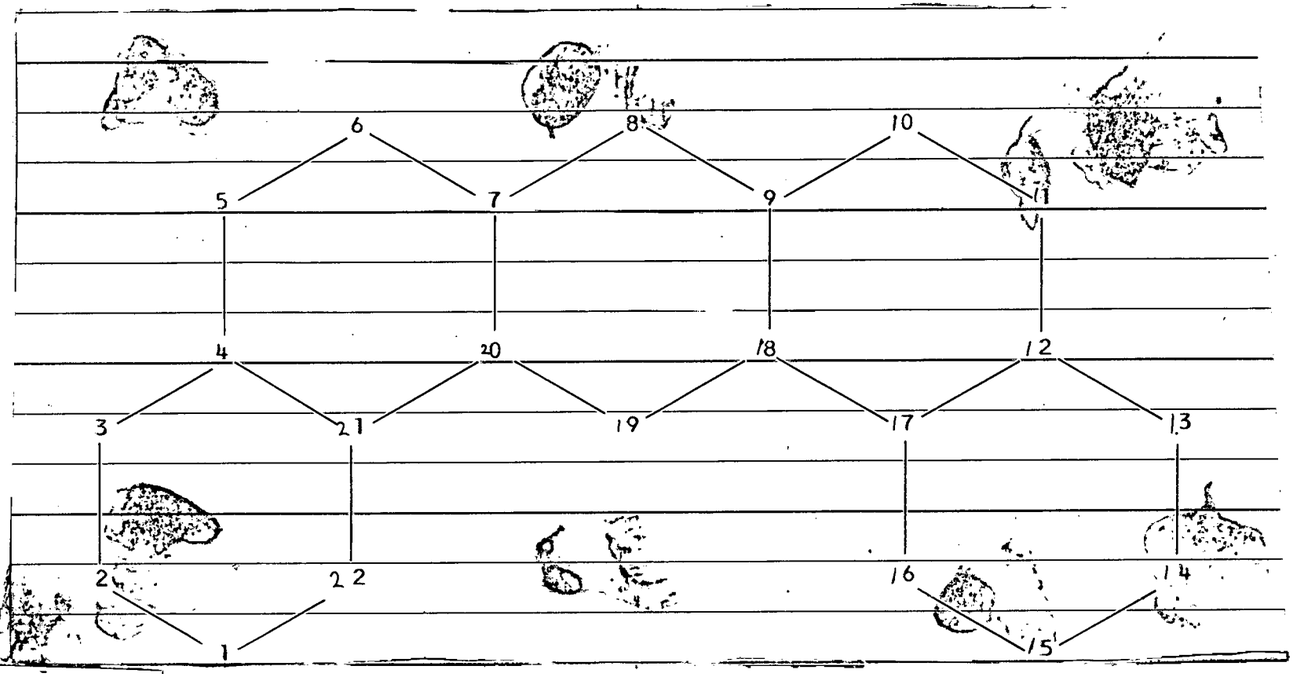
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	11,12	11,13	10,12	10,13	9,14	7,12	7,13	6,12	6,13	4,12
XMOMNT	0.53827	-0.20766	-0.23568	-0.49928	-0.13531	0.36631	0.04499	-0.04777	-0.27117	-0.01696
YMOMNT	-0.34652	-1.06939	-1.08400	-0.39140	0.59619	0.14980	-0.31254	-0.01954	0.16193	0.03546
JUMP E	19.6940	20.9630	21.0372	22.3062	28.1997	30.6676	31.9366	33.4954	34.7643	38.1131
DIAG E	30.7380	31.7770	32.3908	34.8767	46.2088	46.0878	45.9449	48.5093	51.2247	54.6381
DIAG E	30.9900	31.6456	32.7545	34.8571	46.4212	46.5713	46.0450	49.0076	51.3396	54.9041
CORRSP	28.5082	27.9880	33.9965	36.5999	50.3346	43.8498	44.7959	48.3748	52.3629	55.5854
CORRSP	28.6421	28.1293	34.1824	36.7529	45.2513	43.9243	50.5834	48.8295	52.5415	55.6990

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
28.50818	0.09626	0.27309	0.06948	//	0.7929	-0.4003	0.1571	0.4025	-0.1345	-0.0438	-0.0584	0.0252	-0.0097	-0.0145
				//										
18.71257				//	0.7454	-0.1528	0.2321	0.4120	-0.4243	0.0300	0.0953	0.0526	-0.0367	0.0576
				//										
27.98804	0.01806	0.09079	0.08327	//	0.3004	0.6102	-0.6683	0.2729	-0.0245	0.0978	-0.0257	0.0558	-0.0002	0.0484
				//										
27.69844				//	0.3185	0.6882	-0.6233	-0.0238	-0.0260	0.1689	0.0011	0.0438	0.0064	0.0690
				//										
33.99652	2.03783	-0.52185	-1.06642	//	-0.1857	0.4834	0.5824	0.5142	-0.3400	0.0689	-0.0211	-0.0818	0.0082	-0.0282
				//										
23.18615				//	-0.1821	0.6578	0.6459	-0.0853	-0.2838	-0.0017	0.0838	-0.1042	0.0995	0.0380
				//										
36.59994	2.83293	-0.39997	1.28848	//	-0.4892	-0.4477	-0.3618	0.6521	-0.0067	-0.0116	-0.0224	0.0001	-0.0564	0.0170
				//										
26.07686				//	-0.4944	0.0654	-0.1673	0.8221	-0.1742	0.1202	-0.0253	0.0118	-0.0215	0.0371
				//										
50.33456	0.03475	0.03623	0.12216	//	0.0633	0.0366	0.1624	0.1884	0.6520	0.4884	0.5055	-0.0055	-0.1010	-0.0585
				//										
40.45389				//	0.1118	-0.0075	0.1701	0.0458	0.1841	0.4680	-0.7833	-0.2247	0.0773	0.1829
				//										
43.84975	0.37449	0.17200	0.41381	//	-0.0213	-0.0772	0.0416	-0.0447	0.0645	0.6821	-0.6721	0.0450	0.1874	0.1776
				//										
37.92689				//	-0.1722	-0.2411	-0.1257	-0.2985	-0.4584	0.6703	0.2993	-0.0633	0.1600	0.1694
				//										
44.79587	0.22146	0.32204	-0.11200	//	-0.0004	-0.1546	-0.1448	-0.1433	-0.5769	0.4360	0.5063	-0.2159	0.3120	0.1067
				//										
49.00290				//	0.1352	0.0664	0.1720	0.1956	0.5499	0.4435	0.4413	-0.2600	-0.0636	-0.3794
				//										
48.37483	0.07303	0.06095	-0.17829	//	-0.0511	-0.0251	0.0246	-0.0396	-0.2115	0.1442	0.1169	0.9290	-0.0862	-0.2120
				//										
43.82595				//	-0.0622	0.0560	0.1285	-0.0867	-0.0357	0.2789	-0.1125	0.6205	-0.6816	-0.1664
				//										
52.36287	0.55001	-0.44880	0.21350	//	-0.0134	0.0344	0.0368	0.1150	0.2367	-0.2244	0.0326	0.1564	0.9199	-0.0773
				//										
47.39980				//	0.0256	0.0108	0.0715	0.0557	0.1121	0.1110	-0.0597	0.6381	0.6986	-0.2594
				//										
55.58541	0.05560	-0.11588	-0.10046	//	-0.0045	0.0165	0.0873	0.0325	0.0543	-0.1362	0.1291	0.2311	-0.0196	0.9482
				//										
52.30048				//	0.0202	0.0163	0.1286	0.0808	0.3849	-0.0320	-0.2629	0.2646	0.0013	0.8295
				//										

1,2,7,8DIBENZANTHRACENE TBM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	2.5980	3.4640	4.3300	5.1960	6.0620	
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	3.5000	3.0000	3.5000	3.0000	

x	6.0620	6.9280	6.9280	6.0620	5.1960	5.1960	4.3300	3.4640	2.5980	1.7320	1.7320	
y	2.0000	1.5000	0.5000	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	0.5000	

1,2,7,8DIBENZANTHRACENE TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 S	8 A	9 S	10 A	11 S	12 S	13 A
1.622428	1.568342	1.478856	1.399344	1.373255	1.321529	1.310595	1.246811	1.215583	1.152532	1.121372	0.878625	0.847466
0.091758	0.163132	0.235607	-0.300758	-0.107259	-0.122689	0.347108	0.288690	-0.118391	-0.185845	-0.200162	0.200162	0.185844
0.084608	0.163130	0.255902	-0.300745	0.025105	0.122709	0.307674	0.288660	0.265532	0.185900	-0.107491	-0.107491	0.185900
0.121620	0.212523	0.260898	-0.185860	0.145233	0.282560	0.040080	-0.000030	0.350345	0.300748	0.147309	-0.147309	-0.300748
0.222107	0.326262	0.250297	0.000006	0.194534	0.245398	-0.257220	-0.288675	0.040498	-0.000025	0.179927	0.179927	-0.000025
0.160063	0.212520	0.069934	0.185885	0.325005	0.282540	-0.179174	0.000030	-0.111095	-0.300754	-0.263468	0.263468	0.300754
0.181564	0.163132	-0.114602	0.300758	0.296984	0.122688	0.031729	0.288690	-0.137534	-0.185844	-0.309482	-0.309482	-0.185844
0.297817	0.163130	-0.292279	0.300744	0.124127	-0.122710	0.219103	0.288660	-0.009037	0.185900	0.111276	-0.111276	-0.185900
0.236187	0.000000	-0.301293	-0.000000	0.164155	-0.000001	0.348217	0.000000	-0.020694	0.000000	0.452556	0.452556	0.000000
0.297817	-0.163129	-0.292279	-0.300745	0.124127	0.122709	0.219103	-0.288660	-0.009038	-0.185900	0.111275	-0.111275	0.185900
0.181564	-0.163132	-0.114601	-0.300758	0.296984	-0.122689	0.031729	-0.288690	-0.137534	0.185844	-0.309482	-0.309482	0.185845
0.160064	-0.212520	0.069934	-0.185885	0.325004	-0.282540	-0.179175	-0.000030	-0.111095	0.300754	-0.263468	0.263468	-0.300754
0.222107	-0.326261	0.250297	-0.000006	0.194533	-0.245398	-0.257221	0.288675	0.040498	0.000025	0.179927	0.179927	0.000025
0.121621	-0.212522	0.260898	0.185860	0.145233	-0.282561	0.040080	0.000029	0.350345	-0.300748	0.147309	-0.147309	0.300749
0.084609	-0.163129	0.255901	0.300745	0.025105	-0.122710	0.307674	-0.288660	0.265532	-0.185900	-0.107491	-0.107491	-0.185900
0.091758	-0.163132	0.235606	0.300758	-0.107259	0.122688	0.347109	-0.288690	-0.118392	0.185844	-0.200162	0.200162	-0.185845
0.146793	-0.212519	0.201214	0.185885	-0.187313	0.282540	0.129137	-0.000029	-0.368944	0.300754	0.009059	0.009059	0.300754
0.278450	-0.326261	0.154790	0.000006	-0.176026	0.245399	-0.184608	0.288675	-0.203882	0.000025	0.204627	-0.204627	-0.000025
0.333323	-0.212522	-0.151183	-0.185860	0.273435	0.282561	-0.104226	0.000030	0.150342	-0.300748	-0.088357	-0.088357	0.300748
0.264345	0.000000	-0.155846	-0.000000	0.361613	0.000001	-0.165645	0.000000	0.344239	-0.000000	-0.359348	0.359348	-0.000000
0.333322	0.212523	-0.151183	0.185860	-0.273436	-0.282560	-0.104226	-0.000030	0.150342	0.300748	-0.088357	-0.088357	0.300748
0.278449	0.326261	0.154789	-0.000006	-0.176027	-0.245398	-0.184609	-0.288675	-0.203882	-0.000025	0.204627	-0.204627	0.000025
0.146793	0.212520	0.201214	-0.185885	-0.187314	-0.282540	0.129136	0.000030	-0.368944	-0.300754	0.009059	0.009059	-0.300754

OVERLAP EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 S	17 A	18 S	19 A	20 S	21 A	22 S
0.784415	0.753187	0.689403	0.678468	0.626742	0.600654	0.521142	0.431656	0.377570
-0.118394	0.288690	0.347108	-0.122689	0.107259	0.300758	0.235606	-0.163132	-0.091758
-0.265532	-0.288660	-0.307674	-0.122709	0.025105	-0.300745	-0.255901	0.163129	0.084609
0.350345	-0.000030	0.040080	0.282561	-0.145233	0.185860	0.260898	-0.212522	-0.121620
-0.040498	0.288675	0.257220	-0.245399	0.194533	0.000006	-0.250297	0.326261	0.222107
-0.111095	0.000030	-0.179174	0.282540	-0.325005	-0.185885	0.069934	-0.212520	-0.160063
0.137534	-0.288690	-0.031729	-0.122689	0.296984	0.300758	0.114601	0.163132	0.181564
-0.009038	0.288660	0.219103	-0.122710	-0.124127	-0.300745	-0.292279	-0.163129	-0.297817
0.020694	-0.000000	-0.348217	0.000001	0.164156	-0.000000	0.301293	-0.000000	0.236187
-0.009038	-0.288660	0.219104	0.122709	-0.124127	0.300745	-0.292279	0.163129	-0.297817
0.137534	0.288690	-0.031729	0.122689	0.296984	-0.300758	0.114601	-0.163132	0.181564
-0.111095	-0.000030	-0.179175	-0.282540	-0.325005	0.185885	0.069934	0.212520	-0.160063
-0.040498	-0.288675	0.257221	0.245398	0.194533	-0.000006	-0.250297	-0.326261	0.222107
0.350345	0.000030	0.040079	-0.282561	-0.145233	-0.185860	0.260898	0.212522	-0.121620
-0.265533	0.288660	-0.307674	0.122710	0.025105	0.300745	-0.255901	-0.163129	0.084609
-0.118391	-0.288690	0.347109	0.122688	0.107259	-0.300758	0.235606	0.163132	-0.091758
0.368944	0.000030	-0.129137	-0.282540	0.187314	0.185885	-0.201214	-0.212520	0.146793
-0.203882	0.288675	-0.184608	0.245398	0.176026	-0.000006	0.154790	0.326261	-0.278450
-0.150342	-0.000030	0.104225	-0.282561	-0.273435	-0.185860	0.151183	-0.212522	0.333323
0.344239	-0.000000	-0.165644	0.000000	0.361613	-0.000000	-0.155846	-0.000000	-0.264345
-0.150342	0.000030	0.104226	0.282561	-0.273435	0.185860	0.151183	0.212522	0.333323
-0.203882	-0.288675	-0.184609	-0.245398	0.176026	-0.000006	0.154790	-0.326261	-0.278450
0.368944	-0.000030	-0.129136	0.282540	-0.187314	-0.185885	-0.201214	0.212520	0.146793

TBM APPROXIMATION

1,2,7,8DIBENZANTHRACENE

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 S	8 A	9 S	10 A	11 S	12 S	13 A
28.82724	27.23004	24.33090	21.44382	20.42369	18.28198	17.80759	14.87454	13.32628	9.94457	8.13296	-10.38015	-13.52456
0.072038	0.130262	0.193742	-0.254246	-0.091529	-0.106725	0.303201	0.258542	-0.107381	-0.173110	-0.189019	0.213540	0.201877
0.066425	0.130260	0.210431	-0.254235	0.021423	0.106743	0.268755	0.258515	0.240838	0.173162	-0.101508	-0.114676	0.201939
0.095482	0.169701	0.214540	-0.157117	0.123934	0.245795	0.035010	-0.000027	0.317763	0.280141	0.139109	-0.157155	-0.326694
0.174373	0.260523	0.205823	0.000005	0.166004	0.213468	-0.224684	-0.258529	0.036731	-0.000023	0.169911	0.191953	-0.000027
0.125663	0.169699	0.057507	0.157138	0.277341	0.245777	-0.156510	0.000027	-0.100763	-0.280147	-0.248801	0.281077	0.326701
0.142543	0.130262	-0.094238	0.254246	0.253430	0.106724	0.027716	0.258542	-0.124743	-0.173110	-0.292254	-0.330167	-0.201877
0.233812	0.130260	-0.240345	0.254235	0.105923	-0.106743	0.191388	0.258516	-0.008197	0.173163	0.105081	-0.118713	-0.201938
0.185427	0.000000	-0.247757	-0.000000	0.140081	-0.000000	0.304170	0.000000	-0.018769	0.000000	0.427364	0.482803	-0.000000
0.233812	-0.130260	-0.240345	-0.254235	0.105923	0.106743	0.191388	-0.258515	-0.008198	-0.173163	0.105081	-0.118713	0.201939
0.142543	-0.130262	-0.094238	-0.254246	0.253430	-0.106725	0.027715	-0.258542	-0.124744	0.173110	-0.292254	-0.330167	0.201878
0.125664	-0.169699	0.057507	-0.157138	0.277341	-0.245777	-0.156510	-0.000026	-0.100763	0.280147	-0.248801	0.281077	-0.326701
0.174373	-0.260522	0.205823	-0.000005	0.166004	-0.213468	-0.224684	0.258529	0.036732	0.000023	0.169911	0.191953	0.000027
0.095483	-0.169701	0.214540	0.157117	0.123933	-0.245795	0.035010	0.000026	0.317763	-0.280141	0.139109	-0.157154	0.326695
0.066425	-0.130260	0.210431	0.254235	0.021423	-0.106743	0.268755	-0.258516	0.240838	-0.173163	-0.101508	-0.114676	-0.201938
0.072038	-0.130262	0.193742	0.254246	-0.091529	0.106725	0.303201	-0.258542	-0.107381	0.173110	-0.189019	0.213540	-0.201878
0.115245	-0.169699	-0.165461	0.157138	-0.159843	0.245777	0.112802	-0.000026	-0.334633	0.280147	0.008555	0.009665	0.326701
0.218607	-0.260522	-0.127286	0.000005	-0.150211	0.213468	-0.161256	0.258529	-0.184921	0.000023	0.193236	-0.218304	-0.000027
0.261687	-0.169700	-0.124320	-0.157117	-0.233334	0.245796	-0.091042	0.000026	0.136360	-0.280141	-0.083439	-0.094263	-0.326695
0.207534	0.000000	-0.128154	-0.000000	-0.308580	0.000001	-0.144691	-0.000000	0.312225	-0.000000	-0.339344	0.383366	-0.000000
0.261687	0.169701	-0.124320	0.157117	-0.233335	-0.245795	-0.091042	-0.000027	0.136360	0.280141	-0.083439	-0.094262	0.326695
0.218607	0.260522	-0.127285	-0.000005	-0.150211	-0.213468	-0.161257	-0.258529	-0.184921	-0.000023	0.193236	-0.218304	0.000027
0.115245	0.169699	0.165461	-0.157138	-0.159844	-0.245777	0.112801	0.000027	-0.334633	-0.280147	0.008555	0.009664	-0.326701

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 S	17 A	18 S	19 A	20 S	21 A	22 S
-20.65153	-24.62326	-33.85346	-35.61013	-44.75061	-49.95798	-69.04462	-98.93567	123.87197
-0.133674	0.332645	0.418050	-0.148950	0.135484	0.388065	0.326369	-0.248296	-0.149329
-0.299809	-0.332610	-0.370557	-0.148974	0.031711	-0.388048	-0.354482	0.248292	0.137694
0.395570	-0.000034	0.048272	0.343042	-0.183451	0.239814	0.361404	-0.323471	-0.197928
-0.045726	0.332627	0.309791	-0.297925	0.245725	0.000007	-0.346719	0.496588	0.361463
-0.125435	0.000034	-0.215794	0.343017	-0.410530	-0.239846	0.096874	-0.323467	-0.260491
0.155288	-0.332644	-0.038214	-0.148950	0.375136	0.388065	0.158749	0.248296	0.295481
-0.010205	0.332610	0.263883	-0.148975	-0.156791	-0.388048	-0.404874	-0.248292	-0.484675
0.023365	-0.000000	-0.419386	0.000001	0.207353	-0.000000	0.417360	-0.000000	0.384377
-0.010204	-0.332610	0.263884	0.148975	-0.156791	0.388048	-0.404874	0.248292	-0.484675
0.155288	0.332644	-0.038214	0.148950	0.375136	-0.388065	0.158749	-0.248296	0.295481
-0.125435	-0.000034	-0.215795	-0.343016	-0.410530	0.239846	0.096874	0.323467	-0.260491
-0.045726	-0.332627	0.309792	0.297924	0.245725	-0.000008	-0.346719	-0.496588	0.361463
0.395570	0.000034	0.048271	-0.343042	-0.183451	-0.239813	0.361404	0.323471	-0.197928
-0.299809	0.332610	-0.370556	0.148975	0.031712	0.388048	-0.354482	-0.248292	0.137694
-0.133674	-0.332644	0.418051	0.148949	0.135484	-0.388066	0.326369	0.248296	-0.149329
0.416570	0.000034	-0.155530	-0.343016	-0.236605	0.239846	-0.278727	-0.323467	0.238895
-0.230200	0.332627	-0.222338	0.297925	0.222348	-0.000008	0.214419	0.496588	-0.453157
-0.169749	-0.000034	0.125527	-0.343042	-0.345390	-0.239813	0.209423	-0.323471	0.542458
0.388675	-0.000000	-0.199499	0.000000	0.456772	-0.000000	-0.215882	-0.000000	-0.430203
-0.169749	0.000034	0.125528	0.343042	-0.345390	0.239814	0.209423	0.323471	0.542458
-0.230200	-0.332627	-0.222339	-0.297924	0.222348	0.000008	0.214419	-0.496588	-0.453157
0.416570	-0.000034	-0.155529	0.343017	-0.236606	-0.239846	-0.278727	0.323467	0.238895

1,2,7,8DIBENZANTHRACENE TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.00000	0.62606	-0.00000	-0.26365	0.00000	0.17206	-0.00000	-0.06837	-0.00000	0.01613	-0.00000	-0.02278	-0.00000	0.02289	0.00000
	-0.02697	0.00000	0.06093	-0.00000	-0.10892	0.00000	0.69760								
2	0.62606	1.00000	0.70273	0.00000	-0.11835	-0.00000	0.09112	-0.00000	-0.06484	0.00000	0.05152	-0.00000	-0.02183	-0.00000	0.02289
	0.00000	-0.02792	-0.00000	0.10495	0.00000	-0.26881	-0.00000								
3	-0.00000	0.70273	1.00000	0.57926	-0.00000	-0.19930	0.00000	0.09466	0.00000	-0.02945	-0.00000	0.02455	0.00000	-0.02183	-0.00000
	0.02194	-0.00000	-0.04874	-0.00000	0.03619	0.00000	-0.34035								
4	-0.26365	0.00000	0.57926	1.00000	0.49827	0.00000	-0.15957	0.00000	0.08131	0.00000	-0.05642	-0.00000	0.02455	-0.00000	-0.02278
	-0.00000	0.02567	0.00000	-0.11750	-0.00000	0.54390	0.00000								
5	0.00000	-0.11835	-0.00000	0.49827	1.00000	0.77969	-0.00000	-0.21848	-0.00000	0.05512	-0.00000	-0.05642	-0.00000	0.05152	-0.00000
	-0.05817	0.00000	0.13947	-0.00000	-0.22282	0.00000	0.02678								
6	0.17206	-0.00000	-0.19930	0.00000	0.77969	1.00000	0.49796	0.00000	-0.10521	-0.00000	0.05512	0.00000	-0.02945	-0.00000	0.01613
	0.00000	-0.00077	-0.00000	0.03415	0.00000	-0.24165	-0.00000								
7	-0.00000	0.09112	0.00000	-0.15957	-0.00000	0.49796	1.00000	0.61124	-0.00000	-0.10521	0.00000	0.08131	0.00000	-0.06484	0.00000
	0.07352	-0.00000	-0.21130	-0.00000	0.51326	0.00000	-0.09635								
8	-0.06837	-0.00000	0.09466	0.00000	-0.21848	0.00000	0.61124	1.00000	0.61124	0.00000	-0.21848	0.00000	0.09466	0.00000	-0.06837
	-0.00000	0.04555	0.00000	-0.35480	-0.00000	0.04555	0.00000								
9	-0.00000	-0.06484	0.00000	0.08131	-0.00000	-0.10521	-0.00000	0.61124	1.00000	0.49796	0.00000	-0.15957	-0.00000	0.09112	0.00000
	-0.09635	-0.00000	0.51326	0.00000	-0.21130	-0.00000	0.07352								
10	0.01613	0.00000	-0.02945	0.00000	0.05512	-0.00000	-0.10521	0.00000	0.49796	1.00000	0.77969	0.00000	-0.19930	0.00000	0.17206
	0.00000	-0.24165	-0.00000	0.03415	0.00000	-0.00077	-0.00000								
11	-0.00000	0.05152	-0.00000	-0.05642	-0.00000	0.05512	0.00000	-0.21848	0.00000	0.77969	1.00000	0.49827	0.00000	-0.11835	-0.00000
	0.02678	0.00000	-0.22282	-0.00000	0.13947	0.00000	-0.05817								
12	-0.02278	-0.00000	0.02455	-0.00000	-0.05642	0.00000	0.08131	0.00000	-0.15957	0.00000	0.49827	1.00000	0.57926	-0.00000	-0.26365
	-0.00000	0.54390	0.00000	-0.11750	-0.00000	0.02567	0.00000								
13	-0.00000	-0.02183	0.00000	0.02455	-0.00000	-0.02945	0.00000	0.09466	-0.00000	-0.19930	0.00000	0.57926	1.00000	0.70273	0.00000
	-0.34035	-0.00000	0.03619	0.00000	-0.04874	-0.00000	0.02194								
14	0.02289	-0.00000	-0.02183	-0.00000	0.05152	-0.00000	-0.06484	0.00000	0.09112	0.00000	-0.11835	-0.00000	0.70273	1.00000	0.62606
	0.00000	-0.26881	0.00000	0.10495	0.00000	-0.02792	-0.00000								
15	0.00000	0.02289	-0.00000	-0.02278	-0.00000	0.01613	0.00000	-0.06837	0.00000	0.17206	-0.00000	-0.26365	0.00000	0.62606	1.00000
	0.69760	0.00000	-0.10892	-0.00000	0.06093	-0.00000	-0.02697								
16	-0.02697	0.00000	0.02194	-0.00000	-0.05817	0.00000	0.07352	-0.00000	-0.09635	0.00000	0.02678	-0.00000	-0.34035	0.00000	0.69760
	1.00000	0.59380	-0.00000	-0.15294	0.00000	0.03911	0.00000								
17	0.00000	-0.02792	-0.00000	0.02567	0.00000	-0.00077	-0.00000	0.04555	-0.00000	-0.24165	0.00000	0.54390	-0.00000	-0.26881	0.00000
	0.59380	1.00000	0.45346	0.00000	-0.10125	0.00000	0.03911								
18	0.06093	-0.00000	-0.04874	0.00000	0.13947	-0.00000	-0.21130	0.00000	0.51326	-0.00000	-0.22282	0.00000	0.03619	0.00000	-0.10892
	-0.00000	0.45346	1.00000	0.62264	0.00000	-0.10125	-0.00000								
19	-0.00000	0.10495	-0.00000	-0.11750	-0.00000	0.03415	-0.00000	-0.35480	0.00000	0.03415	-0.00000	-0.11750	0.00000	0.10495	-0.00000
	-0.15294	0.00000	0.62264	1.00000	0.62264	0.00000	-0.15294								
20	-0.10892	0.00000	0.03619	-0.00000	-0.22282	0.00000	0.51326	-0.00000	-0.21130	0.00000	0.13947	-0.00000	-0.04874	0.00000	0.06093
	0.00000	-0.10125	0.00000	0.62264	1.00000	0.45346	0.00000								
21	0.00000	-0.26881	0.00000	0.54390	0.00000	-0.24165	0.00000	0.04555	-0.00000	-0.00077	0.00000	0.02567	-0.00000	-0.02792	-0.00000
	0.03911	0.00000	-0.10125	0.00000	0.45346	1.00000	0.59380								
22	0.69760	-0.00000	-0.34035	0.00000	0.02678	-0.00000	-0.09635	0.00000	0.07352	-0.00000	-0.05817	0.00000	0.02194	-0.00000	-0.02697
	0.00000	0.03911	-0.00000	-0.15294	0.00000	0.59380	1.00000								

1,2,7,8DIBENZANTHRACENE TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.76021	-0.45096	-0.05077	-0.24525	0.01926	0.16721	0.00043	-0.06801	-0.00190	0.01621	0.00156	-0.02251	-0.00004	0.02266	0.00096
2	-0.45096	0.75900	0.52550	-0.04090	-0.10960	-0.00544	0.08755	-0.00594	-0.06347	0.00311	0.05086	-0.00044	-0.02166	-0.00025	0.02266
3	-0.05077	0.52550	0.76887	0.41100	-0.05472	-0.18927	0.01406	0.09209	-0.00365	-0.02882	0.00112	0.02428	-0.00065	-0.02166	-0.00004
4	-0.24525	-0.04090	0.41100	0.72261	0.33131	-0.04611	-0.14450	0.01635	0.07825	-0.00564	-0.05540	0.00150	0.02428	-0.00044	-0.02251
5	0.01926	-0.10960	-0.05472	0.33131	0.76989	0.60103	-0.04604	-0.20828	0.00470	0.05387	0.00038	-0.05540	0.00112	0.05086	0.00156
6	0.16721	0.00544	-0.18927	-0.04611	0.60103	0.76996	0.33103	-0.05769	-0.09727	0.01071	0.05387	-0.00564	-0.02882	0.00311	0.01621
7	0.00043	0.08755	0.01406	-0.14450	-0.04604	0.33103	0.72241	0.44203	-0.03684	-0.09727	0.00470	0.07825	-0.00365	-0.06347	-0.00190
8	-0.06801	-0.00594	0.09209	0.01635	-0.20828	-0.05769	0.44203	0.78180	0.44203	-0.05769	-0.20828	0.01635	0.09209	-0.00594	-0.06801
9	-0.00190	-0.06347	-0.00365	0.07825	0.00470	-0.09727	-0.03684	0.44203	0.72241	0.33103	-0.04604	-0.14450	0.01406	0.08755	0.00043
10	0.01621	0.00311	-0.02882	-0.00564	0.05387	0.01071	-0.09727	-0.05769	0.33103	0.76996	0.60103	-0.04611	-0.18927	0.00544	0.16721
11	0.00156	0.05086	0.00112	-0.05540	0.00038	0.05387	0.00470	-0.20828	-0.04604	0.60103	0.76989	0.33131	-0.05472	-0.10960	0.01926
12	-0.02251	-0.00044	0.02428	0.00150	-0.05540	-0.00564	0.07825	0.01635	-0.14450	-0.04611	0.33131	0.72261	0.41100	-0.04090	-0.24525
13	-0.00004	-0.02166	-0.00065	0.02428	0.00112	-0.02882	-0.00365	0.09209	0.01406	-0.18927	-0.05472	0.41100	0.76887	0.52550	-0.05077
14	0.02266	-0.00025	-0.02166	-0.00044	0.05086	0.00311	-0.06347	-0.00594	0.08755	0.00544	-0.10960	-0.04090	0.52550	0.75900	0.45096
15	0.00096	0.02266	-0.00004	-0.02251	0.00156	0.01621	-0.00190	-0.06801	0.00043	0.16721	0.01926	-0.24525	-0.05077	0.45096	0.76021
16	-0.02657	0.00118	0.02180	-0.00062	-0.05716	-0.00346	0.07118	0.00446	-0.08927	0.01424	0.03157	-0.03365	-0.31981	-0.04956	0.52060
17	-0.00258	-0.02743	0.00059	0.02503	-0.00564	-0.00219	0.01137	0.04992	-0.02910	-0.22492	-0.03866	0.38159	-0.03244	-0.25018	-0.04304
18	0.05952	-0.00272	-0.04849	0.00171	0.13539	0.01484	-0.19550	-0.03854	0.35166	-0.03589	-0.20623	-0.03132	0.04022	0.01498	-0.10093
19	0.01022	0.10192	0.00204	-0.11019	0.01748	0.03934	-0.03854	-0.33577	-0.03854	0.03934	0.01748	-0.11019	0.00204	0.10192	0.01022
20	-0.10093	0.01498	0.04022	-0.03132	-0.20623	-0.03589	0.35166	-0.03854	-0.19550	0.01484	0.13539	0.00171	-0.04849	-0.00272	0.05952
21	-0.04304	-0.25018	-0.03244	0.38159	-0.03866	-0.22492	-0.02910	0.04992	0.01137	-0.00219	-0.00564	0.02503	0.00059	-0.02743	-0.00258
22	0.52060	-0.04956	-0.31981	-0.03365	0.03157	0.01424	-0.08927	0.00446	0.07118	-0.00346	-0.05716	-0.00062	0.02180	0.00118	-0.02657
	-0.00279	0.03786	0.00846	-0.14334	-0.04738	0.42457	0.76673								

ENERGIES FOR 1,2,7,8DIBENZANTHRACENE, TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	11,12	11,13	10,13	9,12	9,13	7,12	8,13	5,12	7,13	6,13
XMOMNT	0.00000	0.95170	-0.00000	0.00000	0.12380	-0.00000	-0.00000	-0.00000	-0.09025	0.00000
YMOMNT	0.68954	-0.00000	-0.29631	0.19818	-0.00000	-0.12298	-0.65586	0.13197	0.00000	0.00000
JUMP E	18.5131	21.6575	23.4691	23.7064	26.8508	28.1877	28.3991	30.8038	31.3322	31.8065
DIAG E	30.4061	33.0537	37.5531	38.9644	41.9177	44.0813	43.2571	44.8750	47.8990	47.2225
DIAG E	30.4926	33.0100	37.6243	38.9808	41.8040	44.4110	43.7456	45.2075	48.0985	47.5934
CORRSP	29.2575	32.8751	38.7188	36.9840	42.0856	47.3097	40.6090	43.4587	47.9097	50.0219
CORRSP	29.3901	32.8744	38.7834	37.1371	41.9297	47.6360	41.0401	43.8089	48.1084	50.2594

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	STATE COMPOSITION									
29.25745	0.28722	-0.00000	0.48047	0.9399	-0.0000	0.3047	-0.1000	0.0000	0.0415	0.0870	0.0352	-0.0000	-0.0566
18.23930				0.9529	-0.0000	0.2320	-0.0362	-0.0000	0.1552	-0.0905	0.0295	-0.0000	-0.0615
38.71875	0.09567	-0.00000	-0.24105	-0.2470	-0.0000	0.6895	-0.5161	0.0000	-0.2157	-0.3328	-0.0679	-0.0000	-0.1880
27.77869				-0.1604	-0.0000	0.8039	0.5045	0.0000	-0.0496	0.0617	-0.2510	0.0000	-0.0848
36.98404	0.16612	0.00000	-0.32500	-0.1403	0.0000	0.6043	0.7205	0.0000	-0.0743	0.2943	-0.0616	0.0000	0.0090
37.02828				0.1009	0.0000	-0.2962	0.7033	-0.0000	0.2718	0.3229	0.2885	0.0000	0.3822
47.30965	0.31900	0.00000	0.39819	0.0359	-0.0000	-0.0562	0.2881	-0.0000	0.6607	-0.6531	-0.1069	-0.0000	-0.1951
42.75815				-0.1833	0.0000	-0.0083	0.1145	-0.0000	0.6995	-0.6539	0.0789	-0.0000	-0.1734
40.60901	0.58505	0.00000	-0.58205	-0.1841	0.0000	0.1866	-0.2864	0.0000	0.6536	0.4865	0.4273	0.0000	-0.0525
33.96846				-0.1337	0.0000	0.2990	-0.4036	0.0000	0.5265	0.5892	0.3101	-0.0000	-0.0964
43.45875	0.22750	0.00000	0.35086	0.0249	-0.0000	0.1030	0.1050	-0.0000	-0.1247	-0.3582	0.7058	0.0000	0.5794
38.53430				-0.0680	-0.0000	0.3462	-0.1516	0.0000	-0.2369	-0.3301	0.6348	0.0000	0.5334
50.02189	-0.10678	0.00000	-0.22405	-0.0118	0.0000	0.1340	-0.1685	-0.0000	0.2588	0.0594	-0.5460	0.0000	0.7648
47.12216				-0.0028	0.0000	0.0533	-0.2314	0.0000	0.2774	-0.0058	-0.5895	0.0000	0.7205

ENERGIES FOR 1,2,7,8DIBENZANTHRACENE, TBM APPROXIMATION, PAGE 7

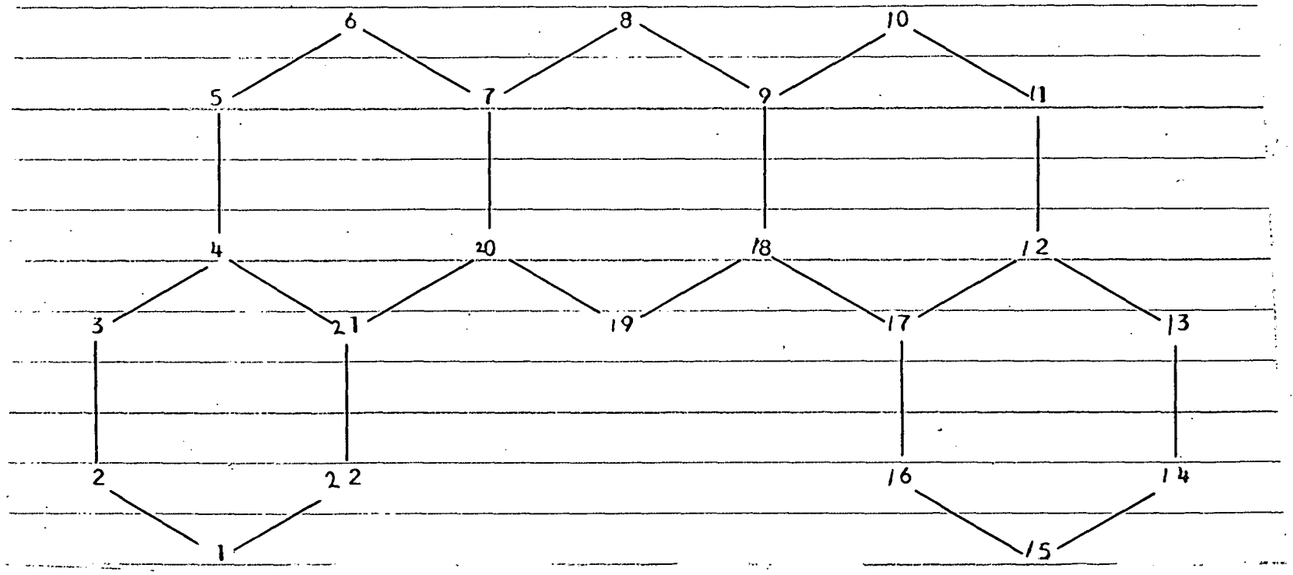
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	10,12	11,13	8,12	9,13	6,12	10,14	7,13	4,12	5,13	8,14
XMOMNT	0.95113	0.95170	0.35032	0.12380	-0.21368	-0.12407	-0.09025	0.06095	0.04574	0.31940
YMOMNT	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.00000	-0.00000
JUMP E	20.3247	21.6575	25.2547	26.8508	28.6621	30.5961	31.3322	31.8240	33.9483	35.5261
DIAG E	31.9843	33.0537	37.9518	41.9177	43.3490	45.3859	47.8990	48.5535	49.9741	51.4528
DIAG E	32.1856	33.0100	38.5703	41.8040	43.8500	45.7812	48.0985	48.7896	50.1765	52.2654
CORRSP	33.2378	27.9099	37.4223	39.3345	42.2409	48.4864	45.0039	50.2485	51.8967	55.7406
CORRSP	33.3725	28.2611	38.0119	39.5319	42.4641	48.6975	45.2789	50.5073	51.9977	56.4081

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
33.23782	1.99110	1.18688	-0.00000	//	0.6706	0.6133	-0.3401	0.1473	-0.1255	-0.1175	-0.0435	0.0048	-0.0248	-0.0682
22.28871				//	0.6654	0.6163	-0.1409	0.2412	-0.1832	-0.2146	-0.0165	-0.0535	-0.0702	0.1080
				//										
27.90987	0.01723	-0.12050	0.00000	//	-0.6708	0.6324	-0.2384	-0.1514	0.1348	-0.1185	-0.0339	-0.1405	0.0762	-0.1066
26.45736				//	-0.5978	0.5202	-0.4520	-0.0345	0.2156	-0.1633	-0.1582	-0.2114	0.0494	0.1458
				//										
37.42226	0.97168	0.78140	-0.00000	//	0.0922	0.3638	0.7654	-0.3041	-0.0937	0.1246	-0.0914	0.2728	0.0265	-0.2705
33.26780				//	-0.2269	0.4151	0.7954	0.0357	0.1159	-0.1709	0.1281	0.2105	0.1784	0.0843
				//										
39.33450	0.07320	0.20919	-0.00000	//	-0.0259	0.1248	0.3723	0.6491	0.4418	-0.4014	0.1813	0.0378	0.1234	-0.1339
29.38012				//	-0.0875	-0.2944	-0.0122	0.7244	0.2006	-0.5377	0.0650	-0.1188	0.0167	-0.1809
				//										
42.24089	0.00240	-0.03655	0.00000	//	0.2341	0.0741	-0.0305	-0.3694	0.6079	0.3680	0.3806	-0.1556	0.2896	-0.2105
40.54027				//	0.2284	0.1141	-0.1533	-0.1027	0.5955	0.1854	0.4779	-0.0556	0.4039	-0.3423
				//										
48.48642	0.01677	0.09020	-0.00000	//	-0.0927	0.1586	0.1338	0.4682	-0.1538	0.6892	0.1107	-0.4049	-0.2245	0.0631
48.39574				//	-0.1816	0.1676	-0.0306	0.6207	-0.1699	0.7109	0.0462	0.1092	0.0441	-0.0495
				//										
45.00395	0.00484	0.05030	0.00000	//	-0.0173	0.0868	0.1675	-0.1965	-0.4567	-0.3006	0.6577	-0.2642	-0.1415	-0.3228
37.97068				//	-0.2200	0.1176	-0.0174	-0.1149	-0.5260	-0.1266	0.6174	-0.2464	-0.2023	-0.3856
				//										
50.24853	0.01679	-0.08865	-0.00000	//	-0.1478	0.0759	-0.1445	0.2088	-0.3217	0.2778	0.2337	0.5903	0.5270	-0.2154
45.61522				//	-0.0740	0.0027	-0.2868	-0.0340	-0.3195	-0.2259	-0.0471	0.6955	0.4829	-0.1972
				//										
51.89668	0.06150	0.16693	-0.00000	//	0.0748	-0.1058	0.1020	0.0268	-0.2279	-0.1230	-0.1494	-0.5280	0.7373	0.2457
50.15548				//	0.0343	-0.1176	0.0917	0.0118	-0.3219	0.0125	-0.0766	-0.5456	0.7219	0.2192
				//										
55.74064	0.00042	0.01338	0.00000	//	-0.0042	-0.1445	-0.1577	0.0539	0.0699	-0.0500	0.5377	0.1386	-0.0443	0.7960
55.25792				//	-0.0254	-0.1476	-0.1660	0.0648	0.0199	-0.0440	0.5781	0.1922	-0.0162	0.7563
				//										

1,2,7,8DIBENZANTHRACENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	0.8660	1.7320	2.5980	3.4640	4.3300	5.1960	6.0620
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	3.5000	3.0000	3.5000	3.0000

6.0620	6.9280	6.9280	6.0620	5.1960	5.1960	4.3300	3.4640	2.5980	1.7320	1.7320
2.0000	1.5000	0.5000	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	0.5000

1,2,7,8DIBENZANTHRACENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 S	8 A	9 S	10 A	11 S	12 S	13 A
1.776465	1.680817	1.533009	1.414031	1.363305	1.276845	1.268576	1.174321	1.149988	1.071860	1.041797	0.821624	0.797460
0.101831	-0.179401	0.254435	-0.304058	-0.124880	-0.100592	0.313718	-0.294694	-0.159163	-0.178244	-0.195503	0.194046	0.190329
0.095312	-0.180151	0.272059	-0.296451	0.006560	0.159990	0.299436	-0.262653	0.243501	0.195893	-0.146168	-0.128985	0.193832
0.128057	-0.222171	0.264039	-0.171091	0.143222	0.306999	0.048010	0.050925	0.361246	0.279104	0.122062	-0.115264	-0.308044
0.221902	-0.319224	0.222712	0.032165	0.208127	0.217514	-0.241721	0.301613	0.062596	-0.029375	0.193289	0.175767	0.008969
0.167267	-0.216160	0.051612	0.222107	0.339366	0.256104	-0.178441	0.001162	-0.119578	-0.310295	-0.243108	0.274727	0.289431
0.186731	-0.167681	-0.118263	0.314333	0.295484	0.097888	0.044790	-0.308255	-0.170401	-0.152896	-0.292160	-0.305089	-0.199480
0.293150	-0.154150	-0.282337	0.277016	0.095361	-0.121023	0.234814	-0.280516	-0.003451	0.225168	0.103755	-0.112866	-0.168470
0.237299	-0.000000	-0.302098	-0.000000	0.120503	0.000000	0.401419	0.000000	0.008797	0.000000	0.440534	0.438287	-0.000000
0.293150	0.154150	-0.282337	-0.277017	0.095361	0.121023	0.234814	0.280516	-0.003452	-0.225168	0.103755	-0.112866	0.168470
0.186731	0.167681	-0.118263	-0.314334	0.295483	-0.097888	0.044790	0.308254	-0.170401	0.152896	-0.292160	-0.305088	0.199480
0.167267	0.216160	0.051612	-0.222108	0.339365	-0.256104	-0.178441	-0.001162	-0.119577	0.310295	-0.243108	0.274727	-0.289431
0.221902	0.319224	0.222711	-0.032165	0.208127	-0.217514	-0.241721	-0.301613	0.062597	0.029375	0.193289	0.175767	-0.008969
0.128057	0.222171	0.264039	0.171091	0.143222	-0.306999	0.048010	-0.050924	0.361246	-0.279104	0.122063	-0.115264	0.308044
0.095312	0.180151	0.272059	0.296451	0.006560	-0.159990	0.299436	0.262653	0.243501	-0.195893	-0.146168	-0.128985	-0.193832
0.101831	0.179401	0.254435	0.304058	-0.124879	0.100592	0.313718	0.294693	-0.159164	0.178244	-0.195504	0.194046	-0.190329
0.155041	0.219370	0.206875	0.192400	-0.202186	0.292938	0.079793	0.010435	-0.370778	0.286568	0.051842	0.024892	0.309176
0.271099	0.313916	0.138538	-0.005891	-0.151926	0.260761	-0.209589	-0.276767	-0.171799	-0.009795	0.227313	-0.220105	-0.013528
0.323674	0.197043	-0.157760	-0.165622	-0.259414	0.281241	-0.120724	-0.013582	0.143619	-0.313871	-0.095793	-0.099060	-0.288989
0.267095	-0.000000	-0.161586	0.000000	-0.375347	0.000000	-0.183099	-0.000000	0.316081	-0.000000	-0.380418	0.361414	0.000000
0.323674	-0.197043	-0.157760	0.165622	-0.259414	-0.281241	-0.120724	0.013582	0.143619	0.313870	-0.095793	-0.099059	0.288989
0.271099	-0.313916	0.138538	0.005891	-0.151926	-0.260761	-0.209589	0.276767	-0.171799	0.009795	0.227313	-0.220105	0.013528
0.155041	-0.219370	0.206875	-0.192399	-0.202187	-0.292938	0.079793	-0.010436	-0.370778	-0.286568	0.051842	0.024892	-0.309176

OVERLAP EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 S	17 A	18 S	19 A	20 S	21 A	22 S
0.755844	0.721759	0.679417	0.671946	0.635391	0.612198	0.562971	0.509345	0.481005
-0.153269	-0.301107	0.337725	-0.119774	-0.122482	-0.288625	-0.223050	-0.148621	-0.085837
-0.234922	0.302334	-0.332969	-0.099386	0.000709	0.293300	0.240235	0.147734	0.078290
0.356822	-0.020601	0.089986	0.265872	0.134290	-0.202507	-0.257414	-0.199035	-0.112552
-0.079077	-0.278575	0.227247	-0.261355	-0.217045	0.032454	0.269623	0.332973	0.222576
-0.100602	0.009993	-0.171617	0.299218	0.323981	0.163337	-0.078968	-0.204912	-0.150663
0.167935	0.272734	-0.027102	-0.143049	-0.293137	-0.291132	-0.101128	0.160312	0.171063
-0.024199	-0.295047	0.220909	-0.096898	0.135926	0.318466	0.294992	-0.170930	-0.302852
0.024878	0.000000	-0.351369	-0.000001	-0.162678	-0.000000	-0.297396	0.000000	0.227017
-0.024198	0.295047	0.220908	0.096899	0.135926	-0.318466	0.294992	0.170930	-0.302852
0.167934	-0.272735	-0.027103	0.143049	-0.293137	0.291132	-0.101128	-0.160312	0.171063
-0.100602	-0.009992	-0.171615	-0.299218	0.323981	-0.163337	-0.078968	0.204912	-0.150664
-0.079077	0.278575	0.227245	0.261357	-0.217045	-0.032454	0.269623	-0.332973	0.222576
0.356822	0.020601	0.089988	-0.265871	0.134290	0.202507	-0.257414	0.199035	-0.112552
-0.234922	-0.302334	-0.332970	0.099384	0.000709	-0.293300	0.240235	-0.147734	0.078291
-0.153268	0.301107	0.337724	0.119776	-0.122482	0.288625	-0.223050	0.148621	-0.085837
0.367638	-0.018182	-0.104592	-0.272498	0.197684	-0.188366	0.198010	-0.202876	0.144052
-0.187166	-0.279294	-0.199014	0.248469	-0.161797	0.012310	-0.170567	0.341544	-0.284188
-0.156426	0.005157	0.112551	-0.285316	0.260692	0.200292	-0.159135	-0.225573	0.344151
0.328236	-0.000000	-0.151023	-0.000001	-0.357872	-0.000000	0.156501	-0.000000	-0.264162
-0.156426	-0.005157	0.112550	0.285317	0.260692	-0.200292	-0.159135	0.225574	0.344151
-0.187165	0.279295	-0.199013	-0.248470	-0.161797	-0.012310	-0.170567	-0.341544	-0.284187
0.367638	0.018182	-0.104594	0.272498	0.197683	0.188367	0.198010	0.202876	0.144051

1,2,7,8DIBENZANTHRACENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A	7 S	8 A	9 S	10 A	11 S	12 S	13 A
32.84312	30.43614	26.12577	22.00154	20.02432	16.29215	15.90853	11.15428	9.80036	5.03768	3.01468	-16.31339	-19.08456
0.076402	-0.138377	0.205497	-0.255698	-0.106954	-0.089021	0.278536	-0.271943	-0.148421	-0.172165	-0.191541	0.214076	0.213133
0.071510	-0.138955	0.219730	-0.249301	0.005618	0.141587	0.265856	-0.242375	0.227067	0.189213	-0.143206	-0.142299	0.217056
0.096078	-0.171367	0.213253	-0.143879	0.122663	0.271686	0.042626	0.046993	0.336865	0.269585	0.119589	-0.127162	-0.344952
0.166488	-0.246227	0.179875	0.027049	0.178251	0.192494	-0.214613	0.278328	0.058372	-0.028373	0.189372	0.193911	0.010044
0.125497	-0.166730	0.041685	0.186781	0.290651	0.226645	-0.158430	0.001072	-0.111507	-0.299713	-0.238182	0.303085	0.324108
0.140100	-0.129337	-0.095516	0.264338	0.253068	0.086628	0.039767	-0.284457	-0.158900	-0.147682	-0.286239	-0.336581	-0.223380
0.219944	-0.118901	-0.228032	0.232957	0.081672	-0.107103	0.208480	-0.258860	-0.003218	0.217489	0.101652	-0.124517	-0.188655
0.178040	-0.000000	-0.243992	-0.000000	0.103205	0.000000	0.356401	0.000000	0.008203	0.000000	0.431606	0.483528	-0.000000
0.219944	0.118900	-0.228032	-0.232957	0.081672	0.107103	0.208480	0.258860	-0.003219	-0.217489	0.101652	-0.124517	0.188655
0.140100	0.129337	-0.095516	-0.264339	0.253067	-0.086628	0.039767	0.284456	-0.158901	0.147682	-0.286239	-0.336581	0.223380
0.125497	0.166730	0.041685	-0.186782	0.290650	-0.226646	-0.158429	-0.001073	-0.111507	0.299713	-0.238182	0.303085	-0.324108
0.166488	0.246227	0.179875	-0.027050	0.178251	-0.192495	-0.214613	-0.278328	0.058373	0.028373	0.189372	0.193911	-0.010044
0.096078	0.171367	0.213253	0.143879	0.122663	-0.271686	0.042626	-0.046992	0.336865	-0.269586	0.119589	-0.127162	0.344952
0.071510	0.138955	0.219730	0.249301	0.005618	-0.141587	0.265856	0.242376	0.227067	-0.189213	-0.143206	-0.142299	-0.217055
0.076402	0.138377	0.205497	0.255698	-0.106953	0.089021	0.278536	0.271943	-0.148422	0.172165	-0.191542	0.214076	-0.213133
0.116324	0.169206	0.167085	0.161799	-0.173163	0.259243	0.070844	-0.009629	-0.345754	0.276795	0.050792	0.027462	0.346219
0.203399	0.242132	0.111891	-0.004954	-0.130117	0.230767	-0.186085	-0.255400	-0.160204	-0.009461	0.222707	-0.242825	-0.015149
0.242845	0.151985	-0.127416	-0.139280	-0.222176	0.248891	-0.107185	-0.012533	0.133926	-0.303167	-0.093851	-0.109285	-0.323614
0.200395	-0.000000	-0.130506	0.000000	-0.321467	0.000000	-0.162566	0.000000	0.294749	-0.000000	-0.372709	0.398720	0.000000
0.242845	-0.151985	-0.127416	0.139280	-0.222176	-0.248891	-0.107185	0.012533	0.133926	0.303167	-0.093851	-0.109285	0.323614
0.203399	-0.242132	0.111891	0.004954	-0.130117	-0.230767	-0.186085	0.255400	-0.160205	0.009461	0.222707	-0.242825	0.015149
0.116324	-0.169206	0.167085	-0.161798	-0.173163	-0.259243	0.070845	-0.009630	-0.345754	-0.276795	0.050792	0.027461	-0.346219

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 S	15 A	16 S	17 A	18 S	19 A	20 S	21 A	22 S
-24.27247	-28.96730	-35.45547	-36.68521	-43.11879	-47.59889	-58.33161	-72.38415	-81.07603
-0.176294	-0.354426	0.409727	-0.146116	-0.153657	-0.368882	-0.297276	-0.208245	-0.123765
-0.270213	0.355870	-0.403957	-0.121243	0.000889	0.374858	0.320180	0.207002	0.112884
0.410427	-0.024249	0.109171	0.324343	0.168470	-0.258817	-0.343075	-0.278884	-0.162285
-0.090957	-0.327904	0.275696	-0.318834	-0.272289	0.041478	0.359348	0.466555	0.320925
-0.115715	0.011762	-0.208206	0.365023	0.406442	0.208756	-0.105247	-0.287118	-0.217237
0.193163	0.321029	-0.032880	-0.174510	-0.367748	-0.372086	-0.134781	0.224627	0.246650
-0.027834	-0.347293	0.268006	-0.118208	0.170523	0.407022	0.393158	-0.239504	-0.436672
0.028616	0.000000	-0.426280	-0.000001	-0.204084	-0.000000	-0.396363	0.000000	0.327328
-0.027833	0.347293	0.268006	0.118210	0.170523	-0.407022	0.393158	0.239504	-0.436673
0.193163	-0.321029	-0.032881	0.174509	-0.367749	0.372086	-0.134781	-0.224626	0.246650
-0.115715	-0.011762	-0.208204	-0.365024	0.406443	-0.208756	-0.105247	0.287118	-0.217237
-0.090956	0.327904	0.275694	0.318835	-0.272289	-0.041478	0.359348	-0.466554	0.320925
0.410426	0.024248	0.109173	-0.324343	0.168471	0.258818	-0.343075	0.278884	-0.162286
-0.270214	-0.355869	-0.403958	0.121241	0.000889	-0.374858	0.320179	-0.207002	0.112885
-0.176294	0.354426	0.409726	0.146118	-0.153657	0.368882	-0.297276	0.208245	-0.123766
0.422867	-0.021402	-0.126891	-0.332427	0.247999	-0.240745	0.263903	-0.284266	0.207703
-0.215283	-0.328750	-0.241444	0.303113	-0.202979	0.015733	-0.227327	0.478564	-0.409761
-0.179925	0.006070	0.136547	-0.348064	0.327045	0.255987	-0.212092	-0.316069	0.496220
0.377547	-0.000000	-0.183221	-0.000001	-0.448959	-0.000000	0.208581	-0.000000	-0.380886
-0.179925	-0.006070	0.136545	0.348065	0.327045	-0.255987	-0.212092	0.316069	0.496220
-0.215283	0.328751	-0.241442	-0.303115	-0.202978	-0.015733	-0.227327	-0.478564	-0.409760
0.422868	0.021401	-0.126893	0.332427	0.247999	0.240745	0.263903	0.284266	0.207703

1,2,7,8DIBENZANTHRACENE

IRM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.01209	0.62143	-0.01544	-0.25670	-0.00237	0.18614	-0.00366	-0.05868	0.00381	0.01513	-0.00417	-0.02455	-0.00041	0.02603	-0.00139
	-0.02779	0.00306	0.05976	-0.00084	-0.12691	-0.00714	0.69812								
2	0.62143	1.01352	0.70127	-0.00897	-0.12365	0.01176	0.10027	-0.00166	-0.07603	-0.00302	0.06443	-0.00017	-0.02337	0.00034	0.02603
	-0.00106	-0.03519	-0.00054	0.11356	-0.00325	-0.26595	-0.01589								
3	-0.01544	0.70127	1.01541	0.58197	0.00863	-0.20982	-0.00480	0.08821	0.00216	-0.03043	0.00022	0.02455	0.00192	-0.02337	-0.00041
	0.02105	-0.00070	-0.04072	-0.00652	0.02885	0.02134	-0.33411								
4	-0.25670	-0.00897	0.58197	0.96790	-0.49844	-0.00984	-0.14866	-0.00175	0.08905	0.00437	-0.06684	-0.00044	0.02455	-0.00017	-0.02455
	0.00106	0.03274	0.00085	-0.12865	0.00857	0.54021	0.02262								
5	-0.00237	-0.12365	0.00863	0.49844	1.01797	0.77407	-0.01245	-0.22957	0.01291	0.06120	-0.01376	-0.06684	0.00022	0.06443	-0.00417
	-0.06616	0.00791	0.15129	-0.00737	-0.20881	0.00657	0.00812								
6	0.18614	0.01176	-0.20982	-0.00984	0.77407	1.01493	0.50044	0.00684	-0.11204	-0.00467	0.06120	0.00437	-0.03043	-0.00302	0.01513
	0.00338	0.00134	-0.00969	0.01431	0.01189	-0.23005	-0.01797								
7	-0.00366	0.10027	-0.00480	-0.14866	-0.01245	0.50044	0.97039	0.61257	-0.00776	-0.11204	0.01291	0.08905	0.00216	-0.07603	0.00381
	0.07757	-0.01063	-0.20250	0.00914	0.50612	0.01396	-0.10494								
8	-0.05868	-0.00166	0.08821	-0.00175	-0.22957	0.00684	0.61257	1.03476	0.61257	0.00684	-0.22957	-0.00175	0.08821	-0.00166	-0.05868
	0.00307	0.03733	0.00762	-0.34268	0.00762	0.03733	0.00307								
9	0.00381	-0.07603	0.00216	0.08905	0.01291	-0.11204	-0.00776	0.61257	0.97039	0.50044	-0.01245	-0.14866	-0.00480	0.10027	-0.00366
	-0.10494	0.01396	0.50612	0.00914	-0.20250	-0.01063	0.07757								
10	0.01513	-0.00302	-0.03043	0.00437	0.06120	-0.00467	-0.11204	0.00684	0.50044	1.01494	0.77407	-0.00984	-0.20982	0.01176	0.18614
	-0.01797	-0.23005	0.01189	0.01431	-0.00969	0.00134	0.00338								
11	-0.00417	0.06443	0.00022	-0.06684	-0.01376	0.06120	0.01291	-0.22957	-0.01245	0.77407	1.01797	0.49844	0.00863	-0.12365	-0.00237
	0.00812	0.00657	-0.20881	-0.00737	0.15129	0.00791	-0.06616								
12	-0.02455	-0.00017	0.02455	-0.00044	-0.06684	0.00437	0.08905	-0.00175	-0.14866	-0.00984	0.49844	0.96790	0.58197	-0.00897	-0.25670
	0.02262	0.54021	0.00857	-0.12865	0.00085	0.03274	0.00106								
13	-0.00041	-0.02337	0.00192	0.02455	0.00022	-0.03043	0.00216	0.08821	-0.00480	-0.20982	0.00863	0.58197	1.01541	0.70127	-0.01544
	-0.33411	0.02134	0.02886	-0.00652	-0.04072	-0.00070	0.02105								
14	0.02603	0.00034	-0.02337	-0.00017	0.06443	-0.00302	-0.07603	-0.00166	0.10027	0.01176	-0.12365	-0.00897	0.70127	1.01352	0.62143
	-0.01589	-0.26595	-0.00325	0.11356	-0.00054	-0.03519	-0.00106								
15	-0.00139	0.02603	-0.00041	-0.02455	-0.00417	0.01513	0.00381	-0.05868	-0.00366	0.18614	-0.00237	-0.25670	-0.01544	0.62143	1.01209
	0.69812	-0.00714	-0.12691	-0.00084	0.05976	0.00306	-0.02779								
16	-0.02779	-0.00106	0.02105	0.00106	-0.06616	0.00338	0.07757	0.00307	-0.10494	-0.01797	0.00812	0.02262	-0.33411	-0.01589	0.69812
	1.01486	0.59718	0.01161	-0.13531	-0.00303	0.04349	0.00212								
17	0.00306	-0.03519	-0.00070	0.03274	0.00791	0.00134	-0.01063	0.03733	0.01396	-0.23005	0.00657	0.54021	0.02134	-0.26595	-0.00714
	0.59718	0.96831	0.45432	0.00929	-0.11769	-0.00478	0.04349								
18	0.05976	-0.00054	-0.04072	0.00085	0.15129	-0.00969	-0.20250	0.00762	0.50612	0.01189	-0.20881	0.00857	0.02886	-0.00325	-0.12691
	0.01161	0.45432	0.97076	0.62651	-0.00545	-0.11769	-0.00303								
19	-0.00084	0.11356	-0.00652	-0.12865	-0.00737	0.01431	0.00914	-0.34268	0.00914	0.01431	-0.00737	-0.12865	-0.00652	0.11356	-0.00084
	-0.13531	0.00929	0.62651	1.03297	0.62651	0.00929	-0.13531								
20	-0.12691	-0.00325	0.02885	0.00857	-0.20881	0.01189	0.50612	0.00762	-0.20250	-0.00969	0.15129	0.00085	-0.04072	-0.00054	0.05976
	-0.00303	-0.11769	-0.00545	0.62651	0.97076	0.45432	0.01161								
21	-0.00714	-0.26595	0.02134	0.54021	0.00657	-0.23005	0.01396	0.03733	-0.01063	0.00134	0.00791	0.03274	-0.00070	-0.03519	0.00306
	0.04349	-0.00478	-0.11769	0.00929	0.45432	0.96831	0.59718								
22	0.69812	-0.01589	-0.33411	0.02262	0.00812	-0.01797	-0.10494	0.00307	0.07757	0.00338	-0.06616	0.00106	0.02105	-0.00106	-0.02779
	0.00212	0.04349	-0.00303	-0.13531	0.01161	0.59718	1.01486								

1,2,7,8DIBENZANTHRACENE IRM DENSITY BOND ORDERS

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.78371	0.44300	-0.09173	-0.26976	0.02311	0.19775	-0.00069	-0.06439	0.00183	0.01624	-0.00267	-0.02662	-0.00022	0.02818	-0.00049
	-0.03015	0.00008	0.06481	0.01047	-0.12730	-0.07312	0.52240								
2	0.44300	0.78445	0.52577	-0.07318	-0.12368	0.02255	0.10679	-0.01099	-0.08191	0.00119	0.06943	-0.00077	-0.02530	0.00024	0.02818
	-0.00001	-0.03793	-0.00401	0.12186	0.01791	-0.27943	-0.09157								
3	-0.09173	0.52577	0.79623	0.41083	-0.06735	-0.21489	0.01341	0.09461	-0.00349	-0.03283	0.00254	0.02670	0.00117	-0.02530	-0.00022
	0.02284	-0.00092	-0.04495	-0.00044	0.03787	-0.03037	-0.35008								
4	-0.26976	-0.07318	0.41083	0.70772	0.32225	-0.08014	-0.15756	0.01975	0.09547	-0.00290	-0.07190	0.00098	0.02670	-0.00077	-0.02662
	0.00046	0.03481	0.00558	-0.13180	-0.04175	0.37941	-0.02931								
5	0.02311	-0.12368	-0.06735	0.32225	0.80023	0.60256	-0.08289	-0.23602	0.02270	0.06444	-0.01531	-0.07190	0.00254	0.06943	-0.00267
	-0.07144	0.00048	0.16179	0.01587	-0.22183	-0.05379	0.01730								
6	0.19775	0.02255	-0.21489	-0.08014	0.60256	0.79678	0.32433	-0.07261	-0.11245	0.00945	0.06444	-0.00290	-0.03283	0.00119	0.01624
	-0.00108	0.00120	0.00942	0.02514	-0.04427	-0.24445	0.00002								
7	-0.00069	0.10679	0.01341	-0.15756	-0.08289	0.32433	0.71008	0.44275	-0.06667	-0.11245	0.02270	0.09547	-0.00349	-0.08191	0.00183
	0.08380	0.00470	-0.21572	-0.05029	0.34374	-0.03288	-0.10626								
8	-0.06439	-0.01099	0.09461	0.01975	-0.23602	-0.07261	0.44275	0.83051	0.44275	-0.07261	-0.23602	0.01975	0.09461	-0.01099	-0.06439
	0.01281	0.04794	-0.05243	-0.36408	-0.05243	0.04794	0.01281								
9	0.00183	-0.08191	-0.00349	0.09547	0.02270	-0.11245	-0.06667	0.44275	0.71008	0.32433	-0.08289	-0.15756	0.01341	0.10679	-0.00069
	-0.10626	-0.03288	0.34374	-0.05029	-0.21572	0.00470	0.08380								
10	0.01624	0.00119	-0.03283	-0.00290	0.06444	0.00945	-0.11245	-0.07261	0.32433	0.79678	0.60256	-0.08014	-0.21489	0.02255	0.19775
	0.00002	-0.24445	-0.04427	0.02514	0.00942	0.00120	-0.00108								
11	-0.00267	0.06943	0.00254	-0.07190	-0.01531	0.06444	0.02270	-0.23602	-0.08289	0.60256	0.80023	0.32225	-0.06735	-0.12368	0.02311
	0.01730	-0.05379	-0.22183	0.01587	0.16179	0.00048	-0.07144								
12	-0.02662	-0.00077	0.02670	0.00098	-0.07190	-0.00290	0.09547	0.01975	-0.15756	-0.08014	0.32225	0.70772	0.41083	-0.07318	-0.26976
	-0.02931	0.37941	-0.04175	-0.13180	0.00558	0.03481	0.00046								
13	-0.00022	-0.02530	0.00117	0.02670	0.00254	-0.03283	-0.00349	0.09461	0.01341	-0.21489	-0.06735	0.41083	0.79623	0.52577	-0.09173
	-0.35008	-0.03037	0.03787	-0.00044	-0.04495	-0.00092	0.02284								
14	0.02818	0.00024	-0.02530	-0.00077	0.06943	0.00119	-0.08191	-0.01099	0.10679	0.02255	-0.12368	-0.07318	0.52577	0.78445	0.44300
	-0.09157	-0.27943	0.01791	0.12186	-0.00401	-0.03793	0.00001								
15	-0.00049	0.02818	-0.00022	-0.02662	-0.00267	0.01624	0.00183	-0.06439	-0.00069	0.19775	0.02311	-0.26976	-0.09173	0.44300	0.78371
	0.52240	-0.07312	-0.12730	0.01047	0.06481	0.00008	-0.03015								
16	-0.03015	0.00001	0.02284	0.00046	-0.07144	-0.00108	0.08380	0.01281	-0.10626	0.00002	0.01730	-0.02931	-0.35008	-0.09157	0.52240
	0.79461	0.42664	-0.05913	-0.15037	0.00619	0.04698	-0.00029								
17	0.00008	-0.03793	-0.00092	0.03481	0.00048	0.00120	0.00470	0.04794	-0.03288	-0.24445	-0.05379	0.37941	-0.03037	-0.27943	-0.07312
	0.42664	0.71587	0.28526	-0.06398	-0.11872	0.00698	0.04698								
18	0.06481	-0.00401	-0.04495	0.00558	0.16179	0.00942	-0.21572	-0.05243	0.34374	-0.04427	-0.22183	-0.04175	0.03787	0.01791	-0.12730
	-0.05913	0.28526	0.71863	0.45719	-0.06742	-0.11872	0.00619								
19	0.01047	0.12186	-0.00044	-0.13180	0.01587	0.02514	-0.05029	-0.36408	-0.05029	0.02514	0.01587	-0.13180	-0.00044	0.12186	0.01047
	-0.15037	-0.06398	0.45719	0.82549	0.45719	-0.06398	-0.15037								
20	-0.12730	0.01791	0.03787	-0.04175	-0.22183	-0.04427	0.34374	-0.05243	-0.21572	0.00942	0.16179	0.00558	-0.04495	-0.00401	0.06481
	0.00619	-0.11872	-0.06742	0.45719	0.71863	0.28526	-0.05913								
21	-0.07312	-0.27943	-0.03037	0.37941	-0.05379	-0.24445	-0.03288	0.04794	0.00470	0.00120	0.00048	0.03481	-0.00092	-0.03793	0.00008
	0.04698	0.00698	-0.11872	-0.06398	0.28526	0.71587	0.42664								
22	0.52240	-0.09157	-0.35008	-0.02931	0.01730	0.00002	-0.10626	0.01281	0.08380	-0.00108	-0.07144	0.00046	0.02284	0.00001	-0.03015
	-0.00029	0.04698	0.00619	-0.15037	-0.05913	0.42664	0.79461								

ENERGIES FOR 1,2,7,8DIBENZANTHRACENE, IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	11,12	11,13	10,13	9,12	9,13	8,13	7,12	7,13	6,13	5,12
XMOMNT	0.00000	0.93623	-0.00000	0.00000	0.20192	0.00000	0.00000	-0.07714	-0.00000	-0.00000
YMOMNT	0.62859	-0.00000	-0.32568	0.29307	-0.00000	0.67139	-0.07088	0.00000	-0.06128	0.14366
JUMP E	19.3281	22.0992	24.1222	26.1137	28.8849	30.2388	32.2219	34.9931	35.3767	36.3377
DIAG E	30.0411	33.3328	37.3661	40.5185	43.7346	45.2213	46.8755	51.1366	50.9960	50.7772
DIAG E	30.1509	33.4027	37.5982	40.4631	43.6394	45.7928	47.2351	51.4563	51.4322	51.0527
CORRSP	29.1639	33.2822	37.4984	39.8118	43.7834	43.4501	50.1619	51.1384	53.8980	47.8117
CORRSP	29.3048	33.3717	37.7684	39.8297	43.6703	43.9214	50.4786	51.4564	54.1727	48.2493

FINAL EXCITED STATES OF A S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
29.16388	0.25681	0.00000	0.45505	//	0.9515	0.0000	0.2971	-0.0355	0.0000	-0.0582	0.0195	-0.0000	-0.0342	0.0173
				//										
19.01243				//	0.9609	-0.0000	0.2105	0.0160	-0.0000	0.0958	0.1447	0.0000	-0.0430	0.0085
				//										
37.49840	0.29129	0.00000	-0.42740	//	-0.2586	0.0000	0.8452	0.4285	0.0000	-0.1794	-0.0509	0.0000	-0.0190	0.0036
				//										
28.88814				//	-0.1939	0.0000	0.8824	0.3933	-0.0000	-0.0521	-0.0048	-0.0000	-0.0307	-0.1595
				//										
39.81180	0.08718	0.00000	0.22692	//	0.1477	0.0000	-0.4296	0.8095	0.0000	-0.3374	0.0665	-0.0000	0.1402	-0.0226
				//										
35.75684				//	0.0666	0.0000	-0.2899	0.6715	-0.0000	0.5078	-0.3910	0.0000	0.0965	-0.2013
				//										
43.45006	0.63073	-0.00000	0.58426	//	0.0764	-0.0000	-0.0198	0.2807	-0.0000	0.6454	-0.6726	0.0000	0.0786	-0.1995
				//										
39.11677				//	-0.0425	0.0000	0.2736	-0.5955	0.0000	0.5860	-0.4616	-0.0000	-0.0909	-0.0632
				//										
50.16189	0.22143	0.00000	0.32219	//	0.0097	0.0000	0.0148	0.2282	-0.0000	0.4743	0.6007	0.0000	-0.4834	-0.3580
				//										
44.39331				//	-0.1716	0.0000	-0.0410	0.0232	-0.0000	0.5570	0.7435	0.0000	-0.3066	-0.1060
				//										
53.89795	0.12645	-0.00000	-0.23488	//	-0.0001	-0.0000	0.0858	-0.1195	0.0000	-0.0255	0.2059	-0.0000	0.6837	-0.6840
				//										
50.48455				//	-0.0134	-0.0000	-0.0113	-0.1919	0.0000	-0.0058	0.1932	-0.0000	0.6746	-0.6859
				//										
47.81166	0.25558	0.00000	0.35454	//	-0.0108	0.0000	0.0700	0.1216	-0.0000	0.4565	0.3701	-0.0000	0.5211	0.6028
				//										
42.94692				//	-0.0558	0.0000	0.1281	0.0463	0.0000	0.2766	0.1516	-0.0000	0.6562	0.6695
				//										

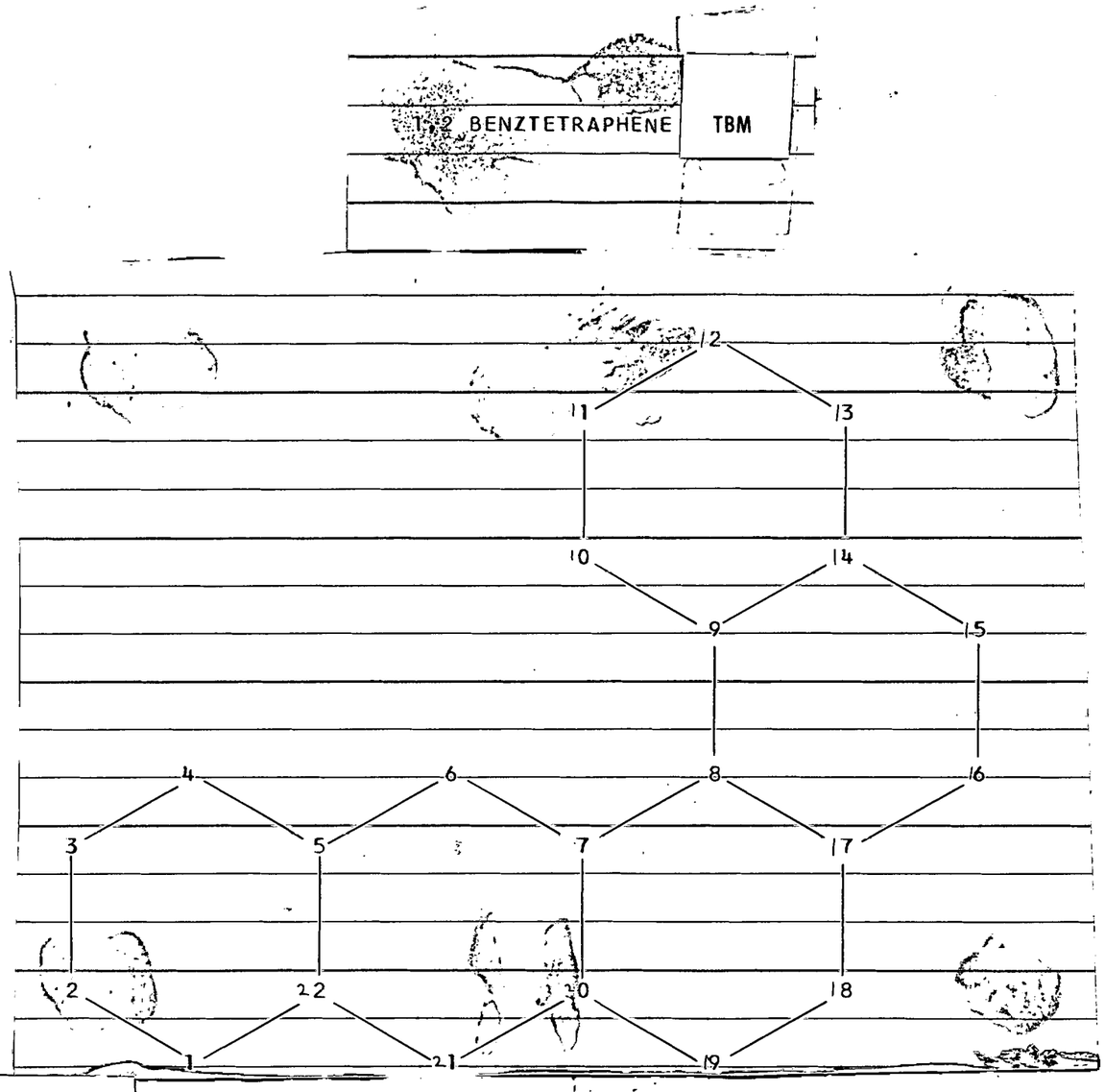
ENERGIES FOR 1,2,7,8DIBENZANTHRACENE, IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	10,12	11,13	8,12	9,13	10,14	6,12	7,13	8,14	4,12	5,13
XMOMNT	1.02487	0.93623	-0.34583	0.20192	-0.13467	-0.22199	-0.07714	-0.30685	-0.00576	0.05462
YMOMNT	0.00000	-0.00000	0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	-0.00000	-0.00000
JUMP E	21.3511	22.0992	27.4677	28.8849	29.3102	32.6055	34.9931	35.4267	38.3149	39.1089
DIAG E	32.1664	33.3328	39.4461	43.7346	43.3313	47.1866	51.1366	51.4540	54.6753	55.6564
DIAG E	32.4383	33.4027	40.0574	43.6394	43.8260	47.6626	51.4563	52.2880	54.8483	55.8920
CORRSP	28.4751	34.3328	38.5911	46.5298	40.2259	44.9233	50.4066	56.1138	54.9315	57.5898
CORRSP	34.5116	28.7958	39.1212	40.5715	46.8831	45.3134	50.6044	57.9237	55.2091	56.5770

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
28.47510	0.01699	0.11844	-0.00000	//	0.6941	-0.6645	-0.1590	-0.0919	-0.1145	-0.0670	0.0301	0.1234	0.0770	-0.0579
26.71279				//	0.6673	-0.5348	-0.3523	-0.0643	0.2150	-0.1619	0.1359	-0.1735	0.1303	-0.0499
34.33284	2.43067	1.29028	-0.00000	//	0.6780	0.6329	0.2795	0.1697	-0.1280	-0.0697	-0.0303	-0.1004	0.0200	-0.0095
23.08030				//	0.6703	0.6156	0.1322	0.2496	-0.2054	-0.1410	-0.0226	-0.1557	-0.0507	-0.0520
38.59113	0.64390	-0.62639	0.00000	//	-0.1351	-0.2815	0.6979	0.3914	-0.3753	0.0687	0.1243	0.2844	-0.1410	-0.0226
35.01353				//	0.1650	-0.3190	0.8884	-0.0269	0.1595	-0.0562	-0.1116	0.0967	-0.1471	-0.0949
46.52983	0.00106	-0.02314	-0.00000	//	-0.0911	-0.0281	0.0586	0.6443	0.5173	0.2856	-0.3532	-0.2849	0.0817	0.1027
29.81212				//	-0.0463	-0.3616	0.0000	0.6609	-0.6166	0.1105	0.0966	0.1532	-0.0712	-0.0011
40.22591	0.23231	-0.36852	0.00000	//	0.0386	-0.0678	0.5928	-0.5015	0.5903	-0.1529	-0.1055	0.0036	-0.0900	-0.0057
48.22924				//	-0.1673	0.1013	-0.0643	0.6547	0.6650	-0.2016	0.1336	0.0350	-0.1429	-0.0810
44.92333	0.01251	-0.08092	0.00000	//	0.1104	0.1411	-0.0521	-0.0946	0.2349	0.7234	0.4555	0.3540	-0.0953	0.1894
43.87460				//	0.1581	0.1568	0.0932	0.0204	0.1862	0.7559	0.3763	0.3148	0.0332	0.3058
50.40662	0.02446	0.10683	-0.00000	//	-0.1009	0.1664	-0.1421	0.3649	0.3920	-0.5294	0.4733	0.2892	-0.1999	-0.1653
40.61405				//	-0.1259	0.1845	0.0665	-0.2198	-0.1686	-0.4245	0.6176	0.5098	-0.1567	-0.1509
56.11377	0.01342	-0.07499	-0.00000	//	-0.0167	0.1331	-0.0781	-0.0132	0.0456	0.1677	-0.4486	0.5225	0.0555	-0.6843
56.77907				//	0.0452	-0.0940	-0.1547	-0.0212	0.0087	-0.0792	-0.5719	0.5789	-0.4381	0.3228
54.93153	0.01994	-0.09239	-0.00000	//	-0.0704	0.0738	0.0617	0.0227	0.0427	-0.1712	-0.0427	0.4032	0.8076	0.3708
50.19670				//	-0.0647	0.0619	0.1664	0.1239	-0.0029	-0.3148	-0.0665	0.1910	0.7276	0.5288
57.58978	0.04434	0.13456	-0.00000	//	0.0536	0.0501	-0.1481	0.0134	-0.0306	-0.1412	-0.4608	0.4100	-0.5046	0.5627
54.76485				//	0.0324	-0.1449	0.0172	-0.0535	-0.0221	-0.2025	0.2946	-0.4254	-0.4317	0.6922



ATOMIC COORDINATES

x	-0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640	4.3300	4.3300	3.4640	3.4640	
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	2.0000	3.0000	3.5000	4.5000	
	4.3300	5.1960	5.1960	6.0620	6.0620	5.1960	5.1960	4.3300	3.4640	2.5980	1.7320	
	5.0000	4.5000	3.5000	3.0000	2.0000	1.5000	0.5000	0.	0.5000	0.	0.5000	

1,2 BENZTETRAPHENE TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1.625176 1.561170 1.485065 1.405023 1.361474 1.328925 1.295739 1.267742 1.208473 1.162913 1.103314 0.896684 0.837085

0.109887-0.245911 0.211488 0.153871-0.213848 0.124711 0.337222 0.078658-0.280008-0.120024 0.291631-0.291631 0.120024
0.072403-0.191327 0.222168 0.254168-0.101864 0.321401 0.188816-0.293867-0.251403 0.058496 0.204653 0.204653 0.058496
0.073515-0.189115 0.225155 0.263237 0.064664 0.303634-0.110981-0.397466 0.067660 0.158644-0.205975 0.205974-0.158644
0.113814-0.238668 0.220347 0.177822 0.196564 0.083268-0.321789-0.137321 0.308540 0.046223-0.290863-0.290863 0.046223
0.214776-0.353539 0.207897 0.028572 0.223218-0.192663-0.274598 0.248500 0.192954-0.128133 0.084220-0.084220 0.128133
0.224283-0.197389-0.005226-0.129272 0.341676-0.184838-0.222491 0.027719-0.160446 0.006913 0.408689 0.408689 0.006913
0.353334-0.095259-0.218168-0.240711 0.277192-0.053670 0.008001-0.218430-0.328477 0.132696 0.086857-0.086857-0.132697
0.377667 0.151431-0.153174 0.036450 0.319955 0.143212 0.213330 0.023159-0.186279-0.160826-0.283114-0.283114-0.160825
0.305672 0.284727 0.170382-0.076819 0.197966 0.086160 0.348908-0.037241 0.312001-0.153091-0.006645 0.006645 0.153091
0.159534 0.192780 0.208500-0.212963 0.072487 0.311201 0.126674 0.208026 0.300432 0.246816 0.189631 0.189631 0.246816
0.098434 0.153599 0.239401-0.272672-0.091807 0.328593-0.197133 0.262921-0.058239 0.316024 0.086028-0.086029-0.316024
0.089808 0.156464 0.262011-0.234508-0.206942 0.126730-0.362879 0.077203-0.349609-0.038205-0.153610-0.153610-0.038204
0.129050 0.202149 0.275536-0.112160-0.211275-0.159701-0.237683-0.179171-0.237065-0.341242-0.150329 0.150329 0.341241
0.237088 0.303173 0.279521 0.050454-0.102490-0.339580 0.078082-0.271583 0.149375-0.187050 0.090687 0.090687-0.187050
0.165830 0.202452 0.103445-0.271768-0.136807-0.379025-0.017676-0.078211-0.051224 0.370849 0.194928-0.194928 0.370848
0.182970 0.157144-0.076222 0.395544-0.097878-0.165554-0.099267 0.186749-0.106114 0.431859-0.009091-0.009091 0.431859
0.297642 0.154853-0.253241 0.377342-0.006551-0.158372-0.101270 0.280793-0.140852-0.085771-0.198723 0.198723 0.085770
0.193303 0.043512-0.268318 0.187240-0.231682-0.233416-0.235421 0.094702 0.173428-0.327665 0.209030 0.209030-0.327665
0.192011-0.055913-0.274104-0.070057-0.332765-0.152709-0.180826-0.178045-0.287334-0.130517 0.286213-0.286212 0.130517
0.293062-0.170640-0.270385-0.302205-0.255677-0.029901 0.018749-0.287846 0.069274 0.241514-0.089222-0.089222 0.241514
0.197001-0.236812-0.039134-0.185170-0.318870-0.138891-0.195291-0.084208-0.099640-0.157244-0.410413-0.410413-0.157245
0.205942-0.367794 0.193475-0.001662-0.211332-0.155199 0.215257 0.379195 0.014889-0.137721-0.082576-0.082576-0.137721

OVERLAP EIGNVALUES AND EIGNVECTORS

0.791524 0.732256 0.704259 0.671073 0.638524 0.594975 0.514933 0.438828 0.374822

-0.280008-0.078658 0.337222-0.124711-0.213847-0.153872 0.211488-0.245911 0.109887
0.251403-0.293867-0.188816 0.321400 0.101863 0.254168-0.222168 0.191327-0.072403
0.067660 0.397466-0.110981-0.303634 0.064665-0.263237 0.225155-0.189115 0.073515
-0.308540-0.137321 0.321788 0.083268-0.196564 0.177822-0.220346 0.238668-0.113813
0.192954-0.248500-0.274598 0.192663 0.223218-0.028572 0.207897-0.353539 0.214775
0.160445 0.027719-0.222491-0.184839-0.341676-0.129272-0.005226 0.197389-0.224283
-0.328477 0.218430 0.008000 0.053671 0.277192 0.240711-0.218168-0.095259 0.353334
0.186280-0.023159-0.213330-0.143210-0.319955-0.036450-0.153173-0.151431-0.377667
0.312001 0.037242 0.348908-0.086159 0.197966 0.076819 0.170382 0.284727 0.305672
-0.300432-0.208025-0.126675-0.311201-0.072488-0.212963-0.208500-0.192779-0.159534
-0.058238-0.262922-0.197132-0.328594-0.091807 0.272672 0.239401 0.153599 0.098434
0.349609 0.077204 0.362879 0.126731-0.206942-0.234508-0.262011-0.156464-0.089808
-0.237065 0.179171-0.237684 0.159699-0.211275 0.112160 0.275536 0.202149 0.129050
-0.149375-0.271583-0.078081-0.339579-0.102491-0.050453-0.279521-0.303173-0.237088
0.051224 0.078211-0.017677 0.379025-0.136808-0.271768 0.103445 0.202452 0.165830
0.106113-0.186749-0.099267-0.165554-0.097879-0.395544-0.076222-0.157144-0.182970
-0.140852-0.280793-0.101270-0.158372-0.006550-0.377342-0.253240 0.154853 0.297642
-0.173428 0.094702 0.235421 0.233417 0.231681-0.187241-0.268318-0.043512-0.193303
0.287334 0.178045-0.180826-0.152711-0.332764 0.070057-0.274104-0.055913 0.192011
-0.069274-0.287846-0.018748-0.029900-0.255677-0.302205-0.270385-0.170640-0.293062
0.099640-0.084207 0.195291 0.138891-0.318870-0.185169-0.039134-0.236812 0.197001
-0.014889-0.379195-0.215257-0.155199-0.211332-0.001662-0.193475-0.367794-0.205942

1,2 BENZTETRAPHENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

28.90556 27.00994 24.54335 21.66085 19.95018 18.59839 17.15025 15.86954 12.96263 10.52660 7.03622 -8.65783 -14.62419

0.086198 -0.196813 0.173545 0.129812 -0.183274 0.108182 0.296249 0.069860 -0.254714 0.111300 0.277641 -0.307974 0.131185
0.056795 -0.153127 0.182309 0.214427 -0.087300 0.278802 0.165875 -0.260997 -0.228692 0.054244 0.194835 0.216122 0.063936
-0.057667 0.151356 0.184761 0.222078 0.055419 0.263390 -0.097497 -0.353008 0.061548 0.147113 -0.196094 0.217517 -0.173396
0.089278 -0.191016 0.180815 0.150018 0.168461 0.072232 -0.282691 -0.121961 0.280668 0.042864 -0.276910 -0.307163 0.050522
-0.168475 0.282952 0.170599 0.024105 -0.191304 0.167127 -0.241234 0.220704 0.175523 0.118820 0.080180 -0.088939 0.140048
0.175932 -0.157978 -0.004289 -0.109060 0.292826 -0.160340 -0.195458 0.024618 -0.145952 0.006411 0.389084 0.431592 0.007556
0.277163 -0.076240 -0.179027 -0.203074 -0.237561 -0.046557 0.007029 -0.193998 -0.298804 -0.123051 -0.082690 -0.091724 -0.145036
0.296250 0.121197 -0.125693 0.030751 0.274211 0.124230 0.187410 0.020569 -0.169452 -0.149136 -0.269533 -0.298979 -0.175780
-0.239776 0.227879 -0.139814 -0.064808 -0.169663 -0.074741 0.306515 -0.033076 0.283817 -0.141963 -0.006326 0.007017 0.167327
0.125142 0.154289 0.171094 -0.179665 0.062124 0.269955 0.111283 0.184757 0.273292 0.228876 0.180534 0.200258 0.269767
-0.077214 0.122932 -0.196451 -0.230038 -0.078682 0.285042 -0.173181 0.233513 -0.052978 0.293053 -0.081901 -0.090850 -0.345410
0.070447 0.125225 0.215005 -0.197841 -0.177355 0.109933 -0.318789 0.068568 -0.318027 -0.035428 -0.146241 -0.162218 -0.041756
-0.101229 0.161788 0.226103 -0.094623 -0.181068 0.138534 -0.208804 0.159130 -0.215649 0.316438 -0.143118 0.158754 -0.372973
0.185977 0.242642 0.229372 0.042565 -0.087837 -0.294572 0.068595 -0.241205 0.135882 -0.173453 0.086337 0.095769 -0.204443
-0.130081 0.162030 0.084886 -0.229275 0.117247 0.328789 -0.015528 0.069462 0.046597 0.343893 0.185577 -0.205852 -0.405332
0.143526 0.125769 -0.062547 0.333698 -0.083885 -0.143611 -0.087206 0.165861 -0.096528 0.400469 -0.008655 -0.009600 0.472017
-0.233477 0.123935 -0.207807 0.318341 -0.005614 0.137382 -0.088966 0.249385 -0.128128 0.079536 -0.189190 0.209860 -0.093746
0.151631 0.034824 -0.220179 0.157964 -0.198558 0.202480 -0.206817 0.084109 0.157762 -0.303848 0.199003 0.220744 -0.358134
-0.150618 0.044750 -0.224927 -0.059103 -0.285189 0.132469 -0.158855 0.158130 0.261378 -0.121030 -0.272483 -0.302252 -0.142654
0.229884 -0.136570 -0.221876 -0.254953 -0.219122 -0.025938 0.016471 -0.255650 0.063016 0.223959 -0.084942 -0.094222 0.263972
-0.154532 0.189530 0.032113 -0.156217 -0.273281 0.120482 -0.171563 0.074789 -0.090639 0.145815 -0.390725 0.433413 -0.171867
0.161545 -0.294360 0.158764 -0.001402 -0.181118 0.134629 0.189103 0.336781 0.013544 -0.127711 -0.078615 -0.087204 -0.150528

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

-19.79113 -27.47493 -31.55433 -36.83066 -42.53845 -51.15204 -70.78337 -96.09065 125.33103

-0.314730 -0.091920 0.401837 -0.152237 -0.267618 -0.199485 0.294721 -0.371219 0.179488
0.282578 -0.343415 -0.224995 0.392339 -0.127476 0.329512 -0.309603 0.288822 -0.118262
0.076050 0.464481 -0.132246 -0.370651 0.080924 -0.341269 0.313766 -0.285482 0.120078
-0.346800 -0.160474 0.383446 0.101647 -0.245989 0.230535 -0.307065 0.360286 -0.185901
0.216881 -0.290398 -0.327214 0.235187 0.279345 -0.037042 0.289716 -0.533691 0.350810
0.180341 0.032392 0.265123 -0.225636 -0.427588 -0.167593 -0.007283 0.297972 -0.366339
-0.369210 0.255259 0.009533 0.065517 0.346890 0.312066 -0.304030 -0.143801 0.577129
0.209379 -0.027064 -0.254207 0.174820 -0.400406 -0.047256 -0.213456 -0.228596 -0.616874
0.350690 0.043521 0.415762 -0.105176 0.247743 0.099591 0.237437 0.429815 0.499280
-0.337687 -0.243100 -0.150947 0.379888 -0.090715 -0.276093 -0.290557 -0.291014 -0.260580
-0.065460 -0.307252 -0.234904 -0.401120 -0.114891 0.353501 0.333619 0.231868 0.160780
0.392962 0.090221 0.432410 0.154703 0.258976 -0.304024 -0.365128 -0.236193 -0.146690
-0.266462 0.209380 -0.283226 0.194948 -0.264399 0.145409 0.383975 0.305158 0.210787
-0.167898 -0.317374 -0.093042 -0.414531 0.128262 0.065409 -0.389528 -0.457661 -0.387255
0.057576 0.091398 -0.021064 0.462682 -0.171207 -0.352329 0.144156 0.305615 0.270864
0.119271 0.218236 0.118287 -0.202095 0.122490 0.512797 0.106220 -0.237220 -0.298860
-0.158318 -0.328137 -0.120674 -0.193328 -0.008197 -0.489199 -0.352905 0.233761 0.486164
-0.194934 0.110670 0.280530 0.284937 0.289936 0.242745 0.373916 -0.065684 -0.315738
0.322965 0.208065 -0.215474 -0.186416 -0.416436 0.090824 -0.381980 -0.084405 0.313627
-0.077864 -0.336379 -0.022341 -0.036500 0.319965 0.391789 0.376797 0.257593 -0.478682
0.111995 -0.098405 0.232710 0.169546 -0.399048 0.240060 -0.054535 -0.357484 0.321777
-0.016735 0.443130 0.256502 0.189454 0.264470 0.002154 0.269610 0.555210 0.336382

1,2-BENZTETRAPHENE | TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1.00000	0.73316	0.00000	-0.36514	-0.00000	-0.09301	-0.00000	-0.02085	-0.00000	-0.01079	-0.00000	-0.01567	-0.00000	-0.01997	-0.00000
	-0.03413	0.00000	0.08209	-0.00000	-0.13859	0.00000	-0.54054								
2	0.73316	1.00000	0.59080	-0.00000	-0.22332	-0.00000	-0.12498	-0.00000	-0.03684	-0.00000	-0.02566	-0.00000	-0.01957	-0.00000	-0.05160
	0.00000	-0.05755	0.00000	0.05151	-0.00000	-0.19212	-0.								
3	-0.00000	-0.59080	1.00000	0.73266	0.00000	-0.19136	-0.00000	0.05145	-0.00000	-0.02197	-0.00000	-0.02177	-0.00000	-0.02478	-0.00000
	0.02818	0.00000	-0.08813	-0.00000	0.12296	-0.00000	-0.22282								
4	-0.36514	-0.00000	-0.73266	1.00000	-0.54180	-0.00000	-0.14193	-0.00000	-0.04153	-0.00000	-0.02586	-0.00000	-0.01656	-0.00000	-0.04820
	0.00000	0.04905	0.00000	-0.01668	0.00000	0.09225	0.00000								
5	-0.00000	-0.22332	0.00000	0.54180	1.00000	-0.59123	-0.00000	-0.10281	0.00000	-0.03764	-0.00000	-0.03107	-0.00000	-0.03467	0.00000
	-0.02733	0.00000	0.12050	0.00000	-0.18932	0.00000	0.49170								
6	-0.09301	-0.00000	-0.19136	-0.00000	-0.59123	1.00000	0.63244	-0.00000	-0.11877	-0.00000	-0.06297	-0.00000	-0.03683	0.00000	-0.12130
	0.00000	-0.14335	0.00000	0.05586	-0.00000	-0.38391	-0.00000								
7	-0.00000	-0.12498	0.00000	-0.14193	-0.00000	0.63244	1.00000	-0.47314	-0.00000	-0.09344	-0.00000	-0.05722	-0.00000	-0.06897	-0.00000
	0.00528	-0.00000	-0.20797	0.00000	0.49368	0.00000	-0.19140								
8	-0.02085	-0.00000	-0.05145	-0.00000	-0.10281	-0.00000	-0.47314	1.00000	-0.49459	-0.00000	-0.13757	-0.00000	0.05867	-0.00000	-0.28132
	0.00000	0.58036	-0.00000	-0.27477	-0.00000	0.06365	0.00000								
9	-0.00000	-0.03684	-0.00000	0.04153	0.00000	-0.11877	-0.00000	-0.49459	1.00000	-0.57568	-0.00000	-0.25417	-0.00000	-0.52998	0.00000
	-0.23418	-0.00000	0.00568	0.00000	-0.06511	-0.00000	0.04675								
10	-0.01079	-0.00000	-0.02197	-0.00000	-0.03764	-0.00000	-0.09344	-0.00000	-0.57568	1.00000	-0.71088	-0.00000	-0.35091	-0.00000	-0.05336
	-0.00000	-0.12520	0.00000	0.09893	0.00000	-0.03222	0.00000								
11	-0.00000	-0.02566	-0.00000	-0.02586	-0.00000	0.06297	0.00000	-0.13757	-0.00000	-0.71088	1.00000	-0.61418	-0.00000	-0.25183	-0.00000
	0.16235	0.00000	-0.03194	0.00000	0.03839	0.00000	-0.03055								
12	-0.01567	-0.00000	-0.02177	-0.00000	-0.03107	-0.00000	-0.05722	-0.00000	-0.25417	-0.00000	-0.61418	-1.00000	0.71325	-0.00000	-0.14285
	0.00000	0.11803	0.00000	-0.09248	0.00000	0.04006	-0.00000								
13	-0.00000	-0.01957	0.00000	0.01656	-0.00000	-0.03683	0.00000	0.05867	-0.00000	-0.35091	0.00000	-0.71325	-1.00000	-0.56802	-0.00000
	-0.18716	0.00000	0.05749	0.00000	-0.03359	0.00000	0.02387								
14	-0.01997	-0.00000	-0.02478	-0.00000	0.03467	0.00000	-0.06897	-0.00000	0.52998	-0.00000	-0.25183	0.00000	0.56802	1.00000	0.52375
	0.00000	-0.18905	0.00000	0.11638	-0.00000	-0.04979	0.00000								
15	-0.00000	0.05160	-0.00000	-0.04820	0.00000	0.12130	-0.00000	-0.28132	0.00000	0.05336	0.00000	-0.14285	-0.00000	0.52375	1.00000
	0.75600	-0.00000	-0.13582	-0.00000	0.09633	-0.00000	-0.06576								
16	-0.03413	-0.00000	-0.02818	-0.00000	-0.02733	0.00000	0.00528	0.00000	-0.23418	-0.00000	0.16235	0.00000	-0.18716	-0.00000	0.75600
	0.00000	0.52795	0.00000	-0.15588	0.00000	0.08036	0.00000								
17	-0.00000	-0.05755	-0.00000	-0.04905	-0.00000	-0.14335	-0.00000	-0.58036	-0.00000	-0.12520	-0.00000	-0.11803	-0.00000	-0.18905	-0.00000
	0.52795	1.00000	0.50786	0.00000	-0.16657	-0.00000	0.08465								
18	-0.08209	-0.00000	-0.08813	-0.00000	-0.12050	-0.00000	-0.20797	-0.00000	0.00568	0.00000	-0.03194	0.00000	0.05749	0.00000	-0.13582
	0.00000	0.50786	1.00000	0.77197	0.00000	-0.22594	-0.00000								
19	-0.00000	-0.05151	-0.00000	-0.01668	-0.00000	-0.05586	-0.00000	-0.27477	-0.00000	-0.09893	-0.00000	-0.09248	-0.00000	-0.11638	-0.00000
	-0.15588	0.00000	0.77197	1.00000	0.50463	0.00000	-0.10801								
20	-0.13859	-0.00000	-0.12296	-0.00000	-0.18932	-0.00000	0.49368	-0.00000	-0.06511	0.00000	-0.03839	-0.00000	-0.03359	-0.00000	-0.09633
	0.00000	-0.16657	0.00000	0.50463	1.00000	0.62257	0.00000								
21	-0.00000	-0.19212	-0.00000	-0.09225	0.00000	-0.38391	0.00000	-0.06365	-0.00000	-0.03222	0.00000	-0.04006	-0.00000	-0.04979	-0.00000
	0.08036	-0.00000	-0.22594	0.00000	0.62257	1.00000	0.59407								
22	-0.54054	-0.	-0.22282	0.00000	0.49170	-0.00000	-0.19140	0.00000	0.04675	0.00000	-0.03055	-0.00000	0.02387	-0.00000	-0.06576
	0.00000	0.08465	-0.00000	-0.10801	0.00000	0.59407	1.00000								

1,2 BENZTETRAPHENE — TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
16	17	18	19	20	21	22									
1	0.77085	0.55577	0.05210	0.34465	0.03093	0.09729	0.01358	0.02214	0.00219	0.01104	0.00115	0.01570	0.00105	0.01995	0.00333
	-0.03343	-0.00618	0.08060	0.01224	-0.13019	-0.05985	0.37269								
2	0.55577	0.76016	0.41602	0.05198	0.20542	0.02087	0.12086	0.00698	0.03604	0.00263	0.02537	0.00145	0.01949	0.00112	0.05098
	0.00137	-0.05654	0.00150	0.05045	0.00278	-0.18259	-0.04141								
3	0.05210	0.41602	0.76028	0.55528	0.04159	0.18186	0.00309	0.05043	0.00104	0.02172	0.00003	0.02158	0.00072	0.02450	0.00083
	0.02788	0.00207	-0.08668	-0.00796	0.11892	0.02123	-0.20494								
4	0.34465	0.05198	0.55528	0.77067	0.37391	0.05937	0.13337	0.01110	0.04025	0.00364	0.02551	0.00220	0.01657	0.00228	0.04760
	-0.00014	0.04817	-0.00739	-0.01821	0.01358	0.09657	-0.03105								
5	0.03093	0.20542	0.04159	0.37391	0.72184	0.42240	0.03778	0.09538	0.00622	0.03647	0.00147	0.03051	0.00079	0.03372	0.00158
	-0.02731	0.00150	0.11664	0.01414	-0.17393	-0.03870	0.33074								
6	0.09729	0.02087	0.18186	0.05937	0.42240	0.78163	0.46235	0.05337	0.11034	0.01206	0.06148	0.00602	0.03711	0.00715	0.11848
	0.00427	-0.13579	0.01847	0.06096	-0.03911	-0.36483	-0.03822								
7	0.01358	0.12086	0.00309	0.13337	0.03778	0.46235	0.72694	0.31161	0.04037	0.08533	0.00751	0.05489	0.00192	0.06269	0.01301
	0.01000	-0.03213	-0.19146	-0.03478	0.33239	-0.03862	-0.17590								
8	0.02214	0.00698	0.05043	0.01110	0.09538	0.05337	0.31161	0.73794	0.33288	0.05027	0.12923	0.01644	0.06262	0.03247	0.26396
	-0.03785	0.41730	-0.03941	-0.25760	-0.03013	0.06807	0.01220								
9	0.00219	0.03604	0.00104	0.04025	0.00622	0.11034	0.04037	0.33288	0.72666	0.40675	0.04221	0.23571	0.03261	0.36785	0.03715
	-0.21734	-0.03108	0.01039	0.01199	-0.05896	0.00347	0.04490								
10	0.01104	0.00263	0.02172	0.00364	0.03647	0.01206	0.08533	0.05027	0.40675	0.76788	0.53377	0.05021	0.33033	0.03316	0.05790
	0.01477	-0.11774	0.00529	0.09631	0.00534	-0.03264	-0.00367								
11	0.00115	0.02537	0.00003	0.02551	0.00147	0.06148	0.00751	0.12923	0.04221	0.53377	0.75988	0.43916	0.05076	0.23352	0.01876
	0.15751	0.00087	-0.03182	-0.00136	0.03731	-0.00180	-0.03003								
12	0.01570	0.00145	0.02158	0.00220	0.03051	0.00602	0.05489	0.01644	0.23571	0.05021	0.43916	0.75933	0.53597	0.04105	0.13392
	0.00487	0.11420	-0.00577	-0.09081	-0.00099	0.03992	0.00155								
13	0.00105	0.01949	0.00072	0.01657	0.00079	0.03711	0.00192	0.06262	0.03261	0.33033	0.05076	0.53597	0.76904	0.39984	0.05495
	-0.17722	0.01466	0.05521	-0.00540	-0.03331	0.00236	0.02374								
14	0.01995	0.00112	0.02450	0.00228	0.03372	0.00715	0.06269	0.03247	0.36785	0.03316	0.23352	0.04105	0.39984	0.72253	0.35656
	-0.04515	-0.17360	0.01503	0.11271	-0.00013	-0.04950	-0.00103								
15	0.00333	0.05098	0.00083	0.04760	0.00158	0.11848	0.01301	0.26396	0.03715	0.05790	0.01876	0.13392	0.05495	0.35656	0.76947
	0.57750	-0.04617	-0.12648	0.00831	0.09280	-0.00699	-0.06447								
16	0.03343	0.00137	0.02788	0.00014	0.02731	0.00427	0.01000	0.03785	0.21734	0.01477	0.15751	0.00487	0.17722	0.04515	0.57750
	0.76845	0.36068	-0.05288	-0.14639	0.01445	0.07784	-0.00422								
17	0.00618	0.05654	0.00207	0.04817	0.00150	0.13579	0.03213	0.41730	0.03108	0.11774	0.00087	0.11420	0.01466	0.17360	0.04617
	0.36068	0.72389	0.34074	-0.04674	-0.15136	0.01723	0.08156								
18	0.08060	0.00150	0.08668	0.00739	0.11664	0.01847	0.19146	0.03941	0.01039	0.00529	0.03182	0.00577	0.05521	0.01503	0.12648
	-0.05288	0.34074	0.76944	0.59341	-0.04597	-0.21572	0.00457								
19	0.01224	0.05045	0.00796	0.01821	0.01414	0.06096	0.03478	0.25760	0.01199	0.09631	0.00136	0.09081	0.00540	0.11271	0.00831
	-0.14639	-0.04674	0.59341	0.77022	0.33759	-0.05863	-0.10005								
20	0.13019	0.00278	0.11892	0.01358	0.17393	0.03911	0.33239	0.03013	0.05896	0.00534	0.03731	0.00099	0.03331	0.00013	0.09280
	0.01445	-0.15136	-0.04597	0.33759	0.72277	0.45326	-0.03681								
21	0.05985	0.18259	0.02123	0.09657	0.03870	0.36483	0.03862	0.06807	0.00347	0.03264	0.00180	0.03992	0.00236	0.04950	0.00699
	0.07784	0.01723	-0.21572	-0.05863	0.45326	0.78321	0.42509								
22	0.37269	0.04141	0.20494	0.03105	0.33074	0.03822	0.17590	0.01220	0.04490	0.00367	0.03003	0.00155	0.02374	0.00103	0.06447
	-0.00422	0.08156	0.00457	-0.10005	-0.03681	0.42509	0.72147								

ENERGIES FOR 1,2 BENZTETRAPHENE ,TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF No SYMMETRY

JUMP	11,12	10,12	9,12	11,13	8,12	10,13	7,12	6,12	5,12	4,12	3,12	2,12	1,12
XMOMNT	-0.09301	-0.70168	0.17995	-0.70244	0.61234	0.27582	-0.16057	-0.07336	-0.04662	0.06874	0.03584	-0.02661	-0.01937
YMOMNT	-0.59577	-0.39163	-0.13810	-0.39205	-0.16689	-0.69938	-0.16363	-0.05166	-0.07750	-0.03306	-0.01357	-0.01044	-0.01538
JUMP E	15.6940	19.1844	21.6205	21.6604	24.5274	25.1508	25.8081	27.2562	28.6080	30.3187	33.2012	35.6678	37.5634
DIAG E	27.1839	32.1340	33.1913	34.1785	37.1696	38.2584	39.9379	43.6563	41.6520	47.1585	50.0442	51.4966	52.5622
DIAG E	27.2703	32.3185	33.5877	34.1885	37.8324	38.3663	40.3100	43.9212	42.1508	47.5325	50.5498	52.1572	53.4147
CORRSP	26.6134	29.0227	32.2570	34.9886	37.3722	39.9019	38.1599	42.5299	43.2949	46.8602	50.1903	51.3418	56.0904
CORRSP	26.7602	29.5891	32.5014	35.2189	37.8332	40.1896	38.5018	43.0578	43.7855	47.2332	51.8096	50.5193	56.6000

FINAL EXCITED STATES OF No SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
26.61339	0.25788	-0.06901	0.47233	//	0.9742	0.0274	-0.0379	-0.0612	-0.0853	0.1764	-0.0610	-0.0186	0.0111	-0.0451
				//	0.0033	-0.0126	-0.0146							
15.08074				//	0.9535	-0.1217	-0.1067	-0.1218	-0.0098	0.1493	-0.1219	-0.0104	0.1104	-0.0015
				//	0.0114	-0.0031	-0.0060							
29.02270	0.28037	-0.44264	-0.17676	//	-0.0993	0.6953	-0.4142	-0.4487	-0.3181	0.0229	-0.0019	0.0532	-0.0021	-0.1093
				//	-0.1306	0.0110	0.0088							
25.53913				//	0.0520	0.5226	-0.5101	-0.1079	-0.5022	-0.3780	0.0770	0.0288	0.0827	-0.1613
				//	-0.1277	0.0233	0.0281							
32.25704	0.54294	-0.43552	-0.45402	//	-0.0398	0.5250	0.7043	0.2960	-0.1324	0.2975	-0.0607	0.0385	-0.1403	-0.0809
				//	0.0348	0.0068	-0.0206							
28.88257				//	0.1604	0.0754	0.7342	0.1239	-0.3534	-0.4654	-0.2158	-0.0284	-0.1056	-0.1103
				//	0.0290	-0.0175	-0.0284							
34.98862	1.23263	-0.64563	-0.64156	//	-0.0279	0.1468	-0.5252	-0.7413	0.0186	0.3356	0.1587	0.0040	0.0995	-0.0096
				//	-0.0562	0.0101	0.0282							
31.54266				//	0.1036	-0.1620	-0.2309	-0.7795	0.2197	-0.3732	0.1102	-0.2338	0.1787	-0.0558
				//	0.0003	0.0680	0.0404							
37.37220	0.09871	0.21851	-0.11984	//	0.0955	0.4072	-0.0521	-0.0316	0.8652	-0.1815	0.0028	-0.0572	-0.0740	0.0932
				//	0.1205	-0.0862	-0.0215							
34.17758				//	0.0732	0.4707	0.0665	-0.3048	0.6518	-0.2567	-0.0621	-0.3395	-0.0969	-0.1254
				//	0.0969	-0.1767	0.0150							
39.90190	0.94832	0.61373	-0.42685	//	-0.1410	-0.0809	0.0269	-0.2812	0.2025	0.6578	-0.2797	-0.1552	0.5524	0.0334
				//	-0.0821	-0.0465	0.0506							
23.43463				//	0.0675	0.6150	0.1606	0.4733	-0.0562	0.5933	-0.0273	-0.0215	-0.0687	-0.0762
				//	-0.0075	-0.0209	-0.0063							

Cont

BENZTETRAPHENE TBM APPROXIMATION (cont.)

38.15992 0.20485 0.34877-0.06779 // -0.0256 -0.1170 0.0394 -0.2705 0.1210 0.4211 0.7851 0.0966 -0.2864 -0.0573
// 0.0661 0.0590 0.0063
33.69285 // 0.1813 -0.0325 0.0498 0.0208 -0.0128 -0.0586 0.7429 0.1088 -0.6227 -0.0755
// 0.0099 0.0313 -0.0363

42.52993 0.15983-0.22643 0.19262 // 0.0706 -0.0932 0.1161 0.0274 0.0070 -0.1938 -0.2352 0.6656 0.5761 0.1562
// 0.0807 0.2707 -0.0055
38.91858 // 0.0730 0.2251 -0.0491 0.1307 0.2641 -0.2326 -0.1612 0.6841 -0.0703 0.4693
// 0.0948 0.1810 -0.1991

43.29489 0.38521-0.29548 0.34917 // 0.0467 0.1038 0.1296 0.0588 -0.0869 -0.2936 0.4123 -0.5762 0.4620 -0.3344
// 0.1011 -0.0755 0.1727
39.36583 // 0.0231 0.1321 0.2855 -0.1150 0.0572 -0.0035 0.5415 0.1481 0.7038 -0.0367
// 0.2000 0.1641 0.0719

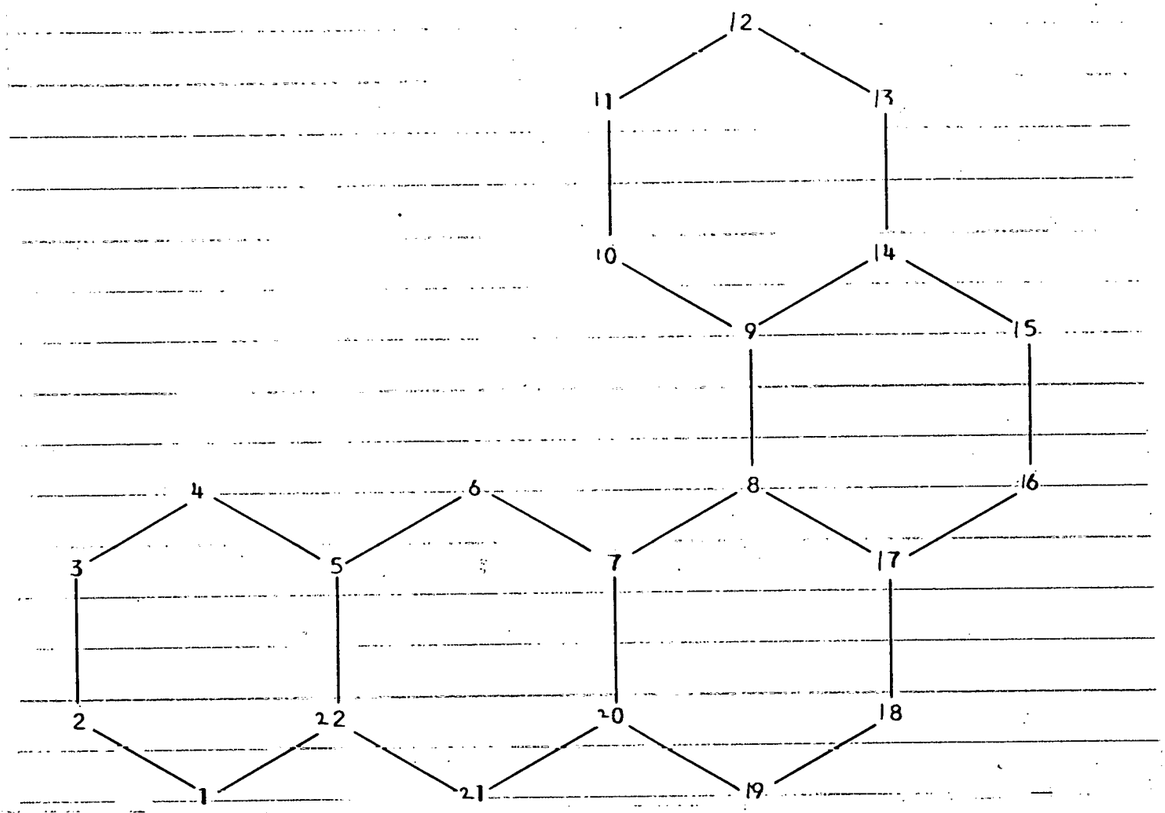
46.86021 0.03669-0.13450 0.01796 // 0.0102 -0.1069 -0.0273 -0.0032 -0.2066 -0.0117 0.1119 -0.3362 0.0068 0.7400
// 0.3930 0.1340 -0.3152
43.69704 // -0.0065 0.0650 -0.0433 -0.0527 -0.2513 0.0244 0.0906 -0.4520 -0.0335 0.5842
// 0.5133 -0.0233 -0.3291

50.19030 0.01731-0.09001-0.00305 // -0.0127 0.0053 -0.0622 0.0103 -0.1383 -0.0120 -0.0060 0.2528 -0.0343 0.0190
// 0.5793 -0.6989 0.2950
48.82871 // -0.0527 -0.0812 -0.1104 -0.0074 0.0035 0.0498 -0.1265 0.1813 -0.0288 -0.6046
// 0.5412 0.0674 -0.5130

51.34179 0.00339 0.01298-0.03722 // -0.0400 -0.0386 -0.1044 0.0125 0.0078 0.0030 -0.1146 0.0578 -0.0293 -0.5299
// 0.5439 0.2208 -0.5858
46.51950 // 0.0106 0.0135 0.0385 0.0097 0.1008 -0.0188 0.0056 -0.2910 0.0240 -0.0252
// -0.4204 0.7313 -0.4360

56.09040 0.00296 0.00873-0.03411 // 0.0003 0.0100 -0.0658 -0.0049 0.0019 0.0159 -0.1473 -0.0568 -0.1738 -0.0373
// 0.3878 0.5936 0.6603
54.67137 // -0.0018 0.0158 -0.0622 0.0001 -0.0049 -0.0029 -0.1435 -0.0648 -0.1820 -0.0489
// 0.4296 0.6019 0.6235

1,2 BENZTETRAPHENE IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	2.5980	3.4640	4.3300	4.3300	3.4640	3.4640
y	0.	0.5000	1.5000	2.0000	1.5000	2.0000	1.5000	2.0000	3.0000	3.5000	4.5000
	4.3300	5.1960	5.1960	6.0620	6.0620	5.1960	5.1960	4.3300	3.4640	2.5980	1.7320
	5.0000	4.5000	3.5000	3.0000	2.0000	1.5000	0.5000	0.	0.5000	0.	0.5000

1,2 BENZTETRAPHENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1.784190 1.666333 1.544112 1.421775 1.340843 1.299776 1.245338 1.199718 1.127892 1.089276 1.028176 0.844178 0.786319

0.115093 0.259740 0.203420 0.169278-0.212233-0.057565 0.381565 0.101329 0.244226 0.118818-0.277764 0.289638-0.141064
0.080760 0.214647 0.225610 0.271788-0.108125-0.298446 0.237115-0.243573 0.230678-0.111926-0.216960-0.205555-0.038088
0.081897 0.212356 0.229706 0.272284-0.049712-0.329000-0.103342-0.346148-0.071408-0.194005-0.204750-0.216372-0.174045
0.119716 0.251329 0.216758 0.170662 0.188182-0.130518-0.362260-0.105082-0.279817-0.011009 0.284657 0.283832-0.086184
0.217426 0.343635-0.180996-0.003961-0.215778-0.164630-0.310050-0.234879-0.141710-0.176654-0.079394-0.090555-0.106229
0.237019 0.181684 0.001801-0.175307 0.352954 0.137322-0.225694 0.045312 0.181242-0.024960-0.413759-0.380716 0.015755
0.342180 0.086855-0.206767-0.238833-0.257513-0.026151-0.017861-0.214856-0.339924-0.170218-0.077243-0.101032-0.133080
0.359033-0.144823-0.154329 0.033468 0.304702-0.127597 0.230891-0.018279 0.201447 0.147766 0.303736 0.282437 0.133767
0.301572-0.268257-0.158903-0.057457-0.209259-0.047030-0.329981-0.090600-0.303922-0.200583-0.042993-0.000149-0.154171
0.181533-0.184711 0.216331-0.230297 0.093834-0.263108 0.184188 0.205345-0.351288-0.182633-0.179292-0.209810-0.238157
0.113662-0.162716-0.260001-0.276691-0.125031-0.307922-0.094532-0.307216-0.001842-0.317807-0.058197-0.140113-0.320421
0.103196-0.168989 0.279326-0.227710-0.256376-0.142355-0.291185 0.103641 0.362750-0.014836 0.157020 0.153309 0.014483
0.136545-0.209289-0.279810-0.089558-0.243362-0.130768-0.243427-0.203962-0.277964-0.297573-0.112734-0.198251-0.318318
0.236705-0.294942 0.253360 0.093104-0.084990 0.314277 0.013959-0.302912-0.140420 0.199083-0.100261-0.065046 0.202649
0.172189-0.205982-0.083552-0.305608-0.088421-0.379134-0.066701-0.064759-0.094776-0.346255-0.217173-0.215890-0.355615
0.185821-0.163702-0.085303 0.399915-0.052090 0.165254-0.098800 0.250774 0.060705-0.415981 0.004285-0.033520-0.444654
0.288085-0.151221-0.255250-0.340203-0.004874-0.162252-0.057574-0.300915-0.154000-0.087774-0.215341-0.195769-0.055770
0.195611-0.043688-0.286094 0.166579-0.230367-0.280569-0.206436 0.125147-0.123264 0.331980-0.206216-0.209871 0.337785
0.195242-0.048684-0.290622-0.063927-0.339412-0.191581-0.168071-0.178314-0.265348-0.118063-0.288445-0.274681-0.168425
0.285752 0.160164-0.271829-0.267203-0.250558 0.043489 0.005330-0.288417-0.075758-0.265883 0.078977 0.087179-0.233795
0.198393 0.235222-0.058020-0.177568-0.311227-0.224085-0.179007-0.057063-0.145975-0.149706-0.397446-0.391759-0.160619
0.207452 0.359619 0.159692-0.005949-0.190310 0.228299 0.197796 0.339765-0.036124 0.179083 0.093927 0.077702 0.133492

OVERLAP EIGNVALUES AND EIGNVECTORS

0.752796 0.709820 0.689422 0.662156 0.645920 0.610599 0.558036 0.512887 0.480412

0.288938-0.023786-0.338416 0.129956 0.201262-0.146781-0.224043-0.230903-0.096455
-0.265862-0.324083-0.138230-0.319988-0.122866 0.234372-0.220872-0.173349-0.061116
-0.053725 0.387901 0.155993 0.313148-0.005808-0.245215-0.220493-0.173333-0.061157
-0.308863-0.113749-0.342585-0.113014-0.145646-0.179893-0.223038-0.230117-0.097400
-0.215776-0.262175 0.269851-0.166249-0.222548-0.047606-0.225564-0.373876-0.204000
-0.154403-0.040764-0.232974-0.166684-0.354312-0.104285-0.015185-0.213227-0.210046
0.321855 0.190098 0.020750 0.001300-0.296497 0.234791 0.231386-0.112278-0.366531
-0.166187-0.036989-0.182481-0.197777-0.313016-0.071649-0.155507-0.152312-0.397722
-0.316419 0.055338-0.305825 0.125361-0.215884 0.073901-0.190569 0.294254-0.315955
-0.297997-0.188477-0.123987-0.321452-0.023979-0.210619-0.202865-0.199902-0.142287
0.060116-0.286749 0.183104 0.293774 0.131799 0.271580-0.222835 0.149930-0.083998
-0.357638-0.140527-0.349506-0.095808-0.204362-0.249861-0.241932-0.144891-0.080695
0.259182 0.132652 0.252576-0.174876 0.179603 0.144832-0.269473 0.188312-0.120188
-0.119613-0.292222-0.041497-0.352753-0.057475-0.019795-0.302240-0.302999-0.242413
-0.029755 0.117076-0.002351-0.400878 0.103089-0.240605-0.115171 0.186955-0.161847
-0.088484-0.167497-0.055447-0.197815-0.116430-0.381442-0.055388-0.145537-0.178360
0.121805-0.296321 0.092280 0.124575 0.081910-0.404363 0.240379 0.151071-0.310331
0.163108-0.104856-0.231193-0.171596-0.287213-0.182549-0.247023-0.036915-0.188137
-0.280641 0.172551 0.177508 0.103655 0.356800 0.083262 0.254994-0.054993-0.185246
0.079169-0.285719-0.014090-0.046759-0.254221-0.322385-0.269247-0.182697-0.299785
-0.093623-0.066765-0.238810 0.159068 0.285492 0.197906 0.021792-0.235890-0.186368
0.008186-0.350880-0.282769-0.150888-0.183019-0.000712-0.226004-0.378057-0.199326

1,2 BENZTETRAPHENE IRM APPROXIMATION

ZEROTH-HAMILTONIAN EIGNVALUES AND EIGNVECTORS

33.02626 30.04755 26.47821 22.29099 19.10097 17.33038 14.80327 12.50888 8.52031 6.15851 2.05913 -3.86995 -20.41956

0.086164 0.201214 0.163702 0.141966 0.183284 0.050492 0.341920 0.092511 0.229963 0.113845 0.273932 0.315238 0.159081
0.060461 0.166281 0.181560 0.227937 0.093376 0.261777 0.212479 0.222377 0.217206 0.107241 0.213967 0.223724 0.042952
0.061313 0.164507 0.184856 0.228353 0.042931 0.288577 0.092605 0.316026 0.067237 0.185885 0.201925 0.235497 0.196274
0.089626 0.194698 0.174436 0.143127 0.162514 0.114482 0.324621 0.095937 0.263475 0.010548 0.280730 0.308919 0.097191
0.162776 0.266205 0.145656 0.003322 0.186346 0.144403 0.277836 0.214440 0.133434 0.169260 0.078298 0.098559 0.119797
0.177445 0.140746 0.001449 0.147023 0.304810 0.120450 0.202244 0.041369 0.170657 0.023915 0.408050 0.414366 0.017768
0.256173 0.067284 0.166396 0.200299 0.222388 0.022938 0.016005 0.196159 0.320072 0.163093 0.076177 0.109961 0.150076
0.268791 0.112191 0.124196 0.028068 0.263140 0.111920 0.206901 0.016689 0.189682 0.141581 0.299545 0.307401 0.150851
0.225772 0.207812 0.127877 0.048187 0.180715 0.041252 0.295695 0.082716 0.286173 0.192188 0.042400 0.000163 0.173861
0.135905 0.143091 0.174092 0.193140 0.081035 0.230781 0.165051 0.187476 0.330772 0.174989 0.176819 0.228354 0.268574
0.085093 0.126052 0.209236 0.232049 0.107976 0.270088 0.084710 0.280482 0.001735 0.304505 0.057394 0.152497 0.361344
0.077258 0.130911 0.224787 0.190971 0.221406 0.124864 0.260931 0.094622 0.341566 0.014215 0.154854 0.166859 0.016333
0.102224 0.162130 0.225177 0.075108 0.210166 0.114701 0.218135 0.186213 0.261731 0.285118 0.111179 0.215774 0.358973
0.177210 0.228484 0.203891 0.078083 0.073397 0.275663 0.012508 0.276552 0.132219 0.190750 0.098878 0.070795 0.228531
0.128910 0.159569 0.067238 0.256300 0.076360 0.332551 0.059770 0.059124 0.089241 0.331762 0.214177 0.234972 0.401034
0.139115 0.126816 0.068648 0.335391 0.044985 0.144950 0.088535 0.228951 0.057160 0.398570 0.004226 0.036483 0.501444
0.215675 0.117147 0.205412 0.285314 0.004209 0.142316 0.051592 0.274729 0.145006 0.084100 0.212370 0.213072 0.062892
0.146445 0.033844 0.230234 0.139703 0.198941 0.246096 0.184988 0.114256 0.116066 0.318085 0.203371 0.228421 0.380926
0.146168 0.037714 0.233878 0.053613 0.293115 0.168042 0.150609 0.162797 0.249852 0.113122 0.284465 0.298959 0.189936
0.213929 0.124075 0.218754 0.224092 0.216381 0.038145 0.004776 0.263318 0.071334 0.254755 0.077888 0.094884 0.263655
0.148527 0.182220 0.046691 0.148919 0.268775 0.196553 0.160408 0.052098 0.137450 0.143440 0.391962 0.426385 0.181133
0.155309 0.278588 0.128512 0.004989 0.164351 0.200249 0.177245 0.310198 0.034014 0.171587 0.092631 0.084570 0.150542

ZEROTH-HAMILTONIAN EIGNVALUES AND EIGNVECTORS

-24.67498 -30.71833 -33.85056 -38.33852 -41.19103 -47.92045 -59.54196 -71.36542 -81.26896

0.333017 -0.028233 -0.407576 0.159704 0.250422 -0.187842 -0.299916 -0.322417 -0.139161
-0.306420 -0.384664 -0.166479 -0.393236 -0.152877 -0.299935 -0.295671 -0.242053 -0.088175
-0.061920 0.460412 0.187873 0.384830 -0.007227 -0.313811 -0.295164 -0.242031 -0.088235
-0.355981 -0.135013 -0.412596 -0.138884 -0.181221 -0.230217 -0.298571 -0.321319 -0.140525
-0.248694 -0.311184 0.324999 -0.204305 -0.276907 -0.060923 -0.301953 -0.522056 -0.294322
-0.177958 -0.048384 -0.280585 -0.204840 -0.440856 -0.133458 -0.020328 -0.297736 -0.303046
0.370956 0.225634 0.024991 0.001598 -0.368919 0.300472 0.309746 -0.156777 -0.528816
-0.191540 -0.043903 -0.219773 -0.243051 -0.389472 -0.091693 -0.208171 -0.212678 -0.573816
-0.364690 0.065683 -0.368324 0.154058 -0.268616 0.094574 -0.255106 0.410876 -0.455846
-0.343458 -0.223709 -0.149326 -0.395035 -0.029836 -0.269538 -0.271566 -0.279129 -0.205285
0.069287 -0.340351 0.220524 0.361022 0.163993 0.347552 -0.298299 0.209353 -0.121188
-0.412197 -0.166796 -0.420932 -0.117740 -0.254280 -0.319757 -0.323864 -0.202316 -0.116423
0.298721 0.157449 0.304193 -0.214907 0.223472 0.185347 -0.360732 0.262947 -0.173402
-0.137860 -0.346848 -0.049978 -0.433502 -0.071514 -0.025332 -0.404595 -0.423087 -0.349742
-0.034294 0.138962 -0.002832 -0.492643 0.128269 -0.307912 -0.154174 0.261052 -0.233506
-0.101983 -0.198808 -0.066778 -0.243097 -0.144869 -0.488147 -0.074145 -0.203219 -0.257341
0.140387 -0.351713 0.111138 0.153091 0.101917 -0.517480 0.321785 0.210946 -0.447733
-0.187991 -0.124457 -0.278440 -0.210876 -0.357367 -0.233616 -0.330679 -0.051545 -0.271437
-0.323454 -0.204806 0.213784 0.127383 0.443952 0.106554 0.341350 -0.076789 -0.268275
-0.091247 -0.339129 -0.016969 -0.057462 -0.316317 -0.412569 -0.360429 -0.255106 -0.432514
-0.107906 -0.079246 -0.287614 -0.195480 0.355226 0.253268 0.029172 -0.329381 -0.268884
-0.009435 -0.416470 -0.340557 -0.185427 -0.227723 -0.000911 -0.302541 -0.527894 -0.287579

1,2 BENZTETRAPHENE IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.01176	0.73235	-0.01216	-0.35594	0.01817	0.07409	-0.01483	-0.02142	0.00064	0.01313	-0.01171	-0.01705	0.01123	0.01944	-0.00798
	-0.03465	0.00920	0.09348	-0.00923	-0.14917	0.01095	-0.54455								
2	0.73235	1.01298	0.58293	-0.01574	-0.21470	0.00314	-0.13972	0.00111	-0.04631	0.00314	0.02731	0.00076	-0.01902	-0.00433	0.06396
	0.00150	-0.06878	-0.00898	0.05778	0.00856	-0.20533	-0.00763								
3	-0.01216	0.58293	1.00915	0.73188	-0.00366	-0.20428	0.00720	0.06209	0.00663	-0.02490	0.01506	0.02432	-0.01446	-0.02607	0.00484
	0.02689	-0.00608	-0.10515	0.00879	0.13580	-0.00416	-0.21427								
4	-0.35594	-0.01574	0.73188	1.01556	0.54563	0.00357	-0.15372	-0.00084	0.04778	-0.00827	-0.02416	-0.00030	0.01380	0.00668	-0.05506
	-0.00451	0.05557	0.01178	-0.01339	-0.01580	0.07392	0.02145								
5	0.01817	-0.21470	-0.00366	0.54563	0.96138	0.59426	-0.00095	-0.11493	-0.01743	0.03174	-0.02102	-0.02960	0.01916	0.03311	-0.00224
	-0.01960	0.00516	0.13013	-0.01272	-0.17956	0.00898	0.48381								
6	0.07409	0.00314	-0.20428	0.00357	0.59426	1.04203	0.63382	-0.00625	-0.11192	0.06005	0.05374	-0.00859	-0.03078	-0.01200	0.12852
	0.00324	-0.15320	-0.00834	0.03572	0.01335	-0.36655	0.00178								
7	-0.01483	0.13972	0.00720	-0.15372	-0.00095	0.63382	0.97679	0.47447	-0.00400	-0.08335	-0.02579	0.06751	0.01486	-0.08291	-0.01174
	-0.00427	0.01815	-0.19441	0.00256	0.48759	0.00907	-0.18380								
8	-0.02142	0.00111	0.06209	-0.00084	-0.11493	-0.00625	0.47447	0.98451	0.49952	-0.00088	-0.15254	0.00058	0.04809	0.01031	-0.27354
	0.00936	0.57781	0.00706	-0.26476	0.01291	0.05246	-0.00478								
9	0.00064	-0.04631	0.00663	0.04778	-0.01743	-0.11192	-0.00400	0.49952	0.97801	0.57702	-0.00252	-0.24996	0.01613	0.52640	0.00088
	-0.22456	0.01957	-0.00721	-0.01216	-0.07626	0.01474	0.05334								
10	0.01313	0.00314	-0.02490	-0.00827	0.03174	0.06005	-0.08335	-0.00088	0.57702	1.01987	0.70948	-0.01802	-0.34313	0.02294	0.03767
	-0.01555	-0.13548	0.00570	0.10531	-0.01433	-0.03041	-0.00286								
11	-0.01171	0.02731	0.01506	-0.02416	-0.02102	0.05374	-0.02579	-0.15254	-0.00252	0.70948	1.00342	0.61004	-0.00805	-0.24539	-0.01234
	0.17755	0.00677	-0.02251	-0.00263	0.03709	0.02712	-0.02981								
12	-0.01705	0.00076	0.02432	-0.00030	-0.02960	-0.00859	0.06751	0.00058	-0.24996	-0.01802	0.61004	1.01414	0.71130	-0.00841	-0.15122
	0.01080	0.12938	-0.00043	-0.10650	0.00561	0.03662	-0.00101								
13	0.01123	-0.01902	-0.01446	0.01380	0.01916	-0.03078	0.01486	0.04809	0.01613	-0.34313	-0.00805	0.71130	1.00893	0.57135	0.01862
	-0.19858	-0.01493	0.05252	0.00913	-0.02743	-0.02592	0.02167								
14	0.01944	-0.00433	-0.02607	0.00668	0.03311	-0.01200	-0.08291	0.01031	0.52640	0.02294	-0.24539	-0.00841	0.57135	0.96645	0.52527
	-0.00972	-0.17861	-0.00620	0.12452	-0.00232	-0.04143	0.00403								
15	-0.00798	0.06396	0.00484	-0.05506	-0.00224	0.12852	-0.01174	-0.27354	0.00088	0.03767	-0.01234	-0.15122	0.01862	0.52527	1.01740
	0.75153	-0.01190	-0.13827	0.01364	0.10180	0.00559	-0.07525								
16	-0.03465	0.00150	0.02689	-0.00451	-0.01960	0.00324	-0.00427	0.00936	-0.22456	-0.01555	0.17755	0.01080	-0.19858	-0.00972	0.75153
	1.01590	0.52791	0.01095	-0.16202	-0.00613	0.07456	0.00139								
17	0.00920	-0.06878	-0.00608	0.05557	0.00516	-0.15320	0.01815	0.57781	0.01957	-0.13548	0.00677	0.12938	-0.01493	-0.17861	-0.01190
	0.52791	0.96951	0.50470	-0.01170	-0.15358	-0.01012	0.09172								
18	0.09348	-0.00898	-0.10515	0.01178	0.13013	-0.00834	-0.19441	0.00706	-0.00721	0.00570	-0.02251	-0.00043	0.05252	-0.00620	-0.13827
	0.01095	0.50470	1.01553	0.76853	-0.00947	-0.23820	0.00840								
19	-0.00923	0.05778	0.00879	-0.01339	-0.01272	0.03572	0.00256	-0.26476	-0.01216	0.10531	-0.00263	-0.10650	0.00913	0.12452	0.01364
	-0.16202	-0.01170	0.76853	1.01707	0.50569	0.01452	-0.11471								
20	-0.14917	0.00856	0.13580	-0.01580	-0.17956	0.01335	0.48759	0.01291	-0.07626	-0.01433	0.03709	0.00561	-0.02743	-0.00232	0.10180
	-0.00613	-0.15358	-0.00947	0.50569	0.96630	0.62411	-0.00346								
21	0.01095	-0.20533	-0.00416	0.07392	0.00898	-0.36655	0.00907	0.05246	0.01474	-0.03041	0.02712	0.03662	-0.02592	-0.04143	0.00559
	0.07456	-0.01012	-0.23820	0.01452	0.62411	1.02729	0.59703								
22	0.54455	-0.00763	-0.21427	0.02145	0.48381	0.00178	-0.18380	-0.00478	0.05334	-0.00286	-0.02981	-0.00101	0.02167	0.00403	0.07525
	0.00139	0.09172	0.00840	-0.11471	-0.00346	0.59703	0.96600								

1,2 BENZTETRAPHENE — IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
16	17	18	19	20	21	22									
1	0.79471	0.55902	0.09014	0.37359	0.03122	0.08800	0.00250	0.02291	0.00280	0.01405	0.01131	0.01813	0.01099	0.02076	0.00386
	-0.03741	0.00165	0.09878	0.00657	-0.15192	-0.07125	0.37084								
2	0.55902	0.78506	0.40187	0.09385	0.22502	0.03132	0.14875	0.00846	0.05073	0.00598	0.02851	0.00071	0.01974	0.00327	0.06887
	0.00419	-0.07371	-0.00851	0.06090	0.01544	-0.21068	-0.07219								
3	0.09014	0.40187	0.78111	0.55842	0.06815	0.20943	0.01426	0.06520	0.00558	0.02504	0.01562	0.02576	0.01430	0.02839	0.00401
	0.02949	-0.00432	-0.11227	-0.00135	0.14454	0.02384	-0.22444								
4	0.37359	0.09385	0.55842	0.79859	0.37222	0.07863	0.15698	0.01447	0.05299	0.01114	0.02422	0.00176	0.01352	0.00438	0.05924
	-0.00598	0.05884	0.00287	-0.01427	0.00125	0.08769	-0.02782								
5	0.03122	0.22502	0.06815	0.37222	0.69985	0.42287	0.06014	0.11457	0.00913	0.02902	0.02143	0.03101	0.01846	0.03696	0.00462
	-0.02281	0.00959	0.13873	0.00550	-0.19115	-0.05069	0.32014								
6	0.08800	0.03132	0.20943	0.07863	0.42287	0.83829	0.46588	0.08291	0.13152	0.04758	0.05095	0.01342	0.02932	0.00363	0.13871
	0.01223	-0.15689	0.01555	0.04732	-0.04606	-0.38935	-0.05802								
7	0.00250	0.14875	0.01426	0.15698	0.06014	0.46588	0.72305	0.30738	0.06748	0.10073	0.01625	0.07368	0.02117	0.08198	0.00582
	0.00264	-0.03225	-0.20646	-0.05326	0.32341	-0.05094	-0.19550								
8	0.02291	0.00846	0.06520	0.01447	0.11457	0.08291	0.30738	0.74331	0.33425	0.07354	0.15302	0.02297	0.05749	0.04104	0.29070
	-0.04992	0.41887	-0.05442	-0.28151	-0.03527	0.06345	0.01163								
9	0.00280	0.05073	0.00558	0.05299	0.00913	0.13152	0.06748	0.33425	0.72420	0.40596	0.06747	0.26232	0.03603	0.36409	0.05818
	-0.23836	-0.02931	-0.00061	0.00382	-0.07478	0.02340	0.05855								
10	0.01405	0.00598	0.02504	0.01114	0.02902	0.04758	0.10073	0.07354	0.40596	0.80014	0.53407	0.09415	0.35948	0.02863	0.04823
	0.00326	-0.13770	0.01586	0.11381	-0.00799	-0.02979	-0.00539								
11	0.01131	0.02851	0.01562	0.02422	0.02143	0.05095	0.01625	0.15302	0.06747	0.53407	0.77446	0.43109	0.08403	0.25783	0.01211
	0.18816	0.01059	-0.02636	-0.00473	0.04164	0.02567	-0.03142								
12	0.01813	0.00071	0.02576	0.00176	0.03101	0.01342	0.07368	0.02297	0.26232	0.09415	0.43109	0.78521	0.53630	0.07253	0.15306
	0.02068	0.13771	-0.00898	-0.11441	0.00441	0.03878	0.00029								
13	0.01099	0.01974	0.01430	0.01352	0.01846	0.02932	0.02117	0.05749	0.03603	0.35948	0.08403	0.53630	0.78964	0.39961	0.05716
	-0.20263	0.00357	0.05697	0.00184	-0.03096	-0.02529	0.02285								
14	0.02076	0.00327	0.02839	0.00438	0.03696	0.00363	0.08198	0.04104	0.36409	0.02863	0.25783	0.07253	0.39961	0.70587	0.35120
	-0.07870	-0.18982	0.01326	0.13297	-0.00025	-0.04580	0.00289								
15	0.00386	0.06887	0.00401	0.05924	0.00462	0.13871	0.00582	0.29070	0.05818	0.04823	0.01211	0.15306	0.05716	0.35120	0.79936
	0.57826	-0.08265	-0.13871	0.02836	0.10866	-0.00423	-0.08118								
16	0.03741	0.00419	0.02949	0.00598	0.02281	0.01223	0.00264	0.04992	0.23836	0.00326	0.18816	0.02068	0.20263	0.07870	0.57826
	0.79614	0.35394	-0.06227	-0.16411	0.01245	0.08018	-0.00483								
17	0.00165	0.07371	0.00432	0.05884	0.00959	0.15689	0.03225	0.41887	0.02931	0.13770	0.01059	0.13771	0.00357	0.18982	0.08265
	0.35394	0.71089	0.32910	-0.08310	-0.16310	0.01194	0.09819								
18	0.09878	0.00851	0.11227	0.00287	0.13873	0.01555	0.20646	0.05442	0.00061	0.01586	0.02636	0.00898	0.05697	0.01326	0.13871
	-0.06227	0.32910	0.79708	0.59650	-0.07943	-0.24496	0.01758								
19	0.00657	0.06090	0.00135	0.01427	0.00550	0.04732	0.05326	0.28151	0.00382	0.11381	0.00473	0.11441	0.00184	0.13297	0.02836
	-0.16411	0.08310	0.59650	0.79969	0.33027	-0.06557	-0.11538								
20	0.15192	0.01544	0.14454	0.00125	0.19115	0.04606	0.32341	0.03527	0.07478	0.00799	0.04164	0.00441	0.03096	0.00025	0.10866
	0.01245	-0.16310	-0.07943	0.33027	0.70584	0.45510	-0.06182								
21	0.07125	0.21068	0.02384	0.08769	0.05069	0.38935	0.05094	0.06345	0.02340	0.02979	0.02567	0.03878	0.02529	0.04580	0.00423
	0.08018	0.01194	-0.24496	-0.06557	0.45510	0.82408	0.42614								
22	0.37084	0.07219	0.22444	0.02782	0.32014	0.05802	0.19550	0.01163	0.05855	0.00539	0.03142	0.00029	0.02285	0.00289	0.08118
	-0.00483	0.09819	0.01758	-0.11538	-0.06182	0.42614	0.70440								

ENERGIES FOR 1,2 BENZTETRAPHENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF No SYMMETRY

JUMPS	11,12	10,12	9,12	11,13	8,12	10,13	7,12	6,12	5,12	4,12	3,12	2,12	1,12
XMOMNT	-0.12542	-0.79442	0.06011	-0.65281	-0.62406	0.38574	0.20917	-0.07727	0.07563	-0.02952	-0.00140	-0.00703	0.01437
YMOMNT	-0.54632	-0.48516	0.06591	-0.39645	-0.24975	-0.67143	-0.13034	-0.06434	0.08599	-0.01751	-0.00103	-0.00383	-0.00762
JUMP E	15.9291	20.0285	22.3903	22.4787	26.3788	26.5781	28.6732	31.2003	32.9709	36.1609	40.3482	43.9175	46.8962
DIAG E	26.5743	32.0052	33.3961	34.1489	39.5373	39.4628	41.8816	47.0551	46.6334	53.1343	57.3894	60.1123	62.8320
DIAG E	26.7092	32.3344	33.8142	34.2362	40.2474	39.7446	42.2786	47.3391	47.1191	53.4817	57.8734	60.7539	63.6491
CORRSP	26.0260	29.6708	32.9002	35.2399	39.4353	40.1772	41.9092	46.5453	47.5479	52.9052	57.6900	59.6185	64.4969
CORRSP	26.1918	30.2224	33.1543	35.5464	39.9106	40.5446	42.3251	47.0780	47.9202	53.2400	58.0931	60.1854	65.1688

FINAL EXCITED STATES OF No SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
26.02603	0.21539	-0.06692	-0.43605	//	0.9773	0.0406	-0.0679	-0.0774	0.0463	0.1680	0.0322	-0.0007	-0.0053	0.0335
				//	0.0007	-0.0098	0.0051							
15.59816				//	0.9567	-0.1021	-0.1253	-0.1622	-0.0213	0.1427	0.0707	0.0234	-0.0752	0.0145
				//	-0.0076	0.0001	-0.0006							
29.67083	0.25586	-0.40606	-0.19466	//	-0.1051	0.7352	-0.4106	-0.4857	0.1832	-0.0136	-0.0135	0.0519	0.0033	0.0506
				//	0.0600	0.0056	0.0000							
24.08213				//	0.1141	0.7307	0.1872	0.4550	0.0503	0.4500	0.0270	-0.0212	0.0355	0.0588
				//	0.0032	-0.0089	0.0016							
32.90017	0.77810	-0.53875	-0.51565	//	-0.0046	0.5643	0.7089	0.2899	0.0975	0.2674	0.0537	0.0381	0.0833	0.0439
				//	-0.0219	0.0105	0.0093							
26.26277				//	-0.0276	-0.5082	0.5324	0.2043	-0.4321	0.4503	0.0961	-0.0570	0.0516	-0.0779
				//	-0.0682	-0.0175	0.0104							
35.23987	1.07811	-0.59007	-0.60929	//	-0.0232	0.2111	-0.5505	0.7686	-0.0425	0.2276	-0.0170	-0.0427	-0.0597	0.0020
				//	0.0392	-0.0140	-0.0064							
32.35587				//	0.0733	-0.2475	-0.4582	0.7819	-0.1244	-0.1951	-0.1026	-0.1686	-0.1338	0.0066
				//	-0.0281	-0.0229	-0.0168							
39.43530	0.02348	-0.11720	0.01632	//	-0.1085	-0.2764	-0.0373	-0.0421	0.8402	0.4369	-0.0654	0.0247	-0.0360	0.0429
				//	0.0528	0.0316	-0.0066							
36.52145				//	-0.1243	-0.2672	-0.1304	0.1097	0.6343	0.3502	0.4890	0.2112	-0.2504	-0.0879
				//	0.0586	0.0398	-0.0050							
40.17716	0.85478	0.58739	-0.39401	//	-0.0878	-0.0530	-0.0140	-0.2209	-0.4137	-0.6430	-0.5883	-0.0605	0.0468	0.0088
				//	-0.0619	-0.0077	-0.0034							
29.47123				//	-0.2110	0.0462	-0.6306	-0.2679	-0.3711	0.5722	-0.1072	0.0135	-0.0399	-0.0680
				//	0.0285	0.0053	-0.0095							

BENZTETRAPHENE IRM APPROXIMATIO N (cont.)

```
41.90916 0.99937 0.63825-0.39166 //  -0.1094 -0.0586 -0.0339 -0.1775 -0.2319  0.4618  0.7449 -0.1262 -0.3283 -0.0049
                                 //  -0.0203 -0.0770 -0.0057
36.74748                         //  -0.0442  0.2150 -0.0295 -0.0671 -0.4250 -0.0439  0.7531 -0.1486 -0.3291  0.0463
                                 //  -0.0321 -0.0750 -0.0112

46.54531 0.03500-0.13208 0.01544 //   0.0146  0.0070  0.0379  0.0254 -0.0399 -0.0157 -0.1224  0.7589 -0.6132 -0.0863
                                 //  -0.0584  0.1335 -0.0150
42.33010                         //   0.0240  0.0789  0.0227  0.1235 -0.2448 -0.1452 -0.0542  0.8759 -0.1396 -0.2880
                                 //  -0.0684  0.1275  0.0533

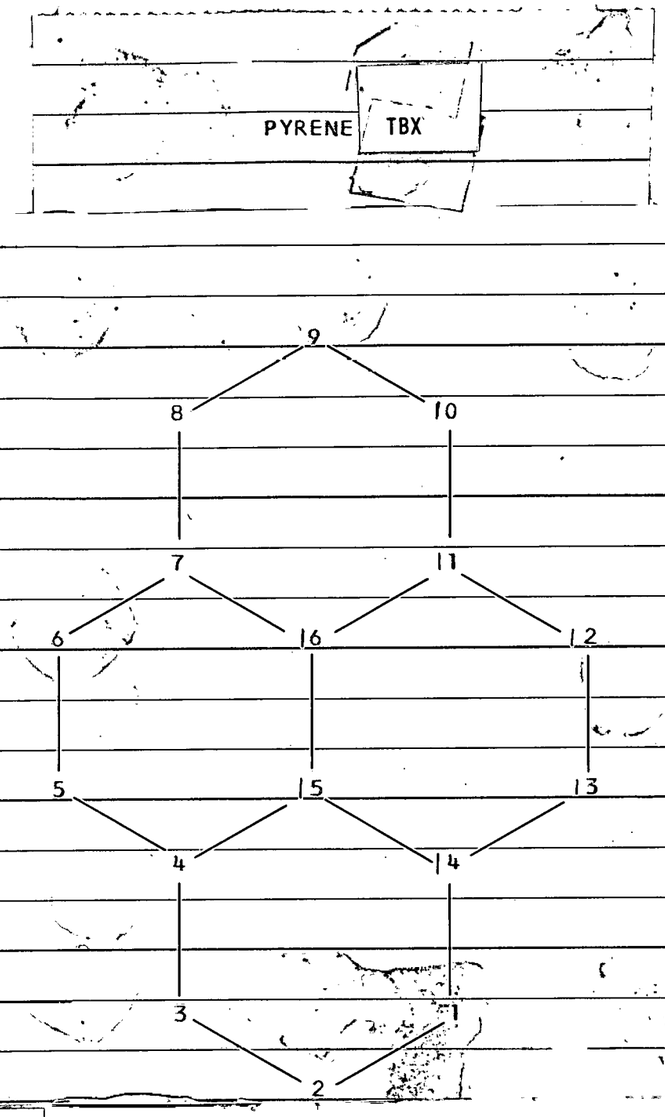
47.54786 0.26698 0.26471-0.24893 //  -0.0299 -0.0846 -0.1020 -0.0165 -0.0919  0.1721  0.2564  0.5998  0.6963 -0.1405
                                 //   0.0792  0.0093  0.0822
43.11075                         //   0.0362 -0.0233 -0.1845  0.0897 -0.0338 -0.0552  0.3818  0.1109  0.8713 -0.1152
                                 //   0.1017 -0.0612  0.0848

52.90525 0.00831 0.06028 0.00778 //  -0.0218 -0.0687  0.0051  0.0144 -0.0825 -0.0133  0.0212  0.1500  0.0245 -0.9353
                                 //   0.2566 -0.0450 -0.1462
49.39901                         //  -0.0272 -0.0935 -0.0056  0.0392 -0.0928  0.0293 -0.0230  0.3037 -0.0328 -0.8531
                                 //   0.3575  0.0308 -0.1708

57.69000 0.01277 0.07215 0.00092 //   0.0149 -0.0132  0.0652 -0.0074 -0.0708  0.0194 -0.0168 -0.0906 -0.0730 -0.2106
                                 //   0.8862  0.3817  0.0267
54.18791                         //   0.0261  0.0202  0.0582  0.0193 -0.0670 -0.0379 -0.0086 -0.1545 -0.0716 -0.2635
                                 //   0.7722  0.5285  0.1229

59.61853 0.00366 0.03091-0.02205 //  -0.0067 -0.0052 -0.0421  0.0018 -0.0140  0.0047  0.0697 -0.0803  0.0385  0.2078
                                 //  -0.2985  0.7675  0.5136
56.33063                         //  -0.0177 -0.0137 -0.0465 -0.0057  0.0059  0.0183  0.0580 -0.0477  0.0490  0.2818
                                 //  -0.4265  0.6332  0.6415

64.49689 0.00222-0.01416 0.02465 //  -0.0050 -0.0077  0.0230  0.0044  0.0064 -0.0160 -0.0643  0.0313 -0.0996  0.0542
                                 //   0.1906 -0.4877  0.8408
62.46215                         //  -0.0042 -0.0146  0.0156  0.0010  0.0027  0.0095 -0.0642  0.0501 -0.1123  0.0540
                                 //   0.2612 -0.5391  0.7864
```



ATOMIC COORDINATES

x	2.6346	1.7691	0.9036	0.9036	0.	0.	0.9036	0.9036	
y	0.5000	0.	0.5000	1.5210	2.0430	3.0430	3.5650	4.5860	

1.7691	2.6346	2.6346	3.5382	3.5382	2.6346	1.7691	1.7691	
5.0860	4.5860	3.5650	3.0430	2.0430	1.5210	2.0210	3.0650	

PYRENE X TBX APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 AA	10SS	11 AS	12 SA	13 AS	14 AA	15 SS	16 AS
1.601039	1.482199	1.419194	1.330202	1.285991	1.239430	1.219266	1.113596	0.886402	0.780732	0.760568	0.714007	0.669796	0.580804	0.517800	0.398960
0.179205	-0.298913	-0.162253	-0.307338	-0.302001	0.011875	-0.184224	0.363963	-0.363963	-0.184224	-0.011875	0.302001	-0.307338	-0.162253	-0.298913	-0.179205
0.147328	-0.306306	-0.000000	-0.459909	0.000000	0.024506	-0.415155	-0.000000	0.000000	0.415155	0.024507	0.000000	-0.459909	-0.000000	0.306306	0.147328
0.179205	-0.298913	0.162253	-0.307338	0.302001	0.011874	-0.184224	-0.363963	0.363963	-0.184224	-0.011875	-0.302001	-0.307338	0.162253	-0.298913	-0.179205
0.303568	-0.291431	0.289543	0.051691	0.367677	-0.013671	0.264680	-0.176006	-0.176006	-0.264680	-0.013671	0.367677	-0.051691	-0.289543	0.291431	0.303568
0.190803	-0.089009	0.373950	0.137992	0.153651	0.413088	0.126443	0.294198	-0.294198	0.126444	-0.413088	-0.153651	0.137992	0.373950	-0.089009	-0.190803
0.190803	0.089009	0.373950	0.137992	-0.153651	0.413088	-0.126445	0.294198	0.294198	0.126444	0.413088	-0.153651	-0.137992	-0.373950	-0.089009	0.190803
0.303568	0.291431	0.289543	0.051690	-0.367677	-0.013672	-0.264680	-0.176006	0.176006	-0.264680	0.013671	0.367677	0.051690	0.289543	0.291431	-0.303568
0.179205	0.298913	0.162253	-0.307338	-0.302001	0.011875	0.184224	-0.363963	-0.363963	-0.184224	0.011875	-0.302001	0.307338	-0.162253	-0.298913	0.179205
0.147328	0.306306	0.000000	-0.459909	0.000000	0.024507	0.415155	0.000000	0.000000	0.415155	-0.024506	0.000000	-0.459909	-0.000000	0.306306	-0.147328
0.179205	0.298913	-0.162253	-0.307338	0.302001	0.011875	0.184224	0.363963	0.363963	-0.184224	0.011875	0.302001	0.307338	0.162253	-0.298913	0.179205
0.303568	0.291431	-0.289543	0.051691	0.367677	-0.013672	-0.264680	-0.176006	-0.176006	-0.264679	0.013671	-0.367677	0.051691	-0.289543	0.291431	-0.303568
0.190803	0.089009	-0.373950	0.137992	0.153651	0.413088	-0.126444	-0.294198	-0.294198	0.126444	0.413088	0.153651	-0.137992	0.373950	-0.089009	0.190803
0.190803	-0.089009	-0.373950	0.137992	-0.153651	0.413088	0.126443	-0.294198	0.294198	0.126444	-0.413088	0.153651	0.137992	-0.373950	-0.089009	-0.190803
0.303568	-0.291431	-0.289543	0.051691	-0.367677	-0.013671	0.264679	0.176006	0.176006	-0.264679	-0.013671	-0.367677	-0.051691	0.289543	0.291431	0.303568
0.396165	-0.204374	-0.000000	0.236944	-0.000000	-0.396812	0.296112	0.000000	0.000000	0.296111	0.396812	0.000000	0.236944	0.000000	-0.204374	-0.396165
0.396164	0.204374	-0.000000	0.236944	-0.000000	-0.396813	-0.296111	-0.000000	0.000000	0.296112	-0.396812	0.000000	-0.236944	0.000000	-0.204374	0.396165

PYRENE X TBX APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 AA	10 SS	11 AS	12 SA	13 AS	14 AA	15 SS	16 AS
28.17381	24.41544	22.16757	18.62975	16.69011	14.49778	13.49640	7.65561	-9.61797	-21.07744	-23.62592	-30.06055	-36.99851	-54.16663	-69.89341	-136.06268
0.141628	-0.245523	-0.136198	-0.266476	-0.266311	0.010666	-0.166839	0.344900	-0.386582	-0.208495	-0.013616	0.357402	-0.375530	-0.212901	-0.415398	-0.283717
0.116435	-0.251595	-0.000000	-0.398762	0.000000	0.022012	-0.375977	-0.000000	0.000000	0.469850	0.028101	0.000000	0.561954	-0.000000	0.425671	0.233249
0.141628	-0.245523	0.136198	-0.266475	0.266311	0.010666	-0.166839	-0.344900	0.386582	-0.208495	-0.013616	-0.357402	-0.375530	0.212901	-0.415398	-0.283717
0.239914	-0.239377	0.243048	0.044818	0.324226	-0.012280	0.239702	-0.166788	-0.186945	-0.299550	-0.015676	0.435126	-0.063160	-0.379925	0.405000	0.480609
0.150794	-0.073111	0.313901	0.119645	0.135493	0.371049	0.114511	0.278789	-0.312481	0.143102	-0.473667	-0.181838	0.168610	0.490681	-0.123695	-0.302079
0.150794	0.073111	0.313901	0.119645	-0.135492	0.371049	-0.114512	0.278789	0.312482	0.143102	0.473668	-0.181837	-0.168610	-0.490681	-0.123695	0.302079
0.239914	0.239377	0.243048	0.044818	-0.324226	-0.012280	-0.239702	-0.166788	0.186944	-0.299550	0.015676	0.435126	0.063160	0.379925	0.405000	-0.480609
0.141628	0.245523	0.136198	-0.266476	-0.266311	0.010667	0.166839	-0.344900	-0.386582	-0.208495	0.013616	-0.357402	0.375530	-0.212901	-0.415398	0.283717
0.116435	0.251595	0.000000	-0.398762	0.000000	0.022013	0.375977	0.000000	0.000000	0.469850	-0.028100	0.000000	-0.561954	-0.000000	0.425671	-0.233249
0.141628	0.245523	-0.136198	-0.266475	0.266311	0.010666	0.166839	0.344900	0.386582	-0.208495	0.013616	0.357402	0.375530	0.212901	-0.415398	0.283717
0.239914	0.239377	-0.243048	0.044818	0.324226	-0.012281	-0.239702	0.166788	-0.186944	-0.299550	0.015676	-0.435126	0.063160	-0.379925	0.405000	-0.480609
0.150794	0.073111	-0.313901	0.119645	0.135493	0.371049	-0.114512	-0.278789	-0.312482	0.143102	0.473667	0.181837	-0.168610	0.490681	-0.123695	0.302079
0.150794	-0.073111	-0.313901	0.119645	-0.135493	0.371049	0.114511	-0.278789	0.312481	0.143102	-0.473667	0.181838	0.168610	-0.490680	-0.123695	-0.302079
0.239914	-0.239377	-0.243048	0.044818	-0.324226	-0.012279	0.239702	0.166788	0.186945	-0.299550	-0.015676	-0.435126	-0.063160	0.379925	0.405000	0.480609
0.313094	-0.167870	-0.000000	0.205441	-0.000000	-0.356429	0.268168	0.000000	0.000000	0.335123	0.455005	0.000000	0.289517	0.000000	-0.284018	-0.627207
0.313094	0.167870	-0.000000	0.205441	-0.000000	-0.356430	-0.268167	-0.000000	0.000000	0.335123	-0.455004	0.000000	-0.289517	0.000000	-0.284018	0.627207

PYRENE X

TBX TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1.00000	0.67216	-0.00000	-0.29075	0.00000	0.17236	-0.00000	-0.12833	0.00000	0.14203	0.00000	-0.19886	-0.00000	0.59756	0.00000	-0.02616
2	0.67216	1.00000	0.67216	0.00000	-0.10092	-0.00000	0.08246	0.00000	-0.06471	0.00000	0.08246	0.00000	-0.10092	-0.00000	-0.24132	-0.00000
3	-0.00000	0.67216	1.00000	0.59756	-0.00000	-0.19886	0.00000	0.14203	-0.00000	-0.12833	0.00000	0.17236	0.00000	-0.29075	0.00000	-0.02616
4	-0.29075	0.00000	0.59756	1.00000	0.46360	0.00000	-0.16070	-0.00000	0.08246	0.00000	-0.07920	-0.00000	0.01165	0.00000	0.55174	0.00000
5	0.00000	-0.10092	0.00000	0.46360	1.00000	0.80992	-0.00000	-0.19886	0.00000	0.17236	0.00000	-0.00121	-0.00000	0.01165	0.00000	-0.22253
6	0.17236	-0.00000	-0.19886	0.00000	0.80992	1.00000	0.46360	0.00000	-0.10092	-0.00000	0.01165	0.00000	-0.00121	-0.00000	-0.22253	0.00000
7	-0.00000	0.08246	0.00000	-0.16070	-0.00000	0.46360	1.00000	0.59756	-0.00000	-0.29075	-0.00000	0.01165	0.00000	-0.07920	0.00000	0.55174
8	-0.12833	0.00000	0.14203	-0.00000	-0.19886	0.00000	0.59756	1.00000	0.67216	0.00000	-0.29075	-0.00000	0.17236	0.00000	-0.02616	-0.00000
9	0.00000	-0.06471	-0.00000	0.08246	0.00000	-0.10092	-0.00000	0.67216	1.00000	0.67216	-0.00000	-0.10092	0.00000	0.08246	0.00000	-0.24132
10	0.14203	0.00000	-0.12833	0.00000	0.17236	-0.00000	-0.29075	0.00000	0.67216	1.00000	0.59756	0.00000	-0.19886	-0.00000	-0.02616	0.00000
11	0.00000	0.08246	0.00000	-0.07920	0.00000	0.01165	-0.00000	-0.29075	-0.00000	0.59756	1.00000	0.46360	-0.00000	-0.16070	0.00000	0.55174
12	-0.19886	0.00000	0.17236	-0.00000	-0.00121	0.00000	0.01165	-0.00000	-0.10092	0.00000	0.46360	1.00000	0.80992	0.00000	-0.22253	-0.00000
13	-0.00000	-0.10092	0.00000	0.01165	-0.00000	-0.00121	0.00000	0.17236	0.00000	-0.19886	-0.00000	0.80992	1.00000	0.46360	-0.00000	-0.22253
14	0.59756	-0.00000	-0.29075	0.00000	0.01165	-0.00000	-0.07920	-0.00000	0.08246	-0.00000	-0.16070	0.00000	0.46360	1.00000	0.55174	0.00000
15	0.00000	-0.24132	0.00000	0.55174	0.00000	-0.22253	0.00000	-0.02616	-0.00000	-0.02616	0.00000	-0.22253	-0.00000	0.55174	1.00000	0.48220
16	-0.02616	-0.00000	-0.02616	0.00000	-0.22253	0.00000	0.55174	-0.00000	-0.24132	0.00000	0.55174	-0.00000	-0.22253	0.00000	0.48220	1.00000

PYRENE X

TBX DENSITY.BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.77545	0.49497	-0.05826	-0.27257	0.01919	0.16814	-0.00232	-0.12704	-0.00303	0.13930	0.01481	-0.18980	-0.05008	0.43532	-0.03546	-0.02136
2	0.49497	0.75542	0.49497	-0.04021	-0.09329	0.00535	0.07938	-0.00303	-0.06321	-0.00303	0.07938	0.00535	-0.09329	-0.04021	-0.22380	0.01055
3	-0.05826	0.49497	0.77545	0.43532	-0.05008	-0.18980	0.01481	0.13930	-0.00303	-0.12704	-0.00232	0.16814	0.01919	-0.27257	-0.03546	-0.02136
4	-0.27257	-0.04021	0.43532	0.73298	0.31132	-0.04420	-0.14654	0.01481	0.07938	-0.00232	-0.07362	0.01234	0.01642	-0.03507	0.38633	-0.03153
5	0.01919	-0.09329	-0.05008	0.31132	0.77561	0.62834	-0.04420	-0.18980	0.00535	0.16814	0.01234	-0.00325	-0.00285	0.01642	-0.03496	-0.20688
6	0.16814	0.00535	-0.18980	-0.04420	0.62834	0.77561	0.31132	-0.05008	-0.09329	0.01919	0.01642	-0.00285	-0.00325	0.01234	-0.20688	-0.03496
7	-0.00232	0.07938	0.01481	-0.14654	-0.04420	0.31132	0.73298	0.43532	-0.04021	-0.27257	-0.03507	0.01642	0.01234	-0.07362	-0.03153	0.38633
8	-0.12704	-0.00303	0.13930	0.01481	-0.18980	-0.05008	0.43532	0.77545	0.49497	-0.05826	-0.27257	0.01919	0.16814	-0.00232	-0.02136	-0.03546
9	-0.00303	-0.06321	-0.00303	0.07938	0.00535	-0.09329	-0.04021	0.49497	0.75542	0.49497	-0.04021	-0.09329	0.00535	0.07938	0.01055	-0.22380
10	0.13930	-0.00303	-0.12704	-0.00232	0.16814	0.01919	-0.27257	-0.05826	0.49497	0.77545	0.43532	-0.05008	-0.18980	0.01481	-0.02136	-0.03546
11	0.01481	0.07938	-0.00232	-0.07362	0.01234	0.01642	-0.03507	-0.27257	-0.04021	0.43532	0.73298	0.31132	-0.04420	-0.14654	-0.03153	0.38633
12	-0.18980	0.00535	0.16814	0.01234	-0.00325	-0.00285	0.01642	0.01919	-0.09329	-0.05008	0.31132	0.77561	0.62834	-0.04420	-0.20688	-0.03496
13	-0.05008	-0.09329	0.01919	0.01642	-0.00285	-0.00325	0.01234	0.16814	0.00535	-0.18980	-0.04420	0.62834	0.77561	0.31132	-0.03496	-0.20688
14	0.43532	-0.04021	-0.27257	-0.03507	0.01642	0.01234	-0.07362	-0.00232	0.07938	0.01481	-0.14654	-0.04420	0.31132	0.73298	0.38633	-0.03153
15	-0.03546	-0.22380	-0.03546	0.38633	-0.03496	-0.20688	-0.03153	-0.02136	0.01055	-0.02136	-0.03153	-0.20688	-0.03496	0.38633	0.73474	0.33436
16	-0.02136	0.01055	-0.02136	-0.03153	-0.20688	-0.03496	0.38633	-0.03546	-0.22380	-0.03546	0.38633	-0.03496	-0.20688	-0.03153	0.33436	0.73474

ENERGIES FOR PyRENE X ,TBX APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OFSA SYMMETRY

JUMP	7, 9	8,10	2, 9	5,11	3,10	6,12	4,12	5,13	1,12
XMOMNT	0.66501	-0.66703	0.01422	0.49558	0.03574	-0.49729	-0.24865	0.24981	0.00911
YMOMNT	-0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.00000
JUMP E	23.1144	28.7330	34.0334	40.3160	43.2450	44.5583	48.6903	53.6886	58.2344
DIAG E	33.0998	37.8587	47.7980	52.1391	57.0744	55.9778	63.6666	68.5234	73.1595
DIAG E	33.8008	37.1991	48.4317	52.5543	56.8112	55.4159	62.8206	69.5371	73.0791
CORRSP	27.8415	39.8472	45.9128	50.9671	56.1253	59.0385	64.2105	70.7547	74.5995
CORRSP	28.2207	39.7499	46.2593	51.0173	56.0924	58.8011	63.5520	71.6827	74.2743

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	E	XMOMNT	YMOMNT	//	STATE COMPOSITION								
27.84147	0.03437	0.17038	-0.00000	//	0.8155	0.5285	-0.1132	0.0026	-0.0698	-0.0336	-0.1358	-0.1338	-0.0225
24.75813				//	0.9459	-0.2220	-0.0667	0.1006	0.0424	0.0632	-0.1800	0.0425	-0.0377
39.84717	0.83975	-0.70397	-0.00000	//	-0.5117	0.8063	0.1660	0.1716	-0.0021	0.1564	-0.0712	-0.0341	-0.0189
29.48206				//	0.2247	0.9242	-0.1553	-0.0246	-0.1338	-0.0505	-0.0122	-0.2223	-0.0233
45.91284	0.00006	0.00552	-0.00000	//	0.1107	-0.0519	0.8238	-0.4669	-0.1325	0.1855	-0.1695	-0.0535	0.0696
39.18755				//	0.0810	0.1481	0.8851	-0.2745	0.0345	-0.0529	-0.2627	0.0971	0.1739
50.96708	0.06397	0.17180	0.00000	//	0.1167	-0.0345	0.4798	0.5864	0.2875	-0.5378	0.0109	0.1293	0.1497
49.15981				//	-0.0589	0.1553	0.1468	0.8163	0.3903	-0.2775	-0.0646	0.2191	0.0547
56.12531	0.37120	-0.39437	-0.00000	//	-0.0095	0.1665	-0.0768	-0.5054	0.7984	-0.1636	0.0862	0.1963	-0.0255
50.39900				//	0.0636	0.0114	-0.1912	-0.4663	0.5448	-0.6491	0.0722	0.1193	-0.0650
59.03849	1.83249	0.85434	-0.00000	//	0.1745	-0.1392	0.0805	0.3866	0.4106	0.7668	-0.0839	0.1469	-0.0950
53.84358				//	-0.0876	0.1622	-0.0834	-0.1368	0.5906	0.6504	-0.2346	0.1976	-0.2728
64.21050	0.03639	-0.11545	0.00000	//	0.1197	0.1209	0.1065	-0.0163	-0.1270	0.1545	0.9123	0.1784	0.2352
62.81096				//	0.1770	0.0717	0.1636	-0.0221	0.1915	0.2387	0.8692	0.1197	0.2697
70.75471	0.13717	0.21352	-0.00000	//	0.0401	0.0709	-0.0463	-0.0529	-0.2661	-0.0299	-0.2126	0.9324	-0.0460
68.82053				//	-0.0078	0.1334	-0.2135	-0.0982	-0.3092	0.0002	-0.0999	0.8724	0.2454
74.59950	0.02335	0.08579	-0.00000	//	-0.0278	0.0019	-0.1578	-0.0281	0.0437	0.1059	-0.2359	0.0006	0.9512
72.05562				//	-0.0409	-0.0325	-0.2247	-0.0361	0.2211	0.1110	-0.2616	-0.2502	0.8679

ENERGIES FOR PYRENE X , TBX APPROXIMATION 1.7

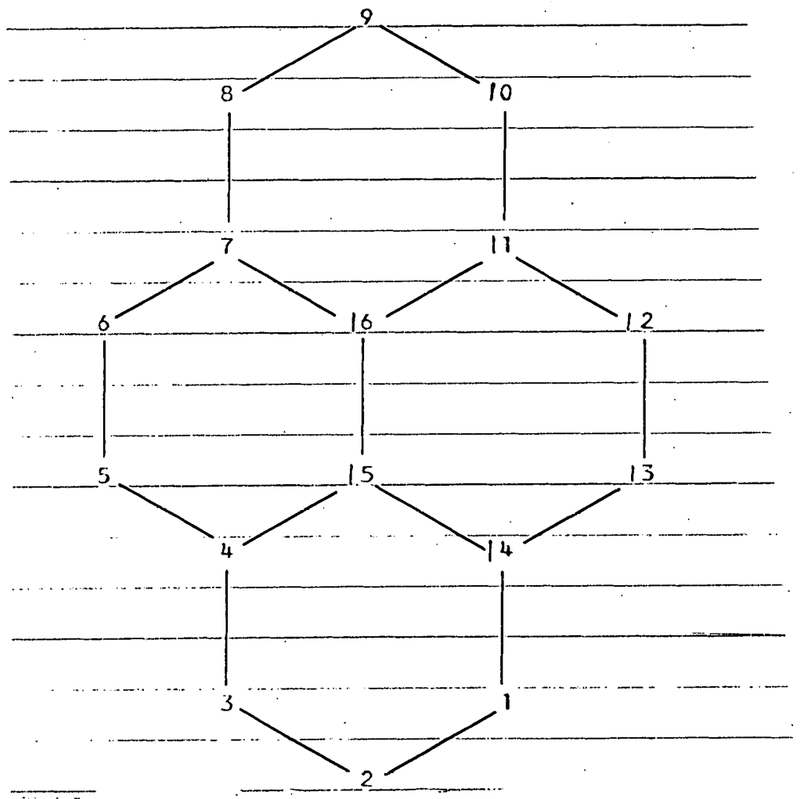
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	8, 9	3, 9	7,10	6,11	4,11	2,10	5,12	6,13	1,11	4,13
XMOMNT	-0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
YMOMNT	1.13636	-0.05574	0.78112	-0.51807	0.04805	-0.03460	0.25036	-0.04844	0.01018	0.23106
JUMP E	17.2736	31.7855	34.5738	38.1237	42.2557	45.4929	46.7507	51.4963	51.7997	55.6283
DIAG E	30.7043	44.9721	46.1102	52.6799	58.5342	60.2004	59.4631	67.2044	66.3240	74.8770
DIAG E	30.8202	45.4844	46.0357	52.7403	58.3105	60.0586	59.2559	67.8634	66.8659	75.2519
CORRSP	28.5346	43.7456	45.8400	52.9273	57.7403	60.3015	60.0603	66.6221	68.4637	76.8338
CORRSP	28.6910	44.2141	45.9225	53.0724	57.4391	60.1212	59.9634	69.0771	67.0388	77.1471

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
28.53461	0.84090	-0.00000	0.83246	//	0.9482	-0.0689	-0.2755	-0.0838	0.0442	0.0594	0.0709	-0.0318	-0.0087	-0.0411
13.48713				//	0.9478	0.0025	-0.1100	0.2102	0.0509	-0.0220	0.1752	-0.0417	0.0196	-0.0974
43.74562	0.17444	-0.00000	-0.30622	//	-0.0223	0.9019	-0.3447	0.1499	0.0277	0.1142	-0.1319	-0.0552	0.0979	-0.0307
31.58513				//	-0.0015	0.6854	0.4613	0.4460	0.1184	0.0215	-0.2295	-0.1032	0.1249	0.1585
45.83999	1.02044	0.00000	0.72352	//	0.2379	0.3560	0.8038	-0.3378	0.1238	-0.0984	-0.0741	-0.0881	0.0851	0.1048
32.32584				//	0.1945	-0.3320	0.7762	-0.4058	0.0816	0.0112	0.0420	-0.0456	0.0229	0.2713
52.92733	2.12075	-0.00000	0.97069	//	0.1758	0.0353	0.3525	0.8651	-0.1593	0.0854	0.1568	0.0322	-0.1618	0.1031
43.38109				//	-0.1292	-0.4563	0.2154	0.7152	-0.2374	0.1245	0.1772	0.1455	-0.2948	0.0762
57.74031	0.01770	0.00000	0.08490	//	-0.0428	-0.1173	0.0100	0.1430	0.8492	0.4242	-0.0677	0.0784	0.1570	0.1653
54.30993				//	-0.1997	-0.0860	0.0588	0.1749	0.5040	-0.3807	0.5783	-0.0605	0.4033	-0.1381
60.30150	0.00588	0.00000	-0.04788	//	-0.0749	0.0666	0.0468	-0.2562	-0.2704	0.7131	0.5557	-0.0739	-0.0776	0.1423
49.72153				//	-0.0399	0.0803	-0.1605	-0.0407	0.2402	0.8042	0.3578	-0.0737	0.0909	0.3441
60.06035	0.03019	0.00000	0.10872	//	-0.0479	0.1236	-0.0498	0.0240	0.2871	-0.4599	0.7933	0.0956	0.1769	-0.1254
56.70200				//	-0.0371	0.3865	0.1427	-0.1873	-0.6016	-0.0694	0.6325	-0.0217	-0.1321	-0.0953
66.62208	0.00676	-0.00000	0.04886	//	0.0545	-0.0230	0.0682	0.0191	-0.2426	0.1277	-0.0668	0.7054	0.6394	-0.0736
66.61059				//	0.0456	-0.0136	0.0637	0.0043	-0.2291	0.1464	-0.0640	0.7348	0.6077	-0.0802
68.46365	0.03416	0.00000	0.10832	//	-0.0097	-0.1391	-0.0184	0.1356	-0.1272	-0.0004	-0.0020	-0.6713	0.6972	0.0942
65.26490				//	-0.0156	-0.2158	-0.0694	0.1138	-0.4353	0.0238	-0.1140	-0.6175	0.5821	0.1104

PYRENE IRX



ATOMIC COORDINATES

x	2.6346	1.7691	0.9036	0.9036	0.	0.	0.9036	0.9036
y	0.5000	0.	0.5000	1.5210	2.0430	3.0430	3.5650	4.5860
	1.7691	2.6346	2.6346	3.5382	3.5382	2.6346	1.7691	1.7691
	5.0860	4.5860	3.5650	3.0430	2.0430	1.5210	2.0210	3.0650

PYRENE X IRX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	3 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 AA	10 SS	11 AS	12 SA	13 AS	14 AA	15 SS	16 AS
1.743501	1.543908	1.444302	1.318246	1.231471	1.178431	1.145341	1.046598	0.831596	0.748856	0.738042	0.699767	0.665307	0.607039	0.563260	0.494321
0.186953	-0.309230	0.152703	0.301497	-0.311758	0.043161	0.166117	0.375854	-0.358424	-0.192259	-0.026365	0.292259	0.311789	-0.156009	0.292099	-0.169925
0.158249	-0.319780	0.000000	0.448088	-0.000000	0.071689	0.410014	0.000000	-0.000000	0.428406	0.027817	0.000000	-0.458063	-0.000000	-0.292408	0.137962
0.186953	-0.309230	-0.152703	0.301497	0.311757	0.043160	0.166117	-0.375854	0.358425	-0.192258	-0.026365	-0.292259	0.311789	0.156010	0.292099	-0.169925
0.300046	-0.278550	-0.281359	-0.052181	0.355871	-0.036597	-0.277291	-0.176360	-0.177663	-0.255571	0.000822	0.373810	0.038658	-0.302972	-0.300988	0.306633
0.198615	-0.083301	-0.384082	-0.188042	0.161751	0.393304	-0.136186	0.278623	-0.299946	0.115382	-0.414452	-0.157638	-0.143031	0.365881	0.084801	-0.179681
0.198615	0.083301	-0.384082	-0.188043	-0.161751	0.393304	0.136186	0.278623	0.299946	0.115380	0.414453	-0.157638	0.143031	-0.365881	0.084801	0.179681
0.300046	0.278550	-0.281359	-0.052181	-0.355871	-0.036597	0.277291	-0.176360	0.177663	-0.255571	-0.000824	0.373811	-0.038658	0.302971	-0.300988	-0.306633
0.186953	0.309230	-0.152703	0.301497	-0.311758	0.043160	-0.166117	-0.375854	-0.358424	-0.192259	0.026364	-0.292260	-0.311789	-0.156010	0.292099	0.169925
0.158249	0.319780	0.000000	0.448089	-0.000000	0.071690	-0.410014	-0.000000	-0.000000	0.428406	-0.027814	0.000000	0.458063	-0.000000	-0.292408	-0.137962
0.186953	0.309230	0.152703	0.301497	0.311757	0.043161	-0.166117	0.375854	0.358425	-0.192259	0.026364	0.292259	-0.311789	0.156010	0.292099	0.169925
0.300046	0.278550	0.281359	-0.052181	0.355871	-0.036597	0.277291	0.176360	-0.177663	-0.255570	-0.000824	-0.373811	-0.038658	-0.302971	-0.300988	-0.306634
0.198615	0.083301	0.384082	-0.188042	0.161751	0.393304	0.136186	-0.278624	-0.299946	0.115379	0.414453	0.157638	0.143031	0.365881	0.084801	0.179681
0.198615	-0.083301	0.384082	-0.188043	-0.161750	0.393304	-0.136186	-0.278624	0.299946	0.115382	-0.414452	0.157638	-0.143031	-0.365881	0.084801	-0.179681
0.300046	-0.278550	0.281359	-0.052181	-0.355871	-0.036597	-0.277291	0.176360	0.177663	-0.255570	0.000822	-0.373811	0.038658	0.302971	-0.300988	0.306633
0.382234	-0.193484	0.000000	-0.203100	0.000000	-0.423178	-0.292958	0.000000	-0.000000	0.292031	0.392802	0.000000	-0.227702	0.000000	0.219736	-0.413035
0.382234	0.193484	0.000000	-0.203100	0.000000	-0.423179	0.292958	0.000000	-0.000000	0.292034	-0.392800	0.000000	0.227702	-0.000000	0.219736	0.413036

PYRENE X IRX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 AA	10 SS	11 AS	12 SA	13 AS	14 AA	15 SS	16 AS
32.00401	26.43923	23.08687	18.11806	14.10643	11.36346	9.52356	3.34145	-15.19791	-25.16920	-26.63768	-32.19952	-37.75469	-48.58219	-58.19155	-76.77332
0.141586	-0.248869	0.127063	0.262594	-0.280934	0.039759	0.155219	0.367392	-0.393044	-0.222171	-0.030689	0.349375	0.382252	-0.200236	0.389202	-0.241687
0.119848	-0.257360	0.000000	0.390270	-0.000000	0.066039	0.383117	0.000000	-0.000000	0.495058	0.032379	0.000000	-0.561584	-0.000000	-0.389614	0.196225
0.141587	-0.248869	-0.127063	0.262594	0.280934	0.039759	0.155219	-0.367391	0.393044	-0.222170	-0.030689	-0.349375	0.382252	0.200237	0.389202	-0.241687
0.227236	-0.224178	-0.234116	-0.045448	0.320686	-0.033713	-0.259101	-0.172389	-0.194823	-0.295333	0.000957	0.446863	0.047395	-0.388860	-0.401047	0.436129
0.150418	-0.067041	-0.319591	-0.163779	0.145758	0.362307	-0.127252	0.272350	-0.328917	0.133334	-0.482430	-0.188445	-0.175356	0.469604	0.112992	-0.255563
0.150418	0.067041	-0.319591	-0.163779	-0.145758	0.362307	0.127252	0.272350	0.328917	0.133331	0.482431	-0.188445	0.175356	-0.469604	0.112992	0.255563
0.227236	0.224178	-0.234116	-0.045448	-0.320686	-0.033713	0.259101	-0.172389	0.194823	-0.295333	-0.000959	0.446863	-0.047395	0.388860	-0.401047	-0.436129
0.141587	0.248869	-0.127063	0.262594	-0.280934	0.039759	-0.155219	0.367391	-0.393044	-0.222171	0.030688	-0.349375	-0.382252	-0.200236	0.389202	0.241687
0.119848	0.257360	0.000000	0.390270	-0.000000	0.066040	-0.383117	-0.000000	-0.000000	0.495059	-0.032375	0.000000	0.561584	-0.000000	-0.389614	-0.196225
0.141587	0.248869	0.127063	0.262594	0.280934	0.039759	-0.155219	0.367391	0.393044	-0.222171	0.030688	0.349375	-0.382252	0.200236	0.389202	0.241687
0.227236	0.224178	0.234116	-0.045448	0.320686	-0.033713	0.259101	0.172389	-0.194823	-0.295333	-0.000959	-0.446864	-0.047395	-0.388860	-0.401047	-0.436129
0.150418	0.067041	0.319591	-0.163779	0.145759	0.362307	0.127252	-0.272350	-0.328917	0.133330	0.482430	0.188445	0.175356	0.469604	0.112992	0.255563
0.150418	-0.067041	0.319591	-0.163779	-0.145758	0.362307	-0.127252	-0.272350	0.328917	0.133334	-0.482429	0.188445	-0.175356	-0.469604	0.112992	-0.255563
0.227236	-0.224178	0.234116	-0.045448	-0.320686	-0.033712	-0.259101	0.172389	0.194824	-0.295333	0.000957	-0.446864	0.047395	0.388860	-0.401047	0.436129
0.289480	-0.155716	0.000000	-0.176894	0.000000	-0.389826	-0.273740	0.000000	-0.000000	0.337466	0.457229	0.000000	-0.279162	0.000000	0.292783	-0.587466
0.289480	0.155716	0.000000	-0.176894	0.000000	-0.389827	0.273740	0.000000	-0.000000	0.337469	-0.457226	0.000000	0.279162	-0.000000	0.292783	0.587466

PYRENE X

IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1.02542	0.66954	-0.02169	-0.28268	-0.00761	0.18155	0.00081	-0.12579	0.00156	0.14378	-0.00597	-0.20444	0.00981	0.59810	-0.00625	-0.03841
2	0.66954	1.00267	0.66954	-0.00628	-0.10767	0.00913	0.09219	0.00156	-0.07881	0.00156	0.09219	0.00913	-0.10767	-0.00628	-0.23820	-0.00522
3	-0.02169	0.66954	1.02542	0.59810	0.00981	-0.20444	-0.00597	0.14378	0.00156	-0.12579	0.00081	0.18155	-0.00761	-0.28268	0.00625	-0.03841
4	-0.28268	-0.00628	0.59810	0.97096	0.46494	-0.00918	-0.15354	-0.00597	0.09219	0.00081	-0.08802	-0.01464	-0.00102	0.02332	0.55180	0.01129
5	-0.00761	-0.10767	0.00981	0.46494	1.01259	0.80599	-0.00918	-0.20444	0.00913	0.18155	-0.01464	0.01005	0.00734	-0.00102	0.00737	-0.21669
6	0.18155	0.00913	-0.20444	-0.00918	0.80599	1.01259	0.46494	0.00981	-0.10767	-0.00761	-0.00102	0.00734	0.01005	-0.01464	-0.21669	0.00737
7	0.00081	0.09219	-0.00597	-0.15354	-0.00918	0.46494	0.97096	0.59810	-0.00628	-0.28268	0.02332	-0.00102	-0.01464	-0.08802	0.01129	0.55180
8	-0.12579	0.00156	0.14378	-0.00597	-0.20444	0.00981	0.59810	1.02542	0.66954	-0.02169	-0.28268	-0.00761	0.18155	0.00081	-0.03841	0.00625
9	0.00156	-0.07881	0.00156	0.09219	0.00913	-0.10767	-0.00628	0.66954	1.00267	0.66954	-0.00628	-0.10767	0.00913	0.09219	-0.00522	-0.23820
10	0.14378	0.00156	-0.12579	0.00081	0.18155	-0.00761	-0.28268	-0.02169	0.66954	1.02542	0.59810	0.00981	-0.20444	-0.00597	-0.03841	0.00625
11	-0.00597	0.09219	0.00081	-0.08802	-0.01464	-0.00102	0.02332	-0.28268	-0.00628	0.59810	0.97096	0.46494	-0.00918	-0.15354	0.01129	0.55180
12	-0.20444	0.00913	0.18155	-0.01464	0.01005	0.00734	-0.00102	-0.00761	-0.10767	0.00981	0.46494	1.01259	0.80599	-0.00918	-0.21669	0.00737
13	0.00981	-0.10767	-0.00761	-0.00102	0.00734	0.01005	-0.01464	0.18155	0.00913	-0.20444	-0.00918	0.80599	1.01259	0.46494	0.00737	-0.21669
14	-0.59810	-0.00628	-0.28268	0.02332	-0.00102	-0.01464	-0.08802	0.00081	0.09219	-0.00597	-0.15354	-0.00918	0.46494	0.97096	0.55180	0.01129
15	0.00625	-0.23820	0.00625	0.55180	0.00737	-0.21669	0.01129	-0.03841	-0.00522	-0.03841	0.01129	-0.21669	0.00737	0.55180	0.97939	0.48634
16	-0.03841	-0.00522	-0.03841	0.01129	-0.21669	0.00737	0.55180	0.00625	-0.23820	0.00625	0.55180	0.00737	-0.21669	0.01129	0.48634	0.97939

PYRENE X

IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.81331	0.49119	-0.10687	-0.29740	0.01626	0.19232	0.00067	-0.13529	-0.00288	0.15350	0.01263	-0.20927	-0.05775	0.43529	-0.04940	-0.03445
2	0.49119	0.76810	0.49119	-0.06860	-0.10693	0.01907	0.09768	-0.00288	-0.08395	-0.00288	0.09768	0.01907	-0.10693	-0.06860	-0.24977	0.00943
3	-0.10687	0.49119	0.81331	0.43529	-0.05775	-0.20927	0.01263	0.15350	-0.00288	-0.13529	0.00067	0.19232	0.01626	-0.29740	-0.04940	-0.03445
4	-0.29740	-0.06860	0.43529	0.71919	0.30405	-0.07492	-0.16172	0.01263	0.09768	0.00067	-0.08848	0.00056	0.00559	-0.03028	0.38559	-0.03775
5	0.01626	-0.10693	-0.05775	0.30405	0.79792	0.63019	-0.07492	-0.20927	0.01907	0.19232	0.00056	0.00992	0.00769	0.00559	-0.04690	-0.22799
6	0.19232	0.01907	-0.20927	-0.07492	0.63019	0.79792	0.30405	-0.05775	-0.10693	0.01626	0.00559	0.00769	0.00992	0.00056	-0.22799	-0.04690
7	0.00067	0.09768	0.01263	-0.16172	-0.07492	0.30405	0.71919	0.43529	-0.06860	-0.29740	-0.03028	0.00559	0.00056	-0.08848	-0.03775	0.38559
8	-0.13529	-0.00288	0.15350	0.01263	-0.20927	-0.05775	0.43529	0.81331	0.49119	-0.10687	-0.29740	0.01626	0.19232	0.00067	-0.03445	-0.04940
9	-0.00288	-0.08395	-0.00288	0.09768	0.01907	-0.10693	-0.06860	0.49119	0.76810	0.49119	-0.06860	-0.10693	0.01907	0.09768	0.00942	-0.24977
10	0.15350	-0.00288	-0.13529	0.00067	0.19232	0.01626	-0.29740	-0.10687	0.49119	0.81331	0.43529	-0.05775	-0.20927	0.01263	-0.03445	-0.04940
11	0.01263	0.09768	0.00067	-0.08848	0.00056	0.00559	-0.03028	-0.29740	-0.06860	0.43529	0.71919	0.30405	-0.07492	-0.16172	-0.03775	0.38559
12	-0.20927	0.01907	0.19232	0.00056	0.00992	0.00769	0.00559	0.01626	-0.10693	-0.05775	0.30405	0.79792	0.63019	-0.07492	-0.22799	-0.04690
13	-0.05775	-0.10693	0.01626	0.00559	0.00769	0.00992	0.00056	0.19232	0.01907	-0.20927	-0.07492	0.63019	0.79792	0.30405	-0.04690	-0.22799
14	0.43529	-0.06860	-0.29740	-0.03028	0.00559	0.00056	-0.08848	0.00067	0.09768	0.01263	-0.16172	-0.07492	0.30405	0.71919	0.38559	-0.03775
15	-0.04940	-0.24977	-0.04940	0.38559	-0.04690	-0.22799	-0.03775	-0.03445	0.00942	-0.03445	-0.03775	-0.22799	-0.04690	0.38559	0.73247	0.33575
16	-0.03445	0.00943	-0.03445	-0.03775	-0.22799	-0.04690	0.38559	-0.04940	-0.24977	-0.04940	0.38559	-0.04690	-0.22799	-0.03775	0.33575	0.73247

ENERGIES FOR "PYRENE" X , IRX - APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	7, 9	8,10	5,11	2, 9	6,12	3,10	4,12	5,13	7,14
XMOMNT	-0.67429	-0.64260	-0.51836	0.03729	0.54786	-0.03900	0.17105	-0.23096	-0.02939
YMOMNT	-0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.00000
JUMP E	24.7215	28.5106	40.7441	41.6371	43.5630	48.2561	50.3176	51.8611	58.1058
DIAG E	34.4270	36.8499	52.4697	55.7414	54.9929	62.4719	64.6101	67.3579	70.3602
DIAG E	35.2106	36.2171	52.8646	56.3549	54.4459	62.2385	63.6539	68.3726	70.5687
CORRSP	28.5844	39.5817	48.3600	55.7937	58.1912	61.1043	64.6318	70.1661	72.8682
CORRSP	28.7567	39.6093	48.4512	55.9760	58.2031	60.9820	64.1091	70.9350	72.9044

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
28.58444	0.01268	-0.10215	-0.00000	//	0.7598	-0.6105	0.0035	0.0389	0.0095	-0.0584	-0.1455	-0.1452	0.0516
25.79680				//	0.8863	0.3835	-0.0998	-0.0133	-0.1003	0.0515	-0.1756	0.0859	0.0803
39.58173	0.82464	-0.69994	-0.00000	//	0.6061	0.7490	0.1633	0.0823	0.1893	-0.0090	0.0251	0.0296	-0.0271
28.97157				//	-0.4001	0.8787	-0.0153	-0.0873	-0.0289	0.0953	0.0590	0.2153	-0.0132
48.36002	0.01781	0.09307	0.00000	//	-0.0205	0.0323	0.7390	-0.3496	-0.5028	-0.1740	-0.1254	-0.1052	0.1428
50.38302				//	0.0369	0.1336	0.6064	0.3403	-0.5308	-0.3286	0.1837	-0.2716	0.0050
55.79369	0.05743	-0.15557	0.00000	//	-0.0065	0.0178	0.0575	0.8326	-0.4867	-0.1400	0.2025	-0.0712	-0.0230
44.66759				//	0.0106	0.0775	-0.5966	0.6834	0.0070	-0.0906	0.3269	-0.1229	-0.2016
58.19115	1.88071	0.87179	0.00000	//	-0.1217	-0.2199	0.6420	0.2895	0.5491	0.3033	0.1959	0.0825	-0.0459
50.67039				//	0.1347	0.1178	0.4648	0.2861	0.7897	0.0956	0.1760	-0.0682	-0.0416
61.10434	0.48907	-0.43384	-0.00000	//	0.1717	-0.0325	-0.0382	-0.1297	-0.4132	0.7316	0.1950	0.4229	-0.1684
57.86951				//	-0.0583	-0.1413	0.1587	0.4316	-0.2420	0.7277	-0.1058	0.3427	0.2202
64.63183	0.06719	0.15636	0.00000	//	0.0894	-0.0900	0.0061	-0.2627	0.0023	-0.3643	0.7948	-0.0116	-0.3876
62.34189				//	0.1731	-0.0930	0.0921	-0.3100	-0.1469	0.2515	0.6859	0.2325	-0.4975
70.16613	0.05025	-0.12977	-0.00000	//	0.0403	-0.0816	0.0242	0.0469	0.0462	-0.3972	-0.0184	0.8569	0.3072
69.25412				//	0.0193	-0.1199	0.0500	0.1421	0.0563	-0.5179	0.0846	0.8101	0.1667
72.86825	0.00025	0.00891	0.00000	//	0.0306	0.0266	-0.0980	-0.0663	0.0090	0.1700	0.4615	-0.2044	0.8370
71.67519				//	0.0339	0.0070	-0.1183	-0.1579	0.0195	0.0451	0.5526	-0.1580	0.7919

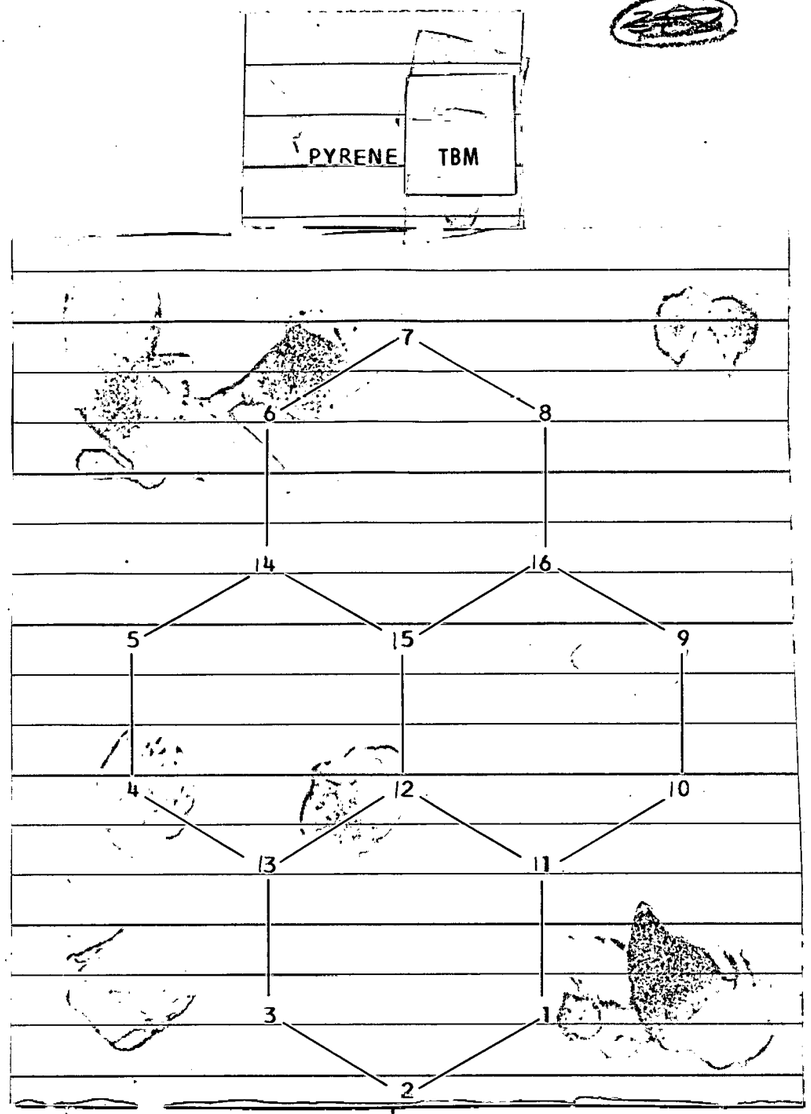
ENERGIES FOR PYRENE X , IRX APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	8,9	7,10	6,11	3,9	4,11	5,12	6,13	2,10	8,14	4,13
XMOMNT	0.00000	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000
YMOMNT	1.14749	-0.81949	0.51255	0.01300	-0.07384	0.26188	0.07781	-0.00202	0.05899	0.19263
JUMP E	18.5394	34.6928	38.0011	38.2848	44.7557	46.3059	49.1181	51.6084	51.9236	55.8727
DIAG E	31.6349	46.3762	52.0218	51.8380	60.2800	58.6834	65.4121	66.6779	62.5049	75.4430
DIAG E	31.7546	46.4065	52.1829	52.3572	60.0318	58.3703	66.1928	66.5389	62.0503	75.8146
CORRSP	29.2242	45.7066	53.2810	50.8581	60.1233	57.1429	66.7706	65.5049	64.5719	77.6884
CORRSP	29.3163	45.8256	53.3147	51.2508	59.8618	56.8316	67.2490	65.6768	64.3725	78.0005

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
29.22418	0.81810	0.00000	0.81135	//	0.9435	0.2934	-0.0959	0.0439	-0.0386	0.0728	0.0267	0.0412	0.0379	-0.0440
14.19688				//	0.9449	0.1179	0.2051	-0.0119	-0.0634	0.1836	0.0305	-0.0281	0.0140	-0.1068
45.70663	1.12567	0.00000	-0.76101	//	-0.2157	0.8504	0.4291	-0.1395	0.0661	-0.0061	-0.0719	0.0683	-0.0327	-0.1066
32.15086				//	-0.1978	0.8766	0.2654	-0.0913	0.0734	0.0168	-0.1098	-0.0652	-0.0537	-0.2979
53.28101	2.55262	0.00000	1.06141	//	0.2075	-0.3935	0.8678	-0.1043	0.0144	0.1364	-0.0175	0.0668	0.0273	0.1175
31.74753				//	-0.0691	-0.2392	0.6639	-0.5329	-0.1511	-0.2672	0.0887	0.0269	-0.3259	0.0647
50.85810	0.00001	-0.00000	-0.00174	//	-0.0600	0.0629	0.1165	0.9329	0.0867	0.2682	-0.1505	-0.0622	-0.0490	-0.0137
46.64587				//	-0.1702	-0.1759	0.6206	0.4904	0.1736	0.4657	-0.1657	0.1144	0.1451	0.0770
60.12330	0.00256	0.00000	-0.03162	//	0.0928	-0.0511	0.0648	0.0911	0.7898	-0.5608	0.0709	-0.1531	0.0381	-0.0897
58.30775				//	0.1464	0.1245	0.0631	0.0015	0.5389	-0.4659	-0.0710	0.5569	0.2213	0.2957
57.14290	0.00137	0.00000	0.02371	//	-0.0580	0.0021	-0.1205	-0.1944	0.4523	0.6507	0.0024	-0.0724	0.5532	-0.0707
53.01938				//	-0.0892	0.1349	-0.1082	-0.4488	-0.2291	0.5564	0.1963	0.4958	0.2271	0.2504
66.77059	0.00244	-0.00000	0.02932	//	-0.0307	0.0674	0.1299	0.1167	-0.2682	-0.0814	0.7032	-0.5423	0.2936	-0.1036
65.85797				//	-0.0494	0.0934	0.1990	0.1951	-0.2075	-0.2470	0.7141	-0.1727	0.5154	0.0416
65.50491	0.00570	-0.00000	-0.04522	//	-0.0581	0.0493	-0.0187	0.1782	0.0055	-0.1523	0.4154	0.7401	0.3601	-0.2981
55.36065				//	0.0256	0.1989	-0.0146	0.4715	-0.5172	-0.1608	0.0690	0.3808	-0.4802	-0.2522
64.57193	0.00477	0.00000	-0.04169	//	0.0110	-0.0017	0.0452	0.0682	-0.2822	-0.3687	-0.5433	-0.1116	0.6854	-0.0125
63.48682				//	0.0115	-0.0130	0.0760	-0.0480	-0.5276	-0.2417	-0.6195	-0.0007	0.5199	0.0278



ATOMIC COORDINATES

x	3.4640	2.5980	1.7320	0.8660	0.8660	1.7320	2.5980	3.4640
y	0.5000	0.	0.5000	2.0000	3.0000	4.5000	5.0000	4.5000

	4.3300	4.3300	3.4640	2.5980	1.7320	1.7320	2.5980	3.4640
	3.0000	2.0000	1.5000	2.0000	1.5000	3.5000	3.0000	3.5000

PYRENE — TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 AA	10 SS	11 AS	12 SA	13 AS	14 AA	15 SS	16 AS
1.624939	1.493617	1.444728	1.332528	1.307760	1.246799	1.217050	1.109830	0.890168	0.782948	0.753200	0.692239	0.667471	0.555270	0.506382	0.375059
0.174322	-0.297042	0.163989	0.310774	0.295499	0.000000	-0.186541	-0.368494	-0.368494	-0.186541	-0.000000	0.295499	0.310774	-0.163989	0.297042	0.174322
0.137693	-0.297046	-0.000000	0.461331	-0.000000	0.000000	-0.424237	-0.000000	0.000000	0.424238	0.000000	0.000000	-0.461331	-0.000000	-0.297046	-0.137693
0.174322	-0.297042	-0.163989	0.310774	-0.295500	0.000000	-0.186541	0.368494	0.368494	-0.186541	-0.000000	0.295499	0.310774	0.163989	0.297042	0.174322
0.198234	-0.099017	-0.368488	-0.122731	-0.163999	0.408248	0.138453	-0.295500	-0.295500	0.138453	0.408248	0.164000	-0.122731	0.368488	0.099017	0.198234
0.198234	0.099017	-0.368488	-0.122731	0.164000	0.408248	-0.138453	-0.295500	0.295500	0.138453	-0.408248	0.163999	0.122731	-0.368488	0.099017	-0.198234
0.174322	0.297042	-0.163989	0.310774	0.295499	-0.000000	0.186541	0.368494	-0.368494	-0.186541	-0.000000	0.295499	-0.310774	-0.163989	0.297042	-0.174322
0.137693	0.297046	0.000000	0.461331	-0.000000	-0.000000	0.424237	-0.000000	0.000000	0.424237	0.000000	-0.000000	0.461331	-0.000000	-0.297046	0.137693
0.174322	0.297041	0.163990	0.310774	-0.295499	-0.000000	0.186541	-0.368494	0.368494	-0.186541	0.000000	-0.295499	-0.310774	0.163989	0.297042	-0.174322
0.198234	0.099017	0.368488	-0.122731	-0.163999	0.408248	-0.138453	0.295500	-0.295500	0.138453	-0.408248	-0.164000	0.122731	0.368488	0.099017	-0.198234
0.198234	-0.099017	0.368488	-0.122731	0.164000	0.408248	0.138453	0.295500	0.295500	0.138453	0.408248	-0.164000	-0.122731	-0.368488	0.099017	0.198234
0.303713	-0.297043	0.295506	-0.042630	0.368489	-0.000000	0.260204	-0.163988	0.163988	-0.260204	-0.000000	0.368489	0.042630	0.295506	-0.297043	-0.303713
0.396468	-0.198034	0.000000	-0.245462	0.000000	-0.408249	0.276905	-0.000000	0.000000	0.276906	-0.408248	-0.000000	-0.245462	0.000000	0.198034	0.396468
0.303713	-0.297043	-0.295506	-0.042630	-0.368489	-0.000000	-0.260204	0.163988	-0.163988	-0.260204	-0.000000	-0.368489	0.042630	-0.295506	-0.297043	-0.303713
0.303713	0.297043	-0.295506	-0.042630	0.368489	-0.000000	-0.260204	0.163988	0.163988	-0.260204	0.000000	-0.368489	-0.042630	0.295506	0.297043	0.303713
0.396468	0.198034	0.000000	-0.245462	0.000000	-0.408248	-0.276906	-0.000000	0.000000	0.276906	0.408248	0.000000	0.245462	-0.000000	0.198034	-0.396468
0.303713	0.297043	0.295506	-0.042630	-0.368489	0.000000	-0.260204	-0.163988	-0.163988	-0.260204	-0.000000	0.368489	-0.042630	-0.295506	-0.297043	0.303713

PYRENE — TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 AA	10 SS	11 AS	12 SA	13 AS	14 AA	15 SS	16 AS
28.86327	24.80251	23.10221	18.72823	17.66155	14.85565	13.38433	7.42696	-9.25981	-20.80537	-24.59127	-33.36591	-37.38892	-60.10863	-73.15741	125.04999
0.136752	-0.243051	0.136434	0.269220	0.258400	0.000000	-0.169091	-0.349785	-0.390566	-0.210818	-0.000000	-0.355164	0.380390	-0.220071	0.417425	0.284644
0.108017	-0.243055	-0.000000	0.399645	-0.000000	0.000000	-0.384552	-0.000000	0.000000	0.479449	0.000000	0.000000	-0.564673	-0.000000	-0.417431	-0.224833
0.136752	-0.243051	-0.136434	0.269219	-0.258400	0.000000	-0.169091	0.349785	0.390566	-0.210818	-0.000000	0.355164	0.380390	0.220071	0.417425	0.284644
0.155511	-0.081019	-0.306571	-0.106321	-0.143410	0.365617	0.125502	-0.280498	-0.313200	0.156472	0.470402	0.197113	-0.150223	0.494506	0.139146	0.323689
0.155511	0.081020	-0.306571	-0.106320	0.143410	0.365617	-0.125501	-0.280498	0.313200	0.156472	-0.470402	0.197113	0.150224	-0.494506	0.139146	-0.323689
0.136752	0.243051	-0.136434	0.269220	0.258400	-0.000000	0.169091	0.349785	-0.390566	-0.210818	-0.000000	0.355164	-0.380390	-0.220071	0.417425	-0.284644
0.108017	0.243055	0.000000	0.399645	-0.000000	-0.000000	0.384552	-0.000000	0.000000	0.479449	0.000000	-0.000000	0.564673	-0.000000	-0.417431	0.224833
0.136752	0.243051	0.136434	0.269219	-0.258400	-0.000000	0.169091	-0.349785	0.390565	-0.210818	0.000000	-0.355164	-0.380390	0.220071	0.417425	-0.284644
0.155511	0.081020	0.306571	-0.106320	-0.143410	0.365617	-0.125501	0.280498	-0.313200	0.156472	-0.470402	-0.197113	0.150223	0.494506	0.139146	-0.323689
0.155511	-0.081020	0.306571	-0.106320	0.143410	0.365617	0.125502	0.280498	0.313200	0.156471	0.470402	-0.197113	-0.150223	-0.494506	0.139146	0.323689
0.238257	-0.243053	0.245852	-0.036930	0.322226	-0.000000	0.235863	-0.155662	0.173810	-0.294067	-0.000000	0.442891	0.052179	0.396565	-0.417427	-0.495923
0.311021	-0.162039	0.000000	-0.212641	0.000000	-0.365617	0.251002	-0.000000	0.000000	0.312944	-0.470402	-0.000000	-0.300447	0.000000	0.278292	0.647379
0.238257	-0.243052	-0.245852	-0.036930	-0.322226	-0.000000	0.235863	0.155662	-0.173810	-0.294067	-0.000000	-0.442891	0.052179	-0.396565	-0.417427	-0.495923
0.238257	0.243053	-0.245851	-0.036929	0.322226	-0.000000	-0.235863	0.155662	0.173810	-0.294067	0.000000	-0.442891	-0.052179	0.396565	-0.417427	0.495923
0.311021	0.162040	0.000000	-0.212641	0.000000	-0.365617	-0.251003	-0.000000	0.000000	0.312943	0.470402	0.000000	0.300447	-0.000000	0.278292	-0.647379
0.238257	0.243052	0.245852	-0.036930	-0.322226	0.000000	-0.235863	-0.155662	-0.173810	-0.294067	-0.000000	0.442891	-0.052179	-0.396565	-0.417427	0.495922

PYRENE

TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1.00000	0.66949	-0.00000	-0.00000	0.17951	-0.14285	-0.00000	0.15860	-0.20819	-0.00000	0.59434	0.00000	-0.27677	0.00000	-0.02868	-0.00000
2	0.66949	1.00000	0.66949	-0.11730	-0.00000	0.00000	-0.07286	0.00000	0.00000	-0.11730	-0.00000	-0.23459	0.00000	0.08861	-0.00000	-0.08861
3	-0.00000	0.66949	1.00000	0.00000	-0.20819	0.15860	0.00000	-0.14285	0.17951	0.00000	-0.27677	0.00000	0.59434	-0.00000	-0.02868	-0.00000
4	-0.00000	-0.11730	0.00000	1.00000	0.77652	-0.20819	0.00000	-0.17951	-0.00831	0.00000	0.02003	-0.00000	0.50348	0.00000	-0.23179	-0.00000
5	0.17951	-0.00000	-0.20819	0.77652	1.00000	0.00000	-0.11730	-0.00000	0.00000	-0.00831	-0.00000	-0.23179	0.00000	0.50348	0.00000	0.02003
6	-0.14285	0.00000	0.15860	-0.20819	0.00000	1.00000	0.66949	-0.00000	-0.00000	0.17951	0.00000	-0.02868	-0.00000	0.59434	0.00000	-0.27677
7	-0.00000	-0.07286	0.00000	0.00000	-0.11730	0.66949	1.00000	0.66949	-0.11730	0.00000	0.08861	-0.00000	0.08861	-0.00000	-0.23459	-0.00000
8	0.15860	0.00000	-0.14285	0.17951	-0.00000	-0.00000	0.66949	1.00000	0.00000	-0.20819	-0.00000	-0.02868	0.00000	-0.27677	0.00000	0.59434
9	-0.20819	0.00000	0.17951	-0.00831	0.00000	-0.00000	-0.11730	0.00000	1.00000	0.77652	-0.00000	-0.23179	-0.00000	0.02003	0.00000	0.50348
10	-0.00000	-0.11730	0.00000	0.00000	-0.00831	0.17951	0.00000	-0.20819	0.77652	1.00000	0.50348	-0.00000	0.02003	-0.00000	-0.23179	-0.00000
11	0.59434	-0.00000	-0.27677	0.02003	-0.00000	0.00000	0.08861	-0.00000	-0.00000	0.50348	1.00000	0.52351	-0.00000	-0.08063	0.00000	-0.16690
12	0.00000	-0.23459	0.00000	-0.00000	-0.23179	-0.02868	-0.00000	-0.02868	-0.23179	-0.00000	0.52351	1.00000	0.52351	0.00000	0.53642	0.00000
13	-0.27677	0.00000	0.59434	0.50348	0.00000	-0.00000	0.08861	0.00000	-0.00000	0.02003	-0.00000	0.52351	1.00000	-0.16690	0.00000	-0.08063
14	0.00000	0.08861	-0.00000	0.00000	0.50348	0.59434	-0.00000	-0.27677	0.02003	-0.00000	-0.08063	0.00000	-0.16690	1.00000	0.52351	-0.00000
15	-0.02868	-0.00000	-0.02868	-0.23179	-0.00000	-0.00000	-0.23459	0.00000	0.00000	-0.23179	0.00000	0.53642	0.00000	0.52351	1.00000	0.52351
16	-0.00000	0.08861	-0.00000	-0.00000	0.02003	-0.27677	-0.00000	0.59434	0.50348	-0.00000	-0.16690	0.00000	-0.08063	-0.00000	0.52351	1.00000

PYRENE TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.77316	0.49293	-0.05778	0.02069	0.17503	-0.14136	-0.00347	0.15542	-0.19834	-0.05623	0.42617	-0.03555	-0.25884	-0.00256	-0.02331	0.01635
2	0.49293	0.75668	0.49293	-0.10852	-0.00575	-0.00347	-0.07114	-0.00347	0.00575	-0.10852	-0.04130	-0.21705	-0.04130	0.08521	0.01151	0.08521
3	-0.05778	0.49293	0.77316	-0.05623	-0.19834	0.15542	-0.00347	-0.14136	0.17503	0.02069	-0.25884	-0.03555	0.42617	0.01635	-0.02331	-0.00256
4	0.02069	-0.10852	-0.05623	0.76942	0.59789	-0.19834	0.00575	0.17503	-0.01050	-0.00351	0.02471	-0.03614	0.33638	-0.04564	-0.21466	0.01237
5	0.17503	0.00575	-0.19834	0.59789	0.76942	-0.05623	-0.10852	0.02069	-0.00351	-0.01050	0.01237	-0.21466	-0.04564	0.33638	-0.03614	0.02471
6	-0.14136	-0.00347	0.15542	-0.19834	-0.05623	0.77316	0.49293	-0.05778	0.02069	-0.17503	-0.00256	-0.02331	0.01635	0.42617	-0.03555	-0.25884
7	-0.00347	-0.07114	-0.00347	0.00575	-0.10852	0.49293	0.75668	0.49293	-0.10852	0.00575	0.08521	0.01151	0.08521	-0.04130	-0.21705	-0.04130
8	0.15542	-0.00347	-0.14136	0.17503	0.02069	-0.05778	0.49293	0.77316	-0.05623	-0.19834	0.01635	-0.02331	-0.00256	-0.25884	-0.03555	0.42617
9	-0.19834	0.00575	0.17503	-0.01050	-0.00351	0.02069	-0.10852	-0.05623	0.76942	0.59789	-0.04564	-0.21466	0.01237	0.02471	-0.03614	0.33638
10	-0.05623	-0.10852	0.02069	-0.00351	-0.01050	0.17503	0.00575	-0.19834	0.59789	0.76942	0.33638	-0.03614	0.02471	0.01237	-0.21466	-0.04564
11	0.42617	-0.04130	-0.25884	0.02471	0.01237	-0.00256	0.08521	0.01635	-0.04564	0.33638	0.72268	0.36108	-0.03133	-0.07484	-0.03326	-0.15146
12	-0.03555	-0.21705	-0.03555	-0.03614	-0.21466	-0.02331	0.01151	-0.02331	-0.21466	-0.03614	0.36108	0.72977	0.36108	-0.03326	0.37273	-0.03326
13	-0.25884	-0.04130	0.42617	0.33638	-0.04564	0.01635	0.08521	-0.00256	0.01237	0.02471	-0.03133	0.36108	0.72268	-0.15146	-0.03326	-0.07484
14	-0.00256	0.08521	0.01635	-0.04564	0.33638	0.42617	-0.04130	-0.25884	0.02471	0.01237	-0.07484	-0.03326	-0.15146	0.72268	0.36108	-0.03133
15	-0.02331	0.01151	-0.02331	-0.21466	-0.03614	-0.03555	-0.21705	-0.03555	-0.03614	-0.21466	-0.03326	0.37273	-0.03326	0.36108	0.72977	0.36108
16	0.01635	0.08521	-0.00256	0.01237	-0.02471	-0.25884	-0.04130	0.42617	0.33638	-0.04564	-0.15146	-0.03326	-0.07484	-0.03133	0.36108	0.72268

ENERGIES FOR PYRENE , TBM APPROXIMATION -1.7-
ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	7, 9	8,10	2, 9	1,11	3,10	6,12	4,12	5,13
XMOMNT	0.67757	0.67958	0.00798	0.48161	-0.01976	-0.48407	-0.24569	0.24638
YMOMNT	0.00000	0.00000	-0.00000	-0.00000	0.00000	-0.00000	0.00000	-0.00000
JUMP E	22.6441	28.2323	34.0623	42.2528	43.9076	48.2216	52.0941	55.0505
DIAG E	32.0995	36.8184	47.1258	53.7570	57.5886	59.2124	66.8883	69.8906
DIAG E	32.7834	36.2089	47.8044	54.1260	57.4268	58.6580	66.0286	70.8918
CORRSP	26.8176	39.0236	46.1128	52.9445	56.8751	61.7071	67.6923	72.2073
CORRSP	27.2007	38.9466	46.5449	52.9347	56.9131	61.3620	66.9344	73.0913

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION							
26.81761	0.03402	0.17270	0.00000	//	0.8168	-0.5338	-0.1170	0.0177	0.0609	0.0468	-0.1150	-0.1216
23.86716				//	0.0574	0.2108	-0.0656	0.0890	-0.0284	-0.0378	-0.1529	0.0329
39.02362	0.90851	0.73991	0.00000	//	0.5146	0.8101	-0.1624	-0.1753	-0.0027	0.1326	0.0615	0.0231
28.51292				//	-0.2069	0.9374	0.1483	-0.0025	-0.1185	-0.0514	0.0096	0.1993
46.11284	0.00201	0.03200	-0.00000	//	0.1361	0.0434	0.8878	-0.3763	0.1027	-0.1259	-0.1470	-0.0430
39.82319				//	0.0776	-0.1545	0.9023	-0.2750	-0.0847	0.0411	-0.2464	0.1042
52.94450	0.16137	0.26772	-0.00000	//	0.1145	0.0663	0.3854	0.6712	-0.3789	0.4600	0.0282	0.1658
50.75607				//	-0.0601	-0.1342	0.1167	0.7795	-0.4905	0.2135	-0.0639	0.2587
56.87515	0.20941	0.29425	-0.00000	//	-0.0057	0.1428	0.0776	0.4850	0.8327	-0.0303	-0.0705	-0.1975
51.72115				//	-0.0482	0.0319	0.2459	0.5295	0.6256	-0.4921	-0.0770	-0.1276
61.70710	1.85515	-0.84081	-0.00000	//	-0.1533	-0.1311	-0.0250	-0.3700	0.2519	0.8595	0.0874	-0.1096
57.23488				//	0.0453	0.1275	0.1293	0.1397	0.4615	0.8239	0.1597	-0.1681
67.69226	0.04157	-0.12017	0.00000	//	0.1094	-0.1100	0.1143	-0.0168	0.1568	-0.1068	0.9244	0.2685
66.35844				//	0.1622	-0.0378	0.2367	0.0197	-0.1036	-0.1628	0.9371	0.0215
72.20731	0.15581	0.22526	-0.00000	//	0.0296	-0.0541	-0.0595	-0.0675	0.2463	0.0415	-0.3058	0.9122
70.39516				//	0.0166	-0.1275	-0.1133	-0.0927	0.3497	0.0340	0.0462	0.9146

ENERGIES FOR PYRENE ,TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	8, 9	3, 9	7,10	6,11	4,11	2,10	5,12	6,13	1,11	4,13
XMOMNT	0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000	-0.00000	0.00000
YMOMNT	-1.16039	0.07393	0.79630	-0.51596	0.00000	-0.04221	0.21989	-0.00000	-0.00000	0.22095
JUMP E	16.6868	32.3620	34.1897	39.4469	43.3195	45.6079	51.0275	52.2446	53.4545	56.1171
DIAG E	29.8491	44.9483	45.7020	53.5766	59.1176	60.0546	63.7420	67.5507	67.5358	75.0844
DIAG E	29.9684	45.5154	45.6570	53.6206	58.8563	60.0043	63.5126	68.2270	68.0276	75.4554
CORRSP	27.4088	43.8771	45.6128	53.9325	58.4449	60.1485	64.2409	67.1495	69.3260	77.0197
CORRSP	27.5620	44.4111	45.7093	54.0366	58.1497	60.0418	64.0842	67.6518	69.8515	77.3463

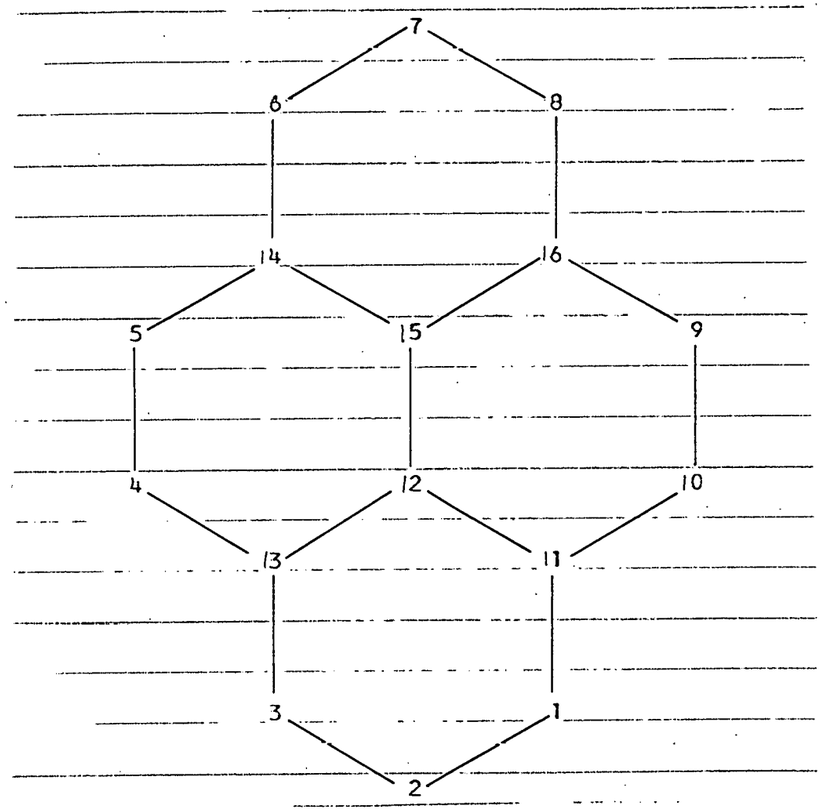
FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
27.40879	0.79605	0.00000	-0.82642	//	0.9449	-0.0548	0.2882	-0.0892	-0.0520	-0.0642	-0.0574	-0.0390	-0.0032	0.0384
12.19275				//	0.9581	0.0020	0.1077	0.1886	-0.0482	0.0255	-0.1446	-0.0399	0.0202	0.0947
43.87715	0.18324	0.00000	0.31338	//	-0.0335	0.9174	0.3135	0.1476	-0.0178	-0.1106	0.1058	-0.0581	0.0976	0.0238
32.74018				//	-0.1162	0.7577	0.1256	0.5990	-0.0198	-0.0214	0.1655	-0.0402	0.0810	0.0381
45.61284	1.16999	-0.00000	0.77665	//	-0.2476	-0.3345	0.8261	0.3100	0.1066	-0.0995	-0.0549	0.0813	-0.0748	0.1088
31.71859				//	-0.1416	-0.1629	0.9080	0.0143	0.0932	0.0334	-0.0954	0.0698	-0.0795	0.3140
53.93254	2.13495	0.00000	-0.96482	//	0.1793	-0.0014	-0.3232	0.8773	0.1617	-0.1297	-0.1260	0.0367	-0.1459	-0.1104
43.28854				//	-0.1062	-0.4728	-0.1790	0.7130	0.2741	-0.0907	-0.1350	0.1745	-0.3026	-0.0362
58.44493	0.00046	0.00000	0.01361	//	0.0557	0.0995	0.0100	-0.1059	0.8412	0.4489	-0.0470	-0.0861	-0.1677	0.1697
55.59443				//	0.1525	0.2341	0.0040	-0.2688	0.7379	-0.2293	0.2854	0.0565	-0.4086	-0.0329
60.14852	0.03867	-0.00000	-0.12296	//	0.0365	0.0247	0.0606	0.2504	-0.4255	0.8380	-0.0142	0.0912	0.1079	0.1677
50.03454				//	0.0052	-0.0241	-0.1605	0.0196	0.1559	0.8618	0.2568	0.0452	-0.0721	0.3648
64.24094	0.01260	0.00000	0.06791	//	0.0619	-0.1174	0.0031	0.1078	0.0311	0.0375	0.9686	-0.1233	-0.1137	-0.0445
59.41689				//	0.1012	-0.2597	0.1303	0.0920	-0.3381	-0.1355	0.8578	0.0631	-0.0863	-0.1303
67.14948	0.01153	0.00000	-0.06355	//	0.0641	-0.0107	-0.0572	0.0083	0.2086	-0.0682	0.1577	0.7923	0.5290	0.1083
65.85281				//	0.0196	0.2182	-0.0725	-0.1260	-0.3787	-0.0240	-0.1461	0.7286	-0.4673	0.1275
69.32603	0.01597	0.00000	-0.07359	//	-0.0096	-0.1369	0.0124	0.1258	0.1420	0.0103	-0.0157	-0.5555	0.7944	-0.0713
67.14941				//	0.0393	-0.0618	-0.0344	0.0074	0.2841	-0.1048	0.1152	0.6195	0.7050	0.0876
77.01969	0.02171	0.00000	0.08142	//	-0.0097	-0.0193	-0.1569	0.0548	-0.0779	-0.2167	0.0285	-0.1409	-0.0059	0.9477
74.12242				//	-0.0418	-0.0412	-0.2587	-0.0095	-0.0796	-0.4055	0.0810	-0.1939	0.0101	0.8453

215

220

PYRENE IRM



ATOMIC COORDINATES

x	3.4640	2.5980	1.7320	0.8660	0.8660	1.7320	2.5980	3.4640
y	0.5000	0.	0.5000	2.0000	3.0000	4.5000	5.0000	4.5000

4.3300	4.3300	3.4640	2.5980	1.7320	1.7320	2.5980	3.4640
3.0000	2.0000	1.5000	2.0000	1.5000	3.5000	3.0000	3.5000

PYRENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 AA	10 SS	11 AS	12 SA	13 AS	14 AA	15 SS	16 AS
1.780323	1.555898	1.475669	1.318542	1.252553	1.177971	1.136972	1.037719	0.829620	0.748032	0.727607	0.679452	0.661255	0.586171	0.553580	0.478622
0.182317	0.309119	0.156185	0.305085	0.306876	0.034640	0.163500	-0.381117	0.362701	0.197104	0.018927	0.283471	0.317346	-0.155804	-0.289195	0.163236
0.149566	0.314775	0.000000	0.452828	-0.000000	0.049730	0.419259	-0.000000	0.000000	-0.438357	-0.007263	0.000000	-0.457416	0.000000	0.279190	-0.125923
0.182317	0.309119	-0.156185	0.305085	-0.306876	0.034641	0.163501	0.381117	-0.362702	0.197103	0.018927	-0.283471	0.317346	0.155803	-0.289195	0.163236
0.205980	0.092157	-0.377788	-0.175361	-0.172207	0.389184	-0.150778	-0.280544	0.300581	-0.127488	0.407283	-0.169030	-0.132918	0.360549	-0.095414	0.187687
0.205980	-0.092157	-0.377788	-0.175361	0.172208	0.389183	0.150779	-0.280544	-0.300581	-0.127488	-0.407283	-0.169030	0.132918	-0.360549	-0.095413	-0.187687
0.182317	-0.309119	-0.156185	0.305085	0.306876	0.034641	-0.163501	0.381117	0.362702	0.197104	-0.018927	-0.283471	-0.317346	-0.155804	-0.289195	-0.163236
0.149565	-0.314775	0.000000	0.452828	-0.000000	0.049731	-0.419259	0.000000	0.000000	-0.438357	0.007263	-0.000000	0.457416	0.000000	0.279190	0.125923
0.182317	-0.309119	0.156185	0.305085	-0.306876	0.034641	-0.163501	-0.381117	-0.362702	0.197104	-0.018927	0.283471	-0.317346	0.155803	-0.289195	-0.163236
0.205979	-0.092157	0.377788	-0.175361	-0.172207	0.389183	0.150779	0.280544	0.300581	-0.127488	-0.407283	0.169030	0.132918	0.360549	-0.095414	-0.187687
0.205980	0.092157	0.377788	-0.175361	0.172208	0.389184	-0.150778	0.280544	-0.300581	-0.127488	0.407283	0.169030	-0.132918	-0.360549	-0.095413	0.187687
0.299668	0.281310	0.287893	-0.045270	0.355207	-0.021506	-0.274817	-0.161385	-0.167627	0.249697	-0.015144	-0.375597	0.026521	0.309402	0.308770	-0.307258
0.383007	0.185877	-0.000000	-0.207825	-0.000000	-0.437348	-0.272471	0.000000	-0.000000	-0.270074	-0.408673	0.000000	-0.229373	-0.000000	-0.214243	0.414227
0.299667	0.281310	-0.287893	-0.045270	-0.355207	-0.021505	-0.274817	0.161385	0.167627	0.249697	-0.015144	0.375597	0.026521	-0.309402	0.308770	-0.307258
0.299667	-0.281311	-0.287892	-0.045269	0.355207	-0.021506	0.274817	0.161385	-0.167627	0.249697	0.015144	0.375596	-0.026520	0.309402	0.308770	0.307258
0.383007	-0.185877	-0.000000	-0.207825	-0.000000	-0.437349	0.272470	0.000000	0.000000	-0.270074	0.408673	0.000000	0.229373	-0.000000	-0.214243	-0.414227
0.299667	-0.281311	0.287892	-0.045270	-0.355207	-0.021506	0.274817	-0.161385	0.167627	0.249697	0.015144	-0.375596	-0.026521	0.309402	0.308770	0.307258

PYRENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 AA	10 SS	11 AS	12 SA	13 AS	14 AA	15 SS	16 AS
32.89431	26.81383	24.19139	18.13084	15.13217	11.33860	9.04122	2.72791	-15.41290	-25.27957	-28.09594	-35.40622	-38.44580	-52.98370	-60.52118	-81.75342
0.136640	0.247819	0.128572	0.265689	0.274198	0.031917	0.153336	-0.374126	0.398208	0.227895	0.022188	0.343898	0.390256	-0.203501	-0.388687	0.235949
0.112094	0.252353	0.000000	0.394354	-0.000000	0.045820	0.393194	-0.000000	0.000000	-0.506836	-0.008515	0.000000	-0.562506	0.000000	0.375240	-0.182016
0.136640	0.247819	-0.128571	0.265689	-0.274198	0.031917	0.153336	0.374126	-0.398208	0.227895	0.022189	-0.343898	0.390255	0.203500	-0.388687	0.235949
0.154374	0.073882	-0.310996	-0.152717	-0.153870	0.358581	-0.141405	-0.275398	0.330006	-0.147404	0.477471	-0.205061	-0.163455	0.470926	-0.128239	0.271293
0.154374	-0.073882	-0.310996	-0.152716	0.153870	0.358581	0.141405	-0.275398	-0.330006	-0.147404	-0.477471	-0.205061	0.163455	-0.470926	-0.128239	-0.271293
0.136640	-0.247819	-0.128571	0.265689	0.274198	0.031917	-0.153336	0.374126	0.398208	0.227895	-0.022189	-0.343898	-0.390256	-0.203501	-0.388687	-0.235949
0.112094	-0.252353	0.000000	0.394354	-0.000000	0.045821	-0.393194	0.000000	0.000000	-0.506836	0.008515	-0.000000	0.562506	0.000000	0.375240	0.182016
0.136640	-0.247819	0.128572	0.265689	-0.274198	0.031917	-0.153336	-0.374126	-0.398208	0.227895	-0.022188	0.343898	-0.390255	0.203500	-0.388687	-0.235949
0.154374	-0.073882	0.310995	-0.152717	-0.153870	0.358581	0.141406	0.275398	0.330006	-0.147404	-0.477472	0.205061	0.163455	0.470926	-0.128239	-0.271293
0.154374	0.073882	0.310995	-0.152717	0.153870	0.358581	-0.141405	0.275398	-0.330006	-0.147404	0.477472	0.205061	-0.163455	-0.470926	-0.128239	0.271293
0.224590	0.225525	0.236993	-0.039424	0.317382	-0.019815	-0.257732	-0.158424	-0.184036	0.288704	-0.017754	-0.455661	0.032614	0.404120	0.414996	-0.444127
0.287050	0.149017	-0.000000	-0.180989	-0.000000	-0.402958	-0.255532	0.000000	-0.000000	-0.312264	-0.479101	0.000000	-0.282070	-0.000000	-0.287950	0.598745
0.224590	0.225525	-0.236993	-0.039424	-0.317382	-0.019814	-0.257732	0.158424	0.184036	0.288704	-0.017754	0.455661	-0.032614	-0.404120	0.414997	-0.444127
0.224590	-0.225525	-0.236993	-0.039424	0.317383	-0.019815	0.257732	0.158424	-0.184036	0.288704	0.017754	0.455661	0.032613	0.404121	0.414996	0.444127
0.287050	-0.149017	-0.000000	-0.180988	-0.000000	-0.402959	0.255531	0.000000	0.000000	-0.312264	0.479101	0.000000	0.282070	-0.000000	-0.287950	-0.598745
0.224590	-0.225525	0.236993	-0.039424	-0.317383	-0.019815	0.257732	-0.158424	0.184036	0.288704	0.017754	-0.455661	-0.032614	-0.404120	0.414997	0.444127

PYRENE

IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1.02724	0.66599	-0.02803	-0.00712	0.18892	-0.14048	0.00258	0.16140	-0.21412	0.01260	0.59516	0.00837	-0.26674	0.00117	-0.04327	-0.00896
2	0.66599	1.00951	0.66599	-0.12691	0.00992	0.00258	-0.08993	0.00258	0.00992	-0.12691	-0.00684	-0.22860	-0.00684	0.09984	-0.00570	0.09984
3	-0.02803	0.66599	1.02724	0.01260	-0.21412	0.16140	0.00258	-0.14048	0.18892	-0.00712	-0.26674	0.00837	0.59516	-0.00896	-0.04327	0.00117
4	-0.00712	-0.12691	0.01260	1.01391	0.77038	-0.21412	0.00992	0.18892	0.00328	0.00957	0.00800	0.00668	0.50662	-0.00750	-0.22617	-0.01677
5	0.18892	0.00992	-0.21412	0.77038	1.01391	0.01260	-0.12691	-0.00712	0.00957	0.00328	-0.01677	-0.22617	-0.00750	0.50662	0.00668	0.00800
6	-0.14048	0.00258	0.16140	-0.21412	0.01260	1.02724	0.66599	-0.02803	-0.00712	0.18892	0.00117	-0.04327	-0.00896	0.59516	0.00837	-0.26674
7	0.00258	-0.08993	0.00258	0.00992	-0.12691	0.66599	1.00951	0.66599	-0.12691	0.00992	0.09984	-0.00570	0.09984	-0.00684	-0.22860	-0.00684
8	0.16140	0.00258	-0.14048	0.18892	-0.00712	-0.02803	0.66599	1.02724	0.01260	-0.21412	-0.00896	-0.04327	0.00117	-0.26674	0.00837	0.59516
9	-0.21412	0.00992	0.18892	0.00328	0.00957	-0.00712	-0.12691	0.01260	1.01391	0.77038	-0.00750	-0.22617	-0.01677	0.00800	0.00668	0.50662
10	0.01260	-0.12691	-0.00712	0.00957	0.00328	0.18892	0.00992	-0.21412	0.77038	1.01391	0.50662	0.00668	0.00800	-0.01677	-0.22617	-0.00750
11	0.59516	-0.00684	-0.26674	0.00800	-0.01677	0.00117	0.09984	-0.00896	-0.00750	0.50662	0.96414	0.52151	0.02375	-0.09021	0.01284	-0.15918
12	0.00837	-0.22860	0.00837	0.00668	-0.22617	-0.04327	-0.00570	-0.04327	-0.22617	0.00668	0.52151	0.97990	0.52151	0.01284	0.54474	0.01284
13	-0.26674	-0.00684	0.59516	0.50662	-0.00750	-0.00896	0.09984	0.00117	-0.01677	0.00800	0.02375	0.52151	0.96414	-0.15918	0.01284	-0.09021
14	0.00117	0.09984	-0.00896	-0.00750	0.50662	0.59516	-0.00684	-0.26674	0.00800	-0.01677	-0.09021	0.01284	-0.15918	0.96414	0.52151	0.02375
15	-0.04327	-0.00570	-0.04327	-0.22617	0.00668	0.00837	-0.22860	0.00837	-0.00668	-0.22617	0.01284	0.54474	0.01284	0.52151	0.97990	0.52151
16	-0.00896	0.09984	0.00117	-0.01677	0.00800	-0.26674	-0.00684	0.59516	0.50662	-0.00750	-0.15918	0.01284	-0.09021	0.02375	0.52151	0.96414

PYRENE IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.81378	0.48877	-0.11296	0.01890	0.20115	-0.15193	-0.00255	0.17334	-0.21981	-0.06453	0.42544	-0.04796	-0.28163	0.00099	-0.03894	0.01185
2	0.48877	0.77693	0.48877	-0.12689	0.02093	-0.00255	-0.09621	-0.00255	0.02093	-0.12689	-0.07141	-0.24106	-0.07141	0.10629	0.01042	0.10629
3	-0.11296	0.48877	0.81378	-0.06453	-0.21981	0.17334	-0.00255	-0.15193	0.20115	0.01890	-0.28163	-0.04796	0.42544	0.01185	-0.03894	0.00099
4	0.01890	-0.12689	-0.06453	0.79485	0.59833	-0.21981	0.02093	0.20115	0.00279	0.00990	0.01557	-0.05079	0.33121	-0.07656	-0.23937	-0.00152
5	0.20115	0.02093	-0.21981	0.59833	0.79485	-0.06453	-0.12689	0.01890	0.00990	0.00279	-0.00152	-0.23937	-0.07656	0.33121	-0.05079	0.01557
6	-0.15193	-0.00255	0.17334	-0.21981	-0.06453	0.81378	0.48877	-0.11296	0.01890	0.20115	0.00099	-0.03894	0.01185	0.42544	-0.04796	-0.28163
7	-0.00255	-0.09621	-0.00255	0.02093	-0.12689	0.48877	0.77693	0.48877	-0.12689	0.02093	0.10629	0.01042	0.10629	-0.07141	-0.24106	-0.07141
8	0.17334	-0.00255	-0.15193	0.20115	0.01890	-0.11296	0.48877	0.81378	-0.06453	-0.21981	0.01185	-0.03894	0.00099	-0.28163	-0.04796	0.42544
9	-0.21981	0.02093	0.20115	0.00279	0.00990	0.01890	-0.12689	-0.06453	0.79485	0.59833	-0.07656	-0.23937	-0.00152	0.01557	-0.05079	0.33121
10	-0.06453	-0.12689	0.01890	0.00990	0.00279	0.20115	0.02093	-0.21981	0.59833	0.79485	0.33121	-0.05079	0.01557	-0.00152	-0.23937	-0.07656
11	0.42544	-0.07141	-0.28163	0.01557	-0.00152	0.00099	0.10629	0.01185	-0.07656	0.33121	0.70334	0.35811	-0.02464	-0.09086	-0.03975	-0.16874
12	-0.04796	-0.24106	-0.04796	-0.05079	-0.23937	-0.03894	0.01042	-0.03894	-0.23937	-0.05079	0.35811	0.73007	0.35811	-0.03975	0.38006	-0.03975
13	-0.28163	-0.07141	0.42544	0.33121	-0.07656	0.01185	0.10629	0.00099	-0.00152	0.01557	-0.02464	0.35811	0.70334	-0.16874	-0.03975	-0.09086
14	0.00099	0.10629	0.01185	-0.07656	0.33121	0.42544	-0.07141	-0.28163	0.01557	-0.00152	-0.09086	-0.03975	-0.16874	0.70334	0.35811	-0.02464
15	-0.03894	0.01042	-0.03894	-0.23937	-0.05079	-0.04796	-0.24106	-0.04796	-0.05079	-0.23937	-0.03975	0.38006	-0.03975	0.35811	0.73007	0.35811
16	0.01185	0.10629	0.00099	-0.00152	0.01557	-0.28163	-0.07141	0.42544	0.33121	-0.07656	-0.16874	-0.03975	-0.09086	-0.02464	0.35811	0.70334

ENERGIES FOR PYRENE IRM APPROXIMATION 5,8

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	7, 9	8,10	2, 9	5,11	6,12	3,10	4,12	5,13
XMOMNT	0.68743	-0.65628	0.03477	0.50548	0.53746	0.02325	0.16161	0.22227
YMOMNT	-0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.00000	-0.00000
JUMP E	24.4541	28.0075	42.2267	43.2281	46.7448	49.4710	53.5371	53.5780
DIAG E	33.4554	35.8346	55.6432	54.5097	57.7893	63.7673	67.4810	69.3473
DIAG E	34.2240	35.2565	56.2921	54.8279	57.2463	63.6538	66.4952	70.3652
CORRSP	27.7003	38.8065	56.5280	50.7496	60.3735	62.7848	68.4087	72.4762
CORRSP	27.9416	38.8329	56.8302	50.8713	60.3160	62.7074	67.5823	73.2792

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION							
27.70032	0.01272	0.10394	-0.00000	//	0.7653	0.6145	-0.0401	0.0156	-0.0287	-0.0481	0.1231	-0.1288
25.20106				//	0.9031	-0.3815	0.0030	0.0943	0.0709	0.0370	0.1381	0.0673
38.80649	0.89717	-0.73733	0.00000	//	-0.6062	0.7556	0.0707	0.1666	0.1672	0.0082	0.0191	-0.0205
27.97067				//	0.3887	0.8899	-0.0913	0.0090	-0.0349	-0.0848	0.0480	-0.1945
56.52802	0.00585	0.04931	-0.00000	//	0.0421	-0.0225	0.8459	0.2834	-0.3969	0.1256	0.1425	0.0911
46.30090				//	0.0363	0.0949	0.7896	-0.5044	-0.0467	0.1128	0.2778	0.1404
50.74960	0.03267	0.12304	-0.00000	//	-0.0015	-0.0128	-0.4719	0.7244	-0.4529	0.1578	-0.1078	0.1039
52.07211				//	-0.0848	0.1319	0.3791	0.8314	-0.0332	0.2016	0.1806	0.2572
60.37354	1.67769	0.80837	-0.00000	//	0.1022	-0.1960	0.1285	0.5908	0.6016	-0.4306	0.1417	-0.1345
53.03504				//	-0.0597	0.0192	0.1379	0.0621	0.9243	-0.3232	0.0607	-0.1034
62.78476	0.74742	0.52909	-0.00000	//	0.1531	-0.0094	0.0455	0.1077	0.4932	0.7397	-0.0712	0.4090
59.58598				//	-0.0138	0.1434	-0.3038	-0.1826	0.3593	0.7615	0.0453	0.3775
68.40872	0.01084	0.06104	-0.00000	//	-0.1051	-0.0876	-0.1741	-0.0236	-0.0298	0.2542	0.9190	-0.2009
67.39616				//	-0.1452	-0.0603	-0.2867	-0.0134	-0.0619	-0.0506	0.9261	-0.1699
72.47623	0.04857	0.12554	-0.00000	//	0.0146	-0.0674	-0.0793	0.0756	-0.0511	-0.3996	0.2878	0.8591
71.19530				//	0.0072	0.1073	-0.1759	-0.0898	-0.0566	-0.5011	0.0735	0.8305

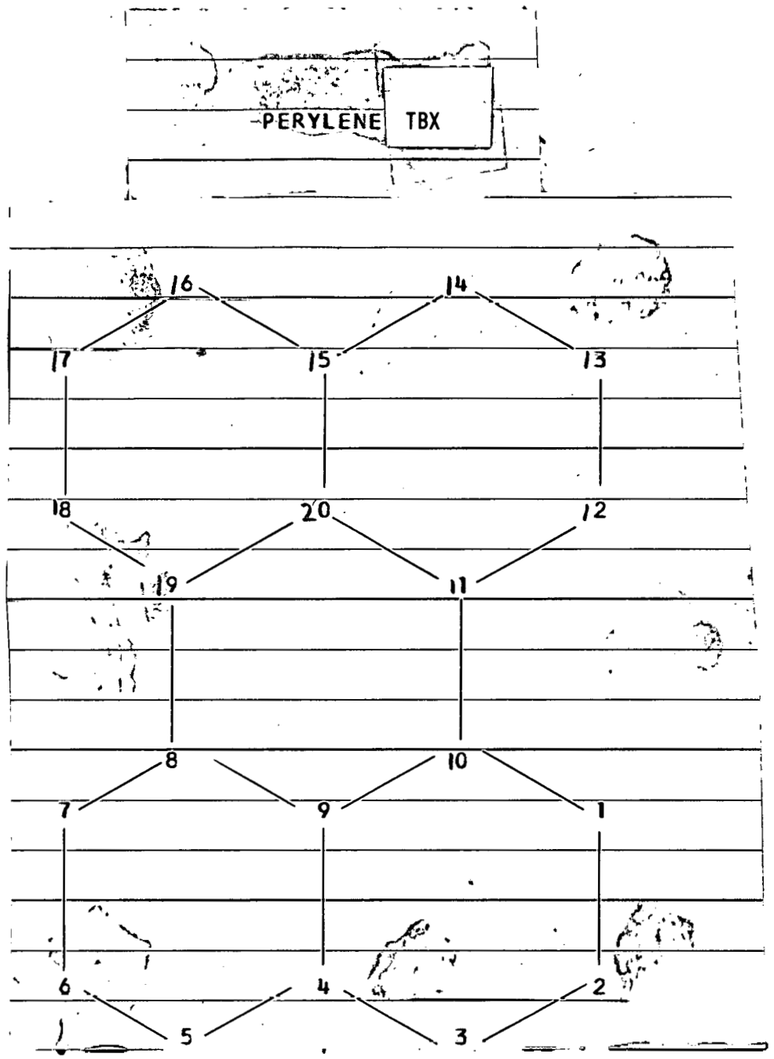
ENERGIES FOR PYRENE , TRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	8, 9	7,10	6,11	3, 9	4,11	6,13	5,12	2,10	8,14	4,13
XMOMNT	0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
YMOMNT	1.17361	0.84167	-0.51508	-0.03442	0.02655	0.03253	-0.23087	-0.00511	-0.07600	0.18195
JUMP E	18.1408	34.3208	39.4345	39.6043	46.2268	49.7844	50.5384	52.0934	55.7116	56.5766
DIAG E	30.9265	46.0414	52.9529	52.6489	60.9418	65.9486	62.9317	67.0344	65.2742	75.8873
DIAG E	31.0380	46.1204	53.0793	53.2249	60.6255	66.7747	62.5804	66.9938	64.7234	76.2706
CORRSP	28.1812	45.7446	54.2697	51.8021	59.3294	66.7339	62.5693	65.8393	68.0225	78.0954
CORRSP	28.2780	45.8741	54.2681	52.3018	58.8826	68.0184	62.3092	66.1281	66.9273	78.4431

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
28.18115	0.76820	-0.00000	0.80063	//	0.9391	-0.3087	0.1027	-0.0357	0.0449	0.0341	-0.0581	0.0431	-0.0291	-0.0421
13.02117				//	0.9560	-0.1156	-0.1821	0.0089	0.0588	0.0302	-0.1509	-0.0328	-0.0110	-0.1052
45.74459	1.30736	0.00000	0.81979	//	0.2364	0.8618	0.4084	-0.0963	0.0687	0.0722	0.0071	-0.0566	-0.0188	0.1086
31.65666				//	0.1709	0.9173	0.1142	0.0028	0.0693	0.0947	0.0584	0.0811	0.0030	0.3042
54.26969	2.55915	-0.00000	-1.05304	//	-0.2120	-0.3586	0.8892	-0.0219	-0.0094	0.0303	0.1070	-0.0853	-0.0130	-0.1239
33.59713				//	0.1073	-0.0777	0.7479	-0.5302	-0.1026	-0.0419	-0.2046	-0.0253	-0.2948	-0.0163
51.80211	0.00126	-0.00000	0.02390	//	0.0496	0.0567	0.0395	0.9605	0.0597	0.1536	0.1851	0.0682	-0.0617	0.0174
47.51284				//	0.1210	-0.1393	0.5879	0.5976	0.2263	0.2164	0.3686	-0.0857	0.1420	-0.0424
59.32943	0.03886	0.00000	-0.12410	//	-0.0138	-0.0488	-0.0326	-0.0890	0.7780	-0.0319	0.3776	0.0905	0.4716	0.0945
59.71775				//	-0.1571	0.1336	-0.0009	0.0902	0.5803	0.0867	-0.5784	-0.4610	-0.0170	-0.2402
66.73395	0.00378	-0.00000	0.03649	//	-0.0195	-0.0299	-0.0809	0.0076	0.0942	0.6780	-0.2816	-0.5932	0.2550	-0.1653
64.74984				//	-0.0389	-0.0217	-0.0105	-0.1323	-0.3600	0.8294	-0.1862	-0.0796	0.3478	-0.0301
62.56927	0.00295	0.00000	-0.03329	//	0.0922	0.0315	-0.0767	-0.1058	-0.5460	0.1581	0.7254	-0.0868	0.3380	-0.0494
56.78685				//	0.0208	-0.1325	-0.0096	-0.5074	0.5778	0.0288	0.2634	0.1557	0.5206	0.1583
65.83928	0.01232	0.00000	-0.06632	//	-0.0716	-0.0488	0.0601	-0.1119	-0.0882	0.6121	-0.1349	0.7084	0.0831	0.2589
54.52220				//	-0.0449	-0.1837	0.0356	0.2301	0.2139	0.1664	-0.4513	0.6880	-0.1558	0.3678
68.02248	0.00116	-0.00000	0.02005	//	0.0236	0.0461	0.1045	0.1830	-0.2481	-0.3239	-0.4287	0.1221	0.7649	-0.0519
67.38870				//	0.0222	0.0795	0.2173	0.1505	-0.2752	-0.4559	-0.3805	0.1136	0.6879	-0.0944
78.09539	0.00348	0.00000	0.03239	//	0.0098	-0.1462	0.0486	0.0349	-0.0891	-0.0621	-0.0290	-0.3141	0.0352	0.9286
76.20255				//	0.0390	-0.2094	-0.0102	0.0543	-0.0914	-0.0982	-0.0950	-0.5050	0.0556	0.8164



ATOMIC COORDINATES

x	3.5412	3.5269	2.6452	1.7706	0.8960	0.0143	0.	0.8602	1.7706	2.6810
y	1.4910	0.4510	0.	0.4580	0.	0.4510	1.4910	1.9850	1.4910	1.9850
z	2.6810	3.5412	3.5269	2.6452	1.7706	0.8960	0.0143	0.	0.8602	1.7706
q	3.0610	3.5550	4.5950	5.0460	4.5880	5.0460	4.5950	3.5550	3.0610	3.5550

PERYLENE X TBX APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 S A	10 A A	11 A S	12 S S	13 S A
1.602067	1.531379	1.440300	1.391656	1.368259	1.257796	1.238198	1.225367	1.224004	1.104327	0.895671	0.775994	0.774630
0.173355	0.141295	0.292730	-0.088114	0.282391	-0.247215	0.036626	0.277481	-0.232613	0.288483	0.288483	-0.232637	-0.277462
0.135165	0.186435	0.222317	0.144341	0.324693	0.015225	-0.280704	0.293752	-0.299358	-0.127887	0.127887	-0.299384	0.293727
0.168221	0.266813	0.127453	0.302324	0.222557	0.235409	-0.297462	0.015494	-0.058786	-0.309419	-0.309419	0.058787	-0.015489
0.264168	0.372558	0.000001	0.322422	-0.000000	0.223587	0.000000	-0.277915	0.245421	0.000000	0.000000	0.245445	-0.277894
0.168221	0.266813	-0.127451	0.302324	-0.222557	0.235408	0.297463	0.015494	-0.058786	0.309419	0.309419	0.058787	-0.015488
0.135165	0.186435	-0.222316	0.144342	-0.324693	0.015224	0.280704	0.293752	-0.299359	0.127886	-0.127887	-0.299383	0.293726
0.173355	0.141295	-0.292730	-0.088112	-0.282391	-0.247214	-0.036627	0.277482	-0.232613	-0.288483	-0.288483	0.232637	-0.277462
0.294374	0.132134	-0.314071	-0.266079	-0.123683	-0.267017	-0.285272	-0.013554	0.060030	-0.233842	0.233842	0.060031	-0.013549
0.321966	0.272872	-0.000000	-0.120213	-0.000000	-0.271816	-0.000000	-0.308832	0.371707	-0.000000	-0.000000	-0.371733	0.308801
0.294375	0.132134	0.314070	-0.266080	0.123682	-0.267018	0.285271	-0.013554	0.060030	0.233842	-0.233842	0.060031	-0.013549
0.294374	-0.132134	0.314070	-0.266080	-0.123683	0.267017	0.285272	-0.013550	-0.060031	-0.233843	-0.233842	0.060030	0.013556
0.173355	-0.141295	0.292730	-0.088113	-0.282392	0.247215	0.036627	0.277465	0.232633	-0.288483	0.288483	0.232609	0.277484
0.135165	-0.186435	0.222316	0.144341	-0.324693	-0.015224	-0.280704	0.293731	0.299379	0.127887	0.127886	-0.299354	-0.293757
0.168221	-0.266813	0.127452	0.302324	-0.222557	-0.235408	-0.297463	0.015490	0.058787	0.309419	-0.309419	0.058786	0.015495
0.264168	-0.372558	0.000000	0.322422	0.000001	-0.223587	-0.000000	-0.277898	-0.245441	-0.000000	0.000000	0.245417	0.277918
0.168221	-0.266812	-0.127451	0.302324	0.222558	-0.235409	0.297462	0.015490	0.058788	-0.309419	0.309419	0.058786	0.015495
0.135165	-0.186435	-0.222316	0.144341	0.324694	-0.015225	0.280703	0.293731	0.299380	-0.127886	-0.127887	-0.299354	-0.293756
0.173355	-0.141295	-0.292730	-0.088112	0.282391	0.247215	-0.036626	0.277465	0.232633	0.288483	-0.288483	0.232609	0.277484
0.294374	-0.132134	-0.314071	-0.266079	0.123683	0.267018	-0.285271	-0.013550	-0.060032	0.233842	0.233842	0.060030	0.013555
0.321966	-0.272872	-0.000000	-0.120212	0.000000	0.271816	0.000000	-0.308806	-0.371729	-0.000000	0.000000	-0.371702	-0.308838

OVERLAP EIGNVALUES AND EIGNVECTORS

14 A A	15 S S	16 A S	17 S A	18 A A	19 S S	20 S A
0.761800	0.742202	0.631739	0.608342	0.559698	0.468619	0.397931
0.036627	-0.247214	0.282391	0.088113	0.292730	-0.141295	-0.173355
0.280703	-0.015224	-0.324693	0.144341	-0.222316	0.186435	0.135165
-0.297463	0.235408	0.222557	-0.302324	0.127452	-0.266812	-0.168221
0.000001	-0.223587	-0.000000	0.322422	-0.000000	0.372558	0.264168
0.297462	0.235409	-0.222557	-0.302324	-0.127452	-0.266812	-0.168221
-0.280704	-0.015225	0.324693	0.144341	0.222316	0.186435	0.135165
-0.036626	-0.247214	-0.282391	0.088113	-0.292730	-0.141295	-0.173355
0.285271	0.267018	0.123683	-0.266079	0.314071	0.132134	0.294375
0.000000	-0.271816	0.000000	0.120212	0.000000	-0.272872	-0.321966
-0.285272	0.267017	-0.123683	-0.266079	-0.314071	0.132134	0.294374
0.285271	0.267018	-0.123682	0.266080	0.314071	0.132134	-0.294375
-0.036627	-0.247215	0.282391	-0.088113	-0.292730	-0.141295	0.173355
-0.280703	-0.015225	-0.324693	-0.144341	0.222316	0.186435	-0.135165
0.297462	0.235409	0.222558	0.302324	-0.127452	-0.266812	0.168221
-0.000000	-0.223587	-0.000000	0.322422	0.000000	0.372558	-0.264168
-0.297463	0.235408	-0.222557	0.302324	0.127452	-0.266812	0.168221
0.280704	-0.015224	0.324693	-0.144342	-0.222316	0.186435	-0.135165
0.036627	-0.247214	-0.282391	-0.088113	0.292730	-0.141295	0.173355
-0.285272	0.267017	0.123683	0.266079	-0.314071	0.132134	-0.294375
0.000001	-0.271816	-0.000000	-0.120212	0.000000	-0.272872	0.321966

PERYLENE X — TBX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 S S	5 A A	6 S A	7 A S	8 S S	9 S A	10 A A	11 A S	12 S S	13 S A
28.12751	25.97102	22.88035	21.06394	20.14431	15.34027	14.39841	13.76549	13.69745	7.07077	-8.71816	-21.60573	-21.77551
0.136961	0.114179	0.243917	-0.074692	0.241416	-0.220429	0.032915	0.250669	-0.210253	0.274519	0.304822	0.264088	-0.315251
0.106789	0.150656	0.185245	0.122355	0.277581	0.013575	-0.252263	0.265368	-0.270583	-0.121696	0.135130	-0.339859	0.333731
0.132905	0.215608	0.106199	0.256275	0.190265	0.209903	-0.267323	0.013997	-0.053135	-0.294441	-0.326943	0.066735	-0.017599
0.208709	0.301059	0.000000	0.273312	-0.000000	0.199361	0.000000	-0.251061	0.221830	0.000000	0.000000	0.278628	-0.315742
0.132905	0.215608	-0.106198	0.256275	-0.190265	0.209901	0.267324	0.013997	-0.053135	0.294441	0.326943	0.066735	-0.017598
0.106789	0.150656	-0.185244	0.122356	-0.277580	0.013574	0.252263	0.265368	-0.270583	0.121696	-0.135130	-0.339859	0.333730
0.136961	0.114179	-0.243917	-0.074691	-0.241416	-0.220429	-0.032916	0.250669	-0.210253	-0.274519	-0.304822	0.264088	-0.315251
0.232573	0.106776	-0.261699	-0.225551	-0.105736	-0.238086	-0.256368	-0.012244	0.054260	-0.222523	0.247086	0.068147	-0.015394
0.254372	0.220504	-0.000000	-0.101902	-0.000000	-0.242365	-0.000000	-0.278991	0.335977	-0.000000	-0.000000	-0.421990	0.350858
0.232573	0.106776	0.261698	-0.225552	0.105736	-0.238087	0.256367	-0.012245	0.054260	0.222523	-0.247087	0.068147	-0.015395
0.232573	-0.106776	0.261698	-0.225552	-0.105737	0.238086	0.256368	-0.012241	-0.054261	-0.222523	-0.247086	0.068146	0.015402
0.136961	-0.114179	0.243916	-0.074692	-0.241417	0.220429	0.032916	0.250654	-0.210271	-0.274518	0.304822	0.264057	0.315276
0.106789	-0.150656	0.185244	0.122356	-0.277581	-0.013574	-0.252263	0.265348	0.270602	0.121696	0.135130	-0.339826	-0.333765
0.132904	-0.215608	0.106199	0.256275	-0.190264	-0.209902	-0.267324	0.013993	0.053136	0.294441	-0.326943	0.066733	0.017606
0.208708	-0.301059	0.000000	0.273312	0.000000	-0.199362	-0.000000	-0.251045	-0.221848	-0.000000	0.000000	0.278596	0.315769
0.132904	-0.215608	-0.106198	0.256275	0.190265	-0.209903	0.267323	0.013993	0.053137	-0.294441	0.326943	0.066733	0.017605
0.106788	-0.150656	-0.185244	0.122356	0.277581	-0.013575	0.252263	0.265348	0.270602	-0.121696	-0.135130	-0.339826	-0.333764
0.136961	-0.114179	-0.243916	-0.074691	0.241417	0.220429	-0.032915	0.250654	0.210271	0.274519	-0.304822	0.264057	0.315276
0.232573	-0.106776	-0.261699	-0.225551	0.105737	0.238087	-0.256367	-0.012241	-0.054261	0.222523	0.247086	0.068146	0.015401
0.254372	-0.220504	-0.000000	-0.101902	0.000000	0.242365	0.000000	-0.278967	-0.335997	-0.000000	0.000000	-0.421955	-0.350900

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 A A	15 S S	16 A S	17 S A	18 A A	19 S S	20 S A
-23.4028	-25.9971	-43.6301	-48.1866	-58.8795	-84.8700	-113.2416
0.041965	-0.286954	0.355290	0.112970	0.391282	-0.206403	-0.274810
0.321608	-0.017672	-0.408512	0.185062	-0.297163	0.272344	0.214270
-0.340810	0.273250	0.280010	-0.387613	0.170361	-0.389759	-0.266671
0.000001	-0.259528	-0.000000	0.413382	-0.000000	0.544232	0.418771
0.340809	0.273251	-0.280010	-0.387613	-0.170360	-0.389759	-0.266671
-0.321609	-0.017673	0.408512	0.185062	0.297163	0.272344	0.214270
-0.041963	-0.286954	-0.355290	-0.112970	-0.391283	-0.206404	-0.274810
0.326841	0.309941	0.155611	-0.341143	0.419808	0.193021	0.466656
0.000000	-0.315511	0.000000	0.154126	0.000000	-0.398611	-0.510395
-0.326842	0.309941	-0.155611	-0.341143	-0.419808	0.193021	0.466655
0.326841	0.309941	-0.155611	0.341144	0.419808	0.193021	-0.466656
-0.041964	-0.286954	0.355289	-0.112971	-0.391283	-0.206403	0.274810
-0.321608	-0.017672	-0.408512	-0.185062	0.297163	0.272344	-0.214270
0.340809	0.273251	0.280010	0.387613	-0.170361	-0.389759	0.266671
-0.000000	-0.259529	-0.000000	-0.413382	0.000000	0.544232	-0.418771
-0.340810	0.273250	-0.280010	0.387613	-0.170360	-0.389759	0.266671
0.321609	-0.017671	0.408512	-0.185062	-0.297163	0.272344	-0.214270
0.041964	-0.286954	-0.355290	-0.112970	0.391283	-0.206403	0.274810
-0.326842	0.309940	0.155611	0.341144	-0.419808	0.193021	-0.466656
0.000001	-0.315511	-0.000000	-0.154126	0.000000	-0.398611	0.510395

PERYLENE X TBX TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20										
1	1.00000	0.58806	-0.00000	-0.23890	0.00000	0.14968	-0.00000	-0.12668	0.00000	0.69241	-0.00000	-0.19264	0.00000	0.13294	0.00000
	-0.07837	-0.00000	0.11110	0.00000	-0.07713										
2	0.58806	1.00000	0.73104	-0.00000	-0.16363	-0.00000	0.14968	0.00000	-0.25818	-0.00000	-0.05141	-0.00000	0.01443	0.00000	0.00245
	0.00000	-0.01132	0.00000	0.03062	0.00000										
3	-0.00000	0.73104	1.00000	0.55044	0.00000	-0.16363	-0.00000	0.05479	0.00000	-0.30384	0.00000	0.13294	-0.00000	-0.10134	0.00000
	0.06084	0.00000	-0.07837	-0.00000	0.05214										
4	-0.23890	-0.00000	0.55044	1.00000	0.55044	-0.00000	-0.23890	0.00000	0.52847	0.00000	-0.01704	0.00000	0.00245	0.00000	0.00389
	-0.00000	0.00245	0.00000	-0.01704	-0.00000										
5	0.00000	-0.16363	0.00000	0.55044	1.00000	0.73104	-0.00000	-0.30384	-0.00000	0.05479	-0.00000	-0.07837	0.00000	0.06084	-0.00000
	-0.10134	-0.00000	0.13294	0.00000	0.05214										
6	0.14968	-0.00000	-0.16363	-0.00000	0.73104	1.00000	0.58806	0.00000	-0.25818	-0.00000	0.03062	0.00000	-0.01132	-0.00000	0.00245
	0.00000	0.01443	-0.00000	-0.05141	-0.00000										
7	-0.00000	0.14968	-0.00000	-0.23890	-0.00000	0.58806	1.00000	0.69241	0.00000	-0.12668	0.00000	0.11110	-0.00000	-0.07837	0.00000
	0.13294	0.00000	-0.19264	-0.00000	-0.07713										
8	-0.12668	0.00000	0.05479	0.00000	-0.30384	0.00000	0.69241	1.00000	0.52380	0.00000	-0.08953	-0.00000	0.03062	0.00000	-0.01704
	-0.00000	-0.05141	0.00000	0.35063	0.00000										
9	0.00000	-0.25818	0.00000	0.52847	-0.00000	-0.25818	0.00000	0.52380	1.00000	0.52380	0.00000	-0.07713	0.00000	0.05214	-0.00000
	0.05214	0.00000	-0.07713	0.00000	-0.14607										
10	0.69241	-0.00000	-0.30384	0.00000	0.05479	-0.00000	-0.12668	0.00000	0.52380	1.00000	0.35063	0.00000	-0.05141	-0.00000	-0.01704
	0.00000	0.03062	-0.00000	-0.08953	0.00000										
11	-0.00000	-0.05141	0.00000	-0.01704	-0.00000	0.03062	0.00000	-0.08953	0.00000	0.35063	1.00000	0.69241	-0.00000	-0.30384	0.00000
	0.05479	0.00000	-0.12668	-0.00000	0.52380										
12	-0.19264	-0.00000	0.13294	0.00000	-0.07837	0.00000	0.11110	-0.00000	-0.07713	0.00000	0.69241	1.00000	0.58806	0.00000	-0.23890
	-0.00000	0.14968	0.00000	-0.12668	-0.00000										
13	0.00000	0.01443	-0.00000	-0.00245	0.00000	-0.01132	-0.00000	0.03062	0.00000	-0.05141	-0.00000	0.58806	1.00000	0.73104	-0.00000
	-0.16363	-0.00000	0.14968	0.00000	-0.25818										
14	0.13294	0.00000	-0.10134	0.00000	0.06084	-0.00000	-0.07837	0.00000	0.05214	-0.00000	-0.30384	0.00000	0.73104	1.00000	0.55044
	0.00000	-0.16363	-0.00000	0.05479	0.00000										
15	0.00000	0.00245	0.00000	-0.00389	-0.00000	0.00245	0.00000	-0.01704	-0.00000	-0.01704	0.00000	-0.23890	-0.00000	0.55044	1.00000
	0.55044	-0.00000	-0.23890	-0.00000	0.52847										
16	-0.07837	0.00000	0.06084	-0.00000	-0.10134	0.00000	0.13294	-0.00000	0.05214	0.00000	0.05479	-0.00000	-0.16363	0.00000	0.55044
	1.00000	0.73104	0.00000	-0.30384	-0.00000										
17	-0.00000	-0.01132	0.00000	0.00245	-0.00000	0.01443	0.00000	-0.05141	0.00000	0.03062	0.00000	0.14968	-0.00000	-0.16363	-0.00000
	0.73104	1.00000	0.58806	-0.00000	-0.25818										
18	0.11110	0.00000	-0.07837	0.00000	0.13294	-0.00000	-0.19264	0.00000	-0.07713	-0.00000	-0.12668	0.00000	0.14968	-0.00000	-0.23890
	0.00000	0.58806	1.00000	0.69241	0.00000										
19	0.00000	0.03062	-0.00000	-0.01704	0.00000	-0.05141	-0.00000	0.35063	-0.00000	-0.08953	-0.00000	-0.12668	0.00000	0.05479	-0.00000
	-0.30384	-0.00000	0.69241	1.00000	0.52380										
20	-0.07713	0.00000	0.05214	-0.00000	0.05214	-0.00000	-0.07713	0.00000	-0.14607	0.00000	0.52380	-0.00000	-0.25818	0.00000	0.52847
	-0.00000	-0.25818	0.00000	0.52380	1.00000										

PERYLENE X | TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20										
1	0.77445	0.42718	-0.05140	-0.22195	0.01977	0.14524	-0.00243	-0.11998	-0.03905	0.51556	-0.04395	-0.18346	0.00835	0.13010	0.00291
	-0.07791	-0.00476	0.10879	0.01342	-0.07087										
2	0.42718	0.76541	0.54946	-0.04571	-0.15356	0.00616	0.14524	0.01217	-0.24064	-0.04352	-0.04529	0.00835	0.01356	-0.00397	0.00215
	0.00218	-0.01081	-0.00476	0.02856	0.00330										
3	-0.05140	0.54946	0.76508	0.37848	-0.05746	-0.15356	0.01977	0.05848	-0.03479	-0.28609	0.01487	0.13010	-0.00397	-0.09998	-0.00140
	0.06065	0.00218	-0.07791	-0.00378	0.04994										
4	-0.22195	-0.04571	0.37848	0.72176	0.37848	-0.04571	-0.22195	-0.02663	0.37576	-0.02663	-0.01350	-0.00291	0.00215	-0.00140	0.00338
	-0.00140	0.00215	0.00291	-0.01350	0.00535										
5	0.01977	-0.15356	-0.05746	0.37848	0.76508	0.54946	-0.05140	-0.28609	-0.03479	0.05848	-0.00378	-0.07791	0.00218	0.06065	-0.00140
	-0.09998	-0.00397	0.13010	0.01487	0.04994										
6	0.14524	0.00616	-0.15356	-0.04571	0.54946	0.76541	0.42718	-0.04352	-0.24064	0.01217	0.02856	-0.00476	-0.01081	0.00218	0.00215
	-0.00397	0.01356	0.00835	-0.04529	0.00330										
7	-0.00243	0.14524	0.01977	-0.22195	-0.05140	0.42718	0.77445	0.51556	-0.03905	-0.11998	0.01342	0.10879	-0.00476	-0.07791	0.00291
	0.13010	0.00835	-0.18346	-0.04395	-0.07087										
8	-0.11998	0.01217	0.05848	-0.02663	-0.28609	-0.04352	0.51556	0.74210	0.37008	-0.03753	-0.07886	0.01342	0.02856	-0.00378	-0.01350
	0.01486	-0.04529	-0.04395	0.21519	-0.02784										
9	-0.03905	-0.24064	-0.03479	0.37576	-0.03479	-0.24064	-0.03905	0.37008	0.74634	0.37008	-0.02784	-0.07087	0.00330	0.04994	0.00535
	0.04994	0.00330	-0.07087	-0.02784	-0.13466										
10	0.51556	-0.04352	-0.28609	-0.02663	0.05848	0.01217	-0.11998	-0.03753	0.37008	0.74210	0.21519	-0.04395	-0.04529	0.01486	-0.01350
	-0.00378	0.02856	0.01342	-0.07886	-0.02784										
11	-0.04395	-0.04529	0.01487	-0.01350	-0.00378	0.02856	0.01342	-0.07886	-0.02784	0.21519	0.74210	0.51556	-0.04352	-0.28609	-0.02663
	0.05848	0.01217	-0.11998	-0.03753	0.37008										
12	-0.18346	0.00835	0.13010	0.00291	-0.07791	-0.00476	0.10879	0.01342	-0.07087	-0.04395	0.51556	0.77445	0.42718	-0.05140	-0.22195
	0.01977	0.14524	-0.00243	-0.11998	-0.03905										
13	0.00835	0.01356	-0.00397	0.00215	0.00218	-0.01081	-0.00476	0.02856	0.00330	-0.04529	-0.04352	0.42718	0.76541	0.54946	-0.04571
	-0.15356	0.00616	0.14524	0.01217	-0.24064										
14	0.13010	-0.00397	-0.09998	-0.00140	0.06065	0.00218	-0.07791	-0.00378	0.04994	0.01486	-0.28609	-0.05140	0.54946	0.76508	0.37848
	-0.05746	-0.15356	0.01977	0.05848	-0.03479										
15	0.00291	0.00215	-0.00140	0.00338	-0.00140	-0.00215	0.00291	-0.01350	0.00535	-0.01350	-0.02663	-0.22195	-0.04571	0.37848	0.72176
	0.37848	-0.04571	-0.22195	-0.02663	0.37576										
16	-0.07791	0.00218	0.06065	-0.00140	-0.09998	-0.00397	0.13010	0.01486	0.04994	-0.00378	0.05848	0.01977	-0.15356	-0.05746	0.37848
	0.76508	0.54946	-0.05140	-0.28609	-0.03479										
17	-0.00476	-0.01081	0.00218	0.00215	-0.00397	0.01356	0.00835	-0.04529	0.00330	0.02856	0.01217	0.14524	0.00616	-0.15356	-0.04571
	0.54946	0.76541	0.42718	-0.04352	-0.24064										
18	0.10879	-0.00476	-0.07791	0.00291	0.13010	0.00835	-0.18346	-0.04395	-0.07087	0.01342	-0.11998	-0.00243	0.14524	0.01977	-0.22195
	-0.05140	0.42718	0.77445	0.51556	-0.03905										
19	0.01342	0.02856	-0.00378	-0.01350	0.01487	-0.04529	-0.04395	0.21519	-0.02784	-0.07886	-0.03753	-0.11998	0.01217	0.05848	-0.02663
	-0.28609	-0.04352	0.51556	0.74210	0.37008										
20	-0.07087	0.00330	0.04994	0.00535	0.04994	0.00330	-0.07087	-0.02784	-0.13466	-0.02784	0.37008	-0.03905	-0.24064	-0.03479	0.37576
	-0.03479	-0.24064	-0.03905	0.37008	0.74634										

ENERGIES FOR PERYLENE X TBXAPPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	8,11	4,11	10,14	1,11	9,13	7,12	6,13	9,15	6,15	5,14
XMOMNT	-0.76325	-0.14447	-0.71919	0.04045	-0.31653	-0.47536	0.23722	-0.34165	0.24200	-0.07276
YMOMNT	-0.00000	-0.00009	0.00000	0.00001	-0.26171	-0.06703	-0.34507	0.23239	0.45878	-0.00002
JUMP E	21.8334	28.1457	30.4360	36.1934	39.3398	39.3400	39.3414	39.3435	39.3451	45.0627
DIAG E	33.0787	40.8563	40.1883	48.8528	53.2936	53.7990	52.7968	52.9510	52.7553	63.1034
DIAG E	33.4881	41.4487	39.7978	49.7599	53.0569	53.9641	53.0190	52.6453	52.9085	62.6060
CORRSP	29.1302	39.6566	41.9368	49.5119	55.6252	52.6284	53.1164	51.7699	54.1627	64.1370
CORRSP	29.4139	40.3281	41.8610	50.1420	55.6435	52.9070	54.5702	51.4256	52.7036	63.6992

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
29.13018	0.12153	-0.31319	0.00434	//	0.8533	-0.0295	-0.4483	0.0848	0.1329	-0.1816	0.0180	0.1073	0.0179	-0.0051
25.73554				//	0.9718	-0.0920	0.0405	0.0455	0.1462	-0.0152	-0.0241	0.1397	-0.0336	-0.0244
39.65662	0.12180	0.26873	-0.00300	//	-0.0653	0.9403	-0.1455	0.1851	-0.0284	-0.0732	-0.1636	-0.0114	-0.1506	0.0211
33.45343				//	0.0602	0.7862	0.4626	0.1027	-0.1194	0.0128	-0.2597	-0.0529	-0.2623	-0.0135
41.93681	1.35149	-0.87053	0.00155	//	0.4643	0.1501	0.8392	0.1728	-0.0783	0.0639	0.0584	-0.0985	0.0619	-0.0252
32.49196				//	-0.0647	-0.4301	0.8353	-0.1181	0.0093	0.3001	0.0737	0.0124	0.0579	-0.0006
49.51187	0.04838	0.15154	0.00345	//	-0.1628	-0.1984	-0.0558	0.9566	0.0814	-0.0355	0.0260	0.0806	0.0275	-0.0100
46.44193				//	-0.0744	-0.1264	0.0328	0.9660	0.0435	0.0912	-0.0832	0.0982	0.0817	0.1036
55.62521	1.20944	-0.70888	-0.09371	//	0.0070	0.0724	0.0802	-0.0493	0.6432	0.5362	-0.0408	0.4726	-0.0291	0.2424
49.73695				//	-0.0143	0.0060	-0.0328	-0.0223	0.7044	0.1549	-0.2784	-0.6198	0.0290	0.1244
52.62840	0.16958	-0.25082	-0.11341	//	0.1558	-0.0934	-0.1649	0.0986	-0.4476	0.6692	-0.1533	-0.2424	-0.3973	0.2045
47.34315				//	-0.0624	0.0022	-0.1865	-0.1796	0.0639	0.5442	-0.4679	0.5099	-0.0690	0.3809
53.11639	0.04010	-0.02142	-0.13151	//	-0.0188	0.0363	0.0425	-0.0221	-0.3623	-0.0922	0.5708	0.6155	-0.3892	-0.0141
51.93087				//	0.0069	0.4119	0.0268	-0.0146	0.2935	0.2491	0.5749	0.1947	0.5405	0.1434
51.76986	0.92649	-0.07293	0.64461	//	0.0195	-0.0026	-0.0003	-0.0013	-0.4585	0.0685	-0.4881	0.5238	0.5211	0.0241
52.96447				//	-0.1844	-0.0184	0.1722	-0.0388	0.5649	-0.5567	-0.1116	0.5225	-0.0823	-0.1149
54.16269	0.34771	0.38698	0.03476	//	-0.0060	0.1929	-0.1818	0.0307	-0.0999	0.3454	0.6146	-0.1801	-0.6228	0.0392
45.71367				//	0.0432	0.0200	0.0705	-0.0628	-0.1965	-0.1980	-0.5263	-0.0296	0.7838	-0.1373

ENERGIES FOR PERYLENE X TBXAPPROXIMATION

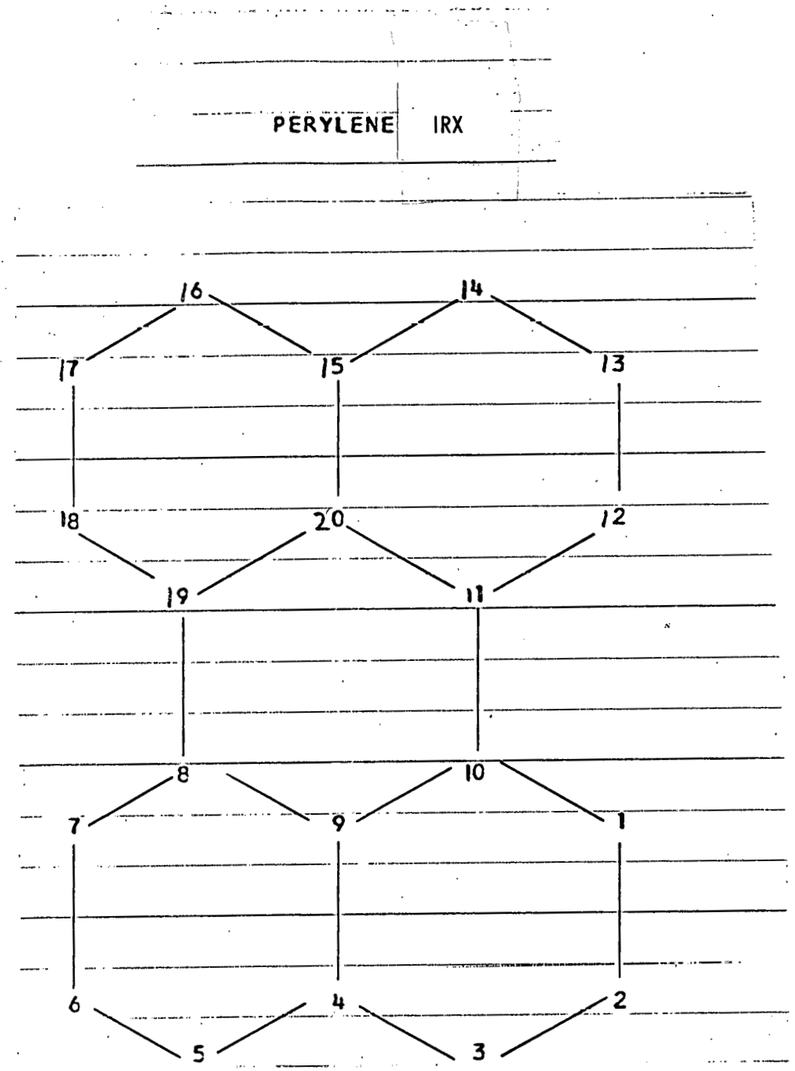
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	10,11	5,11	9,12	7,13	6,12	8,14	7,15	4,14	3,13	3,15
XMOMNT	-0.00001	-0.00010	0.12307	-0.32717	-0.07588	-0.00736	0.16260	-0.00006	-0.00550	-0.02450
YMOMNT	-1.21954	-0.12201	-0.34312	-0.00557	0.38893	0.49193	-0.00632	0.00004	-0.01874	-0.01652
JUMP E	12.9275	27.5543	39.3391	39.3407	39.3407	39.3418	39.3444	45.6541	48.2409	48.2446
DIAG E	24.3055	42.5872	54.7467	54.2569	51.7466	52.3100	53.8342	61.2809	64.5951	64.2405
DIAG E	24.3805	42.5554	54.8566	54.0754	52.3154	52.2539	53.5837	61.4078	64.5635	64.1399
CORRSP	23.2057	41.7083	56.5288	55.1531	49.9949	50.9572	52.0576	63.1795	67.1767	63.9417
CORRSP	23.3057	41.6578	56.6030	55.4849	50.4772	50.9628	51.8574	63.3350	67.1552	63.2930

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
23.20570	1.19365	-0.00057	-1.09981	//	0.9808	-0.0712	-0.1049	-0.0818	0.0214	0.0844	-0.0791	-0.0198	-0.0242	-0.0220
10.72033				//	0.9795	-0.0214	-0.0995	-0.1168	-0.0570	0.0355	-0.1087	-0.0131	-0.0083	-0.0079
41.70835	0.08600	0.03618	-0.21721	//	0.0579	0.9682	0.0310	-0.1163	-0.1153	0.0590	-0.0701	-0.0899	0.0897	0.0830
34.28591				//	0.0201	0.8771	0.3148	-0.2199	0.0048	-0.2111	-0.1367	0.0745	0.0873	0.0799
56.52882	0.06565	0.10587	-0.12688	//	0.0387	-0.0759	0.8441	-0.0058	-0.1317	0.5097	-0.0432	-0.0009	-0.0136	-0.0326
55.34159				//	0.0323	-0.0960	0.7036	0.0026	-0.1546	0.6794	-0.0371	0.0462	0.0383	-0.0645
55.15307	0.07004	-0.15586	-0.07464	//	0.1170	0.1047	0.0376	0.7220	0.1915	0.0676	0.5890	-0.0369	0.1933	0.1605
47.31932				//	-0.0080	0.0927	-0.0628	0.6659	-0.1916	-0.0239	-0.6425	-0.1245	0.2041	-0.1919
49.99493	0.23367	-0.04941	0.32782	//	-0.0156	0.1214	0.1233	-0.0874	0.8970	0.0281	-0.1626	0.3543	-0.0444	-0.0536
45.94557				//	0.0321	-0.1556	0.1633	0.0069	0.8027	-0.0663	-0.3232	0.4301	-0.0028	-0.0995
50.95718	1.31751	-0.02548	0.77933	//	-0.1341	-0.0420	-0.4889	-0.1178	0.0774	0.8415	0.0603	-0.0740	0.0192	0.0616
41.42954				//	-0.1019	0.2871	-0.5717	-0.1749	0.2027	0.6814	-0.1569	-0.0381	0.0992	0.0913
52.05757	0.24448	0.32099	-0.08603	//	0.0252	-0.0099	0.0996	-0.6045	0.0589	-0.0899	0.7305	0.0212	-0.1904	0.2053
50.60205				//	0.1636	0.2121	0.0276	0.6225	0.2962	0.0999	0.5814	-0.0014	0.2249	0.2318
63.17954	0.02965	0.00203	-0.10503	//	0.0256	0.0601	-0.0897	0.0753	-0.3437	0.0741	0.0735	0.9225	-0.0440	-0.0014
61.00365				//	-0.0165	-0.0286	-0.1563	0.0505	-0.4012	0.0146	0.0297	0.8621	0.1987	0.1650
67.17671	0.00719	0.01884	-0.04648	//	0.0045	-0.1432	-0.0453	-0.1792	0.0091	-0.0501	-0.1576	0.0832	0.7144	0.6330
64.39437				//	-0.0258	-0.2450	0.1055	-0.1997	0.0411	-0.1078	-0.1910	-0.2165	0.6541	0.6032

PERYLENE IRX



ATOMIC COORDINATES

x	3.5412	3.5269	2.6452	1.7706	0.8960	0.0143	0.	0.8602	1.7706	2.6810
y	1.4910	0.4510	0.	0.4580	0.	0.4510	1.4910	1.9850	1.4910	1.9850
	2.6810	3.5412	3.5269	2.6452	1.7706	0.8960	0.0143	0.	0.8602	1.7706
	3.0610	3.5550	4.5950	5.0460	4.5880	5.0460	4.5950	3.5550	3.0610	3.5550

PERYLENE X — IRX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 A A	5 S S	6 S A	7 A S	8 S S	9 S A	10 A A	11 A S	12 S S	13 S A
1.747259	1.619605	1.483752	1.379811	1.378752	1.188589	1.181615	1.171128	1.153014	1.026933	0.840426	0.756799	0.743845
0.180358	0.151330	-0.297189	0.277177	-0.084898	-0.283662	-0.062547	0.283559	-0.177808	-0.296249	-0.285591	-0.255487	-0.282150
0.141913	0.195345	-0.232121	0.325358	0.150721	-0.036006	0.274841	0.286054	-0.298857	0.127228	-0.129920	0.303794	0.293470
0.172124	0.267429	-0.142167	0.226686	0.303710	0.234478	0.291333	-0.003054	-0.087397	0.306625	0.304697	-0.046228	-0.028582
0.256349	0.357633	-0.000000	-0.000001	0.309080	0.260145	-0.000004	-0.279338	0.214968	-0.000000	0.000000	-0.261322	-0.263508
0.172124	0.267429	0.142167	-0.226684	0.303712	0.234470	-0.291339	-0.003052	-0.087398	-0.306625	-0.304698	-0.046228	-0.028583
0.141913	0.195345	0.232121	-0.325357	0.150723	-0.036013	-0.274839	0.286055	-0.298858	-0.127228	0.129920	0.303794	0.293471
0.180358	0.151330	0.297189	-0.277178	-0.084896	-0.283660	0.062557	0.283559	-0.177808	0.296249	0.285591	-0.255486	-0.282150
0.290608	0.133913	0.295951	-0.126210	-0.268780	-0.243983	0.292704	-0.020876	0.112169	0.228101	-0.242317	-0.028850	-0.010691
0.317474	0.266600	0.000000	-0.000000	-0.125111	-0.199471	0.000002	-0.310835	0.414102	0.000000	-0.000000	0.332640	0.311813
0.290608	0.133913	-0.295950	-0.126208	-0.268781	-0.243991	-0.292697	-0.020875	0.112168	-0.228101	0.242317	-0.028851	-0.010690
0.290608	-0.133913	-0.295950	-0.126210	-0.268781	-0.243983	-0.292703	-0.020873	-0.112169	0.228101	-0.242317	-0.028850	0.010690
0.180357	-0.151330	-0.297189	-0.277178	-0.084897	0.283660	-0.062555	0.283558	0.177811	0.296249	-0.285591	-0.255483	0.282153
0.141913	-0.195345	-0.232121	-0.325357	0.150723	0.036012	0.274840	0.286051	-0.298861	-0.127228	-0.129920	0.303790	-0.293474
0.172123	-0.267429	-0.142167	-0.226684	0.303712	-0.234470	0.291339	-0.003055	0.087398	-0.306625	0.304697	-0.046227	0.028582
0.256349	-0.357633	-0.000000	0.000001	0.309080	-0.260144	0.000003	-0.279337	-0.214971	0.000000	-0.000000	-0.261319	0.263511
0.172123	-0.267429	0.142167	0.226686	0.303710	-0.234477	-0.291333	-0.003054	0.087397	0.306625	-0.304697	-0.046228	0.028583
0.141913	-0.195345	0.232121	0.325358	0.150721	0.036005	-0.274840	0.286052	0.298860	0.127229	0.129920	0.303790	-0.293475
0.180357	-0.151330	0.297189	0.277177	-0.084898	0.283662	0.062548	0.283558	0.177811	-0.296249	0.285591	-0.255483	0.282153
0.290608	-0.133913	0.295951	-0.126208	-0.268781	0.243991	0.292697	-0.020874	-0.112168	-0.228101	-0.242317	-0.028851	0.010691
0.317474	-0.266601	0.000000	-0.000000	-0.125111	0.199472	-0.000003	-0.310830	-0.414105	-0.000000	0.000000	0.332636	-0.311817

OVERLAP EIGNVALUES AND EIGNVECTORS

14 A A	15 S S	16 A S	17 S A	18 A A	19 S S	20 S A
0.734343	0.715886	0.642344	0.617721	0.591496	0.531851	0.494808
-0.035400	0.214654	0.276049	-0.086143	0.290096	0.136050	-0.167299
-0.285313	0.036865	-0.322030	-0.134969	-0.215759	-0.177956	0.129940
0.295005	-0.240781	0.228191	0.295412	0.132539	0.260790	-0.166673
0.000000	0.209211	-0.000000	-0.338350	-0.000000	-0.385574	0.272568
-0.295005	-0.240781	-0.228191	0.295413	-0.132539	0.260790	-0.166673
0.285313	0.036865	0.322030	-0.134969	0.215759	-0.177956	0.129940
0.035401	0.214654	-0.276049	-0.086143	-0.290096	0.136050	-0.167299
-0.283399	-0.271688	0.134246	0.270619	0.318945	-0.134987	0.294291
-0.000000	0.312699	-0.000000	-0.115058	0.000000	0.280198	-0.327393
0.283399	-0.271688	-0.134246	0.270619	-0.318945	-0.134987	0.294291
-0.283399	-0.271688	-0.134246	-0.270619	0.318945	-0.134987	-0.294290
0.035400	0.214653	0.276049	0.086143	-0.290096	0.136050	0.167299
0.285313	0.036865	-0.322030	0.134969	0.215759	-0.177956	-0.129940
-0.295005	-0.240781	0.228191	-0.295413	-0.132539	0.260790	0.166673
-0.000001	0.209211	0.000000	0.338350	-0.000000	-0.385574	-0.272568
0.295005	-0.240781	-0.228191	-0.295412	0.132539	-0.260790	0.166673
-0.285312	0.036865	0.322030	0.134969	-0.215759	-0.177956	-0.129940
-0.035402	0.214653	-0.276049	0.086143	0.290096	-0.136050	0.167299
0.283399	-0.271688	0.134246	-0.270619	-0.318945	-0.134987	-0.294290
0.000001	0.312699	0.000000	0.115058	-0.000000	0.280198	0.327393

PERYLENE X

IRX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 S A	3 A S	4 A A	5 S S	6 S A	7 A S	8 S S	9 S A	10 A A	11 A S	12 S S	13 S A
32.00965	28.63340	24.40218	20.60226	20.56061	11.87551	11.50383	10.93664	9.93264	1.96296	-14.21116	-24.05203	-25.77436
0.136444	0.118911	-0.243979	0.235965	-0.072303	-0.260187	-0.057540	0.262024	-0.165590	-0.292339	-0.311527	-0.293682	-0.327144
0.107361	0.153496	-0.190561	0.276982	0.128361	-0.033026	0.252839	0.264329	-0.278321	0.125549	-0.141718	0.349212	0.340269
0.130215	0.210138	-0.116713	0.192981	0.258652	0.215073	0.268010	-0.002822	-0.081392	0.302577	0.332368	-0.053139	-0.033140
0.193934	0.281017	-0.000000	0.000001	0.263225	0.238616	-0.000004	-0.258124	0.200197	-0.000000	0.000000	-0.300390	-0.305529
0.130215	0.210138	0.116713	-0.192980	0.258654	0.215065	-0.268016	-0.002820	-0.081392	-0.302577	-0.332368	-0.053139	-0.033141
0.107361	0.153496	0.190561	-0.276981	0.128362	-0.033033	-0.252836	0.264330	-0.278322	-0.125549	0.141718	0.349212	0.340270
0.136444	0.118911	0.243979	-0.235966	-0.072301	-0.260185	0.057549	0.262024	-0.165590	0.292339	0.311527	-0.293682	-0.327144
0.219851	0.105225	0.242962	-0.107444	-0.228905	-0.223791	0.269271	-0.019291	0.104461	-0.225090	-0.264323	-0.033163	-0.012396
0.240176	0.209486	0.000000	-0.000000	-0.106550	-0.182963	0.000001	-0.287229	0.385647	-0.000000	-0.000000	0.382371	0.361537
0.219851	0.105225	-0.242962	0.107443	-0.228905	-0.223799	-0.269266	-0.019290	0.104460	-0.225090	0.264323	-0.033164	-0.012395
0.219851	-0.105225	-0.242962	-0.107444	-0.228905	0.223792	-0.269271	-0.019288	-0.104461	0.225090	-0.264323	-0.033163	0.012395
0.136444	-0.118911	-0.243979	-0.235966	-0.072301	0.260185	-0.057547	0.262023	0.165593	0.292339	-0.311527	-0.293678	0.327148
0.107360	-0.153496	-0.190561	-0.276981	0.128362	0.033032	0.252838	0.264326	0.278325	-0.125549	-0.141718	0.349207	-0.340273
0.130215	-0.210138	-0.116713	-0.192980	0.258654	-0.215066	0.268016	-0.002823	0.081392	-0.302578	0.332368	-0.053138	0.033140
0.193933	-0.281017	-0.000000	0.000001	0.263225	-0.238615	0.000003	-0.258122	0.200200	0.000000	-0.000000	-0.300386	0.305533
0.130215	-0.210138	0.116713	0.192981	0.258652	-0.215073	-0.268010	-0.002822	0.081392	0.302578	-0.332368	-0.053139	0.033141
0.107360	-0.153496	0.190561	0.276982	0.128361	0.033025	-0.252838	0.264327	0.278324	0.125549	0.141718	0.349208	-0.340275
0.136444	-0.118911	0.243979	0.235965	-0.072303	0.260186	0.057541	0.262023	-0.165593	-0.292339	0.311527	-0.293678	0.327148
0.219851	-0.105225	0.242962	0.107443	-0.228905	0.223799	0.269265	-0.019289	-0.104461	0.225090	-0.264323	-0.033164	0.012396
0.240176	-0.209487	0.000000	-0.000000	-0.106550	0.182964	-0.000003	-0.287224	-0.385650	-0.000000	-0.000000	0.382366	-0.361542

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 A A	15 S S	16 A S	17 S A	18 A A	19 S S	20 S A
-27.0763	-29.7041	-41.6740	-46.3186	-51.6906	-65.8811	-76.4164
-0.041310	0.253698	0.344431	-0.109604	0.377194	0.186553	-0.237834
-0.332945	0.043571	-0.401802	-0.171726	-0.280539	-0.244015	0.184725
0.344255	-0.284577	0.284718	0.375866	0.172332	-0.357598	-0.236944
0.000000	0.247265	-0.000000	-0.430497	-0.000000	-0.528704	0.387486
-0.344255	-0.284577	-0.284718	0.375866	-0.172332	0.357598	-0.236944
0.332944	0.043571	0.401802	-0.171727	0.280539	-0.244015	0.184725
0.041311	0.253698	-0.344432	-0.109604	-0.377194	0.186553	-0.237834
-0.330711	-0.321106	0.167501	0.344319	0.414706	-0.185096	0.418368
-0.000000	0.369577	-0.000000	-0.146393	0.000000	0.384211	-0.465427
0.330711	-0.321106	-0.167501	0.344320	-0.414706	-0.185096	0.418368
-0.330712	-0.321106	-0.167501	-0.344319	0.414706	-0.185096	-0.418367
0.041310	0.253697	0.344431	0.109604	-0.377194	0.186553	0.237834
0.332945	0.043571	-0.401802	0.171727	0.280539	-0.244016	-0.184725
-0.344255	-0.284577	0.284718	-0.375866	-0.172332	0.357598	0.236944
-0.000001	0.247265	0.000000	0.430497	-0.000000	-0.528705	-0.387486
0.344255	-0.284577	-0.284718	-0.375866	0.172332	0.357598	0.236944
-0.332943	0.043571	0.401803	0.171726	-0.280539	-0.244016	-0.184725
-0.041312	0.253697	-0.344431	0.109604	0.377194	0.186553	0.237834
0.330711	-0.321106	0.167501	-0.344320	-0.414706	-0.185096	-0.418367
0.000001	0.369577	0.000000	0.146393	-0.000000	0.384211	0.465427

PERYLENE X IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20										
1	1.02390	0.58222	-0.02017	-0.23422	-0.00426	0.16509	-0.00341	-0.13995	0.00607	0.69532	0.00698	-0.17439	0.00060	0.13385	-0.00264
	-0.07428	0.00339	0.11504	-0.00784	-0.08711										
2	0.58222	1.00983	0.73016	-0.00138	-0.17318	0.00399	0.16509	-0.00822	-0.25443	-0.00705	-0.06091	0.00060	0.00657	-0.00057	0.01362
	-0.00179	-0.02293	0.00339	0.03426	0.00356										
3	-0.02017	0.73016	1.01301	0.55340	0.01104	-0.17318	-0.00426	0.04357	0.01186	-0.29456	-0.00443	0.13385	-0.00057	-0.10515	0.00199
	0.05612	-0.00179	-0.07428	0.00304	0.05852										
4	-0.23422	-0.00138	0.55340	0.96213	0.55340	-0.00138	-0.23422	0.01157	0.52403	0.01157	-0.02256	-0.00264	0.01362	0.00199	-0.00503
	0.00199	0.01362	-0.00264	-0.02256	-0.00586										
5	-0.00426	-0.17318	0.01104	0.55340	1.01301	0.73016	-0.02017	-0.29456	0.01186	0.04357	0.00304	-0.07428	-0.00179	0.05612	0.00199
	-0.10515	-0.00057	0.13385	-0.00443	0.05852										
6	0.16509	0.00399	-0.17318	-0.00138	0.73016	1.00983	0.58222	-0.00705	-0.25443	-0.00822	0.03426	0.00339	-0.02293	-0.00179	0.01362
	-0.00057	0.00657	0.00060	-0.06091	0.00356										
7	-0.00341	0.16509	-0.00426	-0.23422	-0.02017	0.58222	1.02390	0.69532	0.00607	-0.13995	-0.00784	0.11504	0.00339	-0.07428	-0.00264
	0.13385	0.00060	-0.17439	0.00698	-0.08711										
8	-0.13995	-0.00822	0.04357	0.01157	-0.29456	-0.00705	0.69532	0.97679	0.52639	0.01191	-0.07643	-0.00784	0.03426	0.00304	-0.02256
	-0.00443	-0.06091	0.00698	0.34478	0.00311										
9	0.00607	-0.25443	0.01186	0.52403	0.01186	-0.25443	0.00607	0.52639	0.99081	0.52639	0.00311	-0.08711	0.00356	0.05852	-0.00586
	0.05852	0.00356	-0.08711	0.00311	-0.13857										
10	0.69532	-0.00705	-0.29456	0.01157	0.04357	-0.00822	-0.13995	0.01191	0.52639	0.97679	0.34478	0.00698	-0.06091	-0.00443	-0.02256
	0.00304	0.03426	-0.00784	-0.07643	0.00311										
11	0.00698	-0.06091	-0.00443	-0.02256	0.00304	0.03426	-0.00784	-0.07643	0.00311	0.34478	0.97679	0.69532	-0.00705	-0.29456	0.01157
	0.04357	-0.00822	-0.13995	0.01191	0.52639										
12	-0.17439	0.00060	0.13385	-0.00264	-0.07428	0.00339	0.11504	-0.00784	-0.08711	0.00698	0.69532	1.02390	0.58222	-0.02017	-0.23422
	-0.00426	0.16509	-0.00341	-0.13995	0.00607										
13	0.00060	0.00657	-0.00057	0.01362	-0.00179	-0.02293	0.00339	0.03426	0.00356	-0.06091	-0.00705	0.58222	1.00983	0.73016	-0.00138
	-0.17318	0.00399	0.16509	-0.00822	-0.25443										
14	0.13385	-0.00057	-0.10515	0.00199	0.05612	-0.00179	-0.07428	0.00304	0.05852	-0.00443	-0.29456	-0.02017	0.73016	1.01301	0.55340
	0.01104	-0.17318	-0.00426	0.04357	0.01186										
15	-0.00264	0.01362	0.00199	-0.00503	0.00199	0.01362	-0.00264	-0.02256	-0.00586	-0.02256	0.01157	-0.23422	-0.00138	0.55340	0.96213
	0.55340	-0.00138	-0.23422	0.01157	0.52403										
16	-0.07428	-0.00179	0.05612	0.00199	-0.10515	-0.00057	0.13385	-0.00443	0.05852	0.00304	0.04357	-0.00426	-0.17318	0.01104	0.55340
	1.01301	0.73016	-0.02017	-0.29456	0.01186										
17	0.00339	-0.02293	-0.00179	0.01362	-0.00057	0.00657	0.00060	-0.06091	0.00356	0.03426	-0.00822	0.16509	0.00399	-0.17318	-0.00138
	0.73016	1.00983	0.58222	-0.00705	-0.25443										
18	0.11504	0.00339	-0.07428	-0.00264	0.13385	0.00060	-0.17439	0.00698	-0.08711	-0.00784	-0.13995	-0.00341	0.16509	-0.00426	-0.23422
	-0.02017	0.58222	1.02390	0.69532	0.00607										
19	-0.00784	0.03426	0.00304	-0.02256	-0.00443	-0.06091	0.00698	0.34478	0.00311	-0.07643	-0.01191	-0.13995	-0.00822	0.04357	0.01157
	-0.29456	-0.00705	0.69532	0.97679	0.52639										
20	-0.08711	0.00356	0.05852	-0.00586	0.05852	0.00356	-0.08711	0.00311	-0.13857	0.00311	0.52639	0.00607	-0.25443	0.01186	0.52403
	0.01186	-0.25443	0.00607	0.52639	0.99081										

PERYLENE X IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20										
1	0.81147	0.41632	-0.09806	-0.24405	0.02140	0.17393	-0.00444	-0.14198	-0.05226	0.52173	-0.05666	-0.19012	0.00997	0.14358	-0.00323
	-0.08030	-0.00319	0.12310	0.00887	-0.08688										
2	0.41632	0.78542	0.55137	-0.06817	-0.17441	0.01453	0.17393	0.00775	-0.26590	-0.07338	-0.05726	0.00997	0.00703	-0.00561	0.01369
	0.00013	-0.02400	-0.00319	0.03587	0.01065										
3	-0.09806	0.55137	0.79030	0.37628	-0.06669	-0.17441	0.02140	0.05227	-0.04438	-0.31246	0.01512	0.14358	-0.00561	-0.11303	-0.00002
	0.06034	0.00013	-0.08030	0.00087	0.06249										
4	-0.24405	-0.06817	0.37628	0.69902	0.37628	-0.06817	-0.24405	-0.03111	0.37018	-0.03111	-0.01944	0.00323	0.01369	-0.00002	-0.00492
	-0.00002	0.01369	0.00323	-0.01944	0.00051										
5	0.02140	-0.17441	-0.06669	0.37628	0.79030	0.55137	-0.09806	-0.31246	-0.04438	0.05227	0.00087	-0.08030	0.00013	0.06034	-0.00002
	-0.11303	-0.00561	0.14358	0.01512	0.06249										
6	0.17393	0.01453	-0.17441	-0.06817	0.55137	0.78542	0.41632	-0.07338	-0.26590	0.00775	0.03587	-0.00319	-0.02400	0.00013	0.01369
	-0.00561	0.00703	0.00997	-0.05726	0.01065										
7	-0.00444	0.17393	0.02140	-0.24405	-0.09806	0.41632	0.81147	0.52173	-0.05226	-0.14198	0.00887	0.12310	-0.00319	-0.08030	0.00323
	0.14358	0.00997	-0.19012	-0.05666	-0.08688										
8	-0.14198	0.00775	0.05227	-0.03111	-0.31246	-0.07338	0.52173	0.73384	0.37202	-0.04115	-0.08058	0.00887	0.03587	0.00087	-0.01944
	-0.01512	-0.05726	-0.05666	0.19672	-0.04108										
9	-0.05226	-0.26590	-0.04438	0.37018	-0.04438	-0.26590	-0.05226	0.37202	0.75524	0.37202	-0.04108	-0.08688	0.01065	0.06249	0.00051
	0.06249	0.01065	-0.08688	-0.04108	-0.14910										
10	0.52173	-0.07338	-0.31246	-0.03111	0.05227	0.00775	-0.14198	-0.04115	0.37202	0.73384	0.19672	-0.05666	-0.05726	0.01512	-0.01944
	0.00087	0.03587	0.00887	-0.08058	-0.04108										
11	-0.05666	-0.05726	0.01512	-0.01944	0.00087	0.03587	0.00887	-0.08058	-0.04108	0.19672	0.73384	0.52173	-0.07338	-0.31246	-0.03111
	0.05227	0.00775	-0.14198	-0.04115	0.37202										
12	-0.19012	0.00997	0.14358	0.00323	-0.08030	-0.00319	0.12310	0.00887	-0.08688	-0.05666	0.52173	0.81147	0.41632	-0.09806	-0.24405
	0.02140	0.17393	-0.00444	-0.14198	-0.05226										
13	0.00997	0.00703	-0.00561	0.01369	0.00013	-0.02400	-0.00319	0.03587	0.01065	-0.05726	-0.07338	0.41632	0.78542	0.55137	-0.06817
	-0.17441	0.01453	0.17393	0.00775	-0.26590										
14	0.14358	-0.00561	-0.11303	-0.00002	0.06034	0.00013	-0.08030	0.00087	0.06249	0.01512	-0.31246	-0.09806	0.55137	0.79030	0.37628
	-0.06669	-0.17441	0.02140	0.05227	-0.04438										
15	0.00323	0.01369	-0.00002	-0.00492	-0.00002	0.01369	0.00323	-0.01944	0.00051	-0.01944	-0.03111	-0.24405	-0.06817	0.37628	0.69903
	0.37628	-0.06817	-0.24405	-0.03111	0.37018										
16	-0.08030	0.00013	0.06034	-0.00002	-0.11303	-0.00561	0.14358	0.01512	0.06249	0.00087	0.05227	0.02140	-0.17441	-0.06669	0.37628
	0.79030	0.55137	-0.09806	-0.31246	-0.04438										
17	-0.00319	-0.02400	0.00013	0.01369	-0.00561	0.00703	0.00997	-0.05726	0.01065	0.03587	0.00775	0.17393	0.01453	-0.17441	-0.06817
	0.55137	0.78542	0.41632	-0.07338	-0.26590										
18	0.12310	-0.00319	-0.08030	0.00323	0.14358	0.00997	-0.19012	-0.05666	-0.08688	0.00887	-0.14198	-0.00444	0.17393	0.02140	-0.24405
	-0.09806	0.41632	0.81147	0.52173	-0.05226										
19	0.00887	0.03587	0.00087	-0.01944	0.01512	-0.05726	-0.05666	0.19672	-0.04108	-0.08058	-0.04115	-0.14198	0.00775	0.05227	-0.03111
	-0.31246	-0.07338	0.52173	0.73384	0.37202										
20	-0.08688	0.01065	0.06249	0.00051	0.06249	0.01065	-0.08688	-0.04108	-0.14910	-0.04108	0.37202	-0.05226	-0.26590	-0.04438	0.37018
	-0.04438	-0.26590	-0.05226	0.37202	0.75524										

ENERGIES FOR PERYLENE X IRXAPPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	6,11	10,15	5,11	7,12	9,14	8,14	7,13	1,11	10,17	4,15
XMOMNT	-0.85455	0.81229	0.09588	-0.62656	0.49067	-0.41824	0.20566	-0.04802	-0.15188	0.08294
YMOMNT	-0.00001	-0.00000	0.00144	-0.00010	0.00288	-0.00216	0.00055	-0.00000	0.00010	-0.00000
JUMP E	24.7065	29.3794	33.7253	38.5546	39.2790	39.9560	40.1970	46.2310	46.6578	50.0222
DIAG E	36.4992	39.8067	46.4724	53.2991	53.8333	53.9622	52.3660	60.2435	56.6787	67.9211
DIAG E	36.8443	39.5712	47.0316	53.5134	54.4067	53.9985	51.7585	61.0477	55.8512	67.6528
CORRSP	29.9713	43.1444	45.5681	52.7333	53.9643	56.2252	50.3740	60.5442	59.5234	69.0337
CORRSP	30.0943	43.1797	46.0255	52.8208	54.1488	56.3763	49.9215	61.2131	59.0935	68.8021

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
29.97128	0.02303	-0.13441	0.00029	//	0.7536	0.5821	0.0014	-0.2236	-0.0476	-0.1976	-0.0161	-0.0333	-0.196	0.0151
27.19592				//	0.9069	-0.3027	-0.0024	0.1055	-0.1789	-0.1854	-0.0886	-0.0110	0.0183	-0.0107
43.14443	1.65742	0.95045	-0.00025	//	-0.5678	0.7081	0.3106	0.0041	-0.2214	-0.0143	-0.1541	0.0304	-0.0752	-0.0105
30.71514				//	0.3176	0.8655	-0.1059	-0.2998	0.0960	-0.1651	0.0983	-0.0343	0.0314	0.0249
45.56811	0.14243	-0.27111	0.00039	//	0.1986	-0.2649	0.8881	-0.1077	-0.2103	0.1547	0.0588	-0.0868	0.1037	-0.0104
48.39458				//	-0.0491	0.0944	0.5024	0.2508	-0.3243	-0.1589	0.5630	-0.0368	0.4519	-0.1430
52.73331	0.19021	-0.29124	-0.00117	//	0.2339	0.1728	0.0192	0.7579	0.0130	0.5356	0.0157	0.0333	-0.1536	-0.1693
46.83016				//	-0.1503	0.2478	-0.2866	0.6244	-0.2674	-0.3628	-0.3189	0.0015	-0.1287	-0.3501
53.96434	0.01005	0.06611	0.00312	//	-0.0403	0.1232	0.2466	0.3189	0.6632	-0.3700	0.0705	0.0260	0.4876	-0.0247
52.41021				//	-0.0775	-0.0913	0.3725	-0.0826	0.5293	-0.5772	-0.3810	-0.0634	0.2750	-0.0438
56.22519	2.51133	1.02486	0.00027	//	-0.0496	0.1587	0.0210	-0.4485	0.5298	0.6471	0.1290	0.1004	-0.0043	0.2110
53.14461				//	0.2072	0.1808	0.2020	0.5574	0.5546	0.4922	0.0049	0.1335	0.0041	-0.0712
50.37396	0.03322	0.12453	-0.00070	//	-0.0671	0.1260	-0.1232	0.0255	-0.3153	0.0551	0.8551	0.0303	0.3561	0.0484
32.77449				//	-0.0095	-0.1819	-0.6683	0.1093	0.3627	-0.2077	0.4409	0.0573	0.3680	0.0188
60.54424	0.04659	-0.13452	0.00049	//	0.0468	-0.0571	0.1098	0.0052	0.0001	-0.1434	0.0940	0.9520	-0.2150	-0.0210
57.20821				//	-0.0161	-0.0023	0.0880	-0.0497	-0.0238	-0.1960	0.0811	0.9562	-0.1630	0.0560
59.52341	0.19353	-0.27650	-0.00176	//	0.0562	0.0025	-0.1592	-0.0499	-0.2760	0.2605	-0.4527	0.2668	0.7405	-0.0196
59.14027				//	-0.0056	0.0840	-0.1397	-0.0569	-0.2388	0.3120	-0.4658	0.2274	0.7342	0.0891

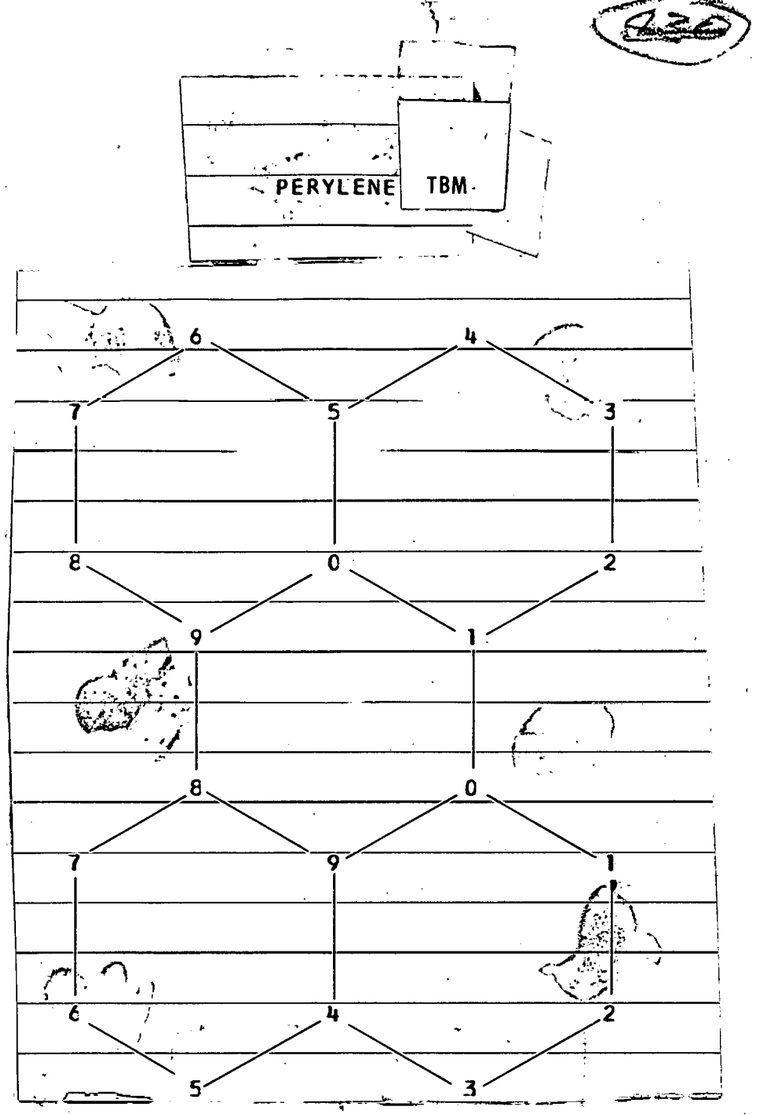
ENERGIES FOR PERYLENE X IRXAPPROXIMATION

CNE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	10,11	4,11	9,12	8,12	9,13	8,13	7,14	6,15	10,16	5,15
XMOMNT	0.00000	-0.00108	0.00016	-0.00034	-0.00232	-0.00180	0.00085	-0.00002	-0.00009	0.00092
YMOMNT	1.20477	0.12853	0.39453	0.41660	0.62466	-0.47257	-0.02701	0.46305	-0.15812	0.00087
JUMP E	13.1316	33.7745	37.4132	38.0903	39.0556	39.7327	40.4204	40.9543	43.6747	49.9730
DIAG E	23.6688	48.0943	50.4687	52.9195	52.4336	50.8900	55.8059	53.7181	57.1110	65.6516
DIAG E	23.6465	48.0392	51.1142	53.0280	52.2574	50.1767	55.9480	53.8500	57.7022	65.9976
CORRSP	22.2909	44.3333	48.4094	48.5640	54.1988	52.6460	54.9886	57.7099	60.1901	67.4303
CORRSP	22.2456	44.2891	48.7642	48.5894	54.1312	52.1732	55.3091	57.8360	60.6376	67.7843

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
22.29095	0.97672	0.00035	1.01507	//	0.9793	-0.0245	-0.0334	-0.1083	-0.0873	0.0140	0.1099	-0.0666	0.0530	0.0208
9.67513				//	0.9695	-0.0036	0.0047	-0.0931	0.1044	-0.1032	0.1595	-0.0600	0.0274	0.0027
44.33334	0.00010	-0.00161	-0.00703	//	-0.0075	0.6416	0.4462	-0.2268	0.1907	0.4644	0.0439	-0.0653	0.1923	0.2062
44.13178				//	0.0068	0.5560	0.4948	-0.3600	-0.1285	0.4249	0.0242	-0.1147	0.1969	0.2584
48.40945	0.24547	0.00052	0.34531	//	0.0322	-0.5554	0.6338	-0.1830	0.1220	-0.0923	-0.2872	0.2495	0.2474	0.1611
36.35935				//	0.1381	-0.1354	0.4949	0.3922	-0.3514	-0.0953	-0.2521	0.5936	0.0783	0.0960
48.56405	0.29251	0.00056	0.37635	//	0.0762	0.1982	0.2608	0.5865	-0.4909	0.0850	-0.0156	0.5379	-0.0583	-0.0425
34.39622				//	0.0102	0.5828	-0.0867	0.4666	0.2241	0.1352	0.3385	0.2706	-0.3898	-0.1636
54.19883	1.96714	-0.00193	0.92384	//	0.1157	0.0490	-0.1475	0.3542	0.8007	-0.0516	0.1284	0.4001	0.1103	-0.0674
45.85761				//	-0.0969	-0.0630	0.3491	-0.0231	0.8697	-0.1832	-0.1091	0.1309	0.1910	0.0937
52.64600	0.44139	-0.00134	-0.44402	//	0.0039	-0.4138	-0.1848	0.1165	0.0325	0.8674	-0.0893	-0.0123	-0.1377	-0.0243
49.43978				//	0.1513	-0.1484	-0.2685	0.2258	0.1885	0.7568	-0.4289	0.0462	0.1764	-0.0803
54.98857	0.07705	0.00077	0.18152	//	-0.0381	-0.1846	0.3973	0.0446	0.0884	-0.0233	0.7114	-0.1170	-0.5247	0.0340
52.98152				//	-0.0487	-0.5512	0.3243	-0.0802	0.0456	0.4142	0.5360	0.0312	-0.3461	0.0234
57.70987	0.16445	0.00059	-0.25886	//	-0.0750	0.0051	-0.2541	-0.6125	-0.1376	0.0711	0.2882	0.6685	-0.0255	-0.0012
57.11560				//	-0.0515	0.0113	-0.3429	-0.4210	-0.0043	0.0585	0.3103	0.6782	0.3725	-0.0630
60.19010	0.51612	0.00064	-0.44905	//	-0.1129	-0.1681	-0.0257	0.1366	-0.1683	0.0724	0.5283	-0.1373	0.7649	-0.1521
58.24843				//	-0.0586	-0.0400	0.0815	0.4549	-0.0655	0.0037	0.4438	-0.2782	0.6898	-0.1641



ATOMIC COORDINATES

x	3.4640	3.4640	2.5981	1.7321	0.8660	0.	0.	0.8660	1.7320	2.5980	
y	1.5000	0.5000	0.	0.5000	0.	0.5000	1.5000	2.0000	1.5000	2.0000	
	2.5980	3.4640	3.4640	2.5980	1.7320	0.8660	0.	0.	0.8660	1.7320	
	3.0000	3.5000	4.5000	5.0000	4.5000	5.0000	4.5000	3.5000	3.0000	3.5000	

PERYLENE (X) TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 A S	3 S A	4 S S	5 A A	6 A S	7 S A	8 S S	9 A S	10 A A	11 S A	12 S S	13 A A
1.638826	1.538518	1.463845	1.393308	1.378135	1.246826	1.246811	1.246799	1.246793	1.085725	0.914273	0.753205	0.753199
0.169590	0.148149	0.288662	0.048159	-0.288659	-0.021416	0.067131	-0.240375	0.366381	0.288690	0.288690	-0.343266	0.089707
0.118661	0.183580	0.214284	-0.167625	-0.328150	-0.276682	-0.217564	-0.194634	0.309447	-0.113989	0.113989	0.286542	-0.171160
0.137521	0.252360	0.114043	-0.315212	-0.214065	-0.255234	-0.284643	0.045734	-0.056926	-0.328201	-0.328201	0.056716	0.081432
0.237264	0.367005	-0.000000	-0.334649	0.000252	0.021485	-0.067046	0.240405	-0.366431	0.000016	-0.000016	-0.343312	0.089760
0.137481	0.252265	-0.114021	-0.314854	0.214515	-0.213409	0.284677	0.079827	-0.136341	0.328276	0.328276	0.124152	-0.348872
0.118628	0.183485	-0.214284	-0.167156	0.328402	-0.234892	0.351709	-0.160535	0.230026	0.114005	-0.114005	0.219100	0.259126
0.169575	0.148087	-0.288708	0.048484	0.288638	-0.021486	0.067034	-0.240364	0.366368	-0.288693	-0.288693	-0.343253	0.089743
0.320290	0.139635	-0.328310	0.244409	0.113832	0.213394	-0.284656	-0.079819	0.136328	-0.214272	0.214272	0.124140	-0.348845
0.339155	0.296208	-0.000046	0.096726	-0.000020	0.490109	-0.067027	0.114848	-0.173174	-0.000003	-0.000003	0.162453	0.177629
0.320297	0.139675	0.328224	0.244360	-0.114116	0.255252	0.284684	-0.045734	0.056923	0.214255	-0.214255	0.056714	0.081455
0.320300	-0.139609	0.328247	0.244530	0.113850	-0.213432	0.284605	0.079800	-0.136295	-0.214280	-0.214280	0.124110	-0.348810
0.169586	-0.148088	0.288670	0.048589	0.288634	-0.156134	-0.010587	-0.300271	-0.286919	-0.288677	0.288677	-0.313907	-0.085242
0.118647	-0.183513	0.214275	-0.167109	0.328377	0.057294	-0.295211	-0.380075	-0.150615	0.114018	0.114018	0.189789	0.434068
0.137518	-0.252325	0.114042	-0.314884	0.214481	0.213415	-0.284627	-0.079799	0.136296	0.328264	-0.328264	0.124110	-0.348819
0.237293	-0.367034	0.000050	-0.334677	0.000226	0.156124	0.010586	0.300282	0.286901	-0.000001	-0.000001	-0.313890	-0.085252
0.137518	-0.252329	-0.113963	-0.315172	-0.214039	0.255240	0.284694	-0.045707	0.056880	-0.328271	0.328271	0.056675	0.081485
0.118646	-0.183522	-0.214226	-0.167568	-0.328151	0.099135	0.274119	-0.345987	-0.230026	-0.114019	-0.114019	0.257219	0.003766
0.169584	-0.148103	-0.288656	0.048146	-0.288730	-0.156101	-0.010568	-0.300278	-0.286909	0.288683	-0.288683	-0.313897	-0.085246
0.320296	-0.139634	-0.328271	0.244283	-0.114223	-0.255239	-0.284677	0.045705	-0.056879	0.214283	0.214283	0.056673	0.081473
0.339170	-0.296191	0.000014	0.096735	-0.000096	-0.312540	0.010522	0.425796	0.093714	0.000006	-0.000006	0.133095	0.352598

OVERLAP EIGNVALUES AND EIGNVECTORS

14 A S	15 A A	16 S A	17 A S	18 A A	19 S S	20 A S
0.753186	0.753172	0.621862	0.606690	0.536153	0.461480	0.361172
-0.208555	-0.166151	-0.288659	0.048160	-0.288662	0.148149	-0.169590
0.332015	-0.189448	0.328150	0.167623	0.214283	-0.183580	0.118660
-0.123447	0.355543	-0.214066	-0.315211	-0.114043	0.252360	-0.137521
-0.208620	-0.166074	-0.000250	0.334649	-0.000001	-0.367005	0.237263
-0.117782	-0.023407	0.214513	-0.314855	0.114021	0.252265	-0.137481
0.326367	0.189448	-0.328401	0.167158	-0.214284	-0.183484	0.118628
-0.208588	-0.166042	0.288639	0.048482	0.288708	0.148087	-0.169575
-0.117775	-0.023405	-0.113834	-0.244409	-0.328310	-0.139635	0.320290
0.449835	-0.166085	-0.000020	0.096725	0.000046	0.296209	-0.339155
-0.123458	0.355580	0.114115	-0.244361	0.328224	-0.139675	0.320297
-0.117813	-0.023361	0.113851	0.244529	-0.328248	-0.139608	-0.320300
0.298518	0.045372	-0.288634	-0.048588	0.288670	0.148087	-0.169586
-0.180710	-0.021998	0.328376	-0.167111	-0.214276	-0.183512	-0.118647
-0.117803	-0.023385	-0.214480	0.314886	0.114043	0.252325	0.137518
0.298520	0.045385	0.000224	-0.334677	-0.000050	-0.367034	-0.237293
-0.123469	0.355565	0.214041	-0.315171	-0.113963	0.252329	-0.137518
-0.175036	-0.400966	-0.328152	-0.167566	0.214225	-0.183522	-0.118646
0.298501	-0.045407	0.288730	-0.048148	-0.288656	0.148104	0.169584
-0.123471	0.355552	-0.114222	0.244284	0.328271	-0.139634	-0.320297
-0.057246	-0.377571	0.000096	-0.096736	0.000014	0.296191	0.339170

PERYLENE (2)

TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 A S	3 S A	4 S S	5 A A	6 A S	7 S A	8 S S	9 A S	10 A A	11 S A	12 S S	13 A A
29.17542	26.19779	23.71620	21.12773	20.53632	14.81674	14.81602	14.81540	14.81515	5.90958	-7.01796	-24.52399	-24.52469
0.132475	0.119439	0.238584	0.040799	-0.245889	-0.019179	0.060120	-0.215274	0.328122	0.277059	0.301921	-0.395526	0.103364
0.092692	0.148004	0.177109	-0.142009	-0.279529	-0.247786	-0.194843	-0.174309	0.277134	-0.109396	0.119213	0.330165	-0.197218
0.107425	0.203455	0.094259	-0.267042	-0.182347	-0.228578	-0.254918	0.040959	-0.050981	-0.314978	-0.343243	0.065351	0.093830
0.185338	0.295883	-0.000000	-0.283508	0.000215	0.019241	-0.060045	0.215301	-0.328167	0.000016	-0.000017	-0.395578	0.103426
0.107393	0.203379	-0.094240	-0.266739	0.182731	-0.191121	0.254948	0.071491	-0.122103	0.315050	0.343322	0.143053	-0.401986
0.092666	0.147927	-0.177110	-0.141612	0.279743	-0.210361	0.314980	-0.143771	0.206006	0.109412	-0.119230	0.252456	0.298577
0.132463	0.119389	-0.238623	0.041075	0.245871	-0.019242	0.060033	-0.215264	0.328111	-0.277061	-0.301924	-0.395511	0.103406
0.250194	0.112575	-0.271354	0.207059	0.096966	0.191108	-0.254930	-0.071484	0.122092	-0.205639	0.224093	0.143039	-0.401955
0.264930	0.238806	-0.000038	0.081944	-0.000017	0.438924	-0.060027	0.102855	-0.155091	-0.000003	-0.000003	0.187185	0.204672
0.250199	0.112607	0.271283	0.207017	-0.097207	0.228595	0.254954	-0.040958	0.050979	0.205623	-0.224075	0.065348	0.093856
0.250202	-0.112554	0.271302	0.207161	0.096981	-0.191142	0.254884	0.071467	-0.122063	-0.205647	-0.224101	0.143005	-0.401915
0.132472	-0.119390	0.238591	0.041164	0.245868	-0.139828	-0.009482	-0.268915	-0.256958	-0.277046	0.301908	-0.361697	-0.098220
0.092681	-0.147950	0.177102	-0.141572	0.279722	0.051310	-0.264383	-0.340386	-0.134888	0.109425	0.119244	0.218683	0.500153
0.107422	-0.203427	0.094258	-0.266764	0.182702	0.191127	-0.254903	-0.071466	0.122063	0.315039	-0.343310	0.143005	-0.401926
0.185361	-0.295907	0.000041	-0.283532	0.000192	0.139819	0.009480	0.268925	0.256942	-0.000001	-0.000001	-0.361677	-0.098232
0.107422	-0.203431	-0.094192	-0.267008	-0.182325	0.228584	0.254964	-0.040934	0.050941	-0.315045	0.343316	0.065303	0.093891
0.092680	-0.147957	-0.177061	-0.141960	-0.279530	0.088782	0.245493	-0.309857	-0.206006	-0.109425	-0.119245	0.296379	0.004339
0.132470	-0.119403	-0.238580	-0.040789	-0.245949	-0.139799	-0.009465	-0.268921	-0.256949	0.277052	-0.301914	-0.361685	-0.098224
0.250199	-0.112575	-0.271322	0.206952	-0.097299	-0.228583	-0.254948	0.040933	-0.050940	0.205649	0.224104	0.065301	0.093877
0.264942	-0.238793	0.000011	0.081952	-0.000082	-0.279900	0.009423	0.381332	0.083928	0.000006	-0.000006	0.153357	0.406279

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 A S	15 A A	16 S A	17 A S	18 A A	19 S S	20 A S
-24.5264	-24.5284	-45.5117	-48.5217	-64.7521	-87.3405	-132.3847
-0.240308	-0.191450	-0.366047	0.061831	-0.394226	0.218083	-0.282191
0.382567	-0.218295	0.416127	0.215205	0.292647	-0.270239	0.197446
-0.142243	0.409681	-0.271457	-0.404686	-0.155748	0.371487	-0.228830
-0.240304	-0.191361	0.000317	0.429642	0.000001	-0.540251	0.394797
-0.135715	-0.026971	0.272023	-0.404229	0.155718	0.371347	-0.228763
0.376058	0.218295	-0.416444	0.214607	-0.292648	-0.270099	0.197393
-0.240347	-0.191324	0.366022	0.062244	0.394289	0.217991	-0.282165
-0.135707	-0.026969	-0.144353	-0.313786	-0.448374	-0.205550	0.532950
0.518324	-0.191374	-0.000025	0.124181	0.000063	0.436035	-0.564340
-0.142255	0.409723	0.144709	-0.313724	0.448256	-0.205609	0.532962
-0.135751	-0.026919	0.144375	0.313941	-0.448288	-0.205511	-0.532967
0.343969	0.052280	-0.366016	-0.062379	0.394238	0.217993	0.282184
-0.208224	-0.025348	0.416413	-0.214547	-0.292636	-0.270140	-0.197424
-0.135740	-0.026946	-0.271981	0.404268	0.155748	0.371436	0.228825
0.343971	0.052295	0.000284	-0.429677	-0.000068	-0.540294	-0.394847
-0.142268	0.409706	0.271425	0.404634	-0.155639	0.371442	0.228825
-0.201686	-0.462020	-0.416129	-0.215130	0.292568	-0.270154	-0.197423
0.343949	0.052321	0.366137	-0.061815	-0.394218	0.218017	0.282182
-0.142270	0.409690	-0.144844	0.313625	0.448320	-0.205549	-0.532961
-0.065962	-0.435062	0.000121	-0.124195	0.000019	0.436009	0.564366

PERYLENE TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20										
1	1.00000	0.62880	-0.00000	-0.23715	0.00000	0.13404	-0.00000	-0.11451	0.00000	0.64362	-0.00000	-0.20895	0.00000	0.16398	0.00000
	-0.09930	-0.00000	0.12438	0.00000	-0.08457										
2	0.62880	1.00000	0.70722	-0.00000	-0.15492	0.00000	0.13404	0.00000	-0.23711	-0.00000	-0.06357	0.00000	0.01861	-0.00000	0.00330
	0.00000	-0.01531	-0.00000	0.04039	0.00000										
3	-0.00000	0.70722	1.00000	0.55225	0.00000	-0.15488	-0.00000	0.05182	-0.00000	-0.31540	0.00000	0.16396	-0.00000	-0.14203	-0.00000
	0.08726	0.00000	-0.09928	-0.00000	0.06468										
4	-0.23715	-0.00000	0.55225	1.00000	0.55221	0.00000	-0.23713	-0.00000	0.52580	0.00000	-0.02318	-0.00000	0.00330	0.00000	0.00660
	-0.00000	0.00330	0.00000	-0.02319	0.00000										
5	0.00000	-0.15492	0.00000	0.55221	1.00000	0.70721	0.00000	-0.31543	-0.00000	0.05184	-0.00000	-0.09930	0.00000	0.08728	-0.00000
	-0.14205	-0.00000	0.16398	0.00000	0.06468										
6	0.13404	0.00000	-0.15488	0.00000	0.70721	1.00000	0.62882	0.00000	-0.23710	-0.00000	0.04039	0.00000	-0.01531	-0.00000	0.00330
	0.00000	0.01862	0.00000	-0.06357	-0.00000										
7	-0.00000	0.13404	-0.00000	-0.23713	0.00000	0.62882	1.00000	0.64361	0.00000	-0.11452	0.00000	0.12439	-0.00000	-0.09930	0.00000
	0.16398	0.00000	-0.20895	0.00000	-0.08456										
8	-0.11451	0.00000	0.05182	-0.00000	-0.31543	0.00000	0.64361	1.00000	0.52907	0.00000	-0.11509	-0.00000	0.04040	-0.00000	-0.02318
	-0.00000	-0.06358	0.00000	0.41364	0.00000										
9	0.00000	-0.23711	-0.00000	0.52580	-0.00000	-0.23710	0.00000	0.52907	1.00000	0.52907	0.00000	-0.08456	0.00000	0.06468	0.00000
	0.06467	0.00000	-0.08456	-0.00000	-0.16911										
10	0.64362	-0.00000	-0.31540	0.00000	0.05184	-0.00000	-0.11452	0.00000	0.52907	1.00000	0.41363	0.00000	-0.06357	-0.00000	-0.02318
	0.00000	0.04039	-0.00000	-0.11508	0.00000										
11	-0.00000	-0.06357	0.00000	-0.02318	-0.00000	0.04039	0.00000	-0.11509	0.00000	0.41363	1.00000	0.64361	-0.00000	-0.31543	0.00000
	0.05184	-0.00000	-0.11453	-0.00000	0.52908										
12	-0.20895	0.00000	0.16396	-0.00000	-0.09930	0.00000	0.12439	-0.00000	-0.08456	0.00000	0.64361	1.00000	0.62884	0.00000	-0.23712
	-0.00000	0.13404	0.00000	-0.11453	-0.00000										
13	0.00000	0.01861	-0.00000	0.00330	0.00000	-0.01531	-0.00000	0.04040	0.00000	-0.06357	-0.00000	0.62884	1.00000	0.70718	-0.00000
	-0.15492	0.00000	0.13404	0.00000	-0.23712										
14	0.16398	-0.00000	-0.14203	0.00000	0.08728	-0.00000	-0.09930	-0.00000	0.06468	-0.00000	-0.31543	0.00000	0.70718	1.00000	0.55226
	0.00000	-0.15492	-0.00000	0.05184	0.00000										
15	0.00000	0.00330	-0.00000	0.00660	-0.00000	0.00330	0.00000	-0.02318	0.00000	-0.02318	0.00000	-0.23712	-0.00000	0.55226	1.00000
	0.55226	0.00000	-0.23712	-0.00000	0.52576										
16	-0.09930	0.00000	0.08726	-0.00000	-0.14205	0.00000	0.16398	-0.00000	0.06467	0.00000	0.05184	-0.00000	-0.15492	0.00000	0.55226
	1.00000	0.70718	0.00000	-0.31542	-0.00000										
17	-0.00000	-0.01531	0.00000	0.00330	-0.00000	0.01862	0.00000	-0.06358	0.00000	0.04039	-0.00000	0.13404	0.00000	-0.15492	0.00000
	0.70718	1.00000	0.62884	0.00000	-0.23712										
18	0.12438	-0.00000	-0.09928	0.00000	0.16398	0.00000	-0.20895	0.00000	-0.08456	-0.00000	-0.11453	0.00000	0.13404	-0.00000	-0.23712
	0.00000	0.62884	1.00000	0.64360	0.00000										
19	0.00000	0.04039	-0.00000	-0.02319	0.00000	-0.06357	0.00000	0.41364	-0.00000	-0.11508	-0.00000	-0.11453	0.00000	0.05184	-0.00000
	-0.31542	0.00000	0.64360	1.00000	0.52908										
20	-0.08457	0.00000	0.06468	0.00000	0.06468	-0.00000	-0.08456	0.00000	-0.16911	0.00000	0.52908	-0.00000	-0.23712	0.00000	0.52576
	-0.00000	-0.23712	0.00000	0.52908	1.00000										

PERYLENE (1) TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20										
1	0.77123	0.45268	-0.05758	-0.21946	0.02209	0.12991	-0.00538	-0.10812	-0.03620	0.47425	-0.04877	-0.19927	0.00952	0.16069	0.00382
	-0.09883	-0.00570	0.12192	0.01568	-0.07734										
2	0.45268	0.75737	0.53031	-0.04075	-0.14584	0.00393	0.12992	0.01279	-0.21942	-0.04374	-0.05607	0.00952	0.01751	-0.00503	0.00288
	0.00290	-0.01462	-0.00570	0.03770	0.00382										
3	-0.05758	0.53031	0.77420	0.38446	-0.05889	-0.14580	0.02209	0.05630	-0.03549	-0.29697	0.01837	0.16066	-0.00503	-0.14026	-0.00214
	0.08707	0.00290	-0.09881	-0.00477	0.06185										
4	-0.21946	-0.04075	0.38446	0.72060	0.38445	-0.04073	-0.21943	-0.03096	0.36324	-0.03095	-0.01837	0.00382	0.00288	-0.00214	0.00577
	-0.00214	0.00289	0.00382	-0.01838	0.00764										
5	0.02209	-0.14584	-0.05889	0.38445	0.77424	0.53033	-0.05758	-0.29700	-0.03548	0.05633	-0.00477	-0.09884	0.00290	0.08709	-0.00214
	-0.14028	-0.00503	0.16069	0.01837	0.06185										
6	0.12991	0.00393	-0.14580	-0.04073	0.53033	0.75738	0.45269	-0.04374	-0.21941	0.01279	0.03770	-0.00570	-0.01462	0.00290	0.00289
	-0.00503	0.01751	0.00952	-0.05607	0.00382										
7	-0.00538	0.12992	0.02209	-0.21943	-0.05758	0.45269	0.77123	0.47424	-0.03620	-0.10813	0.01568	0.12192	-0.00570	-0.09883	0.00382
	0.16069	0.00952	-0.19926	-0.04877	-0.07734										
8	-0.10812	0.01279	0.05630	-0.03096	-0.29700	-0.04374	0.47424	0.72999	0.36608	-0.03868	-0.10124	0.01568	0.03770	-0.00477	-0.01837
	0.01837	-0.05607	-0.04877	0.25368	-0.03309										
9	-0.03620	-0.21942	-0.03549	0.36324	-0.03548	-0.21941	-0.03620	0.36608	0.72964	0.36609	-0.03309	-0.07733	0.00382	0.06184	0.00764
	0.06184	0.00382	-0.07733	-0.03309	-0.15467										
10	0.47425	-0.04374	-0.29697	-0.03095	0.05633	0.01279	-0.10813	-0.03868	0.36609	0.72999	0.25368	-0.04877	-0.05607	0.01837	-0.01837
	-0.00477	0.03770	0.01568	-0.10124	-0.03309										
11	-0.04877	-0.05607	0.01837	-0.01837	-0.00477	0.03770	0.01568	-0.10124	-0.03309	0.25368	0.72999	0.47423	-0.04374	-0.29699	-0.03095
	0.05632	0.01279	-0.10813	-0.03868	0.36610										
12	-0.19927	0.00952	0.16066	0.00382	-0.09884	-0.00570	0.12192	0.01568	-0.07733	-0.04877	0.47423	0.77123	0.45271	-0.05758	-0.21942
	0.02209	0.12992	-0.00537	-0.10813	-0.03620										
13	0.00952	0.01751	-0.00503	0.00288	0.00290	-0.01462	-0.00570	0.03770	0.00382	-0.05607	-0.04374	0.45271	0.75739	0.53030	-0.04074
	-0.14584	0.00393	0.12992	0.01279	-0.21942										
14	0.16069	-0.00503	-0.14026	-0.00214	0.08709	0.00290	-0.09883	-0.00477	0.06184	0.01837	-0.29699	-0.05758	0.53030	0.77422	0.38447
	-0.05890	-0.14584	0.02209	0.05632	-0.03549										
15	0.00382	0.00288	-0.00214	0.00577	-0.00214	0.00289	0.00382	-0.01837	0.00764	-0.01837	-0.03095	-0.21942	-0.04074	0.38447	0.72058
	0.38447	-0.04074	-0.21942	-0.03095	0.36321										
16	-0.09883	0.00290	0.08707	-0.00214	-0.14028	-0.00503	0.16069	0.01837	0.06184	-0.00477	0.05632	0.02209	-0.14584	-0.05890	0.38447
	0.77422	0.53030	-0.05758	-0.29699	-0.03549										
17	-0.00570	-0.01462	0.00290	0.00289	-0.00503	0.01751	0.00952	-0.05607	0.00382	0.03770	0.01279	0.12992	0.00393	-0.14584	-0.04074
	0.53030	0.75739	0.45271	-0.04374	-0.21942										
18	0.12192	-0.00570	-0.09881	0.00382	0.16069	0.00952	-0.19926	-0.04877	-0.07733	0.01568	-0.10813	-0.00537	0.12992	0.02209	-0.21942
	-0.05758	0.45271	0.77123	0.47423	-0.03620										
19	0.01568	0.03770	-0.00477	-0.01838	0.01837	-0.05607	-0.04877	0.25368	-0.03309	-0.10124	-0.03868	-0.10813	0.01279	0.05632	-0.03095
	-0.29699	-0.04374	0.47423	0.72999	0.36610										
20	-0.07734	0.00382	0.06185	0.00764	0.06185	0.00382	-0.07734	-0.03309	-0.15467	-0.03309	0.36610	-0.03620	-0.21942	-0.03549	0.36321
	-0.03549	-0.21942	-0.03620	0.36610	0.72965										

ENERGIES FOR PERYLENE TBMAPPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	10,11	5,11	9,12	8,13	6,12	7,14	9,15	6,15	4,13	3,14
XMOMNT	0.00000	-0.00000	0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	-0.00000
YMOMNT	-1.06232	0.07850	-0.46776	-0.53106	-0.27295	-0.07243	0.27352	-0.62330	0.03533	0.01466
JUMP E	15.7889	28.8625	35.3032	35.5410	36.9460	37.8012	39.6946	41.3374	42.8395	46.2831
DIAG E	27.3440	45.0076	49.0971	48.1925	50.2190	53.6786	52.7784	54.9897	58.0446	64.3300
DIAG E	27.4208	44.9168	49.0865	48.2441	50.4020	53.7540	52.4374	54.8423	58.3577	64.5186
CORRSP	26.1030	41.9347	52.3546	44.6727	47.8030	53.9199	55.2771	54.9884	60.7032	65.9247
CORRSP	26.2037	41.8038	52.1292	44.7401	47.9650	54.2637	55.1546	54.8129	61.0390	65.8679

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
26.10298	0.90514	0.00000	-0.90300	//	0.9742	0.0611	-0.0847	-0.1013	-0.0751	0.1331	0.0695	-0.0039	0.0287	0.0269
14.65925				//	0.9497	0.0315	-0.0903	-0.0933	-0.0117	0.2151	0.0144	0.1823	0.0029	0.0183
41.93469	0.02703	-0.00000	-0.12311	//	0.0013	0.8015	0.0803	0.1692	0.3681	-0.1288	0.3013	0.0687	-0.2253	0.1553
34.49057				//	-0.0005	0.7938	-0.0478	-0.1652	-0.2591	-0.3215	0.3404	0.0750	0.1596	0.1514
52.35459	0.06983	-0.00000	0.17710	//	-0.0321	-0.0407	0.6638	-0.6045	-0.0877	-0.0453	0.4188	0.0103	0.0359	-0.0690
53.94179				//	0.0400	0.2241	0.5161	-0.5386	0.0491	0.0940	-0.5003	-0.3413	-0.0910	0.0734
44.67265	1.07322	0.00000	-0.75162	//	0.1361	-0.1013	0.6559	0.7050	-0.1541	-0.0647	-0.0658	-0.0816	0.0714	-0.0062
31.68438				//	0.1637	0.0888	0.6792	0.6872	-0.0305	-0.1149	0.0387	-0.0606	0.0394	0.1042
47.80305	0.07685	-0.00000	-0.19443	//	0.0542	-0.4931	0.0221	0.1091	0.6820	0.2273	0.2830	-0.1717	-0.3387	0.0216
41.62216				//	-0.0420	0.3581	-0.1195	0.1430	0.7793	0.0546	-0.0384	0.1518	-0.4229	0.1474
53.91991	0.00081	0.00000	-0.01883	//	-0.1333	0.1652	0.1311	-0.0103	-0.1287	0.9095	-0.1013	0.0999	-0.0235	0.2702
49.68403				//	-0.2444	0.0879	0.1969	-0.0488	-0.1517	0.7926	0.2091	0.3405	0.0499	0.2792
55.27710	0.09834	-0.00000	-0.20453	//	-0.0436	-0.1748	-0.2046	0.2559	-0.1873	0.0457	0.6020	0.6631	0.1334	-0.0564
48.70669				//	0.0770	-0.1367	0.1250	-0.1709	0.1444	0.1113	0.7186	-0.5740	-0.2225	-0.0434
54.98841	1.52977	0.00000	-0.80882	//	0.0899	-0.0505	0.2340	-0.1342	0.4209	-0.0861	-0.5057	0.6853	0.0807	0.0111
52.34776				//	-0.0219	-0.2563	0.4314	-0.3762	0.2564	-0.3254	0.2654	0.5742	0.0924	-0.1609
60.70320	0.03294	-0.00000	0.11296	//	-0.0254	0.0740	-0.0339	0.0330	0.3614	0.1030	0.1187	-0.1993	0.8923	-0.0190
59.77760				//	0.0166	-0.0187	-0.0632	-0.0043	0.4528	0.0722	0.0087	-0.2069	0.8377	0.2013

ENERGIES FOR PERYLENE TBMAPPROXIMATION

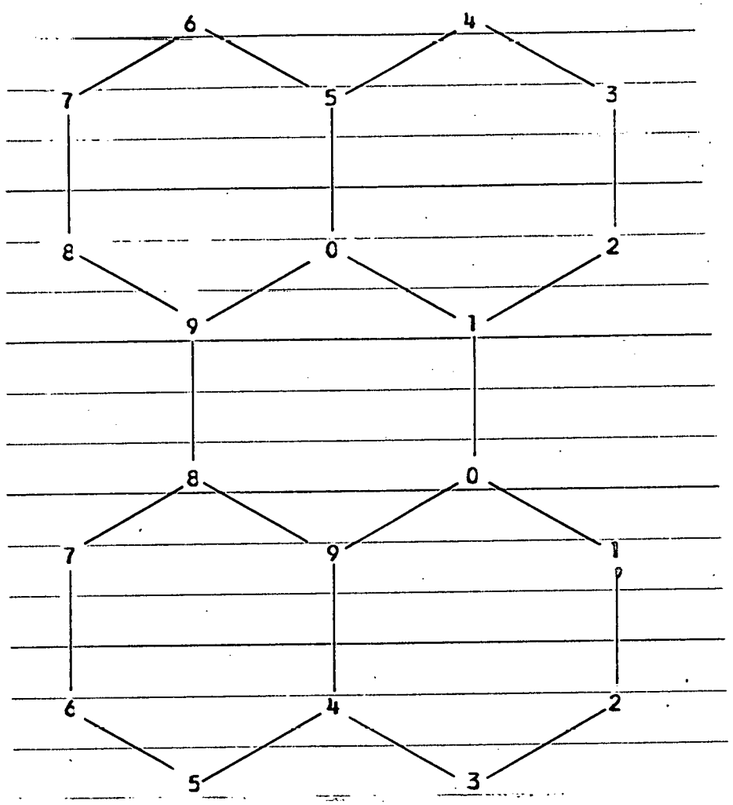
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	8,11	10,13	4,11	7,12	1,11	9,14	6,14	7,15	5,13	3,12
XMOMNT	0.83576	-0.83861	-0.15470	0.66976	0.04468	-0.67029	-0.00175	-0.00175	0.10087	0.11487
YMOMNT	0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
JUMP E	22.4836	28.8463	29.7821	36.0041	36.8457	37.1002	38.7430	40.3955	41.9198	44.4861
DIAG E	35.0532	40.6522	43.4575	50.8858	51.1339	51.9755	52.9552	54.4246	60.1433	60.9540
DIAG E	35.3708	40.4628	44.0367	50.7360	51.9077	52.1902	53.3635	53.9445	59.7864	60.9174
CORRSP	29.0288	43.1804	41.8012	49.5905	51.6680	53.7309	52.5025	56.3264	57.7742	66.0322
CORRSP	29.2575	43.2813	42.4609	49.5118	52.0525	53.6352	56.3277	52.7201	57.8447	65.6239

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
29.02881	0.05091	0.20307	0.00000	//	0.7886	0.5091	-0.0094	-0.2335	-0.0864	-0.2022	-0.0903	0.0738	-0.0039	-0.0476
25.68640				//	0.9135	-0.2149	0.0092	0.1263	-0.0520	-0.3069	0.0024	0.0762	0.0155	0.0176
43.18042	1.57390	-0.92581	-0.00000	//	-0.5332	0.7896	-0.1006	0.0334	0.1801	-0.1863	-0.0123	0.0825	0.0202	0.0805
30.81480				//	0.2487	0.8577	-0.1037	-0.3993	-0.0552	-0.0222	-0.1559	0.0085	-0.0254	-0.0605
41.80123	0.09569	-0.23202	0.00000	//	-0.0822	0.0767	0.9246	-0.0398	-0.1756	-0.1235	0.2673	0.0813	0.0432	-0.0703
33.54214				//	-0.0445	0.1702	0.8245	0.0076	-0.1481	-0.1195	0.3933	0.3063	0.0496	-0.0456
49.59050	0.22569	0.32714	-0.00000	//	0.2096	0.1774	0.1045	0.8082	-0.0165	0.3930	-0.0977	0.1584	0.2142	0.1591
49.67744				//	0.0926	0.2339	-0.0891	0.5913	-0.3182	0.5009	-0.0825	0.3173	-0.0659	0.3394
51.66803	0.01529	0.08341	0.00000	//	0.1849	-0.0121	0.1163	-0.0312	0.8883	0.1241	0.3483	-0.1580	-0.0070	0.0184
48.31396				//	0.0498	0.1781	0.0253	0.2135	0.9108	0.0069	0.1204	0.1678	-0.0936	0.1962
53.73088	2.00867	-0.93760	0.00000	//	-0.0234	0.2388	0.0183	-0.2970	-0.2292	0.7396	0.1895	-0.2232	-0.3480	0.2179
51.95709				//	0.2285	-0.0331	0.3698	0.0285	0.1797	0.5901	-0.2425	-0.4141	0.3266	-0.3029
52.50248	0.24288	0.32982	0.00000	//	0.0526	0.0782	-0.2176	0.2463	-0.2825	-0.2265	0.6191	-0.5702	0.2008	-0.0565
52.57048				//	0.0897	0.1572	-0.1813	0.1219	-0.0817	0.0886	0.7635	-0.5576	-0.0103	0.1047
56.32643	0.04422	-0.13588	-0.00000	//	-0.0042	-0.0206	-0.2476	-0.0984	-0.0802	0.1528	0.5635	0.7111	0.1356	-0.2392
54.63146				//	0.0748	-0.1073	-0.3427	-0.2131	0.0490	0.3178	0.3879	0.5340	0.3049	-0.4337
57.77415	0.67901	-0.52571	-0.00000	//	-0.0742	0.1052	0.0381	-0.1946	0.0251	0.3430	-0.2288	-0.2198	0.5890	-0.6150
43.41683				//	-0.1572	0.2450	-0.1174	0.5255	-0.0088	-0.4279	-0.0863	-0.0560	0.5821	-0.3046

PERYLENE IRM



ATOMIC COORDINATES

x	3.4640	3.4640	2.5981	1.7321	0.8660	0.	0.	0.8660	1.7320	2.5980
y	1.5000	0.5000	0.	0.5000	0.	0.5000	1.5000	2.0000	1.5000	2.0000

2.5980	3.4640	3.4640	2.5980	1.7320	0.8660	0.	0.	0.8660	1.7320
3.0000	3.5000	4.5000	5.0000	4.5000	5.0000	4.5000	3.5000	3.0000	3.5000

PERYLENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 A S	3 S A	4 A A	5 S S	6 S S	7 S A	8 A S	9 A S	10 A A	11 S A	12 S S	13 S S
1.803644	1.629664	1.507216	1.387227	1.385963	1.187623	1.184187	1.175551	1.163181	1.003343	0.853157	0.735520	0.723837
0.177726	0.156908	0.297493	-0.280980	-0.048406	0.295253	-0.036747	0.332971	0.001111	0.299059	-0.282016	0.305312	0.123388
0.129735	0.196517	0.229819	-0.332142	0.169265	0.278181	0.277256	0.196923	0.226795	-0.105434	-0.120820	-0.286507	0.118273
0.146827	0.257975	0.132350	-0.224037	0.311897	-0.023230	0.285817	-0.160605	0.213642	-0.328943	0.321640	-0.021284	-0.266509
0.236690	0.355653	0.000006	-0.003498	0.312384	-0.292974	0.000116	-0.336315	-0.038097	-0.000003	0.000034	0.304202	0.163509
0.146796	0.257895	-0.132340	0.217011	0.316808	-0.023205	-0.285594	-0.160922	0.213801	0.329008	-0.321722	-0.021288	-0.269092
0.129704	0.196424	-0.229838	0.328304	0.176671	0.278219	-0.277310	0.196615	0.226976	0.105449	0.120842	-0.286489	0.121040
0.177708	0.156839	-0.297550	0.282048	-0.042020	0.295235	0.036446	0.332968	0.001134	-0.299053	0.282012	0.305319	0.123195
0.312007	0.134773	-0.301980	0.117000	-0.251919	-0.008828	0.300129	0.130194	-0.220950	-0.203010	-0.228867	-0.038114	-0.256057
0.330649	0.278741	-0.000047	0.001290	-0.111914	-0.289023	-0.000142	-0.051310	-0.454450	-0.000008	0.000006	-0.230368	0.375166
0.312018	0.134822	0.301891	-0.111276	-0.254567	-0.008771	-0.300378	0.129905	-0.220794	0.202994	0.228846	-0.038094	-0.253494
0.312019	-0.134758	0.301915	0.117018	-0.252018	-0.008527	-0.300080	-0.130187	0.220980	-0.203024	0.228870	-0.038083	-0.256069
0.177721	-0.156846	0.297509	0.282047	-0.042118	0.295571	-0.036344	-0.332705	-0.001266	-0.299042	-0.282001	0.305313	0.122260
0.129722	-0.196452	0.229823	0.328281	0.176620	0.278258	0.277358	-0.196396	-0.227113	0.105466	-0.120849	-0.286514	0.121961
0.146826	-0.257944	0.132355	0.216978	0.316825	-0.023516	0.285536	0.160864	-0.213794	0.328998	0.321709	-0.021262	-0.269127
0.236711	-0.355672	0.000049	-0.003511	0.312408	-0.293251	-0.000199	0.335987	0.038230	0.000000	0.000001	0.304130	0.162603
0.146825	-0.257951	-0.132273	-0.224027	0.311881	-0.023461	-0.285858	0.160573	-0.213619	-0.329005	-0.321718	-0.021241	-0.266541
0.129720	-0.196464	-0.229768	-0.332167	0.169230	0.278311	-0.277256	-0.196670	-0.226954	-0.105468	0.120850	-0.286534	0.119257
0.177718	-0.156867	-0.297491	-0.281057	-0.048381	0.295566	0.036746	-0.332654	-0.001309	0.299048	0.282009	0.305310	0.122330
0.312014	-0.134788	-0.301939	-0.111367	-0.254500	-0.008584	0.300375	-0.129876	0.220788	0.203027	-0.228873	-0.038061	-0.253434
0.330660	-0.278727	0.000013	0.001231	-0.111922	-0.288820	0.000093	0.051026	0.454610	0.000006	0.000008	-0.230356	0.376152

OVERLAP EIGNVALUES AND EIGNVECTORS

14 A A	15 A S	16 S A	17 A S	18 A A	19 S S	20 A S
0.722277	0.719839	0.632833	0.617263	0.570950	0.525954	0.470748
-0.011793	0.294422	-0.283922	-0.039935	-0.284849	-0.144302	-0.161869
0.298337	-0.290085	0.325029	-0.159813	0.202689	0.171286	0.108377
-0.283832	0.015819	-0.217507	0.309113	-0.115068	-0.238564	-0.127565
0.000748	0.269898	-0.000223	-0.361967	-0.000008	0.375945	0.234574
0.281484	0.015719	0.217836	0.308800	0.115045	-0.238447	-0.127512
-0.297425	-0.289971	-0.325196	-0.159444	-0.202678	0.171186	0.108342
0.013080	0.294436	0.283920	-0.040162	0.284883	-0.144238	-0.161852
0.283813	-0.004632	-0.127597	0.243179	-0.338497	0.148566	0.327057
0.001668	-0.291935	0.000021	-0.075017	0.000047	-0.316987	-0.350143
-0.286130	-0.004509	0.127785	0.243169	0.338415	0.148598	0.327060
0.283745	0.005372	0.127614	-0.243315	-0.338437	0.148531	-0.327066
0.013015	-0.294860	-0.283916	0.040263	0.284851	-0.144238	0.161864
-0.297302	0.289708	0.325172	0.159407	-0.202670	0.171214	-0.108361
0.281415	-0.014936	-0.217806	-0.308844	0.115064	-0.238520	0.127557
0.000722	-0.270416	0.000184	0.361996	-0.000049	0.375984	-0.234612
-0.283916	-0.014819	0.217475	-0.309052	-0.114993	-0.238524	0.127557
0.298525	0.289583	-0.325012	0.159732	0.202626	0.171222	-0.108361
-0.011982	-0.294852	0.283990	-0.039935	-0.284837	-0.144251	0.161863
-0.286128	0.005488	-0.127907	-0.243089	0.338457	0.148550	-0.327065
0.001787	0.290663	0.000072	0.075037	0.000016	-0.316968	0.350163

PERYLENE (A) IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 A S	3 S A	4 A A	5 S S	6 S S	7 S A	8 A S	9 A S	10 A A	11 S A	12 S S	13 S S
33.34878	28.91863	25.18747	20.89226	20.84304	11.82428	11.64140	11.17708	10.50002	0.24938	-12.88222	-26.91321	-28.55558
0.132335	0.122913	0.242320	-0.238562	-0.041118	0.270928	-0.033769	0.307104	0.001030	0.298561	-0.305323	0.355997	0.145028
0.096601	0.153940	0.187197	-0.282000	0.143778	0.255263	0.254783	0.181625	0.210285	-0.105258	-0.130805	-0.334071	0.139016
0.109328	0.202083	0.107804	-0.190216	0.264932	-0.021317	0.262650	-0.148128	0.198090	-0.328395	0.348222	-0.024817	-0.313250
0.176240	0.278597	0.000005	-0.002970	0.265346	-0.268838	0.000107	-0.310188	-0.035323	-0.000003	0.000037	0.354703	0.192186
0.109305	0.202020	-0.107796	0.184251	0.269104	-0.021293	-0.262445	-0.148421	0.198238	0.328459	-0.348310	-0.024822	-0.316287
0.096578	0.153867	-0.187212	0.278742	0.150068	0.255298	-0.254833	0.181341	0.210454	0.105273	0.130829	-0.334050	0.142268
0.132322	0.122858	-0.242367	0.239469	-0.035693	0.270912	0.033492	0.307101	0.001051	-0.298554	0.305318	0.356006	0.144802
0.232321	0.105573	-0.245975	0.099337	-0.213986	-0.008101	0.275803	0.120080	-0.204866	-0.202672	-0.247781	-0.044441	-0.300965
0.246202	0.218349	-0.000038	0.001095	-0.095063	-0.265212	-0.000131	-0.047324	-0.421368	-0.000008	0.000006	-0.268612	0.440963
0.232330	0.105611	0.245902	-0.094477	-0.216235	-0.008048	-0.276031	0.119814	-0.204721	0.202656	0.247759	-0.044419	-0.297952
0.232330	-0.105562	0.245922	0.099353	-0.214070	-0.007825	-0.275758	-0.120074	0.204894	-0.202685	0.247784	-0.044405	-0.300979
0.132332	-0.122864	0.242333	0.239468	-0.035776	0.271221	-0.033399	-0.306859	-0.001174	-0.298543	-0.305307	0.355998	0.143702
0.096591	-0.153889	0.187200	0.278722	0.150025	0.255334	0.254877	-0.181139	-0.210581	0.105290	-0.130837	-0.334078	0.143351
0.109327	-0.202058	0.107809	0.184222	0.269118	-0.021579	0.262392	0.148367	-0.198231	0.328449	0.348297	-0.024792	-0.316327
0.176256	-0.278613	0.000040	-0.002981	0.265367	-0.269092	-0.000183	0.309886	0.035447	0.000000	0.000001	0.354619	0.191120
0.109327	-0.202063	-0.107742	-0.190207	0.264919	-0.021528	-0.262688	0.148099	-0.198069	-0.328456	-0.348306	-0.024767	-0.313288
0.096590	-0.153898	-0.187155	-0.282022	0.143748	0.255383	-0.254783	-0.181392	-0.210433	-0.105292	0.130838	-0.334102	0.140172
0.132329	-0.122880	-0.242318	-0.238628	-0.041096	0.271216	0.033767	-0.306812	-0.001214	0.298549	0.305315	0.355995	0.143784
0.232327	-0.105585	-0.245941	-0.094554	-0.216178	-0.007877	0.276029	-0.119787	0.204716	0.202688	-0.247788	-0.044379	-0.297882
0.246210	-0.218339	0.000011	0.001045	-0.095069	-0.265026	0.000085	0.047062	0.421517	0.000006	0.000009	-0.268597	0.442123

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 A A	15 A S	16 S A	17 A S	18 A A	19 S S	20 A S
-28.7790	-29.1300	-43.4253	-46.4085	-56.2441	-67.4591	-84.1474
-0.013876	0.347018	-0.356907	-0.050830	-0.376977	-0.198974	-0.235922
0.351038	-0.341906	0.408581	-0.203412	0.268245	0.236183	0.157958
-0.333972	0.018645	-0.273419	0.393444	-0.152285	-0.328950	-0.185924
0.000880	0.318113	-0.000280	0.460717	-0.000010	0.518382	0.341890
0.331208	0.018527	0.273832	0.393044	0.152254	-0.328790	-0.185847
-0.349966	-0.341772	-0.408791	-0.202943	-0.268230	0.236045	0.157907
0.015390	0.347035	0.356904	-0.051119	0.377023	-0.198887	-0.235897
0.333950	-0.005460	-0.160397	0.309522	-0.447976	0.204855	0.476683
0.001963	-0.344087	0.000027	-0.095483	0.000062	-0.437087	-0.510330
-0.336675	-0.005315	0.160633	0.309509	0.447868	0.204899	0.476687
0.333870	0.006332	0.160418	-0.309694	-0.447898	0.204807	-0.476695
0.015315	-0.347535	-0.356900	0.051248	0.376980	-0.198886	0.235915
-0.349821	0.341463	0.408760	-0.202895	-0.268220	0.236084	-0.157936
0.331127	-0.017605	-0.273795	-0.393101	0.152279	-0.328890	0.185913
0.000850	-0.318724	0.000231	0.460754	-0.000065	0.518436	-0.341945
-0.334071	-0.017466	0.273379	-0.393366	-0.152185	-0.328895	0.185913
0.351260	0.341315	-0.408559	0.203310	0.268162	0.236094	-0.157935
-0.014099	-0.347525	0.356992	0.050830	-0.376961	-0.198904	0.235914
-0.336673	0.006468	-0.160786	-0.309407	0.447924	0.204832	-0.476694
0.002103	0.342588	0.000091	0.095508	0.000021	-0.437060	0.510359

PERYLENE IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20										
1	1.02967	0.62726	-0.03035	-0.22960	-0.00087	0.14858	-0.00455	-0.13032	0.00924	0.64435	0.01627	-0.18668	-0.00466	0.16595	-0.00504
	-0.09493	0.00819	0.12873	-0.01553	-0.09535										
2	0.62726	1.00564	0.70331	-0.00340	-0.16534	0.00611	0.14858	-0.01250	-0.23064	-0.00279	-0.07565	-0.00466	0.00981	0.00293	0.01615
	-0.00553	-0.02829	0.00819	0.04499	0.00321										
3	-0.03035	0.70331	1.02994	0.55487	0.00594	-0.16529	-0.00085	0.04096	0.00617	-0.30875	-0.00896	0.16592	0.00293	-0.14968	0.00439
	0.08122	-0.00553	-0.09491	0.00789	0.07425										
4	-0.22960	-0.00340	0.55487	0.96100	0.55482	-0.00344	-0.22958	0.01986	0.52335	0.01985	-0.03076	-0.00503	0.01615	0.00438	-0.00281
	0.00439	0.01615	-0.00504	-0.03077	-0.01139										
5	-0.00087	-0.16534	0.00594	0.55482	1.02998	0.70331	-0.03036	-0.30878	0.00619	0.04098	0.00789	-0.09493	-0.00553	0.08124	0.00439
	-0.14970	0.00292	0.16594	-0.00896	0.07425										
6	0.14858	0.00611	-0.16529	-0.00344	0.70331	1.00566	0.62728	-0.00278	-0.23062	-0.01250	0.04499	0.00819	-0.02829	-0.00553	0.01615
	0.00293	0.00981	-0.00466	-0.07566	0.00321										
7	-0.00455	0.14858	-0.00085	-0.22958	-0.03036	0.62728	1.02965	0.64433	0.00925	-0.13032	-0.01553	0.12873	0.00819	-0.09493	-0.00504
	0.16594	-0.00466	-0.18667	0.01627	-0.09534										
8	-0.13032	-0.01250	0.04096	0.01986	-0.30878	-0.00278	0.64433	0.96199	0.53066	0.01976	-0.09870	-0.01553	0.04500	0.00789	-0.03076
	-0.00896	-0.07567	0.01628	0.40953	0.00542										
9	0.00924	-0.23064	0.00617	0.52335	0.00619	-0.23062	0.00925	0.53066	0.98449	0.53066	0.00542	-0.09533	0.00321	0.07425	-0.01139
	0.07425	0.00321	-0.09533	0.00543	-0.16315										
10	0.64435	-0.00279	-0.30875	0.01985	0.04098	-0.01250	-0.13032	0.01976	0.53066	0.96199	0.40953	0.01628	-0.07566	-0.00896	-0.03076
	0.00789	0.04499	-0.01553	-0.09870	0.00542										
11	0.01627	-0.07565	-0.00896	-0.03076	0.00789	0.04499	-0.01553	-0.09870	0.00542	0.40953	0.96199	0.64433	-0.00279	-0.30877	0.01985
	0.04098	-0.01250	-0.13033	0.01976	0.53068										
12	-0.18668	-0.00466	0.16592	-0.00503	-0.09493	0.00819	0.12873	-0.01553	-0.09533	0.01628	0.64433	1.02965	0.62730	-0.03036	-0.22956
	-0.00087	0.14859	-0.00455	-0.13033	0.00925										
13	-0.00466	0.00981	0.00293	0.01615	-0.00553	-0.02829	0.00819	0.04500	0.00321	-0.07566	-0.00279	0.62730	1.00566	0.70328	-0.00342
	-0.16534	0.00610	0.14859	-0.01250	-0.23064										
14	0.16595	0.00293	-0.14968	0.00438	0.08124	-0.00553	-0.09493	0.00789	0.07425	-0.00896	-0.30877	-0.03036	0.70328	1.02995	0.55487
	0.00596	-0.16534	-0.00087	0.04098	0.00618										
15	-0.00504	0.01615	0.00439	-0.00281	0.00439	0.01615	-0.00504	-0.03076	-0.01139	-0.03076	0.01985	-0.22956	-0.00342	0.55487	0.96098
	0.55487	-0.00342	-0.22956	0.01985	0.52331										
16	-0.09493	-0.00553	0.08122	0.00439	-0.14970	0.00293	0.16594	-0.00896	0.07425	0.00789	0.04098	-0.00087	-0.16534	0.00596	0.55487
	1.02995	0.70328	-0.03036	-0.30877	0.00618										
17	0.00819	-0.02829	-0.00553	0.01615	0.00292	0.00981	-0.00466	-0.07567	0.00321	0.04499	-0.01250	0.14859	0.00610	-0.16534	-0.00342
	0.70328	1.00566	0.62730	-0.00279	-0.23064										
18	0.12873	0.00819	-0.09491	-0.00504	0.16594	-0.00466	-0.18667	0.01628	-0.09533	-0.01553	-0.13033	-0.00455	0.14859	-0.00087	-0.22956
	-0.03036	0.62730	1.02965	0.64432	0.00925										
19	-0.01553	0.04499	0.00789	-0.03077	-0.00896	-0.07566	0.01627	0.40953	0.00543	-0.09870	0.01976	-0.13033	-0.01250	0.04098	0.01985
	-0.30877	-0.00279	0.64432	0.96199	0.53067										
20	-0.09535	0.00321	0.07425	-0.01139	0.07425	0.00321	-0.09534	0.00542	-0.16315	0.00542	0.53068	0.00925	-0.23064	0.00618	0.52331
	0.00618	-0.23064	0.00925	0.53067	0.98449										

PERYLENE (1) IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20										
1	0.81587	0.44710	-0.11613	-0.24154	0.02787	0.15754	-0.00867	-0.13227	-0.04752	0.47795	-0.05505	-0.20657	0.00546	0.17892	0.00239
	-0.10348	0.00064	0.13912	0.00420	-0.09502										
2	0.44710	0.77326	0.52876	-0.06692	-0.16787	0.01459	0.15755	0.00427	-0.24304	-0.06943	-0.07242	0.00545	0.01101	-0.00317	0.01628
	-0.00318	-0.03007	0.00064	0.04801	0.01154										
3	-0.11613	0.52876	0.81849	0.38228	-0.07537	-0.16782	0.02788	0.05086	-0.05039	-0.32649	0.01528	0.17889	-0.00317	-0.16146	0.00130
	0.08805	-0.00318	-0.10346	0.00533	0.07922										
4	-0.24154	-0.06692	0.38228	0.69766	0.38227	-0.06693	-0.24152	-0.02905	0.35971	-0.02905	-0.02695	0.00240	0.01628	0.00129	-0.00234
	0.00130	0.01629	0.00238	-0.02696	-0.00181										
5	0.02787	-0.16787	-0.07537	0.38227	0.81858	0.52878	-0.11613	-0.32652	-0.05036	0.05088	0.00532	-0.10348	-0.00318	0.08807	0.00130
	-0.16148	-0.00317	0.17891	0.01528	0.07922										
6	0.15754	0.01459	-0.16782	-0.06693	0.52878	0.77329	0.44712	-0.06944	-0.24303	0.00426	0.04802	0.00064	-0.03007	-0.00318	0.01628
	-0.00317	0.01102	0.00545	-0.07243	0.01154										
7	-0.00867	0.15755	0.02788	-0.24152	-0.11613	0.44712	0.81585	0.47793	-0.04752	-0.13227	0.00420	0.13911	0.00064	-0.10348	0.00239
	0.17891	0.00546	-0.20657	-0.05505	-0.09501										
8	-0.13227	0.00427	0.05086	-0.02905	-0.32652	-0.06944	0.47793	0.70976	0.36693	-0.03857	-0.10658	0.00420	0.04802	0.00533	-0.02696
	0.01528	-0.07243	-0.05504	0.23796	-0.04788										
9	-0.04752	-0.24304	-0.05039	0.35971	-0.05036	-0.24303	-0.04752	0.36693	0.73492	0.36693	-0.04788	-0.09500	0.01154	0.07921	-0.00181
	0.07921	0.01154	-0.09500	-0.04788	-0.17514										
10	0.47795	-0.06943	-0.32649	-0.02905	0.05088	0.00426	-0.13227	-0.03857	0.36693	0.70975	0.23795	-0.05504	-0.07243	0.01528	-0.02695
	0.00533	0.04802	0.00420	-0.10658	-0.04788										
11	-0.05505	-0.07242	0.01528	-0.02695	0.00532	0.04802	0.00420	-0.10658	-0.04788	0.23795	0.70976	0.47793	-0.06944	-0.32651	-0.02905
	0.05088	0.00427	-0.13228	-0.03857	0.36695										
12	-0.20657	0.00545	0.17889	0.00240	-0.10348	0.00064	0.13911	0.00420	-0.09500	-0.05504	0.47793	0.81585	0.44714	-0.11612	-0.24150
	0.02788	0.15755	-0.00867	-0.13228	-0.04752										
13	0.00546	0.01101	-0.00317	0.01628	-0.00318	-0.03007	0.00064	0.04802	0.01154	-0.07243	-0.06944	0.44714	0.77330	0.52875	-0.06693
	-0.16787	0.01458	0.15755	0.00427	-0.24305										
14	0.17892	-0.00317	-0.16146	0.00129	0.08807	-0.00318	-0.10348	0.00533	0.07921	0.01528	-0.32651	-0.11612	0.52875	0.81854	0.38229
	-0.07538	-0.16787	0.02788	0.05088	-0.05038										
15	0.00239	0.01628	0.00130	-0.00234	0.00130	0.01628	0.00239	-0.02696	-0.00181	-0.02695	-0.02905	-0.24150	-0.06693	0.38229	0.69763
	0.38229	-0.06693	-0.24150	-0.02905	0.35968										
16	-0.10348	-0.00318	0.08805	0.00130	-0.16148	-0.00317	0.17891	0.01528	0.07921	0.00533	0.05088	0.02788	-0.16787	-0.07538	0.38229
	0.81854	0.52875	-0.11612	-0.32651	-0.05038										
17	0.00064	-0.03007	-0.00318	0.01629	-0.00317	0.01102	0.00546	-0.07243	0.01154	0.04802	0.00427	0.15755	0.01458	-0.16787	-0.06693
	0.52875	0.77330	0.44714	-0.06944	-0.24305										
18	0.13912	0.00064	-0.10346	0.00238	0.17891	0.00545	-0.20657	-0.05504	-0.09500	0.00420	-0.13228	-0.00867	0.15755	0.02788	-0.24150
	-0.11612	0.44714	0.81585	0.47792	-0.04752										
19	0.00420	0.04801	0.00533	-0.02696	0.01528	-0.07243	-0.05505	0.23796	-0.04788	-0.10658	-0.03857	-0.13228	0.00427	0.05088	-0.02905
	-0.32651	-0.06944	0.47792	0.70976	0.36694										
20	-0.09502	0.01154	0.07922	-0.00181	0.07922	0.01154	-0.09501	-0.04788	-0.17514	-0.04788	0.36695	-0.04752	-0.24305	-0.05038	0.35968
	-0.05038	-0.24305	-0.04752	0.36694	0.73492										

ENERGIES FOR PERYLENE IRMAPPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	10,11	9,12	4,11	6,12	8,13	7,14	9,15	6,15	10,16	5,13	3,14	2,12	8,17	1,13	2,15
XMOMNT	-0.00000	0.00000	0.00000	0.00001	-0.00000	-0.00000	0.00000	0.00000	-0.00000	-0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000
YMOMNT	-1.04139	0.48949	-0.08841	0.31122	-0.48299	-0.04945	-0.36094	-0.61260	-0.09749	0.03440	0.01215	0.00405	-0.02322	-0.00449	0.05778
JUMP E	16.1741	33.9847	34.8134	35.9275	36.7110	38.5801	39.6367	41.5796	43.6369	46.3350	51.4785	52.6854	57.2553	57.7840	58.3375
DIAG E	27.0451	47.4615	50.4221	49.6013	48.9609	54.0310	52.0180	54.7728	58.4737	61.9211	69.7981	71.5083	70.6556	74.9891	76.7343
DIAG E	27.0644	47.7135	50.3273	49.7937	49.0556	54.1489	51.6672	54.3624	59.1232	62.2617	69.9461	71.6976	70.0897	75.4788	76.3207
CORRSP	25.7374	44.0172	49.2544	42.9448	51.5686	53.8030	54.3887	55.0471	60.1400	62.3361	70.1823	67.9444	73.7089	80.3581	76.9614
CORRSP	25.7496	44.2408	49.3228	42.8758	51.4602	54.4834	54.0098	54.7854	60.6392	62.6734	70.1210	68.1671	73.4240	80.6580	76.4396

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
25.73740	0.84236	0.00000	-0.87729	//	0.9746	0.0885	-0.0398	0.0895	-0.0853	0.1319	-0.0669	-0.0020	-0.0381	0.0240
					0.0172	0.0189	-0.0219	0.0203	0.0015					
14.60035				//	0.9507	0.0860	-0.0278	0.0506	-0.0921	0.2070	0.0221	-0.1786	-0.0284	-0.0008
					0.0071	-0.0227	-0.0100	-0.0164	0.0084					
44.01715	1.02636	0.00000	0.74048	//	-0.1298	0.7537	0.0404	0.0037	-0.6242	0.0867	0.0408	-0.0585	0.0582	-0.0433
					-0.0100	0.0541	-0.0246	0.0433	-0.0199					
31.18325				//	-0.1608	0.7121	0.0708	0.0720	-0.6340	0.1146	0.1439	-0.0458	0.0308	-0.0534
					-0.0882	0.0498	0.0388	0.0511	0.0290					
49.25435	0.02408	-0.00000	-0.10722	//	0.0269	-0.0533	0.7227	-0.4215	0.0293	0.3963	-0.0672	0.2886	0.1760	-0.1029
					-0.0402	0.0319	-0.0113	0.0221	-0.0766					
33.20609				//	0.0033	-0.0097	0.5402	-0.4351	0.1914	0.3714	0.3298	0.1081	0.3608	-0.2215
					-0.1167	-0.0328	0.1615	0.0129	-0.0592					
42.94484	0.02730	0.00001	0.12228	//	-0.0179	-0.1026	0.4243	0.6242	-0.1113	0.0070	0.4634	0.1441	-0.1883	0.2905
					-0.1327	0.0430	0.1784	-0.0195	-0.0026					
42.25978				//	0.0157	-0.2172	0.4997	0.6766	-0.0977	0.0729	0.1384	0.2494	-0.0997	0.2926
					-0.1744	-0.0120	0.1013	-0.0569	-0.0961					
51.56858	0.18027	-0.00000	-0.28671	//	0.0644	0.5279	-0.0451	-0.1917	0.6296	-0.0515	0.4996	0.0890	-0.0572	-0.0290
					0.0335	0.0417	0.1132	-0.0221	0.0400					
53.11804				//	-0.0328	0.5354	0.3040	0.1445	0.6113	-0.0575	-0.2336	-0.3329	-0.1129	0.1217
					-0.0313	0.1117	-0.0966	0.0308	-0.0721					
53.80301	0.01967	-0.00000	-0.09273	//	-0.0579	-0.2059	-0.4143	0.0157	-0.1292	0.6436	0.4133	0.0877	0.3548	0.0020
					0.1869	0.0051	0.0675	0.0118	0.0860					
49.96744				//	-0.2520	-0.2419	-0.1106	0.1915	-0.0593	0.5965	0.0683	-0.6512	0.0712	0.0765
					0.1548	-0.0282	-0.0647	-0.0229	0.0268					
54.38868	0.07555	-0.00000	-0.18073	//	0.1233	-0.2564	-0.0811	-0.4891	-0.4105	-0.4620	0.4547	0.2536	-0.0972	-0.0455
					-0.0472	0.0015	0.0808	-0.0060	0.0066					
45.32877				//	0.0093	0.0329	-0.1411	0.0121	0.1797	-0.2790	0.8156	-0.2049	-0.2549	0.0887
					0.0269	0.1107	0.2015	0.0525	0.1798					
55.04711	1.37263	0.00000	0.76575	//	-0.0242	0.1243	-0.2022	0.2339	0.0444	-0.1453	-0.2676	0.8657	0.1974	-0.0426
					0.0007	-0.0202	0.0457	0.0141	-0.0289					
52.39877				//	-0.0236	0.2744	-0.4524	0.3132	0.3541	0.4099	0.1148	0.4725	0.1525	-0.0844
					0.1499	-0.1170	0.1204	-0.0754	0.0694					
60.14001	0.15802	0.00000	-0.24857	//	0.0677	0.0183	0.1069	-0.0110	0.0467	-0.3252	0.0196	-0.1704	0.7764	0.4439
					-0.0241	0.2048	-0.0398	-0.0000	0.0476					
58.83336				//	0.0372	0.0097	-0.1079	0.2762	0.0280	-0.3943	0.0666	-0.2488	0.7368	-0.1024
					-0.2341	-0.2298	0.0104	-0.1625	-0.0250					

ENERGIES FOR PERYLENE IRMAPPROXIMATION

ONE ELECTRON EXCITATIONS OF AS SYMMETRY.

JUMP	8,11	10,13	5,11	7,12	9,14	6,14	7,15	1,11	4,13	10,17
XMOMNT	-0.86812	0.84337	0.12443	0.70041	0.68627	0.13737	0.02091	-0.05810	0.09362	0.15715
YMOMNT	0.00000	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.00001	0.00000	0.00000	0.00000
JUMP E	25.1478	27.7373	34.7718	35.5559	37.0090	38.9518	41.2079	46.2208	46.3766	48.2816
DIAG E	37.6423	39.4732	48.6942	50.4356	51.8131	53.2288	54.2040	61.2792	64.2691	59.3614
DIAG E	37.9526	39.2769	49.2506	50.4411	52.1774	53.5335	53.6068	61.9846	63.9587	58.5045
CORRSP	30.0127	43.6502	46.7920	49.6910	54.1674	54.7510	52.4272	61.5065	65.3717	62.0312
CORRSP	30.1172	43.7152	47.3602	49.4920	54.3791	54.8194	52.2313	62.2582	65.0883	61.2255

FINAL EXCITED STATES OF AS SYMMETRY.

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
30.01273	0.00598	-0.06848	-0.00000	//	0.7069	0.6114	0.0016	0.2565	-0.1988	-0.1298	-0.0529	-0.0370	0.0108	0.0118
27.16044				//	0.7786	-0.4789	0.0313	-0.2422	-0.3122	-0.0162	-0.0775	-0.0076	-0.0323	0.0071
43.65021	1.65144	0.94323	0.00000	//	-0.6261	0.7158	0.1328	-0.1219	-0.2087	0.0659	-0.0915	0.0513	-0.0415	0.0493
30.11609				//	0.5218	0.7574	-0.0575	0.3289	-0.1144	-0.1636	-0.0025	-0.0409	0.0236	-0.0210
46.79198	0.00721	-0.06019	-0.00000	//	0.0725	-0.1580	0.8631	0.1733	-0.2125	0.3700	-0.0313	-0.1065	0.0012	-0.0220
51.51542				//	0.2034	0.1597	0.4168	-0.3401	0.4243	0.2827	0.5316	-0.0157	-0.0927	-0.3038
49.69095	0.22341	0.32515	-0.00001	//	-0.2720	-0.1302	-0.1975	0.7449	-0.4134	-0.1080	0.2795	0.0183	0.1860	-0.1399
45.15194				//	0.1804	-0.3380	0.1671	0.7084	0.3823	0.1705	0.0207	-0.0232	0.3837	-0.0076
54.16743	2.84915	1.11216	-0.00000	//	-0.0955	0.2236	0.1955	0.3790	0.8217	-0.0358	0.1263	0.0401	0.1922	-0.1676
49.68086				//	0.1979	0.0884	-0.2562	-0.3113	0.6929	-0.0211	-0.4635	0.0514	0.0244	0.3030
54.75096	0.31658	0.36874	0.00000	//	0.0268	0.0197	-0.3200	0.2570	0.1004	0.7200	-0.2752	0.1014	0.0740	0.4588
53.43465				//	0.0520	0.0746	-0.5080	0.0097	-0.1472	0.7461	0.2466	0.1522	0.0606	0.2600
52.42717	0.04225	-0.13766	-0.00001	//	0.1113	0.1390	-0.1189	-0.2353	-0.0237	0.4748	0.7838	0.0368	-0.0568	-0.2322
34.03302				//	0.0520	-0.1636	-0.6521	0.0224	0.1988	-0.4304	0.4317	0.0770	0.0418	-0.3550
61.50649	0.16873	-0.25399	0.00000	//	0.0680	-0.0363	0.0190	-0.0099	-0.0676	0.0929	-0.2340	0.8553	-0.0260	-0.4399
58.31383				//	0.0075	0.0306	0.1637	-0.0038	-0.0350	-0.1053	-0.0087	0.9745	0.1005	0.0067
65.37173	0.09960	-0.18928	0.00000	//	0.0436	0.0097	0.0274	-0.2632	-0.1019	-0.0003	-0.0113	0.0217	0.9574	0.0203
62.66358				//	-0.0407	0.0859	0.0846	-0.3073	-0.1101	-0.1999	0.2445	-0.1269	0.8096	0.3256

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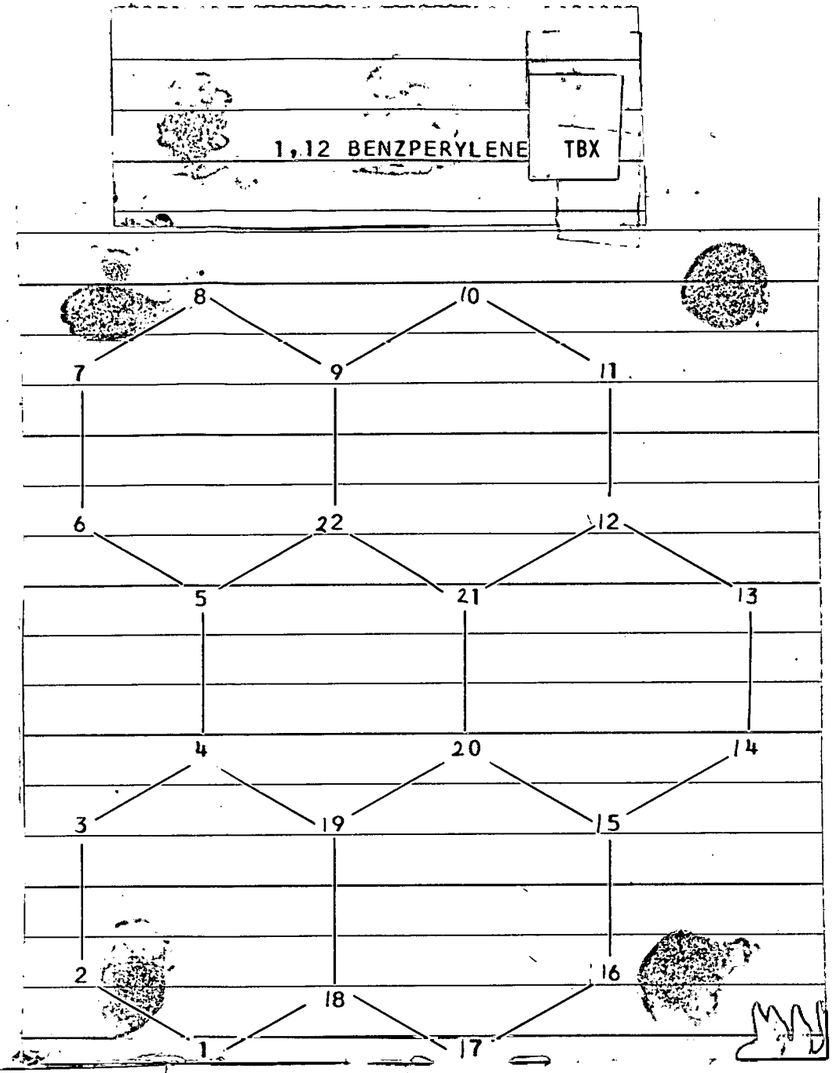


ATOMIC COORDINATES

x	0.8813	0.	0.	0.8777	0.8777	0.	0.	0.8813
y	0.	0.5050	1.5090	2.0150	3.0810	3.5870	4.5910	5.0960

1.7561	2.6439	3.5065	3.5230	4.3885	4.3885	3.5230
4.6040	5.0910	4.5960	3.5690	3.0550	2.0410	1.5270

3.5065	2.6439	1.7561	1.7525	2.6338	2.6338	1.7525
0.5000	0.0050	0.4920	1.5090	2.0360	3.0800	3.5870

1,12 BENZPERYLENE_X TBX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 S	7 A	8 A	9 S	10 S	11 A	12 S	13 A
1.621664	1.528429	1.491921	1.386942	1.382510	1.322586	1.266407	1.241791	1.236298	1.163393	1.111784	0.888214	0.836604
0.130319	-0.246146	0.148675	-0.214661	-0.276057	0.115111	0.103939	-0.213275	-0.299147	-0.061083	0.339525	-0.339525	-0.061083
0.106972	-0.178413	0.191957	-0.297283	-0.098589	0.291676	-0.215140	0.259740	-0.263687	0.215695	0.083068	0.083068	-0.215695
0.145215	-0.146153	0.241580	-0.261659	0.114305	0.272853	-0.335530	0.049393	0.036162	0.203566	-0.292307	0.292307	0.203567
0.267928	-0.140439	0.300456	-0.119346	0.283419	0.069800	-0.153713	-0.215458	0.305098	-0.081378	-0.221401	-0.221401	0.081377
0.267928	0.140438	0.300456	0.119334	0.283424	0.069800	0.153713	0.215465	0.305093	-0.081378	0.221401	-0.221401	-0.081378
0.145215	0.146152	0.241580	0.261654	0.114316	0.272854	0.335529	-0.049392	0.036163	0.203567	0.292307	0.292308	-0.203566
0.106972	0.178413	0.191957	0.297287	-0.098576	0.291677	0.215139	-0.259747	-0.263681	0.215695	-0.083069	0.083068	0.215695
0.130319	0.246146	0.148676	0.214673	-0.276048	0.115111	-0.103939	-0.213283	-0.299141	-0.061083	-0.339525	-0.339525	0.061083
0.227110	0.358150	0.112307	0.050503	-0.335710	-0.131760	-0.322284	0.041724	-0.032578	-0.250449	-0.074365	0.074365	-0.250448
0.146649	0.255408	-0.030624	-0.173571	-0.341448	-0.058533	-0.223731	-0.189704	0.277155	0.075957	0.305867	0.305868	-0.075957
0.147014	0.196622	-0.167918	-0.317091	-0.200700	0.050762	0.070481	-0.223492	0.293226	0.289718	0.208065	-0.208065	0.289717
0.236419	0.173017	-0.323718	-0.342556	0.037066	0.133926	0.322661	-0.028587	0.000038	0.122458	-0.229781	-0.229781	-0.122458
0.150060	0.054797	-0.310798	0.133024	0.062692	0.388505	0.155191	-0.014454	-0.003664	-0.394528	0.159258	0.159259	-0.394528
0.150059	-0.054797	-0.310798	0.133021	0.062697	0.388505	-0.155191	0.014454	-0.003664	-0.394528	0.159259	0.159258	0.394528
0.236418	-0.173016	-0.323719	0.342554	0.037080	0.133926	-0.322661	0.028587	0.000038	0.122458	0.229781	-0.229781	0.122457
0.147014	-0.196622	-0.167919	0.317100	-0.200687	0.050762	-0.070480	0.223500	0.293221	0.289717	-0.208065	-0.208065	-0.289718
0.146649	-0.255408	-0.030625	0.173586	-0.341441	-0.058532	0.223732	0.189711	0.277151	0.075957	-0.305868	0.305867	0.075957
0.227110	-0.358150	0.112307	-0.050488	-0.335712	-0.131760	0.322284	-0.041725	-0.032577	-0.250448	0.074365	0.074365	0.250449
0.312736	-0.286041	0.110505	-0.036279	0.088335	-0.238879	0.028753	-0.454311	0.003824	-0.186290	-0.006231	0.006231	-0.186290
0.328309	-0.139914	-0.192524	0.115099	0.194960	-0.270283	-0.137085	-0.207554	-0.287589	0.209524	0.150939	0.150939	-0.209523
0.328309	0.139914	-0.192524	-0.115107	0.194955	-0.270283	0.137085	0.207547	-0.287595	0.209523	-0.150939	0.150939	0.209523
0.312736	0.286040	0.110505	0.036276	0.088337	-0.238879	-0.028753	0.454310	-0.003836	-0.186290	0.006231	0.006231	0.186290

OVERLAP EIGNVALUES AND EIGNVECTORS

14 A	15 S	16 S	17 A	18 A	19 S	20 A	21 S	22 A
0.763699	0.758207	0.733590	0.677412	0.617487	0.613056	0.508077	0.471568	0.378334
0.299146	0.213277	-0.103939	-0.115111	-0.276053	0.214666	-0.148676	-0.246146	-0.130319
-0.263686	-0.259742	-0.215139	0.291677	0.098584	-0.297285	0.191957	0.178413	0.106972
-0.036162	0.049394	0.335529	-0.272854	0.114310	0.261657	-0.241580	-0.146152	-0.145215
0.305097	0.215458	-0.153713	0.069800	-0.283421	-0.119341	0.300456	0.140438	0.267928
-0.305094	0.215463	-0.153714	-0.069800	0.283422	-0.119339	-0.300456	0.140439	-0.267928
0.036163	0.049393	0.335529	0.272854	-0.114312	0.261656	0.241580	-0.146153	0.145215
0.263682	-0.259746	-0.215139	-0.291677	-0.098581	-0.297286	-0.191957	0.178413	-0.106972
-0.299142	0.213282	-0.103940	0.115111	0.276051	0.214668	0.148675	-0.246146	0.130319
0.032578	0.041725	0.322284	0.131760	-0.335711	-0.050497	-0.112307	0.358150	-0.227110
0.277154	0.189704	-0.223732	-0.058532	0.341445	-0.173577	-0.030625	-0.255408	0.146649
-0.293225	-0.223494	-0.070480	-0.050763	-0.200695	0.317095	0.167918	0.196622	-0.147014
0.000038	0.028588	0.322661	0.133926	-0.037072	-0.342555	-0.323719	-0.173016	0.236418
0.003664	-0.014454	-0.155191	-0.388505	0.062694	0.133023	0.310798	0.054797	-0.150059
-0.003664	-0.014454	-0.155190	0.388505	-0.062695	0.133023	-0.310798	0.054797	0.150059
-0.000038	0.028588	0.322661	-0.133926	0.037075	-0.342555	0.323719	-0.173017	-0.236418
0.293222	-0.223499	-0.070480	0.050763	0.200692	0.317096	-0.167918	0.196622	0.147014
-0.277151	0.189709	-0.223732	0.058532	-0.341444	-0.173580	0.030624	-0.255408	-0.146649
-0.032577	0.041726	0.322284	-0.131760	0.335712	-0.050494	0.112307	0.358150	0.227110
0.003826	-0.454310	-0.028752	0.238879	0.088336	0.036278	-0.110505	-0.286041	-0.312737
-0.287590	0.207552	-0.137086	-0.270284	-0.194958	0.115102	-0.192524	0.139914	0.328309
0.287593	0.207548	-0.137086	0.270284	0.194956	0.115104	0.192524	0.139914	-0.328309
-0.003833	0.454310	-0.028752	-0.238879	-0.088336	0.036277	0.110505	-0.286041	0.312736

1,12 BENZPERYLENE X — TBX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 S	7 A	8 A	9 S	10 S	11 A	12 S	13 A
28.52206	25.72336	24.53214	20.75742	20.58548	18.14710	15.65160	14.48696	14.22078	10.44947	7.48075	-9.36392	-14.53139
0.102336	-0.199100	0.121721	-0.182274	-0.234782	0.100093	0.092362	0.191389	-0.269044	-0.056631	0.322004	-0.360257	-0.066783
0.084002	-0.144313	0.157156	-0.252430	-0.083849	0.253623	-0.191176	0.233086	-0.237152	0.199975	0.078781	0.088141	-0.235820
0.114033	-0.118218	0.197783	-0.222181	0.097215	0.237256	-0.298156	0.044324	0.032523	0.188731	-0.277223	0.310156	0.222560
0.210396	-0.113597	0.245984	-0.101340	0.241043	0.060694	-0.136591	-0.193347	0.274396	-0.075447	-0.209976	-0.234921	0.088970
0.210396	0.113596	0.245984	0.101329	0.241048	0.060693	0.136592	0.193354	0.274391	-0.075447	0.209976	-0.234920	-0.088971
0.114033	0.118218	0.197783	0.222177	0.097224	0.237257	0.298156	-0.044323	0.032524	0.188731	0.277223	0.310157	-0.222559
0.084002	0.144312	0.157156	0.252434	-0.083838	0.253624	0.191176	-0.233091	-0.237146	0.199976	-0.078782	0.088140	0.235820
0.102336	0.199099	0.121721	0.182284	-0.234774	0.100094	-0.092362	-0.191396	-0.269038	-0.056632	-0.322004	-0.360258	0.066782
0.178343	0.289696	0.091946	0.042883	-0.285516	-0.114571	-0.286386	0.037442	-0.029300	-0.232197	-0.070527	0.078906	-0.273816
0.115159	0.206591	-0.025072	-0.147384	-0.290396	-0.050896	-0.198811	-0.170236	0.249265	0.070421	0.290084	0.324545	-0.083044
0.115446	0.159041	-0.137475	-0.269250	-0.170692	0.044140	0.062630	-0.200557	0.263719	0.268604	0.197328	-0.220771	0.316748
0.185653	0.139948	-0.265030	-0.290872	0.031524	0.116454	0.286721	-0.025654	0.000034	0.113533	-0.217924	-0.243812	-0.133883
0.117837	0.044324	-0.254452	-0.112954	0.053318	0.337819	0.137905	-0.012971	-0.003295	-0.365775	-0.151040	0.168984	-0.431338
0.117837	-0.044323	-0.254452	0.112952	0.053323	0.337819	-0.137905	0.012971	-0.003296	-0.365775	0.151040	0.168983	0.431338
0.185653	-0.139947	-0.265030	0.290871	0.031536	0.116454	-0.286722	0.025654	0.000034	0.113533	0.217924	-0.243812	0.133883
0.115446	-0.159041	-0.137476	0.269257	-0.170681	0.044140	-0.062630	0.200564	0.263714	0.268603	-0.197328	-0.220770	-0.316749
0.115159	-0.206591	-0.025073	0.147396	-0.290390	-0.050896	0.198811	0.170242	0.249261	0.070421	-0.290084	0.324545	0.083044
0.178343	-0.289696	0.091946	-0.042871	-0.285518	-0.114570	0.286386	-0.037443	-0.029299	-0.232196	0.070527	0.078906	0.273816
0.245583	-0.231369	0.090471	-0.030806	0.075128	-0.207714	0.025550	-0.407689	-0.003440	-0.172713	-0.005910	0.006612	-0.203671
0.257811	-0.113172	-0.157620	0.097733	0.165810	-0.235021	-0.121816	-0.186254	-0.258649	0.194254	0.143150	0.160156	-0.229072
0.257811	0.113172	-0.157620	-0.097740	0.165806	-0.235021	0.121816	0.186248	-0.258654	0.194254	-0.143150	0.160156	0.229072
0.245583	0.231369	0.090471	0.030803	0.075129	-0.207715	-0.025550	0.407688	-0.003450	-0.172713	0.005910	0.006611	0.203671

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 A	15 S	16 S	17 A	18 A	19 S	20 A	21 S	22 A
-23.02125	-23.72698	-27.01984	-35.43086	-46.08976	-46.96066	-72.03667	-83.37404	122.25557
0.342312	0.244934	-0.121354	-0.139859	-0.351301	0.274166	-0.208581	-0.358443	-0.211870
-0.301735	-0.298297	-0.251184	0.354385	0.125456	-0.379684	0.269302	0.259808	0.173913
-0.041380	0.056725	0.391745	-0.331515	0.145469	0.334182	-0.338919	-0.212830	-0.236088
0.349122	0.247440	-0.179467	0.084806	-0.360677	-0.152420	0.421518	0.204510	0.435594
-0.349118	0.247446	-0.179467	-0.084806	0.360678	-0.152417	-0.421517	0.204510	-0.435594
0.041381	0.056725	0.391745	0.331515	-0.145472	0.334181	0.338919	-0.212831	0.236088
0.301731	-0.298302	-0.251184	-0.354385	-0.125453	-0.379685	-0.269301	0.259809	-0.173913
-0.342308	0.244940	-0.121354	0.139860	0.351298	0.274169	0.208581	-0.358443	0.211870
0.037279	0.047918	0.376281	0.160087	-0.427220	-0.064494	-0.157558	0.521546	-0.369232
0.317147	0.217863	-0.261217	-0.071116	0.434518	-0.221688	-0.042964	-0.371930	0.238419
-0.335537	-0.256668	-0.082288	-0.061677	-0.255401	0.404985	0.235577	0.286325	-0.239013
0.000044	0.032832	0.376721	0.162719	-0.047177	-0.437502	-0.454154	-0.251950	0.384365
0.004193	-0.016600	-0.181192	-0.472030	0.079784	0.169894	0.436027	0.079796	-0.243964
-0.004193	-0.016600	-0.181192	0.472030	-0.079785	0.169893	-0.436027	0.079797	0.243964
-0.000043	0.032832	0.376721	-0.162719	0.047181	-0.437502	0.454154	-0.251951	-0.384365
0.335533	-0.256673	-0.082288	0.061677	0.255397	0.404987	-0.235577	0.286325	0.239013
-0.317144	0.217868	-0.261217	0.071116	-0.434516	-0.221692	0.042964	-0.371930	-0.238419
-0.037278	0.047919	0.376280	-0.160087	0.427221	-0.064490	0.157559	0.521546	0.369232
0.004378	-0.521746	-0.033569	0.290237	0.112414	0.046333	-0.155031	-0.416539	-0.508442
-0.329089	0.238360	-0.160054	-0.328393	-0.248100	0.147006	-0.270097	0.203746	0.533759
0.329092	0.238355	-0.160054	0.328396	0.248098	0.147008	0.270097	0.203746	-0.533759
-0.004387	-0.521746	-0.033569	-0.290237	-0.112414	0.046332	0.155030	-0.416539	0.508442

1,12 BENZPERYLENE X **T BX TOPOLOGICAL BOND ORDERS**

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.00000	0.67589	-0.00000	-0.30766	0.00000	0.12577	-0.00000	-0.11295	0.00000	0.05811	0.00000	-0.07851	-0.00000	0.10383	0.00000
	-0.19990	-0.00000	0.59538	0.00000	0.00985	-0.00000	0.07131								
2	0.67589	1.00000	0.65838	0.00000	-0.07699	-0.00000	0.03655	0.00000	-0.01966	-0.00000	0.01303	0.00000	-0.08241	-0.00000	0.09985
	0.00000	-0.12120	-0.00000	-0.25156	-0.00000	0.08454	0.00000								
3	-0.00000	0.65838	1.00000	0.62961	-0.00000	-0.16115	0.00000	0.12577	-0.00000	-0.06248	-0.00000	0.08735	-0.00000	-0.08226	-0.00000
	0.16509	0.00000	-0.26551	-0.00000	-0.07218	0.00000	-0.08413								
4	-0.30766	0.00000	0.62961	1.00000	0.38786	0.00000	-0.07699	-0.00000	0.00276	0.00000	-0.00594	-0.00000	0.09080	0.00000	-0.09607
	-0.00000	0.03043	0.00000	0.55739	0.00000	-0.15314	0.00000								
5	0.00000	-0.07699	-0.00000	0.38786	1.00000	0.62961	-0.00000	-0.30766	0.00000	0.03043	0.00000	-0.09607	0.00000	-0.09080	-0.00000
	0.00594	-0.00000	0.00276	-0.00000	-0.15314	0.00000	0.55739								
6	0.12577	-0.00000	-0.16115	0.00000	0.62961	1.00000	0.65838	0.00000	-0.26551	-0.00000	0.16509	0.00000	-0.08226	-0.00000	0.08735
	0.00000	-0.06248	-0.00000	-0.08413	-0.00000	-0.07218	0.00000								
7	-0.00000	0.03655	0.00000	-0.07699	-0.00000	0.65838	1.00000	0.67589	-0.00000	-0.12120	0.00000	0.09985	-0.00000	-0.08241	0.00000
	0.01303	0.00000	-0.01966	0.00000	0.08454	0.00000	-0.25156								
8	-0.11295	0.00000	0.12577	-0.00000	-0.30766	0.00000	0.67589	1.00000	0.59538	0.00000	-0.19990	-0.00000	0.10383	0.00000	-0.07851
	-0.00000	0.05811	0.00000	0.07131	0.00000	0.00985	0.00000								
9	0.00000	-0.01966	-0.00000	0.00276	0.00000	-0.26551	-0.00000	0.59538	1.00000	0.49661	-0.00000	-0.17370	0.00000	0.10347	-0.00000
	-0.02758	-0.00000	0.03216	-0.00000	-0.08001	0.00000	0.52815								
10	0.05811	-0.00000	-0.06248	0.00000	0.03043	-0.00000	-0.12120	0.00000	0.49661	1.00000	0.78212	0.00000	-0.17442	-0.00000	0.13360
	0.00000	-0.09985	-0.00000	0.04435	-0.00000	-0.24199	-0.00000								
11	0.00000	0.01303	-0.00000	0.00594	0.00000	0.16509	0.00000	-0.19990	-0.00000	0.78212	1.00000	0.49585	-0.00000	-0.13595	0.00000
	0.05032	-0.00000	-0.02758	0.00000	0.01648	0.00000	-0.23011								
12	-0.07851	0.00000	0.08735	-0.00000	-0.09607	0.00000	0.09985	-0.00000	-0.17370	0.00000	0.49585	1.00000	0.56852	0.00000	-0.22002
	-0.00000	0.13360	0.00000	-0.05346	0.00000	0.54647	0.00000								
13	-0.00000	-0.08241	-0.00000	0.09080	0.00000	-0.08226	-0.00000	0.10383	0.00000	-0.17442	-0.00000	0.56852	1.00000	0.71858	-0.00000
	-0.13595	0.00000	0.10347	-0.00000	-0.26116	-0.00000	-0.00469								
14	0.10383	-0.00000	-0.08226	0.00000	0.09080	-0.00000	-0.08241	0.00000	0.10347	-0.00000	-0.13595	0.00000	0.71858	1.00000	0.56852
	0.00000	-0.17442	-0.00000	-0.00469	-0.00000	-0.26116	-0.00000								
15	0.00000	0.09985	-0.00000	-0.09607	-0.00000	0.08735	0.00000	-0.07851	-0.00000	0.13360	0.00000	-0.22002	-0.00000	0.56852	1.00000
	0.49585	-0.00000	-0.17370	0.00000	0.54647	0.00000	-0.05346								
16	-0.19990	0.00000	0.16509	-0.00000	0.00594	0.00000	0.01303	-0.00000	-0.02758	0.00000	0.05032	-0.00000	-0.13595	0.00000	0.49585
	1.00000	0.78212	0.00000	-0.23011	-0.00000	0.01648	0.00000								
17	-0.00000	-0.12120	0.00000	0.03043	-0.00000	-0.06248	0.00000	0.05811	-0.00000	-0.09985	-0.00000	0.13360	0.00000	-0.17442	-0.00000
	0.78212	1.00000	0.49661	0.00000	-0.24199	0.00000	0.04435								
18	0.59538	-0.00000	-0.26551	0.00000	0.00276	-0.00000	-0.01966	0.00000	0.03216	-0.00000	-0.02758	0.00000	0.10347	-0.00000	-0.17370
	0.00000	0.49661	1.00000	0.52815	0.00000	-0.08001	-0.00000								
19	0.00000	-0.25156	-0.00000	0.55739	-0.00000	-0.08413	0.00000	0.07131	-0.00000	0.04435	0.00000	-0.05346	-0.00000	-0.00469	0.00000
	-0.23011	0.00000	0.52815	1.00000	0.50102	-0.00000	-0.16160								
20	0.00985	-0.00000	-0.07218	0.00000	-0.15314	-0.00000	0.08454	0.00000	-0.08001	-0.00000	0.01648	0.00000	-0.26116	-0.00000	0.54647
	-0.00000	-0.24199	0.00000	0.50102	1.00000	0.53009	0.00000								
21	-0.00000	0.08454	0.00000	-0.15314	0.00000	-0.07218	0.00000	0.00985	0.00000	-0.24199	0.00000	0.54647	-0.00000	-0.26116	0.00000
	0.01648	0.00000	-0.08001	-0.00000	0.53009	1.00000	0.50102								
22	0.07131	-0.00000	-0.08413	0.00000	0.55739	-0.00000	-0.25156	0.00000	0.52815	-0.00000	-0.23011	0.00000	-0.00469	-0.00000	-0.05346
	0.00000	0.04435	-0.00000	-0.16160	0.00000	0.50102	1.00000								

1,12 BENZPERYLENE X

TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.77547	0.50468	-0.05412	-0.28948	0.01510	0.12303	-0.00359	-0.11139	-0.00290	0.05793	0.00353	-0.07778	-0.00527	0.10120	0.01600
	-0.18989	-0.05486	0.42706	-0.03494	0.01449	-0.00116	0.06863								
2	0.50468	0.76194	0.48270	-0.04434	-0.07024	0.00815	0.03541	-0.00359	-0.01976	0.00143	0.01323	-0.00240	-0.08083	-0.00415	0.09653
	0.00586	-0.11286	-0.04093	-0.23413	0.01275	0.08150	0.00272								
3	-0.05412	0.48270	0.77119	0.46294	-0.04229	-0.15303	0.00815	0.12303	0.00326	-0.06220	-0.00425	0.08549	-0.00132	-0.08146	-0.00199
	0.16074	0.01925	-0.24804	-0.03728	-0.06624	0.01358	-0.07787								
4	-0.28948	-0.04434	0.46294	0.74170	0.24848	-0.04229	-0.07024	0.01510	0.00655	-0.00263	0.00423	0.01022	0.08809	0.00091	-0.09031
	0.01219	0.03486	-0.03118	0.39499	-0.03782	-0.14000	-0.02894								
5	0.01510	-0.07024	-0.04229	0.24848	0.74170	0.46294	-0.04434	-0.28948	-0.03118	0.03486	0.01219	-0.09031	0.00091	0.08809	0.01022
	0.00423	0.00263	0.00655	-0.02894	-0.14000	-0.03782	0.39499								
6	0.12303	0.00815	-0.15303	-0.04229	0.46294	0.77119	0.48270	-0.05412	-0.24804	0.01925	0.16074	-0.00199	-0.08146	-0.00132	0.08549
	-0.00424	-0.06220	0.00326	-0.07787	0.01358	-0.06624	-0.03728								
7	-0.00359	0.03541	0.00815	-0.07024	-0.04434	0.48270	0.76194	0.50468	-0.04093	-0.11286	0.00586	0.09653	-0.00415	-0.08083	-0.00240
	0.01323	0.00143	-0.01976	0.00272	0.08150	0.01275	-0.23413								
8	-0.11139	-0.00359	0.12303	0.01510	-0.28948	-0.05412	0.50468	0.77547	0.42706	-0.05486	-0.18989	0.01600	0.10120	-0.00527	-0.07778
	0.00353	0.05793	-0.00290	0.06863	-0.00116	0.01449	-0.03494								
9	-0.00290	-0.01976	0.00326	0.00655	-0.03118	-0.24804	-0.04093	0.42706	0.72767	0.33391	-0.04661	-0.15920	0.01478	0.10010	-0.00067
	-0.02727	-0.00062	0.03105	0.00831	-0.07447	-0.03135	0.37036								
10	0.05793	0.00143	-0.06220	-0.00263	0.03486	0.01925	-0.11286	-0.05486	0.33391	0.76992	0.60037	-0.04625	-0.16505	0.00782	0.13003
	-0.00553	-0.09832	-0.00062	0.04220	0.01265	-0.22601	-0.03521								
11	0.00353	0.01323	-0.00425	0.00423	0.01219	0.16074	0.00586	-0.18989	-0.04661	0.60037	0.77176	0.33761	-0.05165	-0.12724	0.01491
	0.04825	-0.00553	-0.02727	0.00064	0.02076	-0.03387	-0.21415								
12	-0.07778	-0.00240	0.08549	0.01022	-0.09031	-0.00199	0.09653	0.01600	-0.15920	-0.04625	0.33761	0.73341	0.40131	-0.04608	-0.20479
	0.01491	0.13003	-0.00067	-0.04832	-0.03214	0.39031	-0.03093								
13	-0.00527	-0.08083	-0.00132	0.08809	0.00091	-0.08146	-0.00415	0.10120	0.01478	-0.16505	-0.05165	0.40131	0.77224	0.54535	-0.04608
	-0.12724	0.00782	0.10010	0.01174	-0.24466	-0.03642	0.00002								
14	0.10120	-0.00415	-0.08146	0.00091	0.08809	-0.00132	-0.08083	-0.00527	0.10010	0.00782	-0.12724	-0.04608	0.54535	0.77224	0.40131
	-0.05165	-0.16505	0.01478	0.00002	-0.03642	-0.24466	0.01174								
15	0.01600	0.09653	-0.00199	-0.09031	0.01022	0.08549	-0.00240	-0.07778	-0.00067	0.13003	0.01491	-0.20479	-0.04608	0.40131	0.73341
	0.33761	-0.04625	-0.15920	-0.03093	0.39031	-0.03214	-0.04832								
16	-0.18989	0.00586	0.16074	0.01219	0.00423	-0.00424	0.01323	0.00353	-0.02727	-0.00553	0.04825	0.01491	-0.12724	-0.05165	0.33761
	0.77176	0.60037	-0.04661	-0.21415	-0.03387	0.02076	0.00064								
17	-0.05486	-0.11286	0.01925	0.03486	-0.00263	-0.06220	0.00143	0.05793	-0.00062	-0.09832	-0.00553	0.13003	0.00782	-0.16505	-0.04625
	0.60037	0.76992	0.33391	-0.03521	-0.22601	0.01265	0.04220								
18	0.42706	-0.04093	-0.24804	-0.03118	0.00655	0.00326	-0.01976	-0.00290	0.03105	-0.00062	-0.02727	-0.00067	0.10010	0.01478	-0.15920
	-0.04661	0.33391	0.72767	0.37036	-0.03135	-0.07447	0.00831								
19	-0.03494	-0.23413	-0.03728	0.39499	-0.02894	-0.07787	0.00272	0.06863	0.00831	0.04220	0.00064	-0.04832	0.01174	0.00002	-0.03093
	-0.21415	-0.03521	0.37036	0.73701	0.34563	-0.03496	-0.14850								
20	0.01449	0.01275	-0.06624	-0.03782	-0.14000	0.01358	0.08150	-0.00116	-0.07447	0.01265	0.02076	-0.03214	-0.24466	-0.03642	0.39031
	-0.03387	-0.22601	-0.03135	0.34563	0.74211	0.37259	-0.03496								
21	-0.00116	0.08150	0.01358	-0.14000	-0.03782	-0.06624	0.01275	0.01449	-0.03135	-0.22601	-0.03387	0.39031	-0.03642	-0.24466	-0.03214
	0.02076	0.01265	-0.07447	-0.03496	0.37259	0.74211	0.34563								
22	0.06863	0.00272	-0.07787	-0.02894	0.39499	-0.03728	-0.23413	-0.03494	0.37036	-0.03521	-0.21415	-0.03093	0.00002	0.01174	-0.04832
	0.00064	0.04220	0.00831	-0.14850	-0.03496	0.34563	0.73701								

ENERGIES FOR 1,12 BENZPERYLENE X ,TBX APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	10,12	11,13	9,12	10,13	6,12	9,13	8,13	5,12	7,13	6,13
XMOMNT	-0.89241	0.89330	-0.16381	-0.00000	-0.19690	-0.00000	0.13467	-0.11012	-0.20417	-0.00000
YMOMNT	-0.00000	0.00000	-0.00000	0.77488	-0.00000	-0.15751	-0.00000	0.00000	-0.00000	0.05192
JUMP E	19.8134	22.0121	23.5847	24.9809	27.5110	28.7522	29.0184	29.9494	30.1830	32.6785
DIAG E	31.6796	33.5421	36.7780	36.3368	41.5994	41.7204	41.4595	44.1088	43.8843	46.7863
DIAG E	31.8964	33.5002	37.0531	36.4235	41.8652	41.8654	41.9981	44.5852	44.2688	46.9219
CORRSP	26.8470	37.2394	35.7673	36.1357	43.6035	40.7259	39.6642	44.7362	45.1939	47.9819
CORRSP	27.0762	37.3939	36.1306	36.3007	39.9803	41.0207	43.9950	45.0633	45.5277	47.8895

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
26.84702	0.00787	-0.08301	0.00000	//	0.7549	0.6142	-0.1705	-0.0000	0.0394	-0.0000	0.0077	0.0619	-0.1353	0.0000
23.89089				//	0.8131	-0.5466	0.1349	-0.0000	0.0813	-0.0000	0.1143	0.0427	0.0224	0.0000
37.23941	2.08380	1.14711	-0.00000	//	-0.5859	0.7673	-0.1407	-0.0000	0.1603	0.0000	-0.0973	-0.1102	0.0277	-0.0000
26.23289				//	0.5381	0.7055	-0.4035	-0.0000	0.0644	0.0000	-0.0070	-0.0631	-0.2042	0.0000
35.76734	0.16065	-0.32499	0.00000	//	0.1805	-0.0342	0.8568	0.0000	0.3120	-0.0000	0.3496	0.0130	-0.1113	-0.0000
31.31137				//	0.0699	0.3588	0.8735	0.0000	0.2171	-0.0000	0.0182	0.1392	-0.1914	-0.0000
43.60350	0.35398	-0.43692	-0.00000	//	0.0576	-0.1345	-0.0314	0.0000	0.7203	0.0000	-0.5984	0.3100	0.0682	-0.0000
37.34477				//	-0.1746	-0.2406	-0.2206	0.0000	0.6651	0.0002	-0.1404	0.3334	-0.5382	0.0001
39.66421	0.00211	-0.03536	-0.00000	//	-0.0055	-0.0272	-0.3791	-0.0000	0.5411	-0.0000	0.5806	-0.2715	0.3899	-0.0000
36.45134				//	-0.0853	0.0558	-0.0547	-0.0000	0.3959	-0.0000	0.8064	-0.4216	0.0428	-0.0000
44.73620	0.09636	0.22505	0.00000	//	-0.1801	0.0721	-0.1385	-0.0000	-0.0196	-0.0000	0.3976	0.8819	-0.0829	0.0000
41.89075				//	-0.0349	0.0902	-0.0651	-0.0000	0.1968	0.0000	0.2285	0.7126	0.6227	-0.0000
45.19395	0.11676	-0.24648	-0.00000	//	0.1357	0.0934	0.2306	0.0000	-0.2520	0.0000	-0.1225	0.1903	0.8972	-0.0000
39.98011				//	0.0741	0.0749	0.0119	0.0000	0.5517	0.0000	-0.5141	-0.4221	0.4919	0.0000

ENERGIES FOR 1,12 BENZPERYLENE X , TBX APPROXIMATION 1.7

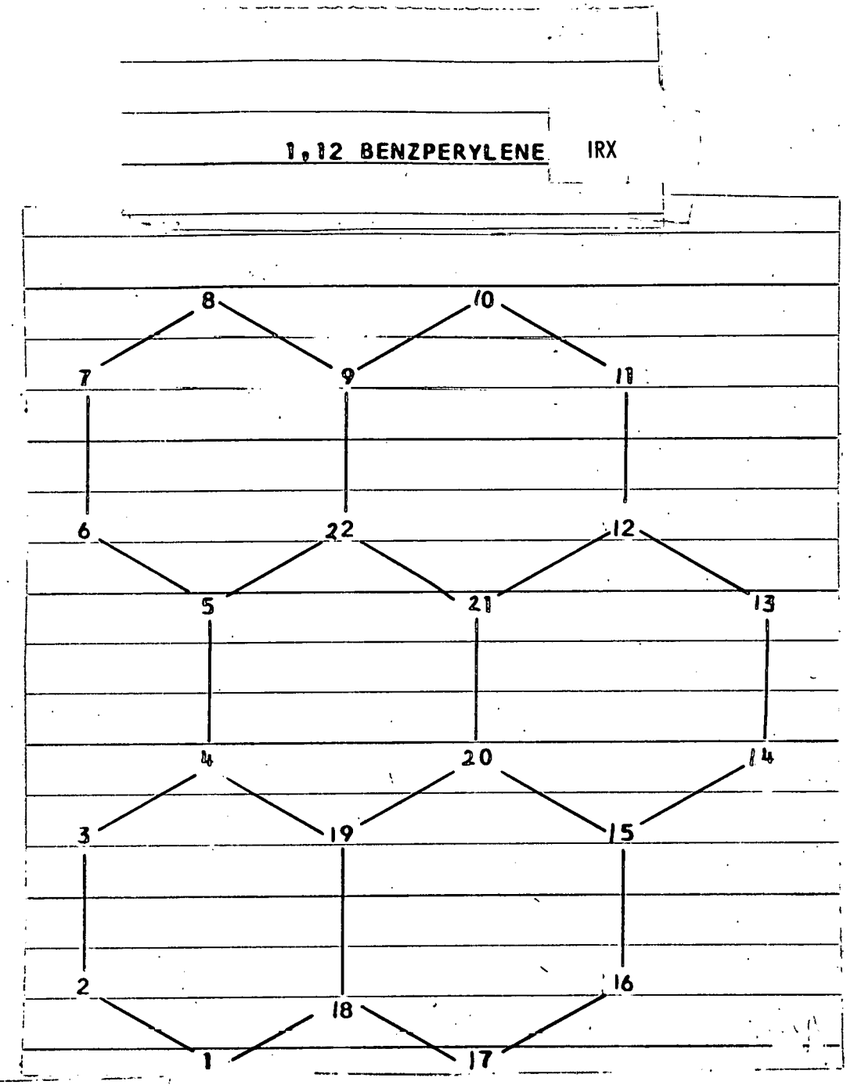
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	11,12	8,12	10,13	7,12	9,13	4,12	6,13	10,14	2,12	5,13
XMOMNT	-0.00000	-0.00000	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000	0.00000
YMOMNT	1.02559	0.15937	0.77488	-0.19482	-0.15751	-0.00222	0.05192	0.15799	-0.01808	0.03652
JUMP E	16.8447	23.8509	24.9809	25.0155	28.7522	30.1213	32.6785	33.4707	35.0873	35.1169
DIAG E	28.5829	32.6395	36.3368	37.9411	41.7204	45.9481	46.7863	46.0437	50.1750	50.7123
DIAG E	28.6712	33.3083	36.4235	38.4558	41.8654	46.1595	46.9219	46.0867	50.7505	51.0585
CORRSP	27.0771	31.3926	37.6830	36.2396	40.9258	45.9856	48.5403	47.1988	52.1339	49.7093
CORRSP	27.2434	32.1840	38.1454	36.3794	41.2753	46.0432	48.5414	47.3017	52.4780	50.1090

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
27.07712	0.52522	-0.00000	0.67538	//	0.9284	-0.0392	-0.3521	-0.0415	0.0182	0.0951	0.0011	-0.0135	-0.0232	-0.0284
18.17412				//	0.9733	0.0055	-0.1692	0.0361	-0.1093	0.0245	0.0224	0.0977	-0.0017	0.0110
31.39256	0.01345	-0.00000	0.10037	//	0.0137	0.9598	-0.0598	-0.0463	-0.0114	0.0177	0.0738	-0.1876	0.1676	-0.0609
29.48255				//	-0.0007	0.8655	-0.2568	-0.1594	0.1776	0.0735	0.1840	-0.2791	0.0650	-0.0813
37.68295	1.48972	0.00000	0.96418	//	0.2608	0.0073	0.7148	-0.4331	-0.4611	0.0169	-0.1023	-0.0754	0.0225	0.0621
26.53433				//	0.1600	0.2866	0.9117	-0.1215	-0.0737	0.0486	-0.1903	-0.0383	0.0264	0.0122
36.23961	0.37833	-0.00000	0.49548	//	0.2332	0.1030	0.5164	0.7733	0.1897	-0.0128	-0.0712	0.1627	-0.0014	-0.0504
31.12520				//	-0.0477	0.2702	0.0288	0.9246	-0.0440	-0.0753	-0.1315	0.1792	-0.0061	-0.1092
40.92584	0.15074	-0.00000	0.29430	//	0.0629	-0.0037	0.2900	-0.3792	0.7215	0.1663	0.4427	0.1518	0.0117	-0.0260
36.86585				//	0.1115	-0.2070	0.1506	0.1612	0.8134	0.3906	0.1830	-0.1127	-0.1101	-0.1531
45.98557	0.05394	0.00000	-0.16608	//	-0.0836	-0.0732	0.0108	0.1276	-0.0225	0.9012	-0.0597	-0.3519	0.0607	0.1660
43.69834				//	-0.0955	0.0382	0.0433	0.0437	-0.3636	0.7289	0.4475	0.3048	0.1249	0.1158
48.54034	0.00200	0.00000	0.03112	//	0.0074	-0.0733	0.0003	0.2108	-0.3761	-0.0325	0.8643	-0.1778	-0.1523	-0.0760
40.54588				//	0.0056	0.0534	0.1802	-0.0297	0.1576	-0.5379	0.6909	0.4087	-0.0054	0.0717
47.19883	0.01740	0.00000	0.09311	//	-0.0478	0.1482	-0.0988	-0.0334	-0.2890	0.3413	0.0924	0.8680	0.0054	0.0532
46.32373				//	-0.0560	0.1798	-0.1002	-0.2616	0.1300	0.1013	-0.3298	0.6963	-0.3937	-0.3322
52.13388	0.00940	0.00000	-0.06510	//	-0.0180	-0.1615	0.0043	-0.0050	-0.0698	0.0798	0.0139	0.0114	0.6550	-0.7300
45.67362				//	-0.0073	0.0705	-0.0754	-0.0505	0.3302	0.0171	-0.3002	0.3475	0.6603	0.4801
49.70932	0.00073	0.00000	-0.01853	//	0.0435	-0.0884	-0.0275	0.0695	-0.0057	-0.1630	0.1537	0.0187	0.7175	0.6476
50.36090				//	-0.0069	0.1063	-0.0245	0.0623	0.0670	0.0470	-0.0467	-0.0274	-0.6134	0.7735

1,12 BENZPERYLENE IRX



ATOMIC COORDINATES

x	0.8813	0.	0.	0.8777	0.8777	0.	0.	0.8813
y	0.	0.5050	1.5090	2.0150	3.0810	3.5870	4.5910	5.0960

1.7561	2.6439	3.5065	3.5230	4.3885	4.3885	3.5230
4.6040	5.0910	4.5960	3.5690	3.0550	2.0410	1.5270

3.5065	2.6439	1.7561	1.7525	2.6338	2.6338	1.7525
0.5000	0.0050	0.4920	1.5090	2.0360	3.0600	3.5870

262

1,12-BENZPERYLENE IRX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 S	7 A	8 S	9 A	10 S	11 A	12 S	13 A
1.779182	1.615721	1.557025	1.396032	1.376388	1.297319	1.203470	1.177707	1.166335	1.090771	1.036025	0.833199	0.789853
0.136833	0.253317	-0.160558	0.216719	0.264467	-0.150145	-0.127174	-0.296403	0.209905	-0.046589	0.339733	0.332830	-0.044967
0.116061	0.192770	-0.204814	0.309736	0.086663	-0.309644	0.203998	-0.203954	0.252102	0.246849	0.071612	-0.073451	-0.228035
0.152787	0.157551	-0.251347	0.269151	-0.122636	-0.258243	0.319511	0.112196	0.032111	0.198533	-0.300955	-0.292583	0.206498
0.265756	0.139723	-0.286517	0.122129	-0.285510	-0.009331	0.137123	0.302530	-0.223630	-0.125998	-0.209421	0.226037	0.089714
0.265756	-0.139723	-0.286517	-0.122131	-0.285509	-0.009331	-0.137123	0.302527	0.223634	-0.125998	0.209421	0.226037	-0.089714
0.152787	-0.157551	-0.251347	-0.269151	-0.122635	-0.258243	-0.319512	0.112197	-0.032109	0.198533	0.300955	-0.292583	-0.206498
0.116061	-0.192770	-0.204814	-0.309735	0.086665	-0.309644	-0.203998	-0.203950	-0.252105	0.246849	-0.071612	-0.073451	0.228034
0.136833	-0.253317	-0.160557	-0.216718	0.264468	-0.150145	0.127174	-0.296400	-0.209909	-0.046589	-0.339733	0.332830	0.044967
0.224422	-0.349057	-0.105682	-0.028059	0.322517	0.109695	0.321993	-0.078097	0.054922	-0.255393	-0.073351	-0.090066	-0.241625
0.152191	-0.257837	0.037296	0.196603	0.351253	0.083177	0.221491	0.265359	-0.188757	0.027616	0.301625	-0.305756	-0.080734
0.153069	-0.202705	0.167246	0.322397	0.212801	-0.017544	-0.098981	0.321919	-0.221570	0.253695	0.195813	0.228475	0.271808
0.235909	-0.169112	0.316441	0.313350	-0.036032	-0.124756	-0.334064	0.014719	-0.017952	0.134146	-0.242297	0.218525	-0.113220
0.156525	-0.051808	0.317200	0.122714	-0.089849	-0.396613	0.171292	-0.006621	-0.016448	0.377700	-0.173758	-0.147824	0.402609
0.156525	0.051808	0.317200	-0.122714	-0.089848	-0.396613	0.171292	-0.006621	0.016447	-0.377699	0.173759	-0.147824	0.402609
0.235909	0.169112	0.316441	-0.313350	-0.036030	-0.124756	0.334064	0.014718	0.017953	0.134146	0.242297	0.218525	0.113221
0.153069	0.202705	0.167246	-0.322396	0.212803	-0.017544	0.098981	0.321915	0.221576	0.253694	-0.195814	0.228476	-0.271808
0.152191	0.257837	0.037296	-0.196602	0.351254	0.083177	-0.221491	0.265356	0.188761	0.027615	-0.301625	-0.305756	0.080734
0.224422	0.349057	-0.105682	0.028061	0.322517	0.109695	-0.321993	-0.078096	-0.054923	-0.255393	0.073351	-0.090066	0.241625
0.305796	0.275018	-0.103575	0.023807	-0.084572	0.244468	-0.035665	-0.048958	-0.456375	-0.179693	-0.003402	0.001499	-0.183208
0.321269	0.134152	0.187069	-0.112008	-0.191797	0.250820	0.128737	-0.289196	-0.211494	0.241480	0.146321	-0.154026	-0.219157
0.321269	-0.134152	0.187069	0.112007	-0.191798	0.250819	-0.128737	-0.289200	0.211490	0.241480	-0.146321	-0.154026	0.219157
0.305796	-0.275018	-0.103575	-0.023808	-0.084572	0.244468	0.035665	-0.048965	0.456374	-0.179694	0.003403	0.001499	0.183207

OVERLAP EIGNVALUES AND EIGNVECTORS

14 A	15 S	16 S	17 A	18 A	19 S	20 A	21 S	22 A
0.734567	0.733371	0.715685	0.669635	0.627306	0.625746	0.557002	0.534429	0.483203
0.293405	-0.223997	0.107345	0.133496	-0.264715	0.212961	-0.148057	0.234866	0.123630
-0.258702	0.288119	0.203021	-0.294850	0.086494	-0.284591	0.182528	-0.167463	-0.099706
-0.040533	-0.089671	-0.320919	0.277057	0.113478	0.251565	-0.236693	0.140812	0.138192
0.303199	-0.194066	0.176496	-0.067476	-0.287824	-0.132067	0.305310	-0.144685	-0.268887
-0.303204	-0.194059	0.176496	0.067476	0.287825	-0.132065	-0.305310	-0.144685	0.268887
0.040531	-0.089672	-0.320920	-0.277056	-0.113479	0.251565	0.236693	0.140812	-0.138192
0.258709	0.288113	0.203022	0.294850	-0.086493	-0.284591	-0.182528	-0.167463	0.099706
-0.293411	-0.223990	0.107344	-0.133496	0.264714	0.212963	0.148057	0.234866	-0.123630
0.046340	-0.052293	-0.318675	-0.113259	-0.354821	-0.059855	-0.116595	-0.367571	0.229008
0.272071	-0.166327	0.253494	0.055925	0.339473	-0.167786	-0.028489	0.245784	-0.139565
-0.312512	0.216212	0.038720	0.053841	-0.196666	0.314223	0.159357	-0.189291	0.138638
0.019804	-0.069751	-0.314975	-0.151026	-0.029258	-0.355798	-0.332032	0.175265	-0.235504
0.007919	0.042424	0.149854	0.381994	0.064766	0.134665	0.300474	-0.050654	0.141059
-0.007919	0.042425	0.149853	-0.381995	-0.064767	0.134665	-0.300474	-0.050654	-0.141059
-0.019805	-0.069751	-0.314975	0.151026	0.029260	-0.355798	0.332032	0.175265	0.235504
0.312517	0.216204	0.038720	-0.053840	0.196665	0.314225	-0.159357	-0.189291	-0.138638
-0.272075	-0.166321	0.253493	-0.055925	-0.339472	-0.167788	0.028489	0.245784	0.139565
-0.046341	-0.052291	-0.318675	0.113259	0.354821	-0.059853	0.116595	-0.367570	-0.229008
0.014506	0.448677	-0.024678	-0.240807	0.074534	0.016364	-0.116324	0.300139	0.321538
-0.280906	-0.189716	0.153403	0.261453	-0.190529	0.124820	-0.204116	-0.145999	-0.336877
0.280901	-0.189723	0.153404	-0.261453	0.190529	0.124821	0.204116	-0.145999	0.336877
-0.014495	0.448678	-0.024678	0.240807	-0.074535	0.016364	0.116324	0.300140	-0.321538

263

1,12 BENZPERYLENE IRX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 S	7 A	8 S	9 A	10 S	11 A	12 S	13 A
32.58401	28.35330	26.61737	21.10672	20.34609	17.05149	12.57915	11.22675	10.61078	6.19158	2.58716	-14.89485	-19.79537
0.102584	0.199288	-0.128672	0.183421	0.225424	-0.131822	-0.115926	-0.273127	0.194361	-0.044609	0.333774	0.364627	-0.050596
0.087011	0.151655	-0.164139	0.262146	0.073869	-0.271856	0.185955	-0.187938	0.233434	0.236354	0.070356	-0.080468	-0.256583
0.114545	0.123948	-0.201431	0.227797	-0.104531	-0.226728	0.291252	0.103385	0.029733	0.190093	-0.295676	-0.320535	0.232350
0.199239	0.109922	-0.229616	0.103365	-0.243361	-0.008193	0.124995	0.278773	-0.207070	-0.120642	-0.205748	0.247631	0.100946
0.199239	-0.109922	-0.229616	-0.103366	-0.243360	-0.008193	-0.124995	0.278770	0.207074	-0.120642	0.205748	0.247631	-0.100946
0.114545	-0.123948	-0.201431	-0.227797	-0.104530	-0.226728	-0.291252	0.103386	-0.029732	0.190093	0.295676	-0.320535	-0.232350
0.087011	-0.151655	-0.164139	-0.262146	0.073871	-0.271857	-0.185955	-0.187934	-0.233437	0.236355	-0.070356	-0.080468	0.256582
0.102584	-0.199288	-0.128672	-0.183420	0.225425	-0.131822	0.115926	-0.273124	-0.194366	-0.044609	-0.333774	0.364627	0.050596
0.168250	-0.274608	-0.084694	-0.023748	0.274905	0.096308	0.293514	-0.071964	0.050855	-0.244536	-0.072064	-0.098671	-0.271875
0.114098	-0.202844	0.029889	0.166396	0.299398	0.073026	0.201901	0.244521	-0.174780	0.026442	0.296334	-0.334966	-0.090841
0.114756	-0.159471	0.134032	0.272862	0.181386	-0.015403	-0.090227	0.296639	-0.205164	0.242910	0.192379	0.250302	0.305836
0.176862	-0.133043	0.253598	0.265205	-0.030713	-0.109531	-0.304518	0.013563	-0.016623	0.128443	-0.238047	0.239401	-0.127395
0.117348	-0.040758	0.254206	0.103859	-0.076584	-0.348211	-0.156142	-0.006101	-0.015230	-0.361643	-0.170711	-0.161947	-0.453012
0.117348	0.040758	0.254206	-0.103860	-0.076584	-0.348211	0.156142	-0.006101	0.015229	-0.361642	0.170711	-0.161947	0.453012
0.176862	0.133043	0.253598	-0.265205	-0.030711	-0.109531	0.304518	0.013563	0.016623	0.128443	0.238047	0.239401	0.127395
0.114756	0.159471	0.134032	-0.272861	0.181387	-0.015403	0.090227	0.296635	0.205169	0.242909	-0.192379	0.250303	-0.305836
0.114098	0.202844	0.029889	-0.166395	0.299399	0.073026	-0.201901	0.244518	0.174784	0.026441	-0.296335	-0.334966	0.090841
0.168250	0.274608	-0.084694	0.023749	0.274905	0.096308	-0.293514	-0.071963	-0.050856	-0.244536	0.072064	-0.098671	0.271875
0.229257	0.216361	-0.083006	0.020150	-0.072087	0.214634	-0.032510	-0.045113	-0.422581	-0.172054	-0.003343	0.001643	-0.206144
0.240857	0.105539	0.149918	-0.094798	-0.163483	0.220210	0.117351	-0.266486	-0.195833	0.231214	0.143755	-0.168741	-0.246594
0.240857	-0.105539	0.149918	0.094797	-0.163483	0.220210	-0.117351	-0.266489	0.195830	0.231214	-0.143755	-0.168740	0.246594
0.229257	-0.216361	-0.083006	-0.020150	-0.072087	0.214634	0.032510	-0.045120	0.422580	-0.172055	0.003343	0.001643	0.206144

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14	15	16	17	18	19	20	21	22
-26.88493	-27.05014	-29.55719	-36.70642	-44.20383	-44.49942	-59.17397	-64.81592	-79.57485
0.342336	-0.261565	0.126888	0.163135	-0.334225	0.269216	-0.198381	0.321273	0.177852
-0.301845	0.336442	0.239983	-0.360315	0.109206	-0.359767	0.244569	-0.229072	-0.143436
-0.047293	-0.104710	-0.379345	0.338571	0.143275	0.318018	-0.317144	0.192617	0.198801
0.353763	-0.226615	0.208629	-0.082458	-0.363402	-0.166953	0.409084	-0.197915	-0.386816
-0.353768	-0.226607	0.208628	0.082457	0.363403	-0.166951	-0.409084	-0.197915	0.386816
0.047291	-0.104711	-0.379346	0.338571	-0.143277	0.318017	0.317144	0.192617	-0.198801
0.301853	0.336435	0.239983	0.360315	-0.109204	-0.359768	-0.244569	-0.229073	0.143436
-0.342342	-0.261557	0.126887	-0.163136	0.334224	0.269218	0.198381	0.321273	-0.177852
0.054068	-0.061063	-0.376693	-0.138405	-0.447991	-0.075666	-0.156225	-0.502800	0.329447
0.317444	-0.194224	0.299644	0.068341	0.428613	-0.212108	-0.038173	0.336209	-0.200776
-0.364629	0.252474	0.045769	0.065795	-0.248308	0.397228	0.213522	-0.258932	0.199442
0.023107	-0.081450	-0.372319	-0.184558	-0.036941	-0.449784	-0.444889	0.239745	-0.338792
0.009240	0.049539	0.177136	0.466808	0.081773	0.170238	0.402604	-0.069290	0.202926
-0.009239	0.049540	0.177135	-0.466808	-0.081774	0.170237	-0.402604	-0.069290	-0.202926
-0.023108	-0.081449	-0.372319	0.184558	0.036944	-0.449784	0.444888	0.239745	0.338792
0.364635	0.252466	0.045769	-0.065795	0.248306	0.397229	-0.213521	-0.258932	-0.199442
-0.317449	-0.194216	0.299644	-0.068342	-0.428612	-0.212111	0.038172	0.336209	0.200776
-0.054069	-0.061062	-0.376692	0.138406	0.447991	-0.075663	0.156226	-0.502800	-0.329448
0.016925	0.523929	-0.029171	-0.294273	0.094106	0.058611	-0.155862	0.410561	0.462560
-0.327751	-0.221535	0.181332	0.319502	-0.240560	0.157792	-0.273494	-0.199713	-0.484626
0.327746	-0.221542	0.181332	-0.319503	-0.240559	0.157794	0.273494	-0.199712	0.484626
-0.016913	0.523929	-0.029171	0.294273	-0.094106	0.058611	0.155862	0.410562	-0.462559

1,12 BENZPERYLENE X IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	1.02760	0.66878	-0.02560	-0.29841	-0.00375	0.12599	-0.00027	-0.11955	0.00541	0.05456	-0.00621	-0.07693	-0.00279	0.10613	-0.00281
	-0.21071	0.00666	0.60078	0.00939	-0.00267	0.00271	0.07975								
2	0.66878	1.00947	0.66026	-0.00754	-0.09298	-0.00157	0.03589	-0.00027	-0.01428	-0.00441	0.00621	0.00523	-0.09435	-0.00030	0.10751
	0.01120	-0.12596	-0.00748	-0.24576	-0.00426	0.09737	0.00298								
3	-0.02560	0.66026	1.02242	0.62703	0.00885	-0.14141	-0.00157	0.12599	-0.00464	-0.05839	0.00687	0.08946	0.00760	-0.08000	-0.00375
	0.17821	-0.00330	-0.26133	0.00708	-0.08479	-0.00997	-0.09177								
4	-0.29841	-0.00754	0.62703	0.97766	0.38922	0.00885	-0.09298	-0.00375	0.00080	0.00580	0.00723	-0.01076	0.09996	0.00265	-0.10512
	-0.01686	0.01619	0.02067	0.55971	0.01131	-0.14618	0.00284								
5	-0.00375	-0.09298	0.00885	0.38922	0.97766	0.62703	-0.00754	-0.29841	0.02067	0.01619	-0.01686	-0.10512	0.00265	0.09996	-0.01076
	0.00723	0.00580	0.00080	0.00284	-0.14618	0.01131	0.55971								
6	0.12599	-0.00157	-0.14141	0.00885	0.62703	1.02242	0.66026	-0.02560	-0.26133	-0.00330	0.17821	-0.00375	-0.08000	0.00760	0.08946
	0.00687	-0.05839	-0.00464	-0.09177	-0.00997	-0.08479	0.00708								
7	-0.00027	0.03589	-0.00157	-0.09298	-0.00754	0.66026	1.00947	0.66878	-0.00748	-0.12596	0.01120	0.10751	-0.00030	-0.09435	0.00524
	0.00621	-0.00441	-0.01428	0.00298	0.09737	-0.00426	-0.24575								
8	-0.11955	-0.00027	0.12599	-0.00375	-0.29841	-0.02560	0.66878	1.02760	0.60078	0.00666	-0.21071	-0.00281	0.10613	-0.00279	-0.07693
	-0.00621	0.05456	0.00541	0.07975	0.00271	-0.00267	0.00939								
9	0.00541	-0.01428	-0.00464	0.00080	0.02067	-0.26133	-0.00748	0.60078	0.96723	0.49631	-0.00648	-0.16351	-0.00514	0.10955	-0.00134
	-0.01971	0.00307	0.02841	-0.00827	-0.09136	0.00696	0.52359								
10	0.05456	-0.00441	-0.05839	0.00580	0.01619	-0.00330	-0.12596	0.00666	0.49631	1.01365	0.77972	-0.01239	-0.18169	0.01735	0.14152
	0.00128	-0.10954	0.00307	0.05268	-0.00950	-0.23333	0.00872								
11	-0.00621	0.00621	0.00687	0.00723	-0.01686	0.17821	0.01120	-0.21071	-0.00648	0.77972	1.01450	0.49445	0.00707	-0.13949	-0.00515
	0.04544	0.00128	-0.01971	0.00353	0.00576	0.00789	-0.22012								
12	-0.07693	0.00523	0.08946	-0.01076	-0.10512	-0.00375	0.10751	-0.00281	-0.16351	-0.01239	0.49445	0.97656	0.57217	-0.01516	-0.21311
	-0.00515	0.14152	-0.00134	-0.06206	0.01259	0.54238	0.01041								
13	-0.00279	-0.09435	0.00760	0.09996	0.00265	-0.08000	-0.00030	0.10613	-0.00514	-0.18169	0.00707	0.57217	1.02147	0.71129	-0.01516
	-0.13949	0.01735	0.10955	-0.00655	-0.25321	0.00556	-0.01807								
14	0.10613	-0.00030	-0.08000	0.00265	0.09996	0.00760	-0.09435	-0.00279	0.10955	0.01735	-0.13949	-0.01516	0.71129	1.02147	0.57217
	0.00707	-0.18169	-0.00514	-0.01807	0.00556	-0.25321	-0.00655								
15	-0.00281	0.10751	-0.00375	-0.10512	-0.01076	0.08946	0.00524	-0.07693	-0.00134	0.14152	-0.00515	-0.21311	-0.01516	0.57217	0.97656
	0.49445	-0.01239	-0.16351	0.01041	0.54238	0.01259	-0.06206								
16	-0.21071	0.01120	0.17821	-0.01686	0.00723	0.00687	0.00621	-0.00621	-0.01971	0.00128	0.04544	-0.00515	-0.13949	0.00707	0.49445
	1.01450	0.77972	-0.00648	-0.22012	0.00789	0.00576	0.00353								
17	0.00666	-0.12596	-0.00330	0.01619	0.00580	-0.05839	-0.00441	0.05456	0.00307	-0.10954	0.00128	0.14152	0.01735	-0.18169	-0.01239
	0.77972	1.01365	0.49631	0.00872	-0.23333	-0.00950	0.05268								
18	0.60078	-0.00748	-0.26133	0.02067	0.00080	-0.00464	-0.01428	0.00541	0.02841	0.00307	-0.01971	-0.00134	0.10955	-0.00514	-0.16351
	-0.00648	0.49631	0.96723	0.52359	0.00696	-0.09136	-0.00827								
19	0.00939	-0.24576	0.00708	0.55971	0.00284	-0.09177	0.00298	0.07975	-0.00827	0.05268	0.00353	-0.06206	-0.00655	-0.01807	0.01041
	-0.22012	0.00872	0.52359	0.98321	0.50566	0.00303	-0.15984								
20	-0.00267	-0.00426	0.08479	0.01131	-0.14618	-0.00997	0.09737	0.00271	-0.09136	-0.00950	0.00576	0.01259	-0.25321	0.00556	0.54238
	0.00789	-0.23333	0.00696	0.50566	0.98622	0.53320	0.00303								
21	0.00271	0.09737	-0.00997	-0.14618	0.01131	-0.08479	-0.00426	-0.00267	0.00696	-0.23333	0.00789	0.54238	0.00556	-0.25321	0.01259
	0.00576	-0.00950	-0.09136	0.00303	0.53320	0.98622	0.50566								
22	0.07975	0.00298	-0.09177	0.00284	0.55971	0.00708	-0.24575	0.00939	0.52359	0.00872	-0.22012	0.01041	-0.01807	-0.00655	-0.06206
	0.00353	0.05268	-0.00827	-0.15984	0.00303	0.50566	0.98321								

1,12 BENZPERYLENE-X — IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22								
1	0.81568	0.49785	-0.10583	-0.31420	0.01598	0.13493	-0.00456	-0.12824	0.00144	0.05878	-0.00270	-0.08332	-0.01029	0.11335	0.01769
	-0.21494	-0.06774	0.43055	-0.04603	0.00393	0.00409	0.08464								
2	0.49785	0.78160	0.48251	-0.07487	-0.09165	0.00727	0.03864	-0.00456	-0.01619	-0.00394	0.00689	0.00234	-0.10079	-0.00656	0.11398
	0.02205	-0.12574	-0.07023	-0.25824	0.01303	0.10352	0.00908								
3	-0.10583	0.48251	0.80648	0.46102	-0.05199	-0.15508	0.00727	0.13493	0.00139	-0.06350	0.00130	0.09632	0.00593	-0.08668	-0.00417
	0.18878	0.02150	-0.27405	-0.05031	-0.08342	0.00723	-0.09176								
4	-0.31420	-0.07487	0.46102	0.73516	0.24075	-0.05199	-0.09165	0.01598	0.00613	0.00549	0.00752	0.00162	0.10689	0.00683	-0.10696
	-0.00168	0.02405	-0.02725	0.39739	-0.04639	-0.15616	-0.04259								
5	0.01598	-0.09165	-0.05199	0.24075	0.73516	0.46102	-0.07487	-0.31420	-0.02725	0.02405	-0.00168	-0.10696	0.00683	0.10689	0.00162
	0.00752	0.00549	0.00613	-0.04259	-0.15616	-0.04639	0.39739								
6	0.13493	0.00727	-0.15508	-0.05199	0.46102	0.80648	0.48251	-0.10583	-0.27405	0.02150	0.18878	-0.00417	-0.08668	0.00593	0.09632
	0.00130	-0.06350	0.00139	-0.09176	0.00723	-0.08342	-0.05031								
7	-0.00456	0.03864	0.00727	-0.09165	-0.07487	0.48251	0.78160	0.49785	-0.07023	-0.12574	0.02205	0.11398	-0.00656	-0.10079	0.00234
	0.00689	-0.00394	-0.01619	0.00908	0.10352	0.01303	-0.25824								
8	-0.12824	-0.00456	0.13493	0.01598	-0.31420	-0.10583	0.49785	0.81568	0.43055	-0.06774	-0.21494	0.01769	0.11335	-0.01029	-0.08332
	-0.00269	0.05878	0.00144	0.08464	0.00409	0.00393	-0.04603								
9	0.00144	-0.01619	0.00139	0.00613	-0.02725	-0.27405	-0.07023	0.43055	0.71042	0.32542	-0.07576	-0.17186	0.01384	0.11615	-0.00053
	-0.02188	0.00235	0.03080	0.00218	-0.09175	-0.04133	0.36492								
10	0.05878	-0.00394	-0.06350	0.00549	0.02405	0.02150	-0.12574	-0.06774	0.32542	0.79467	0.60328	-0.08145	-0.18465	0.03095	0.15056
	-0.00633	-0.11717	0.00235	0.05591	0.00678	-0.24658	-0.04717								
11	-0.00270	0.00689	0.00130	0.00752	-0.00168	0.18878	0.02205	-0.21494	-0.07576	0.60328	0.79680	0.32859	-0.06287	-0.13971	0.01391
	0.04828	-0.00633	-0.02188	0.00722	0.01270	-0.04549	-0.23272								
12	-0.08332	0.00234	0.09632	0.00162	-0.10696	-0.00417	0.11398	0.01769	-0.17186	-0.08145	0.32859	0.72584	0.40117	-0.08445	-0.22499
	0.01391	0.15056	-0.00053	-0.06046	-0.03656	0.38697	-0.03758								
13	-0.01029	-0.10079	0.00593	0.10689	0.00683	-0.08668	-0.00656	0.11335	0.01384	-0.18465	-0.06287	0.40117	0.80506	0.54026	-0.08445
	-0.13971	0.03095	0.11615	0.00888	-0.26761	-0.05150	-0.01255								
14	0.11335	-0.00656	-0.08668	0.00683	0.10689	0.00593	-0.10079	-0.01029	0.11615	0.03095	-0.13971	-0.08445	0.54026	0.80506	0.40117
	-0.06287	-0.18465	0.01384	-0.01255	-0.05150	-0.26761	0.00888								
15	0.01769	0.11398	-0.00417	-0.10696	0.00162	0.09632	0.00234	-0.08332	-0.00053	0.15056	0.01391	-0.22499	-0.08445	0.40117	0.72584
	0.32859	-0.08145	-0.17186	-0.03758	0.38697	-0.03656	-0.06046								
16	-0.21494	0.02205	0.18878	-0.00168	0.00752	0.00130	0.00689	-0.00269	-0.02188	-0.00633	0.04828	0.01391	-0.13971	-0.06287	0.32859
	0.79680	0.60328	-0.07576	-0.23272	-0.04549	0.01270	0.00722								
17	-0.06774	-0.12574	0.02150	0.02405	0.00549	-0.06350	-0.00394	0.05878	0.00235	-0.11717	-0.00633	0.15056	0.03095	-0.18465	-0.08145
	0.60328	0.79467	0.32542	-0.04717	-0.24658	0.00678	0.05591								
18	0.43055	-0.07023	-0.27405	-0.02725	0.00613	0.00139	-0.01619	0.00144	0.03080	0.00235	-0.02188	-0.00053	0.11615	0.01384	-0.17186
	-0.07576	0.32542	0.71042	0.36492	-0.04133	-0.09175	0.00218								
19	-0.04603	-0.25824	-0.05031	0.39739	-0.04259	-0.09176	0.00908	0.08464	0.00218	0.05591	0.00722	-0.06046	0.00888	-0.01255	-0.03758
	-0.23272	-0.04717	0.36492	0.73842	0.34690	-0.05064	-0.16902								
20	0.00393	0.01303	-0.08342	-0.04639	-0.15616	0.00723	0.10352	0.00409	-0.09175	0.00678	0.01270	-0.03656	-0.26761	-0.05150	0.38697
	-0.04549	-0.24658	-0.04133	0.34690	0.74619	0.37454	-0.05064								
21	0.00409	0.10352	0.00723	-0.15616	-0.04639	-0.08342	0.01303	0.00393	-0.04133	-0.24658	-0.04549	0.38697	-0.05150	-0.26761	-0.03656
	0.01270	0.00678	-0.09175	-0.05064	0.37454	0.74619	0.34690								
22	0.08464	0.00908	-0.09176	-0.04259	0.39739	-0.05031	-0.25824	-0.04603	0.36492	-0.04717	-0.23272	-0.03758	-0.01255	0.00888	-0.06046
	0.00722	0.05591	0.00218	-0.16902	-0.05064	0.34690	0.73842								

ENERGIES FOR 1,12 BENZPERYLENE X , IRXAPPROXIMATION
ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	10,12	11,13	10,13	8,12	9,13	8,13	6,12	7,13	5,12	6,13
XMOMNT	0.87289	0.89558	0.00000	0.32813	0.17264	-0.00000	-0.17295	0.22619	-0.07306	-0.00000
YMOMNT	-0.00000	-0.00000	0.79018	0.00000	-0.00000	-0.09408	-0.00000	0.00000	0.00000	-0.03481
JUMP E	21.0864	22.3825	25.9870	26.1216	30.4062	31.0221	31.9463	32.3745	35.2409	36.8469
DIAG E	32.3332	33.3119	36.6814	39.2752	42.9174	43.4743	46.1501	45.6428	49.7652	51.2436
DIAG E	32.6602	33.2701	36.8807	39.5925	43.5271	43.6639	46.3774	46.0626	50.2406	51.3432
CORRSP	27.3013	37.5405	36.6387	38.1729	42.2295	43.0392	47.7432	46.3123	50.0960	51.7214
CORRSP	27.5376	37.6698	36.8599	38.6058	42.6663	43.3300	47.9764	46.7748	50.4998	51.6979

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
27.30132	0.00008	0.00855	0.00000	//	0.7387	-0.6559	-0.0000	-0.0887	-0.0120	0.0000	-0.0397	-0.1172	-0.0273	-0.0000
26.58012				//	0.7093	-0.6354	-0.0000	-0.2105	-0.0342	0.0000	-0.0915	-0.1926	-0.0464	-0.0000
37.54051	2.04768	1.13255	0.00000	//	0.6354	0.7415	0.0000	-0.1476	-0.1094	0.0000	0.0869	-0.0367	-0.0614	0.0000
24.44261				//	0.6838	0.6926	0.0000	0.2006	-0.0945	0.0000	-0.0338	0.0488	-0.0072	0.0000
38.17287	0.18295	0.33571	0.00000	//	0.1010	0.0379	-0.0000	-0.8806	-0.4097	0.0000	-0.1547	-0.1442	-0.0169	-0.0000
33.31374				//	-0.0203	-0.2544	-0.0000	0.9376	-0.0773	0.0000	-0.0873	-0.1819	-0.0956	-0.0000
42.22946	0.04242	0.15370	0.00000	//	0.0429	0.0469	0.0000	0.3263	0.7078	-0.0000	0.4289	-0.4153	-0.1793	-0.0000
38.60825				//	0.0995	0.0115	-0.0000	0.0837	0.9415	-0.0000	0.2034	0.0293	-0.2332	-0.0000
47.74322	0.00414	-0.04518	0.00000	//	0.0490	-0.1081	0.0000	0.1368	-0.1969	0.0000	0.7734	0.5742	-0.0251	-0.0000
43.29507				//	0.0091	0.0354	-0.0000	-0.0216	-0.2209	0.0000	0.8735	-0.3918	-0.1815	0.0000
46.31230	0.71552	0.60275	0.00000	//	0.1724	0.0571	-0.0000	0.2519	0.5119	-0.0000	-0.4227	0.6787	-0.0478	-0.0000
40.23392				//	0.1343	-0.2238	-0.0000	0.1585	-0.0770	-0.0000	-0.4113	0.8169	0.2537	0.0000
50.09602	0.00738	0.05885	0.00000	//	0.0797	0.0375	-0.0000	0.0790	0.1351	-0.0000	0.0794	-0.0363	0.9799	0.0000
46.27383				//	0.0291	0.0187	-0.0000	0.0620	0.2070	0.0000	0.0971	-0.3252	0.9148	0.0001

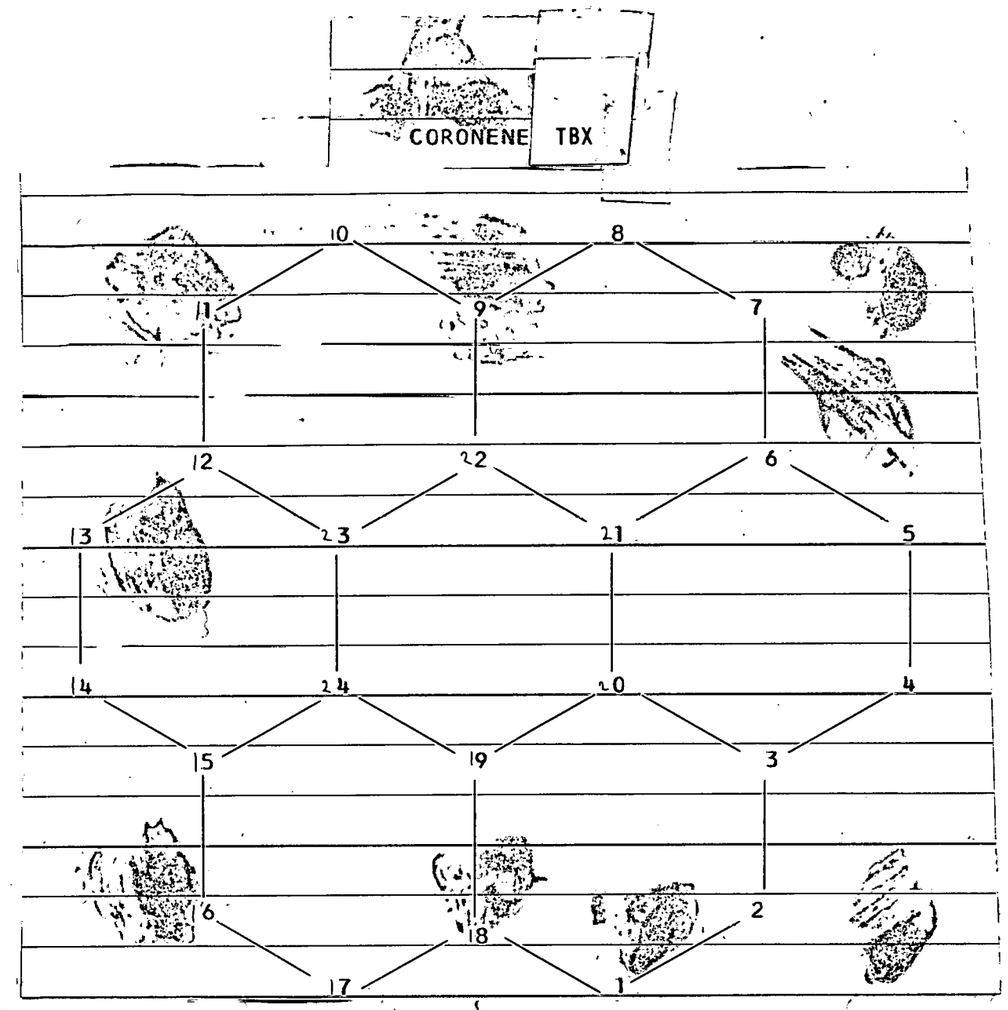
ENERGIES FOR 1,12 BENZPERYLENE X ,IRX APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	11,12	9,12	10,13	7,12	8,13	10,14	4,12	6,13	8,14	5,13
XMOMNT	-0.00000	0.00000	0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	0.00000	0.00000
YMOMNT	-1.01083	-0.18113	0.79018	-0.22490	-0.09408	0.13266	-0.03136	-0.03481	-0.00172	-0.03813
JUMP E	17.4820	25.5056	25.9870	27.4740	31.0221	33.0765	36.0016	36.8469	38.1117	40.1415
DIAG E	28.5931	34.4845	36.6814	40.3532	43.4743	44.9761	51.7400	51.2436	53.6952	55.8111
DIAG E	28.6791	35.2219	36.8807	40.9007	43.6639	45.1312	51.9170	51.3432	53.8406	56.1588
CORRSP	26.8822	33.6512	37.3028	39.2514	43.1087	46.2575	50.4216	52.2469	55.1393	56.7908
CORRSP	27.0101	34.2819	37.3800	39.8368	43.4148	46.4874	50.4936	52.3944	55.3075	57.1304

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
26.88220	0.54924	-0.00000	-0.69315	//	0.9381	-0.0174	0.3172	0.0260	0.0019	0.0380	-0.0480	-0.0020	-0.1199	-0.0147
16.88720				//	0.9513	0.0057	0.1623	-0.0389	0.0939	-0.0634	0.0325	0.0345	-0.2267	0.0262
33.65124	0.00478	0.00000	-0.05782	//	-0.0261	0.9559	0.1058	0.0977	0.0297	0.2324	0.0137	0.0730	0.0326	-0.0582
30.99520				//	0.0142	0.8095	0.2041	0.3176	-0.1825	0.3842	-0.0391	0.1314	-0.0028	-0.0483
37.30278	1.36727	-0.00000	0.92840	//	-0.2931	-0.1708	0.8559	0.3534	0.0608	0.1009	0.0025	0.0519	0.0996	0.0322
27.30009				//	-0.1784	-0.2192	0.9353	-0.1112	-0.0334	-0.0056	0.0324	0.1688	-0.0458	0.0127
39.25144	0.50250	-0.00000	-0.54868	//	0.0884	-0.1024	-0.3669	0.7752	0.4332	0.2303	0.0312	0.0113	-0.0357	0.0553
33.22017				//	0.0434	-0.4465	-0.0109	0.8584	-0.0442	0.2032	-0.0010	0.0721	-0.0358	0.1099
43.10866	0.05872	-0.00000	0.17897	//	-0.0212	-0.0314	0.1001	-0.4629	0.7800	0.2590	0.0618	-0.2983	0.0760	0.0151
39.55825				//	-0.1016	0.2133	0.0889	0.2005	0.8909	-0.1802	0.2302	-0.0552	0.0633	0.0994
46.25750	0.07593	-0.00000	0.19647	//	-0.0318	-0.1790	-0.0610	-0.1135	-0.3688	0.8916	-0.0062	-0.0476	-0.1301	0.0108
42.52294				//	0.0680	-0.1519	0.0890	-0.1640	0.2508	0.6720	-0.3007	-0.5490	0.1525	-0.0889
50.42157	0.00632	-0.00000	0.05429	//	-0.0437	0.0492	0.0617	0.0822	-0.0969	-0.1056	0.7375	-0.4267	-0.4877	-0.0273
43.37391				//	-0.1317	-0.0411	-0.0802	-0.1285	-0.0463	0.3412	0.6538	-0.1322	-0.6160	0.1230
52.24694	0.00459	-0.00000	-0.04547	//	0.0392	-0.0835	-0.0139	-0.1473	0.1414	0.0795	0.5478	0.7913	0.0589	-0.1166
47.67535				//	0.0227	-0.1453	-0.1823	-0.2351	0.2491	0.4439	-0.0399	0.7873	0.0960	0.0131
55.13931	0.02017	0.00000	-0.09275	//	0.0896	-0.0517	-0.0439	0.0910	-0.1216	0.0369	0.2194	-0.2732	0.6212	-0.6739
52.78824				//	0.1182	-0.0749	0.0238	0.0474	-0.0740	0.0482	0.5552	-0.0179	0.4579	-0.6720
56.79083	0.06918	0.00000	-0.16926	//	0.1123	-0.0356	-0.0371	0.0089	-0.1383	0.0218	0.3169	-0.1334	0.5687	-0.7235
54.72761				//	0.1198	-0.0179	0.0314	-0.0853	-0.1690	0.0851	0.3401	-0.0763	0.5653	-0.7072



ATOMIC COORDINATES

X	3.5446	4.4065	4.4317	5.3008	5.3008	4.4317	4.4065	3.5446
Y	0.	0.4980	1.5150	2.0460	3.0420	3.5730	4.5900	5.0880

	2.6504	1.7562	0.8943	0.8691	0.	0.	0.8691	0.8943
	4.6020	5.0880	4.5900	3.5730	3.0420	2.0460	1.5150	0.4980

	1.7562	2.6504	2.6504	3.5410	3.5410	2.6504	1.7598	1.7598
	0.	0.4860	1.5150	2.0290	3.0590	3.5730	3.0590	2.0290

CORONENE X TBX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 AA	5 SS	6 SS	7 AS	8 SA	9 AS	10 SA	11 SS	12 AA	13 SA
1.624499	1.524046	1.523614	1.400129	1.399630	1.368301	1.282308	1.249339	1.238166	1.237321	1.131158	1.131078	0.868920
0.132413	0.250250	0.083639	-0.188364	-0.241012	0.207950	-0.149554	0.289443	0.214614	-0.126161	0.009284	0.328373	-0.328372
0.132433	0.197481	0.175567	-0.302142	-0.043862	0.209056	0.148183	0.289315	0.218878	-0.120025	0.279134	0.172714	0.172655
0.209627	0.173295	0.299905	-0.311902	0.179742	0.106018	0.333978	-0.000270	-0.005934	0.012603	0.144729	-0.250141	0.250172
0.131964	0.052968	0.258184	-0.113523	0.282199	0.210206	0.148511	-0.287248	-0.002849	-0.252492	-0.289552	-0.155700	-0.155639
0.131964	-0.052963	0.258185	0.113527	0.282198	0.210206	-0.148511	-0.287248	0.002905	-0.252491	-0.289736	0.155356	-0.155418
0.209627	-0.173289	0.299907	0.311905	0.179738	0.106018	-0.333978	-0.000270	0.005931	0.012604	0.144431	0.250313	0.250282
0.132432	-0.197478	0.175570	0.302141	-0.043866	0.209055	-0.148184	0.289310	-0.218860	-0.120069	0.279339	-0.172382	0.172441
0.132413	-0.250249	0.083643	0.188360	-0.241015	0.207950	0.149554	0.289439	-0.214594	-0.126204	0.009675	-0.328363	-0.328364
0.209765	-0.345894	0.000003	-0.000003	-0.360650	0.103240	0.334504	0.000000	0.014723	0.000001	-0.288997	-0.000172	0.000111
0.132413	-0.250250	-0.083639	-0.188364	-0.241012	0.207950	0.149554	-0.289443	-0.214614	0.126161	0.009285	0.328374	0.328372
0.132432	-0.197481	-0.175567	-0.302142	-0.043862	0.209055	-0.148183	-0.289314	-0.218878	0.120025	0.279134	-0.172714	-0.172655
0.209627	-0.173295	-0.299904	-0.311902	0.179743	0.106018	-0.333978	0.000270	0.005934	-0.012602	0.144729	-0.250141	-0.250172
0.131964	-0.052967	-0.258183	-0.113523	0.282199	0.210206	-0.148511	0.287248	0.002849	0.252492	-0.289552	-0.155701	0.155639
0.131965	0.052963	-0.258184	0.113527	0.282198	0.210206	0.148511	0.287249	-0.002905	0.252491	-0.289737	0.155356	0.155418
0.209627	0.173289	-0.299907	0.311904	0.179738	0.106019	0.333978	0.000271	-0.005931	-0.012604	0.144431	0.250313	-0.250283
0.132433	0.197477	-0.175571	0.302142	-0.043866	0.209056	0.148184	-0.289310	0.218859	0.120069	0.279340	-0.172382	-0.172441
0.132413	0.250248	-0.083644	0.188361	-0.241015	0.207950	-0.149553	-0.289439	0.214594	0.126204	0.009675	-0.328362	0.328365
0.209765	0.345893	-0.000003	-0.000002	-0.360650	0.103240	-0.334503	-0.000001	-0.014723	-0.000001	-0.288997	-0.000172	-0.000110
0.296349	0.272388	-0.000003	-0.000001	-0.130239	-0.262172	-0.102507	-0.000005	-0.456016	-0.000046	-0.183920	-0.000109	0.000070
0.296071	0.136468	0.235747	-0.114271	0.067308	-0.260633	0.104299	-0.003223	-0.227886	0.394636	0.092109	-0.159941	-0.159960
0.296071	-0.136464	0.235749	0.114272	0.067306	-0.260633	-0.104299	-0.003218	0.227807	0.394682	0.091918	0.160050	-0.160031
0.296349	-0.272388	0.000003	-0.000001	-0.130239	-0.262172	0.102507	0.000004	0.456016	0.000045	-0.183920	-0.000109	-0.000070
0.296071	-0.136468	-0.235747	-0.114272	0.067308	-0.260633	-0.104299	0.003223	0.227886	-0.394636	0.092109	-0.159941	0.159960
0.296071	0.136463	-0.235749	0.114272	0.067306	-0.260633	0.104299	0.003219	-0.227807	-0.394682	0.091919	0.160050	0.160031

OVERLAP EIGNVALUES AND EIGNVECTORS

14 AS	15 AA	16 SS	17 AA	18 SS	19 AS	20 AS	21 SA	22 AA	23 SS	24 AS
0.868839	0.762677	0.761831	0.750659	0.717689	0.631696	0.600368	0.599868	0.476383	0.475951	0.375499
-0.009354	0.126179	0.214606	-0.289441	0.149554	-0.207950	0.241013	0.188363	-0.083646	-0.250247	-0.132413
0.279171	-0.120044	-0.218871	0.289312	0.148183	-0.209055	-0.043863	-0.302142	0.175573	0.197475	0.132432
-0.144676	-0.012603	-0.005932	0.000271	-0.333978	0.106019	-0.179742	0.311903	-0.299909	-0.173286	-0.209627
-0.289585	-0.252491	0.002873	-0.287249	0.148511	0.210206	0.282199	-0.113524	0.258185	0.052960	0.131964
0.289704	0.252491	0.002881	0.287248	0.148511	-0.210206	-0.282198	-0.113526	-0.258183	0.052970	-0.131964
0.144484	0.012603	-0.005932	-0.000270	-0.333978	0.106019	0.179739	0.311904	0.299902	-0.173298	0.209627
-0.279303	0.120051	-0.218867	-0.289312	0.148183	-0.209056	0.043865	-0.302142	-0.175564	0.197483	-0.132432
0.009605	-0.126186	0.214602	0.289441	0.149554	0.207950	-0.241014	0.188361	0.083636	-0.250251	0.132413
0.288997	-0.000000	0.014723	0.000000	-0.334504	-0.103240	0.360650	0.000001	0.000007	0.345893	-0.209765
0.009354	0.126179	0.214606	-0.289441	0.149554	0.207950	-0.241013	-0.188363	-0.083646	-0.250247	0.132413
-0.279171	-0.120044	-0.218871	0.289312	0.148183	-0.209055	0.043863	0.302142	0.175573	0.197475	-0.132432
0.144676	-0.012603	-0.005932	0.000271	-0.333978	0.106019	0.179741	-0.311903	-0.299909	-0.173286	0.209627
0.289585	-0.252491	0.002873	-0.287249	0.148511	-0.210206	-0.282198	0.113524	0.258185	0.052960	-0.131964
-0.289704	0.252491	0.002881	0.287248	0.148511	0.210206	0.282198	0.113526	-0.258183	0.052971	0.131964
-0.144484	0.012603	-0.005932	-0.000270	-0.333978	-0.106019	-0.179739	-0.311904	0.299902	-0.173298	-0.209627
0.279303	0.120051	-0.218867	-0.289312	0.148183	0.209056	-0.043866	0.302142	-0.175565	0.197483	0.132432
-0.009605	-0.126186	0.214602	0.289441	0.149554	-0.207950	0.241015	-0.188361	0.083636	-0.250251	-0.132413
-0.288997	-0.000000	0.014723	0.000000	-0.334503	0.103240	-0.360651	-0.000002	0.000007	0.345893	0.209765
0.183920	0.000007	-0.456016	-0.000000	0.102507	0.262172	0.130239	0.000000	-0.000006	-0.272388	-0.296349
0.092075	0.394655	0.227852	-0.003220	0.104299	-0.260633	0.067308	-0.114271	0.235751	0.136461	0.296071
-0.091953	-0.394663	0.227840	0.003220	0.104300	0.260633	-0.067307	-0.114272	-0.235745	0.136471	-0.296071
-0.183920	0.000007	-0.456016	-0.000000	0.102507	-0.262172	-0.130239	-0.000000	-0.000006	-0.272388	0.296349
-0.092075	0.394655	0.227852	-0.003220	0.104299	0.260633	-0.067308	0.114271	0.235751	-0.136461	-0.296071
0.091952	-0.394662	0.227840	0.003220	0.104300	-0.260633	0.067307	-0.114272	-0.235745	0.136471	0.296071

CORONENE X TBX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 AA	5 SS	6 SS	7 AS	8 SA	9 AS	10 SA	11 SS	12 AA	13 SA
28.46004	25.45628	25.44251	21.15708	21.13820	19.92713	16.29876	14.77519	14.24046	14.19962	8.58412	8.57946	-11.16814
0.103889	0.202710	0.067759	-0.159189	-0.203720	0.177774	-0.132070	0.258954	0.192872	-0.113418	0.008729	0.308760	-0.352270
0.103905	0.159965	0.142235	-0.255345	-0.037075	0.178719	0.130858	0.258839	0.196704	-0.107902	-0.262453	0.162398	0.185220
0.164470	0.140374	0.242966	-0.263593	0.151930	0.090634	0.294931	-0.000242	-0.005333	0.011330	0.136080	-0.235201	0.268379
0.103537	0.042905	0.209166	-0.095940	0.238533	0.179702	0.131148	-0.256991	-0.002560	-0.226990	-0.272248	-0.146401	-0.166966
0.103537	-0.042901	0.209167	0.095944	0.238532	0.179702	-0.131148	-0.256991	0.002611	-0.226989	-0.272421	0.146077	-0.166729
0.164470	-0.140370	0.242968	0.263595	0.151927	0.090634	-0.294932	-0.000242	0.005330	0.011331	0.135800	0.235363	0.268498
0.103904	-0.159963	0.142237	0.255344	-0.037078	0.178719	-0.130859	0.258835	-0.196687	-0.107942	0.262646	-0.162086	0.184991
0.103889	-0.202709	0.067763	0.159186	-0.203721	0.177774	0.132069	0.258950	-0.192854	-0.113457	0.009097	-0.308750	-0.352262
0.164578	-0.280184	0.000003	-0.000002	-0.304845	0.088259	0.295396	0.000000	0.013231	0.000001	-0.271726	-0.000161	0.000119
0.103889	-0.202710	-0.067759	-0.159189	-0.203719	0.177774	0.132069	-0.258954	-0.192872	0.113418	0.008730	0.308761	0.352270
0.103905	-0.159965	-0.142234	-0.255345	-0.037075	0.178719	-0.130859	-0.258839	-0.196704	0.107903	0.262453	0.162398	-0.185220
0.164470	-0.140374	-0.242966	-0.263593	0.151930	0.090634	-0.294932	0.000242	0.005333	-0.011330	0.136079	-0.235201	-0.268379
0.103537	-0.042905	-0.209166	-0.095940	0.238534	0.179702	-0.131148	0.256991	0.002560	0.226990	-0.272248	-0.146401	0.166967
0.103538	0.042901	-0.209167	0.095944	0.238532	0.179702	0.131148	0.256991	-0.002611	0.226989	-0.272422	0.146077	0.166729
0.164470	0.140369	-0.242968	0.263595	0.151927	0.090634	0.294932	0.000242	-0.005330	-0.011331	0.135800	0.235363	-0.268498
0.103905	0.159962	-0.142238	0.255344	-0.037078	0.178719	0.130859	-0.258835	0.196687	0.107942	0.262646	-0.162086	-0.184991
0.103889	0.202708	-0.067763	0.159187	-0.203722	0.177774	-0.132069	-0.258951	0.192854	0.113457	0.009097	-0.308750	0.352262
0.164579	0.280184	-0.000003	-0.000002	-0.304845	0.088259	-0.295396	-0.000001	-0.013231	-0.000001	-0.271727	-0.000162	-0.000118
0.232511	0.220642	-0.000002	-0.000001	-0.110087	-0.224127	-0.090523	-0.000004	-0.409818	-0.000041	-0.172929	-0.000103	0.000075
0.232293	0.110543	0.190989	-0.096572	0.056893	-0.222812	0.092105	-0.002883	-0.204799	0.354777	0.086604	-0.150388	-0.171602
0.232293	-0.110540	0.190991	0.096573	0.056892	-0.222812	-0.092105	-0.002879	0.204728	0.354818	0.086425	0.150491	-0.171677
0.232511	-0.220643	0.000002	-0.000001	-0.110087	-0.224127	0.090523	0.000004	0.409818	0.000041	-0.172929	-0.000103	-0.000075
0.232293	-0.110543	-0.190989	-0.096573	0.056893	-0.222812	-0.092105	0.002883	0.204799	-0.354777	0.086604	-0.150388	0.171602
0.232293	0.110539	-0.190991	0.096573	0.056892	-0.222812	0.092105	0.002880	-0.204728	-0.354818	0.086426	0.150491	0.171677

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 AS	15 AA	16 SS	17 AA	18 SS	19 AS	20 AS	21 SA	22 AA	23 SS	24 AS
-11.17605	-23.03687	-23.14461	-24.59095	-29.12157	-43.16398	-49.27954	-49.38228	-81.37306	-81.51412	123.12542
-0.010036	0.144483	0.245874	-0.334071	0.176534	-0.261640	0.311051	0.243203	-0.121191	-0.362734	-0.216085
0.299503	-0.137458	-0.250760	0.333922	0.174917	-0.263031	-0.056610	-0.390107	0.254378	0.286241	0.216117
-0.155212	-0.014431	-0.006796	0.000312	-0.394230	-0.133392	-0.231974	0.402709	-0.434522	-0.251178	-0.342092
-0.310675	-0.289119	0.003291	-0.331541	0.175303	0.264479	0.364205	-0.146575	0.374070	0.076765	0.215354
0.310802	0.289119	0.003300	0.331540	0.175303	-0.264479	-0.364204	-0.146578	-0.374067	0.076781	-0.215354
0.155007	0.014431	-0.006796	-0.000312	-0.394230	0.133392	0.231971	0.402711	0.434512	-0.251196	0.342092
-0.299644	0.137466	-0.250756	-0.333923	0.174916	-0.263031	0.056613	-0.390106	-0.254366	0.286252	-0.216117
0.010305	-0.144491	0.245869	0.334071	0.176535	0.261640	-0.311053	0.243200	0.121175	-0.362739	0.216085
0.310044	-0.000000	0.016868	0.000000	-0.394850	-0.129896	0.465455	0.000002	0.000010	0.501373	-0.342317
0.010036	0.144483	0.245874	-0.334071	0.176535	0.261640	-0.311051	-0.243203	-0.121190	-0.362734	0.216085
-0.299503	-0.137458	-0.250760	0.333922	0.174917	-0.263031	0.056610	0.390107	0.254378	0.286241	-0.216117
0.155212	-0.014431	-0.006796	0.000312	-0.394230	-0.133392	0.231974	-0.402709	-0.434522	-0.251178	0.342092
0.310675	-0.289119	0.003291	-0.331541	0.175303	-0.264479	-0.364205	0.146575	0.374070	0.076765	-0.215354
-0.310802	0.289119	0.003300	0.331540	0.175303	0.264479	0.364204	0.146578	-0.374067	0.076781	0.215354
-0.155007	0.014431	-0.006796	-0.000312	-0.394230	-0.133392	-0.231971	-0.402711	0.434512	-0.251196	-0.342092
0.299644	0.137466	-0.250756	-0.333923	0.174916	0.263031	-0.056613	0.390106	-0.254366	0.286252	0.216117
-0.010305	-0.144491	0.245869	0.334071	0.176535	-0.261640	0.311053	-0.243200	0.121175	-0.362739	-0.216085
-0.310044	-0.000001	0.016868	0.000000	-0.394850	0.129895	-0.465455	-0.000002	0.000011	0.501373	0.342317
0.197315	0.000008	-0.522458	-0.000000	0.121000	0.329862	0.168086	0.000001	-0.000008	-0.394827	-0.483614
0.098781	0.451906	0.261050	-0.003717	0.123116	-0.327925	0.086868	-0.147540	0.341566	0.197800	0.483161
-0.098649	-0.451914	0.261036	0.003717	0.123116	0.327925	-0.086867	-0.147541	-0.341558	0.197814	-0.483161
-0.197315	0.000008	-0.522458	-0.000000	0.121000	-0.329861	-0.168086	-0.000001	-0.000008	-0.394827	0.483614
-0.098781	0.451906	0.261050	-0.003717	0.123116	0.327926	-0.086868	0.147540	0.341566	-0.197800	-0.483161
0.098649	-0.451914	0.261036	0.003717	0.123116	0.327925	0.086867	0.147541	-0.341558	0.197814	0.483161

CORONENE_X — TBX TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24						
1	1.00000	0.75120	-0.00000	-0.15704	0.00000	0.12508	0.00000	-0.09741	0.00000	0.04904	-0.00000	-0.06225	0.00000	0.08045	-0.00000
	-0.15737	0.00000	0.53371	0.00000	-0.24543	-0.00000	0.05747	0.00000	0.00267						
2	0.75120	1.00000	0.53390	-0.00000	-0.15721	0.00000	0.08031	-0.00000	-0.06207	0.00000	0.04881	0.00000	-0.09749	-0.00000	0.12540
	0.00000	-0.15737	-0.00000	-0.24483	0.00000	0.00218	-0.00000	0.05753	0.00000						
3	-0.00000	0.53390	1.00000	0.53248	-0.00000	-0.20602	-0.00000	0.12508	-0.00000	-0.06225	-0.00000	0.07316	-0.00000	-0.06213	0.00000
	0.12540	0.00000	-0.20676	0.00000	0.54204	-0.00000	-0.06269	-0.00000	-0.06337						
4	-0.15704	-0.00000	0.53248	1.00000	0.75221	0.00000	-0.15721	0.00000	0.12526	-0.00000	-0.09749	-0.00000	0.04883	0.00000	-0.06213
	-0.00000	0.08045	0.00000	0.00206	-0.00000	-0.24492	0.00000	0.05793	-0.00000						
5	0.00000	-0.15721	-0.00000	0.75221	1.00000	0.53248	0.00000	-0.15704	-0.00000	0.08045	0.00000	-0.06213	-0.00000	0.04883	-0.00000
	-0.09749	0.00000	0.12526	-0.00000	-0.24492	0.00000	0.00206	-0.00000	0.05793						
6	0.12508	0.00000	-0.20602	0.00000	0.53248	1.00000	0.53390	-0.00000	-0.20676	0.00000	0.12540	0.00000	-0.06213	-0.00000	0.07316
	0.00000	-0.06225	-0.00000	-0.06269	0.00000	0.54204	-0.00000	-0.06337	0.00000						
7	0.00000	0.08031	-0.00000	-0.15721	0.00000	0.53390	1.00000	0.75120	0.00000	-0.15737	-0.00000	0.12540	0.00000	-0.09749	-0.00000
	0.04881	-0.00000	-0.06207	-0.00000	0.00218	0.00000	-0.24483	-0.00000	0.05753						
8	-0.09741	-0.00000	0.12508	0.00000	-0.15704	-0.00000	0.75120	1.00000	0.53371	0.00000	-0.15737	0.00000	0.08045	0.00000	-0.06225
	0.00000	0.04904	0.00000	0.05747	-0.00000	-0.24543	0.00000	0.00267	-0.00000						
9	0.00000	-0.06207	-0.00000	0.12526	-0.00000	-0.20676	0.00000	0.53371	1.00000	0.53371	0.00000	-0.20676	-0.00000	0.12526	0.00000
	-0.06207	0.00000	0.07299	-0.00000	-0.06267	0.00000	0.54088	0.00000	-0.06267						
10	0.04904	0.00000	-0.06225	-0.00000	0.08045	0.00000	-0.15737	0.00000	0.53371	1.00000	0.75120	-0.00000	-0.15704	-0.00000	0.12508
	0.00000	-0.09741	-0.00000	0.05747	0.00000	0.00267	-0.00000	-0.24543	0.00000						
11	-0.00000	0.04881	-0.00000	-0.09749	0.00000	0.12540	-0.00000	-0.15737	0.00000	0.75120	1.00000	0.53390	0.00000	-0.15721	-0.00000
	0.08031	0.00000	-0.06207	0.00000	0.05753	0.00000	-0.24483	0.00000	0.00218						
12	-0.06225	0.00000	0.07316	-0.00000	-0.06213	0.00000	0.12540	-0.00000	-0.20676	-0.00000	0.53390	1.00000	0.53248	-0.00000	-0.20602
	0.00000	-0.12508	-0.00000	-0.06269	-0.00000	-0.06337	0.00000	0.54204	0.00000						
13	0.00000	-0.09749	-0.00000	0.04883	-0.00000	-0.06213	0.00000	0.08045	-0.00000	-0.15704	0.00000	0.53248	1.00000	0.75221	0.00000
	-0.15720	-0.00000	0.12526	-0.00000	0.05793	0.00000	0.00206	-0.00000	-0.24492						
14	0.08045	-0.00000	-0.06213	0.00000	0.04883	-0.00000	-0.09749	0.00000	0.12526	-0.00000	-0.15721	-0.00000	0.75221	1.00000	0.53248
	0.00000	-0.15704	0.00000	0.00206	0.00000	0.05793	0.00000	-0.24492	-0.00000						
15	-0.00000	0.12540	0.00000	-0.06213	-0.00000	0.07316	-0.00000	-0.06225	0.00000	0.12508	-0.00000	-0.20602	0.00000	0.53248	1.00000
	0.53390	0.00000	-0.20676	0.00000	-0.06337	-0.00000	-0.06269	0.00000	0.54204						
16	-0.15737	0.00000	0.12540	-0.00000	-0.09749	0.00000	0.04881	0.00000	-0.06207	0.00000	0.08031	0.00000	-0.15720	0.00000	0.53390
	1.00000	0.75120	0.00000	-0.24483	-0.00000	0.05753	0.00000	0.00218	0.00000						
17	0.00000	-0.15737	0.00000	0.08045	0.00000	-0.06225	-0.00000	0.04904	0.00000	-0.09741	0.00000	0.12508	-0.00000	-0.15704	0.00000
	0.75120	1.00000	0.53371	0.00000	0.00267	-0.00000	-0.24543								
18	0.53371	-0.00000	-0.20676	0.00000	0.12526	-0.00000	-0.06207	0.00000	0.07299	-0.00000	-0.06207	-0.00000	0.12526	0.00000	-0.20676
	0.00000	0.53371	1.00000	0.54088	0.00000	-0.06267	-0.00000	-0.06267	0.00000						
19	0.00000	-0.24483	0.00000	0.00206	-0.00000	-0.06269	-0.00000	0.05747	-0.00000	0.05747	0.00000	-0.06269	-0.00000	0.00206	0.00000
	-0.24483	0.00000	0.54088	1.00000	0.52153	0.00000	-0.17062	0.00000	0.52153						
20	-0.24543	0.00000	0.54204	-0.00000	-0.24492	0.00000	0.00218	-0.00000	-0.06267	0.00000	0.05753	-0.00000	0.05793	0.00000	-0.06337
	-0.00000	0.00267	0.00000	0.52153	1.00000	0.51971	0.00000	-0.17103	-0.00000						
21	-0.00000	0.00218	-0.00000	-0.24492	0.00000	0.54204	0.00000	-0.24543	0.00000	0.00267	0.00000	-0.06337	0.00000	0.05793	-0.00000
	0.05753	-0.00000	-0.06267	0.00000	0.51971	1.00000	0.52153	-0.00000	-0.17103						
22	0.05747	-0.00000	-0.06269	0.00000	0.00206	-0.00000	-0.24483	0.00000	0.54088	-0.00000	-0.24483	0.00000	0.00206	0.00000	-0.06269
	0.00000	0.05747	-0.00000	-0.17062	0.00000	0.52153	1.00000	0.52153	0.00000						
23	0.00000	-0.05753	-0.00000	0.05793	-0.00000	-0.06337	-0.00000	0.00267	0.00000	-0.24543	0.00000	0.54204	-0.00000	-0.24492	0.00000
	0.00218	-0.00000	-0.06267	0.00000	-0.17103	-0.00000	0.52153	1.00000	0.51971						
24	0.00267	0.00000	-0.06337	-0.00000	0.05793	0.00000	0.05753	-0.00000	-0.06267	0.00000	0.00218	0.00000	-0.24492	-0.00000	0.54204
	0.00000	-0.24543	0.00000	0.52153	-0.00000	-0.17103	0.00000	0.51971	1.00000						

CORONENE X — TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24						
1	0.76979	0.57037	-0.04727	-0.14789	0.00811	0.12157	-0.00491	-0.09581	-0.00157	0.04881	0.00243	-0.06163	-0.00490	0.07813	0.01501
	-0.14822	-0.05096	0.37145	-0.03432	-0.22934	0.01195	0.05511	-0.00015	0.00717						
2	0.57037	0.76969	0.37151	-0.05091	-0.14806	0.01497	0.07799	-0.00491	-0.06145	0.00243	0.04858	-0.00159	-0.09589	-0.00491	0.12187
	0.00809	-0.14822	-0.04721	-0.22876	-0.03448	0.00668	-0.00011	0.05517	0.01200						
3	-0.04727	0.37151	0.73509	0.37052	-0.04713	-0.19114	0.01497	0.12157	-0.00093	-0.06163	-0.00159	0.07158	-0.00159	-0.06151	-0.00091
	0.12187	0.01501	-0.19181	-0.03169	0.38693	-0.03157	-0.05753	0.01014	-0.05818						
4	-0.14789	-0.05091	0.37052	0.77007	0.57152	-0.04713	-0.14806	0.00811	0.12174	-0.00490	-0.09589	-0.00159	0.04860	0.00243	-0.06151
	-0.00491	0.07813	0.01500	0.00657	-0.03442	-0.22888	0.01196	0.05556	-0.00009						
5	0.00811	-0.14806	-0.04713	0.57152	0.77007	0.37052	-0.05091	-0.14789	0.01500	0.07813	-0.00491	-0.06151	0.00243	0.04860	-0.00159
	-0.09589	-0.00490	0.12174	0.01196	-0.22888	-0.03442	0.00657	-0.00009	0.05556						
6	0.12157	0.01497	-0.19114	-0.04713	0.37052	0.73509	0.37151	-0.04727	-0.19181	0.01501	0.12187	-0.00091	-0.06151	-0.00159	0.07158
	-0.00159	-0.06163	-0.00093	-0.05753	-0.03157	0.38693	-0.03169	-0.05818	0.01014						
7	-0.00491	0.07799	0.01497	-0.14806	-0.05091	0.37151	0.76969	0.57037	-0.04721	-0.14822	0.00809	0.12187	-0.00491	-0.09589	-0.00159
	0.04858	0.00243	-0.06145	-0.00011	0.00668	-0.03448	-0.22876	0.01200	0.05517						
8	-0.09581	-0.00491	0.12157	0.00811	-0.14789	-0.04727	0.57037	0.76979	0.37145	-0.05096	-0.14822	0.01501	0.07813	-0.00490	-0.06163
	0.00243	0.04881	-0.00157	0.05511	0.01195	-0.22934	-0.03432	0.00717	-0.00015						
9	-0.00157	-0.06145	-0.00093	0.12174	0.01500	-0.19181	-0.04721	0.37145	0.73516	0.37145	-0.04721	-0.19181	0.01500	0.12174	-0.00093
	-0.06145	-0.00157	0.07141	0.01010	-0.05752	-0.03163	0.38603	-0.03163	-0.05752						
10	0.04881	0.00243	-0.06163	-0.00490	0.07813	0.01501	-0.14822	-0.05096	0.37145	0.76979	0.57037	-0.04727	-0.14789	0.00811	0.12157
	-0.00491	-0.09581	-0.00157	0.05511	-0.00015	0.00717	-0.03432	-0.22934	0.01195						
11	0.00243	0.04858	-0.00159	-0.09589	-0.00491	0.12187	0.00809	-0.14822	-0.04721	0.57037	0.76969	0.37151	-0.05091	-0.14806	0.01497
	0.07799	-0.00491	-0.06145	-0.00011	0.05517	0.01200	-0.22876	-0.03448	0.00668						
12	-0.06163	-0.00159	0.07158	-0.00159	-0.06151	-0.00091	0.12187	0.01501	-0.19181	-0.04727	0.37151	0.73509	0.37052	-0.04713	-0.19114
	0.01497	0.12157	-0.00093	-0.05753	0.01014	-0.05818	-0.03169	0.38693	-0.03157						
13	-0.00490	-0.09589	-0.00159	0.04860	0.00243	-0.06151	-0.00491	0.07813	0.01500	-0.14789	-0.05091	0.37052	0.77007	0.57152	-0.04713
	-0.14806	0.00811	0.12174	0.01196	0.05556	-0.00009	0.00657	-0.03442	-0.22888						
14	0.07813	-0.00491	-0.06151	0.00243	0.04860	-0.00159	-0.09589	-0.00490	0.12174	0.00811	-0.14806	-0.04713	0.57152	0.77007	0.37052
	-0.05091	-0.14789	0.01500	-0.00657	-0.00009	0.05556	0.01196	-0.22888	-0.03442						
15	0.01501	0.12187	-0.00091	-0.06151	-0.00159	0.07158	-0.00159	-0.06163	-0.00093	0.12157	0.01497	-0.19114	-0.04713	0.37052	0.73509
	0.37151	-0.04727	-0.19181	-0.03169	-0.05818	0.01014	-0.05753	-0.03157	0.38693						
16	-0.14822	0.00809	0.12187	-0.00491	-0.09589	-0.00159	0.04858	0.00243	-0.06145	-0.00491	0.07799	0.01497	-0.14806	-0.05091	0.37151
	0.76969	0.57037	-0.04721	-0.22876	0.01200	0.05517	-0.00011	0.00668	-0.03448						
17	-0.05096	-0.14822	0.01501	0.07813	-0.00490	-0.06163	0.00243	0.04881	-0.00157	-0.09581	-0.00491	0.12157	0.00811	-0.14789	-0.04727
	0.57037	0.76979	0.37145	-0.03432	0.00717	-0.00015	0.05511	0.01195	-0.22934						
18	0.37145	-0.04721	-0.19181	0.01500	0.12174	-0.00093	-0.06145	0.00157	0.07141	-0.00157	-0.06145	-0.00093	0.12174	0.01500	-0.19181
	-0.04721	0.37145	0.73516	0.38603	-0.03163	-0.05752	0.01010	-0.05752	-0.03163						
19	-0.03432	-0.22876	-0.03169	0.00657	0.01196	-0.05753	-0.00011	0.05511	0.01010	0.05511	-0.00011	-0.05753	0.01196	0.00657	-0.03169
	-0.22876	-0.03432	0.38603	0.74229	0.36539	-0.03449	-0.15702	-0.03449	0.36539						
20	-0.22934	-0.03448	0.38693	-0.03442	-0.22888	-0.03157	0.00668	0.01195	-0.05752	-0.00015	0.05517	0.01014	0.05556	-0.00009	-0.05818
	0.01200	0.00717	-0.03163	0.36539	0.74257	0.36421	-0.03449	-0.15742	-0.03473						
21	0.01195	0.00668	-0.03157	-0.22888	-0.03442	0.38693	-0.03448	-0.22934	-0.03163	0.00717	0.01200	-0.05818	-0.00009	0.05556	0.01014
	0.05517	-0.00015	-0.05752	-0.03449	0.36421	0.74257	0.36539	-0.03473	-0.15742						
22	0.05511	-0.00011	-0.05753	0.01196	0.00657	-0.03169	-0.22876	-0.03432	0.38603	-0.03432	-0.22876	-0.03169	0.00657	0.01196	-0.05753
	-0.00011	0.05511	0.01010	-0.15702	-0.03449	0.36539	0.74229	0.36539	-0.03449						
23	-0.00015	0.05517	0.01014	0.05556	-0.00009	-0.05818	0.01200	0.00717	-0.03163	-0.22934	-0.03448	0.38693	-0.03442	-0.22888	-0.03157
	0.00668	0.01195	-0.05752	-0.03449	-0.15742	-0.03473	0.36539	0.74257	0.36421						
24	0.00717	0.01200	-0.05818	-0.00009	0.05556	0.01014	0.05517	-0.00015	-0.05752	0.01195	0.00668	-0.03157	-0.22888	-0.03442	0.38693
	-0.03448	-0.22934	-0.03163	0.36539	-0.03473	-0.15742	-0.03449	0.36421	0.74257						

ENERGIES FOR CORONENE X , TBX APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	11,13	12,14	6,13	5,13	4,14	9,15	10,16	8,16	9,17	7,15
XMOMNT	1.01902	1.01902	0.00013	0.04804	0.04752	-0.41160	0.41162	-0.24118	0.24135	-0.48941
YMOMNT	-0.00100	-0.00100	-0.00000	-0.00002	-0.00002	0.00005	-0.00005	-0.00001	0.00002	-0.00001
JUMP E	19.7523	19.7555	31.0953	32.3063	32.3331	37.2773	37.3442	37.9198	38.8314	39.3356
DIAG E	30.7317	30.7342	45.0475	47.8707	47.9210	49.4360	49.4972	54.5663	55.6971	51.6857
DIAG E	31.0461	31.0599	46.2786	48.9073	48.9639	48.9328	48.9850	49.9877	61.9276	51.8542
CORRSP	24.5067	34.6688	43.8559	49.5496	44.9352	45.9398	54.2653	55.2599	57.0818	53.1242
CORRSP	25.1317	34.8299	45.1818	50.0357	45.7669	45.6772	53.9945	50.7362	62.8587	53.7303

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	Γ	XMOMNT	YMOMNT	//	STATE COMPOSITION									
24.50666	0.00000	-0.00025	-0.00000	//	0.6995	-0.6992	0.0011	0.0806	-0.0803	-0.0668	-0.0669	0.0009	0.0011	0.0013
24.43903				//	0.6975	-0.6971	0.0016	0.0973	-0.0973	-0.0661	-0.0654	0.0007	0.0013	0.0016
34.66877	2.21855	1.22671	-0.00132	//	0.6733	0.6737	-0.0705	0.0611	0.0595	0.1941	-0.1929	-0.0541	0.0413	0.0315
21.75620				//	0.6841	0.6846	0.0774	0.0337	0.0339	-0.0374	0.0373	-0.1373	0.1422	-0.1151
43.85590	0.05239	0.16761	-0.00011	//	0.0594	0.0609	0.8937	-0.2133	-0.2059	-0.0302	0.0244	-0.0441	0.3083	0.0870
34.71092				//	-0.0806	-0.0784	0.6390	-0.2859	-0.2826	-0.3653	0.3638	-0.2019	0.2934	0.1573
49.54958	0.00006	-0.00555	0.00000	//	-0.0999	0.0979	0.0020	0.6553	-0.6558	-0.2445	-0.2470	0.0013	0.0034	0.0067
44.17777				//	-0.0541	0.0528	0.0108	0.6232	-0.6075	0.3444	0.3437	-0.0004	-0.0007	0.0019
44.93521	0.06160	0.17954	0.00001	//	-0.0156	-0.0140	0.3310	0.5740	0.5783	-0.0117	-0.0083	0.2092	-0.0207	-0.4263
42.72818				//	-0.0567	-0.0565	0.3726	0.5398	0.5517	-0.2457	0.2323	0.2299	-0.0615	-0.2967
45.93982	0.00001	-0.00205	0.00000	//	0.0325	-0.0355	0.0116	0.2600	-0.2448	0.6620	0.6571	-0.0021	-0.0027	-0.0047
47.06317				//	0.1044	-0.1047	-0.0080	-0.3331	0.3354	0.6032	0.6250	-0.0045	-0.0083	-0.0043
54.26528	2.43898	1.02806	-0.00045	//	0.1947	0.1946	-0.0348	-0.0454	-0.0524	-0.6517	0.6542	-0.0958	-0.1117	-0.2092
46.65027				//	0.0241	0.0276	-0.5824	-0.0134	-0.0342	-0.5611	0.5433	-0.0478	-0.2037	0.0658
55.25995	0.00091	0.01970	-0.00010	//	0.0538	0.0542	-0.0971	-0.2062	-0.2089	-0.0105	0.0185	0.9118	0.1628	-0.2006
54.70544				//	0.0786	0.0791	0.0386	-0.2708	-0.2746	-0.0539	0.0608	0.8877	0.0093	-0.2064
57.08182	0.17977	0.27214	0.00008	//	-0.0362	-0.0361	-0.2730	0.1111	0.1120	-0.0734	0.0795	-0.1479	0.9294	-0.0251
56.56917				//	-0.0682	-0.0679	-0.3113	0.1374	0.1389	-0.0110	0.0188	0.1144	0.9153	0.0661
53.12425	0.17984	-0.28215	-0.00008	//	0.0206	0.0215	0.0376	0.2466	0.2535	-0.1690	0.1736	0.2982	-0.0051	0.8515
51.02490				//	0.1027	0.1035	0.0945	0.1567	0.1666	-0.0098	-0.0069	0.2900	-0.1028	0.9070

ENERGIES FOR CORONENE X ,TBX APPROXIMATION 1.7

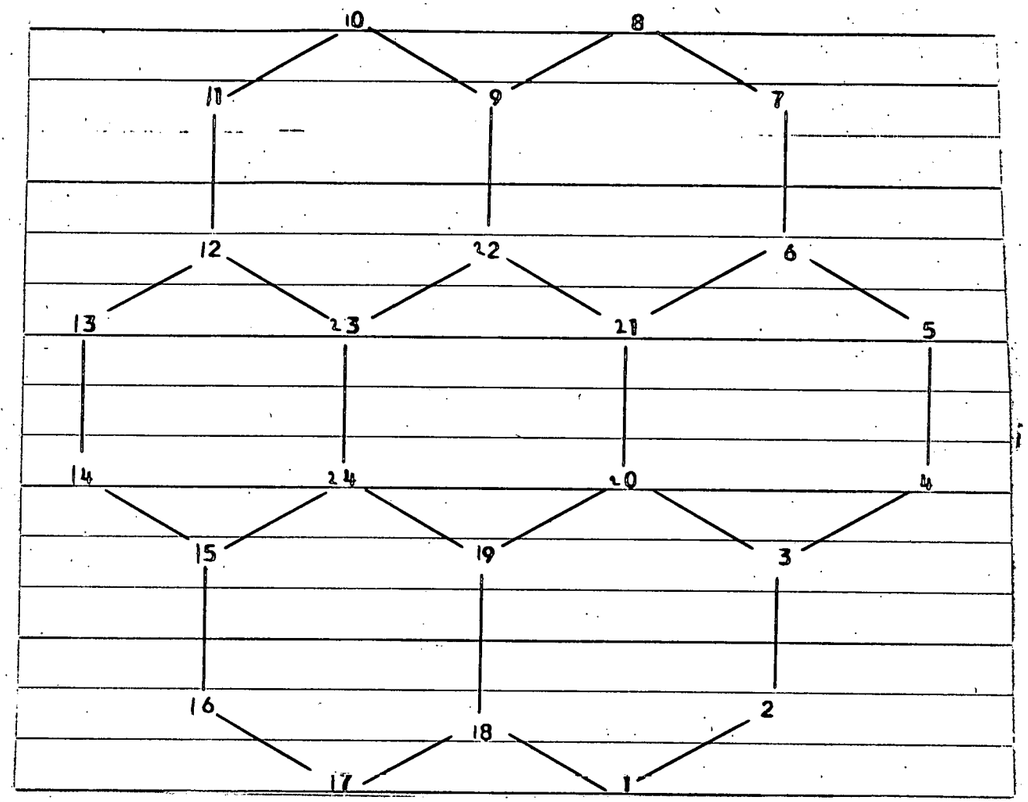
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	12,13	11,14	6,14	5,14	4,13	10,15	9,16	8,15	10,17	8,17
XMOMNT	0.00100	-0.00100	0.00000	-0.00002	0.00002	-0.00005	-0.00005	-0.00000	0.00002	0.00000
YMOMNT	1.01917	-1.01869	-0.00192	-0.04699	0.04697	-0.41497	-0.40863	-0.23630	-0.23648	0.00321
JUMP E	19.7476	19.7602	31.1032	32.3142	32.3252	37.2365	37.3851	37.8121	38.7906	39.3661
DIAG E	31.7097	31.7489	45.0537	48.2997	48.2936	50.8526	51.0302	54.4584	55.6502	60.8537
DIAG E	32.0289	32.0697	46.2913	49.3428	49.3300	50.3469	50.5205	49.8863	61.8781	63.0152
CORRSP	26.2535	34.6692	43.8842	49.5389	46.4056	48.8444	54.1702	55.0775	57.0415	61.9855
CORRSP	26.8035	34.8971	45.3407	50.3215	46.9147	48.5567	53.8921	51.2174	62.8109	63.9551

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
26.25352	0.00001	0.00000	0.00311	//	0.7003	0.6964	0.0000	0.0664	0.0674	0.0377	-0.0354	0.0007	0.0007	0.1140
22.10874				//	0.6858	-0.6890	0.0857	-0.0192	0.0196	-0.0463	-0.0428	-0.1438	-0.1490	0.0008
34.66916	2.27357	-0.00132	-1.24182	//	-0.6709	0.6753	0.0723	0.0672	-0.0661	-0.1941	-0.1930	0.0554	0.0425	-0.0005
17.94433				//	0.6584	0.6543	-0.0003	-0.0464	-0.0458	0.1774	-0.1758	0.0006	0.0006	0.2678
43.88419	0.08510	0.00011	0.21355	//	0.0622	-0.0614	0.9270	0.1361	-0.1398	-0.0364	-0.0251	-0.0216	-0.3042	0.0024
38.66178				//	-0.2080	-0.2075	0.0026	-0.4590	-0.4639	0.4612	-0.4600	-0.0036	-0.0042	0.2519
49.53887	0.00051	0.00001	0.01558	//	-0.0103	-0.0168	-0.0018	0.5025	0.5107	-0.4954	0.4766	0.0035	0.0045	-0.1171
43.30814				//	-0.0489	-0.0499	-0.0211	0.5098	0.3946	0.5327	-0.4727	-0.0335	-0.0187	-0.2653
46.48563	0.01358	-0.00005	-0.08289	//	-0.0383	0.0367	0.2273	-0.6594	0.6616	-0.0025	-0.0183	0.2626	0.0615	-0.0030
43.50494				//	-0.0167	0.0058	0.3133	-0.5472	0.6334	-0.1803	-0.2853	0.2755	0.1019	-0.0279
48.84439	0.00024	-0.00001	-0.01075	//	-0.0572	-0.0539	0.0051	0.4728	0.4594	0.5175	-0.5036	-0.0062	-0.0062	-0.1943
35.09545				//	0.1072	-0.1112	-0.6622	-0.2588	0.2579	0.3831	0.3748	0.1879	0.2856	-0.0024
54.17021	1.95464	-0.00046	-0.92115	//	-0.1977	0.1970	0.0365	-0.0038	0.0090	0.6608	0.6861	-0.0410	-0.1075	0.0033
46.69130				//	-0.0182	0.0200	0.5944	-0.0666	0.0555	0.5358	0.5534	0.0620	-0.2034	0.0032
55.07753	0.05151	0.00006	-0.14829	//	0.0365	-0.0368	-0.0868	0.1635	-0.1633	0.0313	0.0279	0.9508	-0.1750	-0.0047
54.44743				//	0.0996	-0.1006	0.0592	0.2508	-0.2497	-0.0425	-0.0513	0.9196	0.0326	-0.0061
57.04149	0.16087	0.00009	-0.25753	//	0.0375	-0.0378	0.2736	0.1153	-0.1171	0.0852	0.0813	0.1476	0.9271	-0.0075
56.50423				//	0.0709	-0.0712	0.3143	0.1208	-0.1223	0.0266	0.0206	-0.1321	0.9182	-0.0059
61.98547	0.00001	0.00000	0.00172	//	-0.0947	-0.0955	0.0008	0.1474	0.1468	0.0380	-0.0410	0.0059	0.0069	0.9672
59.87562				//	0.1533	-0.1536	0.0014	0.2804	0.2802	-0.0318	0.0320	0.0053	0.0066	0.8909

CORONENE IRX



ATOMIC COORDINATES

X	3.5446	4.4065	4.4317	5.3008	5.3008	4.4317	4.4065	3.5446
y	0.	0.4980	1.5150	2.0460	3.0420	3.5730	4.5900	5.0880
	2.6504	1.7562	0.8943	0.8691	0.	0.	0.8691	0.8943
	4.6020	5.0880	4.5900	3.5730	3.0420	2.0460	1.5150	0.4980
	1.7562	2.6504	2.6504	3.5410	3.5410	2.6504	1.7598	1.7598
	0.	0.4860	1.5150	2.0290	3.0590	3.5730	3.0590	2.0290

CORONENE X IRX APPROXIMATION 30

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 AA	5 SS	6 SS	7 SA	8 AS	9 AS	10 SA	11 SS	12 AA	13 SA
1.785500	1.808146	1.807494	1.409715	1.409006	1.351937	1.219940	1.219711	1.162135	1.161304	1.056601	1.056468	0.815894
0.137634	0.255459	0.089491	-0.202210	0.242825	0.205552	0.288555	-0.157453	-0.212950	-0.125731	-0.009030	0.324177	0.330605
0.137643	0.205124	0.177123	-0.311075	0.054129	0.206051	0.288411	0.156246	-0.215776	-0.121981	0.284988	0.154187	-0.182409
0.208966	0.170987	0.295897	-0.296187	-0.170891	0.102257	-0.000140	0.328527	-0.013930	0.026395	0.151901	-0.262834	-0.246145
0.137197	0.050517	0.265676	-0.108700	-0.296020	0.206604	-0.289062	0.156544	-0.001456	-0.247669	-0.276552	-0.169500	0.148682
0.137197	-0.050507	0.265678	0.108724	-0.296011	0.206605	-0.289054	-0.156558	0.001442	-0.247669	-0.276446	0.169672	0.147904
0.208966	-0.170976	0.295904	0.296201	-0.170867	0.102257	-0.000125	0.328527	0.013931	0.026395	0.152064	0.262739	-0.246518
0.137643	-0.205117	0.177131	0.311070	0.054154	0.206051	0.288419	-0.156232	-0.215783	-0.121969	0.284892	-0.154365	-0.181684
0.137634	-0.255455	0.089501	0.202190	0.242841	0.205552	0.288548	0.157467	-0.212957	-0.125719	-0.009231	-0.324171	0.330555
0.209110	-0.341345	0.000007	-0.000014	0.342166	0.101121	-0.000008	0.328984	0.030390	-0.000001	-0.303574	0.000095	-0.000373
0.137634	-0.255458	-0.089491	-0.202210	0.242824	0.205552	-0.288555	0.157453	-0.212950	0.125731	-0.009029	0.324177	-0.330605
0.137643	-0.205124	-0.177123	-0.311075	0.054129	0.206051	-0.288411	-0.156246	-0.215776	0.121981	0.284988	0.154187	0.182409
0.208966	-0.170987	-0.295897	-0.296187	-0.170891	0.102257	0.000140	-0.328527	0.013930	-0.026395	0.151901	-0.262834	0.246145
0.137197	-0.050517	-0.265676	-0.108700	-0.296020	0.206605	0.289062	-0.156545	0.001456	0.247669	-0.276552	-0.169500	-0.148682
0.137197	0.050506	-0.265678	0.108724	-0.296011	0.206605	0.289055	0.156558	-0.001442	0.247669	-0.276446	0.169672	-0.147904
0.208966	0.170975	-0.295904	0.296200	-0.170867	0.102257	0.000125	0.328527	-0.013931	-0.026395	0.152064	0.262740	0.246518
0.137643	0.205117	-0.177131	0.311071	0.054154	0.206051	-0.288419	0.156233	0.215783	0.121969	0.284892	-0.154365	0.181684
0.137634	0.255455	-0.089501	0.202190	0.242841	0.205552	-0.288548	0.157466	0.212957	0.125719	-0.009231	-0.324171	-0.330555
0.209110	0.341345	-0.000007	-0.000014	0.342166	0.101121	0.000008	-0.328984	-0.030391	0.000001	-0.303573	0.000094	0.000373
0.292003	0.264706	-0.000005	-0.000005	0.129526	-0.267690	0.000002	-0.096334	-0.458172	0.000013	-0.175547	0.000055	-0.000238
0.291762	0.132625	0.229071	-0.113133	-0.065949	-0.266847	-0.000329	0.097989	-0.229055	0.396590	0.087635	-0.152650	0.157696
0.291762	-0.132617	0.229076	0.113139	-0.065940	-0.266847	-0.000325	-0.097989	0.229077	0.396577	0.087730	0.152595	-0.157933
0.292003	-0.264706	0.000005	-0.000005	0.129526	-0.267689	-0.000002	0.096334	0.458172	-0.000013	-0.175547	0.000055	0.000238
0.291762	-0.132625	-0.229071	-0.113133	-0.065949	-0.266847	0.000329	-0.097989	0.229055	-0.396590	0.087635	-0.152650	-0.157695
0.291762	-0.132616	-0.229076	0.113138	-0.065940	-0.266847	0.000325	0.097989	-0.229077	-0.396577	0.087730	0.152595	-0.157934

OVERLAP EIGNVALUES AND EIGNVECTORS

14 AS	15 AA	16 SS	17 AA	18 SS	19 AS	20 AS	21 SA	22 AA	23 SS	24 AS
0.815856	0.736235	0.735437	0.721260	0.701073	0.637900	0.615435	0.615054	0.537907	0.537600	0.482362
0.018565	0.116519	-0.222919	0.289355	-0.149105	0.205967	-0.236684	0.183421	-0.081996	0.240475	0.125663
-0.276084	-0.132082	0.214803	-0.289426	0.147615	-0.207425	0.042161	-0.295678	0.167987	-0.191165	-0.125680
0.142521	0.002928	-0.003111	-0.000262	-0.335355	0.123060	0.183048	0.317899	-0.305292	0.176369	0.209230
0.296319	-0.255047	0.009606	0.287218	0.147893	-0.208808	-0.275261	-0.111921	0.248754	-0.049498	-0.125106
-0.296708	0.255047	0.009611	-0.287218	0.147892	0.208808	0.275249	-0.111953	-0.248754	-0.049496	0.125106
-0.141875	-0.002928	-0.003111	0.000263	-0.335355	-0.123060	-0.183012	0.317920	0.305293	0.176368	-0.209230
0.276562	0.132078	0.214806	0.289426	0.147615	0.207425	-0.042195	-0.295673	-0.167988	-0.191164	0.125680
-0.019432	-0.116515	-0.222922	-0.289356	0.149105	-0.205967	0.236705	0.183394	0.081998	0.240475	-0.125663
-0.284533	-0.000000	0.003036	0.000000	-0.335965	0.119216	-0.367825	0.000021	-0.000001	-0.352038	0.209432
-0.018564	0.116519	-0.222919	0.289356	0.149105	-0.205967	0.236684	-0.183421	-0.081996	0.240475	-0.125663
0.276084	-0.132082	0.214803	-0.289427	0.147614	0.207425	-0.042161	0.295678	0.167987	-0.191165	0.125680
-0.142521	0.002928	-0.003111	-0.000262	-0.335355	-0.123060	-0.183048	-0.317899	-0.305292	0.176370	-0.209229
-0.296319	-0.255047	0.009606	0.287218	0.147893	0.208808	0.275261	0.111921	0.248754	-0.049498	0.125106
0.296708	0.255047	0.009611	-0.287218	0.147892	-0.208808	-0.275248	0.111953	-0.248754	-0.049496	-0.125106
0.141875	-0.002928	-0.003111	0.000262	-0.335355	0.123060	0.183012	-0.317920	0.305293	0.176368	0.209229
-0.276561	-0.132078	0.214806	0.289426	0.147615	-0.207425	0.042195	0.295673	-0.167988	-0.191164	-0.125680
0.019431	-0.116514	-0.222922	-0.289356	0.149105	0.205967	-0.236705	-0.183394	0.081998	0.240475	0.125663
0.284533	-0.000000	0.003036	0.000000	-0.335965	-0.119216	0.367825	-0.000021	-0.000001	-0.352038	-0.209432
-0.181219	-0.000005	0.453395	-0.000000	0.099357	-0.257945	-0.140838	0.000008	0.000001	0.282920	0.302518
-0.091003	0.392330	-0.226437	0.003346	0.101342	0.255799	-0.073260	-0.123855	0.244896	-0.141721	-0.302151
0.090589	-0.392325	-0.226445	-0.003346	0.101343	-0.255799	0.073246	0.123863	-0.244897	-0.141719	0.302151
0.181219	-0.000004	0.453395	-0.000000	0.099357	-0.257945	0.140838	-0.000008	0.000001	0.282920	-0.302518
0.091003	-0.392330	-0.226437	0.003346	0.101342	-0.255799	0.073260	0.123855	0.244897	-0.141721	0.302151
-0.090589	-0.392325	-0.226445	-0.003346	0.101343	-0.255800	-0.073246	-0.123864	-0.244897	-0.141719	-0.302151

CORONENE X IRX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 AA	5 SS	6 SS	7 SA	8 AS	9 AS	10 SA	11 SS	12 AA	13 SA
32.56940	27.99664	27.97796	21.51661	21.49019	19.27221	13.34715	13.33577	10.32866	10.28309	3.96584	3.95703	-16.70542
0.103002	0.201446	0.070584	-0.170308	0.204567	0.176785	0.261252	-0.142569	0.197537	-0.116673	-0.008784	0.315394	0.366009
0.103009	0.161754	0.139701	-0.261999	0.045601	0.177214	0.261122	0.141475	0.200159	-0.113193	0.277249	0.150010	-0.201943
0.156385	0.134834	0.233381	-0.249460	-0.143967	0.087946	-0.000127	0.297470	-0.012922	0.024494	0.147776	-0.255713	-0.272505
0.102675	0.039836	0.209546	-0.091551	-0.249382	0.177689	-0.261711	0.141745	-0.001351	-0.229826	-0.269043	-0.164908	0.164605
0.102675	-0.039828	0.209547	0.091571	-0.249374	0.177690	-0.261704	-0.141758	0.001338	-0.229826	-0.268940	0.165075	0.163743
0.156385	-0.134825	0.233387	0.249471	-0.143947	0.087946	-0.000113	-0.297470	0.012923	0.024493	0.147935	0.255621	-0.272918
0.103009	-0.161748	0.139707	0.261995	0.045622	0.177214	0.261128	-0.141463	-0.200165	-0.113182	0.277156	-0.150183	-0.201141
0.103002	-0.201443	0.070592	0.170292	0.204581	0.176785	0.261245	0.142581	-0.197544	-0.116662	-0.008981	-0.315388	0.365954
0.156493	-0.269173	0.000005	-0.000012	0.288258	0.086969	-0.000007	0.297883	0.028191	-0.000001	-0.295331	0.000092	-0.000413
0.103002	-0.201445	-0.070584	-0.170308	0.204567	0.176784	-0.261252	0.142568	-0.197537	0.116673	-0.008784	0.315394	-0.366009
0.103009	-0.161754	-0.139701	-0.261999	0.045601	0.177213	-0.261122	-0.141475	-0.200159	0.113193	0.277250	0.150010	0.201943
0.156385	-0.134834	-0.233382	-0.249459	-0.143967	0.087946	0.000127	-0.297469	0.012922	-0.024494	0.147776	-0.255713	0.272505
0.102675	-0.039836	-0.209546	-0.091551	-0.249382	0.177690	-0.261711	-0.141746	0.001351	0.229826	-0.269043	-0.164908	-0.164605
0.102675	0.039828	-0.209547	0.091571	-0.249374	0.177690	0.261704	0.141758	-0.001338	0.229826	-0.268940	0.165075	-0.163743
0.156385	0.134825	-0.233387	0.249471	-0.143947	0.087946	0.000113	0.297470	-0.012923	-0.024493	0.147935	0.255622	0.272917
0.103009	0.161748	-0.139707	0.261995	0.045622	0.177214	-0.261128	0.141463	0.200165	0.113182	0.277156	-0.150183	0.201141
0.103002	-0.201443	-0.070592	0.170292	0.204581	0.176785	-0.261246	-0.142580	0.197544	0.116662	-0.008980	-0.315389	-0.365954
0.156493	0.269173	-0.000005	-0.000011	0.288258	0.086969	0.000007	-0.297884	-0.028191	0.000001	-0.295331	0.000092	0.000413
0.218528	0.208737	-0.000004	-0.000004	0.109119	-0.230226	0.000002	-0.087227	-0.425011	0.000012	-0.170781	0.000053	-0.000263
0.218348	0.104584	0.180674	-0.095285	-0.055559	-0.229501	-0.000298	0.088726	-0.212477	0.368018	0.085256	-0.148514	0.174583
0.218348	-0.104577	0.180678	0.095289	-0.055551	-0.229501	-0.000294	-0.088726	0.212497	0.368006	0.085348	0.148461	0.174847
0.218528	-0.208737	0.000004	-0.000004	0.109119	-0.230225	-0.000002	0.087227	0.425011	-0.000012	-0.170781	0.000053	0.000263
0.218348	-0.104584	-0.180674	-0.095285	-0.055559	-0.229501	0.000298	-0.088726	0.212477	-0.368018	0.085256	-0.148514	-0.174583
0.218348	0.104577	-0.180678	0.095289	-0.055551	-0.229501	0.000294	0.088726	-0.212497	-0.368006	0.085348	0.148461	-0.174847

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 AS	15 AA	16 SS	17 AA	18 SS	19 AS	20 AS	21 SA	22 AA	23 SS	24 AS
-16.70969	-26.52305	-26.63223	-28.61082	-31.56644	-42.02422	-46.26055	-46.33511	-63.59842	-63.67700	-79.44691
0.020553	0.135797	-0.259941	0.340711	0.178078	0.257883	-0.301702	0.233880	-0.111800	0.327975	0.180934
-0.305657	-0.153934	0.250477	-0.340794	0.176298	-0.259708	0.053743	-0.377018	0.229045	-0.260723	-0.180959
0.157788	0.003412	-0.003628	-0.000308	-0.400519	0.154078	0.233332	0.405353	-0.416257	0.240544	0.301257
0.328060	-0.297244	0.011202	0.338194	0.176630	-0.261439	-0.350876	-0.142710	0.339169	-0.067508	-0.180133
-0.328490	0.297244	0.011208	-0.338194	0.176629	0.261439	0.350860	-0.142751	-0.339170	-0.067506	0.180133
-0.157072	-0.003413	-0.003628	0.000309	-0.400519	-0.154078	-0.233286	0.405379	0.416259	0.240541	-0.301257
0.306186	0.153929	0.250480	0.340794	0.176299	0.259708	-0.053786	-0.377012	-0.229047	-0.260722	0.180959
-0.021513	-0.135791	-0.259944	-0.340711	0.178078	0.257882	0.301728	0.233845	0.111802	0.327974	-0.180934
-0.315011	-0.000000	0.003541	0.000000	-0.401248	0.149265	-0.468867	0.000027	-0.000001	-0.480131	0.301549
-0.020553	0.135797	-0.259941	0.340711	0.178078	-0.257883	0.301701	-0.233879	-0.111800	0.327975	-0.180934
0.305657	-0.153934	0.250477	-0.340794	0.176298	0.259708	-0.053743	0.377018	0.229046	-0.260723	0.180959
-0.157788	0.003412	-0.003628	-0.000308	-0.400519	-0.154078	-0.233332	-0.405353	-0.416258	0.240544	-0.301257
-0.328059	-0.297243	0.011202	0.338194	0.176630	0.261440	0.350876	0.142710	0.339169	-0.067508	0.180132
0.328490	0.297244	0.011207	-0.338194	0.176629	-0.261439	-0.350860	0.142751	-0.339170	-0.067506	-0.180132
0.157072	-0.003413	-0.003628	0.000309	-0.400519	0.154078	0.233286	-0.405379	0.416259	0.240541	0.301257
-0.306186	0.153929	0.250480	0.340794	0.176298	-0.259708	0.053786	0.377012	-0.229047	-0.260722	-0.180959
0.021513	-0.135791	-0.259944	-0.340711	0.178078	0.257883	-0.301728	-0.233845	0.111801	0.327974	0.180934
0.315011	-0.000000	0.003540	0.000000	-0.401248	-0.149265	0.468868	-0.000027	-0.000001	-0.480131	-0.301549
-0.200631	-0.000005	0.528693	-0.000000	0.118663	-0.322962	-0.179526	0.000010	0.000001	0.385864	0.435577
-0.100751	0.457239	-0.264043	0.003940	0.121034	0.320275	-0.093385	-0.157928	0.333910	-0.193287	-0.435048
0.100293	-0.457233	-0.264052	-0.003940	0.121035	-0.320275	0.093367	-0.157938	-0.333911	-0.193286	0.435048
0.200631	-0.000005	0.528693	-0.000000	0.118663	0.322962	0.179526	-0.000010	0.000001	0.385864	-0.435577
0.100751	0.457239	-0.264043	0.003940	0.121034	-0.320275	0.093385	0.157928	-0.333910	-0.193287	0.435048
-0.100293	-0.457233	-0.264052	-0.003940	0.121035	0.320275	-0.093367	0.157938	-0.333911	-0.193286	-0.435048

CORONENE X — IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16.	17	18	19	20	21	22	23	24						
1	1.01740	0.74583	-0.01259	-0.16310	0.01710	0.13268	-0.00081	-0.10810	0.00580	0.04748	-0.00681	-0.06102	-0.00090	0.08285	-0.00390
	-0.16346	0.00519	0.53591	0.00688	-0.23579	-0.00806	0.06600	0.00335	-0.01157						
2	0.74583	1.01715	0.53606	0.00541	-0.16324	-0.00390	0.08269	-0.00081	-0.06083	-0.00681	0.04722	0.00587	-0.10822	-0.00081	0.13306
	0.01714	-0.16346	-0.01259	-0.23518	0.00686	-0.01207	0.00329	0.06609	-0.00816						
3	-0.01259	0.53606	0.97764	0.53465	-0.01276	-0.19894	-0.00390	0.13268	-0.00255	-0.06102	0.00587	0.07519	0.00583	-0.06087	-0.00252
	0.13306	-0.00390	-0.19973	0.00965	0.53641	0.00970	-0.07032	-0.00883	-0.07107						
4	-0.16310	0.00541	0.53465	1.01741	0.74685	-0.01276	-0.16324	0.01710	0.13290	-0.00090	-0.10822	0.00584	0.04724	-0.00682	-0.06087
	-0.00081	0.08285	-0.00397	-0.01219	0.00692	-0.23529	-0.00800	0.06650	0.00326						
5	0.01710	-0.16324	-0.01276	0.74685	1.01741	0.53465	0.00541	-0.16310	-0.00397	0.08285	-0.00081	-0.06087	-0.00682	0.04724	0.00584
	-0.10822	-0.00090	0.13290	-0.00800	-0.23529	0.00692	-0.01219	0.00326	0.06650						
6	0.13268	-0.00390	-0.19894	-0.01276	0.53465	0.97764	0.53606	-0.01259	-0.19973	-0.00390	0.13306	-0.00252	-0.06087	0.00584	0.07519
	0.00587	-0.06102	-0.00255	-0.07032	0.00970	0.53641	0.00965	-0.07107	-0.00883						
7	-0.00081	0.08269	-0.00390	-0.16324	0.00541	0.53606	1.01715	0.74583	-0.01259	-0.16346	0.01714	0.13306	-0.00081	-0.10822	0.00587
	0.04722	-0.00681	-0.06083	0.00329	-0.01207	0.00686	-0.23518	-0.00816	0.06609						
8	-0.10810	-0.00081	0.13268	0.01710	-0.16310	-0.01259	0.74583	1.01740	0.53591	0.00519	-0.16346	-0.00390	0.08285	-0.00090	-0.06102
	-0.00681	0.04748	0.00580	0.06600	-0.00806	-0.23579	0.00688	-0.01157	0.00335						
9	0.00580	-0.06083	-0.00255	0.13290	-0.00397	-0.19973	-0.01259	0.53591	0.97772	0.53591	-0.01259	-0.19973	-0.00397	0.13290	-0.00255
	-0.06083	0.00580	0.07503	-0.00874	-0.07030	0.00968	0.53515	0.00968	-0.07030						
10	0.04748	-0.00681	-0.06102	-0.00090	0.08285	-0.00390	-0.16346	0.00519	0.53591	1.01740	0.74583	-0.01259	-0.16310	0.01710	0.13268
	-0.00081	-0.10810	0.00580	0.06600	0.00335	-0.01157	0.00688	-0.23579	-0.00806						
11	-0.00681	0.04722	0.00587	-0.10822	-0.00081	0.13306	0.01714	-0.16346	-0.01259	0.74583	1.01715	0.53606	0.00541	-0.16324	-0.00390
	0.08269	-0.00081	-0.06083	0.00329	0.06609	-0.00816	-0.23518	0.00686	-0.01207						
12	-0.06102	0.00587	0.07519	0.00584	-0.06087	-0.00252	0.13306	-0.00390	-0.19973	-0.01259	0.53606	0.97764	0.53465	-0.01276	-0.19894
	-0.00390	0.13268	-0.00255	-0.07032	-0.00883	-0.07107	0.00965	0.53641	0.00970						
13	-0.00090	-0.10822	0.00583	0.04724	-0.00682	-0.06087	-0.00081	0.08285	-0.00397	-0.16310	0.00541	0.53465	1.01741	0.74685	-0.01276
	-0.16324	0.01710	-0.13290	-0.00800	0.06650	0.00326	-0.01219	0.00692	-0.23529						
14	0.08285	-0.00081	-0.06087	-0.00682	0.04724	0.00584	-0.10822	-0.00090	0.13290	0.01710	-0.16324	-0.01276	0.74685	1.01741	0.53465
	0.00541	-0.16310	-0.00397	-0.01219	0.00326	0.06650	-0.00800	-0.23529	0.00692						
15	-0.00390	0.13306	-0.00252	-0.06087	0.00584	0.07519	0.00587	-0.06102	-0.00255	0.13268	-0.00390	-0.19894	-0.01276	0.53465	0.97764
	0.53606	-0.01259	-0.19973	0.00965	-0.07107	-0.00883	-0.07032	0.00970	0.53641						
16	-0.16346	0.01714	0.13306	-0.00081	-0.10822	0.00587	0.04722	-0.00681	-0.06083	-0.00081	0.08269	-0.00390	-0.16324	0.00541	0.53606
	1.01715	0.74583	-0.01259	-0.23518	-0.00816	0.06609	0.00329	-0.01207	0.00686						
17	0.00519	-0.16346	-0.00390	0.08285	-0.00090	-0.06102	-0.00681	0.04748	0.00580	-0.10810	-0.00081	0.13268	0.01710	-0.16310	-0.01259
	0.74583	1.01740	0.53591	0.00688	-0.01157	0.00335	0.06600	-0.00806	-0.23579						
18	0.53591	-0.01259	-0.19973	-0.00397	0.13290	-0.00255	-0.06083	0.00580	0.07503	0.00580	-0.06083	-0.00255	0.13290	-0.00397	-0.19973
	-0.01259	0.53591	0.97772	0.53515	0.00968	-0.07030	-0.00874	-0.07030	0.00968						
19	0.00688	-0.23518	0.00965	-0.01219	-0.00800	-0.07032	0.00329	0.06600	-0.00874	0.06600	0.00329	-0.07032	-0.00800	-0.01219	0.00965
	-0.23518	0.00688	0.53515	0.98758	0.52662	0.00415	-0.16951	0.00415	0.52662						
20	-0.23579	0.00686	0.53641	0.00692	-0.23529	0.00970	-0.01207	-0.00806	-0.07030	0.00335	0.06609	-0.00883	0.06650	0.00326	-0.07107
	-0.00816	-0.01157	0.00968	0.52662	0.98775	0.52474	0.00415	-0.16990	0.00437						
21	-0.00806	-0.01207	0.00970	-0.23529	0.00692	0.53641	0.00686	-0.23579	0.00968	-0.01157	-0.00816	-0.07107	0.00326	0.06650	-0.00883
	0.06609	0.00335	-0.07030	0.00415	0.52474	0.98775	0.52662	0.00437	-0.16990						
22	0.06600	0.00329	-0.07032	-0.00800	-0.01219	0.00965	-0.23518	0.00688	0.53515	0.00688	-0.23518	0.00965	-0.01219	-0.00800	-0.07032
	0.00329	0.06600	-0.00874	-0.16951	0.00415	0.52662	0.98758	0.52662	0.00415						
23	0.00335	0.06609	-0.00883	0.06650	0.00326	-0.07107	-0.00816	-0.01157	0.00968	-0.23579	0.00686	0.53641	0.00692	-0.23529	0.00970
	-0.01207	-0.00806	-0.07030	0.00415	-0.16990	0.00437	0.52662	0.98775	0.52474						
24	-0.01157	-0.00816	-0.07107	0.00326	0.06650	-0.00883	0.06609	0.00335	-0.07030	-0.00806	-0.01207	0.00970	-0.23529	0.00692	0.53641
	0.00686	-0.23579	0.00968	0.52662	0.00437	-0.16990	0.00415	0.52474	0.98775						

CORONENE X

IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24						
1	0.79808	0.56801	-0.08295	-0.16460	0.03098	0.14086	-0.00764	-0.11553	0.00392	0.05098	-0.00495	-0.06608	-0.00773	0.08824	0.01531
	-0.16496	-0.06320	0.36842	-0.04765	-0.24925	0.00740	0.07024	0.00601	-0.00580						
2	0.56801	0.79773	0.36841	-0.06295	-0.16475	0.01525	0.08808	-0.00764	-0.06588	-0.00495	0.05070	0.00398	-0.11565	-0.00764	0.14127
	0.03099	-0.16496	-0.08286	-0.24860	-0.04789	-0.00634	0.00599	0.07033	0.00736						
3	-0.08295	0.36841	0.72855	0.36740	-0.08292	-0.20918	0.01525	0.14086	-0.00217	-0.06608	0.00398	0.08094	0.00395	-0.06593	-0.00211
	0.14127	0.01531	-0.20999	-0.03869	0.38145	-0.03844	-0.06944	0.00377	-0.07021						
4	-0.16460	-0.06295	0.36740	0.79834	0.56919	-0.08292	-0.16475	0.03098	0.14109	-0.00773	-0.11565	0.00395	0.05073	-0.00497	-0.06593
	-0.00764	0.08824	0.01522	-0.00645	-0.04768	-0.24869	0.00747	0.07077	0.00599						
5	0.03098	-0.16475	-0.08292	0.56919	0.79834	0.36740	-0.06295	-0.16460	0.01522	0.08824	-0.00764	-0.06593	-0.00497	0.05073	0.00395
	-0.11565	-0.00773	0.14109	0.00747	-0.24869	-0.04768	-0.00645	0.00599	0.07077						
6	0.14086	0.01525	-0.20918	-0.08292	0.36740	0.72855	0.36841	-0.08295	-0.20999	0.01531	0.14127	-0.00211	-0.06593	0.00395	0.08094
	0.00398	-0.06608	-0.00217	-0.06944	-0.03844	0.38145	-0.03869	-0.07021	0.00377						
7	-0.00764	0.08808	0.01525	-0.16475	-0.06295	0.36841	0.79773	0.56801	-0.08286	-0.16496	0.03099	0.14127	-0.00764	-0.11565	0.00398
	0.05070	-0.00495	-0.06588	0.00599	-0.00634	-0.04789	-0.24860	0.00736	0.07033						
8	-0.11553	-0.00764	0.14086	0.03098	-0.16460	-0.08295	0.56801	0.79808	0.36842	-0.06320	-0.16496	0.01531	0.08824	-0.00773	-0.06608
	-0.00495	0.05098	0.00392	0.07024	0.00740	-0.24925	-0.04765	-0.00580	0.00601						
9	0.00392	-0.06588	-0.00217	0.14109	0.01522	-0.20999	-0.08286	0.36842	0.72870	0.36842	-0.08286	-0.20999	0.01522	0.14109	-0.00217
	-0.06588	0.00392	0.08077	0.00383	-0.06941	-0.03857	0.38044	-0.03857	-0.06941						
10	0.05098	-0.00495	-0.06608	-0.00773	0.08824	0.01531	-0.16496	-0.06320	0.36842	0.79808	0.56801	-0.08295	-0.16460	0.03098	0.14086
	-0.00764	-0.11553	0.00392	0.07024	0.00601	-0.00580	-0.04765	-0.24925	0.00740						
11	-0.00495	0.05070	0.00398	-0.11565	-0.00764	0.14127	0.03099	-0.16496	-0.08286	0.56801	0.79773	0.36841	-0.06295	-0.16475	0.01525
	0.08808	-0.00764	-0.06588	0.00599	0.07033	0.00736	-0.24860	-0.04789	-0.00634						
12	-0.06608	0.00398	0.08094	0.00395	-0.06593	-0.00211	0.14127	0.01531	-0.20999	-0.08295	0.36841	0.72855	0.36740	-0.08292	-0.20918
	0.01525	0.14086	-0.00217	-0.06944	0.00377	-0.07021	-0.03869	0.38145	-0.03844						
13	-0.00773	-0.11565	0.00395	0.05073	-0.00497	-0.06593	-0.00764	0.08824	0.01522	-0.16460	-0.06295	0.36740	0.79834	0.56919	-0.08292
	-0.16475	0.03098	0.14109	0.00747	0.07077	0.00599	-0.00645	-0.04768	-0.24869						
14	0.08824	-0.00764	-0.06593	-0.00497	0.05073	0.00395	-0.11565	-0.00773	0.14109	0.03098	-0.16475	-0.08292	0.56919	0.79834	0.36740
	-0.06295	-0.16460	0.01522	-0.00645	0.00599	0.07077	0.00747	-0.24869	-0.04768						
15	0.01531	0.14127	-0.00211	-0.06593	0.00395	0.08094	0.00398	-0.06608	-0.00217	0.14086	0.01525	-0.20918	-0.08292	0.36740	0.72855
	0.36841	-0.08295	-0.20999	-0.03869	-0.07021	0.00377	-0.06944	-0.03844	0.38145						
16	-0.16496	0.03099	0.14127	-0.00764	-0.11565	0.00398	0.05070	-0.00495	-0.06588	-0.00764	0.08808	0.01525	-0.16475	-0.06295	0.36841
	0.79773	0.56801	-0.08286	-0.24860	0.00736	0.07033	0.00599	-0.00634	-0.04789						
17	-0.06320	-0.16496	0.01531	0.08824	-0.00773	-0.06608	-0.00495	0.05098	0.00392	-0.11553	-0.00764	0.14086	0.03098	-0.16460	-0.08295
	0.56801	0.79808	0.36842	-0.04765	-0.00580	0.00601	0.07024	0.00740	-0.24925						
18	0.36842	-0.08286	-0.20999	0.01522	0.14109	-0.00217	-0.06588	0.00392	0.08077	0.00392	-0.06588	-0.00217	0.14109	0.01522	-0.20999
	-0.08286	0.36842	0.72870	0.38044	-0.03857	-0.06941	0.00383	-0.06941	-0.03857						
19	-0.04765	-0.24860	-0.03869	-0.00645	0.00747	-0.06944	0.00599	0.07024	0.00383	0.07024	0.00599	-0.06944	0.00747	-0.00645	-0.03869
	-0.24860	-0.04765	0.38044	0.74729	0.36864	-0.04896	-0.17997	-0.04896	0.36864						
20	-0.24925	-0.04789	0.38145	-0.04768	-0.24869	-0.03844	-0.00634	0.00740	-0.06941	0.00601	0.07033	0.00377	0.07077	0.00599	-0.07021
	0.00736	-0.00580	-0.03857	0.36864	0.74775	0.36739	-0.04896	-0.18040	-0.04907						
21	0.00740	-0.00634	-0.03844	-0.24869	-0.04768	0.38145	-0.04789	-0.24925	-0.03857	-0.00580	0.00736	-0.07021	0.00599	0.07077	0.00377
	0.07033	0.00601	-0.06941	-0.04896	0.36739	0.74775	0.36864	-0.04907	-0.18040						
22	0.07024	0.00599	-0.06944	0.00747	-0.00645	-0.03869	-0.24860	-0.04765	0.38044	-0.04765	-0.24860	-0.03869	-0.00645	0.00747	-0.06944
	0.00599	0.07024	0.00383	-0.17997	-0.04896	0.36864	0.74729	0.36864	-0.04896						
23	0.00601	-0.07033	0.00377	0.07077	0.00599	-0.07021	0.00736	-0.00580	-0.03857	-0.24925	-0.04789	0.38145	-0.04768	-0.24869	-0.03844
	-0.00634	0.00740	-0.06941	-0.04896	-0.18040	-0.04907	0.36864	0.74775	0.36739						
24	-0.00580	0.00736	-0.07021	0.00599	0.07077	0.00377	0.07033	-0.00601	-0.06941	0.00740	-0.00634	-0.03844	-0.24869	-0.04768	0.38145
	-0.04789	-0.24925	-0.03857	0.36864	-0.04907	-0.18040	-0.04896	0.36739	0.74775						

ENERGIES FOR CORONENE X , TRX APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	12,14	11,13	6,13	9,15	10,16	5,13	4,14	9,17	8,15	7,16
XMOMNT	-1.03600	-1.03592	-0.02593	-0.43916	-0.44078	0.01594	-0.01576	-0.23185	-0.50577	0.18159
YMOMNT	0.00104	0.00104	-0.00003	-0.00002	-0.00002	-0.00002	0.00002	0.00001	0.00000	0.00001
JUMP E	20.6667	20.6713	35.9776	36.8517	36.9153	38.1956	38.2263	38.9395	39.8588	39.9794
DIAG E	31.1821	31.1814	50.1362	48.7756	48.8330	53.7725	53.8312	56.4810	51.6405	55.2996
DIAG E	31.7570	31.7453	51.6498	48.4236	48.4708	54.7776	54.8467	63.0430	51.7301	50.6815
CORRSP	35.0270	24.9851	48.2715	45.4704	53.8560	54.9685	54.3507	58.4479	48.8224	56.9296
CORRSP	35.3096	25.6372	50.5620	45.1901	53.9125	55.8204	56.5408	64.2287	48.5769	51.3471

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
35.02700	2.13368	-1.19685	0.00140	//	0.6686	0.6685	-0.0556	-0.2172	-0.2154	-0.0239	0.0230	0.0470	-0.0403	-0.0672
24.82091				//	0.7004	-0.7018	-0.0010	-0.0662	0.0655	0.0639	0.0641	-0.0014	0.0016	-0.0001
24.98512	0.00000	0.00055	-0.00000	//	-0.7026	0.7028	0.0005	0.0663	-0.0664	-0.0429	-0.0428	0.0010	-0.0013	0.0005
22.17110				//	0.6872	0.6858	0.0648	0.0395	0.0405	-0.0081	0.0084	0.1385	0.1161	-0.1308
48.27146	0.00021	0.01014	0.00001	//	0.0239	0.0227	0.6231	0.0560	0.0594	0.3521	-0.3498	0.3717	-0.4468	-0.1410
37.06168				//	-0.0846	-0.0866	0.5243	0.4880	0.4865	0.2122	-0.2107	0.2829	-0.1550	-0.2051
45.47440	0.00009	-0.00696	0.00000	//	0.0625	-0.0592	0.0040	0.7011	-0.6974	0.0838	0.0873	0.0061	0.0034	0.0011
45.40325				//	0.0514	-0.0531	-0.0046	0.7144	-0.6662	0.1098	0.1644	-0.0098	0.0291	0.0184
53.85604	1.15841	0.71120	0.00038	//	0.1890	0.1891	0.0325	0.5821	0.5862	-0.2232	0.2274	-0.0745	-0.2777	0.2466
45.88531				//	-0.0164	-0.0084	-0.0646	0.3630	0.4499	-0.4304	0.4157	-0.2256	0.4207	0.2746
54.96845	0.00362	0.03935	-0.00001	//	-0.0541	0.0465	0.0009	-0.0975	0.0648	0.6944	0.7052	-0.0012	-0.0204	0.0369
50.82715				//	-0.0796	0.0711	-0.0163	-0.1296	0.1329	0.7070	0.6725	-0.0002	0.0365	-0.0192
54.35067	1.67276	0.85073	-0.00017	//	-0.0913	-0.0978	0.0609	-0.3123	-0.3219	-0.2621	0.1962	0.0128	-0.5481	0.6078
48.75312				//	-0.0751	-0.0743	0.6844	-0.3049	-0.2997	-0.1692	0.1724	0.2820	0.4397	0.0802
58.44794	0.03396	-0.11690	-0.00009	//	-0.0539	-0.0538	-0.3549	0.0234	0.0302	-0.2056	0.2119	0.8648	-0.0479	-0.1717
58.23403				//	-0.0694	-0.0695	-0.3836	0.0213	0.0278	-0.2455	0.2503	0.8372	-0.1074	-0.0816
48.82244	0.24479	-0.34337	0.00005	//	0.0243	0.0254	0.6610	-0.0389	-0.0292	-0.2981	0.2972	0.1992	0.5570	0.1797
51.63796				//	-0.0926	-0.0979	-0.2985	0.0414	0.0298	0.2300	-0.3004	0.0531	0.7357	-0.4506
56.92962	0.19852	-0.28636	0.00013	//	0.0659	0.0650	-0.2025	0.0769	0.0776	0.3671	-0.3833	0.2576	0.3288	0.6945
56.31696				//	0.0413	0.0406	-0.1082	0.0432	0.0448	0.3345	-0.3415	0.2581	0.1931	0.8054

ENERGIES FOR CORONENE X , TRX APPROXIMATION 5.8

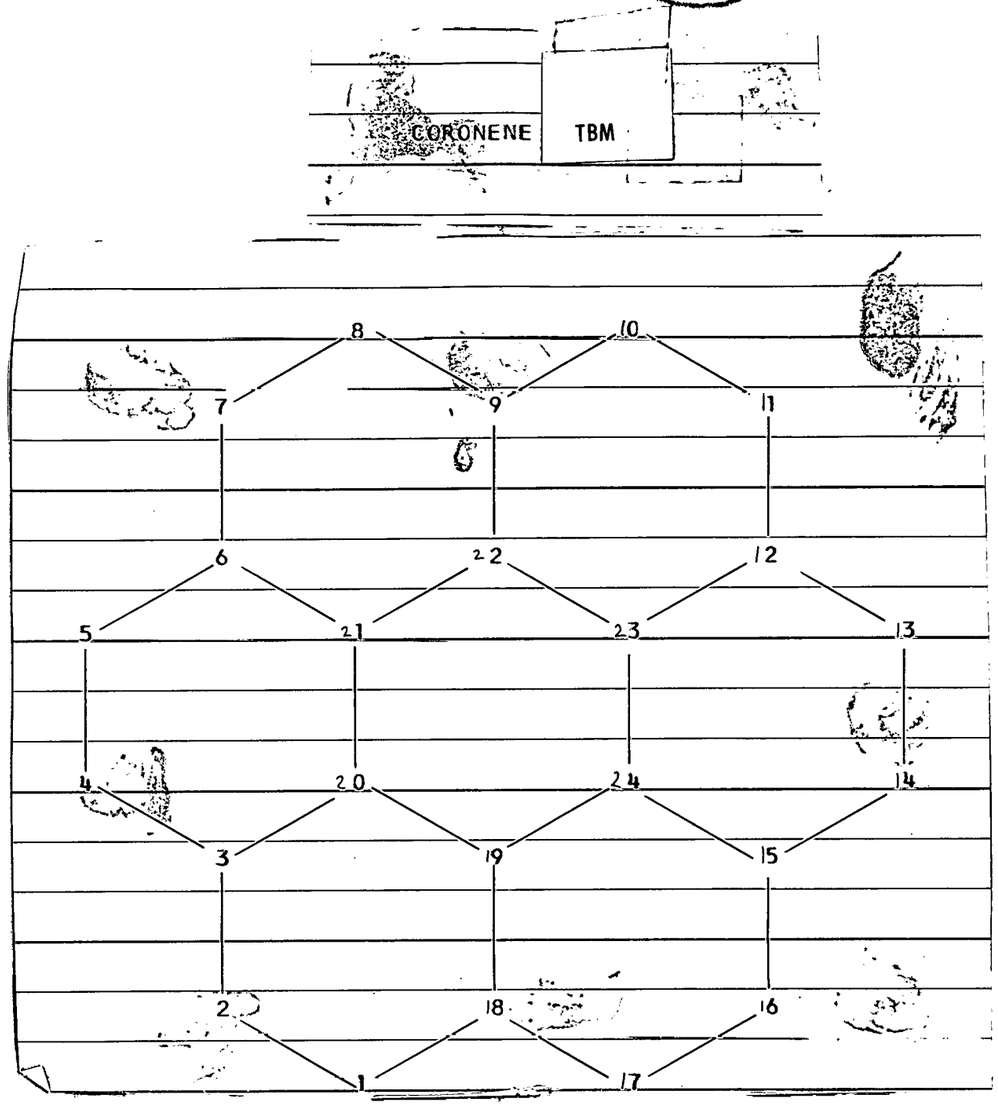
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	12,13	11,14	6,14	10,15	9,16	5,14	4,13	10,17	7,15	8,16
XMOMNT	-0.00104	0.00104	0.00003	0.00002	-0.00002	-0.00002	-0.00002	0.00001	0.00001	-0.00000
YMOMNT	-1.03598	1.03555	-0.02459	-0.44064	0.43579	-0.01494	-0.01523	0.22655	-0.18263	-0.50672
JUMP E	20.6625	20.6755	35.9819	36.8061	36.9609	38.1999	38.2220	38.8939	39.8702	39.9680
DIAG E	32.1683	32.2093	50.1447	50.1218	50.3093	54.2286	54.2337	56.4274	55.1957	51.7359
DIAG E	32.7343	32.7820	51.6672	49.7673	49.9496	55.2426	55.2403	62.9869	50.5853	51.8178
CORRSP	27.1438	35.0124	48.2391	48.3489	53.8247	55.6939	54.3504	58.4083	56.8959	48.8572
CORRSP	27.7928	35.2978	50.5658	47.9570	53.8990	56.6331	56.5574	64.1842	51.3365	48.5495

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
27.14376	0.00001	-0.00000	-0.00307	//	0.7067	0.7026	-0.0002	-0.0411	-0.0386	-0.0424	0.0434	-0.0002	-0.0012	-0.0001
20.94848				//	0.6884	0.6801	-0.0003	-0.1782	-0.1761	0.0204	-0.0192	-0.0016	-0.0019	0.0007
35.01245	2.13549	0.00140	1.19761	//	-0.6661	0.6707	0.0570	0.2171	-0.2151	-0.0240	-0.0234	0.0498	-0.0674	0.0404
22.16177				//	-0.6828	0.6902	-0.0645	-0.0420	0.0386	-0.0072	-0.0080	0.1388	-0.1320	-0.1152
48.23909	0.00063	-0.00002	-0.01751	//	0.0448	-0.0057	0.5632	0.3880	0.2635	-0.2943	-0.3197	-0.3308	0.1276	-0.3825
48.78031				//	-0.0737	0.0744	0.6841	-0.2942	0.3019	0.1754	0.1781	-0.2869	-0.0857	0.4372
48.34893	0.00029	-0.00000	-0.01189	//	0.0285	0.0450	-0.2992	0.6045	0.6464	0.1820	0.1304	0.1791	-0.0633	0.1954
39.73065				//	0.1787	0.1760	-0.0105	0.6649	0.6729	-0.1404	0.1493	0.0116	-0.0042	0.0017
53.82470	1.18994	0.00039	0.72102	//	-0.1906	0.1917	-0.0244	-0.5803	0.5982	-0.2146	-0.2211	-0.0851	0.2419	0.2665
37.07245				//	0.0816	-0.0902	-0.5244	-0.4995	0.4791	0.2137	0.2090	0.2758	-0.2063	0.1525
55.69385	0.00035	-0.00000	-0.01220	//	0.0431	0.0392	-0.0036	-0.0251	-0.0374	0.6996	-0.7107	-0.0032	-0.0017	0.0058
49.98610				//	0.0188	0.0163	0.0032	0.1413	0.1490	0.6873	-0.6962	-0.0031	-0.0071	-0.0078
54.35041	1.60967	0.00016	0.83453	//	-0.0900	0.0895	0.0573	-0.2986	0.3105	0.2241	0.2111	-0.0239	-0.6269	-0.5537
51.66905				//	0.0953	-0.0976	0.2951	-0.0382	0.0350	0.2503	0.2612	0.0494	-0.4549	-0.7425
58.40829	0.03475	-0.00009	0.11829	//	0.0536	-0.0540	0.3574	-0.0369	0.0315	-0.2074	-0.2092	0.8638	-0.1697	0.0482
58.19644				//	0.0695	-0.0698	0.3855	-0.0349	0.0284	-0.2485	-0.2483	0.8351	-0.0828	0.1096
56.89586	0.21900	0.00013	0.30086	//	-0.0655	0.0673	0.2036	-0.0811	0.0821	0.3907	0.3763	0.2548	0.6774	-0.3441
56.25763				//	-0.0390	0.0414	0.1117	-0.0458	0.0453	0.3469	0.3362	0.2603	0.7997	-0.1989
48.85718	0.24204	-0.00005	0.34131	//	0.0251	-0.0250	0.6457	-0.0270	0.0402	0.3107	0.3074	0.1924	-0.1895	0.5617
45.88363				//	-0.0101	0.0083	0.0668	0.4045	0.4096	0.4317	0.4174	0.2339	-0.2818	0.4115

508



ATOMIC COORDINATES

x	2.5980	1.7320	1.7320	0.8660	0.8660	1.7320	1.7320	2.5980	3.4640	4.3300	5.1960	5.1960	6.0620	6.0620
	5.1960	5.1960	4.3300	3.4640	3.4640	2.5980	2.5980	3.4640	4.3300	4.3300				
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	4.5000	5.0000	4.5000	5.0000	4.5000	3.5000	3.0000	2.0000
	1.5000	0.5000	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	2.0000				

CORONENE TBM APPROXIMATION (1)

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 AS	9 SA	10 SA	11 SS	12 AA	13 AS
1.660243	1.546513	1.546508	1.413435	1.413433	1.379883	1.299703	1.246813	1.246808	1.246798	1.133084	1.133066	0.866932
0.123304	0.243455	0.073899	-0.234020	0.185123	0.213358	0.150336	0.224267	0.315741	-0.001404	0.335655	0.015894	0.015139
0.123301	0.190567	0.168562	-0.023072	0.297464	0.213393	-0.150260	0.224320	0.315737	-0.001405	0.180413	0.283505	-0.283099
0.206548	0.178525	0.299358	0.195382	0.313175	0.115094	-0.332814	0.000055	-0.000007	-0.000001	-0.238385	0.136963	0.137499
0.123302	0.057730	0.247785	0.277272	0.110079	0.213448	-0.150305	-0.000576	-0.159497	-0.352929	-0.154066	-0.298634	0.298287
0.123303	-0.050698	0.249319	0.269091	-0.128789	0.213448	0.150307	-0.000631	-0.159497	-0.352928	0.155319	-0.297984	-0.298333
0.206548	-0.169986	0.304288	0.173500	-0.325807	0.115094	0.332814	-0.000055	-0.000006	0.000001	0.237808	0.137963	-0.137427
0.123301	-0.185723	0.173884	-0.043368	-0.295189	0.213393	0.150260	-0.222942	0.316713	-0.001081	-0.181602	0.282745	0.283153
0.123304	-0.241267	0.080755	-0.246136	-0.168679	0.213358	-0.150336	-0.222889	0.316716	-0.001082	-0.335719	0.014484	-0.015240
0.206547	-0.348512	0.004930	-0.368936	0.012635	0.115000	-0.332813	0.000051	-0.000001	-0.000001	0.000577	-0.274936	-0.274937
0.123304	-0.243455	-0.073899	-0.234019	0.185123	0.213358	-0.150336	-0.224267	-0.315741	0.001405	0.335655	0.015894	-0.015139
0.123301	-0.190567	-0.168562	-0.023072	0.297464	0.213393	0.150261	-0.224320	-0.315737	0.001405	0.180413	0.283506	0.283099
0.206548	-0.178525	-0.299358	0.195382	0.313175	0.115094	0.332814	-0.000055	0.000007	0.000001	-0.238385	0.136963	-0.137499
0.123302	-0.057729	-0.247785	0.277272	0.110079	0.213448	0.150305	0.000575	0.159497	0.352929	-0.154066	-0.298634	-0.298287
0.123302	0.050698	-0.249319	0.269092	-0.128789	0.213448	-0.150307	0.000631	0.159497	0.352928	0.155319	-0.297985	0.298334
0.206548	0.169986	-0.304287	0.173500	-0.325807	0.115095	-0.332814	0.000055	0.000006	-0.000001	0.237808	0.137963	0.137427
0.123301	0.185723	-0.173884	-0.043368	-0.295189	0.213393	-0.150260	0.222942	-0.316713	0.001081	-0.181602	0.282745	-0.283153
0.123304	0.241267	-0.080755	-0.246136	-0.168679	0.213358	0.150336	0.222889	-0.316716	0.001082	-0.335719	0.014484	0.015240
0.206546	0.348512	-0.004930	-0.368936	0.012634	0.114999	0.332813	-0.000051	0.000000	0.000001	0.000577	-0.274936	0.274937
0.305938	0.287000	-0.004060	-0.137859	0.004721	-0.249726	0.103468	-0.447230	0.000975	0.000324	0.000375	-0.178617	-0.178618
0.305937	0.147020	0.246522	0.073084	0.117071	-0.249682	-0.103578	-0.223677	-0.156231	0.354334	-0.154879	0.088986	-0.089334
0.305937	-0.139988	0.250581	0.064904	-0.121797	-0.249681	0.103577	0.223506	-0.157206	0.354010	0.154504	0.089636	0.089288
0.305938	-0.287000	0.004059	-0.137859	0.004721	-0.249726	-0.103468	0.447230	-0.000976	-0.000324	0.000375	-0.178618	0.178618
0.305937	-0.147020	-0.246522	0.073084	0.117071	-0.249681	0.103578	0.223678	0.156231	-0.354334	-0.154880	0.088986	0.089334
0.305937	0.139988	-0.250582	0.064904	-0.121797	-0.249681	-0.103577	-0.223506	0.157206	-0.354011	0.154504	0.089636	-0.089288

OVERLAP EIGNVALUES AND EIGNVECTORS

14 SA	15 AA	16 AA	17 SS	18 SS	19 AS	20 SA	21 AS	22 SS	23 AA	24 AS
0.866914	0.753199	0.753189	0.753184	0.700295	0.620115	0.586564	0.586562	0.453489	0.453485	0.339755
-0.335690	-0.001741	0.315470	-0.224645	-0.150336	-0.213358	0.176025	-0.240937	0.077432	-0.242354	-0.123304
0.181051	0.001741	-0.315467	0.224698	-0.150260	0.213393	-0.296362	0.034446	-0.171315	0.188095	0.123301
0.238076	-0.000000	-0.000007	-0.000055	0.332814	-0.115094	0.320427	0.183246	0.301923	-0.174152	-0.206548
-0.154737	-0.354385	0.156235	-0.000393	-0.150306	0.213448	-0.120616	-0.272853	-0.248599	0.054119	0.123302
-0.154647	0.354385	-0.156235	0.000449	-0.150306	-0.213448	-0.118390	0.273826	0.248555	0.054319	-0.123302
0.238118	-0.000000	0.000006	-0.000055	0.332814	0.115094	0.318924	-0.185849	-0.301783	-0.174394	0.206548
0.180965	-0.001606	0.316978	0.222563	-0.150261	-0.213393	-0.296633	-0.032031	0.171164	0.188232	-0.123301
-0.335685	0.001607	-0.316981	-0.222509	-0.150336	0.213358	0.177982	0.239495	-0.077237	-0.242416	0.123304
0.000042	-0.000000	-0.000000	-0.000051	0.332813	-0.115000	-0.001503	-0.369149	-0.000140	0.348547	-0.206547
0.335690	-0.001741	0.315470	-0.224645	-0.150336	0.213359	-0.176025	0.240937	0.077432	-0.242354	0.123304
-0.181051	0.001741	-0.315467	0.224698	-0.150260	-0.213393	0.296362	-0.034446	-0.171315	0.188095	-0.123301
-0.238076	-0.000000	-0.000007	-0.000055	0.332814	0.115094	-0.320427	-0.183246	0.301923	-0.174152	0.206548
0.154737	-0.354385	0.156235	-0.000394	-0.150306	-0.213448	0.120616	0.272853	-0.248598	0.054119	-0.123302
0.154647	0.354385	-0.156235	0.000449	-0.150306	0.213448	0.118390	-0.273826	0.248555	0.054319	0.123302
-0.238118	-0.000000	0.000006	-0.000055	0.332814	-0.115094	-0.318924	0.185849	-0.301783	-0.174394	-0.206548
-0.180966	-0.001606	0.316978	0.222562	-0.150260	0.213393	0.296633	0.032031	0.171164	0.188233	0.123301
0.335685	0.001607	-0.316981	-0.222510	-0.150336	-0.213358	-0.177981	-0.239495	-0.077237	-0.242416	-0.123304
-0.000041	-0.000000	-0.000000	-0.000051	0.332813	0.115000	0.001503	0.369149	-0.000140	0.348547	0.206546
0.000027	-0.000135	0.001511	-0.447228	-0.103468	0.249726	-0.000562	-0.137939	0.000115	-0.287029	-0.305938
-0.154679	0.352644	-0.159222	-0.224238	-0.103577	-0.249681	-0.119784	-0.068547	-0.248634	0.143419	0.305937
-0.154706	-0.352779	-0.160733	-0.222944	-0.103578	0.249681	-0.119222	0.069520	0.248519	0.143618	-0.305937
-0.000027	0.000135	-0.001511	0.447228	-0.103468	-0.249726	0.000562	0.137939	0.000115	-0.287029	0.305938
0.154679	0.352644	0.159222	-0.224238	-0.103577	0.249681	0.119784	0.068547	-0.248634	0.143419	-0.305937
0.154706	-0.352779	-0.160732	-0.222945	-0.103578	-0.249681	0.119222	-0.069520	0.248519	0.143618	0.305937

CORONENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 AS	9 SA	10 SA	11 SS	12 AA	13 AS
29.44120	28.16196	26.16182	21.65485	21.65477	20.38125	17.07143	14.65517	14.65493	14.65445	8.69535	8.69430	-11.36352
0.095695	0.194908	0.062187	-0.202054	0.148884	0.181630	0.131868	0.200229	0.283206	-0.001258	-0.014269	0.315361	0.016315
0.095693	0.151307	0.137698	-0.027958	0.249395	0.181660	-0.131802	0.200277	0.283203	-0.001258	-0.265979	0.170048	-0.304080
0.160301	0.140137	0.242728	0.155229	0.268891	0.097979	-0.291931	0.000049	-0.000006	-0.000001	-0.129138	-0.223680	0.147636
0.095694	0.043599	0.199887	0.229915	0.100518	0.181707	-0.131841	-0.000204	-0.142842	-0.316074	0.280244	-0.145325	0.320388
0.095694	-0.043599	0.199887	0.229915	-0.100518	0.181707	0.131843	-0.000253	-0.142842	-0.316074	0.280244	0.145325	-0.320387
0.160301	-0.140137	0.242728	0.155229	-0.268891	0.097979	0.291931	-0.000049	-0.000006	0.000001	-0.129138	0.223680	-0.147637
0.095693	-0.151307	0.137699	-0.027959	-0.249394	0.181660	0.131802	-0.200278	0.283203	-0.000968	-0.265980	-0.170048	0.304079
0.095695	-0.194908	0.062187	-0.202054	-0.148883	0.181630	-0.131869	0.200231	0.283205	-0.000969	-0.014269	-0.315361	-0.016312
0.160300	-0.280275	-0.000000	-0.310504	0.000000	0.097898	-0.291930	0.000045	-0.000000	-0.000001	0.258287	-0.000000	-0.295284
0.095695	-0.194908	-0.062187	-0.202054	0.148884	0.181630	-0.131868	-0.200229	0.283206	0.001258	-0.014269	0.315361	-0.016314
0.095693	-0.151307	-0.137699	-0.027958	0.249395	0.181660	0.131802	-0.200277	0.283202	0.001258	-0.265980	0.170048	0.304080
0.160301	-0.140137	-0.242728	0.155229	0.268891	0.097979	0.291931	-0.000050	0.000006	0.000001	-0.129138	-0.223680	-0.147636
0.095694	-0.043599	-0.199887	0.229915	0.100518	0.181707	0.131841	0.000204	0.142842	0.316074	0.280244	-0.145326	-0.320388
0.095694	0.043599	-0.199887	0.229915	-0.100518	0.181707	-0.131843	0.000253	0.142842	0.316074	0.280244	0.145325	0.320387
0.160301	0.140137	-0.242728	0.155229	-0.268891	0.097979	-0.291931	0.000050	0.000006	0.000001	-0.129138	0.223680	0.147637
0.095693	0.151307	-0.137698	-0.027959	-0.249395	0.181660	-0.131802	0.200278	-0.283203	0.000968	-0.265980	-0.170047	-0.304079
0.095695	0.194908	-0.062187	-0.202054	-0.148884	0.181630	0.131869	0.200231	-0.283206	0.000969	-0.014270	-0.315361	0.016313
0.160299	0.280275	-0.000000	-0.310504	0.000000	0.097898	0.291930	-0.000046	-0.000000	0.000001	0.258287	-0.000000	0.295284
0.237436	0.230807	-0.000000	-0.116025	-0.000000	-0.212590	0.090758	-0.400526	0.000000	0.000290	0.167801	0.000000	-0.191837
0.237436	0.115407	0.199887	0.058067	0.100518	-0.212552	-0.090855	-0.200013	-0.140352	0.317332	-0.083902	-0.145325	-0.095920
0.237436	-0.115406	0.199887	0.058067	-0.100518	-0.212552	0.090853	0.200472	-0.140352	0.317043	-0.083902	0.145325	0.095921
0.237436	-0.230807	-0.000000	-0.116025	0.000000	-0.212590	-0.090758	0.400526	-0.000000	-0.000290	0.167801	-0.000000	0.191837
0.237436	-0.115406	-0.199887	0.058067	0.100518	-0.212552	0.090854	0.200013	0.140352	-0.317332	-0.083902	-0.145325	0.095920
0.237436	0.115407	-0.199887	0.058067	-0.100518	-0.212552	-0.090853	-0.200472	0.140352	-0.317043	-0.083902	0.145325	-0.095921

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 ss	15 AA	16 AA	17 SS	18 SS	19 AS	20 SA	21 AS	22 SS	23 AA	24 AS
-11.36530	-24.25829	-24.25960	-24.26028	-31.68376	-45.35281	-52.18149	-52.18195	-89.21866	-89.22021	143.86767
-0.360535	-0.361881	-0.034314	-0.258849	-0.179648	-0.270940	0.231114	-0.313652	0.359934	0.114840	-0.211540
0.194406	0.361877	0.034314	0.258910	-0.179558	0.270984	-0.387139	0.043400	-0.279417	-0.254287	0.211536
0.255721	0.000008	0.000001	-0.000064	0.397705	-0.146156	0.417403	0.240966	0.258790	0.448244	-0.354355
-0.166142	-0.143006	-0.422729	-0.000453	-0.179612	0.271054	-0.156036	-0.356902	-0.080514	-0.369130	0.211538
-0.166143	0.143006	0.422729	0.000517	-0.179612	-0.271054	-0.156036	0.356902	-0.080514	0.369130	-0.211538
0.255720	-0.000007	-0.000001	-0.000064	0.397705	0.146156	0.417403	-0.240966	0.258790	-0.448243	0.354355
0.194407	-0.363625	-0.034314	0.256449	-0.179558	-0.270984	-0.387139	-0.043400	-0.279417	0.254287	-0.211536
-0.360535	0.363629	0.034315	-0.256388	-0.179648	0.270941	0.231115	0.313652	0.359933	-0.114840	0.211540
-0.000001	0.000000	-0.000000	-0.000058	0.397704	-0.146037	-0.000000	-0.482001	-0.517580	-0.000000	-0.354352
0.360535	-0.361881	-0.034314	-0.258849	-0.179648	0.270941	-0.231114	0.313652	0.359934	0.114840	0.211540
-0.194405	0.361877	0.034314	0.258910	-0.179558	-0.270985	0.387139	-0.043400	-0.279417	-0.254287	-0.211536
-0.255721	0.000008	0.000001	-0.000064	0.397705	0.146156	-0.417403	-0.240966	0.258790	0.448243	0.354355
0.166142	-0.143006	-0.422729	-0.000454	-0.179612	-0.271054	0.156036	0.356902	-0.080514	-0.369130	-0.211538
0.166144	0.143006	0.422729	0.000517	-0.179612	0.271054	0.156036	-0.356902	-0.080514	0.369130	0.211538
-0.255720	-0.000007	-0.000001	-0.000064	0.397705	-0.146156	-0.417403	0.240966	0.258790	-0.448244	-0.354355
-0.194407	-0.363625	-0.034314	0.256449	-0.179558	0.270984	0.387139	0.043400	-0.279417	0.254287	0.211536
0.360535	0.363629	0.034315	-0.256388	-0.179648	-0.270940	-0.231114	-0.313652	0.359934	-0.114840	-0.211540
0.000001	0.000000	-0.000000	-0.000058	0.397704	0.146037	-0.000000	0.482001	-0.517581	0.000000	0.354352
-0.000000	-0.001748	-0.000000	0.515322	-0.123642	0.317123	0.000000	-0.180108	0.426229	0.000000	-0.524868
-0.166143	-0.218860	0.388416	-0.258380	-0.123773	-0.317066	-0.156036	-0.090138	-0.213120	-0.369130	0.524867
-0.166142	0.220608	-0.388416	-0.256889	-0.123773	0.317066	-0.156036	0.090138	-0.213120	0.369130	-0.524867
0.000001	-0.001748	-0.000000	0.515322	-0.123642	-0.317123	-0.000000	0.180108	0.426229	-0.000000	0.524868
0.166143	-0.218860	0.388416	-0.258380	-0.123773	0.317066	0.156036	0.090138	-0.213120	-0.369130	-0.524867
0.166142	0.220608	-0.388416	-0.256889	-0.123773	-0.317066	0.156036	-0.090138	0.213120	0.369130	0.524867

CORONENE

TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24						
1	1.00000	0.74505	-0.00000	-0.16090	0.00000	0.12449	0.00000	-0.10142	0.00000	0.05071	-0.00000	-0.06224	0.00000	-0.08531	0.00000
	-0.16091	-0.00000	0.53802	-0.00000	-0.24620	-0.00000	0.05946	0.00000	0.00000						
2	0.74505	1.00000	0.53800	0.00000	-0.16090	0.00000	0.08531	0.00000	-0.06226	-0.00000	0.05073	0.00000	-0.10144	0.00000	0.12450
	0.00000	-0.16091	-0.00000	-0.24621	0.00000	0.00001	-0.00000	0.05946	-0.00000						
3	-0.00000	0.53800	1.00000	0.53803	-0.00000	-0.20009	0.00000	0.12449	0.00000	-0.06224	0.00000	0.07099	0.00000	-0.06225	0.00000
	0.12450	0.00000	-0.20009	0.00000	0.53802	-0.00000	-0.06224	-0.00000	-0.06225						
4	-0.16090	0.00000	0.53803	1.00000	0.74503	-0.00000	-0.16090	0.00000	0.12450	-0.00000	-0.10144	-0.00000	0.05072	-0.00000	-0.06225
	-0.00000	0.08531	0.00000	-0.00001	-0.00000	-0.24622	0.00000	0.05947	0.00000						
5	0.00000	-0.16090	-0.00000	0.74503	1.00000	0.53803	0.00000	-0.16090	0.00000	0.08531	0.00000	-0.06225	-0.00000	0.05072	0.00000
	-0.10144	0.00000	0.12450	0.00000	-0.24622	0.00000	-0.00001	0.00000	0.05947						
6	0.12449	0.00000	-0.20009	-0.00000	0.53803	1.00000	0.53800	-0.00000	-0.20009	0.00000	0.12450	0.00000	-0.06225	-0.00000	0.07099
	0.00000	-0.06224	-0.00000	-0.06224	0.00000	0.53802	-0.00000	-0.06225	-0.00000						
7	0.00000	0.08531	0.00000	-0.16090	0.00000	0.53800	1.00000	0.74505	0.00000	-0.16091	0.00000	0.12450	-0.00000	-0.10144	-0.00000
	0.05073	-0.00000	-0.06226	0.00000	0.00001	-0.00000	-0.24621	0.00000	0.05946						
8	-0.10142	0.00000	0.12449	0.00000	-0.16090	-0.00000	0.74505	1.00000	0.53802	0.00000	-0.16091	-0.00000	0.08531	0.00000	-0.06224
	-0.00000	0.05071	0.00000	0.05946	-0.00000	-0.24620	0.00000	0.00000	0.00000						
9	0.00000	-0.06226	0.00000	0.12450	0.00000	-0.20009	0.00000	0.53802	1.00000	0.53802	0.00000	-0.20009	0.00000	0.12450	0.00000
	-0.06226	0.00000	0.07100	-0.00000	-0.06225	0.00000	0.53801	0.00000	-0.06225						
10	0.05071	-0.00000	-0.06224	-0.00000	0.08531	0.00000	-0.16091	0.00000	0.53802	1.00000	0.74505	-0.00000	-0.16090	0.00000	0.12449
	0.00000	-0.10142	-0.00000	0.05946	0.00000	0.00000	-0.00000	-0.24620	0.						
11	-0.00000	0.05073	0.00000	-0.10144	0.00000	0.12450	0.00000	-0.16091	0.00000	0.74505	1.00000	0.53800	0.00000	-0.16090	-0.00000
	0.08531	0.00000	-0.06226	0.00000	0.05946	-0.00000	-0.24621	0.00000	0.00001						
12	-0.06224	0.00000	0.07099	-0.00000	-0.06225	0.00000	0.12450	-0.00000	-0.20009	-0.00000	0.53800	1.00000	0.53803	-0.00000	-0.20009
	0.	0.12449	0.00000	-0.06224	-0.00000	-0.06225	0.00000	0.53802	0.00000						
13	0.00000	-0.10144	0.00000	0.05072	-0.00000	-0.06225	-0.00000	0.08531	0.00000	-0.16090	0.00000	0.53803	1.00000	0.74503	0.00000
	-0.16090	-0.00000	0.12450	-0.00000	0.05947	0.00000	-0.00001	-0.00000	-0.24622						
14	0.08531	0.00000	-0.06225	-0.00000	0.05072	-0.00000	-0.10144	0.00000	0.12450	0.00000	-0.16090	-0.00000	0.74503	1.00000	0.53803
	0.00000	-0.16090	-0.00000	-0.00001	0.00000	0.05947	-0.00000	-0.24622	0.00000						
15	0.00000	0.12450	0.00000	-0.06225	0.00000	0.07099	-0.00000	-0.06224	0.00000	0.12449	-0.00000	-0.20009	0.00000	0.53803	1.00000
	0.53800	-0.00000	-0.20009	0.00000	-0.06225	-0.00000	-0.06224	0.00000	0.53802						
16	-0.16091	0.00000	0.12450	-0.00000	-0.10144	0.00000	0.05073	-0.00000	-0.06226	0.00000	0.08531	0.	-0.16090	0.00000	0.53800
	1.00000	0.74505	0.00000	-0.24621	-0.00000	0.05946	0.00000	0.00001	0.00000						
17	-0.00000	-0.16091	0.00000	0.08531	0.00000	-0.06224	-0.00000	0.05071	0.00000	-0.10142	0.00000	0.12449	-0.00000	-0.16090	-0.00000
	0.74505	1.00000	0.53802	-0.00000	0.00000	0.00000	0.05946	-0.00000	-0.24620						
18	0.53802	-0.00000	-0.20009	0.00000	0.12450	-0.00000	-0.06226	0.00000	0.07100	-0.00000	-0.06226	0.00000	0.12450	-0.00000	-0.20009
	0.00000	0.53802	1.00000	0.53801	0.00000	-0.06225	-0.00000	-0.06225	0.00000						
19	-0.00000	-0.24621	0.00000	-0.00001	0.00000	-0.06224	0.00000	0.05946	-0.00000	0.05946	0.00000	-0.06224	-0.00000	-0.00001	0.00000
	-0.24621	-0.00000	0.53801	1.00000	0.52190	0.00000	-0.17243	-0.00000	0.52190						
20	-0.24620	0.00000	0.53802	-0.00000	-0.24622	0.00000	0.00001	-0.00000	-0.06225	0.00000	0.05946	-0.00000	0.05947	0.00000	-0.06225
	-0.00000	0.00000	0.00000	0.52190	1.00000	0.52188	0.00000	-0.17243	-0.00000						
21	-0.00000	0.00001	-0.00000	-0.24622	0.00000	0.53802	-0.00000	-0.24620	0.00000	0.00000	-0.00000	-0.06225	0.00000	0.05947	-0.00000
	0.05946	0.00000	-0.06225	0.00000	0.52188	1.00000	0.52190	0.00000	-0.17243						
22	0.05946	-0.00000	-0.06224	0.00000	-0.00001	-0.00000	-0.24621	0.00000	0.53801	-0.00000	-0.24621	0.00000	-0.00001	-0.00000	-0.06224
	0.00000	0.05946	-0.00000	-0.17243	0.00000	0.52190	1.00000	0.52190	0.00000						
23	0.00000	0.05946	-0.00000	0.05947	0.00000	-0.06225	-0.00000	0.00000	0.00000	-0.24620	0.00000	0.53802	-0.00000	-0.24622	0.00000
	0.00001	-0.00000	-0.06225	-0.00000	-0.17243	0.00000	0.52190	1.00000	0.52188						
24	0.00000	-0.00000	-0.06225	-0.00000	0.05947	-0.00000	0.05946	0.00000	-0.06225	0.	-0.00001	0.00000	-0.24622	0.00000	0.53802
	0.00000	-0.24620	0.00000	0.52190	-0.00000	-0.17243	0.00000	0.52188	1.00000						

CORONENE (D) TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.76868	-0.56667	-0.04594	-0.15142	0.00757	-0.12077	-0.00521	-0.09968	-0.00188	0.05050	0.00275	-0.06162	-0.00521	0.08272	-0.01571
	-0.15143	-0.05409	0.37058	-0.03617	-0.22907	0.01271	0.05680	-0.00006	0.00507						
2	-0.56667	0.76868	0.37057	-0.05409	-0.15143	0.01571	0.08272	-0.00521	-0.06163	0.00275	0.05051	-0.00188	-0.09969	-0.00520	0.12078
	0.00756	-0.15143	-0.04595	-0.22908	-0.03617	0.00507	-0.00006	0.05681	0.01271						
3	-0.04594	0.37057	0.72437	0.37059	-0.04594	-0.18442	0.01571	-0.12077	-0.00064	-0.06162	-0.00188	0.06925	-0.00188	-0.06162	-0.00064
	0.12078	0.01571	-0.18442	-0.03324	0.37565	-0.03323	-0.05656	0.01083	-0.05657						
4	-0.15142	-0.05409	0.37059	0.76868	0.56666	-0.04594	-0.15143	0.00757	0.12078	-0.00521	-0.09969	-0.00188	0.05050	0.00274	-0.06162
	-0.00520	0.08272	0.01571	0.00506	-0.03617	-0.22909	0.01271	0.05681	-0.00006						
5	0.00757	-0.15143	-0.04594	0.56666	0.76868	0.37059	-0.05409	-0.15142	0.01571	0.08272	-0.00520	-0.06162	0.00274	0.05050	-0.00188
	-0.09969	-0.00521	0.12078	0.01271	-0.22909	-0.03617	0.00506	-0.00006	0.05681						
6	0.12077	0.01571	-0.18442	-0.04594	0.37059	0.72437	0.37057	-0.04594	-0.18442	0.01571	0.12078	-0.00064	-0.06162	-0.00188	0.06925
	-0.00188	-0.06162	-0.00064	-0.05656	-0.03323	0.37565	-0.03324	-0.05657	0.01083						
7	-0.00521	0.08272	0.01571	-0.15143	-0.05409	0.37057	0.76868	0.56667	-0.04595	-0.15143	0.00756	0.12078	-0.00520	-0.09969	-0.00188
	0.05051	0.00275	-0.06163	-0.00006	0.00507	-0.03617	-0.22908	0.01271	0.05681						
8	-0.09968	-0.00521	0.12077	0.00757	-0.15142	-0.04594	0.56667	0.76868	0.37058	-0.05409	-0.15143	0.01571	0.08272	-0.00521	-0.06162
	0.00275	0.05050	-0.00188	0.05680	0.01271	-0.22907	-0.03617	0.00507	-0.00006						
9	-0.00188	-0.06163	-0.00064	0.12078	0.01571	-0.18442	-0.04595	0.37058	0.72436	0.37058	-0.04595	-0.18442	0.01571	0.12078	-0.00064
	-0.06163	-0.00188	0.06925	0.01083	-0.05656	-0.03323	0.37564	-0.03323	-0.05656						
10	0.05050	0.00275	-0.06162	-0.00521	0.08272	0.01571	-0.15143	-0.05409	0.37058	0.76868	0.56667	-0.04594	-0.15142	0.00757	0.12077
	-0.00521	-0.09968	-0.00188	0.05680	-0.00006	0.00507	-0.03617	-0.22907	0.01271						
11	0.00275	0.05051	-0.00188	-0.09969	-0.00520	0.12078	0.00756	-0.15143	-0.04595	0.56667	0.76868	0.37057	-0.05409	-0.15143	0.01571
	0.08272	-0.00521	-0.06163	-0.00006	0.05681	0.01271	-0.22908	-0.03617	0.00507						
12	-0.06162	-0.00188	0.06925	-0.00188	-0.06162	-0.00064	0.12078	0.01571	-0.18442	-0.04594	0.37057	0.72437	0.37059	-0.04594	-0.18442
	0.01571	0.12077	-0.00064	-0.05656	0.01083	-0.05657	-0.03324	0.37565	-0.03323						
13	-0.00521	-0.09969	-0.00188	0.05050	-0.00274	-0.06162	-0.00520	0.08272	0.01571	-0.15142	-0.05409	0.37059	0.76868	0.56666	-0.04594
	-0.15143	0.00757	0.12078	0.01271	0.05681	-0.00006	0.00506	-0.03617	-0.22909						
14	0.08272	-0.00520	-0.06162	0.00274	-0.05050	-0.00188	-0.09969	-0.00521	0.12078	0.00757	-0.15143	-0.04594	0.56666	0.76868	0.37059
	-0.05409	-0.15142	0.01571	0.00506	-0.00006	0.05681	0.01271	-0.22909	-0.03617						
15	0.01571	0.12078	-0.00064	-0.06162	-0.00188	0.06925	-0.00188	-0.06162	-0.00064	0.12077	0.01571	-0.18442	-0.04594	0.37059	0.72437
	0.37057	-0.04594	-0.18442	-0.03324	-0.05657	0.01083	-0.05656	-0.03323	0.37565						
16	-0.15143	0.00756	0.12078	-0.00520	-0.09969	-0.00188	0.05051	0.00275	-0.06163	-0.00521	0.08272	0.01571	-0.15143	-0.05409	0.37057
	0.76868	0.56667	-0.04595	-0.22908	0.01271	0.05681	-0.00006	0.00507	-0.03617						
17	-0.05409	-0.15143	0.01571	0.08272	-0.00521	-0.06162	0.00275	0.05050	-0.00188	-0.09968	-0.00521	0.12077	0.00757	-0.15142	-0.04594
	0.56667	0.76868	0.37058	-0.03617	0.00507	-0.00006	0.05680	0.01271	-0.22907						
18	0.37058	-0.04595	-0.18442	0.01571	0.12078	-0.00064	-0.06163	-0.00188	0.06925	-0.00188	-0.06163	-0.00064	0.12078	0.01571	-0.18442
	-0.04595	0.37058	0.72436	0.37564	-0.03323	-0.05656	0.01083	-0.05656	-0.03323						
19	-0.03617	-0.22908	-0.03324	0.00506	0.01271	-0.05656	-0.00006	0.05680	0.01083	0.05680	-0.00006	-0.05656	0.01271	0.00506	-0.03324
	-0.22908	-0.03617	0.37564	0.73024	0.35868	-0.03569	-0.15748	-0.03569	0.35868						
20	-0.22907	-0.03617	0.37565	-0.03617	-0.22909	-0.03323	0.00507	0.01271	-0.05656	-0.00006	0.05681	0.01083	0.05681	-0.00006	-0.05657
	0.01271	0.00507	-0.03323	0.35868	0.73024	0.35867	-0.03569	-0.15749	-0.03570						
21	0.01271	0.00507	-0.03323	-0.22909	-0.03617	0.37565	-0.03617	-0.22907	-0.03323	0.00507	0.01271	-0.05657	-0.00006	0.05681	0.01083
	0.05681	-0.00006	-0.05656	-0.03569	0.35867	0.73024	0.35868	-0.03570	-0.15749						
22	0.05680	-0.00006	-0.05656	0.01271	0.00506	-0.03324	-0.22908	-0.03617	0.37564	-0.03617	-0.22908	-0.03324	0.00506	0.01271	-0.05656
	-0.00006	0.05680	0.01083	-0.15748	-0.03569	0.35868	0.73024	0.35868	-0.03569						
23	-0.00006	0.05681	0.01083	0.05681	-0.00006	-0.05657	0.01271	0.00507	-0.03323	-0.22907	-0.03617	0.37565	-0.03617	-0.22909	-0.03323
	0.00507	0.01271	-0.05656	-0.03569	-0.15749	-0.03570	0.35868	0.73024	0.35867						
24	0.00507	-0.01271	-0.05657	-0.00006	0.05681	0.01083	0.05681	-0.00006	-0.05656	0.01271	-0.00507	-0.03323	-0.22909	-0.03617	0.37565
	-0.03617	-0.22907	-0.03323	0.35868	-0.03570	-0.15749	-0.03569	0.35867	0.73024						

ENERGIES FOR CORONENE ,TBM APPROXIMATION 1.7
ONE ELECTRON EXCITATIONS OF SA SYMMETRY.

JUMP	12,13	11,14	6,14	5,13	4,14	8,15	10,17	8,16	9,17	1,14
XMOMNT	1.00476	1.00477	-0.00002	-0.06764	-0.06763	-0.40410	0.28417	0.24572	-0.37805	0.01075
YMOMNT	-0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00136	-0.00013	-0.00037	0.00035	0.00000
JUMP E	20.0578	20.0606	31.7466	33.0183	33.0201	38.9135	38.9147	38.9148	38.9152	40.8065
DIAG E	31.1173	31.1201	45.7226	48.3025	48.3048	54.7830	51.5960	51.9732	54.7963	55.7573
DIAG E	31.5083	31.5112	47.1137	49.7713	49.7736	59.2623	50.5279	53.1163	51.0968	58.9774
CORRSP	24.8804	35.0496	43.8527	50.2974	46.9467	57.3648	55.5259	47.4168	55.6900	56.4484
CORRSP	25.6322	35.3543	45.9622	50.9640	47.9312	62.9208	47.4310	55.4633	52.0812	58.9185

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	E	XMOMNT	YMOMNT	//	STATE COMPOSITION									
24.88042	0.00000	0.00017	-0.00004	//	0.6991	-0.6989	0.0000	-0.0884	0.0884	0.0295	0.0547	-0.0521	-0.0242	0.0000
24.79833				//	0.6962	-0.6968	0.0001	-0.1069	0.1069	0.0290	0.0536	-0.0510	-0.0236	0.0000
35.04961	2.27499	1.23545	0.00003	//	0.6751	0.6753	0.0636	-0.0645	-0.0645	0.0513	-0.1942	-0.1858	0.0232	0.0214
22.21373				//	0.6851	0.6844	-0.0968	-0.0164	-0.0163	-0.1620	-0.0171	-0.0371	-0.1559	-0.0129
43.85274	0.06591	-0.18799	-0.00044	//	-0.0489	-0.0489	0.9045	-0.1250	-0.1250	0.2967	-0.0255	0.1297	0.0242	-0.1995
35.62338				//	0.1211	0.1212	0.6718	-0.2782	-0.2782	0.4393	-0.2300	-0.1379	0.3113	-0.0524
50.29737	0.00000	-0.00002	0.00022	//	0.1066	-0.1066	-0.0000	0.5959	-0.5962	-0.1798	-0.3339	0.3179	0.1478	0.0000
44.75374				//	0.0791	-0.0791	-0.0008	0.6538	-0.6561	0.1253	0.2332	-0.2211	-0.1026	0.0003
46.94668	0.00683	0.05847	0.00005	//	0.0408	0.0408	0.1976	0.6658	0.6639	-0.0671	-0.1019	-0.0481	-0.2148	-0.1013
44.07168				//	0.0141	0.0138	0.3725	0.5807	0.5780	0.0260	-0.2929	-0.2204	-0.1587	-0.1714
57.36483	0.28576	-0.34226	-0.00110	//	0.0216	0.0217	-0.2059	0.1492	0.1492	0.8051	-0.0204	0.2978	0.2932	0.2983
56.73207				//	0.0735	0.0735	-0.3429	0.1296	0.1296	0.7965	-0.0596	0.4264	-0.0825	-0.1064
55.52588	0.74979	0.56351	0.00010	//	0.1712	0.1712	-0.0435	0.0787	0.0787	-0.1722	0.6589	0.4357	0.3425	-0.3952
48.69870				//	-0.0927	0.0927	-0.0002	-0.2441	0.2441	0.3236	0.6008	-0.5721	-0.2658	0.0000
47.41683	0.00000	0.00015	0.00037	//	0.0049	-0.0047	0.0005	-0.3685	0.3715	-0.2968	-0.5512	0.5243	0.2433	-0.0002
48.04726				//	0.0135	0.0135	0.5264	0.0321	0.0320	-0.1055	0.4998	0.6061	-0.3037	-0.0056
55.68998	1.02539	-0.65801	0.00056	//	-0.0966	-0.0966	0.0444	-0.0831	0.0831	-0.0479	-0.1342	-0.5371	0.7940	-0.1625
55.45238				//	0.0771	0.0770	-0.0649	0.1695	0.1694	-0.0750	0.4133	0.0478	0.7401	-0.4472
56.44844	0.10314	0.20729	0.00046	//	0.0309	0.0309	0.3043	0.0533	0.0533	-0.3216	0.2833	0.0257	0.1937	0.8233
53.73102				//	0.0689	0.0689	0.0404	0.2004	0.2003	0.0873	0.1365	0.0285	0.3537	0.8697

ENERGIES FOR CORONENE TBM APPROXIMATION 1.7

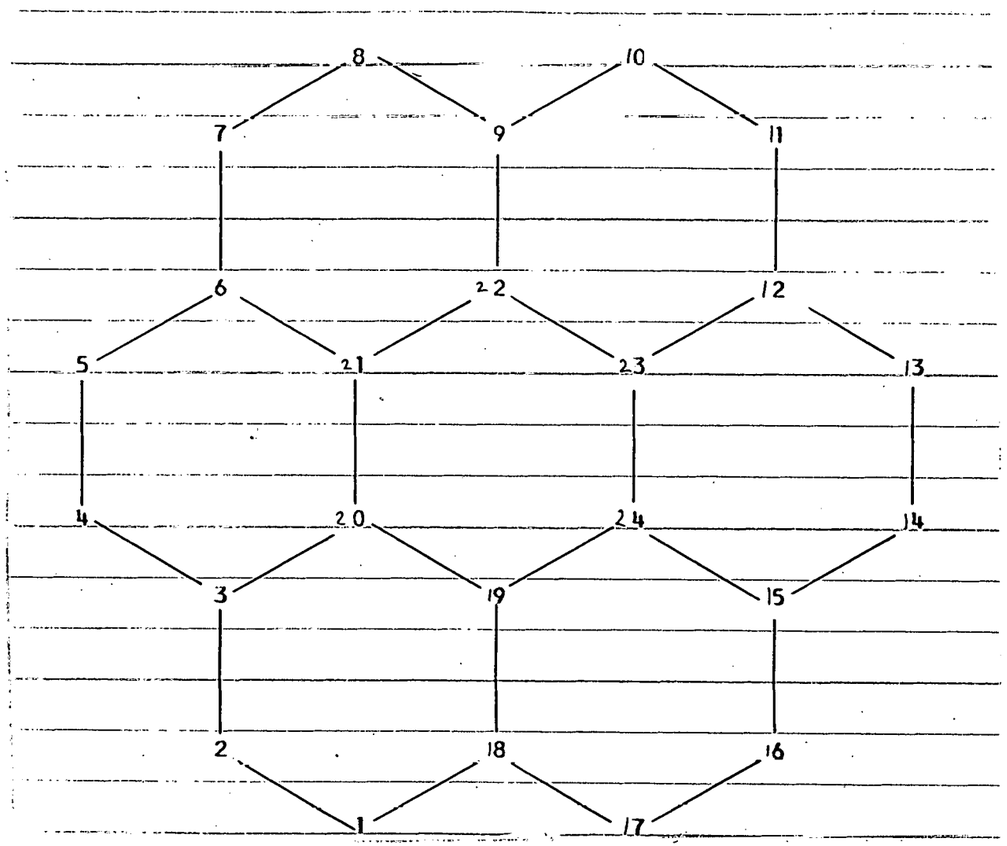
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	11,13	12,14	6,13	4,13	5,14	10,15	9,15	10,16	9,16	8,17
XMOMNT	0.00000	0.00000	0.00000	-0.00000	-0.00000	-0.00067	0.00128	-0.00018	-0.00000	-0.00117
YMOMNT	-1.00481	1.00473	0.00002	0.06764	-0.06765	0.04819	0.10295	-0.51370	0.00770	0.41259
JUMP E	20.0589	20.0596	31.7448	33.0184	33.0201	38.9127	38.9132	38.9140	38.9145	38.9154
DIAG E	32.1178	32.1185	45.7202	48.7117	48.7137	55.1986	58.3228	54.3817	55.6069	52.5851
DIAG E	32.5089	32.5096	47.1113	50.1805	50.1825	59.0371	59.5299	54.8841	53.4779	52.1578
CORRSP	26.6024	35.0587	44.3306	47.0609	49.4665	57.2690	61.3283	55.6370	55.7598	50.9637
CORRSP	27.2702	35.3627	45.9964	51.1730	47.9701	62.7411	63.2576	50.2295	52.1160	55.4626

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
26.60241	0.00000	0.00007	-0.00011	//	0.6977	0.6976	-0.0000	-0.0731	-0.0731	0.0309	0.1014	0.0447	0.0453	0.0259
22.21927				//	0.6846	-0.6848	0.0978	-0.0166	0.0166	0.0755	-0.1138	0.1624	0.0701	-0.0480
35.05866	2.27250	0.00038	1.23462	//	-0.6751	0.6752	0.0691	0.0641	-0.0641	-0.1086	0.0789	0.1085	-0.1026	-0.1871
17.73610	1			//	0.6549	0.6547	0.0000	0.0519	0.0519	0.0256	0.2605	0.1895	0.0699	-0.1666
44.33057	0.07979	-0.00031	-0.20573	//	0.0601	-0.0600	0.9054	0.1750	-0.1750	0.2435	-0.1203	0.1831	-0.0588	-0.0329
48.04720				//	-0.0138	0.0137	0.5275	-0.0337	0.0335	0.4402	-0.1541	-0.3943	0.1025	0.5792
47.06087	0.00262	-0.00020	-0.03618	//	0.0325	-0.0325	-0.2826	0.6546	-0.6541	0.0002	-0.1303	0.1010	0.1855	0.0109
44.80134				//	0.0608	0.0608	0.0006	0.3892	0.3907	0.3363	0.0758	-0.4008	0.3040	-0.5626
49.46652	0.00000	0.00032	0.00010	//	0.0537	0.0538	0.0001	0.6607	0.6612	0.1648	0.1667	-0.0845	0.1728	-0.1690
39.72272				//	-0.2041	-0.2041	-0.0000	0.5111	0.5110	-0.0745	0.3104	0.3711	-0.0073	0.3933
57.26902	0.33544	-0.00079	-0.37113	//	-0.0196	0.0196	-0.2849	-0.1348	0.1349	0.5831	-0.3755	0.6074	-0.0610	-0.1676
56.70391	1			//	-0.0709	0.0709	-0.3335	-0.1264	0.1264	0.7387	-0.2479	0.3799	-0.3075	-0.0287
61.32830	0.00000	0.00068	0.00005	//	-0.1020	-0.1020	-0.0000	-0.1606	-0.1606	0.3136	0.7750	0.2346	0.4132	0.0544
59.43610				//	-0.1608	-0.1608	-0.0000	-0.2899	-0.2900	0.3256	0.6953	0.1490	0.4090	-0.0335
55.63701	1.78762	0.00131	-0.86922	//	0.1946	-0.1946	0.0007	0.0207	-0.0208	-0.4633	0.2340	0.4062	-0.2309	-0.6601
35.67000				//	-0.1224	0.1224	0.6684	0.2839	-0.2839	0.0619	-0.1329	0.4776	-0.0248	-0.3345
55.75982	0.03361	-0.00020	-0.11906	//	0.0353	0.0353	0.1203	-0.1360	0.1361	-0.3858	-0.3365	0.2325	0.7936	-0.0123
55.08944				//	0.1028	0.1029	-0.0607	-0.2424	0.2425	-0.1179	-0.4435	0.2952	0.7456	0.0629
50.96374	-0.00000	-0.00053	-0.00032	//	-0.0049	-0.0050	0.0001	0.1789	0.1789	-0.3147	-0.1214	0.5407	-0.2493	0.6838
44.36681				//	0.0202	-0.0200	-0.3879	0.5863	-0.5854	0.1083	-0.1847	-0.0459	0.2625	0.2131

CORONENE IRM



ATOMIC COORDINATES

x	2.5980	1.7320	1.7320	0.8660	0.8660	1.7320	1.7320	2.5980	3.4640	4.3300	5.1960	5.1960	6.0620	6.0620
	5.1960	5.1960	4.3300	3.4640	3.4640	2.5980	2.5980	3.4640	4.3300	4.3300				
y	0.	0.5000	1.5000	2.0000	3.0000	3.5000	4.5000	5.0000	4.5000	5.0000	4.5000	3.5000	3.0000	2.0000
	1.5000	0.5000	0.	0.5000	1.5000	2.0000	3.0000	3.5000	3.0000	2.0000				

CORONENE IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 SA	10 AS	11 SS	12 AA	13 AS
1.841892	1.638602	1.638593	1.421978	1.421975	1.364978	1.230039	1.212106	1.163200	1.163179	1.050624	1.050602	0.807919
0.130960	0.251146	0.084770	-0.243398	0.194790	0.209613	-0.160451	0.288692	-0.219719	0.125523	0.330783	0.009384	0.027564
0.130959	0.199203	0.174863	-0.043769	0.308629	0.209649	0.160357	0.288694	-0.218237	0.128201	0.161086	-0.289082	-0.280093
0.207452	0.172299	0.298004	0.175552	0.300389	-0.108320	0.325710	-0.000005	0.012111	-0.021174	-0.252486	-0.147987	0.133059
0.130961	0.052160	0.259885	0.290332	0.113363	0.209716	0.160413	-0.288639	-0.001179	0.253132	-0.173522	0.281777	0.307563
0.130961	-0.051838	0.259950	0.289107	-0.116452	0.209716	-0.160412	-0.288640	0.001990	0.253127	0.169813	0.284028	-0.307500
0.207452	-0.171929	0.298217	0.172339	-0.302244	0.108320	-0.325710	-0.000006	-0.012179	-0.021136	0.254405	-0.144664	-0.133159
0.130959	-0.198986	0.175110	-0.047058	-0.308145	0.209649	-0.160358	0.288693	0.218648	0.127500	-0.157282	-0.291169	0.280009
0.130960	-0.251041	0.085081	-0.245461	-0.192183	0.209613	0.160450	0.288692	0.220122	0.124817	-0.330878	0.005046	-0.027416
0.207450	-0.344226	0.000213	-0.347949	0.001855	0.108225	0.325702	0.000000	-0.024483	0.000039	-0.001919	0.292660	-0.266232
0.130960	-0.251146	-0.084770	-0.243397	0.194790	0.209612	0.160450	-0.288692	0.219719	-0.125523	0.330784	0.009384	-0.027563
0.130959	-0.199203	-0.174863	-0.043769	0.308630	0.209649	-0.160357	-0.288694	0.218237	-0.128201	0.161086	-0.289082	0.280092
0.207452	-0.172298	-0.298004	0.175552	0.300389	0.108320	-0.325710	0.000006	-0.012111	0.021174	-0.252486	-0.147987	-0.133060
0.130961	-0.052160	-0.259885	0.290332	0.113363	0.209715	-0.160413	0.288639	0.001179	-0.253132	-0.173523	0.281778	-0.307563
0.130961	0.051838	-0.259950	0.289107	-0.116452	0.209716	0.160412	0.288639	-0.001990	-0.253126	0.169813	0.284028	0.307500
0.207451	0.171929	-0.298217	0.172339	-0.302244	0.108320	0.325710	0.000006	0.012179	0.021135	0.254405	-0.144664	0.133159
0.130959	0.198986	-0.175110	-0.047058	-0.308145	0.209649	0.160358	-0.288693	-0.218648	-0.127500	-0.157282	-0.291169	-0.280009
0.130960	0.251041	-0.085082	-0.245461	-0.192183	0.209613	-0.160449	-0.288692	-0.220121	-0.124817	-0.330878	0.005046	0.027416
0.207450	0.344226	-0.000214	-0.347949	0.001855	0.108225	-0.325702	-0.000001	0.024483	-0.000039	-0.001919	0.292660	0.266232
0.298881	0.272616	-0.000169	-0.133896	0.000714	-0.258924	-0.095412	-0.000001	0.452370	-0.000725	-0.001110	0.169288	-0.175431
0.298880	0.136457	0.236009	0.067639	0.115648	-0.258880	0.095548	-0.000045	0.225531	-0.392108	-0.146060	-0.085606	-0.087684
0.298880	-0.136164	0.236178	0.066402	-0.116363	-0.258880	-0.095548	-0.000045	-0.226788	-0.391382	0.147170	-0.083683	0.087750
0.298881	-0.272616	0.000169	-0.133897	0.000714	-0.258924	0.095412	0.000001	-0.452370	0.000726	-0.001110	0.169288	0.175431
0.298880	-0.136457	-0.236009	0.067639	0.115648	-0.258879	-0.095548	0.000046	-0.225531	0.392108	-0.146061	-0.085606	0.087684
0.298880	0.136164	-0.236178	0.066402	-0.116363	-0.258879	0.095548	0.000045	0.226788	0.391382	0.147170	-0.083683	-0.087749

OVERLAP EIGNVALUES AND EIGNVECTORS

14 sa	15 SS	16 AA	17 AA	18 SS	19 AS	20 AS	21 SA	22 SS	23 AA	24 AS
0.807902	0.725410	0.725402	0.718491	0.684001	0.627896	0.602405	0.602405	0.520491	0.520490	0.459388
0.339231	-0.120252	0.233967	-0.288736	0.149104	0.211598	0.244115	-0.153606	0.080546	0.225678	-0.113231
-0.193370	0.144000	-0.220162	0.288739	0.149059	-0.211612	-0.048894	0.284226	-0.165264	-0.173503	0.113229
-0.230588	-0.023282	0.013358	-0.000003	-0.334521	0.137759	-0.167235	-0.339699	0.312198	0.168630	-0.203981
0.145746	0.262963	-0.012756	-0.288548	0.149086	-0.211643	0.255052	0.134590	-0.235712	-0.043083	0.113229
0.145880	-0.262858	-0.014769	0.288548	0.149087	0.211643	-0.270568	0.099793	0.232892	-0.056372	-0.113229
-0.230530	0.023179	0.013536	0.000003	-0.334521	-0.137760	0.210557	-0.314688	-0.302139	0.186052	0.203981
-0.193491	-0.142310	-0.221257	-0.288740	0.149059	0.211612	0.010999	0.288191	0.155165	-0.182590	-0.113229
0.339243	0.118458	0.234880	0.288737	0.149104	-0.211598	-0.221735	-0.184446	-0.067627	0.229880	0.113231
0.000058	0.000102	-0.026799	-0.000000	-0.334521	0.137711	0.377822	0.025013	-0.010059	-0.354686	-0.203980
-0.339231	-0.120252	0.233967	-0.288736	0.149104	-0.211598	-0.244115	0.153606	0.080546	0.225678	0.113231
0.193370	0.144000	-0.220162	0.288740	0.149059	0.211612	0.048894	-0.284226	-0.165264	-0.173503	-0.113229
0.230588	-0.023282	0.013358	-0.000003	-0.334521	-0.137760	0.167236	0.339699	0.312198	0.168630	0.203981
-0.145746	0.262963	-0.012756	-0.288548	0.149086	0.211643	-0.255052	-0.134590	-0.235712	-0.043083	-0.113229
-0.145880	-0.262858	-0.014769	0.288548	0.149087	-0.211643	0.270569	-0.099793	0.232892	-0.056372	0.113229
0.230530	0.023178	0.013536	0.000003	-0.334521	0.137760	-0.210557	0.314688	-0.302139	0.186052	-0.203981
0.193491	-0.142310	-0.221257	-0.288740	0.149059	-0.211612	-0.010999	-0.288191	0.155165	-0.182590	0.113229
-0.339243	0.118458	0.234880	0.288737	0.149104	0.211598	0.221735	0.184446	-0.067627	0.229880	-0.113231
-0.000058	0.000102	-0.026800	-0.000000	-0.334521	-0.137711	-0.377822	-0.025012	-0.010058	-0.354686	0.203980
0.000038	0.001687	-0.440614	-0.000001	0.101499	-0.241120	0.153306	0.010149	0.008626	0.304171	-0.315305
0.151953	-0.382413	0.218834	-0.000171	0.101563	0.241090	0.067895	0.137870	-0.267736	-0.144618	0.315304
0.151914	0.380727	0.221754	0.000172	0.101563	-0.241090	0.085478	0.127717	0.259109	-0.159559	-0.315304
-0.000038	0.001686	-0.440614	-0.000001	0.101498	0.241120	-0.153306	-0.010150	0.008626	0.304171	0.315305
-0.151952	-0.382413	0.218834	-0.000171	0.101563	-0.241090	-0.067895	-0.137870	-0.267736	-0.144618	-0.315303
0.151914	0.380727	0.221755	0.000172	0.101563	0.241090	0.085478	-0.127717	0.259110	-0.159559	0.315303

CORONENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 SS	7 AS	8 SA	9 SA	10 AS	11 SS	12 AA	13 AS
33.83885	28.85229	28.85203	21.96951	21.96940	19.79541	13.84540	12.95497	10.38700	10.38584	3.56727	3.56577	-17.60106
0.096496	0.196155	0.066344	-0.204981	0.162259	0.179413	-0.144671	0.262219	-0.116057	-0.203912	-0.007039	0.322772	-0.030585
0.096495	0.155533	0.136700	-0.038085	0.258617	0.179444	-0.144587	0.262221	-0.118543	-0.202541	0.283056	0.155306	-0.311569
0.152857	0.134456	0.232885	0.145872	0.252688	0.092714	0.293678	-0.000005	0.019615	0.011261	0.142760	-0.247272	0.148089
0.096496	0.040622	0.203049	0.242961	0.096363	0.179501	0.144637	-0.262171	-0.234701	-0.001469	-0.276009	-0.167486	0.342142
0.096496	-0.040622	0.203049	0.242962	-0.096362	0.179501	-0.144637	-0.262172	-0.234701	0.001469	-0.276009	0.167486	-0.342141
0.152857	-0.134455	0.232885	0.145873	-0.252687	0.092714	-0.293678	-0.000006	0.019615	-0.011261	0.142760	-0.247272	-0.148091
0.096495	-0.155533	0.136700	-0.038083	-0.258617	0.179444	-0.144588	0.262220	-0.118542	0.202542	0.283055	-0.155306	0.311567
0.096496	-0.196155	0.066344	-0.204980	-0.162260	0.179414	0.144670	0.262219	-0.116058	0.203912	-0.007039	-0.322772	-0.030582
0.152855	-0.268910	-0.000000	-0.291793	-0.000001	0.092633	0.293671	0.000000	-0.000000	-0.022701	-0.285528	0.000000	-0.296194
0.096496	-0.196155	-0.066344	-0.204981	0.162259	0.179413	0.144671	-0.262219	0.116057	0.203912	-0.007039	0.322772	-0.030585
0.096495	-0.155533	-0.136700	-0.038085	0.258617	0.179444	-0.144587	-0.262221	0.118543	0.202541	0.283055	0.155306	0.311568
0.152857	-0.134455	-0.232885	0.145872	0.252688	0.092714	-0.293678	0.000005	-0.019615	-0.011261	0.142760	-0.247272	-0.148089
0.096496	-0.040622	-0.203049	0.242961	0.096363	0.179501	-0.144637	0.262171	0.234701	0.001469	-0.276009	-0.167486	-0.342142
0.096496	0.040622	-0.203049	0.242962	-0.096362	0.179501	0.144637	0.262171	0.234701	-0.001469	-0.276009	0.167486	0.342141
0.152857	0.134455	-0.232885	0.145873	-0.252687	0.092714	0.293678	0.000006	-0.019615	0.011261	0.142760	0.247272	0.148091
0.096495	0.155533	-0.136700	-0.038083	-0.258617	0.179444	0.144588	-0.262220	0.118543	-0.202542	0.283055	-0.155306	-0.311567
0.096496	0.196155	-0.066344	-0.204980	-0.162260	0.179413	-0.144670	-0.262219	0.116058	-0.203912	-0.007039	-0.322772	0.030582
0.152855	0.268910	-0.000000	-0.291793	-0.000001	0.092633	-0.293671	-0.000001	0.000000	0.022701	-0.285528	-0.000000	0.296194
0.220225	0.212968	-0.000000	-0.112287	-0.000001	-0.221620	-0.086029	-0.000001	-0.000000	0.419441	-0.165163	0.000000	-0.195174
0.220224	0.106486	0.184437	0.056204	0.097284	-0.221582	0.086151	-0.000041	0.363226	0.209697	0.082582	-0.143044	-0.097588
0.220224	-0.106486	0.184437	0.056204	-0.097284	-0.221582	-0.086151	-0.000041	0.363226	-0.209697	0.082582	0.143044	0.097589
0.220225	-0.212968	-0.000000	-0.112287	-0.000000	-0.221620	0.086029	0.000001	-0.000000	-0.419441	-0.165163	-0.000000	0.195174
0.220224	-0.106486	-0.184437	0.056204	0.097284	-0.221582	-0.086151	0.000041	-0.363226	-0.209697	0.082582	-0.143044	0.097588
0.220224	0.106486	-0.184437	0.056204	-0.097284	-0.221582	0.086151	0.000041	-0.363226	0.209697	0.082582	0.143044	-0.097589

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

14 SA	15 SS	16 AA	17 AA	18 SS	19 AS	20 AS	21 SA	22 SS	23 AA	24 AS
-17.60304	-28.02367	-28.02477	-29.00649	-34.20207	-43.87330	-48.86249	-48.86251	-68.20350	-68.20369	-87.12238
0.377419	-0.275241	-0.140138	-0.340636	0.180285	0.267034	-0.300761	0.218253	-0.315851	0.102732	-0.167062
-0.215200	0.259139	0.168082	0.340640	0.180231	-0.267052	0.038668	-0.369563	0.246889	-0.222162	0.167058
-0.256510	-0.015789	-0.027275	-0.000003	-0.404478	0.173851	0.243910	0.422484	-0.245911	0.425936	-0.300954
0.162223	0.016158	0.308689	-0.340414	0.180264	-0.267091	-0.339350	-0.151322	0.068955	-0.324896	0.167058
0.162226	0.016159	-0.308689	0.340414	0.180265	0.267091	-0.339350	-0.151322	0.068955	0.324896	-0.167058
-0.256509	-0.015789	0.027275	0.000003	-0.404478	-0.173852	-0.243909	0.422484	-0.245911	-0.425936	0.300954
-0.215203	0.259138	-0.168082	-0.340641	0.180231	0.267053	-0.038668	-0.369562	0.246889	0.222162	-0.167058
0.377419	-0.275240	0.140138	0.340637	0.180285	-0.267035	0.300761	0.218252	-0.315851	-0.102732	0.167062
0.000001	0.031466	-0.000000	-0.000000	-0.404478	0.173790	-0.487857	0.000000	0.491827	-0.000000	-0.300953
-0.377419	-0.275242	-0.140138	-0.340636	0.180286	-0.267034	0.300760	-0.218253	-0.315851	0.102733	0.167062
0.215200	0.259139	0.168082	0.340640	0.180231	0.267052	-0.038668	0.369563	0.246889	-0.222162	-0.167058
0.256510	-0.015789	-0.027275	-0.000003	-0.404478	-0.173851	-0.243910	-0.422484	-0.245911	0.425937	0.300953
-0.162223	0.016158	0.308689	-0.340414	0.180264	0.267091	0.339350	0.151322	0.068955	-0.324896	-0.167058
-0.162226	0.016160	-0.308689	0.340414	0.180265	-0.267091	-0.339350	0.151322	0.068955	0.324896	0.167058
0.256509	-0.015789	0.027275	0.000003	-0.404478	0.173852	0.243909	-0.422484	-0.245911	-0.425936	-0.300953
0.215203	0.259138	-0.168081	-0.340641	0.180231	-0.267053	0.038668	0.369562	0.246889	0.222162	0.167058
-0.377419	-0.275241	0.140138	0.340637	0.180285	0.267035	-0.300761	-0.218252	-0.315851	-0.102733	-0.167062
-0.000001	0.031466	-0.000000	0.000000	-0.404478	-0.173790	0.487857	-0.000001	0.491827	0.000000	0.300953
0.000001	0.517332	0.000000	-0.000001	0.122725	-0.304291	-0.197955	-0.000000	-0.421780	-0.000000	-0.465201
0.169035	-0.258651	-0.448010	-0.000202	0.122803	0.304253	-0.099020	-0.171467	0.210894	-0.365276	0.465200
0.169034	-0.258651	0.448010	0.000203	0.122802	-0.304253	0.099020	-0.171468	0.210894	0.365276	-0.465200
-0.000001	0.517332	0.000000	-0.000001	0.122724	0.304291	0.197955	0.000000	-0.421780	0.000000	0.465201
-0.169034	-0.258651	-0.448010	-0.000202	0.122803	-0.304254	0.099020	0.171467	0.210894	-0.365276	-0.465199
-0.169033	-0.258651	0.448010	-0.000203	-0.122802	-0.304253	-0.099020	0.171468	0.210894	0.365276	0.465199

CORONENE — IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24						
1	1.02232	0.73790	-0.01659	-0.16826	0.01932	0.13246	-0.00065	-0.11388	0.00742	0.04880	-0.00814	0.06041	-0.00065	0.08826	-0.00507
	-0.16828	0.00986	0.54065	0.00619	-0.23603	-0.00842	0.06909	0.00332	-0.01580						
2	0.73790	1.02234	0.54063	0.00985	-0.16827	-0.00506	0.08827	-0.00065	-0.06042	-0.00814	0.04882	0.00742	-0.11390	-0.00065	0.13248
	0.01931	-0.16828	-0.01659	-0.23604	0.00618	-0.01579	0.00333	0.06909	-0.00842						
3	-0.01659	0.54063	0.97329	0.54066	-0.01660	-0.19026	-0.00506	0.13246	-0.00410	-0.06041	0.00742	0.07259	0.00742	-0.06041	-0.00410
	0.13248	-0.00507	-0.19027	0.01446	0.53224	0.01446	-0.07089	-0.01175	-0.07090						
4	-0.16826	0.00985	0.54066	1.02233	0.73788	-0.01660	-0.16827	0.01932	0.13248	-0.00065	-0.11390	0.00742	0.04880	-0.00814	-0.06041
	-0.00065	0.08826	-0.00507	-0.01581	0.00619	-0.23604	-0.00842	0.06910	0.00332						
5	0.01932	-0.16827	-0.01660	0.73788	1.02233	0.54066	0.00985	-0.16826	-0.00507	0.08826	-0.00065	-0.06041	-0.00814	0.04880	0.00742
	-0.11390	-0.00065	0.13248	-0.00842	-0.23604	0.00619	-0.01581	0.00332	0.06910						
6	0.13246	-0.00506	-0.19026	-0.01660	0.54066	0.97329	0.54063	-0.01659	-0.19027	-0.00507	0.13248	-0.00410	-0.06041	0.00742	0.07259
	0.00742	-0.06041	-0.00410	-0.07089	0.01446	0.53224	0.01446	-0.07090	-0.01175						
7	-0.00065	0.08827	-0.00506	-0.16827	0.00985	0.54063	1.02234	0.73790	-0.01659	-0.16828	0.01931	0.13248	-0.00065	-0.11390	0.00742
	0.04881	-0.00814	-0.06042	0.00333	-0.01579	0.00618	-0.23604	-0.00842	0.06909						
8	-0.11388	-0.00065	0.13246	0.01932	-0.16826	-0.01659	0.73790	1.02232	0.54065	0.00986	-0.16828	-0.00507	0.08826	-0.00065	-0.06041
	-0.00814	0.04880	0.00742	0.06909	-0.00842	-0.23603	0.00619	-0.01580	0.00332						
9	0.00742	-0.06042	-0.00410	0.13248	-0.00507	-0.19027	-0.01659	0.54065	0.97329	0.54065	-0.01659	-0.19027	-0.00507	0.13248	-0.00410
	-0.06042	0.00742	0.07260	-0.01175	-0.07089	0.01446	0.53222	0.01446	-0.07089						
10	0.04880	-0.00814	-0.06041	-0.00065	0.08826	-0.00507	-0.16828	0.00986	0.54065	1.02232	0.73790	-0.01659	-0.16826	0.01932	0.13246
	-0.00065	-0.11388	0.00742	0.06909	0.00332	-0.01580	0.00619	-0.23603	-0.00842						
11	-0.00814	0.04882	0.00742	-0.11390	-0.00065	0.13248	0.01931	-0.16828	-0.01659	0.73790	1.02234	0.54063	0.00985	-0.16827	-0.00506
	0.08827	-0.00065	-0.06042	0.00333	0.06909	-0.00842	-0.23604	0.00618	-0.01579						
12	-0.06041	0.00742	0.07259	0.00742	-0.06041	-0.00410	0.13248	-0.00507	-0.19027	-0.01659	0.54063	0.97329	0.54066	-0.01660	-0.19027
	-0.00506	0.13246	-0.00410	-0.07089	-0.01175	-0.07090	0.01446	0.53224	0.01446						
13	-0.00065	-0.11390	0.00742	0.04880	-0.00814	-0.06041	-0.00065	0.08826	-0.00507	-0.16826	0.00985	0.54066	1.02233	0.73788	-0.01660
	-0.16827	0.01932	0.13248	-0.00842	0.06910	0.00332	-0.01581	0.00619	-0.23604						
14	0.08826	-0.00065	-0.06041	-0.00814	0.04880	0.00742	-0.11390	-0.00065	0.13248	0.01932	-0.16827	-0.01660	0.73788	1.02233	0.54066
	0.00985	-0.16826	-0.00507	-0.01581	0.00332	0.06910	-0.00842	-0.23604	0.00619						
15	-0.00507	0.13248	-0.00410	-0.06041	0.00742	0.07259	0.00742	-0.06041	-0.00410	0.13246	-0.00506	-0.19027	-0.01660	0.54066	0.97329
	0.54063	-0.01659	-0.19027	0.01446	-0.07090	-0.01175	-0.07089	0.01446	0.53224						
16	-0.16828	0.01931	0.13248	-0.00065	-0.11390	0.00742	0.04881	-0.00814	-0.06042	-0.00065	0.08827	-0.00506	-0.16827	0.00985	0.54063
	1.02234	0.73790	-0.01659	-0.23604	-0.00842	0.06909	0.00333	-0.01579	0.00618						
17	0.00986	-0.16828	-0.00507	0.08826	-0.00065	-0.06041	-0.00814	0.04880	0.00742	-0.11388	-0.00065	0.13246	0.01932	-0.16826	-0.01659
	0.73790	1.02232	0.54065	0.00619	-0.01580	0.00332	0.06909	-0.00842	-0.23603						
18	0.54065	-0.01659	-0.19027	-0.00507	0.13248	-0.00410	-0.06042	0.00742	0.07260	0.00742	-0.06042	-0.00410	0.13248	-0.00507	-0.19027
	-0.01659	0.54065	0.97329	0.53222	0.01446	-0.07089	-0.01175	-0.07089	0.01446						
19	0.00619	-0.23604	0.01446	-0.01581	-0.00842	-0.07089	0.00333	0.06909	-0.01175	0.06909	0.00333	-0.07089	-0.00842	-0.01581	0.01446
	-0.23604	0.00619	0.53222	0.98204	0.52682	0.00541	-0.17020	0.00541	0.52682						
20	-0.23603	0.00618	0.53224	0.00619	-0.23604	0.01446	-0.01579	-0.00842	-0.07089	0.00332	0.06909	-0.01175	0.06910	0.00332	-0.07090
	-0.00842	-0.01580	0.01446	0.52682	0.98205	0.52679	0.00541	-0.17021	0.00541						
21	-0.00842	-0.01579	0.01446	-0.23604	0.00619	0.53224	0.00618	-0.23603	0.01446	-0.01580	-0.00842	-0.07090	0.00332	0.06910	-0.01175
	0.06909	0.00332	-0.07089	0.00541	0.52679	0.98205	0.52682	0.00541	-0.17021						
22	0.06909	0.00333	-0.07089	-0.00842	-0.01581	0.01446	-0.23604	0.00619	0.53222	0.00619	-0.23604	0.01446	-0.01581	-0.00842	-0.07089
	0.00333	0.06909	-0.01175	-0.17020	0.00541	0.52682	0.98204	0.52682	0.00541						
23	0.00332	0.06909	-0.01175	0.06910	0.00332	-0.07090	-0.00842	-0.01580	0.01446	-0.23603	0.00618	0.53224	0.00619	-0.23604	0.01446
	-0.01579	-0.00842	-0.07089	0.00541	-0.17021	0.00541	0.52682	0.98205	0.52679						
24	-0.01580	-0.00842	-0.07090	0.00332	0.06910	-0.01175	0.06909	0.00332	-0.07089	-0.00842	-0.01579	0.01446	-0.23604	0.00619	0.53224
	0.00618	-0.23603	0.01446	0.52682	0.00541	-0.17021	0.00541	0.52679	0.98205						

CORONENE | IRM AUGMENTED DENSITY | BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24						
1	0.80339	0.56378	-0.08714	-0.17092	0.03340	0.14174	-0.00815	-0.12260	0.00517	0.05292	-0.00613	-0.06619	-0.00815	0.09492	0.01542
	-0.17093	-0.06517	0.36759	-0.05128	-0.25051	0.00837	0.07395	0.00655	-0.00925						
2	0.56378	0.80341	0.36758	-0.06517	-0.17092	0.01542	0.09492	-0.00815	-0.06620	-0.00613	0.05293	0.00517	-0.12262	-0.00814	0.14176
	0.03340	-0.17093	-0.08714	-0.25052	-0.05129	-0.00924	0.00656	0.07395	0.00836						
3	-0.08714	0.36758	0.71537	0.36760	-0.08714	-0.20241	0.01542	0.14174	-0.00308	-0.06619	0.00517	0.07908	0.00518	-0.06619	-0.00309
	0.14176	0.01542	-0.20241	-0.03750	0.37023	-0.03750	-0.06987	0.00201	-0.06989						
4	-0.17092	-0.06517	0.36760	0.80340	0.56376	-0.08714	-0.17092	0.03340	0.14175	-0.00815	-0.12262	0.00518	0.05292	-0.00614	-0.06619
	-0.00814	0.09492	0.01541	-0.00927	-0.05128	-0.25052	0.00837	0.07396	0.00655						
5	0.03340	-0.17092	-0.08714	0.56376	0.80340	0.36760	-0.06517	-0.17092	0.01541	0.09492	-0.00814	-0.06619	-0.00614	0.05292	0.00518
	-0.12262	-0.00815	0.14175	0.00837	-0.25052	-0.05128	-0.00927	0.00655	0.07396						
6	0.14174	0.01542	-0.20241	-0.08714	0.36760	0.71537	0.36758	-0.08714	-0.20241	0.01542	0.14176	-0.00308	-0.06619	0.00518	0.07908
	0.00517	-0.06619	-0.00308	-0.06987	-0.03750	0.37023	-0.03750	-0.06989	0.00201						
7	-0.00815	0.09492	0.01542	-0.17092	-0.06517	0.36758	0.80341	0.56378	-0.08714	-0.17093	0.03340	0.14176	-0.00814	-0.12262	0.00517
	0.05293	-0.00613	-0.06620	0.00656	-0.00924	-0.05129	-0.25052	0.00836	0.07395						
8	-0.12260	-0.00815	0.14174	0.03340	-0.17092	-0.08714	0.56378	0.80339	0.36759	-0.06517	-0.17093	0.01542	0.09492	-0.00815	-0.06619
	-0.00613	0.05292	0.00517	0.07395	0.00837	-0.25051	-0.05128	-0.00925	0.00655						
9	0.00517	-0.06620	-0.00308	0.14175	0.01541	-0.20241	-0.08714	0.36759	0.71537	0.36759	-0.08714	-0.20241	0.01541	0.14175	-0.00308
	-0.06620	0.00517	0.07909	0.00200	-0.06988	-0.03749	0.37022	-0.03749	-0.06988						
10	0.05292	-0.00613	-0.06619	-0.00815	0.09492	0.01542	-0.17093	-0.06517	0.36759	0.80339	0.56378	-0.08714	-0.17092	0.03340	0.14174
	-0.00815	-0.12260	0.00517	0.07395	0.00655	-0.00925	-0.05128	-0.25051	0.00837						
11	-0.00613	0.05293	0.00517	-0.12262	-0.00814	0.14176	0.03340	-0.17093	-0.08714	0.56378	0.80341	0.36758	-0.06517	-0.17092	0.01542
	0.09492	-0.00815	-0.06620	0.00656	0.07395	0.00836	-0.25052	-0.05129	-0.00924						
12	-0.06619	0.00517	0.07908	0.00518	-0.06619	-0.00308	0.14176	0.01542	-0.20241	-0.08714	0.36758	0.71537	0.36760	-0.08714	-0.20241
	0.01542	0.14174	-0.00308	-0.06987	0.00201	-0.06989	-0.03750	0.37023	-0.03750						
13	-0.00815	-0.12262	0.00518	0.05292	-0.00614	-0.06619	-0.00814	0.09492	0.01541	-0.17092	-0.06517	0.36760	0.80340	0.56376	-0.08714
	-0.17092	0.03340	0.14175	0.00837	0.07396	0.00655	-0.00927	-0.05128	-0.25052						
14	0.09492	-0.00814	-0.06619	-0.00614	0.05292	0.00518	-0.12262	-0.00815	0.14175	0.03340	-0.17092	-0.08714	0.56376	0.80340	0.36760
	-0.06517	-0.17092	0.01541	-0.00927	0.00655	0.07396	0.00837	-0.25052	-0.05128						
15	0.01542	0.14176	-0.00309	-0.06619	0.00518	0.07908	0.00517	-0.06619	-0.00308	0.14174	0.01542	-0.20241	-0.08714	0.36760	0.71537
	0.36758	-0.08714	-0.20241	-0.03750	-0.06989	0.00201	-0.06987	-0.03750	0.37023						
16	-0.17093	0.03340	0.14176	-0.00814	-0.12262	0.00517	0.05293	-0.00613	-0.06620	-0.00815	0.09492	0.01542	-0.17092	-0.06517	0.36758
	0.80341	0.56378	-0.08714	-0.25052	0.00836	0.07395	0.00656	-0.00924	-0.05129						
17	-0.06517	-0.17093	0.01542	0.09492	-0.00815	-0.06619	-0.00613	0.05292	0.00517	-0.12260	-0.00815	0.14174	0.03340	-0.17092	-0.08714
	0.56378	0.80339	0.36759	-0.05128	-0.00925	0.00655	0.07395	0.00837	-0.25051						
18	0.36759	-0.08714	-0.20241	0.01541	0.14175	-0.00308	-0.06620	0.00517	0.07909	0.00517	-0.06620	-0.00308	0.14175	0.01541	-0.20241
	-0.08714	0.36759	0.71537	0.37022	-0.03749	-0.06988	0.00200	-0.06988	-0.03749						
19	-0.05128	-0.25052	-0.03750	-0.00927	0.00837	-0.06987	0.00656	0.07395	0.00200	0.07395	0.00656	-0.06987	0.00837	-0.00927	-0.03750
	-0.25052	-0.05128	0.37022	0.73238	0.36176	-0.05113	-0.18237	-0.05113	0.36176						
20	-0.25051	-0.05129	0.37023	-0.05128	-0.25052	-0.03750	-0.00924	0.00837	-0.06988	0.00655	0.07395	0.00201	0.07396	0.00655	-0.06989
	0.00836	-0.00925	-0.03749	0.36176	0.73237	0.36173	-0.05113	-0.18236	-0.05113						
21	0.00837	-0.00924	-0.03750	-0.25052	-0.05128	0.37023	-0.05129	-0.25051	-0.03749	-0.00925	0.00836	-0.06989	0.00655	0.07396	0.00201
	0.07395	0.00655	-0.06988	-0.05113	0.36173	0.73237	0.36176	-0.05113	-0.18236						
22	0.07395	0.00656	-0.06987	0.00837	-0.00927	-0.03750	-0.25052	-0.05128	0.37022	-0.05128	-0.25052	-0.03750	-0.00927	0.00837	-0.06987
	0.00656	0.07395	0.00200	-0.18237	-0.05113	0.36176	0.73238	0.36176	-0.05113						
23	0.00655	0.07395	0.00201	0.07396	0.00655	-0.06989	0.00836	-0.00925	-0.03749	-0.25051	-0.05129	0.37023	-0.05128	-0.25052	-0.03750
	-0.00924	0.00837	-0.06988	-0.05113	-0.18236	-0.05113	0.36176	0.73237	0.36173						
24	-0.00925	0.00836	-0.06989	0.00655	0.07396	0.00201	0.07395	0.00655	-0.06988	0.00837	-0.00924	-0.03750	-0.25052	-0.05128	0.37023
	-0.05129	-0.25051	-0.03749	0.36176	-0.05113	-0.18236	-0.05113	0.36173	0.73237						

ENERGIES FOR CORONENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	12,13	11,14	6,14	10,16	9,15	10,17	5,13	4,14	8,15	7,16
XMOMNT	1.02393	1.02392	0.02702	0.44300	0.44303	0.21858	-0.03115	0.03114	-0.17125	-0.50195
YMOMNT	-0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000	-0.00000	-0.00000
JUMP E	21.1668	21.1703	37.3985	38.4106	38.4107	39.3923	39.5705	39.5726	40.9786	41.8702
DIAG E	31.7318	31.7348	51.7430	50.4395	50.4393	57.0512	55.0276	55.0300	55.6492	53.5631
DIAG E	32.4791	32.4822	53.5421	50.3002	50.2998	63.5179	56.5159	56.5183	51.3473	53.8795
CORRSP	25.5690	35.5533	49.4772	47.2225	55.5473	59.3369	56.1915	57.8786	55.2067	50.4263
CORRSP	26.4085	35.9983	52.0290	55.6828	47.1584	64.9301	57.5124	58.3282	50.0925	52.7419

FINAL EXCITED STATES OF SA SYMMETRY

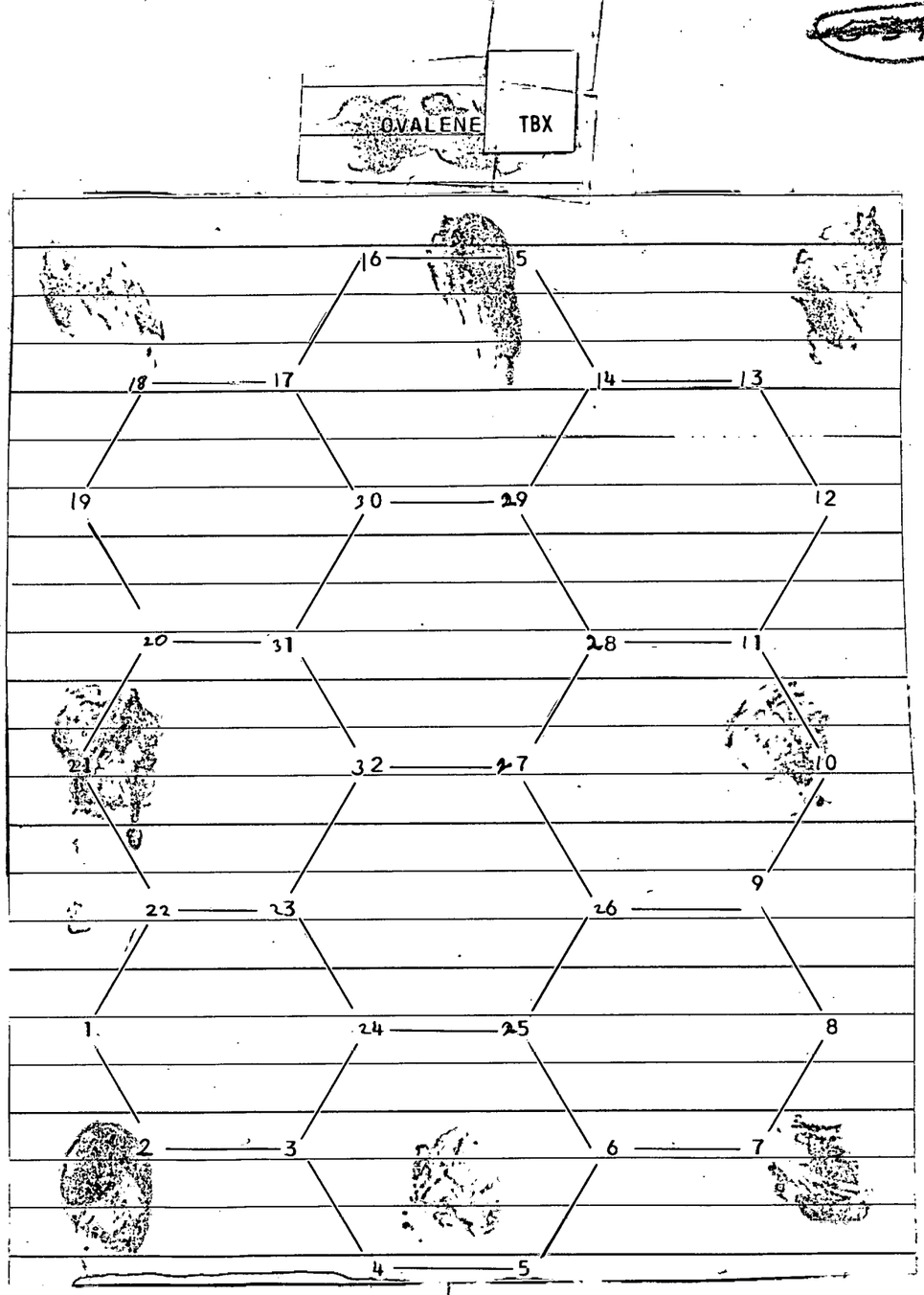
ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
25.56898	0.00000	0.00023	-0.00000	//	0.7034	-0.7032	-0.0000	-0.0597	0.0597	-0.0001	-0.0430	-0.0430	-0.0000	-0.0001
25.34907				//	0.7010	-0.7018	-0.0001	-0.0592	0.0591	-0.0002	-0.0671	-0.0670	0.0001	-0.0001
35.55334	2.12896	1.18664	-0.00001	//	0.6699	0.6701	-0.0513	-0.2110	-0.2110	0.0534	-0.0158	0.0158	-0.0725	0.0440
22.48427				//	0.6855	0.6847	0.0729	0.0455	0.0456	0.1465	0.0006	-0.0007	-0.1396	-0.1043
49.47715	0.00318	0.03887	0.00000	//	0.0203	0.0202	0.6710	0.0707	0.0706	0.4286	0.3274	-0.3272	-0.1240	0.3543
38.37292				//	-0.1034	-0.1035	0.5294	0.4575	0.4577	0.3082	0.2321	-0.2320	-0.2302	0.1545
47.22248	0.00000	0.00006	0.00000	//	0.0536	-0.0536	-0.0000	0.6988	-0.6988	0.0002	-0.0940	-0.0937	0.0001	-0.0002
47.13268				//	0.0429	-0.0430	-0.0001	0.6903	-0.6856	-0.0009	-0.1600	-0.1556	0.0015	-0.0021
55.54727	2.41414	1.01094	-0.00000	//	0.1529	0.1530	0.0073	0.5310	0.5311	-0.0965	0.0000	-0.0010	-0.5308	-0.3132
47.27579				//	-0.0027	-0.0020	-0.0493	0.4411	0.4485	-0.2291	-0.4053	0.4063	0.2793	-0.3769
59.33686	0.03312	0.11456	0.00000	//	-0.0503	-0.0503	-0.3915	0.0425	0.0428	0.8463	-0.2208	0.2209	-0.1416	0.0649
59.19880				//	-0.0665	-0.0665	-0.4109	0.0342	0.0346	0.8170	-0.2547	0.2546	-0.0833	0.1258
56.19155	0.00000	0.00075	0.00000	//	0.0505	-0.0503	0.0001	0.0904	-0.0898	-0.0001	0.6994	0.6997	-0.0004	-0.0005
52.01252				//	0.0786	-0.0783	0.0008	0.1524	-0.1525	0.0001	0.6853	0.6867	0.0011	0.0008
57.87864	0.44612	-0.42574	0.00000	//	-0.0734	-0.0734	0.2360	-0.1200	-0.1201	-0.2300	-0.4189	0.4188	-0.5209	0.4792
50.35617				//	-0.0679	-0.0678	0.6643	-0.2939	-0.2933	0.3022	-0.2017	0.2008	0.1290	-0.4338
55.20667	0.19749	0.29004	-0.00000	//	0.1371	0.1370	0.0216	0.3878	0.3877	-0.0611	-0.2139	0.2140	0.5914	0.4651
56.93088				//	0.0306	-0.0306	-0.1628	0.0534	0.0535	0.2675	0.3724	-0.3723	0.7373	-0.2711
50.42627	0.23796	-0.33312	0.00000	//	-0.0247	-0.0248	-0.5810	0.0440	0.0437	-0.1769	0.3503	-0.3500	-0.2377	0.5695
53.06287				//	0.0999	0.1000	0.2746	-0.0212	-0.0208	-0.0241	-0.1948	0.1925	0.5314	0.7387

ENERGIES FOR CORONENE ,TRM APPROXIMATION 5.8
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	11,13	12,14	6,13	10,15	9,16	9,17	4,13	5,14	8,16	7,15
XMOMNT	0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000
YMOMNT	1.02398	-1.02388	-0.02700	-0.44284	0.44312	-0.21822	0.03116	0.03116	0.17117	-0.50209
JUMP E	21.1683	21.1688	37.3965	38.4095	38.4118	39.3935	39.5706	39.5724	40.9797	41.8691
DIAG E	32.7412	32.7415	51.7405	51.8075	51.8101	57.0515	55.4410	55.4430	55.6502	53.5620
DIAG E	33.4885	33.4888	53.5396	51.6681	51.6707	63.5182	56.9292	56.9313	51.3485	53.8783
CORRSP	27.7245	35.5534	49.4755	49.9713	55.5468	59.3367	56.8689	57.8790	55.2066	50.4256
CORRSP	28.5582	35.9984	52.0275	49.8272	55.6824	64.9304	58.2755	58.3279	50.0923	52.7413

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
27.72448	0.00000	0.00000	0.00013	//	0.7053	0.7052	0.0000	0.0287	0.0287	-0.0000	0.0426	-0.0426	0.0001	0.0000
22.48457				//	0.6842	-0.6860	-0.0729	-0.0458	0.0455	-0.1465	-0.0006	-0.0006	0.1396	-0.1043
35.55339	2.12924	-0.00001	-1.18672	//	-0.6700	0.6700	-0.0514	-0.2110	0.2109	0.0536	-0.0158	-0.0158	-0.0725	-0.0441
21.22773				//	0.6872	0.6855	-0.0001	0.1671	0.1672	-0.0002	-0.0315	0.0315	0.0003	-0.0001
49.47554	0.00323	-0.00000	-0.03917	//	-0.0203	0.0203	0.6715	0.0715	-0.0705	0.4285	0.3271	0.3270	-0.1239	-0.3541
38.37103				//	0.1035	-0.1034	0.5295	0.4578	-0.4578	0.3078	0.2320	0.2319	-0.2301	-0.1544
49.97128	0.00000	0.00000	0.00015	//	-0.0308	-0.0308	-0.0009	0.7057	0.7055	-0.0002	0.0345	-0.0346	-0.0002	-0.0001
41.57003				//	-0.1700	-0.1699	-0.0001	0.6691	0.6689	0.0002	-0.1535	0.1533	0.0001	0.0001
55.54681	2.41162	0.00000	1.01042	//	0.1527	-0.1527	-0.0071	-0.5302	0.5305	0.0969	-0.0012	-0.0006	0.5316	-0.3141
47.27682				//	-0.0023	0.0024	0.0495	-0.4444	0.4448	0.2295	0.4061	0.4056	-0.2793	-0.3770
59.33673	0.03312	-0.00000	-0.11456	//	0.0503	-0.0503	-0.3914	0.0428	-0.0432	0.8463	-0.2207	-0.2208	-0.1417	-0.0648
59.19849				//	0.0665	-0.0665	-0.4109	0.0346	-0.0349	0.8171	-0.2545	-0.2545	-0.0833	-0.1257
56.86886	0.00000	-0.00000	0.00031	//	-0.0411	-0.0411	0.0001	-0.0363	-0.0363	-0.0001	0.7047	-0.7053	0.0006	-0.0004
51.44258				//	-0.0063	-0.0066	0.0002	0.1564	0.1565	0.0001	0.6893	-0.6898	-0.0005	0.0009
57.87901	0.44598	-0.00000	-0.42567	//	-0.0734	0.0734	-0.2358	0.1200	-0.1201	0.2299	0.4190	0.4187	0.5211	0.4790
50.35535				//	-0.0679	0.0679	-0.6642	0.2937	-0.2934	-0.3024	0.2017	0.2009	-0.1289	-0.4338
55.20658	0.19943	-0.00000	-0.29146	//	-0.1373	0.1372	0.0215	0.3885	-0.3885	-0.0616	-0.2146	-0.2138	0.5905	-0.4645
56.93173				//	-0.0307	0.0306	-0.1627	0.0534	-0.0535	0.2674	0.3726	0.3721	0.7374	0.2710
50.42564	0.23793	-0.00000	-0.33310	//	-0.0247	0.0247	0.5806	-0.0435	0.0444	0.1766	-0.3504	-0.3503	0.2376	0.5698
53.06247				//	0.1000	-0.0999	-0.2747	0.0209	-0.0212	0.0241	0.1933	0.1904	-0.5313	0.7387



ATOMIC COORDINATES

x	0.0036	0.5044	1.5231	2.0446	3.0418	3.5633	4.5820	5.0828	4.5936	5.0864	4.5936	5.0828	4.5820	3.5633
	3.0418	2.0446	1.5231	0.5044	0.0036	0.4928	0.	0.4928	1.5231	2.0360	3.0504	3.5633	3.0569	3.5633
	3.0504	2.0360	1.5231	2.0295										
y	1.7450	0.9090	0.8680	0.	0.	0.8680	0.9090	1.7450	2.6560	3.5310	4.4060	5.3170	6.1530	6.1940
	7.0620	7.0620	6.1940	6.1530	5.3170	4.4060	3.5310	2.6560	2.6380	1.7450	1.7450	2.6380	3.5310	4.4240
	5.3170	5.3170	4.4240	3.5310										

OVALENE X TBX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS —

1 SS	2 SA	3 AS	4 SS	5 AA	6 SS	7 AS	8 SA	9 SA	10 AS	11 AA	12 SS	13 SS	14 AA	15 SA	16 AS
1.642859	1.578858	1.545065	1.477259	1.466216	1.407537	1.360218	1.358882	1.320146	1.268159	1.262143	1.241344	1.212274	1.189339	1.146825	1.089442
0.103137	0.110938	-0.186986	0.001951	-0.231084	0.230794	-0.086932	0.152309	0.282063	-0.204707	-0.098457	0.023522	0.210580	0.267370	-0.018808	0.238265
0.100582	0.154204	-0.142442	0.126270	-0.245010	0.148285	-0.259743	0.012847	0.244615	-0.113059	0.145678	0.035030	0.284263	0.186259	-0.223334	0.139210
0.159734	0.255436	-0.121655	0.253482	-0.229479	-0.000012	-0.300351	-0.149632	0.018892	0.098782	0.271374	0.009736	0.022060	-0.147397	-0.118215	-0.211853
0.097029	0.185216	-0.036735	0.265401	-0.076938	-0.000018	-0.118235	-0.324556	0.063105	0.045816	0.127351	-0.329798	-0.146221	-0.080675	0.278801	-0.150237
0.097029	0.185217	0.036734	0.265400	0.076940	-0.000017	0.118242	-0.324553	0.063105	-0.045817	-0.127353	-0.329797	-0.146221	0.080675	0.278802	0.150238
0.159734	0.255437	0.121653	0.253480	0.229481	-0.000012	0.300355	-0.149626	0.018891	-0.098782	-0.271374	0.009738	0.022060	0.147397	-0.118215	0.211852
0.100582	0.154205	0.142441	0.126267	0.245819	0.148285	0.259744	0.012853	0.244614	0.113058	-0.145677	0.035031	0.284263	-0.186259	-0.223334	-0.139211
0.103138	0.110939	0.186985	0.001949	0.231084	0.230794	0.086930	0.152311	0.282063	0.204706	0.098458	0.023521	0.210580	-0.267370	-0.018808	-0.238266
0.175476	0.104669	0.283729	-0.141090	0.190410	0.242493	-0.161144	0.225229	0.115250	0.111039	0.280815	-0.015351	-0.130559	-0.008129	0.244649	0.066482
0.133405	0.000001	0.254406	-0.144481	-0.000001	0.290805	-0.218632	-0.000003	0.000000	0.202370	-0.000001	-0.031085	-0.300595	0.000001	-0.000000	0.363263
0.175475	-0.104668	0.283730	-0.141088	-0.190412	0.242492	-0.161140	-0.225232	-0.115250	0.111036	-0.280816	-0.015349	-0.130558	0.008129	-0.244649	0.066482
0.103137	-0.110938	0.186985	0.001951	-0.231084	0.230794	0.086933	-0.152309	-0.282063	0.204705	-0.098460	0.023521	0.210581	0.267369	0.018809	-0.238266
0.100582	-0.154205	0.142442	0.126270	-0.245818	0.148284	0.259743	-0.012847	-0.244614	0.113060	0.145677	0.035030	0.284263	0.186258	0.223335	-0.139211
0.159733	-0.255436	0.121655	0.253483	-0.229479	-0.000012	0.300351	0.149632	-0.018892	-0.098778	0.271375	0.009736	0.022059	-0.147397	0.118215	0.211853
0.097029	-0.185216	0.036735	0.265401	-0.076938	-0.000017	0.118235	0.324555	-0.063105	-0.045816	0.127351	-0.329798	-0.146221	-0.080675	-0.278802	0.150238
0.097029	-0.185217	-0.036734	0.265401	0.076940	-0.000017	-0.118242	0.324553	-0.063105	0.045815	-0.127354	-0.329797	-0.146221	0.080675	-0.278802	-0.150238
0.159733	-0.255437	-0.121654	0.253480	0.229481	-0.000011	-0.300354	0.149626	-0.018891	0.098778	-0.271375	0.009737	0.022060	0.147397	0.118215	-0.211853
0.100582	-0.154205	-0.142441	0.126267	0.245819	0.148285	-0.259743	-0.012852	-0.244614	-0.113061	-0.145676	0.035031	0.284263	-0.186260	0.223335	0.139210
0.103137	-0.110939	-0.186985	0.001949	0.231084	0.230794	-0.086930	-0.152311	-0.282063	-0.204706	0.098460	0.023522	0.210580	-0.267370	0.018808	0.238266
0.175475	-0.104669	-0.283729	-0.141090	0.190410	0.242492	0.161144	-0.225229	-0.115251	-0.111035	0.280816	-0.015351	-0.130558	-0.008128	-0.244649	-0.066482
0.133405	-0.000001	-0.254406	-0.144481	-0.000001	0.290805	0.218632	0.000002	-0.000001	-0.202369	0.000001	-0.031084	-0.300596	-0.000000	-0.000000	-0.363263
0.175475	0.104667	-0.283730	-0.141088	-0.190412	0.242492	0.161140	0.225232	0.115250	-0.111038	-0.280815	-0.015349	-0.130559	0.008129	0.244649	-0.066482
0.246915	0.153771	-0.217225	-0.141374	-0.157348	-0.107976	0.106305	0.200882	-0.119040	0.288631	-0.222857	-0.006381	-0.009659	-0.258402	0.175031	0.124325
0.234835	0.282415	-0.100672	0.116198	-0.128755	-0.147048	-0.078392	0.088488	-0.280734	0.177369	0.026443	0.307564	-0.114807	-0.220790	-0.132565	-0.066330
0.234435	0.282416	0.100670	0.116196	0.128756	-0.147048	0.078389	0.088490	-0.280734	-0.177367	-0.026441	0.307565	-0.114807	0.220791	-0.132564	0.066330
0.246916	0.153773	0.217224	-0.141375	0.157346	-0.107976	-0.106310	0.200879	-0.119040	-0.288631	0.222857	-0.006382	-0.009659	0.258402	0.175031	-0.124325
0.278207	0.000000	0.129711	-0.266570	-0.000001	-0.284174	-0.083314	-0.000001	0.000000	-0.267890	0.000000	-0.296656	0.234454	-0.000001	-0.000000	-0.179669
0.246915	-0.153772	0.217225	-0.141374	-0.157348	-0.107976	-0.106305	-0.200881	0.119041	-0.288633	-0.222854	-0.006380	-0.009660	-0.258402	-0.175031	-0.124324
0.234435	-0.282415	0.100671	0.116198	-0.128755	-0.147048	0.078392	-0.088488	0.280734	-0.177366	0.026445	0.307565	-0.114808	-0.220791	0.132564	0.066331
0.234434	-0.282416	-0.100670	0.116196	0.128756	-0.147048	-0.078389	-0.088489	0.280734	0.177368	-0.026443	0.307564	-0.114807	0.220791	0.132565	-0.066331
0.246915	-0.153773	-0.217224	-0.141375	0.157347	-0.107976	0.106310	-0.200879	0.119040	0.288633	0.222854	-0.006383	-0.009658	0.258403	-0.175031	0.124324
0.278206	-0.000001	-0.129711	-0.266570	-0.000001	-0.284173	0.083314	0.000001	0.000000	0.267889	-0.000003	-0.296657	0.234455	-0.000000	0.000000	0.179669

(527
334-340
Cont.

298

S AND EIGNVECTORS — TBX APPROXIMATION (cont.) — OVERLAP EIGNVALUES AND EIGNVECTORS — OVALENE TBX

17 BS	18 AA	19 SA	20 AS	21 AS	22 SA	23 SS	24 AA	25 AA	26 SS	27 AS	28 SA	29 AS	30 SS	31 AA	32 AS
0.910554	0.853171	0.810657	0.787725	0.758652	0.737854	0.731837	0.679851	0.641115	0.639779	0.592460	0.533781	0.522738	0.454932	0.421139	0.357137
-0.238266	-0.018809	-0.267370	0.210580	-0.023521	0.098458	-0.204706	0.282063	-0.152310	0.086933	-0.230794	0.231084	0.001950	0.186985	0.110938	-0.103137
0.139210	0.223335	0.186259	-0.284263	0.035029	0.145678	0.113059	-0.244614	0.012847	-0.259743	0.148285	-0.245818	-0.126269	-0.142441	-0.154205	0.100582
0.211853	-0.118215	0.147397	0.022060	-0.009737	-0.271374	0.098781	0.018892	0.149633	0.300351	-0.000011	-0.229480	0.253482	0.121654	0.255437	-0.159733
-0.150237	-0.278802	-0.080675	0.146222	-0.329797	0.127352	-0.045817	-0.063105	-0.324555	-0.118235	-0.000017	0.076939	-0.265401	-0.036735	-0.185216	0.097029
-0.150238	0.278802	-0.080675	-0.146222	0.329797	0.127352	-0.045816	0.063105	0.324553	-0.118242	0.000017	0.076939	0.265401	-0.036735	0.185216	-0.097029
0.211853	0.118215	0.147397	-0.022060	0.009736	-0.271374	0.098781	-0.018891	-0.149626	0.300355	-0.000012	-0.229480	-0.253481	0.121654	-0.255437	0.159733
0.139211	-0.223335	0.186259	0.284263	-0.035029	0.145678	0.113059	0.244614	-0.012853	-0.259743	-0.148285	0.245819	0.126268	-0.142441	0.154205	-0.100582
-0.238266	0.018809	-0.267370	-0.210580	0.023521	0.098458	-0.204706	-0.282063	0.152312	0.086930	0.230794	-0.231084	-0.001950	0.186985	-0.110938	0.103137
-0.066482	0.244649	0.008129	-0.130558	0.015349	-0.280815	0.111038	0.115250	-0.225229	0.161144	-0.242492	0.190411	-0.141089	-0.283730	0.104668	-0.175475
0.363263	-0.000000	-0.000000	0.300596	-0.031083	-0.000001	-0.202370	-0.000000	-0.000002	-0.218632	0.290805	0.000000	0.144480	0.254406	0.000000	0.133405
-0.066481	-0.244649	-0.008129	-0.130559	0.015350	0.280816	0.111036	-0.115250	0.225232	0.161140	-0.242493	-0.190411	-0.141088	-0.283730	-0.104668	-0.175475
-0.238266	-0.018809	0.267370	-0.210580	0.023521	-0.098459	-0.204706	0.282063	-0.152310	0.086933	0.230794	0.231084	-0.001950	0.186985	0.110938	0.103137
0.139210	0.223334	-0.186259	0.284263	-0.035029	-0.145677	-0.113060	-0.244614	0.012847	-0.259743	-0.148285	-0.245819	0.126269	-0.142441	-0.154205	-0.100582
0.211853	-0.118215	-0.147397	-0.022060	0.009737	0.271375	0.098779	0.018891	0.149632	0.300351	-0.000012	-0.229480	-0.253482	0.121654	0.255437	0.159733
-0.150237	-0.278802	0.080675	0.146222	0.329797	-0.127352	-0.045815	-0.063105	-0.324555	-0.118235	0.000017	0.076939	0.265401	-0.036735	-0.185216	-0.097029
-0.150238	0.278802	0.080675	0.146223	-0.329797	-0.127352	-0.045816	0.063105	0.324553	-0.118242	-0.000017	-0.076939	-0.265401	-0.036735	0.185216	0.097029
0.211852	0.118215	-0.147397	0.022060	-0.009737	0.271375	0.098779	-0.018891	-0.149626	0.300355	0.000012	0.229480	0.253481	0.121654	-0.255437	-0.159733
0.139211	-0.223334	-0.186259	-0.284264	0.035029	-0.145677	-0.113060	0.244614	-0.012853	-0.259743	0.148284	-0.245819	-0.126268	-0.142441	0.154205	0.100582
-0.238266	0.018808	0.267370	0.210580	-0.023521	-0.098459	-0.204706	-0.282063	-0.152311	0.086930	-0.230794	0.231084	0.001950	0.186985	-0.110938	-0.103137
-0.066482	0.244649	-0.008129	0.130559	-0.015350	0.280816	0.111036	0.115250	-0.225229	0.161144	0.242492	-0.190411	0.141089	-0.283730	0.104668	0.175475
0.363263	0.000000	-0.000000	-0.300596	0.031083	-0.000001	-0.202370	-0.000000	-0.000002	-0.218632	-0.290805	-0.000000	-0.144480	0.254406	0.000000	-0.133405
-0.066481	-0.244649	0.008129	0.130558	-0.015349	-0.280815	0.111038	-0.115250	0.225232	0.161139	0.242493	0.190411	0.141088	-0.283730	-0.104668	0.175475
-0.124324	0.175031	0.258402	-0.009659	0.006381	0.222856	0.288632	-0.119040	-0.200881	-0.106305	0.107976	-0.157347	-0.141374	0.217225	0.153773	-0.246915
-0.066331	0.132564	-0.220791	0.114806	0.307565	0.026442	-0.177367	0.280734	0.088487	-0.078392	-0.147048	0.128755	-0.116197	-0.100671	-0.282416	0.234435
-0.066331	-0.132565	-0.220791	-0.114806	-0.307565	0.026442	-0.177367	-0.280734	-0.088489	-0.078390	0.147048	0.128756	0.116197	-0.100671	0.282416	-0.234435
-0.124324	-0.175031	0.258402	0.009659	-0.006381	0.222856	0.288631	0.119040	0.200879	-0.106310	-0.107976	0.157347	0.141374	0.217225	-0.153773	0.246915
0.179669	0.000000	-0.000000	0.234454	0.296657	-0.000001	-0.267889	-0.000000	0.000001	0.083314	0.284173	-0.000000	-0.266570	-0.129711	-0.000000	-0.278207
-0.124325	0.175031	-0.258402	0.009659	-0.006382	-0.222854	-0.288633	-0.119040	0.200881	-0.106305	-0.107976	0.157347	0.141374	0.217225	0.153773	0.246915
-0.066331	0.132564	0.220791	-0.114806	-0.307565	-0.026443	-0.177367	0.280734	0.088487	-0.078392	0.147048	-0.128756	0.116197	-0.100671	-0.282416	-0.234435
-0.066330	-0.132564	0.220791	0.114806	0.307565	-0.026443	-0.177367	-0.280734	-0.088489	-0.078390	-0.147048	-0.128756	-0.116197	-0.100671	0.282416	0.234435
-0.124324	-0.175031	-0.258402	-0.009659	0.006381	-0.222854	0.288633	0.119040	-0.200879	-0.106310	0.107976	0.157347	-0.141375	0.217225	-0.153773	-0.246915
0.179669	0.000000	0.000000	-0.234454	-0.296657	-0.000001	-0.267090	-0.000000	0.000001	0.083314	-0.284173	0.000000	0.266570	-0.129711	0.000000	0.278207

(10)

OVALENE X TBX — TBX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 AS	4 SS	5 AA	6 SS	7 AS	8 SA	9 SA	10 AS	11 AA	12 SS	13 SS	14 AA	15 SA	16 AS
28.77052	26.95635	25.93782	23.75359	23.37874	21.28821	19.47101	19.41787	17.83027	15.54714	15.27078	14.29476	12.87430	11.70487	9.41314	6.03628
0.080467	0.088289	-0.150430	0.001605	-0.190841	0.194533	-0.074538	0.130658	0.245491	-0.181780	-0.087638	0.021112	0.191257	0.245165	-0.017563	0.228275
0.078473	0.122723	-0.114595	0.103889	-0.203009	0.124987	-0.222710	0.011021	0.212898	-0.100396	0.129670	0.031441	0.258179	0.170791	-0.208548	0.133373
0.124622	0.203288	-0.097872	0.208555	-0.189515	-0.000010	-0.257529	-0.128362	0.016442	0.087718	0.241554	0.008738	0.020035	-0.135156	-0.110389	-0.202970
0.075701	0.147403	-0.029554	0.218361	-0.063539	-0.000015	-0.101378	-0.278419	0.054923	0.040685	0.113357	-0.296007	-0.132804	-0.073975	0.260343	-0.143938
0.075701	0.147404	0.029553	0.218360	0.063541	-0.000015	0.101384	-0.278416	0.054922	-0.040686	-0.113359	-0.296006	-0.132804	0.073975	0.260343	0.143939
0.124622	0.203288	0.097870	0.208553	0.189517	-0.000010	0.257531	-0.128356	0.016441	-0.087718	-0.241554	0.008740	0.020036	0.135156	-0.110389	0.202970
0.078473	0.122724	0.114594	0.103887	0.203010	0.124988	0.222711	0.011026	0.212897	0.100396	-0.129670	0.031442	0.258179	-0.170791	-0.208549	-0.133374
0.080467	0.088290	0.150429	0.001603	0.190841	0.194534	0.074536	0.130660	0.245491	0.181779	0.087639	0.021111	0.191257	-0.245166	-0.017563	-0.228275
0.136904	0.083300	0.228261	-0.116083	0.157250	0.204394	-0.138169	0.193211	0.100307	0.098602	0.249957	-0.013778	-0.118578	-0.007454	0.228452	0.063694
0.104081	0.000000	0.204670	-0.118872	-0.000001	0.245116	-0.187460	-0.000002	0.000000	0.179704	-0.000001	-0.027900	-0.273012	0.000001	-0.000000	0.348032
0.136904	-0.083299	0.228261	-0.116081	-0.157252	0.204394	-0.138165	-0.193215	-0.100307	0.098600	-0.249959	-0.013776	-0.118578	0.007454	-0.228452	0.063694
0.080467	-0.088289	0.150430	0.001605	-0.190841	0.194533	0.074538	-0.130658	-0.245491	0.181778	-0.087641	0.021111	0.191258	0.245165	0.017564	-0.228276
0.078473	-0.122723	0.114595	0.103889	-0.203009	0.124987	0.222710	-0.011021	-0.212898	0.100397	0.129669	0.031440	0.258179	0.170790	0.208549	-0.133374
0.124622	-0.203288	0.097872	0.208555	-0.189515	-0.000010	0.257528	0.128361	-0.016442	-0.087715	0.241555	0.008739	0.020035	-0.135156	0.110388	0.202970
0.075701	-0.147403	0.029553	0.218361	-0.063539	-0.000015	0.101377	0.278418	-0.054923	-0.040684	0.113357	-0.296007	-0.132804	-0.073975	-0.260344	0.143938
0.075701	-0.147404	-0.029553	0.218360	0.063541	-0.000014	-0.101384	0.278416	-0.054922	0.040684	-0.113359	-0.296006	-0.132803	0.073976	0.260344	-0.143938
0.124622	-0.203288	-0.097870	0.208553	0.189517	-0.000009	-0.257531	0.128356	-0.016441	0.087715	-0.241555	0.008740	0.020036	0.135156	0.110389	-0.202970
0.078473	-0.122724	-0.114594	0.103887	0.203010	0.124988	-0.222710	-0.011025	-0.212897	-0.100398	-0.129669	0.031442	0.258178	-0.170791	0.208549	0.133374
0.080467	-0.088290	0.150429	0.001603	0.190841	0.194534	-0.074536	-0.130660	-0.245491	-0.181779	0.087640	0.021112	0.191257	-0.245166	0.017563	0.228276
0.136904	-0.083300	-0.228261	-0.116083	0.157250	0.204394	0.138169	-0.193212	-0.100307	-0.098599	0.249958	-0.013778	-0.118578	-0.007453	-0.228452	-0.063694
0.104081	-0.000001	-0.204670	-0.118873	-0.000001	0.245116	0.187461	0.000002	-0.000001	-0.179704	0.000001	-0.027899	-0.273013	-0.000000	-0.000000	-0.348032
0.136904	0.083299	-0.228261	-0.116081	-0.157252	0.204394	0.138165	0.193214	0.100307	-0.098602	-0.249957	-0.013776	-0.118579	0.007454	0.228452	-0.063694
0.192641	0.122378	-0.174758	-0.116316	-0.129946	-0.091012	0.091149	0.172325	-0.103606	0.256305	-0.198368	-0.005728	-0.008772	-0.236943	0.163443	0.119112
0.182903	0.224759	-0.080991	0.095602	-0.106332	-0.123945	-0.067215	0.075909	-0.244334	0.157503	0.023537	0.276051	-0.104272	-0.202454	-0.123788	-0.063549
0.182904	0.224759	0.080989	0.095601	0.106333	-0.123945	0.067213	0.075911	-0.244334	-0.157502	-0.023535	0.276052	-0.104272	0.202455	-0.123788	0.063549
0.192641	0.122380	0.174757	-0.116318	0.129944	-0.091012	-0.091153	0.172323	-0.103605	-0.256305	0.198368	-0.005728	-0.008773	0.236942	0.163443	-0.119112
0.217054	0.000000	-0.104353	-0.219323	-0.000001	-0.239527	-0.071435	-0.000001	0.000000	-0.237887	0.000000	-0.266261	0.212941	-0.000001	-0.000000	-0.172136
0.192641	-0.122379	0.174758	-0.116316	-0.129946	-0.091012	-0.091149	-0.172325	0.103606	-0.256307	-0.198365	-0.005726	-0.008773	-0.236943	-0.163443	-0.119111
0.182903	-0.224759	0.080990	-0.095603	-0.106332	-0.123945	-0.067215	-0.075909	0.244334	-0.157501	0.023539	0.276052	-0.104273	-0.202455	0.123788	-0.063550
0.182903	-0.224759	-0.080989	0.095601	-0.106333	-0.123945	-0.067213	-0.075910	0.244334	0.157503	-0.023537	0.276051	-0.104272	0.202455	0.123788	-0.063550
0.192640	-0.122380	-0.174757	-0.116318	0.129945	-0.091012	0.091153	-0.172323	0.103605	0.256307	0.198365	-0.005729	-0.008772	0.236943	-0.163443	0.119111
0.217054	-0.000001	-0.104353	-0.219323	-0.000001	-0.239526	0.071435	0.000001	0.000000	0.237885	-0.000002	-0.266262	0.212941	-0.000000	0.000000	0.172136

NVALUES AND EIGNVECTORS OVALENE — TBX APPROXIMATION (cont)

17 SS	18 AA	19 SA	20 AS	21 AS	22 SA	23 SS	24 AA	25 AA	26 SS
-7.22248	-12.65338	-17.17290	-19.81324	-23.39019	-26.12194	-26.94111	-34.62354	-41.15776	-41.39725
-0.249694	-0.020363	-0.296957	0.237263	0.027004	0.114621	-0.239290	0.342089	-0.190221	0.108685
0.145888	0.241790	0.206870	-0.320282	-0.040217	0.169593	0.132159	-0.296671	0.016045	-0.324735
0.222014	-0.127983	0.163708	0.024855	-0.011179	-0.315925	0.115469	0.022912	0.186878	0.375504
-0.157444	-0.301841	-0.089603	0.164750	-0.378639	0.148259	-0.053557	-0.076535	-0.405341	-0.147819
-0.157444	0.301841	-0.089603	-0.164750	0.378639	0.148259	-0.053557	0.076535	0.405338	-0.147828
0.222014	0.127984	0.163708	-0.024855	0.011178	-0.315925	0.115469	-0.022911	-0.186870	0.375508
0.145888	-0.241790	0.206870	0.320283	-0.040217	0.169593	0.132159	0.296671	-0.016052	-0.324735
-0.249695	0.020363	-0.296957	-0.237263	0.027004	0.114621	-0.239290	-0.342089	0.190224	0.108681
-0.069671	0.264865	0.009029	-0.147102	0.017622	-0.326915	0.129797	0.139777	-0.281291	0.201465
0.380687	-0.000000	-0.000000	0.338685	-0.035686	-0.000001	-0.236558	-0.000000	-0.000003	-0.273337
-0.069670	-0.264865	-0.009029	-0.147102	0.017623	0.326916	0.129795	-0.139777	0.281296	0.201459
-0.249694	-0.020363	0.296957	-0.237263	0.027004	-0.114623	-0.239289	0.342089	-0.190221	0.108685
0.145888	0.241790	-0.206871	0.320283	-0.040217	-0.169592	0.132160	-0.296671	0.016045	-0.324735
0.222014	-0.127984	-0.163708	-0.024855	0.011179	0.315925	0.115467	0.022912	0.186878	0.375504
-0.157444	-0.301840	0.089603	-0.164750	0.378640	-0.148259	-0.053556	-0.076535	-0.405341	-0.147819
-0.157444	0.301840	0.089603	0.164751	-0.378640	-0.148259	-0.053556	0.076535	0.405338	-0.147828
0.222014	0.127984	-0.163709	0.024855	-0.011178	0.315925	0.115467	-0.022911	-0.186870	0.375508
0.145888	-0.241790	-0.206870	-0.320283	0.040217	-0.169592	0.132160	0.296671	-0.016052	-0.324735
-0.249694	0.020363	0.296957	0.237263	-0.027004	-0.114623	-0.239289	-0.342089	0.190224	0.108681
-0.069671	0.264865	-0.009029	0.147102	-0.017623	-0.326916	0.129795	0.139777	-0.281291	0.201465
0.380687	0.000000	-0.000000	-0.338685	0.035687	-0.000001	-0.236558	-0.000000	-0.000003	-0.273337
-0.069670	-0.264865	0.009029	0.147102	-0.017623	-0.326915	0.129797	-0.139777	0.281296	0.201459
-0.130288	0.189495	0.286997	-0.010883	0.007326	0.259442	0.337393	-0.144373	-0.250883	-0.132905
-0.069513	0.143519	-0.245224	0.129353	0.353114	0.030783	-0.207332	0.340477	0.110513	-0.098007
-0.069512	-0.143519	-0.245223	-0.129353	-0.353114	0.030783	-0.207332	-0.340478	-0.110515	-0.098004
-0.130287	-0.189495	0.286997	0.010883	-0.007326	0.259442	0.337393	0.144374	0.250880	-0.132910
0.188287	0.000000	-0.000000	0.264161	0.340591	-0.000001	-0.313147	-0.000000	0.000001	0.104160
-0.130288	0.189495	-0.286997	0.010883	-0.007327	-0.259439	0.337395	-0.144373	-0.250883	-0.132905
-0.069512	0.143519	0.245224	-0.129353	-0.353114	-0.030784	-0.207332	0.340478	0.110513	-0.098007
-0.069512	-0.143519	0.245224	0.129353	0.353115	-0.030784	-0.207331	-0.340478	-0.110515	-0.098004
-0.130288	-0.189495	-0.286997	-0.010883	0.007326	-0.259439	-0.337395	0.144374	0.250880	-0.132910
0.188287	0.000000	0.000000	-0.264161	-0.340591	-0.000001	-0.313147	-0.000000	0.000001	0.104160

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

27 AS	28 SA	29 AS	30 SS	31 AA	32 AS
-50.57588	-64.21838	-67.12819	-88.09193	101.06052	132.34722
-0.299844	-0.316292	0.002697	0.277226	0.170950	-0.172583
0.192649	0.336460	-0.174644	-0.211185	-0.237621	0.168308
0.000015	-0.314096	0.350594	0.180366	0.393614	-0.267287
-0.000023	0.105309	-0.367079	-0.054463	-0.285408	0.162362
0.000023	0.105309	0.367079	-0.054463	0.285408	-0.162362
-0.000015	0.314097	-0.350594	0.180366	-0.393614	0.267287
0.192649	-0.336460	0.174644	-0.211185	0.237621	-0.168307
-0.299844	0.316292	0.002697	0.277226	-0.170950	-0.172583
0.315042	-0.260622	0.195142	-0.420660	0.161288	-0.293628
-0.377809	-0.000000	-0.199833	0.377185	0.000000	0.223231
0.315042	0.260622	0.195141	-0.420660	-0.161288	0.293628
0.140281	-0.215366	-0.195537	0.322059	0.236955	-0.413172
-0.191042	0.176232	-0.160714	-0.149256	-0.435188	0.392287
0.191042	0.176232	0.160714	-0.149256	0.435188	-0.392287
-0.140281	-0.215366	0.195537	0.322059	-0.236955	0.413172
0.369193	-0.000000	-0.368697	-0.192311	-0.000000	-0.465532
-0.140281	0.215367	0.195537	0.322059	0.236955	0.413172
0.191042	0.176232	0.160714	-0.149255	-0.435188	-0.392287
-0.191042	0.176232	-0.160714	-0.149256	0.435188	0.392287
0.140281	0.215366	-0.195537	0.322059	-0.236955	-0.413171
-0.369193	0.000000	0.368697	-0.192311	-0.000000	0.465532

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	31	32													
1	1.00000	0.79116	-0.00000	-0.17743	0.00000	0.13976	-0.00000	-0.10311	0.00000	0.06625	0.00000	-0.02646	0.00000	0.03496	0.00000
	-0.04679	-0.00000	0.05306	0.00000	-0.11155	-0.00000	0.47903	0.00000	-0.23343	-0.00000	0.03549	-0.00000	-0.05080	0.00000	0.02164
	-0.00000	0.01993													
2	0.79116	1.00000	0.49269	0.00000	-0.12915	0.00000	0.05496	-0.00000	-0.03708	-0.00000	0.02222	0.00000	-0.01431	0.00000	0.05036
	0.00000	-0.05523	-0.00000	0.05306	0.00000	-0.19296	0.00000	-0.21565	-0.00000	0.00083	0.00000	0.03376	-0.00000	-0.04414	0.00000
	0.11968	0.00000													
3	-0.00000	0.49269	1.00000	0.56177	-0.00000	-0.23073	0.00000	0.13976	-0.00000	-0.08900	0.00000	0.03496	0.00000	-0.04648	-0.00000
	0.04892	0.00000	-0.05523	-0.00000	0.09177	0.00000	-0.17790	0.00000	0.54652	-0.00000	-0.04155	0.00000	0.06820	0.00000	-0.00761
	-0.00000	-0.08338													
4	-0.17743	0.00000	0.56177	1.00000	0.72541	0.00000	-0.12915	-0.00000	0.10199	-0.00000	-0.07215	0.00000	0.05036	-0.00000	-0.04541
	-0.00000	0.04892	0.00000	-0.04679	0.00000	0.11520	-0.00000	-0.02189	-0.00000	-0.24858	0.00000	0.07922	0.00000	0.00011	0.00000
	-0.05846	-0.00000													
5	0.00000	-0.12915	-0.00000	0.72541	1.00000	0.56177	-0.00000	-0.17743	0.00000	0.11520	0.00000	-0.04679	-0.00000	0.04892	0.00000
	-0.04541	-0.00000	0.05036	0.00000	-0.07215	-0.00000	0.10199	0.00000	-0.24858	0.00000	-0.02189	-0.00000	-0.05846	0.00000	0.00011
	0.00000	0.07922													
6	0.13976	0.00000	-0.23073	0.00000	0.56177	1.00000	0.49269	0.00000	-0.17790	-0.00000	0.09177	-0.00000	-0.05523	0.00000	0.04892
	0.00000	-0.04648	-0.00000	0.03496	0.00000	-0.08900	-0.00000	-0.04155	0.00000	0.54652	0.00000	-0.08338	0.00000	-0.00761	0.00000
	0.06820	-0.00000													
7	-0.00000	0.05496	0.00000	-0.12915	-0.00000	0.49269	1.00000	0.79116	-0.00000	-0.19296	0.00000	0.05306	-0.00000	-0.05523	-0.00000
	0.05036	0.00000	-0.01431	-0.00000	0.02222	0.00000	-0.03708	0.00000	0.00083	-0.00000	-0.21565	0.00000	0.11968	0.00000	-0.04414
	0.00000	0.03376													
8	-0.10311	-0.00000	0.13976	-0.00000	-0.17743	0.00000	0.79116	1.00000	0.47903	0.00000	-0.11155	0.00000	0.05306	0.00000	-0.04679
	-0.00000	0.03496	0.00000	-0.02646	-0.00000	0.06625	0.00000	0.03549	-0.00000	-0.23343	0.00000	0.01993	-0.00000	0.02164	-0.00000
	-0.05080	0.00000													
9	0.00000	-0.03708	-0.00000	0.10199	0.00000	-0.17790	-0.00000	0.47903	1.00000	0.61614	-0.00000	-0.11155	0.00000	0.09177	-0.00000
	-0.07215	0.00000	0.02222	0.00000	-0.03215	0.00000	0.04641	-0.00000	-0.06377	0.00000	0.51556	-0.00000	-0.20797	0.00000	0.05860
	0.00000	-0.03415													
10	0.06625	-0.00000	-0.08900	-0.00000	0.11520	-0.00000	-0.19296	0.00000	0.61614	1.00000	0.61614	0.00000	-0.19296	-0.00000	0.11520
	0.00000	-0.08900	-0.00000	0.06625	0.00000	-0.14175	-0.00000	0.10027	0.00000	-0.01330	-0.00000	-0.27306	0.00000	-0.01330	-0.00000
	0.10027	-0.00000													
11	0.00000	0.02222	0.00000	-0.07215	0.00000	0.09177	0.00000	-0.11155	-0.00000	0.61614	1.00000	0.47903	0.00000	-0.17790	-0.00000
	0.10199	-0.00000	-0.03708	-0.00000	0.04641	0.00000	-0.03215	0.00000	0.05860	-0.00000	-0.20797	0.00000	0.51556	0.00000	-0.06377
	-0.00000	-0.03415													
12	-0.02646	0.00000	0.03496	0.00000	-0.04679	-0.00000	0.05306	0.00000	-0.11155	0.00000	0.47903	1.00000	0.79116	0.00000	-0.17743
	-0.00000	0.13976	0.00000	-0.10311	-0.00000	0.06625	0.00000	-0.05080	-0.00000	0.02164	0.00000	-0.01993	-0.00000	-0.23343	-0.00000
	0.03549	0.00000													
13	0.00000	-0.01431	0.00000	0.05036	-0.00000	-0.05523	-0.00000	0.05306	0.00000	-0.19296	0.00000	0.79116	1.00000	0.49269	0.00000
	-0.12915	-0.00000	0.05496	0.00000	-0.03708	-0.00000	0.02222	0.00000	-0.04414	0.00000	0.11968	0.00000	-0.21565	-0.00000	0.00083
	-0.00000	0.03376													
14	0.03496	0.00000	-0.04648	-0.00000	0.04892	0.00000	-0.05523	0.00000	0.09177	-0.00000	-0.17790	0.00000	0.49269	1.00000	0.56177
	0.00000	-0.23073	-0.00000	0.13976	-0.00000	-0.08900	0.00000	0.06820	0.00000	-0.00761	-0.00000	-0.08338	0.00000	0.54652	-0.00000
	-0.04155	-0.00000													
15	0.00000	0.05036	-0.00000	-0.04541	0.00000	0.04892	-0.00000	-0.04679	-0.00000	0.11520	-0.00000	-0.17743	0.00000	0.56177	1.00000
	0.72541	0.00000	-0.12915	-0.00000	0.10199	0.00000	-0.07215	0.00000	0.00011	0.00000	-0.05846	-0.00000	-0.02189	0.00000	-0.24858
	-0.00000	0.07922													
16	-0.04679	0.00000	0.04892	-0.00000	-0.04541	0.00000	0.05036	-0.00000	-0.07215	0.00000	0.10199	-0.00000	-0.12915	0.00000	0.72541
	1.00000	0.56177	0.00000	-0.17743	-0.00000	0.11520	-0.00000	-0.05846	0.00000	0.00011	0.00000	0.07922	-0.00000	-0.24858	0.00000
	-0.02189	0.00000													
17	-0.00000	-0.05523	0.00000	0.04892	-0.00000	-0.04648	0.00000	0.03496	0.00000	-0.08900	-0.00000	0.13976	-0.00000	-0.23073	0.00000
	0.56177	1.00000	0.49269	0.00000	-0.17790	0.00000	0.09177	-0.00000	-0.00761	0.00000	0.06820	-0.00000	-0.04155	0.00000	0.54652
	0.00000	-0.08338													
18	0.05306	-0.00000	-0.05523	0.00000	0.05036	-0.00000	-0.01431	0.00000	0.02222	-0.00000	-0.03708	0.00000	0.05496	-0.00000	-0.12915
	0.00000	0.49269	1.00000	0.79116	0.00000	-0.19296	0.00000	0.11968	-0.00000	-0.04414	0.00000	0.03376	0.00000	0.00083	-0.00000
	-0.21565	0.00000													

TBX TOPOLOGICAL BOND ORDERS (cont.)

19 0.00000 0.05306-0.00000-0.04679 0.00000 0.03496-0.00000-0.02646 0.00000 0.06625-0.00000-0.10311 0.00000 0.13976-0.00000
-0.17743 0.00000 0.79116 1.00000 0.47903-0.00000-0.11155-0.00000 0.02164-0.00000-0.05080 0.00000 0.03549-0.00000-0.23343
0.00000 0.01993
20-0.11155 0.00000 0.09177 0.00000-0.07215 0.00000 0.02222-0.00000-0.03215 0.00000 0.04641-0.00000-0.03708-0.00000 0.10199
-0.00000-0.17790 0.00000 0.47903 1.00000 0.61614-0.00000-0.20797-0.00000 0.05860-0.00000-0.03415-0.00000-0.06377 0.00000
0.51556 0.00000
21-0.00000-0.19296 0.00000 0.11520-0.00000-0.08900 0.00000 0.06625 0.00000-0.14175 0.00000 0.06625-0.00000-0.08900 0.00000
0.11520-0.00000-0.19296-0.00000 0.61614 1.00000 0.61614 0.00000-0.01330-0.00000 0.10027-0.00000 0.10027-0.00000-0.01330
-0.00000-0.27306
22 0.47903 0.00000-0.17790-0.00000 0.10199-0.00000-0.03708 0.00000 0.04641-0.00000-0.03215 0.00000 0.02222 0.00000-0.07215
-0.00000 0.09177 0.00000-0.11155-0.00000 0.61614 1.00000 0.51556 0.00000-0.06377-0.00000-0.03415 0.00000 0.05860-0.00000
-0.20797 0.00000
23 0.00000-0.21565 0.00000-0.02189 0.00000-0.04155 0.00000 0.03549-0.00000 0.10027 0.00000-0.05080 0.00000 0.06820 0.00000
-0.05846 0.00000 0.11968-0.00000-0.20797 0.00000 0.51556 1.00000 0.51161 0.00000-0.19379 0.00000-0.06423 0.00000-0.05975
0.00000 0.54677
24-0.23343-0.00000 0.54652-0.00000-0.24858 0.00000 0.00083-0.00000-0.06377 0.00000 0.05860-0.00000-0.04414 0.00000 0.00011
0.00000-0.00761 0.00000 0.02164-0.00000-0.01330 0.00000 0.51161 1.00000 0.52734 0.00000-0.16850-0.00000 0.05555 0.00000
-0.05975 0.00000
25 0.00000 0.00083-0.00000-0.24858 0.00000 0.54652-0.00000-0.23343 0.00000-0.01330-0.00000 0.02164 0.00000-0.00761 0.00000
0.00011-0.00000-0.04414-0.00000 0.05860-0.00000-0.06377 0.00000 0.52734 1.00000 0.51161 0.00000-0.05975 0.00000 0.05555
-0.00000-0.16850
26 0.03549 0.00000-0.04155 0.00000-0.02189 0.00000-0.21565 0.00000 0.51556-0.00000-0.20797 0.00000 0.11968-0.00000-0.05846
0.00000 0.06820 0.00000-0.05080-0.00000 0.10027-0.00000-0.19379 0.00000 0.51161 1.00000 0.54677 0.00000-0.05975-0.00000
-0.06423 0.00000
27-0.00000 0.03376 0.00000 0.07922-0.00000-0.08338 0.00000 0.01993-0.00000-0.27306 0.00000 0.01993 0.00000-0.08338-0.00000
0.07922-0.00000 0.03376 0.00000-0.03415-0.00000-0.03415 0.00000-0.16850 0.00000 0.54677 1.00000 0.54677 0.00000-0.16850
0.00000 0.48875
28-0.05080-0.00000 0.06820 0.00000-0.05846 0.00000 0.11968-0.00000-0.20797 0.00000 0.51556-0.00000-0.21565 0.00000-0.02189
-0.00000-0.04155 0.00000 0.03549-0.00000 0.10027 0.00000-0.06423-0.00000-0.05975 0.00000 0.54677 1.00000 0.51161 0.00000
-0.19379 0.00000
29 0.00000-0.04414 0.00000 0.00011-0.00000-0.00761 0.00000 0.02164 0.00000-0.01330 0.00000-0.23343-0.00000 0.54652 0.00000
-0.24858 0.00000 0.00083-0.00000-0.06377 0.00000 0.05860 0.00000 0.05555 0.00000-0.05975 0.00000 0.51161 1.00000 0.52734
0.00000-0.16850
30-0.02164 0.00000-0.00761 0.00000 0.00011 0.00000-0.04414-0.00000 0.05860-0.00000-0.06377-0.00000 0.00083-0.00000-0.24858
0.00000 0.54652-0.00000-0.23343 0.00000-0.01330-0.00000-0.05975 0.00000 0.05555-0.00000-0.16850 0.00000 0.52734 1.00000
0.51161 0.00000
31-0.00000 0.11968-0.00000-0.05846 0.00000 0.06820 0.00000-0.05080 0.00000 0.10027-0.00000 0.03549-0.00000-0.04155-0.00000
-0.02189 0.00000-0.21565 0.00000 0.51556-0.00000-0.20797 0.00000-0.05975-0.00000-0.06423 0.00000-0.19379 0.00000 0.51161
1.00000 0.54677
32 0.01993 0.00000-0.08338-0.00000 0.07922-0.00000 0.03376 0.00000-0.03415-0.00000-0.03415 0.00000 0.03376-0.00000 0.07922
0.00000-0.08338 0.00000 0.01993 0.00000-0.27306-0.00000 0.54677 0.00000-0.16850 0.00000 0.48875 0.00000-0.16850 0.00000
0.54677 1.00000

OVALENE X | TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	31	32													
1	0.76866	0.60165	-0.04994	-0.16772	0.00907	0.13605	-0.00549	-0.10152	-0.00067	0.06606	0.00146	-0.02645	-0.00130	0.03489	0.00310
	-0.04613	-0.00599	0.05184	0.01007	-0.10382	-0.05380	0.32400	-0.02997	-0.21750	0.01190	0.03328	-0.00160	-0.05041	-0.00154	0.02030
	0.01359	0.02410													
2	0.60165	0.76403	0.33270	-0.04981	-0.12040	0.01508	0.05284	-0.00549	-0.03666	0.00353	0.02223	-0.00130	-0.01437	0.00171	-0.04978
	0.00066	-0.05436	-0.00076	0.05184	0.00625	-0.18316	-0.04636	-0.19988	-0.03442	0.00549	-0.00017	0.03158	-0.00250	-0.04313	-0.00353
	0.11625	0.01208													
3	-0.04994	0.33270	0.73417	0.39760	-0.04723	-0.21512	0.01508	0.13605	-0.00107	-0.08834	-0.00166	0.03489	0.00171	-0.04603	-0.00101
	0.04844	0.00301	-0.05436	-0.00599	0.08882	0.01819	-0.16326	-0.03358	0.38760	-0.03300	-0.03627	0.01101	0.06662	-0.00258	-0.00758
	-0.00058	-0.07801													
4	-0.16772	-0.04981	0.39760	0.76919	0.54565	-0.04723	-0.12040	0.00907	0.09862	-0.00679	-0.07084	0.00310	0.04978	-0.00101	-0.04507
	-0.00041	0.04844	0.00066	-0.04613	-0.00368	0.11252	0.01462	-0.01705	-0.03526	-0.23191	0.01293	0.07667	-0.00157	0.00030	0.00174
	-0.05794	-0.00036													
5	0.00907	-0.12040	-0.04723	0.54565	0.76919	0.39760	-0.04981	-0.16772	0.01462	0.11252	-0.00368	-0.04613	0.00066	0.04844	-0.00041
	-0.04507	-0.00101	0.04978	0.00310	-0.07084	-0.00679	0.09862	0.01293	-0.23191	-0.03526	-0.01705	-0.00036	-0.05794	0.00174	0.00030
	-0.00157	0.07667													
6	0.13605	0.01508	-0.21512	-0.04723	0.39760	0.73417	0.33270	-0.04994	-0.16326	0.01819	0.08882	-0.00599	-0.05436	0.00301	0.04844
	-0.00101	-0.04603	0.00171	0.03489	-0.00166	-0.08834	-0.00107	-0.03627	-0.03300	0.38760	-0.03358	-0.07801	-0.00058	-0.00758	-0.00258
	0.06662	0.01101													
7	-0.00549	0.05284	0.01508	-0.12040	-0.04981	0.33270	0.76403	0.60165	-0.04636	-0.18316	0.00625	0.05184	-0.00076	-0.05436	0.00066
	0.04978	0.00171	-0.01437	-0.00130	0.02223	0.00353	-0.03666	-0.00017	0.00549	-0.03442	-0.19988	0.01208	0.11626	-0.00353	-0.04313
	-0.00250	0.03158													
8	-0.10152	-0.00549	0.13605	0.00907	-0.16772	-0.04994	0.60165	0.76866	0.32400	-0.05380	-0.10382	0.01007	0.05184	-0.00599	-0.04613
	0.00310	0.03489	-0.00130	-0.02645	0.00146	0.06606	-0.00067	0.03328	0.01190	-0.21750	-0.02997	0.02410	0.01359	0.02030	-0.00154
	-0.05041	-0.00160													
9	-0.00067	-0.03666	-0.00107	0.09862	0.01462	-0.16326	-0.04636	0.32400	0.73400	0.44682	-0.04113	-0.10382	0.00625	0.08882	-0.00368
	-0.07084	-0.00166	0.02223	0.00146	-0.03197	-0.00320	0.04507	0.00990	-0.05855	-0.03036	0.36141	-0.03219	-0.19334	0.00992	0.05636
	0.00116	-0.02927													
10	0.06606	0.00353	-0.08834	-0.00679	0.11252	0.01819	-0.18316	-0.05380	0.44682	0.78162	0.44682	-0.05380	-0.18316	0.01819	0.11252
	-0.00679	-0.08834	0.00353	0.06606	-0.00320	-0.14018	-0.00320	0.09757	0.00054	-0.00831	-0.04107	-0.25733	-0.04107	-0.00831	0.00054
	0.09757	0.01430													
11	0.00146	0.02223	-0.00166	-0.07084	-0.00368	0.08882	0.00625	-0.10382	-0.04113	0.44682	0.73400	0.32400	-0.04636	-0.16326	0.01462
	0.09862	-0.00107	-0.03666	-0.00067	0.04507	-0.00320	-0.03197	0.00116	0.05636	0.00992	-0.19334	-0.03219	0.36141	-0.03036	-0.05855
	0.00990	-0.02927													
12	-0.02645	-0.00130	0.03489	0.00310	-0.04613	-0.00599	0.05184	0.01007	-0.10382	-0.05380	0.32400	0.76866	0.60165	-0.04994	-0.16772
	0.00907	0.13605	-0.00549	-0.10152	-0.00067	0.06606	0.00146	-0.05041	-0.00154	0.02030	0.01359	0.02410	-0.02997	-0.21750	0.01190
	0.03328	-0.00160													
13	-0.00130	-0.01437	0.00171	0.04978	0.00066	-0.05436	-0.00076	0.05184	0.00625	-0.18316	-0.04636	0.60165	0.76403	0.33270	-0.04981
	-0.12040	0.01508	0.05284	-0.00549	-0.03666	0.00353	0.02223	-0.00250	-0.04313	-0.00353	0.11626	0.01208	-0.19988	-0.03442	0.00549
	-0.00017	0.03158													
14	0.03489	0.00171	-0.04603	-0.00101	0.04844	0.00301	-0.05436	-0.00599	0.08882	0.01819	-0.16326	-0.04994	0.33270	0.73417	0.39760
	-0.04723	-0.21512	0.01508	0.13605	-0.00107	-0.08834	-0.00166	0.06662	-0.00258	-0.00758	-0.00058	-0.07801	-0.03358	0.38760	-0.03300
	-0.03627	0.01101													
15	0.00310	0.04978	-0.00101	-0.04507	-0.00041	0.04844	0.00066	-0.04613	-0.00368	0.11252	0.01462	-0.16772	-0.04981	0.39760	0.76919
	0.54565	-0.04723	-0.12040	0.00907	0.09862	-0.00679	-0.07084	-0.00157	0.00030	0.00174	-0.05794	-0.00036	-0.01705	-0.03526	-0.23191
	0.01293	0.07667													
16	-0.04613	0.00066	0.04844	-0.00041	-0.04507	-0.00101	0.04978	0.00310	-0.07084	-0.00679	0.09862	0.00907	-0.12040	-0.04723	0.54565
	0.76919	0.39760	-0.04981	-0.16772	0.01462	0.11252	-0.00368	-0.05794	0.00174	0.00030	-0.00157	0.07667	0.01293	-0.23191	-0.03526
	-0.01705	-0.00036													
17	-0.00599	-0.05436	0.00301	0.04844	-0.00101	-0.04603	0.00171	0.03489	-0.00166	-0.08834	-0.00107	0.13605	0.01508	-0.21512	-0.04723
	0.39760	0.73417	0.33270	-0.04994	-0.16326	0.01819	0.08882	-0.00058	-0.00758	-0.00258	0.06662	0.01101	-0.03627	-0.03300	0.38760
	-0.03358	-0.07801													
18	0.05184	-0.00076	-0.05436	0.00066	0.04978	0.00171	-0.01437	-0.00130	0.02223	0.00353	-0.03666	-0.00549	0.05284	0.01508	-0.12040
	-0.04981	0.33270	0.76403	0.60165	-0.04636	-0.18316	0.00625	0.11625	-0.00353	-0.04313	-0.00250	0.03158	-0.00017	0.00549	-0.03442
	-0.19988	0.01208													

TBX DENSITY BOND ORDERS (cont,)

19 0.01007 0.05184-0.00599-0.04613 0.00310 0.03489-0.00130-0.02645 0.00146 0.06606-0.00067-0.10152-0.00549 0.13605 0.00907
-0.16772-0.04994 0.60165 0.76866 0.32400-0.05380-0.10382 0.01359 0.02030-0.00154-0.05041-0.00160 0.03328 0.01190-0.21750
-0.02997 0.02410

20-0.10382 0.00625 0.08882-0.00368-0.07084-0.00166 0.02223 0.00146-0.03197-0.00320 0.04507-0.00067-0.03666-0.00107 0.09862
0.01462-0.16326-0.04636 0.32400 0.73400 0.44682-0.04113-0.19334 0.00992 0.05636 0.00116-0.02927 0.00990-0.05855-0.03036
0.36141-0.03219

21-0.05380-0.18316 0.01819 0.11252-0.00679-0.08834 0.00353 0.06606-0.00320-0.14018-0.00320 0.06606 0.00353-0.08834-0.00679
0.11252 0.01819-0.18316-0.05380 0.44682 0.78162 0.44682-0.04107-0.00831 0.00054 0.09757 0.01430 0.09757 0.00054-0.00831
-0.04107-0.25733

22 0.32400-0.04636-0.16326 0.01462 0.09862-0.00107-0.03666-0.00067 0.04507-0.00320-0.03197 0.00146 0.02223-0.00166-0.07084
-0.00368 0.08882 0.00625-0.10382-0.04113 0.44682 0.73400 0.36141-0.03036-0.05855 0.00990-0.02927 0.00116 0.05636 0.00992
-0.19334-0.03219

23-0.02997-0.19988-0.03358-0.01705 0.01293-0.03627-0.00017 0.03328 0.00990 0.09757 0.00116-0.05041-0.00250 0.06662-0.00157
-0.05794-0.00058 0.11625 0.01359-0.19334-0.04107 0.36141 0.74452 0.35668-0.03509-0.17991-0.03488-0.05888 0.01070-0.05447
-0.03347 0.39001

24-0.21750-0.03442 0.38760-0.03526-0.23191-0.03300 0.00549 0.01190-0.05855 0.00054 0.05636-0.00154-0.04313-0.00258 0.00030
0.00174-0.00758-0.00353 0.02030 0.00992-0.00831-0.03036 0.35668 0.73821 0.36713-0.03509-0.15493 0.01070 0.05331 0.00161
-0.05447-0.03421

25 0.01190 0.00549-0.03300-0.23191-0.03526 0.38760-0.03442-0.21750-0.03036-0.00831 0.00992 0.02030-0.00353-0.00758 0.00174
0.00030-0.00258-0.04313-0.00154 0.05636 0.00054-0.05855-0.03509 0.36713 0.73821 0.35668-0.03421-0.05447 0.00161 0.05331
0.01070-0.15493

26 0.03328-0.00017-0.03627 0.01293-0.01705-0.03358-0.19988-0.02997 0.36141-0.04107-0.19334 0.01359 0.11626-0.00058-0.05794
-0.00157 0.06662-0.00250-0.05041 0.00116 0.09757 0.00990-0.17991-0.03509 0.35668 0.74452 0.39001-0.03347-0.05447 0.01070
-0.05888-0.03488

27-0.00160 0.03158 0.01101 0.07667-0.00036-0.07801 0.01208 0.02410-0.03219-0.25733-0.03219 0.02410 0.01208-0.07801-0.00036
0.07667 0.01101 0.03158-0.00160-0.02927 0.01430-0.02927-0.03488-0.15493-0.03421 0.39001 0.74208 0.39001-0.03421-0.15493
-0.03488 0.33323

28-0.05041-0.00250 0.06662-0.00157-0.05794-0.00058 0.11626 0.01359-0.19334-0.04107 0.36141-0.02997-0.19988-0.03358-0.01705
0.01293-0.03627-0.00017 0.03328 0.00990 0.09757 0.00116-0.05888 0.01070-0.05447-0.03347 0.39001 0.74452 0.35668-0.03509
-0.17991-0.03488

29-0.00154-0.04313-0.00258 0.00030 0.00174-0.00758-0.00353 0.02030 0.00992-0.00831-0.03036-0.21750-0.03442 0.38760-0.03526
-0.23191-0.03300 0.00549 0.01190-0.05855 0.00054 0.05636 0.01070 0.05331 0.00161-0.05447-0.03421 0.35668 0.73821 0.36713
-0.03509-0.15493

30 0.02030-0.00353-0.00758 0.00174 0.00030-0.00258-0.04313-0.00154 0.05636 0.00054-0.05855 0.01190 0.00549-0.03300-0.23191
-0.03526 0.38760-0.03442-0.21750-0.03036-0.00831 0.00992-0.05447 0.00161 0.05331 0.01070-0.15493-0.03509 0.36713 0.73821
0.35668-0.03421

31 0.01359 0.11625-0.00058-0.05794-0.00157 0.06662-0.00250-0.05041 0.00116 0.09757 0.00990 0.03328-0.00017-0.03627 0.01293
-0.01705-0.03358-0.19988-0.02997 0.36141-0.04107-0.19334-0.03347-0.05447 0.01070-0.05888-0.03488-0.17991-0.03509 0.35668
0.74452 0.39001

32 0.02410 0.01208-0.07801-0.00036 0.07667 0.01101 0.03158-0.00160-0.02927 0.01430-0.02927-0.00160 0.03158 0.01101 0.07667
-0.00036-0.07801 0.01208 0.02410-0.03219-0.25733-0.03219 0.39001-0.03421-0.15493-0.03488 0.33323-0.03488-0.15493-0.03421
0.39001 0.74208

ENERGIES FOR OVALENE X , TBX APPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	15,17	16,18	9,17	8,17	10,18	13,19	12,19	7,18	2,17	6,19
XMOMNT	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000
YMOMNT	1.23243	-1.23343	0.05612	0.07448	0.10055	-0.53340	0.07863	-0.10410	0.00701	0.01244
JUMP E	16.6356	18.6897	25.0528	26.6404	28.2005	30.0472	31.4677	32.1244	34.1788	38.4611
DIAG E	28.1124	29.7424	39.0856	42.5064	41.9455	46.3795	46.8066	48.9421	51.3098	56.6759
DIAG E	28.4700	29.5096	39.3666	42.8000	42.3236	45.8672	46.8287	49.0961	51.9957	56.6622
CORRSP	23.0093	33.0144	37.9787	43.1474	40.7408	45.2062	48.7194	49.8602	52.0889	57.7406
CORRSP	23.2902	33.1520	38.4218	43.3934	40.8989	45.3088	48.6014	49.8130	52.5312	57.5889

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
23.00928	0.04067	-0.00000	0.20388	//	0.7706	0.6130	0.0573	0.1152	0.0383	-0.0151	-0.0951	0.0562	0.0002	-0.0017
21.10461				//	0.9461	-0.2530	0.0322	0.1238	-0.0096	-0.1105	-0.1103	-0.0015	-0.0053	0.0093
33.01438	3.35444	0.00000	-1.54574	//	-0.5613	0.7510	-0.1948	-0.0194	0.1101	-0.1106	0.2369	0.0375	0.0201	-0.0178
23.75918				//	0.2492	0.9563	0.0626	0.0665	0.0604	0.0614	-0.0312	0.0818	0.0001	0.0002
37.97875	0.40373	0.00000	-0.49998	//	-0.1653	0.1870	0.8435	-0.3029	-0.2622	0.1034	-0.1225	-0.0102	-0.1843	0.0779
34.22965				//	-0.0276	-0.0633	0.8594	-0.0560	-0.1044	0.3784	-0.2571	-0.0933	-0.0668	0.1422
43.14744	0.18363	0.00000	-0.31635	//	-0.0919	0.0680	-0.0321	0.6363	-0.7125	0.2103	0.0394	-0.1448	0.0795	0.0175
37.57455				//	-0.0580	-0.0155	0.0607	0.8091	-0.3856	0.1150	0.3848	-0.0023	0.1336	0.1015
40.74077	0.00081	0.00000	0.02156	//	-0.0687	-0.0458	0.4096	0.5744	0.6134	0.2098	0.2002	-0.1768	0.0559	-0.0283
39.76008				//	-0.0323	-0.0745	0.0942	0.3549	0.9006	0.1367	0.0994	-0.1214	0.0239	-0.0599
45.20623	0.94886	0.00000	-0.70255	//	-0.0835	0.1161	-0.2054	-0.1734	0.1117	0.7917	-0.4270	-0.1504	0.0087	-0.2512
42.97567				//	0.0208	-0.0166	-0.4382	0.1129	-0.0966	0.6802	-0.4732	-0.2454	0.1290	-0.1474
48.71944	0.10131	0.00000	0.22114	//	0.1974	-0.0144	-0.0601	-0.3107	-0.0979	0.2167	0.6850	-0.5665	-0.1186	0.0011
48.64350				//	0.1603	-0.0653	-0.0330	-0.2948	0.0063	0.5654	0.6064	0.3430	-0.2035	-0.1883
49.86020	0.01862	0.00000	-0.09372	//	0.0597	-0.0665	-0.0005	0.0170	-0.0503	0.3720	0.4435	0.7549	-0.2612	-0.1267
46.11257				//	-0.0944	-0.0826	-0.0149	0.2230	0.0646	0.0076	-0.3984	0.8772	-0.0415	-0.0140
52.08895	0.00128	0.00000	-0.02400	//	0.0337	-0.0039	0.1428	-0.1809	-0.0576	0.1166	0.1703	0.1606	0.9348	-0.0164
50.02858				//	0.0431	-0.0180	0.0756	-0.2037	0.0531	0.0541	0.1057	0.1461	0.9508	-0.0918
57.74064	0.06765	0.00000	-0.16598	//	-0.0096	0.0189	-0.1111	-0.0161	0.0765	0.2510	-0.0318	0.0630	-0.0005	0.9556
55.83504				//	0.0285	-0.0063	-0.2119	-0.0750	0.0959	0.1535	-0.0355	0.0354	-0.1156	0.9487

ENERGIES FOR OVALENE X , TBX APPROXIMATION 1.7

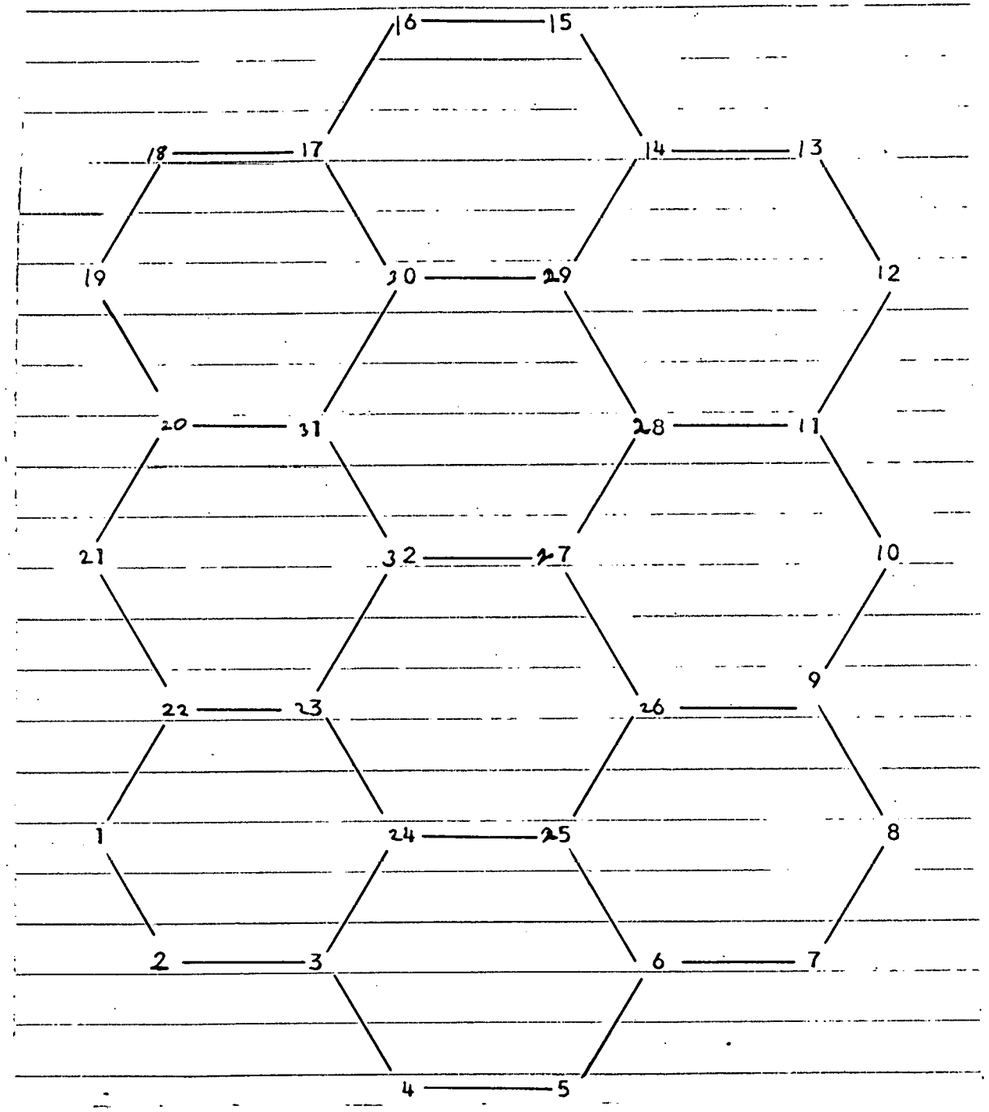
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	16,17	15,18	10,17	7,17	14,19	9,18	8,18	11,19	13,20	3,17
XMOMNT	1.21758	0.91260	-0.00463	0.02100	0.70470	0.04540	0.03874	-0.37488	0.01250	0.01951
YMOMNT	0.00000	0.00000	-0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000
JUMP E	13.2588	22.0665	22.7696	26.6935	28.8778	30.4837	32.0712	32.4437	32.6875	33.1603
DIAG E	25.1830	34.3269	33.8435	42.6056	44.4201	46.5949	49.1999	47.1979	51.7893	49.1597
DIAG E	25.2631	34.3717	34.5345	43.0724	44.4306	46.5631	49.2606	47.6265	52.0831	49.7535
CORRSP	22.7273	35.2805	32.1829	40.9495	46.0989	45.6139	50.7931	47.9170	53.1529	49.6046
CORRSP	22.9312	35.5357	32.7905	41.3548	46.1989	45.7104	50.7766	48.2391	53.3666	50.0551

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	CF	XMOMNT	YMOMNT	//	STATE COMPOSITION									
22.72728	0.56673	0.76576	0.00000	//	0.9171	-0.3551	0.0919	0.0746	-0.0493	-0.0445	-0.0502	-0.0332	-0.1020	-0.0198
13.03045				//	0.9619	-0.0833	0.0695	-0.0209	0.1396	0.0348	0.0150	-0.0464	-0.1975	0.0214
35.28051	1.66375	1.05306	0.00000	//	0.3469	0.7935	-0.4512	0.0448	-0.1607	0.0267	0.1248	-0.0269	-0.0115	0.0370
26.91104				//	0.1200	0.9420	0.1313	0.1250	-0.1341	0.0100	0.0692	-0.1281	0.1614	-0.0100
32.18288	0.05194	0.19482	-0.00000	//	0.0481	0.3858	0.8423	0.0633	-0.3270	-0.0514	0.0569	-0.0492	0.0849	-0.1136
29.98133				//	-0.0154	-0.1551	0.9103	-0.0776	-0.3545	-0.0717	-0.0472	0.0823	0.0304	-0.0186
40.94952	0.00264	0.03092	-0.00000	//	-0.0821	-0.0772	-0.0662	0.8685	0.0481	0.0904	0.1780	-0.3928	0.1114	-0.1406
35.07692				//	0.0833	-0.2389	-0.0440	0.7893	-0.1980	-0.2035	0.0215	-0.3563	0.3073	-0.0924
46.09891	1.84685	0.97062	0.00000	//	0.1178	0.2661	0.2475	0.0705	0.8851	0.1813	-0.0440	0.1209	-0.1236	0.0319
40.13399				//	-0.1317	0.0442	0.3474	0.3156	0.7797	0.2995	-0.0736	0.0409	-0.0083	-0.2358
45.61389	0.00055	-0.01683	0.00000	//	-0.0135	-0.0158	0.0249	-0.1427	-0.1715	0.8714	-0.2093	-0.2932	-0.2446	-0.0150
44.10477				//	-0.0704	-0.0559	-0.0185	0.0545	-0.3197	0.7761	0.1582	-0.3728	-0.3321	-0.0993
50.79312	0.21092	-0.31249	-0.00000	//	-0.0060	-0.1199	0.0241	0.0348	-0.0815	0.2788	0.7918	0.4762	-0.2037	-0.0654
43.91556				//	-0.1001	-0.0299	0.1193	-0.1312	0.2103	-0.3205	0.8068	-0.3561	-0.1788	0.0315
47.91703	0.28113	-0.37144	0.00000	//	-0.0067	0.0266	-0.0449	0.3808	-0.1643	0.1838	-0.5018	0.7156	0.1205	-0.1142
47.98329				//	-0.0006	0.0029	0.0201	0.3688	-0.0346	0.2041	0.3408	0.5222	-0.0506	0.6552
53.15292	0.08983	0.19936	0.00000	//	-0.1242	-0.0534	-0.0195	-0.1834	0.0987	0.2812	0.1483	-0.0045	0.9144	-0.0273
51.73066				//	0.1256	-0.1363	-0.0059	-0.2954	0.0633	0.3401	0.2496	-0.0360	0.8332	0.0278
49.60462	0.00953	-0.06722	-0.00000	//	-0.0026	-0.0190	0.0959	0.1702	-0.0798	0.0609	0.0233	0.0452	0.0508	0.9728
46.76872				//	-0.0711	-0.0086	0.1082	-0.1086	0.1951	-0.0088	-0.3639	-0.5534	0.0220	0.7029

OVALENE IRX



ATOMIC COORDINATES

x	0.0036	0.5044	1.5231	2.0446	3.0418	3.5633	4.5820	5.0828	4.5936	5.0864	4.5936	5.0828	4.5820	3.5633
	3.0418	2.0446	1.5231	0.5044	0.0036	0.4928	0.	0.4928	1.5231	2.0360	3.0504	3.5633	3.0569	3.5633
	3.0504	2.0360	1.5231	2.0295										
y	1.7450	0.9090	0.8680	0.	0.	0.8680	0.9090	1.7450	2.6560	3.5310	4.4060	5.3170	6.1530	6.1940
	7.0620	7.0620	6.1940	6.1530	5.3170	4.4060	3.5310	2.6560	2.6380	1.7450	1.7450	2.6380	3.5310	4.4240
	5.3170	5.3170	4.4240	3.5310										

OVALENE X — IRX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 SA	3 AS	4 SS	5 AA	6 SS	7 SA	8 AS	9 SA	10 AS	11 AA	12 SS	13 SS	14 AA	15 SA	16 AS
1.817153	1.699937	1.641058	1.526432	1.511333	1.409867	1.348955	1.340774	1.283148	1.196180	1.188921	1.185041	1.144176	1.107788	1.066185	1.014275
0.107618	0.117204	-0.191550	-0.001079	0.240510	-0.234711	0.199919	-0.098426	-0.250999	0.209790	-0.122463	-0.133205	0.158522	-0.256066	0.005552	0.232028
0.105237	0.158686	-0.148832	0.120019	0.253704	-0.155240	0.065126	-0.268270	-0.240671	0.103531	0.140759	-0.185261	0.215469	-0.188165	0.221114	0.120929
0.159342	0.253621	-0.120385	0.248247	0.220118	-0.005510	-0.134836	-0.282974	-0.039125	0.111331	0.277888	-0.026402	-0.000336	0.137048	-0.129914	-0.221909
0.101371	0.192834	-0.034919	0.275456	0.072738	0.006474	-0.323636	-0.114968	-0.104892	-0.052246	0.142258	0.348129	0.064108	0.075368	0.264988	-0.164973
0.101371	0.192834	0.034919	0.275456	-0.072740	0.006474	-0.323636	0.114967	-0.104892	0.052247	-0.142259	0.348128	0.064108	-0.075368	0.264988	0.164972
0.159342	0.253621	0.120385	0.248245	-0.220120	-0.005511	-0.134836	0.282974	-0.039126	0.111330	-0.277888	-0.026403	-0.000335	-0.137048	-0.129914	0.221909
0.105237	0.158687	0.148832	0.120018	-0.253705	-0.155241	0.065125	0.268270	-0.240671	-0.103531	-0.140758	-0.185262	0.215468	0.188165	-0.221114	-0.120929
0.107618	0.117204	0.191550	-0.001081	-0.240509	-0.234712	0.199918	0.098427	-0.250999	-0.209790	0.122463	-0.133204	0.158521	0.256067	0.005551	-0.232028
0.176351	0.103599	0.281869	-0.142758	-0.188116	-0.231040	0.223326	-0.160619	-0.070213	-0.101789	0.277610	0.092373	-0.100215	-0.023718	0.258553	0.060645
0.136851	0.000000	0.256285	-0.156410	0.000001	-0.282152	0.000000	-0.236702	-0.000000	-0.205511	-0.000001	0.211877	-0.238691	-0.000001	-0.000000	0.363256
0.176351	-0.103599	0.281869	-0.142756	0.188117	-0.231039	-0.223326	-0.160619	0.070213	-0.101788	-0.277611	0.092371	-0.100215	0.023718	-0.258553	0.060645
0.107618	-0.117204	0.191550	-0.001079	0.240510	-0.234711	-0.199919	0.098426	0.250999	-0.209789	-0.122464	-0.133205	0.158522	-0.256066	-0.005551	-0.232028
0.105237	-0.158686	0.148832	0.120019	0.253704	-0.155240	-0.065126	0.268270	0.240671	-0.103532	0.140759	-0.185261	0.215469	-0.188165	0.221115	-0.120929
0.159342	-0.253620	0.120385	0.248247	0.220118	-0.005511	0.134836	0.282974	0.039126	0.111329	0.277889	-0.026402	-0.000336	0.137048	0.129914	0.221909
0.101372	-0.192833	0.034919	0.275457	0.072738	0.006474	0.323635	0.114967	0.104891	0.052246	0.142258	0.348129	0.064108	0.075368	-0.264989	0.164972
0.101372	-0.192833	-0.034919	0.275456	-0.072740	0.006474	0.323635	-0.114967	0.104891	-0.052245	-0.142259	0.348128	0.064108	-0.075368	-0.264988	-0.164972
0.159342	-0.253620	-0.120385	0.248246	-0.220120	-0.005511	0.134836	-0.282974	0.039125	-0.111329	-0.277889	-0.026403	-0.000335	-0.137048	0.129914	-0.221909
0.105237	-0.158686	-0.148832	0.120018	-0.253705	-0.155241	-0.065126	-0.268270	0.240670	0.103531	-0.140758	-0.185261	0.215468	0.188166	0.221114	0.120929
0.107618	-0.117204	-0.191550	-0.001080	-0.240509	-0.234712	-0.199919	-0.098427	0.250999	0.209789	0.122464	-0.133204	0.158521	0.256067	-0.005551	0.232028
0.176351	-0.103599	-0.281869	-0.142757	-0.188116	-0.231039	-0.223326	0.160618	0.070213	0.101788	0.277611	0.092372	-0.100215	-0.023718	-0.258553	0.060645
0.136851	-0.000000	-0.256285	-0.156410	0.000001	-0.282152	-0.000000	0.236702	0.000000	0.205512	0.000000	0.211877	-0.238691	-0.000000	-0.000000	0.363257
0.176351	0.103599	-0.281869	-0.142756	0.188117	-0.231040	0.223325	0.160619	-0.070213	0.101790	-0.277610	0.092372	-0.100215	0.023718	0.258552	-0.060645
0.244995	0.151356	-0.213586	-0.141369	0.151381	0.111357	0.175238	0.106049	0.161653	-0.288362	-0.198448	0.004771	0.002333	0.276615	0.171942	-0.132030
0.230998	0.275557	-0.097619	0.111868	0.125466	0.147455	0.047828	-0.074931	0.292373	-0.175498	0.035791	-0.195663	-0.268079	0.217905	-0.132542	-0.055742
0.230998	0.275557	0.097619	0.111867	-0.125467	0.147455	0.047828	0.074931	0.292373	0.175498	-0.035791	-0.195663	-0.268078	-0.217906	-0.132542	0.055742
0.244995	0.151356	0.213586	-0.141370	-0.151380	0.111357	0.175238	-0.106048	0.161653	-0.288362	0.198448	0.004771	0.002334	-0.276614	0.171942	-0.132030
0.275066	-0.000000	0.126538	-0.256829	0.000001	0.294656	0.000000	-0.093577	-0.000000	0.263494	0.000001	0.116261	0.357582	0.000001	0.000000	-0.172540
0.244995	-0.151356	0.213586	-0.141369	0.151381	0.111357	-0.175238	-0.106048	-0.161654	0.288362	-0.198446	0.004770	0.002333	0.276615	-0.171942	-0.132030
0.230998	-0.275557	0.097619	0.111868	0.125466	0.147455	-0.047828	0.074931	-0.292373	0.175497	0.035792	-0.195664	-0.268079	0.217905	0.132542	0.055742
0.230999	-0.275557	-0.097619	0.111867	-0.125467	0.147454	-0.047828	-0.074931	-0.292373	-0.175498	-0.035791	-0.195664	-0.268078	-0.217906	0.132542	-0.055742
0.244995	-0.151356	-0.213586	-0.141370	-0.151381	0.111357	-0.175238	0.106048	-0.161653	-0.288362	0.198447	0.004771	0.002333	-0.276615	-0.171942	0.132030
0.275066	-0.000000	-0.126538	-0.256829	0.000001	0.294656	-0.000000	0.093577	-0.000000	-0.263494	-0.000001	0.116261	0.357582	0.000000	0.000000	0.172540

IRX APPROXIMATION (cont.)

17 SS	18 AA	19 SA	20 AS	21 AS	22 SA	23 SS	24 AA	25 AA	26 SS
0.847528	0.801080	0.768197	0.748291	0.729489	0.714992	0.712673	0.668176	0.641087	0.640187

OVERLAP EIGNVALUES AND EIGNVECTORS

27 AS	28 SA	29 AS	30 SS	31 AA	32AS
0.610606	0.570391	0.563908	0.525074	0.504828	0.472209
0.241614	0.028638	-0.268033	-0.206341	-0.056234	0.106433	0.206079	0.271653	-0.159776	-0.091493	0.225305	0.223818	0.008099	-0.176738	0.106980	-0.095942
-0.153032	-0.218068	0.193290	0.287447	0.056867	0.137679	-0.105405	-0.247079	0.018284	0.257697	0.142317	-0.239679	-0.124107	0.136877	-0.146558	0.094977
-0.215204	0.112262	0.128523	-0.025414	0.002960	-0.279229	-0.093747	0.040405	0.159400	-0.302823	0.006292	0.233667	0.259926	-0.124318	0.256703	-0.159812
0.149153	0.288625	-0.062529	-0.108136	-0.347343	0.132240	0.037985	-0.075501	-0.314555	0.116780	0.001328	-0.073869	-0.254496	0.034311	-0.175610	0.092235
0.149153	-0.288625	-0.062530	0.108136	0.347343	0.132240	0.037985	0.075502	0.314562	0.116760	-0.001328	-0.073870	0.254495	0.034311	0.175610	-0.092235
-0.215204	-0.112262	0.128523	0.025414	-0.002960	-0.279229	-0.093747	-0.040406	-0.159419	-0.302813	-0.006292	0.233668	-0.259925	-0.124319	-0.256703	0.159811
-0.153032	0.218068	0.193290	-0.287448	-0.056867	0.137679	-0.105406	0.247079	-0.018268	0.257698	0.142317	-0.239680	0.124106	0.136878	0.146558	-0.094977
0.241614	-0.028638	-0.268033	0.206342	0.056234	0.106433	0.206079	-0.271653	0.159770	-0.091502	-0.225305	0.223818	-0.008099	-0.176738	-0.106980	0.095942
0.069544	-0.241732	0.008692	0.126815	0.026887	-0.282614	-0.124809	0.117044	-0.232071	-0.156143	0.256104	-0.194082	-0.136282	0.285952	0.104850	-0.172469
-0.348940	0.000000	-0.000000	-0.277690	-0.073941	0.000002	0.218915	0.000000	0.000007	0.212053	-0.292156	-0.000000	0.141792	-0.246338	0.000000	0.126729
0.069544	0.241732	-0.008692	0.126816	0.026887	0.282612	-0.124813	0.117045	0.232060	-0.156157	0.256104	0.194082	-0.136282	0.285952	-0.104850	-0.172469
0.241614	0.028637	0.268034	0.206341	0.056234	-0.106430	0.206081	0.271653	-0.159776	-0.091493	-0.225306	-0.223818	-0.008099	-0.176738	0.106980	0.095942
-0.153032	-0.218067	-0.193290	-0.287448	-0.056867	-0.137681	-0.105403	-0.247079	0.018284	0.257697	0.142317	0.239679	0.124106	0.136878	-0.146558	-0.094977
-0.215204	0.112263	-0.128523	0.025414	-0.002960	0.279227	-0.093751	0.040405	0.159400	-0.302824	-0.006292	-0.233667	-0.259926	-0.124318	0.256703	0.159811
0.149153	0.288625	0.062530	0.108136	0.347343	-0.132240	0.037987	-0.075502	-0.314555	0.116780	-0.001329	0.073869	0.254496	0.034311	-0.175610	-0.092235
0.149153	-0.288625	0.062529	-0.108137	-0.347342	-0.132239	0.037987	0.075502	0.314562	0.116760	0.001329	0.073870	-0.254496	0.034311	0.175610	0.092235
-0.215204	-0.112262	-0.128523	-0.025414	0.002960	0.279227	-0.093751	-0.040406	-0.159419	-0.302813	0.006292	-0.233668	0.259925	-0.124319	-0.256703	-0.159811
-0.153032	0.218068	-0.193290	0.287448	0.056867	-0.137681	-0.105403	0.247079	-0.018267	0.257698	-0.142317	0.239680	-0.124106	0.136878	0.146558	0.094977
0.241614	-0.028638	0.268033	-0.206342	-0.056234	-0.106430	0.206081	-0.271653	0.159770	-0.091503	0.225305	-0.223818	0.008099	-0.176738	-0.106980	-0.095942
0.069544	-0.241732	-0.008693	-0.126815	-0.026887	0.282612	-0.124813	0.117044	-0.232070	-0.156142	-0.256104	0.194082	0.136282	0.285952	0.104850	0.172469
-0.348940	-0.000000	0.000000	0.277690	0.073940	0.000002	0.218915	0.000000	0.000007	0.212053	0.292156	0.000000	-0.141792	-0.246338	0.000000	-0.126729
0.069544	0.241732	0.008692	-0.126815	-0.026886	-0.282614	-0.124809	-0.117045	0.232061	-0.156157	-0.256104	-0.194082	0.136281	0.285952	-0.104850	0.172469
0.117557	-0.170700	0.266774	0.009208	0.003535	0.208282	-0.284459	-0.126272	-0.202920	0.107973	-0.094671	0.161666	-0.144834	-0.226210	0.157879	-0.250026
0.069712	-0.134708	-0.221641	-0.152232	0.289785	0.031751	0.172212	0.279605	0.068907	0.082048	0.144628	-0.136375	-0.123694	0.104798	-0.290553	0.239962
0.069711	0.134708	-0.221640	0.152232	-0.289785	0.031751	0.172212	-0.279605	-0.068901	0.082053	-0.144628	-0.136376	0.123694	0.104799	0.290553	-0.239962
0.117557	0.170699	0.266774	-0.009209	-0.003534	0.208282	-0.284459	0.126272	0.202926	0.107960	0.094671	0.161666	-0.144835	-0.226210	-0.157879	0.250026
-0.174634	0.000000	-0.000000	-0.262908	0.266472	0.000002	0.268611	-0.000000	-0.000003	-0.096233	-0.285640	0.000000	-0.273130	0.135143	-0.000000	-0.282336
0.117557	-0.170699	-0.266774	-0.009209	-0.003535	-0.208287	-0.284456	-0.126272	-0.202920	0.107973	0.094671	-0.161666	0.144835	-0.226210	0.157879	0.250026
0.069712	-0.134708	0.221641	0.152231	-0.289785	-0.031748	0.172212	0.279605	0.068907	0.082048	-0.144628	0.136375	0.123694	0.104799	-0.290553	-0.239962
0.069712	0.134708	0.221641	-0.152232	0.289785	-0.031748	0.172213	-0.279605	-0.068902	0.082053	0.144628	0.136376	-0.123694	0.104799	0.290553	0.239962
0.117557	0.170700	-0.266774	0.009209	0.003535	-0.208287	-0.284456	0.126272	0.202926	0.107960	-0.094671	-0.161666	-0.144835	-0.226210	-0.157879	-0.250026
-0.174634	-0.000000	0.000000	0.262908	-0.266472	0.000002	0.268611	0.000000	-0.000003	-0.096233	0.285640	-0.000000	0.273130	0.135142	-0.000000	0.282336

OVALENE X — IRX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS — ZEROTH HAMILTONIAN EIG

1 SS	2 SA	3 AS	4 SS	5 AA	6 SS	7 SA	8 AS	9 SA	10 AS	11 AA	12 SS	13 SS	14 AA	15 SA	16 AS
33.06312	30.27320	28.72140	25.35695	24.87573	21.37454	19.01972	18.68716	16.22439	12.05844	11.68312	11.48067	9.26474	7.15397	4.56413	1.03480
0.079835	0.089893	-0.149527	-0.000873	0.195638	-0.197672	0.172129	-0.085003	-0.221582	0.191817	-0.112312	-0.122364	0.148199	-0.243290	0.005376	0.230389
0.078068	0.121709	-0.116181	0.097143	0.206370	-0.130742	0.056073	-0.231683	-0.212464	0.094661	-0.129092	-0.170184	0.201436	-0.178776	-0.214141	0.120075
0.118205	0.194522	-0.093975	0.200930	0.179051	-0.004641	-0.116093	-0.244382	-0.034540	-0.101793	0.254855	-0.024253	-0.000314	0.130210	-0.125818	-0.220342
0.075200	0.147899	-0.027258	0.222953	0.059167	0.005453	-0.278649	-0.099288	-0.092598	-0.047770	0.130467	0.319796	0.059933	0.071608	0.256632	-0.163807
0.075200	0.147899	0.027258	0.222953	-0.059169	0.005453	-0.278649	0.099288	-0.092598	0.047770	-0.130467	0.319796	0.059933	-0.071608	0.256632	0.163807
0.118205	0.194522	0.093975	0.200929	-0.179052	-0.004641	-0.116094	0.244381	-0.034540	0.101792	-0.254855	-0.024254	-0.000313	-0.130210	-0.125817	0.220342
0.078068	0.121709	0.116181	0.097142	-0.206371	-0.130743	0.056073	0.231683	-0.212464	-0.094662	-0.129091	-0.170184	0.201436	0.178777	-0.214142	-0.120075
0.079834	0.089893	0.149527	-0.000875	-0.195637	-0.197672	0.172129	0.085003	-0.221581	-0.191817	0.112313	-0.122363	0.148198	0.243290	0.005376	-0.230389
0.130822	0.079459	0.220031	-0.115547	-0.153019	-0.194580	0.192283	-0.138713	-0.061984	-0.093069	0.254600	0.084855	-0.093689	-0.022535	0.250399	0.060217
0.101520	0.000000	0.200061	-0.126598	0.000001	-0.237626	0.000000	-0.204421	-0.000000	-0.187905	-0.000001	0.194634	-0.223146	-0.000001	-0.000000	0.360691
0.130822	-0.079458	0.220031	-0.115546	0.153020	-0.194579	-0.192282	-0.138713	0.061984	-0.093068	-0.254601	0.084854	-0.093688	0.022534	-0.250399	0.060217
0.079834	-0.089893	0.149527	-0.000873	0.195638	-0.197672	-0.172129	0.085003	0.221582	-0.191816	-0.112313	-0.122364	0.148199	-0.243290	-0.005376	-0.230389
0.078068	-0.121709	0.116181	0.097143	0.206370	-0.130742	-0.056073	0.231683	0.212464	-0.094662	0.129092	-0.170183	0.201436	-0.178776	0.214142	-0.120075
0.118205	-0.194522	0.093975	0.200930	0.179050	-0.004641	0.116093	0.244381	0.034540	0.101791	0.254856	-0.024253	-0.000314	0.130210	0.125817	0.220342
0.075200	-0.147899	0.027258	0.222954	0.059167	0.005452	0.278649	0.099288	0.092598	0.047770	0.130467	0.319796	0.059933	0.071608	-0.256632	0.163807
0.075200	-0.147899	-0.027258	0.222953	-0.059169	0.005452	0.278649	-0.099288	0.092598	-0.047769	-0.130468	0.319796	0.059933	-0.071608	-0.256632	-0.163807
0.075200	-0.147899	0.027258	0.222954	0.059167	0.005452	0.278649	0.099288	0.092598	0.047770	0.130467	0.319796	0.059933	0.071608	-0.256632	0.163807
0.075200	-0.147899	-0.027258	0.222953	-0.059169	0.005452	0.278649	-0.099288	0.092598	-0.047769	-0.130468	0.319796	0.059933	-0.071608	-0.256632	-0.163807
0.118205	-0.194522	-0.093975	0.200929	-0.179052	-0.004641	0.116094	-0.244381	0.034540	-0.101791	-0.254856	-0.024254	-0.000313	-0.130210	-0.125818	-0.220342
0.078068	-0.121709	-0.116181	0.097142	-0.206371	-0.130743	-0.056073	-0.231683	0.212464	0.094662	-0.129091	-0.170184	0.201436	0.178777	0.214141	0.120075
0.079835	-0.089893	-0.149527	-0.000875	-0.195637	-0.197672	-0.172129	-0.085003	0.221581	0.191816	0.112314	-0.122364	0.148198	0.243291	-0.005376	0.230389
0.130822	-0.079458	-0.220031	-0.115547	-0.153019	-0.194580	-0.192283	0.138713	0.061984	0.093068	0.254601	0.084854	-0.093688	-0.022535	-0.250399	-0.060217
0.101520	-0.000000	-0.200061	-0.126598	0.000000	-0.237626	-0.000000	0.204421	0.000000	0.187905	0.000000	0.194633	-0.223146	-0.000000	-0.000000	-0.360691
0.130822	0.079458	-0.220032	-0.115546	0.153020	-0.194580	0.192282	0.138714	-0.061984	0.093069	-0.254600	0.084854	-0.093688	0.022535	0.250399	-0.060217
0.181744	0.116087	-0.166729	-0.114423	0.123138	0.093784	0.150879	0.091586	0.142707	-0.263657	-0.181999	0.004382	0.002181	0.262813	0.166520	0.131098
0.171361	0.211347	-0.076203	0.090545	0.102058	0.124185	0.041180	-0.064712	0.258107	-0.160463	0.032824	-0.179739	-0.250620	0.207032	-0.128362	-0.055348
0.171361	0.211347	0.076203	0.090545	-0.102058	0.124185	0.041180	0.064712	0.258107	0.160463	-0.032824	-0.179739	-0.250620	-0.207033	-0.128362	0.055348
0.181744	0.116087	0.166729	-0.114424	-0.123137	0.093784	0.150879	-0.091585	0.142707	0.263657	0.181999	0.004383	0.002182	-0.262813	0.166520	-0.131098
0.204052	-0.000000	0.098778	-0.207876	0.000001	0.248157	0.000000	-0.080815	-0.000000	-0.240920	0.000001	0.106799	0.334295	0.000001	-0.000000	-0.171321
0.181744	-0.116087	0.166729	-0.114423	0.123138	0.093784	-0.150879	-0.091585	0.142708	0.263658	-0.181998	0.004382	0.002181	0.262813	-0.166520	-0.131097
0.171362	-0.211347	0.076203	0.090546	0.102058	0.124185	-0.041180	0.064712	-0.258107	0.160462	-0.032825	-0.179739	-0.250621	0.207033	0.128362	0.055348
0.171362	-0.211347	-0.076203	0.090545	-0.102058	0.124185	-0.041179	-0.064712	-0.258106	-0.160462	-0.032825	-0.179739	-0.250620	-0.207033	0.128362	-0.055348
0.181744	-0.116087	-0.166729	-0.114424	-0.123137	0.093784	-0.150879	0.091585	-0.142707	-0.263658	0.181998	0.004382	-0.002182	-0.262813	-0.166520	0.131097
0.204052	-0.000000	-0.098778	-0.207876	0.000000	0.248157	-0.000000	0.080815	-0.000000	-0.240920	-0.000001	0.106799	0.334295	0.000000	0.000000	0.171321

IRX APPROXIMATION (cont.) RS

17 SS	18 AA	19 SA	20 AS	21 AS	22 SA	23 SS	24 AA	25 AA	26 SS
-13.22722	-18.25720	-22.18592	-24.73204	-27.26460	-29.30808	-29.64278	-36.51320	-41.16274	-41.32401

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

27 AS	28 SA	29 AS	30 SS	31 AA	32 AS
-46.88776	-55.37742	-56.05940	-66.50241	-72.11822	-82.17867
0.262449	0.031997	-0.305810	-0.238534	-0.065840	0.125872	0.244112	0.332330	-0.199551	-0.114349	0.288331	0.296353	0.010786	-0.243904	0.150567	-0.139618
-0.166229	-0.243643	0.220532	0.332294	0.066581	0.162824	-0.124858	0.302267	0.022835	0.322075	-0.182127	-0.317354	0.165269	0.188895	-0.206271	0.138214
-0.233762	0.125428	0.146638	-0.029379	0.003466	-0.330225	-0.111048	0.049430	0.199081	-0.378474	0.008052	0.309393	0.346135	-0.171563	0.361293	-0.232563
0.162015	0.322475	-0.071342	-0.125007	-0.406676	0.156391	0.044995	-0.092366	-0.392860	0.145954	0.001700	-0.097808	-0.338904	0.047350	-0.247160	0.134224
0.162015	-0.322475	-0.071343	0.125007	0.406676	0.156391	0.044995	0.092366	0.392869	0.145929	-0.001700	-0.097809	0.338903	0.047351	0.247160	-0.134224
-0.233762	-0.125429	0.146638	0.029379	-0.003466	-0.330225	-0.111048	-0.049431	-0.199105	-0.378461	-0.008052	0.309394	-0.346134	-0.171564	-0.361293	0.232563
-0.166228	0.243643	0.220533	-0.332295	-0.066581	0.162824	-0.124859	0.302267	-0.022815	0.322075	0.182128	-0.317355	0.165268	0.188896	0.206270	-0.138214
0.262450	-0.031996	-0.305811	0.238535	0.065840	0.125871	0.244112	-0.332330	0.199543	-0.114361	-0.288331	0.296353	-0.010785	-0.243905	-0.150567	0.139618
0.075541	-0.270082	0.009917	0.146601	0.031479	-0.334228	-0.147843	0.143187	-0.289842	-0.195150	0.327744	-0.256980	-0.181482	0.394624	0.147569	-0.250983
-0.379031	0.000000	-0.000000	-0.321014	-0.086571	0.000002	0.259317	0.000000	0.000009	0.265028	-0.373881	-0.000000	0.188819	-0.339954	0.000000	0.184420
0.075541	0.270082	-0.009917	0.146601	0.031479	0.334225	-0.147848	-0.143188	0.289829	-0.195168	0.327745	0.256980	-0.181482	0.394624	-0.147570	-0.250983
0.262450	0.031996	0.305811	0.238534	0.065840	-0.125868	0.244114	0.332329	-0.199550	-0.114349	-0.288331	-0.296352	-0.010785	-0.243905	0.150567	0.139618
-0.166229	-0.243642	-0.220533	-0.332295	-0.066581	-0.162826	-0.124855	-0.302266	0.022835	0.322075	0.182128	0.317354	0.165269	0.188896	-0.206271	-0.138214
-0.233762	0.125429	-0.146638	0.029380	-0.003466	0.330223	-0.111054	0.049430	0.199081	-0.378474	-0.008052	-0.309393	-0.346135	-0.171564	0.361293	0.232563
0.162015	0.322475	0.071343	0.125008	0.406676	-0.156391	0.044998	-0.092366	-0.392860	0.145954	-0.001700	-0.097808	0.338904	0.047350	-0.247160	-0.134224
0.162015	-0.322475	0.071342	-0.125008	-0.406676	-0.156390	0.044997	0.092366	0.392869	0.145929	0.001700	-0.097809	-0.338904	0.047350	0.247160	0.134224
-0.233762	-0.125428	-0.146638	-0.029379	0.003466	0.330223	-0.111053	-0.049431	-0.199105	-0.378462	0.008052	-0.309394	0.346134	-0.171564	-0.361293	-0.232563
-0.166229	0.243643	-0.220532	0.332295	0.066581	-0.162826	-0.124856	0.302267	-0.022815	0.322076	-0.182127	0.317354	-0.165268	0.188896	0.206270	0.138214
0.262450	-0.031996	0.305810	-0.238535	-0.065840	-0.125867	0.244114	-0.332330	0.199543	-0.114361	0.288331	-0.296352	0.010785	-0.243905	-0.150567	-0.139618
-0.075541	-0.270082	-0.009918	-0.146601	-0.031479	0.334225	-0.147848	0.143187	-0.289842	-0.195150	-0.327745	0.256979	0.181482	0.394624	0.147569	0.250983
-0.379031	-0.000000	0.000000	0.321014	0.086571	0.000002	0.259317	0.000000	0.000008	0.265027	0.373882	0.000000	-0.188819	-0.339954	0.000000	-0.184420
0.075541	0.270082	0.009918	-0.146601	-0.031479	-0.334228	-0.147843	-0.143188	0.289830	-0.195167	-0.327744	-0.256980	0.181481	0.394624	-0.147570	0.250983
0.127694	-0.190719	0.304373	0.010645	0.004138	0.246321	-0.336957	-0.154477	-0.253434	0.134946	-0.121153	0.214059	-0.192871	-0.312178	0.222205	-0.363846
0.075723	-0.150506	-0.252879	-0.175983	0.339286	0.037550	0.203994	0.342058	0.086060	0.102545	0.185086	-0.180572	-0.164720	0.144625	-0.408935	0.349200
0.075723	0.150506	-0.252879	0.175983	-0.339287	0.037550	0.203995	-0.342058	-0.086054	0.102551	-0.185085	-0.180572	0.164719	0.144626	0.408935	-0.349200
0.127694	0.190719	0.304374	-0.010645	-0.004138	0.246321	-0.336958	0.154477	0.253443	0.134930	-0.121153	0.214058	0.192872	-0.312178	-0.222204	0.363846
-0.189693	0.000000	-0.000000	-0.303926	0.311991	0.000003	0.318184	-0.000000	-0.000004	-0.120274	-0.365543	0.000000	-0.363719	0.186501	-0.000000	-0.410864
0.127694	-0.190719	-0.304374	-0.010645	-0.004139	-0.246327	-0.336953	-0.154477	-0.253434	0.134946	0.121153	-0.214058	0.192872	-0.312178	0.222205	0.363846
0.075723	-0.150506	0.252879	0.175982	-0.339286	-0.037546	0.203995	0.342058	0.086061	0.102545	-0.185085	0.180571	0.164720	0.144626	-0.408935	-0.349200
0.075723	0.150506	0.252879	-0.175983	0.339286	-0.037546	0.203995	-0.342058	-0.086054	0.102551	0.185086	-0.180572	-0.164719	0.144626	0.408934	0.349200
0.127694	0.190719	-0.304374	0.010645	0.004139	-0.246326	-0.336953	0.154477	0.253443	0.134930	-0.121153	-0.214058	-0.192872	-0.312178	-0.222204	-0.363846
-0.189693	-0.000000	0.000000	0.303926	-0.311991	0.000002	0.318184	0.000000	-0.000004	-0.120274	0.365543	-0.000001	0.363719	0.186501	-0.000000	0.410864

OVALENE X

IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	31	32													
1	1.01784	0.78784	-0.01322	-0.18376	0.01808	0.14724	0.00122	-0.11272	0.00477	0.06088	-0.00595	-0.02601	0.00588	0.03504	-0.00162
	-0.04965	-0.00404	0.05679	-0.00275	-0.11676	-0.00064	0.47930	0.00752	-0.22450	-0.00977	0.04555	0.00427	-0.04754	-0.00074	0.02458
	-0.00460	0.00340													
2	0.78784	1.01122	0.49297	0.00639	-0.13352	-0.00559	0.05503	0.00122	-0.03391	-0.00649	0.01999	0.00588	-0.01157	-0.00733	0.05897
	0.00450	-0.06215	-0.01206	0.05679	0.01151	-0.19852	-0.00890	-0.20494	0.00940	-0.01295	0.00356	0.04115	0.00323	-0.05261	0.00280
	0.12734	-0.00959													
3	-0.01322	0.49297	0.97863	0.56508	-0.01505	-0.22401	-0.00559	0.14724	-0.00254	-0.08517	0.00623	0.03504	-0.00733	-0.04983	-0.00045
	0.05270	-0.00284	-0.06215	0.00404	0.09861	0.00124	-0.17006	0.00779	0.54106	0.01190	-0.05059	-0.00908	0.06937	0.00474	-0.00552
	-0.00094	-0.08988													
4	-0.18376	0.00639	0.56508	1.02047	0.71810	-0.01505	-0.13352	0.01808	0.10866	-0.00701	-0.08175	-0.00162	0.05897	-0.00045	-0.04964
	0.00305	0.05270	0.00450	-0.04965	-0.00141	0.11669	-0.00318	-0.03663	0.00556	-0.23855	-0.00535	0.08696	0.00485	-0.00346	-0.00447
	-0.05546	0.00281													
5	0.01808	-0.13352	-0.01505	0.71810	1.02047	0.56508	0.00639	-0.18376	-0.00318	0.11669	-0.00141	-0.04965	0.00450	0.05270	0.00305
	-0.04964	-0.00045	0.05897	-0.00162	-0.08175	-0.00701	0.10866	-0.00535	-0.23855	0.00556	-0.03663	0.00281	-0.05546	-0.00447	-0.00346
	0.00485	0.08696													
6	0.14724	-0.00559	-0.22401	-0.01505	0.56508	0.97863	0.49297	-0.01322	-0.17006	0.00124	0.09861	0.00404	-0.06215	-0.00284	0.05270
	-0.00045	-0.04983	-0.00733	0.03504	0.00623	-0.08517	-0.00254	-0.05059	0.01190	0.54106	0.00779	-0.08988	-0.00094	-0.00552	0.00474
	0.06937	-0.00908													
7	0.00122	0.05503	-0.00559	-0.13352	0.00639	0.49297	1.01122	0.78784	-0.00890	-0.19852	0.01151	0.05679	-0.01206	-0.06215	0.00450
	0.05897	-0.00733	-0.01157	0.00588	0.01999	-0.00649	-0.03391	0.00356	-0.01295	0.00940	-0.20494	-0.00959	0.12734	0.00280	-0.05261
	0.00323	0.04115													
8	-0.11272	0.00122	0.14724	0.01808	-0.18376	-0.01322	0.78784	1.01784	0.47930	-0.00064	-0.11676	-0.00275	0.05679	0.00404	-0.04965
	-0.00162	-0.03504	0.00588	-0.02601	-0.00595	0.06088	0.00477	0.04555	-0.00977	-0.22450	0.00752	0.00340	-0.00460	0.02458	-0.00074
	-0.04754	0.00427													
9	0.00477	0.03391	-0.00254	0.10866	-0.00318	-0.17006	-0.00890	0.47930	0.97625	0.61670	-0.00537	-0.11676	0.01151	0.09861	-0.00141
	-0.08175	0.00623	0.01999	-0.00595	-0.03044	0.00387	0.04703	-0.00844	-0.07182	0.00751	0.51159	0.01082	-0.20062	-0.00556	0.06579
	0.00039	-0.04283													
10	0.06088	-0.00649	-0.08517	-0.00701	0.11669	0.00124	-0.19852	-0.00064	0.61670	1.04114	0.61670	-0.00064	-0.19852	0.00124	0.11669
	-0.00701	-0.08517	-0.00649	0.06088	0.00387	-0.14247	0.00387	0.10411	0.00716	-0.02699	-0.00542	-0.25658	-0.00542	-0.02699	0.00716
	0.10411	-0.00759													
11	-0.00595	0.01999	0.00623	-0.08175	-0.00141	0.09861	0.01151	-0.11676	-0.00537	0.61670	0.97625	0.47930	-0.00890	-0.17006	-0.00318
	0.10866	-0.00254	-0.03391	0.00477	0.04703	0.00387	-0.03044	0.00039	0.06579	-0.00556	-0.20061	0.01082	0.51159	0.00751	-0.07182
	-0.00844	-0.04283													
12	-0.02601	0.00588	0.03504	-0.00162	-0.04965	0.00404	0.05679	-0.00275	-0.11676	-0.00064	0.47930	1.01784	0.78784	-0.01322	-0.18376
	0.01808	0.14724	0.00122	-0.11272	0.00477	0.06088	-0.00595	-0.04754	-0.00074	0.02458	-0.00460	0.00340	0.00752	-0.22450	-0.00977
	0.04555	0.00427													
13	0.00588	-0.01157	-0.00733	0.05897	0.00450	-0.06215	-0.01206	0.05679	0.01151	-0.19852	-0.00890	0.78784	1.01122	0.49297	0.00639
	-0.13352	-0.00559	0.05503	0.00122	-0.03391	-0.00649	0.01999	0.00323	-0.05261	0.00280	-0.12734	-0.00959	-0.20494	0.00940	-0.01295
	0.00356	-0.04115													
14	0.03504	-0.00733	-0.04983	-0.00045	0.05270	-0.00284	-0.06215	0.00404	0.09861	0.00124	-0.17006	-0.01322	0.49297	0.97863	0.56508
	-0.01505	-0.22401	-0.00559	0.14724	-0.00254	-0.08517	0.00623	0.06937	0.00474	-0.00552	-0.00094	-0.08988	0.00779	0.54106	0.01190
	-0.05059	-0.00908													
15	-0.00162	0.05897	-0.00045	-0.04964	0.00305	0.05270	0.00450	-0.04965	-0.00141	0.11669	-0.00318	-0.18376	0.00639	0.56508	1.02047
	0.71810	-0.01505	-0.13352	0.01808	0.10866	-0.00701	-0.08175	0.00485	-0.00346	-0.00447	-0.05546	0.00281	-0.03663	0.00556	-0.23855
	-0.00535	0.08696													
16	-0.04965	0.00450	0.05270	0.00305	-0.04964	-0.00045	0.05897	-0.00162	-0.08175	-0.00701	0.10866	0.01808	-0.13352	-0.01505	0.71810
	1.02047	0.56508	0.00639	-0.18376	-0.00318	0.11669	-0.00141	-0.05546	-0.00447	-0.00346	0.00485	0.08696	-0.00535	-0.23855	0.00556
	-0.03663	0.00281													
17	0.00404	-0.06215	-0.00284	0.05270	-0.00045	-0.04983	-0.00733	0.03504	0.00623	-0.08517	-0.00254	0.14724	-0.00559	-0.22401	-0.01505
	0.56508	0.97863	0.49297	-0.01322	-0.17006	0.00124	0.09861	-0.00094	-0.00552	0.00474	0.06937	-0.00908	-0.05059	0.01190	0.54106
	0.00779	-0.08988													
18	0.05679	-0.01206	-0.06215	0.00450	0.05897	-0.00733	-0.01157	0.00588	0.01999	-0.00649	-0.03391	0.00122	0.05503	-0.00559	-0.13352
	0.00639	0.49297	1.01122	0.78784	-0.00890	-0.19852	0.01151	0.12734	0.00280	-0.05261	0.00323	0.04115	0.00356	-0.01295	0.00940
	-0.20494	-0.00959													

IRX AUGMENTED TOPOLOGICAL BOND ORDERS (cont.)

19-0.00275 0.05679 0.00404-0.04965-0.00162 0.03504 0.00588-0.02601-0.00595 0.06088 0.00477-0.11272 0.00122 0.14724 0.01808
-0.18376-0.01322 0.78784 1.01784 0.47930-0.00064-0.11676-0.00460 0.02458-0.00074-0.04754 0.00427 0.04555-0.00977-0.22450
0.00752 0.00340
20-0.11676 0.01151-0.09861-0.00141-0.08175 0.00623 0.01999-0.00595-0.03044 0.00387 0.04703 0.00477-0.03391-0.00254-0.10866
-0.00318-0.17006-0.00890 0.47930 0.97625 0.61670-0.00537-0.20061-0.00556 0.06579 0.00039-0.04283-0.00844-0.07182 0.00751
0.51159 0.01082
21-0.00064-0.19852 0.00124 0.11669-0.00701-0.08517-0.00649 0.06088 0.00387-0.14247 0.00387 0.06088-0.00649-0.08517-0.00701
0.11669 0.00124-0.19852-0.00064 0.61670 1.04114 0.61670-0.00542-0.02699 0.00716 0.10411-0.00759 0.10411 0.00716-0.02699
-0.00542-0.25658
22 0.47930-0.00890-0.17006-0.00318 0.10866-0.00254-0.03391 0.00477 0.04703 0.00387-0.03044-0.00595 0.01999 0.00623-0.08175
-0.00141 0.09861 0.01151-0.11676-0.00537 0.61670 0.97625 0.51159 0.00751-0.07182-0.00844-0.04283 0.00039 0.06579-0.00556
-0.20062 0.01082
23 0.00752-0.20494 0.00779-0.03663-0.00535-0.05059 0.00356 0.04555-0.00844 0.10411 0.00039-0.04754 0.00323 0.06937 0.00485
-0.05546-0.00094 0.12734-0.00460-0.20061-0.00542 0.51159 0.99602 0.51704 0.00377-0.18903 0.00437-0.07103-0.00581-0.06988
0.00352 0.54722
24-0.22450 0.00940 0.54106 0.00556-0.23855 0.01190-0.01295-0.00977-0.07182 0.00716 0.06579-0.00074-0.05261 0.00474-0.00346
-0.00447-0.00552 0.00280 0.02458-0.00556-0.02699 0.00751 0.51704 0.98519 0.53096 0.00377-0.16463-0.00581 0.06391 0.00209
-0.06988 0.00323
25-0.00977-0.01295 0.01190-0.23855 0.00556 0.54106 0.00940-0.22450 0.00751-0.02699-0.00556 0.02458 0.00280-0.00552-0.00447
-0.00346 0.00474-0.05261-0.00074 0.06579 0.00716-0.07182 0.00377 0.53096 0.98519 0.51704 0.00323-0.06988 0.00209 0.06391
-0.00581-0.16463
26 0.04555 0.00356-0.05059-0.00535-0.03663 0.00779-0.20494 0.00752 0.51159-0.00542-0.20061-0.00460 0.12734-0.00094-0.05546
0.00485 0.06937 0.00323-0.04754 0.00039 0.10411-0.00844-0.18903 0.00377 0.51704 0.99602 0.54722 0.00352-0.06988-0.00581
-0.07103 0.00437
27 0.00427 0.04115-0.00908 0.08696 0.00281-0.08988-0.00959 0.00340 0.01082-0.25658 0.01082 0.00340-0.00959-0.08988 0.00281
0.08696-0.00908 0.04115 0.00427-0.04283-0.00759-0.04283 0.00437-0.16463 0.00323 0.54722 0.98759 0.54722 0.00323-0.16463
0.00437 0.49172
28-0.04754 0.00323 0.06937 0.00485-0.05546-0.00094 0.12734-0.00460-0.20062-0.00542 0.51159 0.00752-0.20494 0.00779-0.03663
-0.00535-0.05059 0.00356 0.04555-0.00844 0.10411 0.00039-0.07103-0.00581-0.06988 0.00352 0.54722 0.99602 0.51704 0.00377
-0.18903 0.00437
29-0.00074-0.05261 0.00474-0.00346-0.00447-0.00552 0.00280 0.02458-0.00556-0.02699 0.00751-0.22450 0.00940 0.54106 0.00556
-0.23855 0.01190-0.01295-0.00977-0.07182 0.00716 0.06579-0.00581 0.06391 0.00209-0.06988 0.00323 0.51704 0.98519 0.53096
0.00377-0.16463
30 0.02458 0.00280-0.00552-0.00447-0.00346 0.00474-0.05261-0.00074 0.06579 0.00716-0.07182-0.00977-0.01295 0.01190-0.23855
0.00556 0.54106 0.00940-0.22450 0.00751-0.02699-0.00556-0.06988 0.00209 0.06391-0.00581-0.16463 0.00377 0.53096 0.98519
0.51704 0.00323
31-0.00460 0.12734-0.00094-0.05546 0.00485 0.06937 0.00323-0.04754 0.00039 0.10411-0.00844 0.04555 0.00356-0.05059-0.00535
-0.03663 0.00779-0.20494 0.00752 0.51159-0.00542-0.20062 0.00352-0.06988-0.00581-0.07103 0.00437-0.18903 0.00377 0.51704
0.99602 0.54722
32 0.00340-0.00959-0.08988 0.00281 0.08696-0.00908 0.04115 0.00427-0.04283-0.00759-0.04283 0.00427 0.04115-0.00908 0.08696
0.00281-0.08988-0.00959 0.00340 0.01082-0.25658 0.01082 0.54722 0.00323-0.16463 0.00437 0.49172 0.00437-0.16463 0.00323
0.54722 0.98759

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	31	32													
1	0.79751	0.60289	-0.08632	-0.18635	0.03319	0.15664	-0.00614	-0.12063	0.00385	0.06564	-0.00524	-0.02766	0.00526	0.03762	0.00228
	-0.05327	-0.00314	0.05933	0.00985	-0.11708	-0.07243	0.31640	-0.04219	-0.23723	0.00567	0.04834	0.00547	-0.05201	-0.00351	0.02631
	0.01272	0.01010													
2	0.60289	0.78577	0.32576	-0.06042	-0.13334	0.01370	0.05870	-0.00614	-0.03714	-0.00348	0.02158	0.00526	-0.01226	-0.00580	0.06328
	0.00620	-0.06631	-0.01490	0.05933	0.02287	-0.20204	-0.07839	-0.21803	-0.04596	-0.00715	0.00649	0.04387	-0.00022	-0.05673	-0.00183
	0.13580	0.00595													
3	-0.08632	0.32576	0.72945	0.39773	-0.08607	-0.23627	0.01370	0.15664	-0.00226	-0.09235	0.00445	0.03762	-0.00580	-0.05377	-0.00151
	0.05694	0.00023	-0.06631	-0.00314	0.10496	0.02441	-0.17818	-0.04348	0.38196	-0.03845	-0.04798	0.00439	0.07482	0.00167	-0.00669
	0.00024	-0.09038													
4	-0.18635	-0.06042	0.39773	0.80115	0.53968	-0.08607	-0.13334	0.03319	0.11523	-0.01656	-0.08766	0.00228	0.06328	-0.00151	-0.05353
	0.00273	0.05694	0.00620	-0.05327	-0.00689	0.12449	0.01561	-0.03244	-0.05086	-0.25238	0.01183	0.09285	0.00268	-0.00356	-0.00321
	-0.06047	0.00531													
5	0.03319	-0.13334	-0.08607	0.53968	0.80115	0.39773	-0.06042	-0.18635	0.01561	0.12449	-0.00689	-0.05327	0.00620	0.05694	-0.00273
	-0.05353	-0.00151	0.06328	0.00228	-0.08766	-0.01656	0.11523	0.01183	-0.25238	-0.05086	-0.03244	0.00531	-0.06047	-0.00321	-0.00356
	0.00268	0.09285													
6	0.15664	0.01370	-0.23627	-0.08607	0.39773	0.72945	0.32576	-0.08632	-0.17818	0.02441	0.10496	-0.00314	-0.06631	0.00023	0.05694
	-0.00151	-0.05377	-0.00580	0.03762	0.00445	-0.09235	-0.00226	-0.04798	-0.03845	0.38196	-0.04348	-0.09038	0.00024	-0.00669	0.00167
	0.07482	0.00439													
7	-0.00614	0.05870	0.01370	-0.13334	-0.06042	0.32576	0.78577	0.60289	-0.07839	-0.20204	0.02287	0.05933	-0.01490	-0.06631	0.00620
	0.06328	-0.00580	-0.01226	0.00526	0.02158	-0.00348	-0.03714	0.00649	-0.00715	-0.04596	-0.21803	0.00595	0.13580	-0.00183	-0.05673
	-0.00022	0.04387													
8	-0.12063	-0.00614	0.15664	0.03319	-0.18635	-0.08632	0.60289	0.79751	0.31640	-0.07243	-0.11708	0.00985	0.05933	-0.00314	-0.05327
	0.00228	0.03762	0.00526	-0.02766	-0.00524	0.06564	0.00385	0.04834	0.00567	-0.23723	-0.04219	0.01010	0.01272	0.02631	-0.00351
	-0.05201	0.00547													
9	0.00385	-0.03714	-0.00226	0.11523	0.01561	-0.17818	-0.07839	0.31640	0.72564	0.44630	-0.06865	-0.11708	0.02287	0.10496	-0.00689
	-0.08766	0.00445	0.02158	-0.00524	-0.03344	-0.00003	0.05089	0.00389	-0.07105	-0.03859	0.35612	-0.03925	-0.21263	0.00743	0.07037
	0.00395	-0.04007													
10	0.06564	-0.00348	-0.09235	-0.01656	0.12449	0.02441	-0.20204	-0.07243	0.44630	0.83539	0.44630	-0.07243	-0.20204	0.02441	0.12449
	-0.01656	-0.09235	-0.00348	0.06564	-0.00003	-0.15348	-0.00003	0.11154	0.01107	-0.02161	-0.06747	-0.27306	-0.06747	-0.02161	0.01107
	0.11154	0.01007													
11	-0.00524	0.02158	0.00445	-0.08766	-0.00689	0.10496	0.02287	-0.11708	-0.06865	0.44630	0.72564	0.31640	-0.07839	-0.17818	0.01561
	0.11523	-0.00226	-0.03714	0.00385	0.05089	-0.00003	-0.03344	0.00395	0.07037	0.00743	-0.21263	-0.03925	0.35612	-0.03859	-0.07105
	0.00389	-0.04007													
12	-0.02766	0.00526	0.03762	0.00228	-0.05327	-0.00314	0.05933	0.00985	-0.11708	-0.07243	0.31640	0.79751	0.60289	-0.08632	-0.18635
	0.03319	0.15664	-0.00614	-0.12063	0.00385	0.06564	-0.00524	-0.05201	-0.00351	0.02631	0.01272	0.01010	-0.04219	-0.23723	0.00567
	0.04834	0.00547													
13	0.00526	-0.01226	-0.00580	0.06328	0.00620	-0.06631	-0.01490	0.05933	0.02287	-0.20204	-0.07839	0.60289	0.78577	0.32576	-0.06042
	-0.13334	0.01370	0.05870	-0.00614	-0.03714	-0.00348	0.02158	-0.00022	-0.05673	-0.00183	0.13580	0.00595	-0.21803	-0.04596	-0.00715
	0.00649	0.04387													
14	0.03762	-0.00580	-0.05377	-0.00151	0.05694	0.00023	-0.06631	-0.00314	0.10496	0.02441	-0.17818	-0.08632	0.32576	0.72945	0.39773
	-0.08607	-0.23627	0.01370	0.15664	-0.00226	-0.09235	0.00445	0.07482	0.00167	-0.00669	0.00024	-0.09038	-0.04348	0.38196	-0.03845
	-0.04798	0.00439													
15	0.00228	0.06328	-0.00151	-0.05353	0.00273	0.05694	0.00620	-0.05327	-0.00689	0.12449	0.01561	-0.18635	-0.06042	0.39773	0.80115
	0.53968	-0.08607	-0.13334	0.03319	0.11523	-0.01656	-0.08766	0.00268	-0.00356	-0.00321	-0.06047	0.00531	-0.03244	-0.05086	-0.25238
	0.01183	0.09285													
16	-0.05327	0.00620	0.05694	0.00273	-0.05353	-0.00151	0.06328	0.00228	-0.08766	-0.01656	0.11523	0.03319	-0.13334	-0.08607	0.53968
	0.80115	0.39773	-0.06042	-0.18635	0.01561	0.12449	-0.00689	-0.06047	-0.00321	-0.00356	0.00268	0.09285	0.01183	-0.25238	-0.05086
	-0.03244	0.00531													
17	-0.00314	-0.06631	0.00023	0.05694	-0.00151	-0.05377	-0.00580	0.03762	0.00445	-0.09235	-0.00226	0.15664	0.01370	-0.23627	-0.08607
	0.39773	0.72945	0.32576	-0.08632	-0.17818	0.02441	0.10496	0.00024	-0.00669	0.00167	0.07482	0.00439	-0.04798	-0.03845	0.38196
	-0.04348	-0.09038													
18	0.05933	-0.01490	-0.06631	0.00620	0.06328	-0.00580	-0.01226	0.00526	0.02158	-0.00348	-0.03714	-0.00614	0.05870	0.01370	-0.13334
	-0.06042	0.32576	0.78577	0.60289	-0.07839	-0.20204	0.02287	0.13580	-0.00183	-0.05673	-0.00022	0.04387	0.00649	-0.00715	-0.04596
	-0.21803	0.00595													

IRX AUGMENTED DENSITY BOND ORDERS (cont.)

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 19 0.00985 0.05933-0.00314-0.05327 0.00228 0.03762 0.00526-0.02766-0.00524 0.06564 0.00385-0.12063-0.00614 0.15664 0.03319
   -0.18635-0.08632 0.60289 0.79751 0.31640-0.07243-0.11708 0.01272 0.02631-0.00351-0.05201 0.00547 0.04834 0.00567-0.23723
   -0.04219 0.01010
 20-0.11708 0.02287 0.10496-0.00689-0.08766 0.00445 0.02158-0.00524-0.03344-0.00003 0.05089 0.00385-0.03714-0.00226 0.11523
    0.01561-0.17818-0.07839 0.31640 0.72564 0.44630-0.06865-0.21263 0.00743 0.07037 0.00395-0.04007 0.00389-0.07105-0.03859
    0.35612-0.03925
 21-0.07243-0.20204 0.02441 0.12449-0.01656-0.09235-0.00348 0.06564-0.00003-0.15348-0.00003 0.06564-0.00348-0.09235-0.01656
    0.12449 0.02441-0.20204-0.07243 0.44630 0.83539 0.44630-0.06747-0.02161 0.01107 0.11154 0.01007 0.11154 0.01107-0.02161
   -0.06747-0.27306
 22 0.31640-0.07839-0.17818 0.01561 0.11523-0.00226-0.03714 0.00385 0.05089-0.00003-0.03344-0.00524 0.02158 0.00445-0.08766
   -0.00689 0.10496 0.02287-0.11708-0.06865 0.44630 0.72564 0.35612-0.03859-0.07105 0.00389-0.04007 0.00395 0.07037-0.00743
   -0.21263-0.03925
 23-0.04219-0.21803-0.04348-0.03244 0.01183-0.04798 0.00649 0.04834 0.00389 0.11154 0.00395-0.05201-0.00022 0.07482 0.00268
   -0.06047 0.00024 0.13580 0.01272-0.21263-0.06747 0.35612 0.75905 0.36027-0.05106-0.20193-0.04902-0.06985 0.00813-0.06857
   -0.04772 0.39038
 24-0.23723-0.04596 0.38196-0.05086-0.25238-0.03845-0.00715 0.00567-0.07105 0.01107 0.07037-0.00351-0.05673 0.00167-0.00356
   -0.00321-0.00669-0.00183 0.02631 0.00743-0.02161-0.03859 0.36027 0.74145 0.36880-0.05106-0.17498 0.00813 0.06838 0.00619
   -0.06857-0.04908
 25 0.00567-0.00715-0.03845-0.25238-0.05086 0.38196-0.04596-0.23723-0.03859-0.02161 0.00743 0.02631-0.00183-0.00669-0.00321
   -0.00356 0.00167-0.05673-0.00351 0.07037 0.01107-0.07105-0.05106 0.36880 0.74145 0.36027-0.04908-0.06857 0.00619 0.06838
    0.00813-0.17498
 26 0.04834 0.00649-0.04798 0.01183-0.03244-0.04348-0.21803-0.04219 0.35612-0.06747-0.21263 0.01272 0.13580 0.00024-0.06047
    0.00268 0.07482-0.00022-0.05201 0.00395 0.11154 0.00389-0.20193-0.05106 0.36027 0.75905 0.39038-0.04772-0.06857 0.00813
   -0.06985-0.04902
 27 0.00547 0.04387 0.00439 0.09285 0.00531-0.09038 0.00595 0.01010-0.03925-0.27306-0.03925 0.01010 0.00595-0.09038 0.00531
    0.09285 0.00439 0.04387 0.00547-0.04007 0.01007-0.04007-0.04902-0.17498-0.04908 0.39038 0.74654 0.39038-0.04908-0.17498
   -0.04902 0.33182
 28-0.05201-0.00022 0.07482 0.00268-0.06047 0.00024 0.13580 0.01272-0.21263-0.06747 0.35612-0.04219-0.21803-0.04348-0.03244
    0.01183-0.04798 0.00649 0.04834 0.00389 0.11154 0.00395-0.06985 0.00813-0.06857-0.04772 0.39038 0.75905 0.36027-0.05106
   -0.20193-0.04902
 29-0.00351-0.05673 0.00167-0.00356-0.00321-0.00669-0.00183 0.02631 0.00743-0.02161-0.03859-0.23723-0.04596 0.38196-0.05086
   -0.25238-0.03845-0.00715 0.00567-0.07105 0.01107 0.07037 0.00813 0.06838 0.00619-0.06857-0.04908 0.36027 0.74145 0.36880
   -0.05106-0.17498
 30 0.02631-0.00183-0.00669-0.00321-0.00356 0.00167-0.05673-0.00351 0.07037 0.01107-0.07105 0.00567-0.00715-0.03845-0.25238
   -0.05086 0.38196-0.04596-0.23723-0.03859-0.02161 0.00743-0.06857 0.00619 0.06838 0.00813-0.17498-0.05106 0.36880 0.74145
    0.36027-0.04908
 31 0.01272 0.13580 0.00024-0.06047 0.00268 0.07482-0.00022-0.05201 0.00395 0.11154 0.00389 0.04834 0.00649-0.04798 0.01183
   -0.03244-0.04348-0.21803-0.04219 0.35612-0.06747-0.21263-0.04772-0.06857 0.00813-0.06985-0.04902-0.20193-0.05106 0.36027
    0.75905 0.39038
 32 0.01010 0.00595-0.09038 0.00531 0.09285 0.00439 0.04387 0.00547-0.04007 0.01007-0.04007 0.00547 0.04387 0.00439 0.09285
    0.00531-0.09038 0.00595 0.01010-0.03925-0.27306-0.03925 0.39038-0.04908-0.17498-0.04902 0.33182-0.04902-0.17498-0.04908
    0.39038 0.74654
```

ENERGIES FOR OVALENE X ,IRX APPROXIMATION

ONE ELECTRON EXCITATIONS OF (SA) SYMMETRY

JUMP	15,17	16,18	9,17	10,18	13,19	7,17	12,19	8,18	2,17	6,19
XMOMNT	-0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000	-0.00000	-0.00000	0.00000
YMOMNT	-1.29814	1.25383	-0.01854	0.11134	-0.50978	-0.02016	0.15040	0.07263	0.00163	0.01353
JUMP E	17.7914	19.2920	29.4516	30.3156	31.4507	32.2469	33.6666	36.9444	43.5004	43.5605
DIAG E	28.9891	29.9327	43.4521	44.3764	45.8411	48.3046	49.6644	53.6478	61.2517	61.4312
DIAG E	29.4417	29.7425	43.8371	44.8065	45.9168	48.5952	49.1188	53.7903	61.9349	61.4152
CORRSP	23.5690	33.7882	42.1553	44.2141	46.2308	47.6355	51.4524	54.1434	61.4827	62.2197
CORRSP	23.8134	33.9293	42.5625	44.4068	46.2672	48.0195	51.1654	54.2437	62.0101	62.1812

FINAL EXCITED STATES OF (SA) SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
23.56901	0.02465	-0.00000	-0.15684	//	0.7532	0.6475	-0.0194	-0.0162	-0.0418	0.0614	-0.0790	0.0321	0.0022	-0.0055
21.74531				//	0.9323	-0.3238	0.0086	0.0012	0.0335	0.0594	-0.1453	0.0052	-0.0040	0.0035
33.78821	3.66979	0.00000	1.59814	//	-0.6000	0.7360	0.1229	-0.0599	0.2331	-0.0219	0.1569	0.0053	-0.0001	-0.0137
23.90056				//	0.3247	0.9393	-0.0376	-0.0207	-0.0670	0.0584	-0.0020	0.0495	0.0004	0.0012
42.15535	-0.59743	0.00000	-0.57729	//	0.1468	-0.1496	0.7527	-0.5213	0.2703	0.1560	0.0879	0.0167	0.0897	-0.0659
37.46258				//	0.0031	0.0698	0.7425	-0.1108	0.6347	-0.0549	0.0315	0.1016	0.0097	-0.1192
44.21407	0.01949	0.00000	-0.10181	//	0.0377	-0.0077	0.5196	0.7206	0.1778	-0.3045	-0.2594	0.1289	-0.0000	0.0314
41.33108				//	0.0090	0.0004	-0.0213	0.8188	0.2072	0.4265	0.2879	0.0428	0.0506	0.1300
46.23080	0.94176	0.00000	-0.69212	//	0.1044	-0.0904	-0.3563	-0.1634	0.8212	-0.2468	-0.2049	0.1448	-0.0300	0.1678
45.13020				//	-0.0063	0.0323	-0.6345	-0.1046	0.7187	-0.1888	-0.0548	0.0930	-0.0485	0.1384
47.63554	0.16372	-0.00000	-0.28429	//	0.0755	-0.0678	-0.0565	0.4107	0.3582	0.7102	0.3889	-0.1519	0.0309	0.0998
43.17782				//	0.0125	-0.0501	-0.0883	-0.5398	0.0714	0.6763	0.4699	-0.1082	0.0500	0.0272
51.45237	0.08230	-0.00000	-0.19394	//	0.1811	-0.0518	0.0002	0.0610	0.0495	-0.5377	0.8085	-0.0961	-0.0577	-0.0541
49.91608				//	0.1332	0.0208	-0.0015	0.0662	0.0276	-0.4671	0.5993	-0.6277	0.0251	-0.0680
54.14338	0.03593	-0.00000	0.12493	//	-0.0142	-0.0260	-0.0399	0.0113	-0.0801	0.1373	0.2023	0.9607	-0.0503	-0.0761
51.89484				//	0.0838	-0.0627	-0.0411	-0.0320	-0.1450	-0.2772	0.5531	0.7517	-0.0500	-0.1227
61.48268	0.00186	-0.00000	0.02669	//	-0.0035	0.0057	-0.0860	0.0385	-0.0002	-0.0659	0.0260	0.0464	0.9895	-0.0694
59.15396				//	0.0108	-0.0024	0.0630	-0.0662	0.0302	-0.1207	0.0119	0.0764	0.8567	0.4859
62.21967	0.05901	-0.00000	0.14934	//	-0.0125	0.0221	0.0940	-0.0666	0.1666	-0.0338	0.0743	0.0610	0.0717	0.9710
60.67437				//	0.0122	-0.0000	0.1751	-0.0693	-0.0649	-0.0741	0.0774	0.0107	-0.5053	0.8326

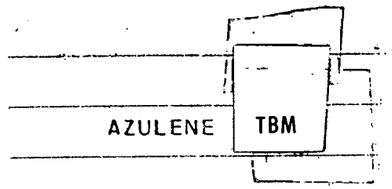
ENERGIES FOR OVALENE X , IRX APPROXIMATION

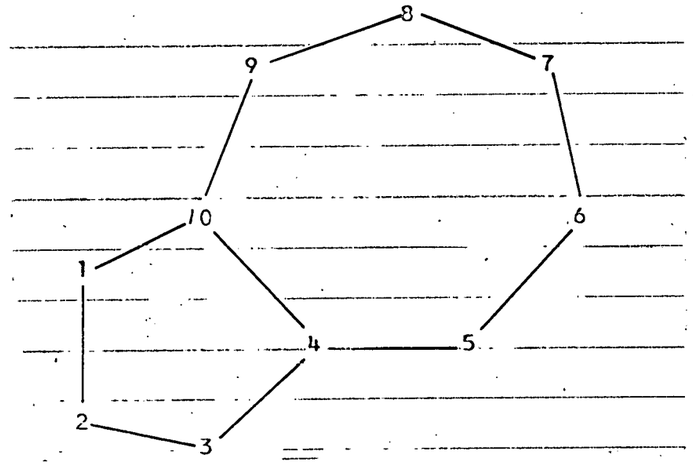
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	16,17	15,18	10,17	14,19	8,17	11,19	13,20	9,18	12,20	7,18
XMOMNT	-1.20382	-0.92632	-0.04604	-0.67911	-0.00256	-0.44174	-0.10799	0.05655	-0.06958	-0.00198
YMOMNT	0.00000	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.00000	0.00000	-0.00000	0.00000
JUMP E	14.2620	22.8213	25.2857	29.3399	31.9144	33.8690	33.9968	34.4816	36.2127	37.2769
DIAG E	25.4659	34.4275	36.8202	44.2903	47.8309	48.1866	50.5783	50.3030	54.9959	54.7254
DIAG E	25.5783	34.5774	37.5529	44.3490	48.2761	48.5924	51.3237	50.3854	55.1199	54.7134
CORRSP	23.1608	33.8906	36.4817	45.7138	44.8341	50.1520	53.7898	47.9091	57.1242	54.5674
CORRSP	23.3368	34.2252	36.9773	45.9780	45.2376	50.5236	54.2500	48.2747	57.1268	54.5382

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
23.16080	0.55602	-0.75136	0.00000	//	0.9235	-0.3580	-0.0439	-0.0459	0.0351	0.0269	-0.0906	0.0268	0.0541	-0.0330
13.79969				//	0.9646	-0.0804	-0.0291	0.1418	-0.0394	0.0576	-0.1546	-0.0301	0.1089	0.0244
33.89065	0.68983	-0.69185	0.00000	//	0.2450	0.7383	-0.4786	-0.3888	0.0376	0.0237	-0.0267	0.0423	-0.0914	0.0430
26.99424				//	0.1149	0.9622	-0.0608	-0.1166	0.0848	0.1138	0.0400	-0.0055	-0.1480	0.0077
36.48171	1.04677	-0.82142	0.00000	//	0.2290	0.4964	0.8164	0.0992	-0.0112	-0.0089	-0.1364	-0.0503	-0.0464	0.0363
32.38549				//	-0.0494	0.1071	0.8663	0.4665	0.0369	0.0793	-0.0534	-0.0781	0.0067	0.0366
45.71377	1.12863	-0.76195	-0.00000	//	0.0426	0.1406	-0.2412	0.6910	0.4263	0.3377	-0.2672	-0.2160	-0.1640	0.0460
41.96206				//	-0.0713	-0.0301	-0.4074	0.6932	0.5109	0.2164	0.1450	-0.0334	-0.1310	-0.0203
44.83415	0.05116	0.16381	-0.00000	//	-0.0610	-0.1129	0.1944	-0.4085	0.5741	0.5596	0.2928	0.0377	0.0583	0.2137
37.82053				//	0.1329	-0.1808	0.2594	-0.4626	0.5667	0.3993	0.3508	0.2313	-0.0939	0.0487
50.15204	0.47027	-0.46958	-0.00000	//	0.0172	0.0612	-0.0425	0.1405	-0.6230	0.6662	-0.0097	0.2028	0.2628	0.1795
46.60368				//	-0.1388	0.0102	-0.1074	0.0278	-0.2717	0.6927	-0.1948	0.0546	0.3296	0.5148
53.78977	0.50760	-0.47107	-0.00000	//	0.1385	0.0953	-0.0358	0.1708	-0.1555	-0.0350	0.7272	-0.6170	0.0571	0.0549
50.24614				//	0.0252	0.0291	-0.0015	-0.0851	0.1708	-0.2335	0.3757	-0.6927	0.3434	0.4107
47.90908	0.33986	-0.40843	-0.00000	//	0.0927	0.1296	-0.0287	0.3776	0.1749	-0.2232	0.4751	0.6995	0.1110	0.1529
46.11788				//	0.0605	0.0842	-0.0070	0.2069	-0.2031	-0.2775	0.5705	0.6108	0.2494	0.2597
57.12422	0.08679	-0.18902	-0.00000	//	-0.0218	0.1348	-0.0128	0.0324	0.1839	0.0423	-0.0221	-0.0369	0.7380	-0.6309
56.07301				//	-0.0767	0.1173	-0.0039	-0.0237	0.2611	0.0046	-0.1520	0.1032	0.8070	-0.4760
54.56741	0.03512	0.12302	0.00000	//	-0.0227	0.0072	-0.0500	-0.0068	0.0960	-0.2736	-0.2452	-0.1854	0.5718	0.7010
50.93701				//	-0.0419	0.0302	0.0086	-0.0530	0.4419	-0.3997	-0.5476	0.2680	-0.0171	0.5172





ATOMIC COORDINATES

x	0.	0.	0.9511	1.5388	2.5378	3.1958	3.0172	2.1366	1.2171	0.9511
y	1.3090	0.3090	0.	0.8090	0.7640	1.5170	2.5010	2.9750	2.5820	1.6180

AZULENE TBM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 S	3 A	4 S	5 A	6 S	7 A	8 S	9 S	10 A
1.570184	1.407574	1.334578	1.218890	1.117791	0.901208	0.817931	0.610272	0.538706	0.482860
0.323276	0.267735	-0.220715	0.258603	0.[illegible]	-0.063196	0.299149	-0.436405	0.250096	-0.258987
0.279869	0.324263	-0.000092	0.582954	-0.[illegible]	0.315726	-0.000057	0.552645	-0.267567	-0.000080
0.323335	0.267787	0.220610	0.258449	-0.[illegible]	-0.063191	-0.299132	-0.436328	0.250033	0.259177
0.467090	0.117981	0.299121	-0.353630	-0.259033	-0.290361	0.220699	0.136398	-0.199762	-0.542913
0.288640	-0.190907	0.484076	-0.218456	0.160168	0.469940	0.357056	0.084483	0.323250	0.335520
0.199767	-0.433234	0.357124	0.159862	0.335459	0.102236	-0.484083	-0.269794	-0.404416	-0.160140
0.172905	-0.524640	0.000051	0.360312	-0.000066	-0.510972	0.000049	0.341614	0.432712	0.000024
0.199764	-0.433321	-0.357046	0.159757	-0.335482	0.102335	0.484035	-0.269748	-0.404500	0.160086
0.288615	-0.191028	-0.484047	-0.218547	-0.160039	0.469890	-0.357101	0.084398	0.323378	-0.335437
0.467039	0.117894	-0.299151	-0.353625	0.259143	-0.290454	-0.220649	0.136504	-0.199905	0.542802

AZULENE TBM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 S	3 A	4 S	5 A	6 S	7 A	8 S	9 S	10 A
27.76940	22.14303	19.17148	13.73292	-8.05852	-8.38299	-17.0[illegible]	-48.83609	-65.48282	-81.90087
0.257987	0.225667	-0.191056	0.234235	0.513432	-0.066570	0.330772	-0.558635	0.340747	-0.372706
0.223347	0.273314	-0.000079	0.528022	-0.000038	0.332581	-0.000063	0.707432	-0.364549	-0.000116
0.258035	0.225712	0.190964	0.234095	-0.513494	-0.066565	-0.330753	0.558537	0.340660	0.372980
0.372757	0.099443	0.258925	-0.320307	-0.245005	-0.305862	0.244029	-0.174601	-0.272168	-0.781303
0.230347	-0.160911	0.419027	-0.197871	0.151494	0.495029	0.394801	0.108145	0.440415	0.482845
0.159422	-0.365163	0.309134	0.144798	0.317292	0.107694	-0.535256	-0.345359	-0.551001	-0.230457
0.137985	-0.442207	0.000044	0.326360	-0.000063	-0.538250	0.000055	0.437295	0.589553	0.000034
0.159420	-0.365236	-0.309067	0.144703	-0.317314	0.107798	0.535202	-0.345301	-0.551115	0.230379
0.230327	-0.161013	-0.419002	-0.197953	-0.151372	0.494975	-0.394850	0.108037	0.440590	-0.482726
0.372716	0.099370	-0.258951	-0.320303	0.245109	-0.305960	-0.243974	0.174736	-0.272363	0.781143

AZULENE TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	1.17289	0.65609	-0.20067	-0.23099	-0.06839	0.18641	0.01712	-0.22685	0.01121	0.59559
2	0.65609	1.04662	0.65598	-0.07437	-0.21705	0.01715	0.17663	0.01715	-0.21704	-0.07438
3	-0.20067	0.65598	1.17291	0.59568	0.01117	-0.22688	0.01717	0.18641	-0.06844	-0.23099
4	-0.23099	-0.07437	0.59568	1.02744	0.58572	0.01118	-0.21704	-0.06842	0.17245	0.40100
5	-0.06839	-0.21705	0.01117	0.58572	0.85493	0.66410	0.14273	-0.24217	-0.18486	0.17249
6	0.18641	0.01715	-0.22688	0.01118	0.66410	0.98645	0.63886	0.02625	0.24215	-0.06842
7	0.01712	0.17663	0.01717	-0.21704	0.14273	0.63886	0.86994	0.63889	0.14273	-0.21709
8	-0.22685	0.01715	0.18641	-0.06842	-0.24217	0.02625	0.63889	0.98645	0.66407	0.01118
9	0.01121	-0.21704	-0.06844	0.17245	-0.18486	-0.24215	0.14273	0.66407	0.85494	0.58577
10	0.59559	-0.07438	-0.23099	0.40100	0.17249	-0.06842	-0.21709	0.01118	0.58577	1.02744

AZULENE TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	0.94493	0.48595	-0.25558	-0.26336	-0.05102	0.19297	0.02442	-0.22254	-0.04190	0.43775
2	0.48595	0.80678	0.48587	-0.11741	-0.19410	0.02444	0.16456	0.02445	-0.19410	-0.11742
3	-0.25558	0.48587	0.94494	0.43780	-0.04195	-0.22257	0.02447	0.19298	-0.05107	-0.26338
4	-0.26336	-0.11741	0.43780	0.75701	0.40924	-0.04193	-0.19410	-0.05105	0.12369	0.24862
5	-0.05102	-0.19410	-0.04195	0.40924	0.63328	0.48887	0.07674	-0.22144	-0.16074	0.12374
6	0.19297	0.02444	-0.22257	-0.04193	0.48887	0.75193	0.46145	-0.03297	-0.22141	0.05105
7	0.02442	0.16456	0.02447	-0.19410	0.07674	0.46145	0.64220	0.46148	0.07674	-0.19415
8	-0.22254	0.02445	0.19298	-0.05105	-0.22144	-0.03297	0.46148	0.75192	0.48883	-0.04193
9	-0.04190	-0.19410	-0.05107	0.12369	-0.16074	-0.22141	0.07674	0.48883	0.63327	0.40930
10	0.43775	-0.11742	-0.26338	0.24862	0.12374	-0.05105	-0.19415	-0.04193	0.40930	0.75704

ENERGIES FOR AZULENE ,TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	4, 6	5, 7	2, 6	4, 7	1, 6	3, 7	2, 7	1, 7
XMOMNT	-0.62070	-0.64693	0.13759	-0.31049	-0.00569	-0.17627	0.07383	0.00243
YMOMNT	-0.45097	-0.47006	0.09984	-0.42734	-0.00417	-0.12001	-0.10167	-0.00332
JUMP E	22.1159	25.0809	30.5260	30.7553	36.1524	36.1939	39.1655	44.7918
DIAG E	27.0902	30.2750	42.2754	33.1228	41.3263	45.8038	51.0897	50.5040
DIAG E	27.2424	30.4087	42.0997	33.4570	41.6980	46.0239	51.0959	51.0578
CORRSP	21.7683	32.2537	46.3297	32.4720	36.2441	50.1748	56.4648	45.7798
CORRSP	21.8562	32.4329	46.3661	32.7292	36.6964	50.1211	56.5189	46.3626

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION							
21.76830	0.01069	-0.08695	-0.06315	//	0.7732	-0.5978	0.1782	0.0000	0.0509	0.1024	0.0000	0.0000
13.52186				//	0.9427	-0.3032	0.0866	-0.0001	-0.0946	-0.0530	-0.0000	-0.0000
32.25372	1.12984	-0.73466	-0.53292	//	0.5569	0.7329	0.2101	0.0015	0.0641	-0.3234	0.0002	-0.0000
16.80947				//	0.2990	-0.9494	-0.0269	0.0000	-0.0413	-0.0829	-0.0000	-0.0000
46.32973	0.04280	-0.11921	-0.08668	//	-0.0163	0.1649	0.5005	-0.0000	-0.6555	0.5407	0.0003	0.0003
30.41050				//	0.0168	0.0518	0.7564	0.0001	0.6462	0.0857	0.0000	-0.0000
36.24407	0.04078	-0.13166	-0.09553	//	-0.1980	0.0350	0.6135	-0.0000	0.7114	0.2778	-0.0000	0.0000
39.25076				//	0.0724	-0.0515	-0.5259	-0.0000	0.6838	-0.4980	-0.0000	0.0000
50.17479	0.89840	-0.52502	-0.38132	//	0.2295	-0.2776	-0.5452	0.0001	0.2401	0.7179	0.0001	0.0001
33.81845				//	0.1276	0.0380	-0.3783	0.0000	0.3228	0.8573	0.0000	0.0000

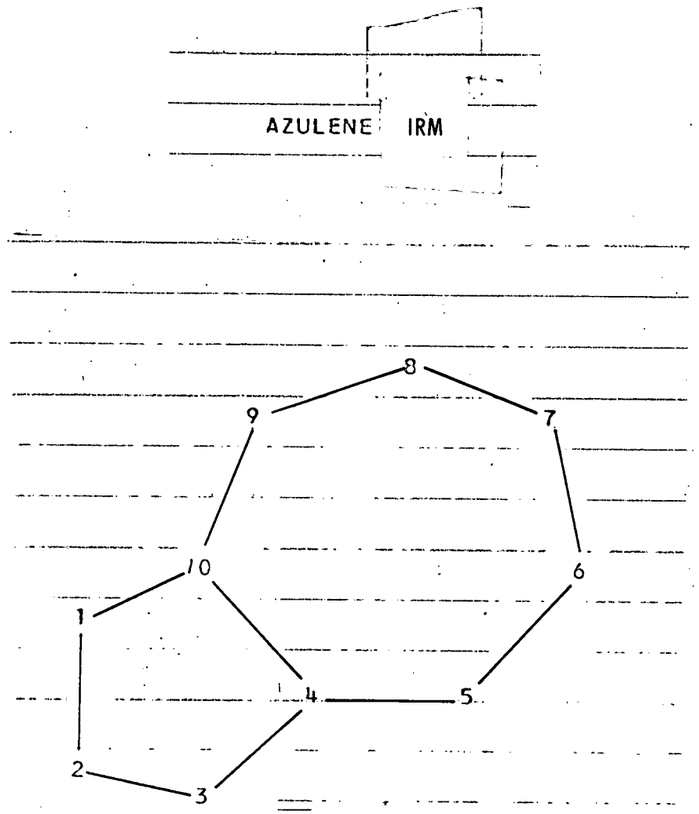
ENERGIES FOR AZULENE ,TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	5, 6	3, 6	4, 7	2, 7	1, 7	5, 8
XMOMNT	0.21386	0.28007	-0.31049	0.07383	0.00243	0.13236
YMOMNT	-0.29423	-0.38559	-0.42734	-0.10167	-0.00332	-0.18215
JUMP E	16.4415	27.5545	30.7553	39.1655	44.7918	56.8946
DIAG E	13.0709	37.0808	33.1228	51.0897	50.5040	68.1815
DIAG E	13.0226	37.1190	33.4570	51.0959	51.0578	68.5986
CORRSP	10.9019	39.2622	30.3108	56.7718	46.9059	68.8971
CORRSP	10.9532	39.1881	30.5546	56.7992	47.5234	69.3321

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
10.90185	0.01325	-0.09944	-0.13673	//	0.9671	-0.2058	0.1362	-0.0258	-0.0384	-0.0413
8.89858				//	0.9914	-0.1165	-0.0481	-0.0236	0.0003	-0.0250
39.26222	0.53730	0.33342	-0.45895	//	0.1953	0.7604	-0.4100	-0.3990	-0.1908	-0.1412
24.10003				//	0.0473	0.7121	-0.6835	-0.0851	0.1195	-0.0436
30.31076	0.05254	-0.11870	0.16330	//	-0.0108	0.5071	0.8572	0.0857	-0.0198	0.0110
27.01604				//	0.1128	0.6750	0.7176	0.0592	0.0403	-0.1081
56.77179	0.17178	0.15676	-0.21583	//	0.0480	0.1337	-0.1678	0.7430	-0.6316	0.0276
39.22336				//	0.0016	-0.0687	-0.0694	0.8203	0.5048	-0.2503
46.90592	0.28041	0.22037	-0.30334	//	0.1387	0.3080	-0.2154	0.5255	0.7502	-0.0231
47.39789				//	-0.0157	-0.0964	0.1019	-0.4916	0.8527	0.1066
68.89707	0.29906	0.18781	-0.25846	//	0.0703	0.0978	-0.0628	-0.0675	0.0065	0.9884
58.77431				//	0.0430	0.0986	0.0192	0.2721	0.0472	0.9549



ATOMIC COORDINATES

x	0.	0.	-0.9511	-1.5388	2.5378	3.1958	3.0172	2.1366	1.2171	0.9511
y	1.3090	0.3090	0.	0.8090	0.7640	1.5170	2.5010	2.9750	2.5820	1.6180

AZULENE — IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 S	3 A	4 S	5 A	6 S	7 A	8 S	9 S	10 A
1.689059	1.434824	1.308616	1.150408	1.040124	0.844996	0.780222	0.631992	0.579216	0.540539
0.341283	-0.267937	-0.199904	0.236299	0.549522	0.051154	-0.316335	0.462675	-0.198167	-0.240704
-0.308103	-0.326457	-0.000066	-0.549878	-0.000042	-0.357427	-0.000080	-0.577145	-0.187833	-0.000065
0.341327	-0.267962	0.199836	0.236120	-0.549588	0.051169	0.316307	0.462611	-0.198128	0.240884
-0.453175	-0.100270	-0.280158	-0.350226	-0.264191	-0.311599	-0.215582	-0.164886	-0.193910	-0.552519
0.278617	0.207368	0.494843	-0.258218	0.119484	-0.445646	-0.359502	-0.047558	-0.334358	0.334137
-0.195567	-0.434146	-0.369754	-0.160076	-0.337485	-0.114807	-0.473546	-0.222423	-0.430057	-0.158698
0.172228	0.516405	0.000039	0.395134	-0.000069	0.499225	-0.000048	-0.284581	-0.466176	0.000015
-0.195565	-0.434210	-0.369693	-0.159991	-0.337505	-0.114905	-0.473496	-0.222358	-0.430137	-0.158663
0.278592	0.207462	-0.494822	-0.258278	-0.119360	-0.445594	0.359535	-0.047445	-0.334469	-0.334070
-0.453135	-0.100205	-0.280189	-0.350213	-0.264296	-0.311692	-0.215532	-0.164996	-0.194012	-0.552403

AZULENE — IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 S	3 A	4 S	5 A	6 S	7 A	8 S	9 S	10 A
31.19704	23.17486	18.03465	9.99816	2.95003	-14.02779	-21.54113	-44.52949	-55.55476	-65.00165
0.262599	-0.223683	-0.174749	0.220311	0.538818	0.055649	-0.358128	0.581996	-0.260383	0.327394
0.237068	-0.272538	-0.000058	-0.512673	-0.000041	-0.388830	-0.000090	-0.725988	-0.246803	-0.000088
0.262632	-0.223704	0.174690	0.220144	-0.538883	0.055665	0.358096	0.581916	-0.260331	0.327638
0.348693	-0.083709	0.244904	-0.326529	-0.259045	-0.338976	-0.244064	-0.207409	-0.254788	-0.751508
0.214380	0.173118	0.432575	-0.240747	0.117157	-0.484801	-0.406998	-0.059823	-0.439331	0.454477
0.150478	-0.362440	-0.323226	-0.149245	-0.330912	-0.124894	-0.536109	-0.279785	-0.565074	-0.215853
0.132520	0.431113	0.000034	0.368399	-0.000068	0.543087	-0.000054	-0.357973	-0.612533	0.000021
0.150476	-0.362493	-0.323173	-0.149165	-0.330931	-0.125000	-0.536053	-0.279703	-0.565179	-0.215805
0.214361	0.173196	-0.432556	-0.240803	-0.117035	-0.484743	0.407036	-0.059681	-0.439477	-0.454385
0.348662	-0.083655	0.244932	-0.326518	-0.259148	-0.339077	-0.244007	-0.207548	-0.254922	-0.751351

AZULENE — IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	1.17208	0.64509	-0.19576	-0.20483	-0.10951	0.19957	0.02748	-0.24671	0.02357	0.59998
2	0.64509	1.00774	0.64498	-0.04046	-0.24776	-0.01302	-0.20351	-0.01303	-0.24775	-0.04049
3	-0.19576	0.64498	1.17208	0.60007	0.02357	-0.24675	0.02751	0.19957	-0.10954	-0.20484
4	-0.20483	-0.04046	0.60007	0.97273	0.60594	-0.00692	-0.22417	-0.05071	-0.17762	-0.37946
5	-0.10951	-0.24776	0.02357	0.60594	0.89290	0.65295	0.10610	-0.24010	-0.14357	0.17767
6	0.19957	-0.01302	-0.24675	-0.00692	0.65295	1.00593	0.64224	-0.00354	-0.24007	-0.05070
7	0.02748	0.20351	0.02751	-0.22417	0.10610	0.64224	0.90493	0.64227	0.10610	-0.22423
8	-0.24671	-0.01303	-0.19957	-0.05071	-0.24010	-0.00354	0.64227	1.00593	0.65292	-0.00692
9	0.02357	-0.24775	-0.10954	-0.17762	-0.14357	-0.24007	0.10610	0.65292	0.89291	0.60600
10	0.59998	-0.04049	-0.20484	-0.37946	-0.17767	-0.05070	-0.22423	-0.00692	-0.60600	-0.97276

AZULENE — IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10
1	0.97678	0.47230	-0.30676	-0.28804	-0.09587	0.22628	0.03897	-0.26109	-0.04595	0.44154
2	0.47230	0.78662	0.47221	-0.12386	-0.23963	-0.02675	0.20558	-0.02677	-0.23962	-0.12388
3	-0.30676	0.47221	0.97679	0.44160	-0.04598	-0.26112	0.03901	0.22629	-0.09591	-0.28807
4	-0.28804	-0.12386	0.44160	0.72460	0.42893	-0.06633	-0.22029	-0.04000	0.12652	0.21616
5	-0.09587	-0.23963	-0.04598	0.42893	0.66947	0.47532	0.02872	-0.23893	-0.13383	0.12656
6	0.22628	-0.02675	-0.26112	-0.06633	0.47532	0.78052	0.46233	-0.07536	-0.23890	-0.04000
7	0.03897	0.20558	0.03901	-0.22029	0.02872	0.46233	0.67828	0.46236	0.02871	-0.22035
8	-0.26109	-0.02677	0.22629	-0.04000	-0.23893	-0.07536	0.46236	0.78050	0.47528	-0.06634
9	-0.04595	-0.23962	-0.09591	0.12652	-0.13383	-0.23890	0.02871	0.47528	0.66947	0.42899
10	0.44154	-0.12388	-0.28807	0.21616	0.12656	-0.04000	-0.22035	-0.06634	0.42899	0.72465

ENERGIES FOR AZULENE , IRM APPROXIMATION 5.0

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	4, 6	5, 7	4, 7	2, 6	3, 7	2, 7	1, 6	1, 7	4, 8
XMOMNT	0.67699	0.67433	0.32435	0.07670	-0.18122	0.05377	0.04422	0.01188	0.15083
YMOMNT	0.49183	0.48996	-0.44643	0.05562	-0.13161	-0.07102	-0.03216	-0.01639	-0.10964
JUMP E	24.0260	24.4912	31.5393	37.2026	39.5758	44.7160	45.2248	52.7382	54.5277
DIAG E	31.9904	31.2350	35.5044	48.9068	49.7527	56.4603	52.3722	60.2316	68.2569
DIAG E	32.0831	31.3939	35.9388	48.6689	49.9622	56.4841	52.6362	60.7573	68.7982
CORRSP	36.8181	24.2436	35.3374	45.1889	52.3875	54.2872	55.1417	62.6516	68.7342
CORRSP	36.9822	24.3402	35.6644	45.2398	52.6045	54.6171	55.0525	62.8987	69.3233

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	E	XMOMNT	YMOMNT	//	STATE COMPOSITION							
36.81807	1.65971	0.83299	0.60521	//	0.6938	0.6485	-0.0001	-0.0896	-0.2807	0.0000	-0.0099	-0.0000	-0.1055
15.77658				//									
24.24359	0.00077	0.02215	0.01615	//	-0.6820	0.7181	-0.0000	0.1047	-0.0753	0.0000	-0.0277	-0.0000	0.0431
17.54006				//	0.6932	0.7171	-0.0000	-0.0071	-0.0470	0.0000	-0.0461	-0.0000	-0.0302
45.18890	0.02962	-0.10040	-0.07302	//	0.0429	-0.1349	0.0000	0.7519	-0.4406	0.0000	-0.4686	-0.0000	0.0296
36.74444				//	0.0431	-0.0428	-0.0001	0.8606	0.3081	-0.0001	-0.2715	0.0000	-0.2950
52.38754	0.53705	0.39728	0.28850	//	0.1713	0.1977	-0.0001	0.2169	0.8190	0.0001	-0.4619	-0.0001	0.0222
38.43986				//	0.0796	0.0059	0.0000	-0.1982	0.9156	0.0000	0.3296	-0.0000	0.0857
55.14171	0.20224	0.23761	0.17260	//	0.1099	0.0700	-0.0000	0.6066	0.2238	-0.0002	0.7511	0.0002	-0.0284
46.98651				//	0.0543	-0.0071	0.0000	0.3714	-0.2470	0.0006	0.8933	-0.0001	0.0123
68.73421	0.25829	-0.24045	-0.17479	//	0.1014	0.0394	-0.0001	0.0240	-0.0254	-0.0000	0.0460	-0.0001	0.9924
58.97638				//	0.0198	0.0165	-0.0000	0.2805	0.0153	-0.0002	-0.1265	0.0001	0.9510

ENERGIES FOR AZULENE , IRM APPROXIMATION 5.8

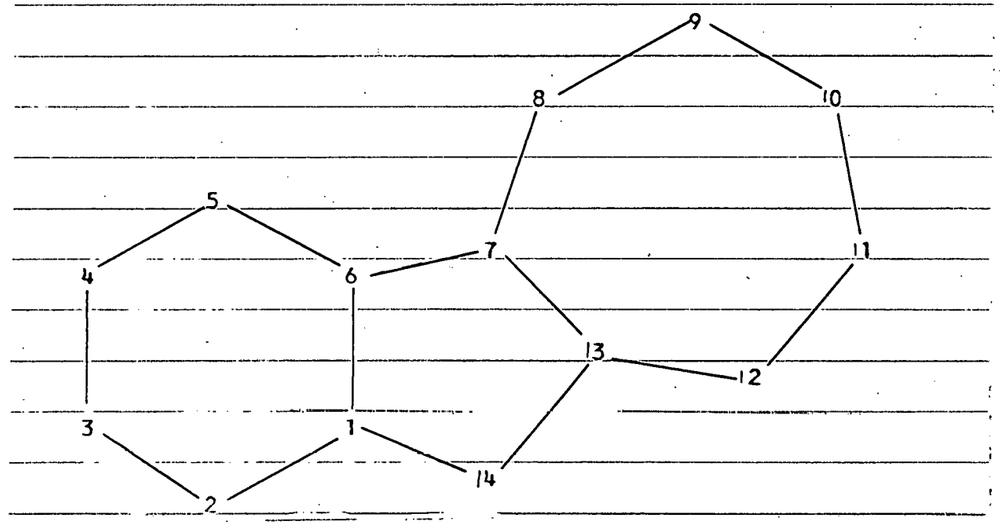
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	5, 6	4, 7	3, 6	2, 7	5, 8	1, 7	5, 9
XMOMNT	-0.18755	0.32435	-0.28174	0.05377	-0.14868	0.01188	0.18198
YMOMNT	0.25803	-0.44643	0.38789	-0.07402	0.20463	-0.01639	-0.25047
JUMP E	16.9778	31.5393	32.0624	44.7160	47.4795	52.7382	58.5048
DIAG E	13.7320	35.5844	42.2018	56.4603	58.7609	60.2316	63.6602
DIAG E	13.6292	35.9388	42.1495	56.4841	59.1067	60.7573	63.9760
CORRSP	12.3763	33.0772	43.6649	54.7696	58.0900	62.1281	66.5249
CORRSP	12.2914	33.3434	43.5748	55.1428	58.6006	62.3450	66.7436

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION						
12.37631	0.01305	-0.09260	0.12734	//	0.9814	0.1320	-0.1212	0.0233	-0.0328	-0.0273	0.0478
10.46233				//	0.9968	-0.0428	-0.0535	0.0181	-0.0205	0.0024	0.0308
33.07722	0.09186	0.15023	-0.20673	//	-0.0577	0.8848	0.4531	-0.0512	0.0284	-0.0096	-0.0705
26.97105				//	0.0188	0.9180	-0.3850	-0.0559	0.0064	-0.0623	0.0404
43.66491	0.56893	-0.32532	0.44784	//	0.1351	-0.3888	0.8298	0.2731	-0.2382	-0.0846	0.0595
31.11726				//	0.0613	0.3808	0.8963	-0.0216	-0.2038	0.0724	-0.0259
54.76961	0.27497	0.20196	-0.27798	//	-0.0924	0.1693	-0.2606	0.7632	-0.1818	-0.5277	-0.0302
50.51661				//	-0.0439	-0.0067	-0.1193	0.6139	-0.5637	0.3041	0.4435
58.09002	0.04337	-0.07786	0.10720	//	0.0131	-0.0463	0.1200	0.0480	0.7925	-0.3091	0.5073
42.45885				//	0.0108	0.0827	0.1524	0.6852	0.6703	-0.2074	0.0889
62.12813	0.04778	-0.07907	0.10878	//	0.0332	0.0011	0.0131	0.5596	0.3977	0.6756	-0.2665
54.45964				//	0.0040	0.0337	0.0215	-0.2260	0.4326	0.8146	0.3108
66.52487	0.72001	-0.29653	0.40815	//	-0.0734	0.1330	-0.0947	0.1562	-0.3494	0.4020	0.8123
60.55165)				//	-0.0151	-0.0489	0.0877	-0.3140	0.0612	-0.4380	0.8340

1,2 BENZAZULENE TBM



ATOMIC COORDINATES

x	1.7320	0.8660	0.	0.	0.8660	1.7320	2.6830
y	0.5000	0.	0.5000	1.5000	2.0000	1.5000	1.8090
	2.9490	3.8686	4.7492	4.9277	4.2698	3.2708	2.6830
	2.7730	3.1660	2.6920	1.7080	0.9550	1.0000	0.1910

1,2 BENZAZULENE — TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1.607511 1.469684 1.372061 1.344483 1.275061 1.207718 1.079813 0.904141 0.835177 0.741847 0.673961 0.556571 0.487654 0.444308

0.381330 0.255693-0.151368 0.138735 0.412937 0.297635-0.010341 0.189152 0.153303 0.178449-0.366687 0.100451-0.320307 0.386739
0.216332 0.298334 0.113026 0.284455 0.374702-0.175085 0.342941 0.077836-0.271192-0.494721-0.083700-0.139618 0.233773-0.276299
0.151156 0.312036 0.321751 0.258287 0.004652-0.444907 0.121241-0.219382 0.027800 0.339003-0.477255 0.150389-0.164971 0.235341
0.155734 0.295486 0.372022 0.076049-0.369537-0.199430-0.303750 0.007370 0.252640 0.140149-0.546780-0.130580 0.108688-0.253576
0.232181 0.250290 0.239076-0.152130-0.416404 0.277123-0.219461 0.216508-0.196512-0.485574 0.245064 0.084222-0.060657 0.335591
0.415763 0.180815-0.011623-0.288382-0.094617 0.432658 0.232781-0.091459-0.121409 0.367735 0.223051-0.020735 0.017227-0.501998
0.409844-0.161864-0.105228-0.389068-0.101870-0.210596 0.305052-0.370097 0.124283-0.077490-0.173031-0.147403 0.345157 0.407887
0.219922-0.247336 0.198435-0.391627 0.193382-0.306368 0.042746 0.401179 0.385574-0.170650 0.094568 0.349916-0.194939-0.237713
0.131548-0.308891 0.404425-0.157611 0.317433-0.047277-0.291248 0.214282-0.381827 0.256019 0.048097-0.481368 0.059557 0.127385
0.103936-0.340599 0.411343 0.171607 0.160452 0.266577-0.136950-0.484429-0.130544-0.097183-0.158118 0.515089 0.071287-0.049144
0.124333-0.339398 0.215786 0.397172-0.138577-0.271672 0.246948-0.026097 0.469015-0.154346 0.160818-0.444234-0.207565-0.016715
0.202094-0.305298-0.085963 0.382720-0.314817-0.037880 0.216753 0.494407-0.182666 0.258568-0.054344 0.283090 0.359551-0.086756
0.373121-0.241559-0.345430 0.136960-0.212273-0.303614-0.176903-0.165933-0.347122-0.116091-0.089058-0.064316-0.538826-0.178626
0.306517 0.007444-0.329558 0.197532 0.180096-0.007059-0.579004-0.059840 0.290193-0.059638 0.345023-0.020119 0.413874-0.092452

1,2 BENZAZULENE — TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

28.63689 24.21628 20.54785 19.41506 16.34647 13.03272 5.60082 -8.03385-14.95425-26.36874-36.65732-60.37105-79.61189-94.77098

0.300763 0.210915-0.129225 0.119649 0.365695 0.270832-0.009952 0.198926 0.167750 0.207184-0.446661 0.134646-0.458680 0.580197
0.170626 0.246088 0.096492 0.245322 0.331834-0.159318 0.330024 0.081858-0.296748-0.574385-0.101955-0.187146 0.334764-0.414512
0.119219-0.257391 0.274684 0.222754 0.004120-0.404916 0.116674-0.230719 0.030420 0.393592 0.581344 0.201584-0.236239 0.353065
0.122831 0.243739 0.317601 0.065586-0.327259-0.181471-0.292309 0.007751 0.276448 0.162718-0.666032-0.175032 0.155641-0.380423
0.183126 0.206458 0.204103-0.131201-0.368836 0.252168-0.211195 0.227697-0.215031-0.563766 0.298512 0.112893-0.086861 0.503464
0.327921 0.149150-0.009923-0.248708-0.083793 0.393697 0.224013-0.096185-0.132850 0.426951 0.271699-0.027793 0.024669-0.753112
0.323253-0.133518-0.089835-0.335543-0.090215-0.191632 0.293562-0.389222 0.135995-0.089968-0.210769-0.197581 0.494266 0.611924
0.173457-0.204021 0.169407-0.337750 0.171258-0.278779 0.041136 0.421910 0.421908-0.198129 0.115193 0.469033-0.279153-0.356623
0.103754-0.254796 0.345264-0.135928-0.281116-0.043020-0.280278 0.225356-0.417809 0.297245 0.058586-0.645233 0.085286 0.191106
0.081976-0.280952 0.351170 0.147999-0.142095 0.242572-0.131792-0.509463-0.142846-0.112833-0.192604 0.690433 0.102083-0.073728
0.098064-0.279961 0.184220 0.342532-0.122723 0.247208 0.237647-0.027446 0.513213-0.179201 0.195892-0.595458-0.297233-0.025076
0.159396-0.251833-0.073388 0.330068-0.278800-0.034469 0.208589 0.519956-0.199879 0.300205-0.066196 0.379458 0.514879 0.130154
0.294288-0.199256-0.294899 0.118118-0.187987-0.276273-0.170239-0.174508-0.379833-0.134785-0.108482-0.086210-0.771601-0.267980
0.241756 0.006140-0.281349 0.170357 0.159492-0.006424-0.557195-0.062933 0.317539-0.069241 0.420272-0.026968 0.592669-0.138700

1,2 BENZAZULENE — TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.02432	0.56040	-0.01444	-0.23927	0.01602	0.50765	-0.06210	-0.15104	0.01624	0.12221	0.00830	-0.15681	-0.04877	0.54866
2	0.56040	1.03631	0.71372	-0.04439	-0.34239	0.05833	0.04225	0.05115	-0.07096	-0.03468	0.09642	0.02958	-0.15696	-0.08475
3	-0.01444	0.71372	1.00637	0.61056	-0.00207	-0.24741	0.01464	0.12234	0.00024	-0.09675	-0.01338	0.09629	0.03585	-0.14516
4	-0.23927	-0.04439	0.61056	1.04869	0.70558	-0.06021	-0.13151	-0.03629	0.09655	0.02153	-0.09685	-0.00712	0.12273	0.10617
5	0.01602	-0.34239	-0.00207	0.70558	0.99055	0.58220	0.01159	-0.15730	-0.01499	0.09645	0.02779	-0.07043	-0.06831	0.02859
6	0.50765	0.05833	-0.24741	-0.06021	0.58220	1.07837	0.48817	-0.03289	-0.15739	-0.00873	0.12284	-0.03339	-0.15297	-0.15845
7	-0.06210	0.04225	0.01464	-0.13151	0.01159	0.48817	1.00881	0.63903	0.02290	-0.25317	-0.07821	0.19711	0.41337	-0.22248
8	-0.15104	0.05115	0.12234	-0.03629	-0.15730	0.03289	0.63903	0.87075	0.62145	0.13005	-0.20182	-0.17399	0.12805	-0.12989
9	0.01624	-0.07096	0.00024	0.09655	-0.01499	-0.15739	0.02290	0.62145	0.97789	0.67281	0.03421	-0.27094	-0.07819	0.19949
10	0.12221	-0.03468	-0.09675	0.02153	0.09645	-0.00873	-0.25317	0.13005	0.67281	0.88205	0.60362	0.13002	-0.17660	0.06794
11	0.00830	0.09642	-0.01338	-0.09685	0.02779	0.12284	-0.07821	-0.20182	0.03421	0.60362	0.97790	0.69813	0.02296	-0.25387
12	-0.15681	0.02958	0.09629	-0.00712	-0.07043	-0.03339	0.19711	-0.17399	-0.27094	0.13002	0.69813	0.87088	0.54250	-0.03666
13	-0.04877	-0.15696	0.03585	0.12273	-0.06831	-0.15297	0.41337	0.12805	-0.07819	-0.17660	0.02296	0.54250	1.00837	0.63961
14	0.54866	-0.08475	-0.14516	0.10617	0.02859	-0.15845	-0.22248	-0.12989	0.19949	0.06794	-0.25387	-0.03666	0.63961	1.21873

1,2 BENZAZULENE — TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.74628	0.39004	-0.05604	-0.22152	-0.01587	0.35073	-0.09458	-0.13290	0.02105	0.11340	0.01466	-0.13913	-0.08630	0.38575
2	0.39004	0.80716	0.53843	-0.09696	-0.32541	0.02817	0.05758	0.05540	-0.07478	-0.03989	0.09593	0.04186	-0.14570	-0.14507
3	-0.05604	0.53843	0.76624	0.43451	-0.05291	-0.22853	0.03245	0.11570	-0.00555	-0.09225	-0.01268	0.08939	0.04067	-0.14137
4	-0.22152	-0.09696	0.43451	0.81029	0.53142	-0.10467	-0.12978	-0.02850	0.09824	0.02166	-0.09877	-0.01388	0.12617	0.12970
5	-0.01587	-0.32541	-0.05291	0.53142	0.75853	0.40865	-0.03946	-0.14724	-0.00128	0.09171	0.02046	-0.06200	-0.05462	0.04599
6	0.35073	0.02817	-0.22053	-0.10467	0.40865	0.80787	0.33661	-0.01224	-0.15375	-0.00249	0.12845	-0.02027	-0.18164	-0.20019
7	-0.09458	0.05758	0.03245	-0.12978	-0.03946	0.33661	0.74804	0.46294	-0.03449	-0.23038	-0.05788	0.14796	0.25704	-0.26258
8	-0.13290	0.05540	0.11570	-0.02850	-0.14724	-0.01224	0.46294	0.64645	0.44597	0.06467	-0.18102	-0.14888	0.07934	-0.11667
9	0.02105	-0.07478	-0.00555	0.09824	-0.00128	-0.15375	-0.03449	0.44597	0.74560	0.49534	-0.02638	-0.24971	-0.05963	0.20901
10	0.11340	-0.03989	-0.09225	0.02166	0.09171	-0.00249	-0.23038	0.06467	0.49534	0.65456	0.42658	0.06286	-0.15453	0.07809
11	0.01466	0.09593	-0.01268	-0.09877	0.02046	0.12845	-0.05788	-0.18102	-0.02638	0.42658	0.74382	0.52188	-0.02981	-0.25013
12	-0.13913	0.04186	0.08939	-0.01388	-0.06200	-0.02027	0.14796	-0.14888	-0.24971	0.06286	0.52188	0.65117	0.36828	-0.09321
13	-0.08630	-0.14570	0.04067	0.12617	-0.05462	-0.18164	0.25704	0.07934	-0.05963	-0.15453	-0.02981	0.36828	0.73575	0.47933
14	0.38575	-0.14507	-0.14137	0.12970	0.04599	-0.20019	-0.26258	-0.11667	0.20901	0.07809	-0.25013	-0.09321	0.47933	1.00522

ENERGIES FOR 1,2 BENZAZULENE , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF NO SYMMETRY

JUMP	7, 8	7, 9	6, 8	5, 8	4, 8	6, 9	3, 8	5, 9	7,10	2, 8	4, 9	3, 9	1, 8	2, 9	6,10
XMOMNT	0.37928	0.72825	-0.69289	-0.24263	0.13270	0.47255	-0.24113	0.03728	-0.00861	0.04826	0.23210	-0.06751	-0.00078	-0.01747	0.22873
YMOMNT	-0.19373	0.63870	-0.42812	0.04793	-0.41664	-0.33447	-0.10182	-0.15959	0.05050	0.05725	-0.00598	-0.11695	0.01368	0.06503	-0.10347
JUMP E	13.6347	20.5551	21.0666	24.3803	27.4489	27.9870	28.5817	31.3007	31.9696	32.2501	34.3693	35.5021	36.6707	39.1705	39.4015
DIAG E	11.7088	26.1123	26.1290	30.6324	36.9811	33.6231	39.0083	39.7722	40.7398	43.8446	44.4821	47.3478	42.2874	52.5470	52.2314
DIAG E	11.5956	26.3919	27.6743	31.0015	37.5945	35.5612	38.9175	40.5340	41.0204	43.9673	45.4883	47.6498	44.6989	53.0625	54.1705
CORRSP	9.6178	20.0429	28.9279	28.1630	39.8421	30.9676	37.2151	35.4485	41.7866	42.4399	50.3125	46.6888	46.3978	56.6257	52.9708
CORRSP	9.8988	21.3319	30.4165	28.1180	40.3467	33.5053	38.5166	36.4305	41.9656	42.8328	50.0542	47.4553	46.9041	54.5051	57.0467

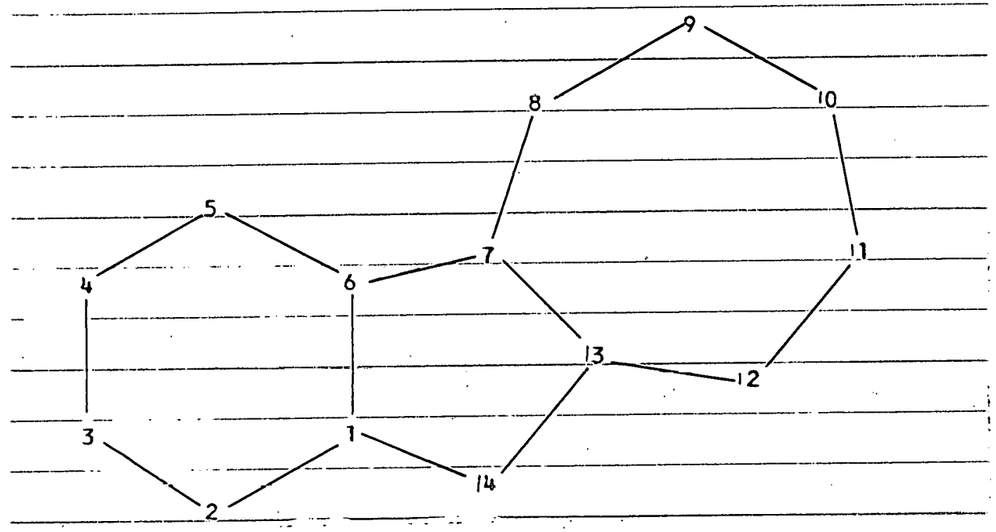
FINAL EXCITED STATES OF NO SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
9.61782	0.02311	0.21704	-0.09688	//	0.9551	0.0806	0.1642	-0.0041	-0.1312	-0.0886	0.1358	-0.0353	0.0725	0.0385
				//	-0.0273	-0.0136	-0.0313	-0.0150	0.0268					
6.62847				//	0.9782	0.0042	-0.0373	-0.1279	-0.1069	-0.0094	0.0427	0.0157	0.0993	-0.0194
				//	-0.0321	0.0041	0.0182	0.0069	0.0119					
20.04294	0.01850	0.00335	0.14728	//	-0.1465	0.6889	0.6566	0.1244	0.0275	0.0771	-0.0526	-0.0069	-0.1266	0.1195
				//	-0.0783	0.0521	0.0856	0.0289	0.0230					
13.59273				//	0.0102	0.9713	0.0227	0.0532	-0.0699	0.0685	0.0069	-0.0639	-0.1478	0.0224
				//	-0.0748	0.1007	0.0068	0.0064	-0.0360					
28.92791	0.73734	-0.58331	-0.50905	//	0.0063	-0.5085	0.3676	0.5940	-0.1621	0.3871	-0.0493	0.1028	0.0638	0.1479
				//	0.1080	-0.0114	0.1026	0.0647	-0.1089					
16.50462				//	0.0726	-0.0374	0.9270	0.2166	0.0777	0.1658	0.1116	0.0310	0.0135	0.1853
				//	0.0537	0.0049	-0.0249	0.0446	0.0116					
28.16297	0.14154	0.28229	0.19621	//	0.1235	0.2296	-0.3683	0.6866	0.4178	-0.2798	-0.2083	0.0361	-0.1292	0.0047
				//	0.0674	0.0504	0.0373	-0.0268	-0.0399					
23.58597				//	0.1143	-0.0926	-0.1700	0.8340	-0.1123	-0.2441	0.1350	-0.1731	-0.3019	0.0817
				//	-0.0799	-0.0142	-0.0209	-0.0943	0.1405					
39.84213	0.58817	0.32299	-0.49277	//	0.1152	-0.0320	0.1312	-0.2429	0.6787	0.2865	-0.1477	0.3175	0.2021	0.0042
				//	0.1781	-0.4059	-0.0518	0.0611	-0.0196					
27.51308				//	0.0946	0.0915	0.0030	-0.0438	0.8880	-0.3165	-0.0594	-0.1507	-0.0168	-0.0286
				//	0.0020	-0.0610	-0.1289	-0.0416	0.2067					
30.96763	0.84175	0.76074	0.24590	//	0.0706	0.3605	-0.4383	0.0667	-0.1901	0.6733	0.1696	0.2726	-0.0053	-0.0444
				//	-0.1471	0.0876	-0.0735	0.1313	-0.1483					
25.77174				//	0.0798	-0.0493	-0.2536	0.2494	0.3335	0.8331	-0.0662	0.1346	-0.0931	0.0226
				//	0.0396	0.0152	-0.0494	0.1488	-0.0375					
37.21507	0.07263	-0.18251	0.11218	//	-0.0842	0.0364	0.0667	0.0470	-0.0971	-0.2514	0.4931	0.4546	-0.2242	0.0646
				//	0.5236	-0.0209	-0.3556	0.0615	-0.0570					
29.51343				//	-0.0598	0.0896	-0.1096	0.0798	0.0453	-0.0756	0.6757	0.5246	0.3404	-0.0309
				//	-0.0100	0.0586	-0.3025	0.0359	0.1318					
35.44849	0.04694	0.10157	0.14431	//	0.0368	0.0693	-0.0180	-0.0913	-0.3962	-0.2187	-0.5489	0.5741	0.0790	-0.1789
				//	0.1001	-0.0620	0.3039	0.0463	-0.0542					
30.42277				//	0.0305	0.0979	-0.0004	0.3170	0.0632	-0.2295	-0.5280	0.5783	0.3015	-0.0015
				//	0.1654	-0.0196	0.2748	0.0720	-0.1405					

BENZAZULENE TBM APPROXIMATION (cont.)

41.78658	0.13448	-0.09504	0.25816	//	-0.1211	-0.1534	-0.0106	-0.1179	-0.0369	-0.1663	-0.1358	0.0069	0.9193	0.1006
				//	0.0457	-0.1553	-0.1028	0.0183	-0.0894					
37.99706				//	-0.0144	-0.0218	-0.0158	0.1977	0.0508	0.0052	-0.0202	-0.4160	0.5306	-0.1573
				//	0.0167	0.5927	-0.1192	0.0346	-0.3326					
42.43991	0.01570	0.05981	0.07159	//	0.0022	-0.0267	-0.1459	-0.1420	0.0931	-0.0765	0.2325	0.1358	-0.0466	0.6942
				//	-0.0220	0.0734	0.6113	0.0827	-0.0185					
38.36338				//	-0.0309	0.0140	-0.1161	-0.0271	-0.0483	0.0179	-0.1806	-0.0889	0.3254	0.7991
				//	-0.3675	-0.0994	-0.1896	0.0353	0.1221					
50.31247	0.82716	0.54045	0.30744	//	0.0214	0.1759	-0.1665	-0.0542	-0.2444	0.1549	-0.3375	-0.4241	0.0077	0.3602
				//	0.5932	-0.2504	-0.1252	0.0173	-0.0103					
35.61736				//	0.0417	0.0426	-0.0936	-0.0248	-0.0383	-0.0876	0.0238	-0.0805	-0.1040	0.3287
				//	0.7870	-0.1233	-0.3631	0.0275	-0.2914					
46.68876	0.11579	-0.05521	-0.23510	//	0.0682	-0.1204	0.0583	-0.1699	0.1352	-0.0260	-0.3522	0.0686	-0.0909	0.2807
				//	-0.0759	0.5856	-0.3974	0.4248	-0.1637					
41.61637				//	0.0309	-0.1210	-0.0052	-0.1506	0.0610	-0.1640	-0.0325	0.2861	-0.4913	0.2449
				//	-0.1220	0.6677	-0.0613	0.2699	-0.0978					
46.39781	0.04657	0.09389	-0.12160	//	0.0566	0.0214	0.0448	-0.0901	0.1541	0.1140	0.1205	-0.2039	0.0129	-0.4615
				//	0.4936	0.4197	0.4393	0.2211	-0.1367					
40.80853				//	-0.0158	0.0072	-0.1042	-0.0422	0.1580	0.0074	0.3991	-0.1006	0.0699	0.3410
				//	0.1913	0.0839	0.7876	-0.0475	-0.0720					
56.62573	0.38541	-0.27442	0.29112	//	-0.0344	0.0176	0.0015	0.0561	-0.0718	-0.1987	0.1111	-0.1723	-0.0207	-0.0963
				//	-0.1868	-0.4538	0.0449	0.6995	-0.4085					
47.61862				//	-0.0280	0.0324	-0.0145	0.0057	-0.1408	-0.0015	-0.0774	-0.1599	0.1265	-0.0606
				//	0.2954	0.1102	0.0740	0.6158	0.6654					
52.97082	0.09458	0.20366	-0.02265	//	-0.0145	-0.0001	-0.0499	0.0960	-0.0352	-0.0307	0.0253	0.0340	0.0668	-0.0361
				//	0.0262	-0.0222	0.0118	0.4910	0.8579					
48.81381				//	-0.0019	0.0004	0.0040	-0.0492	-0.0664	0.1435	-0.1559	0.0960	0.0261	0.0682
				//	0.2483	0.3748	-0.0300	-0.7079	0.4791					

1,2 BENZAZULENE IRM



ATOMIC COORDINATES

x	1.7320	0.8660	0.	0.	0.8660	1.7320	2.6830
y	0.5000	0.	0.5000	1.5000	2.0000	1.5000	1.8090

2.9490	3.8686	4.7492	4.9277	4.2698	3.2708	2.6830
2.7730	3.1660	2.6920	1.7080	0.9550	1.0000	0.1910

1,2 BENZAZULENE | IRM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1.748675 1.523080 1.376160 1.316891 1.221686 1.129564 1.004964 0.852513 0.791748 0.713816 0.670858 0.586603 0.545225 0.518206

0.385269-0.222698-0.153074-0.110911 0.382955 0.321856-0.010822 0.187407-0.167487 0.206102-0.368794 0.116577-0.355530 0.366366
0.225367-0.294793 0.139629-0.240735 0.432937-0.132072-0.334227 0.127796 0.241315-0.486973-0.086686-0.141259 0.256221-0.251883
0.168155-0.320946 0.341774-0.215913 0.082998-0.439736-0.077530-0.258621 0.001372 0.324254 0.478709 0.135042-0.182074 0.215512
0.171366-0.308267 0.374379-0.057535-0.339310-0.207737 0.326648-0.030426-0.251195 0.123280-0.549462-0.109033 0.138451-0.234440
0.238139-0.254373 0.226444 0.146910-0.451264 0.271841 0.167760 0.259948 0.167608-0.466153 0.260098 0.062607-0.096708 0.325819
0.410589-0.160979-0.054511 0.255391-0.151744 0.407097-0.256021-0.091439 0.138885 0.387836 0.207936-0.017473 0.070394-0.506399
0.394578 0.161766-0.144160 0.357493-0.110627-0.210793-0.296777-0.399142-0.074243-0.093186-0.171742-0.148088 0.327926 0.438562
0.213883 0.252291 0.168497 0.444958 0.155319-0.303449-0.078675 0.347419-0.416160-0.153958 0.091107 0.346113-0.187886-0.246658
0.130624 0.317153 0.384250 0.232826 0.297878-0.012010 0.297334 0.251353 0.350384 0.264828 0.038704-0.475426 0.060688 0.126177
0.106871 0.346888 0.415819-0.124225 0.153743 0.306828 0.148422-0.455098 0.167586-0.132306-0.135555 0.512652 0.066135-0.042827
0.124732 0.343105 0.248845-0.400654-0.136088 0.237720-0.259631-0.058137-0.471199-0.116592 0.144962-0.450460-0.194353-0.033617
0.197243 0.305892-0.044386-0.421252-0.291936-0.130089-0.198655 0.478750 0.162438 0.261956-0.049181 0.300750 0.341216 0.113937
0.365648 0.229713-0.320871-0.162869-0.168681-0.312228 0.191846-0.142387 0.364649-0.154382-0.093582-0.089752-0.527078-0.222718
0.315846 0.007245-0.330568-0.181872 0.190511 0.033082 0.577403-0.040481-0.303799-0.079063 0.353069-0.010874 0.398013-0.060648

1,2 BENZAZULENE | IRM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

32.44218 26.02383 20.71238 18.23418 13.75004 8.69162 0.37428-13.10928-19.93094-30.37984-37.17731-53.40090-63.20436-70.45068

0.291346-0.180449-0.130487-0.096649 0.346472 0.302835-0.010795 0.202972-0.188230 0.243943-0.450265 0.152210-0.481492 0.508938
0.170426-0.238867 0.119026-0.209780 0.391693-0.124267-0.333401 0.138410 0.271201-0.576384-0.105836-0.184435 0.346999-0.349903
0.127161-0.260058 0.291343-0.188150 0.075091-0.413749-0.077338-0.280100 0.001542 0.383788 0.584462 0.176318-0.246581 0.299378
0.129590-0.249784 0.319137-0.050136-0.306985-0.195460 0.325841-0.032953-0.282304 0.145915-0.670845-0.142359 0.187503-0.325672
0.180084-0.206115 0.193031 0.128019-0.408273 0.255776 0.167345 0.281537 0.188365-0.551741 0.317556 0.081742-0.130970 0.452611
0.310494-0.130439-0.046468 0.222551-0.137288 0.383038-0.255388-0.099033 0.156085 0.459045 0.253871-0.022814 0.095334-0.703464
0.298386 0.131077-0.122888 0.311525-0.100088-0.198336-0.296043-0.432292-0.083438-0.110296-0.209682-0.193351 0.444108 0.609228
0.161741 0.204428 0.143634 0.387743 0.140523-0.285516-0.078481 0.376273-0.467700-0.182225 0.111234 0.451904-0.254452-0.342645
0.098780 0.256984 0.327551 0.202888 0.269500-0.011300 0.296599 0.272229 0.393778 0.313452 0.047254-0.620741 0.082189 0.175278
0.080817-0.281079 0.354462-0.108251 0.139096 0.288695 0.148055-0.492895 0.188341-0.156599-0.165501 0.669346 0.089567-0.059494
0.094324 0.278013 0.212126-0.349136-0.123123 0.223672-0.258989-0.062965-0.529555-0.137999 0.176986-0.588145-0.263211-0.046698
0.149158 0.247860-0.037836-0.367085-0.264124-0.122401-0.198164 0.518511 0.182556 0.310052-0.060045 0.392676 0.462106 0.158276
0.276508-0.186133-0.273524-0.141927-0.152611-0.293776 0.191371-0.154213 0.409809-0.182727-0.114256-0.117185-0.713817-0.309389
0.238848 0.005870-0.281791-0.158486 0.172361 0.031127 0.575975-0.043843-0.341423-0.093580 0.431067-0.014197 0.539026-0.084250

1,2 BENZAZULENE — IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.96824	0.56942	-0.00204	-0.23318	0.02061	0.49948	-0.01717	-0.17252	0.00409	0.14015	0.01039	-0.18027	-0.02054	0.53640
2	0.56942	1.06346	0.70426	-0.06604	-0.32487	0.07401	0.02837	0.04771	-0.07056	-0.02756	0.10925	0.01335	-0.17364	-0.09641
3	-0.00204	0.70426	1.00196	0.61198	-0.00528	-0.24965	-0.01101	0.13787	0.01637	-0.11619	-0.02658	0.11831	0.04337	-0.13285
4	-0.23318	-0.06604	0.61198	1.06570	0.69399	-0.06365	-0.14481	-0.03800	0.10724	0.01355	-0.11239	0.01663	0.13170	0.11138
5	0.02061	-0.32487	-0.00528	0.69399	0.99991	0.60019	0.03105	-0.15099	-0.03232	0.10410	0.04479	-0.07945	-0.08903	-0.01663
6	0.49948	0.07401	-0.24965	-0.06365	0.60019	1.03399	0.48416	0.04940	-0.17024	-0.00555	0.12798	-0.06244	-0.12316	-0.12636
7	-0.01717	0.02837	-0.01101	-0.14481	0.03105	0.48416	0.95038	0.66023	0.02404	-0.26361	-0.06478	0.20358	0.39402	-0.18195
8	-0.17252	0.04771	0.13787	-0.03800	-0.15099	0.04940	0.66023	0.91634	0.60563	0.08852	-0.19190	-0.13159	0.12615	-0.18624
9	0.00409	-0.07056	0.01637	0.10724	-0.03232	-0.17024	0.02404	0.60563	0.99357	0.68215	0.01371	-0.27364	-0.06010	0.20445
10	0.14015	-0.02756	-0.11619	0.01355	0.10410	-0.00555	-0.26361	0.08852	0.68215	0.91980	0.59815	0.09356	-0.17538	0.09309
11	0.01039	0.10925	-0.02658	-0.11239	0.04479	0.12798	-0.06478	-0.19190	0.01371	0.59815	0.99633	0.69534	0.01751	-0.27097
12	-0.18027	0.01335	0.11831	0.01663	-0.07945	-0.06244	0.20358	-0.13159	-0.27364	0.09356	0.69534	0.90702	0.55398	-0.03765
13	-0.02054	-0.17364	0.04337	0.13170	-0.08903	-0.12316	0.39402	0.12615	-0.06010	-0.17538	0.01751	0.55398	0.95739	0.64230
14	0.53640	-0.09641	-0.13285	0.11138	-0.01663	-0.12636	-0.18195	-0.18624	0.20445	0.09309	-0.27097	-0.03765	0.64230	1.22589

1,2 BENZAZULENE — IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.71136	0.39835	-0.06860	-0.24608	-0.02741	0.33948	-0.08467	-0.16583	0.01361	0.14211	0.02250	-0.17459	-0.09505	0.36709
2	0.39835	0.84860	0.52910	-0.14867	-0.34290	0.03126	0.04742	0.06235	-0.08009	-0.03844	0.11697	0.03308	-0.17439	-0.17875
3	-0.06860	0.52910	0.77378	0.43294	-0.08155	-0.26209	0.01376	0.14210	0.00992	-0.11927	-0.02915	0.11738	0.05812	-0.13583
4	-0.24608	-0.14867	0.43294	0.84433	0.51975	-0.13822	-0.15176	-0.03322	0.11818	0.01585	-0.12466	0.00837	0.15158	0.15236
5	-0.02741	-0.34290	-0.08155	0.51975	0.77735	0.42721	-0.03306	-0.15035	-0.01853	0.10602	0.04014	-0.07032	-0.08069	0.00219
6	0.33948	0.03126	-0.26209	-0.13822	0.42721	0.79180	0.32793	-0.01088	-0.17999	0.00308	0.14837	-0.05194	-0.19550	-0.21524
7	-0.08467	0.04742	0.01376	-0.15176	-0.03306	0.32793	0.71072	0.48799	-0.05285	-0.26267	-0.05123	0.15333	0.22638	-0.27329
8	-0.16583	0.06235	0.14210	-0.03322	-0.15835	-0.01088	0.48799	0.69270	0.42409	0.00994	-0.18731	-0.11918	0.07174	-0.18393
9	0.01361	-0.08009	0.00992	0.11818	-0.01853	-0.17999	-0.05285	0.42409	0.76996	0.50499	-0.06623	-0.27403	-0.04858	0.23516
10	0.14211	-0.03844	-0.11927	0.01585	0.10602	0.00308	-0.26267	0.00994	0.50499	0.69502	0.41571	0.01327	-0.16926	0.11292
11	0.02250	0.11697	-0.02915	-0.12466	0.04014	0.14837	-0.05123	-0.18731	-0.06623	0.41571	0.77069	0.51916	-0.05425	-0.28742
12	-0.17459	0.03308	0.11738	0.00837	-0.07032	-0.05194	0.15333	-0.11918	-0.27403	0.01327	0.51916	0.68776	0.37634	-0.11510
13	-0.09505	-0.17439	0.05812	0.15158	-0.08069	-0.19550	0.22638	0.07174	-0.04858	-0.16926	-0.05425	0.37634	0.70456	0.48297
14	0.36709	-0.17875	-0.13583	0.15236	0.00219	-0.21524	-0.27329	-0.18393	0.23516	0.11292	-0.28742	-0.11510	0.48297	1.01806

ENERGIES FOR 1,2 BENZAZULENE , TRM APPROXIMATION = 5.8

ONE ELECTRON EXCITATIONS OF NO SYMMETRY

JUMP	7, 8	7, 9	6, 8	5, 8	6, 9	7,10	4, 8	5, 9	3, 8	7,11	4, 9	6,10	2, 8	3, 9	5,10
XMOMNT	-0.24122	0.80179	-0.87421	-0.17305	-0.38887	-0.07480	-0.15644	-0.00821	-0.15369	0.39458	0.26450	-0.19322	-0.07667	-0.04696	-0.00363
YMOMNT	0.21360	0.62714	-0.38628	0.00775	0.40966	-0.01512	0.45177	0.14335	0.11892	-0.26302	-0.01831	-0.08170	-0.05085	0.07303	0.46342
JUMP E	13.4836	20.3052	21.8009	26.8593	28.6226	30.7541	31.3435	33.6810	33.8217	37.5516	38.1651	39.0715	39.1331	40.6433	44.1299
DIAG E	12.0449	26.7305	28.9520	33.9334	34.4401	38.7291	42.6061	42.3112	44.8993	51.2500	48.8455	51.2447	51.6869	52.0243	58.0434
DIAG E	11.8724	26.9864	30.4530	34.0294	36.3695	38.6460	42.8711	42.8356	44.6957	51.3068	49.5388	52.8351	51.5836	52.2491	58.2289
CORRSP	10.5435	21.2786	33.8032	32.4749	31.4856	38.7940	43.6979	39.5002	44.4498	56.5141	50.0577	48.9345	53.8647	52.5479	59.7945
CORRSP	10.4586	22.0847	36.1478	31.3069	33.2755	39.0296	43.6750	39.7896	44.7436	49.6706	50.3354	57.6044	52.4506	53.9510	59.9775

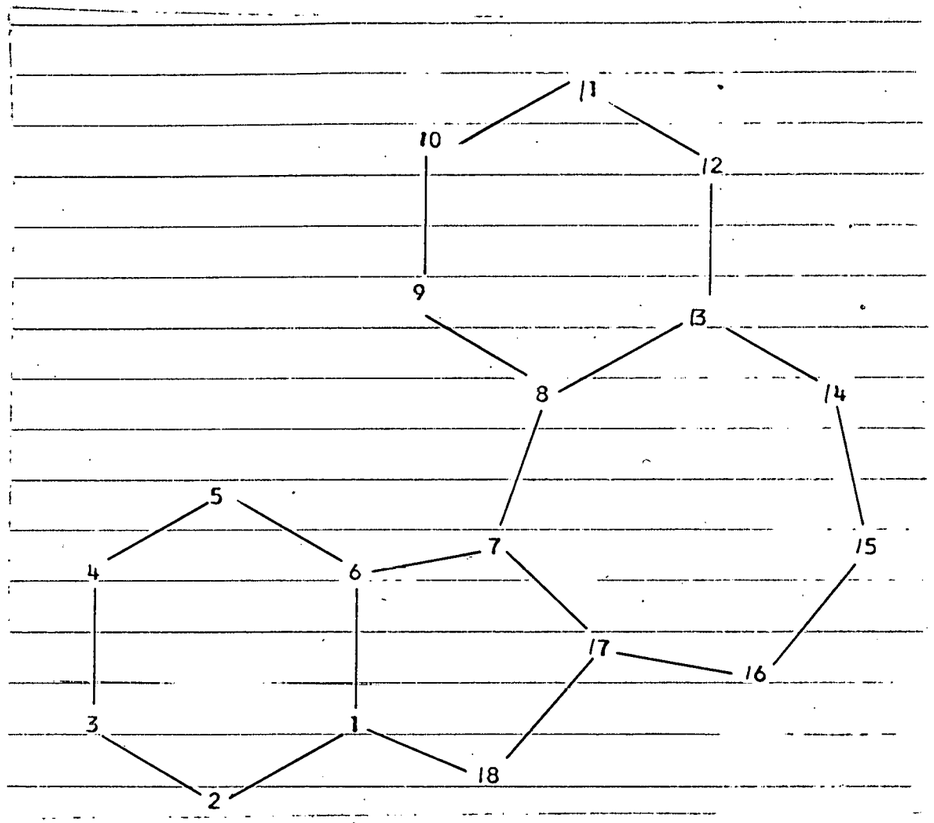
FINAL EXCITED STATES OF NO SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
10.54351	0.01573	-0.15087	0.11098	//	0.9676	-0.1171	-0.1395	0.0133	-0.0754	0.0910	-0.0662	-0.0219	-0.0909	0.0308
				//	0.0213	-0.0282	0.0258	-0.0106	0.0176					
7.26777				//	0.9786	0.0074	0.0934	0.1032	-0.0136	0.0985	-0.0277	-0.0008	-0.0034	0.0271
				//	0.0446	0.0004	-0.0128	0.0094	0.0962					
21.27863	0.04323	0.06123	0.20984	//	0.1592	0.7527	0.6146	0.0446	-0.0716	0.1045	-0.0543	0.0166	-0.0422	0.0115
				//	-0.0380	0.0454	-0.0543	-0.0235	0.0084					
13.39544				//	-0.0214	0.9784	0.0266	-0.0001	-0.0303	0.0791	0.0794	0.0750	0.0082	-0.0857
				//	-0.0172	-0.0217	-0.0133	-0.0750	0.0925					
33.80318	1.95661	-1.08252	-0.43508	//	0.0358	-0.5281	0.6401	0.2513	0.4090	0.0697	-0.0464	0.1377	-0.1087	0.0915
				//	0.1675	0.0506	-0.0495	0.0025	0.0215					
18.28186				//	-0.1146	-0.0310	0.9567	0.1156	-0.1700	-0.0304	-0.0330	-0.0313	0.0805	0.0249
				//	0.0612	0.0266	-0.0963	-0.0035	0.0681					
32.47487	0.07574	-0.01445	-0.23375	//	-0.0818	-0.0767	-0.0104	0.7919	-0.5199	0.1411	0.0799	-0.1745	-0.0339	-0.0162
				//	0.0228	-0.1588	-0.0431	-0.0564	0.0319					
24.92725				//	-0.1057	-0.0380	-0.0509	0.7371	0.0903	0.5656	-0.0277	0.2129	0.0062	-0.0056
				//	-0.0711	0.1397	-0.0283	-0.0050	-0.2046					
31.48558	0.33916	0.36291	0.34872	//	-0.0358	0.3014	-0.3858	0.4127	0.6227	0.2043	-0.3524	-0.0474	-0.1327	0.0437
				//	0.0594	-0.0017	0.0311	-0.0470	-0.0812					
27.10188				//	0.0099	-0.0022	0.1790	-0.0602	0.9454	-0.0661	0.2058	0.0846	0.0304	-0.0375
				//	-0.0540	0.0557	0.0053	0.0303	0.0856					
38.79397	0.02004	-0.09800	-0.05042	//	-0.0529	-0.0434	0.0415	-0.2460	0.0886	0.6669	0.3430	-0.5474	-0.0489	0.0997
				//	0.1153	-0.1175	0.0356	-0.0264	-0.1475					
30.79906				//	0.0187	-0.0425	0.1332	-0.4894	0.0325	0.3859	-0.3576	0.4921	-0.3024	-0.2554
				//	0.0424	-0.0802	0.0341	-0.0238	-0.2321					
43.69792	0.36162	-0.02181	0.44060	//	0.0580	0.0923	-0.1064	0.1342	0.1764	0.0632	0.6266	0.4475	0.1494	0.3508
				//	-0.2430	-0.0696	-0.0252	-0.3476	-0.0042					
31.82944				//	-0.0019	-0.1355	0.0272	-0.0915	-0.1803	0.2325	0.8426	0.1755	-0.1293	-0.1239
				//	0.0495	-0.3155	-0.0225	-0.0456	0.0926					
39.50021	0.05522	-0.00919	-0.18107	//	-0.0639	-0.0946	-0.0406	-0.0798	-0.2105	0.6549	-0.3258	0.5015	0.2882	-0.1368
				//	-0.0810	0.1830	-0.0674	0.0274	-0.0300					
37.70449				//	-0.0052	-0.0523	-0.0843	0.3114	-0.0528	-0.5108	-0.0798	0.6035	0.0007	-0.3225
				//	0.2735	-0.0387	-0.0892	-0.0549	0.2599					

BENZAZULENE IRM APPROXIMATION (cont.)

44.44981	0.09694	-0.02261	0.22534	//	0.0922	0.0642	0.0025	0.0730	0.1069	-0.1162	0.0210	-0.1567	0.8180	-0.0218
				//	0.4838	-0.0125	-0.1322	-0.0684	0.0784					
36.15884				//	0.0350	-0.0500	-0.0283	-0.2453	-0.1255	0.0909	0.1212	0.3286	0.7475	-0.0190
				//	-0.2628	0.3994	0.0201	0.0012	0.0203					
56.51406	0.87751	0.41215	-0.44189	//	-0.0402	-0.0564	-0.0214	-0.0223	-0.1569	-0.0453	-0.2185	-0.2388	-0.0094	0.5590
				//	-0.0353	0.6481	-0.0448	-0.3549	0.0314					
44.53106				//	-0.0018	0.0128	0.0311	0.0470	0.0457	-0.0673	-0.1081	0.2935	0.1710	0.6035
				//	-0.1259	-0.5317	0.2946	-0.3333	-0.0490					
50.05769	0.45252	0.45907	0.04278	//	-0.0623	0.1006	-0.0599	-0.0414	-0.1442	0.0603	0.0454	0.2691	-0.1864	0.2961
				//	0.6061	-0.0327	0.5708	0.1425	0.2118					
39.56695				//	-0.0784	0.0182	-0.0826	-0.0997	0.0718	0.2923	-0.0835	-0.0122	0.2923	0.2558
				//	0.7473	-0.1142	-0.1448	0.3001	0.2137					
48.93446	0.36236	-0.09820	0.40557	//	0.0551	0.0445	-0.0595	0.1708	0.1027	0.0303	0.4151	-0.0301	-0.0318	-0.4560
				//	0.0234	0.6931	0.1526	0.2311	0.1048					
48.87284				//	0.0258	0.0160	0.0008	-0.0756	-0.0066	-0.0870	0.1906	0.0626	-0.2003	0.2941
				//	0.4012	0.5311	-0.0242	-0.5513	-0.2671					
53.86472	0.26664	-0.31784	-0.12403	//	0.0324	-0.0504	0.1130	0.1076	0.0696	-0.0122	-0.0943	-0.1611	0.3820	0.2191
				//	-0.5007	-0.0432	0.5984	0.3556	-0.0335					
46.32279				//	-0.0117	0.0246	0.0680	0.0485	-0.0537	-0.0232	0.0796	0.0376	-0.1027	-0.0262
				//	0.1531	0.2146	0.8973	0.3028	0.0597					
52.54792	0.33069	0.33675	0.18597	//	-0.0015	0.0496	-0.0951	0.0286	0.0119	0.0453	0.0909	0.0292	-0.0251	0.4095
				//	-0.0101	0.0357	-0.5076	0.7055	0.2263					
41.88039				//	-0.0029	0.0571	-0.0010	-0.0373	-0.0747	-0.1148	0.0930	0.3214	-0.3487	0.5309
				//	-0.2316	0.2277	-0.2531	0.5366	0.0610					
59.79454	0.52364	-0.16031	0.42454	//	-0.0282	-0.0184	0.0019	-0.0573	0.0906	0.1194	-0.0614	-0.1200	-0.0064	-0.1111
				//	-0.1820	-0.1113	0.0193	-0.2077	-0.9239					
54.99767				//	-0.0943	-0.1017	-0.0440	-0.0489	-0.0163	0.2746	-0.1409	-0.0270	-0.1965	0.0790
				//	-0.1599	0.1831	0.0444	-0.3209	0.8193					

1,2 4,5 DIBENZAZULENE TBM



ATOMIC COORDINATES

X	1.7320	0.8660	0.	0.	0.8660	1.7320	2.6830	2.9490	2.1490
y	0.5000	0.	0.5000	1.5000	2.0000	1.5000	1.8090	2.7730	3.3730

2.2685	3.1881	3.9882	3.8686	4.7492	4.9277	4.2698	3.2708	2.6830
4.3660	4.7590	4.1590	3.1660	2.6920	1.7080	0.9550	1.0000	0.1910

1,2 4,5 DIBENZAZULENE | TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1.621994	1.527233	1.432856	1.374964	1.324648	1.277604	1.246794	1.183781	1.069839	0.945416	0.820624	0.753205	0.732670
0.318520	-0.312470	0.080877	0.005888	-0.299089	0.366620	-0.000328	-0.285861	0.071277	0.156647	-0.150576	-0.000327	-0.255893
0.173219	-0.240415	0.215237	0.218188	-0.265874	0.173548	0.353372	-0.021058	-0.333507	0.084698	0.285833	-0.353081	0.314981
0.118012	-0.201097	0.296602	0.325589	-0.050633	-0.171420	0.353674	0.270180	-0.165649	-0.175379	-0.057158	0.353382	-0.085272
0.124190	-0.189172	0.304957	0.276470	0.199284	-0.366373	0.000276	0.222251	0.286649	-0.045915	-0.244305	-0.000276	-0.222632
0.194967	-0.203018	0.238243	0.094450	0.312762	-0.240671	-0.353379	-0.104674	0.246753	0.185524	0.234708	-0.353088	0.326407
0.367150	-0.244509	0.112872	-0.132979	0.212113	0.095676	-0.353630	-0.300193	-0.216826	0.004886	0.073728	0.353339	-0.130908
0.411752	-0.006840	-0.121153	-0.302338	0.265296	-0.018316	0.000103	0.166975	-0.379348	-0.343214	-0.137710	0.000102	0.071256
0.327952	0.307442	0.082169	-0.204603	0.284461	0.089391	0.353563	0.057980	0.019369	0.200229	-0.306040	-0.353752	-0.101374
0.172208	0.256788	0.187889	-0.258516	-0.041453	-0.230143	0.353678	-0.289530	0.211947	0.207698	0.046984	0.354072	0.363119
0.106096	0.241222	0.247461	-0.188235	-0.339121	-0.348395	0.000107	-0.273686	0.040624	-0.246259	0.271996	-0.000313	-0.292062
0.095258	0.258663	0.246232	-0.027574	-0.404708	-0.161848	-0.353481	0.085627	-0.200396	-0.153175	-0.244686	-0.353669	-0.046629
0.134017	0.311446	0.184468	0.146344	-0.193328	0.166331	-0.353648	0.337476	-0.097346	0.280156	-0.094140	0.354041	0.342595
0.242615	0.406889	0.077381	0.250014	0.150384	0.349053	-0.000225	0.165762	0.172883	0.091224	0.313190	-0.000430	-0.324607
0.149602	0.250550	-0.130853	0.438208	0.106661	0.137002	-0.000240	-0.271914	0.126881	-0.500495	0.172499	0.000240	0.110533
0.134476	0.128438	-0.306912	0.415855	-0.010056	-0.194924	-0.000015	0.368271	-0.136969	0.019485	-0.438575	0.000190	0.204858
0.189295	0.023860	-0.407377	0.193628	-0.119852	-0.356171	0.000225	-0.002359	-0.165593	0.496025	0.146256	-0.000430	-0.332354
0.342580	-0.077493	-0.407534	-0.121754	-0.147605	-0.205674	0.000240	0.366593	0.090138	-0.129195	0.332368	0.000240	0.155109
0.262335	-0.182564	-0.186244	-0.076263	-0.339611	0.143128	-0.000088	0.108369	0.570442	-0.124216	-0.250102	0.000087	0.093075

OVERLAP EIGNVALUES AND EIGNVECTORS

0.668829	0.633199	0.497803	0.471859	0.416665
0.322796	-0.090836	-0.088147	0.455847	0.207274
0.113607	0.126262	0.042574	-0.344693	-0.136691
-0.475232	-0.096808	0.001519	0.281743	0.115791
0.524080	0.017610	-0.045668	-0.258206	-0.136985
-0.227996	0.070632	0.091402	0.270793	0.207975
-0.218158	-0.122580	-0.140311	-0.321248	-0.354559
0.197921	0.202353	0.282211	-0.039191	0.422714
-0.165436	-0.073864	0.041694	0.198787	-0.434063
0.126031	-0.274085	-0.081521	-0.160588	0.260270
-0.003681	0.481401	0.124237	0.144921	-0.181180
-0.121059	-0.441549	-0.171334	-0.149617	0.168087
0.166156	0.174937	0.224457	0.175305	-0.216175
-0.101962	0.181547	-0.285549	-0.225649	0.343035
0.136167	-0.370886	0.315041	-0.108902	-0.160730
-0.080781	0.369753	-0.355601	-0.007432	0.036923
-0.027746	-0.178667	0.408514	-0.092966	0.073423
0.118031	-0.104285	-0.475606	0.206381	-0.210478
-0.328555	0.131295	0.277060	-0.309489	0.001344

1,2 4,5 DIBENZAZULENE | TBM APPROXIMATION

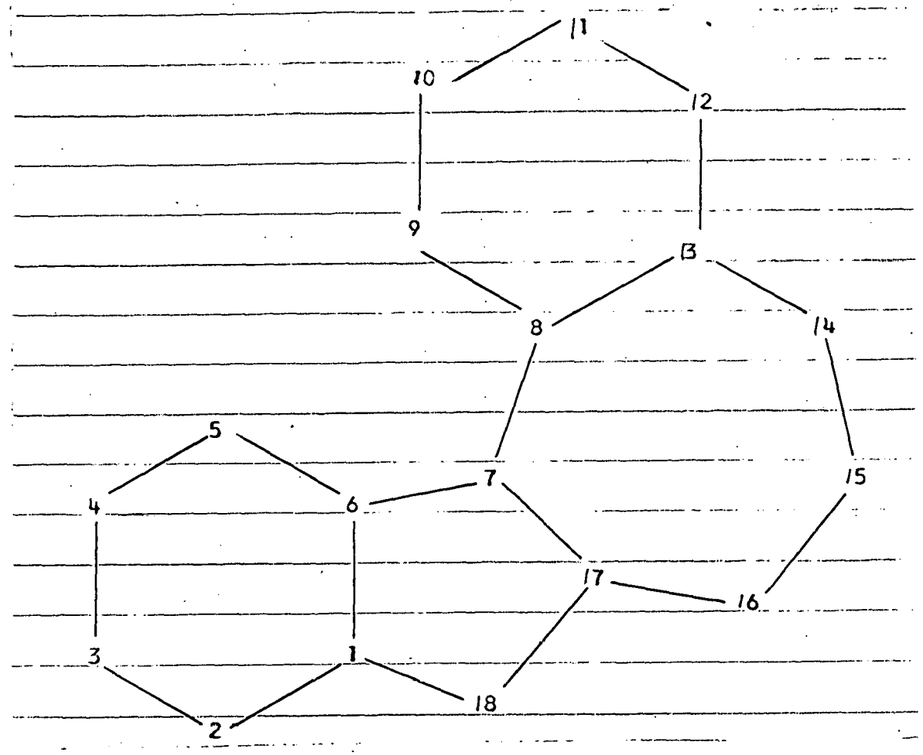
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

28.90935	26.02546	22.77414	20.55886	18.47624	16.38063	14.92246	11.70387	4.92131	-4.35255	-16.47860	-24.70161	-27.50681
0.250099	-0.252846	0.067566	0.005022	-0.259867	0.324353	-0.000294	-0.262735	0.068911	0.161106	-0.166220	-0.000377	-0.298953
0.136010	-0.194540	0.179810	0.186074	-0.231007	0.153540	0.316472	-0.019354	-0.322438	0.087109	0.315530	-0.406834	0.367986
0.092662	-0.162724	0.247784	0.277667	-0.043993	-0.151657	0.316742	0.248324	-0.160151	-0.180371	-0.063096	0.407182	-0.099622
0.097513	-0.153075	0.254763	0.235778	0.173150	-0.324135	0.000247	0.204272	0.277135	-0.047222	-0.269687	-0.000318	-0.260096
0.153086	-0.164279	0.199030	0.080548	0.271746	-0.212925	-0.316478	-0.096206	0.238563	0.190805	0.259093	-0.406843	0.381333
0.288283	-0.197853	0.094294	-0.113407	0.184296	0.084645	-0.316703	-0.275909	-0.209629	0.005025	0.081388	0.407132	-0.152936
0.323304	-0.005535	-0.101212	-0.257838	0.230505	-0.016204	0.000092	0.153467	-0.366757	-0.352983	-0.152018	0.000118	0.083247
0.257505	0.248777	0.068645	-0.174488	0.247157	0.079085	0.316643	0.053290	0.018726	0.205928	-0.337836	-0.407607	-0.118433
0.135216	0.207789	0.156964	-0.220466	-0.036017	-0.203611	0.316746	-0.266108	0.204912	0.213610	0.051865	0.407976	0.424223
0.083306	0.195193	0.206731	-0.160529	-0.294648	-0.308229	0.000096	-0.251546	0.039276	-0.253268	0.300255	-0.000360	-0.341210
0.074796	0.209306	0.205704	-0.023515	-0.351635	-0.143189	-0.316570	0.078700	-0.193744	-0.157535	-0.270108	-0.407513	-0.054475
0.105229	0.252017	0.154106	0.124805	-0.167975	0.147155	-0.316718	0.310175	-0.094115	0.288130	-0.103920	0.407941	0.400246
0.190499	0.329248	0.064645	0.213215	0.130662	0.308812	-0.000202	0.152353	0.167144	0.093820	0.345729	-0.000496	-0.379231
0.117466	0.202741	-0.109316	0.373710	0.092674	0.121207	-0.000215	-0.249917	0.122670	-0.514741	0.190421	0.000277	0.129133
0.105589	0.103930	-0.256397	0.354647	-0.008737	-0.172452	-0.000013	-0.338479	-0.132423	0.020040	-0.484141	0.000219	0.239331
0.148633	0.019307	-0.340326	0.165129	-0.104135	-0.315109	0.000201	-0.002169	-0.160097	0.510143	0.161451	-0.000496	-0.388282
0.268990	-0.062706	-0.340457	-0.103834	-0.128248	-0.181962	0.000215	0.336937	0.087146	-0.132872	0.366899	0.000277	0.181210
0.205983	-0.147728	-0.155590	-0.065038	-0.295075	0.126627	-0.000079	0.099602	0.551508	-0.127752	-0.276086	0.000101	0.108738

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECT

-37.32823	-43.67076	-76.05327	-84.37990	105.54373
0.394703	-0.114153	-0.124933	0.663610	0.321109
0.138914	0.158673	0.060342	-0.501795	-0.211761
-0.581096	-0.121659	0.002153	0.410153	0.179383
-0.640826	0.022131	-0.064726	-0.375890	-0.212217
-0.278785	0.088763	0.129547	0.394213	0.322195
-0.266755	-0.154045	-0.198868	-0.467665	-0.549281
0.242011	0.254296	0.399986	-0.057053	0.654868
-0.202289	-0.092825	0.059094	0.289389	-0.672449
0.154106	-0.344441	-0.115543	-0.233781	0.403210
-0.004501	0.604974	0.176085	0.210972	-0.280683
-0.148027	-0.554893	-0.242837	-0.217809	0.260400
0.203169	0.219842	0.318130	0.255204	-0.334897
-0.124676	0.228149	-0.404718	-0.328494	0.531429
0.166500	-0.466091	0.446518	0.158536	-0.249002
-0.098776	0.464666	-0.504004	-0.010819	0.057201
-0.033927	-0.224530	0.579000	-0.135337	0.113746
0.144324	-0.131054	-0.674092	-0.300445	-0.326072
-0.401745	0.164998	0.392686	-0.450547	0.002083

1,2 4,5 DIBENZAZULENE IRM



ATOMIC COORDINATES

X	1.7320	0.8660	0.	0.	0.8660	1.7320	2.6830	2.9490	2.1490
y	0.5000	0.	0.5000	1.5000	2.0000	1.5000	1.8090	2.7730	3.3730

2.2685	3.1881	3.9882	3.8686	4.7492	4.9277	4.2698	3.2708	2.6830
4.3660	4.7590	4.1590	3.1660	2.6920	1.7080	0.9550	1.0000	0.1910

1,2 4,5 DIBENZAZULENE | IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1.775404	1.611817	1.467740	1.375075	1.284616	1.227176	1.176794	1.105842	0.987332	0.882582	0.777334	0.728307	0.710196	0.666231	0.634771	0.551249	0.535197	0.502319
0.324286	-0.297129	0.049497	-0.030033	0.300524	-0.307285	0.026575	0.319719	0.060251	-0.160812	0.161175	-0.070722	-0.275935	-0.308795	-0.131366	-0.133356	0.459671	0.192959
0.181592	-0.241767	0.213134	0.211094	0.278270	-0.168408	0.386755	0.052968	-0.303343	-0.124455	-0.267240	-0.255057	0.381996	-0.125930	0.137386	0.078978	-0.339354	-0.119895
0.133309	-0.211000	0.303631	0.334680	0.059190	0.122301	0.334422	-0.302876	-0.123182	0.211844	0.043472	0.334779	-0.145166	0.472211	-0.075913	-0.031202	0.276046	0.102270
0.139477	-0.197811	0.315033	0.295336	-0.195823	0.300266	-0.074468	-0.263878	0.291407	0.076622	0.241278	-0.088814	-0.212672	-0.515270	-0.013962	-0.004839	-0.263602	-0.118044
0.207409	-0.194548	0.248184	0.105156	-0.315882	0.209345	-0.397548	0.118750	0.182803	-0.223008	-0.223630	-0.239182	0.392842	0.231365	-0.100699	0.050027	0.289183	0.190354
0.367357	-0.229178	0.086524	-0.133702	-0.192434	-0.087829	-0.328839	0.309292	-0.253965	0.016267	-0.071341	0.302072	-0.244641	0.215432	-0.108247	-0.090916	-0.354624	-0.354288
0.394871	-0.009377	-0.135972	-0.278674	-0.266765	-0.027538	0.007756	-0.174403	-0.369824	0.370159	0.108271	0.008116	0.080454	-0.203206	0.197019	0.282386	-0.004736	0.439909
0.311782	0.293560	0.066682	-0.174838	-0.324312	-0.108676	0.333560	-0.106128	0.000440	-0.179504	0.309780	-0.361797	-0.013018	0.164003	-0.059721	0.045257	0.207502	-0.455263
0.193133	0.255342	0.200128	-0.252593	-0.061800	0.255181	0.357068	0.238769	0.222951	-0.218702	-0.015211	0.434032	0.256321	-0.129344	-0.279096	-0.092234	-0.160500	0.243833
0.120505	0.261841	0.254942	-0.193093	0.288229	0.379989	0.050841	0.251288	0.071364	0.246759	-0.287936	-0.083601	-0.297563	-0.017145	0.463561	0.122551	0.143112	-0.162275
0.107776	0.281982	0.246377	-0.049638	0.414147	0.162658	-0.317939	-0.066785	-0.221249	0.171982	0.235752	-0.346285	0.086354	0.149104	-0.437485	-0.146943	-0.147731	0.153832
0.139147	0.327852	0.172760	0.130702	0.235013	-0.206089	-0.348608	-0.286888	-0.115888	-0.269500	0.098704	0.441986	0.206723	-0.193616	0.204239	0.193617	0.180416	-0.203858
0.230424	0.392901	0.049925	0.237544	-0.118075	-0.378792	-0.007646	-0.142158	0.174483	-0.122040	-0.289801	-0.110042	-0.325693	0.120957	0.161300	-0.276178	-0.253917	0.356394
0.148133	0.248441	-0.149672	0.441669	-0.090828	-0.156811	-0.003113	0.284655	-0.161840	0.465052	-0.209597	0.028577	0.135866	-0.116585	-0.368673	0.299521	0.126940	-0.154822
0.132731	0.130404	-0.311124	0.419763	0.000364	0.233436	0.027679	0.350758	-0.134230	0.009180	0.448263	0.047491	0.158714	0.057151	0.374309	-0.349056	-0.039781	0.028386
0.184116	0.030739	-0.399048	0.196576	0.106545	0.397792	0.016588	-0.066959	-0.174089	-0.474397	-0.133905	-0.061196	-0.306477	0.041035	-0.198223	0.414697	-0.045634	0.083248
0.333172	-0.078219	-0.390036	-0.125519	0.132852	0.183611	-0.022828	-0.375329	0.086696	0.118742	-0.348860	0.027197	0.171246	-0.126391	-0.082431	-0.502842	0.146977	-0.227229
0.270514	-0.179028	-0.200038	-0.124134	0.335275	-0.122610	-0.022410	-0.074969	0.583024	0.085628	0.250528	0.016043	0.115782	0.326006	0.140166	0.295238	-0.262524	0.009638

1,2 4,5 DIBENZAZULENE | IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
32.92548	28.61587	24.02460	20.56331	16.70272	13.95585	11.32580	7.21552	-0.96727	-10.02958	-21.59467	-28.12327	-30.76288	-37.76785	-43.37600	-61.37032	-65.47203	-74.69177
0.243377	-0.234039	0.040856	-0.025611	0.265150	-0.277388	0.024498	0.304034	0.060636	-0.171175	0.182808	-0.082870	-0.327429	-0.378318	-0.164882	-0.179613	0.628333	0.272254
0.136285	-0.190432	0.175925	0.180017	0.245516	-0.152023	0.356522	0.050369	-0.305282	-0.132476	-0.303108	-0.298868	0.453283	-0.154283	0.172439	0.106373	-0.463870	-0.169166
0.100049	-0.166198	0.250623	0.285408	0.052223	0.110402	0.308279	-0.288017	-0.123970	0.225496	0.049307	0.392284	-0.172256	0.578527	-0.095282	-0.042025	0.377333	0.144297
0.104678	-0.155809	0.260035	0.251857	-0.172773	0.271052	-0.068647	-0.250932	0.293270	0.081560	0.273661	-0.104070	-0.252361	-0.631280	-0.017524	-0.006518	-0.360323	-0.166554
0.155661	-0.153239	0.204856	0.089675	-0.278700	0.188977	-0.366471	0.112924	0.183972	-0.237379	-0.253644	-0.280267	0.466153	0.283456	0.126391	0.067379	0.395290	0.268579
0.275702	-0.180516	0.071419	-0.114019	-0.169784	-0.079284	-0.303133	0.294118	-0.255589	0.017315	-0.080916	0.353960	-0.290295	0.263935	-0.135865	-0.122452	-0.484743	-0.499881
0.296351	-0.007386	-0.112234	-0.237647	-0.235365	-0.024859	0.007149	-0.165847	-0.372189	0.394013	0.122803	0.009510	0.095468	-0.248957	0.247286	0.380337	-0.006474	0.620688
0.233993	0.231227	0.055041	-0.149098	-0.286138	-0.098103	0.307485	-0.100922	0.000443	-0.191072	0.351358	-0.423943	-0.015447	0.200927	-0.074958	0.060955	0.283639	-0.642351
0.144947	0.201124	0.165190	-0.215406	-0.054526	0.230354	0.329155	0.227056	0.224377	-0.232796	-0.017253	0.508586	0.304155	-0.158465	-0.350304	-0.124227	-0.219390	0.344036
0.090439	0.206244	0.210434	-0.164666	0.254302	0.343018	0.046867	0.238960	0.071820	0.262661	-0.326582	-0.097961	-0.353093	-0.021005	0.581833	0.165060	0.195623	-0.228962
0.080886	0.222107	0.203364	-0.042330	0.365400	0.146832	-0.293085	-0.063508	-0.222663	0.183065	0.267394	-0.405766	0.102469	0.182674	-0.549105	-0.197913	-0.201936	0.217049
0.104430	0.258238	0.142599	0.111460	0.207351	-0.186038	-0.321357	-0.272813	-0.116629	-0.286867	0.111952	0.517906	0.245301	-0.237207	0.256349	0.260778	0.246614	-0.287633
0.172934	0.309474	0.041210	0.202573	-0.104177	-0.341938	-0.007048	-0.135184	0.175598	-0.129905	-0.328697	-0.128944	-0.386473	0.148190	0.202454	-0.371977	-0.347084	0.502853
0.111174	0.195689	-0.123543	0.376646	-0.080137	-0.141554	-0.002869	0.270690	0.162875	0.495022	-0.237728	0.033486	0.161221	-0.142834	-0.462736	0.403417	0.173517	-0.218445
0.099615	0.102714	-0.256808	0.357965	0.000321	0.210724	-0.025515	0.333550	-0.135089	-0.009771	0.508427	0.055648	0.188333	0.070018	0.469809	-0.470133	-0.054377	0.040051
0.138180	0.024212	-0.329383	0.167636	0.094004	0.359089	-0.015291	-0.063674	-0.175202	-0.504968	-0.151878	-0.071707	-0.363671	0.050274	-0.248797	0.558543	-0.062378	0.117458
0.250046	-0.061611	-0.321944	-0.107040	0.117215	0.165747	-0.021044	-0.356915	0.087251	0.126394	-0.395683	0.031869	0.203204	-0.154847	-0.103462	-0.677264	0.200905	-0.320607
0.203021	-0.141014	-0.165115	-0.105859	0.295811	-0.110681	-0.020658	-0.071291	0.586753	0.091147	0.284153	0.018799	0.137389	0.399405	0.175928	0.397648	-0.358849	0.013598

1,2 4,5 DIBENZAZULENE — IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.97619	-0.55849	-0.00852	-0.21835	0.02670	0.47905	-0.03413	-0.13335	0.01306	0.07108	-0.00760	-0.04336	-0.00182	0.15023	-0.01892	-0.19351	-0.03226	0.56749
2	0.55849	1.06322	0.71424	-0.06719	-0.33256	0.07963	0.04503	0.02851	-0.02877	-0.00062	0.04379	-0.00870	-0.04968	-0.01183	0.09133	0.00156	-0.15835	-0.10396
3	-0.00852	-0.07142	1.00740	0.59817	-0.01056	-0.23129	0.00376	0.10501	-0.00944	-0.06153	-0.00275	0.03772	0.01633	-0.12409	-0.03135	0.12983	0.05233	-0.16041
4	-0.21835	-0.06719	0.59817	1.06731	0.70582	-0.07096	-0.17313	-0.02209	0.05795	-0.00669	-0.06645	0.01514	0.07723	-0.00443	-0.09008	0.03245	0.11424	-0.12469
5	0.02670	-0.33256	-0.01056	0.70582	1.00538	0.58325	0.01555	-0.11943	0.02718	0.05640	0.00935	-0.02469	-0.03044	0.10435	0.04790	-0.08582	-0.09771	-0.00649
6	0.47905	0.07963	-0.23129	-0.07096	0.58325	1.05175	0.52777	0.01147	-0.09438	-0.02765	0.09805	0.00333	-0.12522	0.00938	0.09747	-0.07522	-0.09787	-0.15588
7	-0.03413	-0.04503	-0.00376	-0.17313	0.01555	0.52777	0.98265	0.54092	-0.01036	-0.18581	-0.00742	0.05026	0.03291	-0.25508	-0.08265	0.21741	-0.42606	-0.23698
8	-0.13335	0.02851	0.10501	-0.02209	-0.11943	0.01147	0.54092	0.91583	0.55771	0.04149	-0.21912	-0.02282	0.48210	0.09448	-0.13602	-0.11954	0.09214	-0.10904
9	0.01306	-0.02877	-0.00944	0.05795	0.02718	-0.09438	0.01036	0.55771	1.01901	0.72629	-0.01645	-0.34756	0.01536	0.03813	0.02778	-0.08012	-0.08355	-0.09986
10	0.07108	-0.00062	-0.06153	-0.00669	0.05640	-0.02765	-0.18581	0.04149	0.72629	0.96731	0.58332	0.02552	-0.20825	-0.08676	0.11709	0.08801	-0.07352	0.06073
11	-0.00760	0.04379	-0.00275	-0.06645	0.00935	0.09805	-0.00742	-0.21912	-0.01645	0.58332	1.01353	0.72593	-0.00212	-0.17946	-0.02164	0.13396	0.04403	-0.12480
12	-0.04336	-0.00870	0.03772	0.01514	-0.02469	0.00333	0.05026	-0.02282	-0.34756	0.02552	0.72593	0.97749	0.54819	0.09114	-0.16082	-0.06178	0.07180	-0.01204
13	-0.00182	-0.04968	0.01633	0.07723	-0.03044	-0.12522	0.03291	0.48210	0.01536	-0.20825	-0.00212	0.54819	0.94904	0.57422	0.00807	-0.20594	-0.03966	0.14386
14	0.15023	-0.01183	-0.12409	-0.00443	0.10435	0.00938	-0.25508	0.09448	0.03813	-0.08676	-0.17946	0.09114	0.57422	0.88242	0.65084	0.12423	-0.20147	0.06514
15	0.01892	0.09133	-0.03135	-0.09008	0.04790	0.09747	-0.08265	-0.13602	0.02778	0.11709	-0.02164	-0.16082	0.00807	0.65084	1.00786	0.65671	-0.00335	-0.22197
16	-0.19351	0.00156	-0.12983	0.03245	-0.08582	-0.07522	0.21741	-0.11954	-0.08012	0.08801	0.13396	-0.06178	-0.20594	0.12423	0.65671	0.87476	0.57352	-0.02035
17	-0.03226	-0.15835	-0.05233	0.11424	-0.09771	-0.09787	0.42606	0.09214	-0.08355	-0.07352	0.04403	0.07180	-0.03966	-0.20147	0.00335	0.57352	0.97055	0.59792
18	0.56749	-0.10396	-0.16041	0.12469	0.00649	-0.15588	-0.23698	-0.10904	0.09986	0.06073	-0.12480	-0.01204	0.14386	0.06514	-0.22197	-0.02035	0.59792	1.26827

(613)

(614)

335

340

1,2 4,5 DIBENZAZULENE | IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.72059	-0.38624	-0.07627	-0.23015	-0.01997	0.31731	-0.10595	-0.12576	0.02564	0.07398	-0.01347	-0.04671	0.00551	0.15337	0.03204	-0.18815	-0.10755	0.40182
2	0.38624	0.84885	0.54008	-0.15049	-0.35141	0.03825	0.06616	0.03954	-0.03276	-0.00493	0.04912	-0.00662	-0.05635	-0.02262	0.09692	0.02134	-0.15726	-0.18842
3	-0.07627	0.54008	0.78035	0.41815	-0.08804	-0.24231	0.03199	0.10850	-0.01632	-0.06323	0.00180	0.03867	0.01163	-0.12743	-0.03495	0.12884	-0.06787	-0.16639
4	-0.23015	-0.15049	0.41815	0.84658	0.53235	-0.14653	-0.18193	-0.01516	0.06126	-0.00499	-0.07299	0.01182	0.08568	-0.00120	-0.10041	0.02380	-0.13273	0.16780
5	-0.01997	-0.35141	-0.08804	0.53235	0.78401	0.40920	-0.05193	-0.12779	0.02257	0.05557	0.00321	-0.02310	-0.01972	0.10590	0.04491	-0.07602	-0.09015	0.02800
6	0.31731	0.03825	-0.24231	-0.14653	0.40920	0.81106	0.37646	-0.04588	-0.11867	-0.02229	0.10990	0.01236	-0.13209	0.01449	0.11580	-0.06385	-0.16933	-0.24883
7	-0.10595	0.06616	0.03199	-0.18193	-0.05193	0.37646	0.75809	0.37090	-0.07517	-0.18723	0.02245	0.05745	-0.02754	-0.25459	-0.07531	0.16545	0.26198	-0.33737
8	-0.12576	0.03954	-0.10850	-0.01516	-0.12779	-0.04588	0.37090	0.65942	0.38606	-0.02221	-0.22996	-0.07407	0.31799	0.03399	-0.13418	-0.11254	0.04458	-0.10218
9	0.02564	-0.03276	-0.01632	0.06126	0.02257	-0.11867	-0.07517	0.38606	0.80285	0.55154	-0.09569	-0.36286	-0.03244	0.04551	0.03583	-0.07353	-0.08575	0.12727
10	0.07398	-0.00493	-0.06323	-0.00499	0.05557	-0.02229	-0.18723	-0.02221	0.55154	0.73780	0.40255	-0.05071	-0.21805	-0.06058	0.12154	-0.08114	-0.06712	0.06672
11	-0.01347	0.04912	-0.00180	-0.07299	0.00321	0.10990	0.02245	-0.22996	-0.09569	0.40255	0.78722	0.55203	-0.06838	-0.18259	-0.00806	0.13624	0.04435	-0.14445
12	-0.04671	-0.00662	0.03867	0.01182	-0.02310	0.01236	0.05745	-0.07407	-0.36286	-0.05071	0.55203	0.75851	0.37422	0.00861	-0.16474	-0.04405	0.07958	-0.02195
13	0.00551	-0.05635	0.01163	0.08568	-0.01972	-0.13209	-0.02754	0.31799	-0.03244	-0.21805	-0.06838	0.37422	0.69070	0.39955	-0.06027	-0.20614	-0.03189	0.16613
14	0.15337	-0.02262	-0.12743	-0.00120	0.10590	0.01449	-0.25459	0.03399	0.04551	-0.06058	-0.18259	0.00861	0.39955	0.66810	0.47217	0.03951	-0.20000	0.08759
15	0.03204	0.09692	-0.03495	-0.10041	0.04491	0.11580	-0.07531	-0.13418	0.03583	0.12154	-0.00806	-0.16474	-0.06027	0.47217	0.77825	0.47873	-0.06693	-0.23310
16	-0.18815	-0.02134	0.12884	0.02380	-0.07602	-0.06385	0.16545	-0.11254	-0.07353	-0.08114	-0.13624	-0.04405	-0.20614	0.03951	0.47873	0.65808	0.39763	-0.09847
17	-0.10755	-0.15726	-0.06787	0.13273	-0.09015	-0.16933	0.26198	0.04458	-0.08575	-0.06712	0.04435	0.07958	-0.03189	-0.20000	-0.06693	0.39763	0.71616	0.43469
18	0.40182	-0.18842	-0.16639	0.16780	0.02800	-0.24883	-0.33737	-0.10218	0.12727	0.06672	-0.14445	-0.02195	0.16613	0.08759	-0.23310	-0.09847	0.43469	1.09823

ENERGIES FOR 1,2 4,5 DIBENZAZULENE , IRM APPROXIMATION

ONE ELECTRON EXCITATIONS OF No SYMMETRY

JUMP	9,10	8,10	9,11	7,10	6,10	5,10	8,11	4,10	7,11	3,10	6,11	2,10	1,10
XMOMNT	0.33411	0.76332	-0.55450	-0.14050	-0.43086	-0.22240	0.60941	-0.02780	-0.00435	-0.01227	0.18250	0.04115	0.01776
YMOMNT	-0.22733	0.56893	-0.75558	-0.05662	0.39618	0.42249	-0.44119	0.07684	-0.06518	-0.11743	0.00477	-0.00025	0.00895
JUMP E	9.0623	17.2451	20.6274	21.3554	23.9854	26.7323	28.8102	30.5929	32.9205	34.0542	35.5505	38.6454	42.9551
DIAG E	7.0162	23.0393	24.2509	27.1341	33.9607	34.4756	37.3028	42.4701	42.3043	45.2179	47.4273	50.3463	50.9317
DIAG E	7.0801	23.4092	24.0383	27.1899	34.1407	34.7264	37.3963	42.5221	42.0837	45.2663	47.3308	50.6616	51.5456
CORRSP	5.3357	18.5143	27.0498	26.0209	31.4859	38.0853	32.5678	40.8694	45.3042	46.4824	51.0253	47.8916	55.2442
CORRSP	5.4342	18.7684	27.0506	26.0622	31.5040	32.9213	38.2092	41.1319	45.2705	46.4756	50.8260	48.1959	55.5411

FINAL EXCITED STATES OF No SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
5.33573	0.01218	0.17168	-0.15562	//	0.9625	-0.1936	-0.1123	-0.0286	0.0243	0.1140	-0.0544	-0.0237	0.0156	-0.0656	0.0044
				//	-0.0197	0.0241									
1.93586				//	0.9930	0.0222	-0.0140	-0.0332	-0.0553	0.0872	-0.0209	0.0183	-0.0229	0.0004	0.0127
				//	-0.0067	-0.0051									
18.51429	0.04709	0.24336	-0.02425	//	0.1893	0.7133	0.5989	-0.2417	-0.0806	0.0861	-0.1175	-0.0329	0.0022	0.0173	-0.0355
				//	-0.0806	0.0368									
13.33278				//	-0.0416	0.9545	-0.1409	-0.1219	-0.1800	0.0174	-0.0849	0.0430	-0.0020	0.0956	-0.0145
				//	-0.0368	-0.0005									
27.04984	1.55314	-0.85471	-0.78719	//	-0.0354	-0.5328	0.7556	0.2128	0.0891	0.2072	0.1273	0.0983	-0.0663	-0.1022	0.0810
				//	0.0181	-0.0144									
15.62214				//	0.0054	0.1198	0.9726	-0.1444	0.0316	-0.0137	-0.1076	-0.0072	-0.0708	0.0129	-0.0135
				//	-0.0233	-0.0041									
26.02093	0.07966	0.18063	0.19840	//	0.0327	0.2636	-0.0935	0.8313	-0.3205	0.3454	-0.0275	-0.0216	-0.0517	0.0035	-0.0582
				//	-0.0071	0.0166									
23.27815				//	-0.0049	0.0793	0.1143	0.9212	-0.1446	0.2523	-0.1909	0.0790	-0.0090	0.0394	-0.0150
				//	0.0423	-0.0331									
31.48594	0.02060	-0.10738	0.06209	//	0.1153	0.1954	0.0770	0.3971	0.7110	-0.4465	0.0593	0.0936	-0.0063	0.1273	-0.1626
				//	0.1184	-0.1055									
25.44055				//	0.0390	0.1255	-0.0788	0.0456	0.8752	-0.0355	-0.4124	0.1615	0.0311	-0.0659	-0.0300
				//	0.0426	-0.0545									
38.08532	0.55837	-0.39294	0.43630	//	-0.0685	-0.0146	-0.0583	-0.0421	0.2379	0.4192	-0.3329	0.4285	0.6328	0.2248	-0.0062
				//	-0.0524	-0.0969									
29.05229				//	-0.0850	-0.0751	-0.0165	-0.2653	-0.0601	0.8560	-0.1897	0.0825	0.2894	-0.1778	-0.0424
				//	-0.1408	0.0192									
32.56778	0.25683	0.36706	0.22519	//	-0.0211	0.1456	-0.1426	-0.1555	0.2808	0.4909	0.7209	-0.0577	-0.0882	-0.0971	-0.2548
				//	-0.0936	0.0042									
28.59522				//	-0.0135	0.1653	0.0602	0.1257	0.3645	0.2882	0.7861	-0.0840	-0.1803	-0.0843	-0.2666
				//	-0.0371	-0.0061									

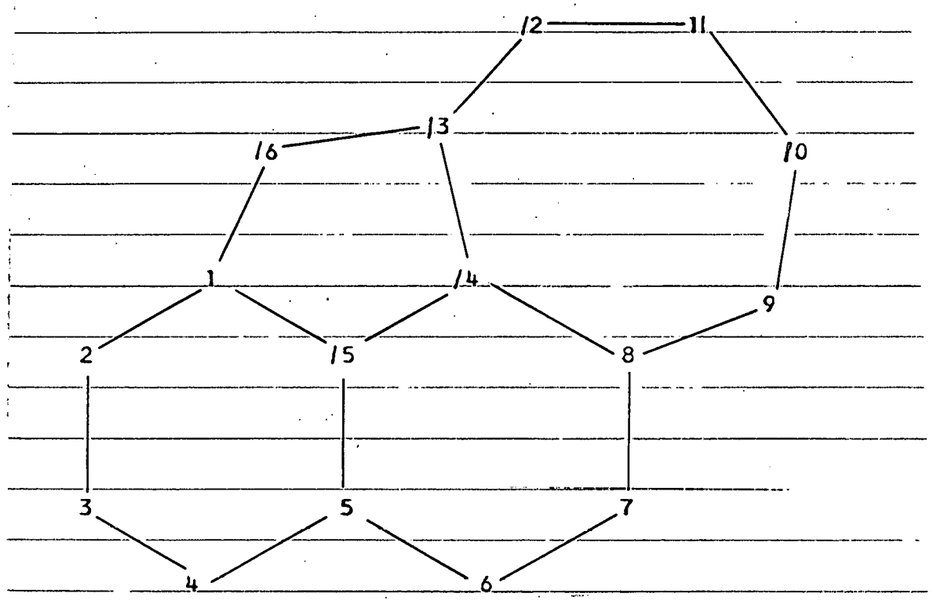
cont.

DIBENZAZULENE IRM APPROXIMATION (cont.)

40.86940	0.47519	0.33787	-0.39907	//	0.0994	-0.0266	0.0325	-0.0332	-0.3784	-0.2473	0.2304	0.6939	-0.2001	0.4014	-0.1670
				//	-0.0664	-0.1217									
34.73089				//	-0.0113	-0.0514	0.0388	-0.0484	-0.0380	-0.0203	0.2296	0.8877	0.1170	0.2781	0.1074
				//	0.0520	-0.2136									
45.30424	0.88377	0.32132	-0.59622	//	0.0618	-0.0274	0.1184	0.0499	-0.3043	-0.2626	-0.4011	-0.2450	0.6940	0.0009	-0.2143
				//	0.2542	-0.0658									
38.16316				//	0.0433	-0.0070	0.0495	0.0432	0.0372	-0.1339	0.0500	-0.2026	0.7343	0.3954	-0.4741
				//	0.0132	-0.1019									
46.48238	0.09874	0.03228	-0.22116	//	0.0218	-0.0612	0.0336	0.0504	0.0669	0.0113	0.1731	-0.3244	0.0585	0.7139	0.2749
				//	-0.3699	0.3562									
40.33011				//	-0.0292	-0.0960	-0.0566	-0.0803	0.0862	0.2493	-0.1097	-0.1959	-0.4075	0.8085	0.0580
				//	-0.1532	-0.1170									
51.02534	0.53395	0.49601	-0.00729	//	0.0347	0.1667	-0.0523	0.0935	0.0122	-0.1731	0.2734	0.3233	0.1969	-0.3691	0.7220
				//	-0.1500	0.1772									
43.56839				//	0.0155	0.0802	0.0590	0.0882	0.1681	0.0326	0.2299	-0.2064	0.3973	0.1122	0.8199
				//	-0.0901	0.0807									
47.89164	0.09895	0.21519	0.04778	//	0.0399	0.0837	-0.0207	-0.0617	0.0094	0.1813	0.1149	-0.1191	-0.1278	0.3050	0.4760
				//	0.5281	-0.5585									
44.81610				//	-0.0125	0.0270	0.0032	-0.0752	-0.0291	0.1268	0.0091	-0.1925	-0.0187	-0.0625	0.1147
				//	0.7101	-0.6463									
55.24422	0.02303	0.03069	0.09413	//	-0.0015	0.0270	-0.0091	-0.0464	0.0273	0.0906	-0.0181	0.1644	-0.0649	0.0938	-0.0112
				//	0.6782	0.6983									
50.63448				//	-0.0028	0.0015	0.0113	-0.0466	0.0275	0.1167	0.0108	0.0674	0.0032	0.2055	-0.0192
				//	0.6591	0.7082									

Delenzajul IRM

NAPTHYLAZULENE | TBM



ATOMIC COORDINATES

x	0.8725	0.	0.	0.8500	1.7321	2.6095	3.4641	3.4641
y	2.0350	1.5500	0.5500	0.0210	0.5000	0.0210	0.5500	1.5500

4.3695	4.5370	3.8987	2.8930	2.3700	2.5700	1.7321	1.2695
1.9780	2.9690	3.7400	3.7710	2.9900	2.0350	1.5000	2.9620

NAPTHYLAZULENE TBM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS — OVERLAP EIGNVALUES A

1.625180 1.485690 1.437441 1.357872 1.316309 1.228356 1.203508 1.062801 0.905066 0.878535 0.735331 0.695043 0.637791 0.537584 0.489432 0.404047

0.310140 0.240415 0.306288-0.027796 0.339517-0.276623 0.265964-0.020997-0.176612 0.146432 0.071308 0.196942 0.415550 0.157733-0.354991-0.261483
0.177484 0.273257 0.201606 0.247541 0.354629-0.188822 0.148541-0.332799 0.341601 0.111805-0.305548 0.268274-0.248746-0.173065 0.282675 0.177255
0.138174 0.296350 0.049787 0.386858 0.113591-0.452476-0.144576-0.063602 0.045941-0.202062 0.256067-0.529245-0.052200 0.165879-0.228329-0.165459
0.173004 0.310796-0.113672 0.314284-0.209619-0.230471-0.268492 0.317483-0.360257-0.012392 0.031027 0.386741 0.326248-0.138111 0.190200 0.222892
0.303109 0.318891-0.253353 0.070548-0.385319 0.240097-0.077899 0.145494 0.093581 0.209446-0.291195 0.050367-0.430528 0.094171-0.167240-0.376518
0.194264 0.127729-0.371365-0.012358-0.257420 0.032453 0.458789-0.020934 0.405375-0.125405-0.116958-0.222948 0.462161 0.075640 0.047620 0.254195
0.190992-0.068609-0.409503-0.089587 0.056392-0.212790 0.461740-0.152751-0.252578-0.149676 0.421857 0.227768-0.250342-0.238798 0.069693-0.239807
0.291844-0.261238-0.358852-0.117694 0.326651-0.228958-0.072616-0.018183-0.303425 0.197586-0.336824-0.061127-0.089288 0.372677-0.191234 0.327877
0.156809-0.280482-0.244894 0.231417 0.345270 0.116781-0.150255 0.329663 0.265537 0.403145 0.134492-0.184360 0.142064-0.431185 0.056248-0.157261
0.107643-0.295107-0.077351 0.458253 0.118375 0.340235-0.052145 0.103224 0.202631-0.400029 0.193723 0.292161-0.120938 0.441688 0.075101 0.053617
0.117970-0.304241 0.105138 0.436753-0.189904 0.199839 0.105718-0.300170-0.341098-0.201963-0.341402-0.179207 0.037180-0.402337-0.211411 0.025995
0.194219-0.308706 0.267378 0.178630-0.366778-0.156841 0.141235-0.181997-0.072018 0.505823 0.175339-0.071109 0.067071 0.317678 0.367705-0.117966
0.327179-0.267909 0.322457-0.149305-0.246361-0.297898 0.010679 0.217309 0.316892-0.043439 0.129285 0.230331-0.117632-0.172999-0.480971 0.225746
0.408161-0.172807 0.018230-0.324534 0.018920-0.120193-0.387190-0.187838 0.108975-0.363715-0.202694 0.032789 0.249680-0.030984 0.280979-0.411473
0.401904 0.191655 0.035300-0.196860-0.028424 0.418123-0.257279-0.256722-0.084621 0.034715 0.398580-0.222444-0.154088-0.115250 0.109786 0.433839
0.221456 0.012874 0.312277-0.099646 0.108781 0.040297 0.326395 0.589680-0.196752-0.222400-0.159858-0.302637-0.214664-0.010034 0.350800 0.032757

NAPTHYLAZULENE TBM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS — ZEROTH HAMILTONIAN EIGNVALU

28.87013 24.53442 22.83887 19.77945 18.03429 13.95190 12.69049 4.43466 -7.87202-10.37613-27.01248-32.92848-42.62127-64.55537-78.29003110.69430

0.243280 0.197241 0.255467-0.023853 0.295926 0.249589 0.242437-0.020367-0.185643 0.156227 0.083157 0.236229 0.520336 0.215130-0.507424-0.411365
0.139222 0.224185 0.168155 0.212431 0.309098-0.170369 0.135401-0.322817 0.359070 0.119283-0.356318 0.321790-0.311470-0.236041 0.404056 0.278857
0.108387 0.243131 0.041526 0.331988 0.099007-0.408257-0.131787-0.061695 0.048290-0.215578 0.298615-0.634820-0.065363 0.226239-0.326373-0.260300
0.135708 0.254983-0.094811 0.269707-0.182705-0.207948-0.244741 0.307960-0.378680-0.013221 0.036182 0.463889 0.408515-0.188367 0.271873 0.350654
0.237765 0.261624-0.211315 0.060541-0.335847 0.216633-0.071008 0.141130 0.098367 0.223456-0.339580 0.060414-0.539092 0.128439-0.239053-0.592339
0.152385 0.104791-0.309747-0.010605-0.224370 0.029282 0.418204-0.020306 0.426105-0.133793-0.136391-0.267423 0.578701 0.103164 0.068068 0.399900
0.149818-0.056288-0.341556-0.076880 0.049152-0.191995 0.420894-0.148169-0.265495-0.159688 0.491953 0.273204-0.313469-0.325692 0.099619-0.377264
0.228929-0.214324-0.299309-0.101001 0.284711-0.206583-0.066193-0.017638-0.318942 0.210803-0.392792-0.073321-0.111804 0.508288-0.273350 0.515816
0.123004-0.230113-0.204260 0.198593 0.300940 0.105369-0.136963 0.319775 0.279116 0.430112 0.156839-0.221137 0.177888-0.588086 0.080401-0.247402
0.084437-0.242112-0.064517 0.393256 0.103177 0.306984-0.047533 0.100128 0.212994-0.426788 0.225912 0.350442-0.151434 0.602411 0.107349 0.084351
0.092538-0.249605 0.087693 0.374806-0.165522 0.180309 0.096366-0.291166-0.358541-0.215473-0.398129-0.214956 0.046555-0.548740-0.302191 0.040895
0.152350-0.253268 0.223013 0.153294-0.319686-0.141513 0.128742-0.176538-0.075701 0.539658 0.204473-0.085294 0.083984 0.433275 0.525597-0.185584
0.256646-0.219798 0.268953-0.128128-0.214730-0.268785 0.009735 0.210791 0.333097-0.046345 0.150767 0.276278-0.147294-0.235950-0.687500 0.355144
0.320170-0.141774 0.015205-0.278504 0.016491-0.108447-0.352939-0.182204 0.114547-0.388044-0.236373 0.039330 0.312640-0.042258 0.401631-0.647330
0.315262 0.157238 0.029443-0.168938-0.024774 0.377261-0.234520-0.249021-0.088948 0.037037 0.464808-0.266818-0.192943-0.157187 0.156929 0.682515
0.173715 0.010562 0.260462-0.085512 0.094814 0.036359 0.297522 0.571992-0.206813-0.237277-0.186420-0.363008-0.268794-0.013685 0.501434 0.051533

NAPTHYLAZULENE | TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1.02308	0.58055	-0.01024	-0.25635	0.00587	0.04319	0.01220	-0.10059	0.00481	0.08856	0.01746	-0.12716	-0.05559	-0.05243	0.45996	0.58540
2	0.58055	1.00465	0.67343	-0.01169	-0.26930	-0.06170	0.18003	0.06654	-0.14508	-0.05611	0.15527	0.05866	-0.17788	-0.03407	0.08056	-0.07136
3	-0.01024	0.67343	1.00328	0.66206	0.00133	-0.13500	-0.00668	0.10374	0.00603	-0.07736	-0.01570	0.07646	0.03110	-0.01001	-0.20193	-0.15832
4	-0.25635	-0.01169	0.66206	1.01632	0.59012	0.05658	-0.21027	-0.05776	0.17248	0.04653	-0.15753	-0.03853	0.15237	-0.03821	-0.07924	0.08598
5	-0.00587	-0.26930	0.00133	0.59012	0.99217	0.52205	0.00486	-0.18012	-0.01775	0.09121	0.02432	-0.05705	-0.04861	0.01556	0.50828	0.02643
6	-0.04319	-0.06170	-0.13500	0.05658	0.52205	0.94072	0.75028	0.06719	-0.15641	-0.07847	0.09954	0.10946	-0.06893	-0.25604	0.00021	0.08127
7	0.01220	0.18003	-0.00668	-0.21027	0.00486	0.75028	1.00380	0.53509	0.00726	-0.14828	0.00531	0.07697	-0.03314	-0.02405	-0.20673	-0.03869
8	-0.10059	0.06654	0.10374	-0.05776	-0.18012	0.06719	0.53509	0.92154	0.54128	0.09002	-0.17046	-0.14098	0.10067	0.52230	-0.00788	-0.09437
9	0.00481	-0.14508	0.00603	0.17248	-0.01775	-0.15641	0.00726	0.54128	0.96178	0.69422	0.04417	-0.26654	-0.07377	0.04331	-0.10379	-0.23840
10	-0.08856	-0.05611	-0.07736	0.04653	0.09121	-0.07847	-0.14828	0.09002	0.69422	0.91560	0.60702	0.10050	-0.17545	-0.18610	0.03915	0.04132
11	0.01746	0.15527	-0.01570	-0.15753	0.02432	0.09954	0.00531	-0.17046	0.04417	0.60702	0.97113	0.66167	0.02390	-0.10252	0.09130	-0.28717
12	-0.12716	0.05866	0.07646	-0.03853	-0.05705	0.10946	0.07697	-0.14098	-0.26654	0.10050	0.66167	0.89723	0.60968	0.14187	-0.10320	-0.00541
13	-0.05559	-0.17788	0.03110	0.15237	-0.04861	-0.06893	-0.03314	0.10067	-0.07377	-0.17545	0.02390	0.60968	1.00373	0.44072	-0.11034	0.55481
14	-0.05243	-0.03407	0.01001	-0.03821	0.01556	-0.25604	-0.02405	0.52230	0.04331	-0.18610	-0.10252	0.14187	0.44072	1.00423	0.58500	-0.22746
15	0.45996	0.08056	-0.20193	-0.07924	0.50828	0.00021	-0.20673	-0.00788	-0.10379	0.03915	0.09130	-0.10320	-0.11034	0.58500	1.09198	-0.19898
16	0.58540	-0.07136	-0.15832	0.08598	0.02643	0.08127	-0.03869	-0.09437	0.23840	0.04132	-0.28717	-0.00541	0.55481	-0.22746	-0.19898	1.24874

NAPTHYLAZULENE TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.74596	0.40866	-0.05256	-0.23784	-0.02277	0.04316	0.02321	-0.08726	0.00651	0.08103	0.02411	-0.10938	-0.08343	-0.08717	0.30861	0.42107
2	0.40866	0.78031	0.49867	-0.07238	-0.25362	-0.04158	0.17439	0.06394	-0.14666	-0.05800	0.15290	0.06843	-0.16569	-0.01842	0.04982	-0.13813
3	-0.05256	0.49867	0.76090	0.48473	-0.04068	-0.12484	-0.00046	0.09816	-0.00014	-0.07372	-0.01464	0.07027	0.03439	0.02413	-0.18533	-0.15226
4	-0.23784	-0.07238	0.48473	0.79305	0.42499	0.00041	-0.20014	-0.04147	0.17210	0.04337	-0.15764	-0.04349	0.15277	-0.03890	-0.11739	0.11392
5	-0.02277	-0.25362	-0.04068	0.42499	0.71596	0.35519	-0.04096	-0.16534	0.00168	0.08707	0.01515	-0.05046	-0.03626	-0.02145	0.34240	0.03896
6	0.04316	-0.04158	-0.12484	0.00041	0.35519	0.71353	0.57184	0.01791	-0.14483	-0.06553	0.09088	0.10196	-0.05155	-0.23720	-0.03845	0.08082
7	0.02321	0.17439	-0.00046	-0.20014	-0.04096	0.57184	0.77314	0.36954	-0.04917	-0.14126	0.02019	0.08185	-0.03455	-0.05551	-0.18830	-0.03761
8	-0.08726	0.06394	0.09816	-0.04147	-0.16534	0.01791	0.36954	0.65312	0.37179	0.03630	-0.15008	-0.12053	0.05666	0.36187	-0.03670	-0.08423
9	0.00651	-0.14666	-0.00014	0.17210	0.00168	-0.14483	-0.04917	0.37179	0.74385	0.51860	-0.02355	-0.24658	-0.05021	-0.00559	-0.10436	0.24655
10	0.08103	-0.05800	-0.07372	0.04337	0.08707	-0.06553	-0.14126	0.03630	0.51860	0.68346	0.42905	0.03971	-0.15376	-0.16441	0.03937	0.05151
11	0.02411	0.15290	-0.01464	-0.15764	0.01515	0.09088	0.02019	-0.15008	-0.02355	0.42905	0.74602	0.49107	-0.03837	-0.08256	0.10244	-0.28557
12	-0.10938	0.06843	0.07027	-0.04349	-0.05046	0.10196	0.08185	-0.12053	-0.24658	0.03971	0.49107	0.66111	0.41166	0.08437	-0.08564	-0.05873
13	-0.08343	-0.16569	0.03439	0.15277	-0.03626	-0.05155	-0.03455	0.05666	-0.05021	-0.15376	-0.03837	0.41166	0.73163	0.27374	-0.14988	0.43321
14	-0.08717	-0.01842	0.02413	-0.03890	-0.02145	0.23720	-0.05551	0.36187	-0.00559	-0.16441	-0.08256	0.08437	0.27374	0.74040	0.42593	-0.25942
15	-0.30861	0.04982	-0.18533	-0.11739	0.34240	-0.03845	-0.18830	-0.03670	-0.10436	0.03937	-0.10244	-0.08564	-0.14988	0.42593	0.82694	-0.24461
16	0.42107	-0.13813	-0.15226	0.11392	0.03896	0.08082	-0.03761	-0.08423	0.24655	0.05151	-0.28557	-0.05873	0.43321	-0.25942	-0.24461	1.06290

ENERGIES FOR NAPTHYLAZULENE , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF NO SYMMETRY

JUMP	8, 9	8,10	7, 9	6, 9	7,10	6,10	5, 9	4, 9	5,10	4,10	3, 9	8,11	2, 9	3,10	2,10
XMOMNT	0.97880	0.45711	-0.35383	0.41935	-0.22688	-0.58208	-0.08132	0.03162	0.16920	-0.18720	-0.10010	-0.20062	-0.02014	-0.08466	-0.01611
YMOMNT	0.38575	-0.30719	-0.57086	-0.39670	0.24294	-0.57365	0.19735	-0.12184	-0.27635	-0.06513	-0.05070	0.24156	0.03600	0.08954	-0.02413
JUMP E	12.3067	14.8108	20.5625	21.8239	23.0666	24.3280	25.9063	27.6515	28.4104	30.1556	30.7109	31.4471	32.4064	33.2150	34.9106
DIAG E	17.3297	14.7210	27.4053	27.7244	29.7286	32.2282	36.0954	41.2682	38.1634	42.9599	41.3598	35.7802	44.9950	43.5612	47.4823
DIAG E	16.8738	14.4073	27.9969	29.4272	30.4624	34.0732	37.5591	41.2461	39.7693	43.0800	42.5675	33.7170	46.0560	44.9112	48.6855
CORRSP	15.9792	10.1216	25.4719	24.5213	30.4255	31.8843	38.5884	36.8256	41.0659	41.9767	45.6562	35.1109	50.1689	44.0557	48.9501
CORRSP	17.5002	9.2267	25.7584	27.2629	31.6215	39.0230	34.8750	42.1097	37.4147	42.6420	46.8356	32.4839	48.1577	45.0906	50.8299

FINAL EXCITED STATES OF NO SYMMETRY

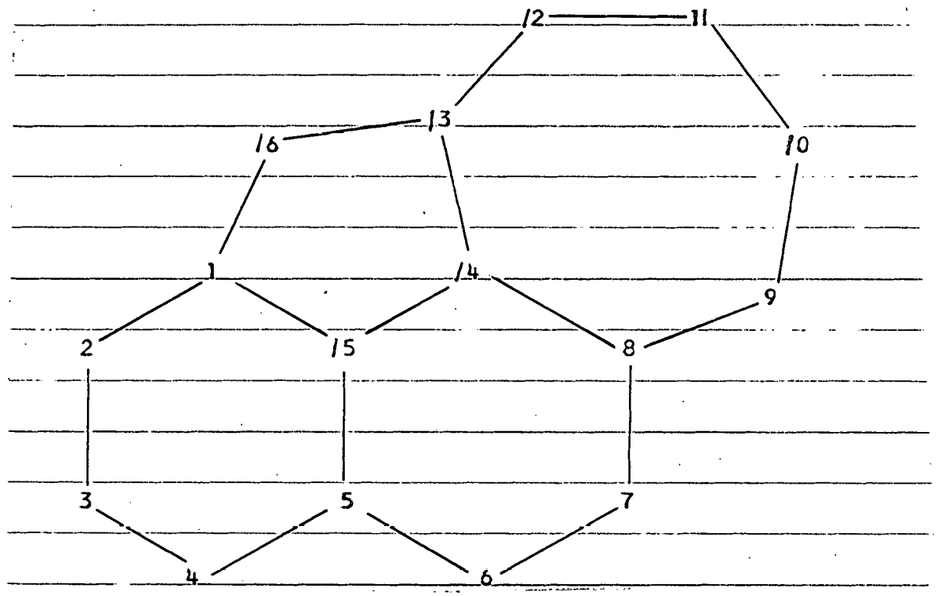
ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
15.97924	0.21825	0.56665	-0.00967	//	0.6329	0.6232	0.2564	-0.2866	0.1598	0.1368	-0.0127	0.0513	-0.0338	0.0101
				//	0.0475	0.0287	-0.0549	0.0906	0.0243					
5.17042				//	0.9099	0.3746	0.0409	-0.0324	0.0338	0.0091	-0.0633	-0.0116	0.0512	-0.0252
				//	0.0415	0.1348	-0.0177	0.0112	-0.0032					
10.12158	0.03219	-0.16387	-0.21892	//	-0.6273	0.7191	-0.2012	-0.0173	0.0983	-0.1527	-0.0026	-0.0253	-0.0258	-0.0287
				//	-0.0611	-0.0487	0.0043	0.0755	-0.0407					
8.02001				//	-0.3797	0.9071	-0.0433	0.0253	0.1326	0.0064	0.0563	-0.0181	0.0739	-0.0087
				//	-0.0219	0.0254	-0.0017	0.0515	-0.0004					
25.47195	0.12329	-0.06732	-0.33059	//	-0.1029	0.0238	0.7233	0.4302	0.2260	-0.3599	0.2196	0.0127	-0.0221	0.0815
				//	0.1577	-0.0193	0.1192	0.0318	-0.0636					
18.28164				//	-0.0295	0.0133	0.8723	0.3797	-0.0655	-0.1025	0.2201	0.0015	0.0085	-0.0519
				//	0.0941	0.0855	0.1027	0.0156	-0.0300					
24.52131	0.06440	0.23231	-0.08830	//	0.1491	0.0560	-0.3184	0.6299	0.5173	0.3578	-0.0788	-0.1399	0.0599	0.0722
				//	-0.0478	0.1004	0.0968	0.1225	0.0976					
20.70055				//	0.0514	0.0122	-0.3563	0.8529	-0.0740	-0.2074	-0.2000	-0.1201	-0.0889	-0.0422
				//	-0.0240	-0.0914	0.1248	-0.0027	-0.0755					
30.42554	0.28696	-0.33798	0.32796	//	-0.0989	-0.2337	0.0194	-0.4264	0.6909	-0.2233	-0.2087	0.1620	0.3618	0.0344
				//	-0.1264	-0.0317	-0.0471	0.0711	0.0009					
23.83475				//	0.0145	-0.1274	-0.0834	-0.0069	0.7629	-0.4222	0.2433	-0.0425	-0.1469	0.0830
				//	0.0857	0.2540	0.0102	0.2264	-0.0602					
31.88425	0.97445	-0.79088	-0.30528	//	-0.2943	-0.0438	0.1941	-0.2346	0.0630	0.5605	0.5357	-0.0207	0.2024	0.0994
				//	0.1223	0.3438	-0.0417	0.0175	0.1648					
22.88835				//	0.0092	-0.0896	-0.0017	0.2779	0.4094	0.7822	0.0395	-0.0878	0.2102	0.1983
				//	0.0472	0.0575	0.0061	0.0091	0.1917					
38.58839	1.41194	0.50513	0.77799	//	0.1885	0.0004	-0.3657	-0.0542	0.0608	-0.4801	0.3728	-0.1228	-0.1061	0.4495
				//	0.1089	0.4415	-0.0988	-0.0385	-0.0906					
26.28646				//	-0.0150	-0.0395	-0.2902	0.0701	-0.3246	0.0056	0.6243	-0.0859	0.2515	-0.1382
				//	0.1814	0.5200	0.0144	-0.1336	0.0529					
36.82562	0.13497	-0.26635	0.12347	//	-0.0686	-0.0626	-0.0143	-0.0476	0.1262	-0.1200	0.0089	0.6625	-0.5977	0.1011
				//	-0.1809	0.1600	0.3018	0.0269	-0.0453					
32.83901				//	0.0730	0.0078	-0.0950	0.0341	-0.0844	-0.1108	0.2478	0.6324	0.3498	0.1649
				//	0.1857	-0.4235	0.3536	-0.1222	-0.0177					

cont.

NAPTHYLAZULENE TBM APP ROXIMATION (cont.)

41.06587	0.44036	0.47907	-0.15051	//	0.1212	-0.1096	-0.0735	0.1270	-0.3092	-0.1113	0.1220	0.3499	-0.6163	0.1192
				//	-0.2796	-0.0399	0.4543	0.1537	0.0512					
30.20380				//	-0.0829	-0.0865	0.0743	-0.0076	0.1255	-0.2115	-0.4572	0.0720	0.6896	-0.1895
				//	-0.2402	0.3426	0.0545	-0.0821	0.0957					
41.97674	0.13005	-0.16939	-0.21015	//	-0.0187	0.0300	-0.1806	0.0061	-0.0082	0.1050	0.0243	-0.2124	-0.0660	0.4756
				//	-0.7169	-0.1865	-0.1496	-0.3272	0.0231					
35.65709				//	-0.0002	0.0233	0.0299	0.0141	-0.1299	-0.0829	0.0051	-0.0190	0.0188	0.8373
				//	-0.3270	0.2301	-0.0033	-0.2019	-0.2687					
45.65619	0.36147	-0.32732	-0.28113	//	-0.1082	-0.0198	0.0673	-0.0109	-0.1569	0.0567	-0.3549	0.0760	-0.0223	0.6333
				//	0.3076	-0.1376	-0.1193	0.3977	0.3691					
37.75888				//	-0.1033	0.0236	0.0051	-0.0449	-0.0593	0.0072	-0.4215	0.1057	-0.1242	0.1916
				//	0.7939	0.3036	0.0935	-0.0989	-0.0333					
35.11086	0.05703	0.15596	-0.11778	//	-0.0841	0.0295	0.2282	0.0573	-0.1419	-0.0206	-0.5105	-0.1009	0.0506	-0.0963
				//	-0.1937	0.7652	-0.0875	0.0343	-0.0405					
33.52777				//	-0.0249	0.0103	-0.0333	0.0271	-0.0571	0.2141	-0.0737	0.5417	-0.4009	-0.1559
				//	-0.3250	0.4235	0.3737	0.1993	0.0105					
50.16892	0.31152	-0.15401	0.34972	//	0.0038	-0.0673	0.0326	-0.2442	0.0441	-0.1027	0.0158	-0.5196	-0.2310	-0.0861
				//	-0.1193	0.0149	0.6374	0.2189	0.3501					
43.95416				//	0.0003	-0.0117	0.0003	-0.1641	0.0963	0.1447	-0.0042	-0.3803	0.0452	-0.1895
				//	-0.0013	-0.0489	0.6216	-0.1627	-0.5872					
44.05573	0.06733	-0.01794	0.18872	//	0.0286	-0.1038	0.0176	0.0304	-0.0513	-0.0347	0.2376	-0.0374	-0.1067	-0.1656
				//	-0.3633	-0.0459	-0.3428	0.7792	-0.1670					
41.41028				//	0.0002	-0.0356	-0.0288	-0.0200	-0.2305	0.0400	-0.0132	-0.0625	0.2742	0.1575
				//	0.0975	-0.0323	0.0447	0.8852	-0.2062					
48.95011	0.24454	0.31899	0.12539	//	0.0429	0.0288	-0.0340	0.1166	0.0104	-0.2296	0.1304	0.2036	-0.0427	-0.2799
				//	-0.1442	0.0594	-0.3069	-0.1316	0.8095					
43.54786				//	0.0171	0.0225	0.0059	-0.1138	-0.0875	-0.1547	-0.0053	-0.3312	-0.0581	0.2089
				//	-0.0356	-0.0510	0.5553	0.0755	0.6928					

NAPTHYLAZULENE IRM



ATOMIC COORDINATES

x	0.8725	0.	0.	0.8500	1.7321	2.6095	3.4641	3.4641
y	2.0350	1.5500	0.5500	0.0210	0.5000	0.0210	0.5500	1.5500

4.3695	4.5370	3.8987	2.8930	2.3700	2.5700	1.7321	1.2695
1.9780	2.9690	3.7400	3.7710	2.9900	2.0350	1.5000	2.9620

NAPTHYLAZULENE IRM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

OVERLAP EIGNVALUES

1.780260 1.541127 1.463237 1.350738 1.276368 1.152598 1.124928 0.987727 0.846458 0.830486 0.709170 0.684551 0.638601 0.575295 0.544110 0.494335

0.312439-0.231646-0.292042-0.037725-0.319351 0.294951 0.240841 0.026628 0.129796 0.211544-0.043973-0.225981 0.426807-0.170988-0.358807-0.244074
0.185327-0.285910-0.179449 0.262889-0.333753-0.167823 0.252795 0.322413-0.342215 0.031974 0.300655-0.220183-0.281328 0.178561 0.286346 0.158600
0.152904-0.311106-0.040006 0.404895-0.096489-0.446123-0.049863 0.016867 0.016383-0.251294-0.282027 0.507937-0.005733-0.164241-0.231142-0.147631
0.183741-0.311933 0.114208 0.323508 0.219688-0.210900-0.272952-0.336634 0.329760 0.077657 0.031893-0.412771 0.282875-0.134334 0.213244 0.202394
0.302953-0.285814 0.254240-0.057961 0.370219 0.256027-0.151673-0.085200-0.149029 0.202192 0.252483 0.008294-0.456596-0.088297-0.211235-0.371284
0.203769-0.104653 0.386115-0.053648 0.286074 0.112514 0.426621-0.033874-0.364007-0.224804 0.142380 0.196370 0.458039-0.069102 0.068427 0.238295
0.200049 0.078711 0.422790-0.118197-0.037169-0.166958 0.480469 0.068143 0.293075-0.077546-0.424914-0.247343-0.240625 0.225659 0.044417-0.227771
0.281701 0.257274 0.346155-0.105281-0.313670-0.262554-0.060085 0.037414 0.250636 0.241770 0.344462 0.083648-0.085685-0.389740-0.174014 0.338779
0.156357 0.295605 0.236583 0.231187-0.367252 0.085965-0.168012-0.305071-0.342202 0.339556-0.126844 0.189956 0.155104 0.427757 0.043675-0.147226
0.111936 0.315073 0.064182 0.447421-0.128071 0.356939-0.078274-0.088241-0.113924-0.419337-0.178462-0.299255-0.133829-0.434924 0.083929 0.042829
0.120175 0.320107-0.114577 0.420045 0.210628 0.204811-0.128314 0.287548 0.397832-0.111171 0.309368 0.187889 0.042262 0.399925-0.208106 0.037275
0.182751 0.307224-0.267970 0.165663 0.383561-0.181587 0.179646 0.129910-0.055773 0.489849-0.176710 0.076586 0.067611-0.320991 0.370142-0.137673
0.313692 0.254140-0.323395-0.150679 0.233451-0.293941-0.003072-0.205809-0.319068-0.113579-0.111441-0.247988-0.114656 0.171223-0.481097 0.252813
0.392236 0.167496-0.031396-0.297942-0.037144-0.179616-0.363761 0.231832-0.023918-0.377244 0.210250-0.049933 0.226666 0.049910 0.268219-0.439588
0.402171-0.170849-0.043726-0.189170 0.013096 0.351424-0.287338 0.304603 0.078404-0.062473-0.432212 0.209358-0.101711 0.107049-0.140683 0.435972
0.243735-0.011783-0.321029-0.157486-0.107561 0.120157 0.252276-0.614802 0.231568-0.163073 0.159955 0.301064-0.227866-0.009440 0.310411-0.012285

NAPTHYLAZULENE IRM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

ZEROTH HAMILTONIAN EIGNVALUE

32.89281 26.35152 23.75929 19.48754 16.25011 9.93610 8.33448 -0.93256-13.61342-15.31861-30.77749-34.58343-42.47198-55.40400-62.88087-76.76923

0.234166-0.186598-0.241428-0.032460-0.282670 0.274733 0.227074 0.026793 0.141078 0.232132-0.052217-0.273130 0.534093-0.225434-0.486427-0.347146
0.138898-0.230309-0.148349 0.226197-0.295418-0.156319 0.238345 0.324410-0.371960 0.035085 0.357020-0.266121-0.352045 0.235419 0.388193 0.225576
0.114598-0.250605-0.033073 0.348383-0.085406-0.415543-0.047013 0.016971 0.017807-0.275750-0.334900 0.613913-0.007174-0.216538-0.313354-0.209975
0.137710-0.251271 0.094415 0.278355 0.194455-0.196443-0.257350-0.338719 0.358422 0.085215 0.037872-0.498891 0.353981 0.177109 0.289090-0.287864
0.227056-0.230231 0.210177 0.049871 0.327696 0.238477-0.143003-0.085727-0.161982 0.221870 0.299817 0.010024-0.571370-0.116413-0.286367-0.528075
0.152720-0.084301 0.319197-0.046161 0.253216 0.104801 0.402235-0.034084-0.395646-0.246682 0.169073 0.237340 0.573175-0.091105 0.092765 0.338925
0.149932 0.063404 0.349516-0.101700-0.032900-0.155513 0.453005 0.068565 0.318549-0.085093-0.504575-0.298949-0.301110 0.297514 0.060215-0.323958
0.211128 0.207242 0.286163-0.090587-0.277642-0.244557-0.056651 0.037646 0.272421 0.265299 0.409041 0.101100-0.107224-0.513842-0.235908 0.481844
0.117186 0.238118 0.195581 0.198920-0.325070 0.080073-0.158409-0.306960-0.371947 0.372602-0.150624 0.229589 0.194092 0.563965 0.059209-0.209398
0.083894 0.253801 0.053059 0.384974-0.113361 0.332472-0.073800-0.088788-0.123827-0.460148-0.211919-0.361692-0.167470-0.573414 0.113781 0.060916
0.090068 0.257855-0.094719 0.361418-0.186435 0.190772 0.120979 0.289329 0.432411-0.121990 0.367367 0.227090 0.052886 0.527270-0.282125 0.053016
0.136968 0.247477-0.221528 0.142541 0.339505-0.169140 0.169378-0.130715-0.060621 0.537522-0.209839 0.092565 0.084606-0.423202 0.501794-0.195812
0.235105 0.204717-0.267347-0.129648 0.206637-0.273792-0.002897-0.207083-0.346801-0.124633-0.132334-0.299729-0.143477 0.225744-0.652212 0.359575
0.293972 0.134923-0.025954-0.256358-0.032878-0.167304-0.342968 0.233267-0.025997-0.413958 0.249666-0.060351 0.283643 0.065803-0.363618-0.625224
0.301418-0.137624-0.036148-0.162767 0.011592 0.327335-0.270913 0.306489 0.085219 0.068553-0.513242 0.253038-0.127278 0.141136 0.190721 0.620080
0.182674-0.009491-0.265392-0.135505-0.095207 0.111920 0.237856-0.618610 0.251696-0.178944 0.189942 0.363878-0.285144 0.012446 0.420818-0.017473

NAPTHYLAZULENE IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.97137	0.58635	0.00784	-0.24591	0.00583	0.04169	0.01083	-0.11889	-0.00677	0.10268	0.02543	-0.14277	-0.05641	-0.03678	0.44703	0.58551
2	0.58635	1.04963	0.66163	-0.05535	-0.24973	-0.06628	0.18297	0.06896	-0.13981	-0.05726	0.16443	0.05485	-0.18364	-0.04512	0.08744	-0.10793
3	0.00784	0.66163	0.99363	0.66476	0.00945	-0.14619	-0.00682	0.11516	0.03280	-0.09356	-0.03959	0.09479	0.05224	-0.01150	-0.19755	-0.15233
4	-0.24591	-0.05535	0.66476	1.05866	0.58005	0.06180	-0.20957	-0.06550	0.17615	0.04403	-0.16743	-0.01894	0.15217	-0.05836	-0.06870	0.09996
5	0.00583	-0.24973	0.00945	0.58005	0.94869	0.51919	0.00712	-0.16742	-0.05210	0.09894	0.05317	-0.06755	-0.07877	0.04278	0.52208	-0.01696
6	0.04169	-0.06628	-0.14619	0.06180	0.51919	0.96417	0.75073	0.04721	-0.15373	-0.07254	0.10503	0.10854	-0.08017	-0.25523	0.00696	0.09319
7	0.01083	0.18297	-0.00682	-0.20957	0.00712	0.75073	1.00737	0.52915	0.05006	-0.15402	-0.01926	0.07819	-0.02253	-0.02803	-0.21116	-0.01206
8	-0.11889	0.06896	0.11516	-0.06550	-0.16742	0.04721	0.52915	0.89757	0.53792	0.07113	-0.16894	-0.11649	0.10821	0.52685	0.01281	-0.12977
9	0.00677	-0.13981	0.03280	0.17615	-0.05210	-0.15373	0.05006	0.53792	0.96962	0.69410	0.02878	-0.26399	-0.06975	0.04625	-0.12190	0.23454
10	0.10268	-0.05726	-0.09356	0.04403	0.09894	-0.07254	-0.15402	0.07113	0.69410	0.94765	0.61121	0.06943	-0.17881	-0.17996	0.04623	0.04734
11	0.02543	0.16443	-0.03959	-0.16743	0.05317	0.10503	-0.01926	-0.16894	0.02878	0.61121	0.98387	0.64920	0.04441	-0.09084	0.08929	-0.29262
12	-0.14277	0.05485	0.09479	-0.01894	-0.06755	0.10854	0.07819	-0.11649	-0.26399	0.06943	0.64920	0.91256	0.62547	0.13067	-0.13890	0.00647
13	-0.05641	0.18364	0.05224	0.15217	-0.07877	-0.08017	-0.02253	0.10821	-0.06975	-0.17881	0.04441	0.62547	0.94709	0.43637	-0.07333	0.53268
14	-0.03678	-0.04512	-0.01150	-0.05836	0.04278	-0.25523	-0.02803	0.52685	0.04625	-0.17996	-0.09084	0.13067	0.43637	0.98274	0.59679	-0.20251
15	0.44703	0.08744	-0.19755	-0.06870	0.52208	0.00696	-0.21116	0.01281	-0.12190	0.04623	0.08929	-0.13890	-0.07333	0.59679	1.05529	-0.15015
16	0.58551	-0.10793	-0.15233	0.09996	-0.01696	0.09319	-0.01206	-0.12977	0.23454	0.04734	-0.29262	0.00647	0.53268	-0.20251	-0.15015	1.31008

NAPTHYLAZULENE IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.71331	0.41469	-0.05994	-0.25829	-0.03623	0.04713	0.02695	-0.11188	-0.00195	0.10246	0.03809	-0.13144	-0.10846	-0.10010	0.28724	0.41623
2	0.41469	0.83853	0.48366	-0.14401	-0.26263	-0.04708	0.19122	0.07523	-0.15281	-0.06494	0.17345	0.07211	-0.18055	-0.02917	0.04474	-0.19417
3	-0.05994	0.48366	0.76174	0.48795	-0.05535	-0.14535	0.00320	0.11975	0.02663	-0.09628	-0.04246	0.09241	0.06412	0.00767	-0.21111	-0.15035
4	-0.25829	-0.14401	0.48795	0.85172	0.41112	-0.00764	-0.21249	-0.05063	0.19188	0.04332	-0.18217	-0.02636	0.16892	-0.06301	-0.13755	0.14518
5	-0.03623	-0.26263	-0.05535	0.41112	0.68656	0.34448	-0.06139	-0.17715	-0.03130	0.10254	0.04737	-0.05968	-0.07164	-0.00836	0.35747	-0.00873
6	0.04713	-0.04708	-0.14535	-0.00764	0.34448	0.74501	0.57812	-0.01941	-0.15221	-0.05988	0.10221	0.10936	-0.06236	-0.26939	-0.05713	0.10924
7	0.02695	0.19122	0.00320	-0.21249	-0.06139	0.57812	0.78837	0.35622	-0.02754	-0.15886	-0.00234	0.09026	-0.02352	-0.08528	-0.22522	-0.00226
8	-0.11188	0.07523	0.11975	-0.05063	-0.17715	-0.01941	0.35622	0.63828	0.36025	0.00325	-0.16354	-0.10734	0.05852	0.36815	-0.03374	-0.12954
9	-0.00195	-0.15281	0.02663	0.19188	-0.03130	-0.15221	-0.02754	0.36025	0.75931	0.51928	-0.05597	-0.26171	-0.05370	-0.01896	0.13124	0.26481
10	0.10246	-0.06494	-0.09628	0.04332	0.10254	-0.05988	-0.15886	0.00325	0.51928	0.71838	0.42957	-0.00281	-0.17654	-0.17692	0.05215	0.06409
11	0.03809	0.17345	-0.04246	-0.18217	0.04737	0.10221	-0.00234	-0.16354	-0.05597	0.42957	0.76739	0.47598	-0.04309	-0.08195	0.11353	-0.31287
12	-0.13144	0.07211	0.09241	-0.02636	-0.05968	0.10936	0.09026	-0.10734	-0.26171	-0.00281	0.47598	0.67809	0.42503	0.06480	-0.13044	-0.05936
13	-0.10846	-0.18055	0.06412	0.16892	-0.07164	-0.06236	-0.02352	0.05852	-0.05370	-0.17654	-0.04309	0.42503	0.69204	0.25722	-0.15291	0.41325
14	-0.10010	-0.02917	0.00767	-0.06301	-0.00836	-0.26939	-0.08528	0.36815	-0.01896	-0.17692	-0.08195	0.06480	0.25722	0.74426	0.44394	-0.29485
15	0.28724	0.04474	-0.21111	-0.13755	0.35747	-0.05713	-0.22522	-0.03374	-0.13124	0.05215	0.11353	-0.13044	-0.15291	0.44394	0.82441	-0.26097
16	0.41623	-0.19417	-0.15035	-0.14518	-0.00873	0.10924	-0.00226	-0.12954	0.26481	0.06409	-0.31287	-0.05936	0.41325	-0.29485	-0.26097	1.16620

ENERGIES FOR NAPTHYLAZULENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF NO SYMMETRY

JUMP	8, 9	8,10	7, 9	6, 9	7,10	6,10	8,11	5, 9	5,10	4, 9	8,12	4,10	3, 9	3,10	7,11
XMOMNT	0.99626	-0.24958	0.54733	-0.24877	-0.08856	-0.75208	0.23523	0.02459	-0.19177	0.01962	0.12145	-0.10732	-0.08188	0.07339	-0.42442
YMOMNT	0.30291	0.27104	0.44703	0.59656	0.46219	-0.48705	-0.18922	0.17073	0.32327	0.10574	-0.24379	-0.01967	-0.01250	-0.07991	0.21063
JUMP E	12.6809	14.3861	21.9479	23.5495	23.6531	25.2547	29.8449	29.8635	31.5687	33.1010	33.6509	34.8062	37.3727	39.0779	39.1120
DIAG E	16.8008	11.3335	28.8790	29.6444	30.9410	33.5689	32.6541	40.4571	41.7424	45.6162	42.0866	47.1746	48.3411	49.9194	49.3288
DIAG E	16.9269	10.5814	29.9145	31.8509	31.0983	34.8972	30.5942	42.1560	42.5631	45.9219	43.1146	46.6021	49.9346	50.6347	48.1782
CORRSP	14.4935	9.1796	26.8433	25.5593	31.9058	36.2396	30.8081	41.0405	39.4402	46.8128	44.6107	47.5606	51.0208	53.2729	49.6998
CORRSP	15.7762	7.8945	28.2842	26.4250	32.5555	37.2990	29.6861	42.1048	39.9855	47.3977	45.2246	47.7404	52.1689	53.2745	49.1514

FINAL EXCITED STATES OF NO SYMMEITRY

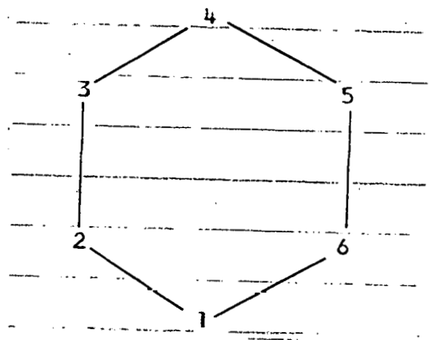
ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
14.49350	0.21092	0.58378	0.03769	//	0.8492	-0.3862	-0.2450	0.0948	0.0334	0.2167	0.0037	-0.0199	0.0186	-0.0150
				//	-0.0538	-0.0210	0.0574	-0.0553	0.0437					
4.19599				//	0.9443	-0.2753	0.0150	-0.0081	0.0118	0.0253	0.1401	-0.0095	-0.0521	0.0462
				//	0.0585	-0.0269	0.0450	-0.0114	-0.0248					
9.17956	0.01688	0.09624	0.18435	//	0.3851	0.8993	-0.0893	-0.0709	-0.0767	0.0724	0.0368	0.0125	-0.0112	-0.0119
				//	0.0925	0.0416	0.0288	0.0760	0.0117					
7.20028				//	0.2802	0.9488	-0.0174	0.0144	-0.0615	-0.0434	-0.0204	-0.0529	0.0481	0.0006
				//	0.0774	0.0216	0.0168	0.0485	0.0232					
26.84327	0.08925	0.13742	0.24352	//	0.0927	0.0117	0.7581	0.3784	-0.2579	0.4115	-0.0086	-0.1264	0.0099	-0.0127
				//	0.0637	-0.0806	-0.1020	0.0109	0.0103					
19.83653				//	0.0189	0.0271	0.8789	0.2994	0.1720	0.1525	-0.1219	-0.1834	-0.0490	-0.0546
				//	-0.1513	0.0205	-0.0690	0.0154	-0.0420					
25.55933	0.02986	-0.15404	0.06120	//	-0.0692	0.0159	-0.3584	0.6672	-0.5355	-0.2750	-0.1048	0.0524	0.0628	-0.1205
				//	0.0498	-0.0463	0.0259	0.0904	-0.1155					
22.65098				//	-0.0018	0.0120	-0.3280	0.8651	0.0864	0.3016	0.1074	0.1327	-0.0183	-0.1146
				//	-0.0057	-0.0062	-0.0007	-0.0208	0.0481					
31.90579	0.28403	-0.13084	0.43843	//	0.0149	0.1129	0.0146	0.4405	0.6751	-0.1008	-0.4566	-0.1426	-0.2542	-0.1335
				//	0.0681	-0.0377	-0.0744	-0.0471	-0.0422					
24.45024				//	-0.0537	0.0348	0.0593	0.0866	0.6684	-0.5397	0.4073	0.1119	0.1406	0.0726
				//	0.1483	0.0012	0.0812	-0.1213	-0.0051					
36.23962	1.11716	-0.73952	-0.42192	//	-0.1694	0.0017	-0.1607	-0.0340	-0.0075	0.5759	-0.4231	0.6187	0.0926	-0.0403
				//	0.0608	0.0675	0.1266	0.0315	-0.1236					
23.93353				//	-0.0389	0.0937	-0.0516	-0.3636	0.4896	0.7265	0.2119	0.0946	-0.1160	0.0175
				//	0.0214	0.1244	0.0444	-0.0434	-0.0068					
30.80812	0.22110	-0.40911	0.03729	//	-0.1758	0.0376	-0.2277	0.3129	0.2697	0.3639	0.7370	0.0623	-0.1415	-0.0774
				//	0.0797	0.0147	-0.0309	-0.0723	-0.1640					
26.67462				//	-0.1095	0.0411	0.2722	-0.0045	-0.4686	0.0654	0.7172	0.3574	-0.1059	0.0906
				//	0.0817	-0.0959	0.0224	0.1006	-0.0183					
41.04049	0.70742	0.51933	0.36828	//	0.1391	-0.0615	0.2410	0.1199	0.0100	-0.3281	0.1484	0.5564	-0.4281	0.2482
				//	0.2094	0.3138	0.1423	-0.0353	0.2375					
33.64722				//	0.0722	0.0180	-0.1132	-0.0288	0.0992	-0.0922	-0.3936	0.8186	-0.1721	-0.0245
				//	-0.0733	0.0532	-0.1071	0.1558	0.2517					

cont.

NAPTHYLAZULENE IRM APPROXIM ATION (cont.)

39.44020	0.19624	0.20957	0.27034	//	0.0677	-0.0627	0.1215	0.0034	0.1806	-0.1726	0.0885	0.0678	0.6260	-0.3252
				//	0.5971	0.2147	0.0325	0.0239	-0.0057					
36.78541				//	0.0665	0.0027	-0.0088	-0.0795	-0.0543	0.0057	0.1254	0.1634	0.5697	-0.4683
				//	-0.5198	0.2560	0.1028	-0.0172	-0.2310					
46.81279	0.48227	0.05860	0.48870	//	0.0143	0.0518	0.0819	0.1860	0.2168	-0.0805	0.0540	0.0272	0.3892	-0.6164
				//	-0.1311	-0.2475	0.4771	0.1479	-0.1979					
41.77344				//	-0.0114	0.0375	-0.0507	0.0802	0.0070	0.0339	-0.0426	-0.0045	0.0695	0.7385
				//	-0.4792	-0.0816	0.3934	0.0053	-0.2125					
44.61073	0.81286	-0.14463	-0.63841	//	-0.0806	-0.0776	-0.1829	-0.1153	-0.1340	0.1728	-0.1109	-0.3147	-0.2845	0.3177
				//	0.7268	-0.2245	0.1353	-0.0028	0.0523					
31.33003				//	-0.0194	-0.0668	0.1360	0.0429	-0.0861	0.1983	-0.1920	0.1356	0.6439	0.1963
				//	0.6103	0.0088	0.1888	-0.0491	-0.0953					
47.56063	0.17457	-0.27756	-0.09629	//	-0.0362	-0.0396	-0.1290	0.0834	0.0315	0.1493	-0.0659	-0.2204	0.1069	0.3889
				//	-0.0268	0.6221	-0.3821	0.4481	0.0126					
40.83140				//	0.0205	-0.0414	-0.0091	0.0463	-0.0533	-0.0280	0.0862	-0.0530	0.1402	0.3530
				//	-0.0482	0.7275	-0.3877	0.1258	0.3739					
51.02083	0.18967	-0.24267	-0.16890	//	-0.0670	0.0177	0.0202	0.0252	-0.0898	0.0896	-0.0656	-0.3170	-0.0810	-0.1080
				//	-0.0968	0.5753	0.6141	-0.3568	-0.1012					
45.26968				//	-0.0327	-0.0555	0.0098	-0.0038	0.0240	0.0063	0.0951	-0.2778	0.0517	-0.1616
				//	0.0160	0.0099	0.5956	0.5295	0.4945					
53.27290	1.17061	0.64591	-0.31549	//	0.0951	-0.0952	0.1321	-0.1747	-0.0118	-0.0793	0.0303	-0.0262	-0.2768	-0.2766
				//	0.0364	-0.0120	0.1892	0.5923	-0.6202					
47.68302				//	0.0109	-0.0188	-0.0703	-0.0009	0.1658	0.0056	-0.0082	0.0352	0.1214	0.0699
				//	0.0093	-0.2124	-0.3941	0.7914	-0.3455					
49.69977	0.60612	-0.53496	0.02466	//	-0.1086	-0.0135	-0.0587	0.0645	0.0656	0.1350	0.0471	-0.0999	-0.0001	-0.2679
				//	-0.1007	-0.0934	0.3689	0.5213	0.6687					
39.38765				//	0.0362	0.0131	0.0077	-0.0662	0.0426	0.1004	0.0510	0.0168	0.3703	0.0923
				//	-0.2413	-0.5693	-0.3332	-0.1435	0.5655					

BENZENE, TOLUENE, M XYLENE, MESITYLENE | TBM, IRM



ATOMIC COORDINATES

x	0.8660	0.	0.	0.8660	1.7320	1.7320
y	0.	0.5000	1.5000	2.0000	1.5000	0.5000

BENZENE, TOLUENE, M XYLENE, MESITYLENE , TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A
1.493617	1.246817	1.246800	0.753200	0.753183	0.506383
0.408253	0.577347	0.000216	-0.000249	-0.577347	-0.408253
0.408246	0.288866	-0.499892	-0.499875	0.288894	0.408246
0.408246	-0.288491	-0.500108	0.500124	0.288463	-0.408246
0.408253	-0.577347	-0.000216	-0.000249	-0.577347	0.408253
0.408246	-0.288866	0.499892	-0.499875	0.288894	-0.408246
0.408246	0.288491	0.500108	0.500124	0.288463	0.408246

BENZENE, TOLUENE, M XYLENE, MESITYLENE, TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6
1	1.00000	0.66667	0.00000	-0.33332	0.00000	0.66667
2	0.66667	1.00000	0.66666	0.00000	-0.33334	-0.00000
3	0.00000	0.66666	1.00000	0.66667	-0.	-0.33334
4	-0.33332	0.00000	0.66667	1.00000	0.66667	0.00000
5	-0.00000	-0.33334	-0.	0.66667	1.00000	0.66666
6	0.66667	-0.00000	-0.33334	0.00000	0.66666	1.00000

BENZENE, TOLUENE, M XYLENE, MESITYLENE , TBM DENSITY BOND ORDERS

	1	2	3	4	5	6
1	0.75787	0.49052	-0.04418	-0.31151	-0.04418	0.49052
2	0.49052	0.75787	0.49052	-0.04418	-0.31153	-0.04418
3	-0.04418	0.49052	0.75787	0.49052	-0.04418	-0.31153
4	-0.31151	-0.04418	0.49052	0.75787	0.49052	-0.04418
5	-0.04418	-0.31153	-0.04418	0.49052	0.75787	0.49052
6	0.49052	-0.04418	-0.31153	-0.04418	0.49052	0.75787

BENZENE TBX & TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 AA	5 SS	6 AS
25.81018	15.46010	15.45925	-25.59031	-25.59264	-76.12920
0.334049	0.517054	0.000194	-0.000287	-0.665253	-0.573706
0.334043	0.258699	-0.447690	-0.575979	0.332880	0.573697
0.334043	-0.258363	-0.447884	0.576266	0.332384	-0.573697
0.334049	-0.517054	-0.000194	-0.000287	-0.665253	0.573707
0.334043	-0.258699	0.447690	-0.575979	0.332880	-0.573697
0.334043	0.258363	0.447884	-0.576266	0.332384	0.573697

TOLUENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1	2	3	4	5	6
24.9145	14.9236	14.9228	-24.7022	-24.7045	-73.4873
0.334049	0.517054	0.000194	-0.000287	-0.665253	-0.573706
0.334043	0.258699	-0.447690	-0.575979	0.332880	0.573697
0.334043	-0.258363	-0.447884	0.576266	0.332384	-0.573697
0.334049	-0.517054	-0.000194	-0.000287	-0.665253	0.573707
0.334043	-0.258699	0.447690	-0.575979	0.332880	-0.573697
0.334043	0.258363	0.447884	0.576266	0.332384	0.573697

M XYLENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A
24.4666	14.6553	14.6545	-24.2582	-24.2604	-72.1663
0.334049	0.517054	0.000194	-0.000287	-0.665253	-0.573706
0.334043	0.258699	-0.447690	-0.575979	0.332880	0.573697
0.334043	-0.258363	-0.447884	0.576266	0.332384	-0.573697
0.334049	-0.517054	-0.000194	-0.000287	-0.665253	0.573707
0.334043	-0.258699	0.447690	-0.575979	0.332880	-0.573697
0.334043	0.258363	0.447884	0.576266	0.332384	0.573697

MESITYLENE TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A
24.0188	14.3871	14.3863	-23.8142	-23.8163	-70.8453
0.334049	0.517054	0.000194	-0.000287	-0.665253	-0.573706
0.334043	0.258699	-0.447690	-0.575979	0.332880	0.573697
0.334043	-0.258363	-0.447884	0.576266	0.332384	-0.573697
0.334049	-0.517054	-0.000194	-0.000287	-0.665253	0.573707
0.334043	-0.258699	0.447690	-0.575979	0.332880	-0.573697
0.334043	0.258363	0.447884	0.576266	0.332384	0.573697

BENZENE, TOLUENE, M-XYLENE, MESITYLENE, IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A
1.578467	1.196670	1.196646	0.733948	0.733935	0.560333
0.408250	0.577346	-0.000546	0.000367	-0.577349	-0.408254
0.408247	0.288206	-0.500273	-0.500184	0.288358	0.408245
0.408247	-0.289152	-0.499727	0.499816	0.288995	-0.408245
0.408250	-0.577346	0.000546	0.000367	-0.577349	0.408254
0.408247	-0.288206	0.500273	-0.500184	0.288358	-0.408245
0.408247	0.289152	0.499727	0.499816	0.288995	0.408245

BENZENE, TOLUENE, M XYLENE, MESITYLENE, IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6
1	0.99999	0.66667	-0.00000	-0.33332	-0.00000	0.66667
2	0.66667	1.00000	0.66666	-0.00000	-0.33334	0.00000
3	-0.00000	0.66666	1.00000	0.66667	0.00000	-0.33334
4	-0.33332	-0.00000	0.66667	0.99999	0.66667	-0.00000
5	-0.00000	-0.33334	0.00000	0.66667	1.00000	0.66666
6	0.66667	0.00000	-0.33334	-0.00000	0.66666	1.00000

BENZENE, TOLUENE, M XYLENE, MESITYLENE, IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6
1	0.76827	0.48973	-0.06738	-0.34592	-0.06738	0.48973
2	0.48973	0.76829	0.48973	-0.06738	-0.34594	-0.06738
3	-0.06738	0.48973	0.76829	0.48973	-0.06738	-0.34594
4	-0.34592	-0.06738	0.48973	0.76827	0.48973	-0.06738
5	-0.06738	-0.34594	-0.06738	0.48973	0.76829	0.48973
6	0.48973	-0.06738	-0.34594	-0.06738	0.48973	0.76829

BENZENE IRX & IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SA	4 SS	5 AA	6 AS
28.62091	12.83523	12.83394	-28.31014	-28.31205	-61.27982
0.324944	0.527775	0.000000	0.673916	-0.000000	-0.545391
0.324942	0.263894	-0.457075	-0.336961	-0.583635	0.545378
0.324942	-0.263894	-0.457075	-0.336960	0.583635	-0.545378
0.324944	-0.527775	0.000000	0.673916	-0.000000	0.545391
0.324942	-0.263894	0.457075	-0.336961	-0.583635	-0.545378
0.324942	0.263894	0.457075	-0.336961	0.583635	0.545378

TOLUENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A
27.62766	12.38980	12.38856	-27.32768	-27.32952	-59.15320
0.324944	0.527775	-0.000499	0.000429	-0.673922	-0.545391
0.324942	0.263461	-0.457324	-0.583844	0.336592	0.545378
0.324942	-0.264326	-0.456825	0.583415	0.337335	-0.545378
0.324944	-0.527775	0.000499	0.000429	-0.673922	0.545391
0.324942	-0.263461	0.457324	-0.583844	0.336592	-0.545378
0.324942	0.264326	0.456825	0.583415	0.337335	0.545378

M XYLENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A
27.1310	12.1671	12.1659	-26.8365	-26.8383	-58.0899
0.324944	0.527775	-0.000499	0.000429	-0.673922	-0.545391
0.324942	0.263461	-0.457324	-0.583844	0.336592	0.545378
0.324942	-0.264326	-0.456825	0.583415	0.337335	-0.545378
0.324944	-0.527775	0.000499	0.000429	-0.673922	0.545391
0.324942	-0.263461	0.457324	-0.583844	0.336592	-0.545378
0.324942	0.264326	0.456825	0.583415	0.337335	0.545378

MESITYLENE IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 A	5 S	6 A
26.6344	11.9444	11.9432	-26.3452	-26.3470	-57.0266
0.324944	0.527775	-0.000499	0.000429	-0.673922	-0.545391
0.324942	0.263461	-0.457324	-0.583844	0.336592	0.545378
0.324942	-0.264326	-0.456825	0.583415	0.337335	-0.545378
0.324944	-0.527775	0.000499	0.000429	-0.673922	0.545391
0.324942	-0.263461	0.457324	-0.583844	0.336592	-0.545378
0.324942	0.264326	0.456825	0.583415	0.337335	0.545378

ENERGIES FOR TOLUENE , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF NO SYMMETRY

JUMP	3, 4	2, 4	3, 5	2, 5
XMOMNT	0.00042	0.51595	0.51595	-0.00042
YMOMNT	-0.51596	0.00042	0.00042	0.51595
JUMP E	48.7422	48.7432	48.7450	48.7460
DIAG E	60.0836	55.8720	55.8737	60.0873
DIAG E	58.1851	53.9735	53.9750	58.1886
CORRSP	56.3523	47.9264	63.8193	63.8186
CORRSP	54.4537	46.0277	61.9207	61.9200

FINAL EXCITED STATES OF NO SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION			
56.35231	0.00000	0.00000	-0.00019	//	0.7073	0.0000	-0.0000	0.7069
37.73564				//	0.7074	0.0000	-0.0000	0.7068
47.92636	0.00000	0.00004	0.00000	//	-0.0000	0.7071	-0.7071	-0.0000
42.83089				//	0.0000	0.7072	0.7070	0.0000
63.81933	1.44493	0.72967	0.00059	//	0.0000	0.7071	0.7071	-0.0000
47.92636				//	0.0000	-0.7070	0.7072	0.0000
63.81860	1.44493	-0.00059	0.72967	//	-0.7069	0.0000	-0.0000	0.7073
42.83112				//	-0.7068	-0.0000	0.0000	0.7074

ENERGIES FOR TOLUENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF NO SYMMETRY

JUMP	3, 4	2, 4	3, 5	2, 5	1, 4	1, 5
XMOMNT	-0.00081	0.51500	0.51500	0.00081	-0.00000	0.00000
YMOMNT	-0.51501	-0.00081	-0.00081	0.51500	0.00000	-0.00000
JUMP E	39.7162	39.7175	39.7181	39.7193	54.9553	54.9572
DIAG E	50.8909	46.7140	46.7141	50.8940	65.7069	65.7089
DIAG E	51.2433	47.6253	46.1552	50.8940	66.4064	65.4970
CORRSP	47.1636	38.8062	54.6219	54.6212	65.7069	65.7088
CORRSP	54.7962	54.8266	38.9464	47.3323	66.4140	65.5057

FINAL EXCITED STATES OF NO SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
47.16364	0.00000	-0.00000	-0.00016	//	0.7073	0.0002	-0.0002	0.7070	0.0000	-0.0000
28.61551				//	0.7073	0.0002	-0.0002	0.7069	0.0000	0.0000
38.80623	0.00000	0.00001	-0.00000	//	-0.0002	0.7071	-0.7071	-0.0002	0.0000	-0.0000
33.71076				//	-0.0025	0.7071	0.7071	0.0025	0.0000	0.0000
54.62188	1.23214	0.72832	0.00016	//	-0.0013	0.7071	0.7071	0.0013	-0.0000	-0.0000
38.80623				//	0.0002	-0.7071	0.7071	0.0002	0.0000	0.0000
54.62123	1.23214	-0.00016	0.72833	//	-0.7070	-0.0013	-0.0013	0.7073	-0.0000	0.0000
33.71097				//	-0.7069	-0.0025	-0.0025	0.7073	0.0000	0.0000
65.70694	0.00000	-0.00000	0.00000	//	-0.0000	-0.0000	0.0000	0.0000	1.0000	-0.0002
53.94786				//	-0.0000	-0.0000	-0.0000	-0.0000	1.0000	-0.0003
65.70085	0.00000	0.00000	-0.00000	//	0.0000	0.0000	0.0000	-0.0000	0.0002	1.0000
53.94957				//	-0.0000	-0.0000	-0.0000	-0.0000	0.0003	1.0000

ENERGIES FOR M XYLENE TBMAPPROXIMATION

ONE ELECTRON EXCITATIONS

JUMP	3, 4	2, 4	3, 5	2, 5	1, 4	1, 5
XMOMNT	0.00042	0.51595	0.51595	-0.00042	-0.00000	0.
YMOMNT	-0.51596	0.00042	0.00042	0.51595	-0.00000	-0.00000
JUMP E	38.9127	38.9135	38.9149	38.9157	48.7248	48.7270
DIAG E	50.2541	46.0424	46.0436	50.2571	59.1131	59.1155
DIAG E	50.5177	46.5738	45.8638	50.3451	59.5549	59.1140
CORRSP	46.5225	38.0965	53.9895	53.9887	59.1131	59.1155
CORRSP	54.1849	54.1580	38.2373	46.6898	59.7934	58.9058

FINAL EXCITED STATES OF SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
46.52247	0.00000	0.00000	-0.00015	//	0.7072	0.0000	-0.0000	-0.7070	0.0000	0.0000
27.90579				//	0.7073	0.0000	-0.0000	0.7069	0.0000	-0.0000
38.09651	0.00000	0.00003	-0.00000	//	-0.0000	0.7071	-0.7071	-0.0000	-0.0000	0.0000
33.00104				//	0.0004	0.7072	0.7070	-0.0004	-0.0000	0.0000
53.98948	1.22237	0.72967	0.00059	//	0.0000	0.7071	0.7071	0.0000	0.0000	-0.0000
38.09651				//	0.0000	-0.7070	0.7072	0.0000	0.0000	0.0000
53.98875	1.22237	-0.00059	0.72967	//	-0.7070	0.0000	-0.0000	0.7072	0.0000	0.0000
33.00127				//	-0.7069	0.0004	0.0004	0.7073	0.0000	0.0000
59.11312	0.00000	-0.00000	-0.00000	//	-0.0000	0.0000	-0.0000	-0.0000	1.0000	-0.0002
47.68103				//	0.0000	0.0000	-0.0000	-0.0000	1.0000	-0.0005
59.11553	0.00000	0.00000	-0.00000	//	0.0000	-0.0000	0.0000	-0.0000	0.0002	1.0000
47.68309				//	-0.0000	-0.0000	-0.0000	-0.0000	0.0005	1.0000

ENERGIES FOR M XYLENE IRMAPPROXIMATION

ONE ELECTRON EXCITATIONS

JUMP	3, 4	2, 4	3, 5	2, 5	1, 4	1, 5
XMOMNT	-0.00081	0.51500	0.51500	0.00081	-0.00000	0.00000
YMOMNT	-0.51501	-0.00081	-0.00081	0.51500	0.00000	-0.00000
JUMP E	39.0023	39.0035	39.0041	39.0053	53.9675	53.9693
DIAG E	50.1770	46.0000	46.0002	50.1800	64.7191	64.7210
DIAG E	50.4413	46.5448	45.8078	50.2681	65.1912	64.7364
CORRSP	46.4497	38.0923	53.9079	53.9073	64.7191	64.7210
CORRSP	54.1126	54.0826	38.2319	46.6188	65.4275	64.5162

FINAL EXCITED STATES OF SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
46.44969	0.00000	-0.00000	-0.00015	//	0.7072	0.0002	-0.0002	-0.7070	0.0000	-0.0000
27.90156				//	0.7073	0.0002	-0.0002	0.7069	0.0000	-0.0000
38.09228	0.00000	0.00001	-0.00000	//	-0.0002	0.7071	-0.7071	-0.0002	0.0000	-0.0000
32.99682				//	-0.0025	0.7071	0.7071	0.0025	0.0000	0.0000
53.90793	1.21603	0.72832	0.00016	//	-0.0013	0.7071	0.7071	0.0013	-0.0000	-0.0000
38.09228				//	0.0002	-0.7071	0.7071	0.0002	0.0000	0.0000
53.90728	1.21604	-0.00016	0.72833	//	-0.7070	-0.0013	-0.0013	0.7072	-0.0000	0.0000
32.99703				//	-0.7069	-0.0025	-0.0025	0.7073	0.0000	0.0000
64.71909	0.00000	-0.00000	0.00000	//	-0.0000	-0.0000	0.0000	0.0000	1.0000	-0.0002
52.96001				//	-0.0000	-0.0000	-0.0000	-0.0000	1.0000	-0.0004
64.72096	0.00000	0.00000	-0.00000	//	0.0000	0.0000	0.0000	-0.0000	0.0002	1.0000
52.96168				//	-0.0000	-0.0000	-0.0000	-0.0000	0.0004	1.0000

ENERGIES FOR MESITYLENE TBMAPPROXIMATION

ONE ELECTRON EXCITATIONS

JUMP	3, 4	2, 4	3, 5	2, 5	1, 4	1, 5
XMOMNT	0.00042	0.51595	0.51595	-0.00042	-0.00000	0.
YMOMNT	-0.51596	0.00042	0.00042	0.51595	-0.00000	-0.00000
JUMP E	38.2004	38.2012	38.2026	38.2034	47.8329	47.8351
DIAG E	49.5419	45.3301	45.3313	49.5447	58.2212	58.2236
DIAG E	49.7177	45.5059	45.5071	49.7205	58.4414	58.4437
CORRSP	45.8102	37.3842	53.2772	53.2764	58.2212	58.2236
CORRSP	45.9860	37.5600	53.4530	53.4522	58.4414	58.4437

FINAL EXCITED STATES OF • SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
45.81016	0.00000	0.00000	-0.00015	//	0.7072	0.0000	-0.0000	0.7070	-0.0000	0.0000
27.19349				//	0.7073	0.0000	-0.0000	0.7069	0.0000	-0.0000
37.38421	0.00000	0.00003	-0.00000	//	-0.0000	0.7071	-0.7071	-0.0000	-0.0000	0.0000
32.28873				//	0.0004	0.7072	0.7070	-0.0004	-0.0000	0.0000
53.27717	1.20625	0.72967	0.00059	//	0.0000	0.7071	0.7071	0.0000	0.0000	-0.0000
37.38421				//	0.0000	-0.7070	0.7072	0.0000	0.0000	0.0000
53.27644	1.20625	-0.00059	0.72967	//	-0.7070	0.0000	-0.0000	0.7072	0.0000	0.0000
32.28896				//	-0.7069	0.0004	0.0004	0.7073	0.0000	0.0000
58.22124	0.00000	-0.00000	-0.00000	//	-0.0000	0.0000	-0.0000	-0.0000	1.0000	-0.0002
46.78915				//	0.0000	0.0000	-0.0000	-0.0000	1.0000	-0.0005
58.22361	0.00000	0.00000	-0.00000	//	0.0000	-0.0000	0.0000	-0.0000	0.0002	1.0000
46.79117				//	-0.0000	-0.0000	-0.0000	-0.0000	0.0005	1.0000

ENERGIES FOR MESITYLENE IRMAPPROXIMATION

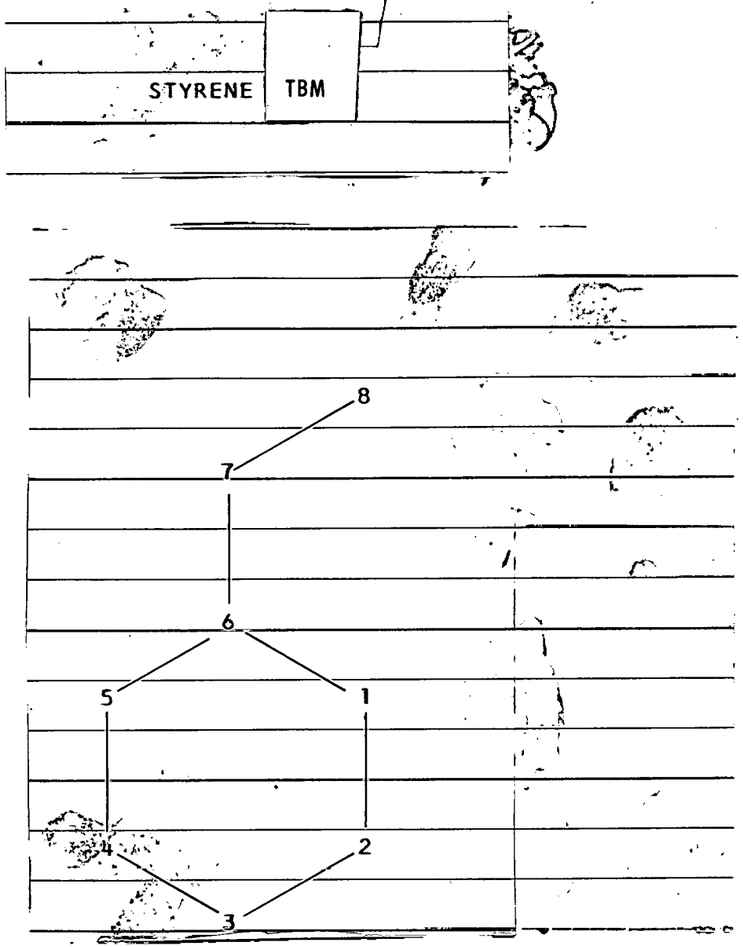
ONE ELECTRON EXCITATIONS

JUMP	3, 4	2, 4	3, 5	2, 5	1, 4	1, 5
XMOMNT	-0.00081	0.51500	0.51500	0.00081	-0.00000	0.00000
YMOMNT	-0.51501	-0.00081	-0.00081	-0.51500	0.00000	-0.00000
JUMP E	38.2884	38.2896	38.2902	38.2914	52.9796	52.9814
DIAG E	49.4631	45.2861	45.2862	49.4660	63.7312	63.7331
DIAG E	49.6393	45.4623	45.4624	49.6422	63.9750	63.9769
CORRSP	45.7357	37.3783	53.1940	53.1933	63.7312	63.7331
CORRSP	45.9119	37.5545	53.3702	53.3695	63.9750	63.9769

FINAL EXCITED STATES OF SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
45.73574	0.00000	-0.00000	-0.00015	//	0.7072	0.0002	-0.0002	0.7070	0.0000	-0.0000
27.18762				//	0.7073	0.0002	-0.0002	0.7069	0.0000	0.0000
37.37833	0.00000	0.00001	-0.00000	//	-0.0002	0.7071	-0.7071	-0.0002	0.0000	-0.0000
32.28287				//	-0.0025	0.7071	0.7071	0.0025	0.0000	0.0000
53.19398	1.19993	0.72832	0.00017	//	-0.0013	0.7071	0.7071	0.0013	-0.0000	-0.0000
37.37833				//	0.0002	-0.7071	0.7071	0.0002	0.0000	0.0000
53.19334	1.19993	-0.00017	0.72833	//	-0.7070	-0.0013	-0.0013	0.7072	-0.0000	0.0000
32.28308				//	-0.7069	-0.0025	-0.0025	0.7073	0.0000	0.0000
63.73124	0.00000	-0.00000	0.00000	//	-0.0000	-0.0000	0.0000	0.0000	1.0000	-0.0002
51.97216				//	-0.0000	-0.0000	-0.0000	-0.0000	1.0000	-0.0004
63.73308	0.00000	0.00000	-0.00000	//	0.0000	0.0000	0.0000	-0.0000	0.0002	1.0000
51.97380				//	-0.0000	-0.0000	-0.0000	-0.0000	0.0004	1.0000

STYRENE TBM



ATOMIC COORDINATES

x	1.7320	1.7320	0.8660	0.	0.	0.8660	0.8660	1.7320
y	1.5000	0.5000	0.	0.5000	1.5000	2.0000	3.0000	3.5000

0.2468127 20 0.22996

STYRENE TBM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1.527126 1.349041 1.246799 1.163433 0.836567 0.753200 0.650958 0.472873
0.394103 0.000013 0.500000-0.307706-0.307706-0.500000-0.000013-0.394103
0.328596-0.353553 0.500000 0.130478-0.130478 0.500000-0.353553 0.328596
0.307712-0.500006-0.000000 0.394090 0.394090-0.000000 0.500006-0.307712
0.328596-0.353553-0.500000 0.130478-0.130478-0.500000-0.353553 0.328596
0.394103 0.000013-0.500000-0.307706-0.307706 0.500000-0.000013-0.394103
0.513120 0.353553-0.000000-0.334227 0.334227-0.000000 0.353553 0.513120
0.307700 0.499993-0.000000 0.394116 0.394116-0.000000-0.499994-0.307700
0.144072 0.353553-0.000000 0.595183-0.595183 0.000000 0.353553 0.144072

STYRENE TBM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

26.95753 20.20652 15.45923 10.97079-15.25741-25.59032-41.87591-87.05846
0.318913 0.000011 0.447787-0.285276-0.336423-0.576122-0.000016-0.573109
0.265904-0.304398 0.447787 0.120967-0.142655 0.576123-0.438206 0.477848
0.249005-0.430490-0.000000 0.365363 0.430869-0.000000 0.619725-0.447479
0.265904-0.304398-0.447787 0.120967-0.142655-0.576122-0.438206 0.477848
0.318913 0.000011-0.447787-0.285276-0.336423 0.576123-0.000016-0.573109
0.415223 0.304399-0.000000-0.309864 0.365419-0.000000 0.438206 0.746185
0.248995 0.430479-0.000000 0.365387 0.430897-0.000000-0.619709-0.447461
0.116585 0.304398-0.000000 0.551798-0.650729 0.000000 0.438206 0.209511

STYRENE TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8
1	1.00000	0.67869	-0.00000	-0.32131	0.00000	0.61014	0.00000	-0.25272
2	0.67869	1.00000	0.65862	-0.00000	-0.32131	-0.00000	-0.04848	-0.00000
3	-0.00000	0.65862	1.00000	0.65862	-0.00000	-0.30120	0.00000	0.20422
4	-0.32131	-0.00000	0.65862	1.00000	0.67869	0.00000	-0.04848	-0.00000
5	0.00000	-0.32131	-0.00000	0.67869	1.00000	0.61014	0.00000	-0.25272
6	0.61014	-0.00000	-0.30120	0.00000	0.61014	1.00000	0.40587	0.00000
7	0.00000	-0.04848	0.00000	-0.04848	0.00000	0.40587	1.00000	0.91135
8	-0.25272	-0.00000	0.20422	-0.00000	-0.25272	0.00000	0.91135	1.00000

STYRENE TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8
1	0.76720	0.50160	-0.04965	-0.30045	-0.03485	0.44164	-0.04965	-0.24046
2	0.50160	0.75702	0.48290	-0.04503	-0.30045	-0.03946	-0.04126	0.01018
3	-0.04965	0.48290	0.76163	0.48290	-0.04965	-0.28172	0.02037	0.19919
4	-0.30045	-0.04503	0.48290	0.75702	0.50160	-0.03946	-0.04126	0.01018
5	-0.03485	-0.30045	-0.04965	0.50160	0.76720	0.44164	-0.04965	-0.24046
6	0.44164	-0.03946	-0.28172	-0.03946	0.44164	0.72217	0.24241	-0.05983
7	-0.04965	-0.04126	0.02037	-0.04126	-0.04965	0.24241	0.76164	0.72337
8	-0.24046	0.01018	0.19919	0.01018	-0.24046	-0.05983	0.72337	0.82146

ENERGIES FOR STYRENE , TBM APPROXIMATION 1.7

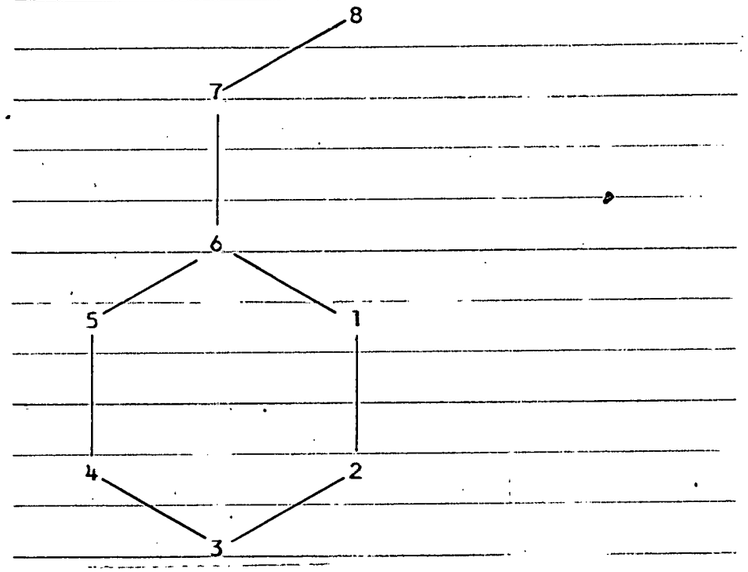
ONE ELECTRON EXCITATIONS OF NO SYMMETRY

JUMP	4, 5	3, 5	2, 5	4, 6	3, 6	1, 5	2, 6	1, 6	4, 7	3, 7
XMOMNT	-0.31096	-0.38705	-0.18746	0.38847	0.00000	-0.07765	-0.31928	-0.06031	0.18997	-0.32250
YMOMNT	-0.74021	-0.00000	0.14105	-0.00000	-0.51596	0.00000	-0.00000	0.00000	-0.14294	0.00000
JUMP E	26.2282	30.7166	35.4639	36.5611	41.0496	42.2149	45.7968	52.5478	52.8467	57.3351
DIAG E	39.5677	41.2375	49.2670	46.4011	52.5977	54.4785	56.3055	63.1390	65.5284	67.2638
DIAG E	40.2300	43.5948	51.6243	44.7061	52.5977	58.1270	56.3055	64.4303	63.8334	67.2638
CORRSP	38.5778	36.2546	46.9707	49.5992	52.7800	55.8870	57.3592	63.2689	66.2385	68.8502
CORRSP	38.6792	36.5468	49.9592	47.7754	54.2749	58.5699	56.8623	64.3533	65.7165	69.9752

FINAL EXCITED STATES OF NO SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION								
38.57781	0.74263	-0.20201	-0.64177	//	0.9534	0.0313	-0.1098	0.1486	-0.1621	-0.1583	-0.0508	-0.0245	0.0296	0.0228
19.37325				//	0.9414	-0.0005	0.2660	0.0016	-0.1234	0.0250	0.0040	0.0011	-0.1649	0.0036
36.25458	0.01481	-0.05796	0.07905	//	-0.1127	0.7979	0.0134	0.4990	0.0097	0.0448	-0.2551	-0.0448	0.0088	0.1795
31.60558				//	-0.0431	0.8432	0.1388	-0.3990	0.0731	0.0931	0.1826	0.0872	-0.0589	0.2242
46.97071	0.06845	0.12373	-0.13770	//	0.1081	-0.3185	0.7410	0.4387	0.3150	0.1963	-0.0764	-0.0342	-0.0023	0.0255
30.86251				//	-0.1504	-0.1438	0.6148	0.1075	0.6252	0.2981	-0.0425	-0.0197	-0.2893	-0.0388
49.59919	0.78110	0.59252	0.13873	//	-0.1941	-0.4661	-0.4898	0.6667	-0.0984	-0.1753	-0.0836	-0.0026	-0.0938	0.0672
37.15365				//	0.0165	0.4499	-0.0415	0.7933	-0.0013	0.0078	-0.3873	-0.0751	0.0285	0.0984
52.78004	0.53742	-0.06606	-0.48485	//	0.0689	0.0791	-0.1789	-0.0715	0.8498	-0.4302	0.0244	0.0171	-0.2087	0.0146
34.12983				//	0.2893	0.0307	-0.5179	-0.0416	0.7595	-0.1176	0.0342	0.0052	0.2306	0.0186
55.88696	0.26339	-0.05995	-0.32746	//	0.1474	0.0143	-0.3859	0.0629	0.3205	0.8213	0.2012	-0.0543	-0.0102	-0.0662
49.31396				//	0.0661	-0.0271	-0.2412	-0.0154	-0.1055	0.9376	-0.0138	0.0028	0.2079	-0.0537
57.35916	0.10890	-0.19733	0.07553	//	-0.0277	0.1650	0.1014	0.2519	-0.0810	-0.1796	0.9087	-0.1111	0.0076	-0.1460
59.25338				//	0.0123	0.0186	0.2215	0.3306	-0.0005	-0.0377	0.5592	0.5565	0.4389	-0.1572
63.26889	0.01774	-0.06551	-0.04798	//	0.0216	0.0344	0.0040	0.0772	0.0254	0.0249	0.1020	0.9807	0.1360	0.0214
47.38424				//	0.0042	0.0354	0.0056	-0.2269	0.0155	-0.0271	-0.6301	0.6835	-0.0022	-0.2865
66.23850	0.21156	0.16967	-0.21522	//	-0.0296	-0.0599	-0.0836	0.0050	0.1758	-0.0886	0.0245	-0.1373	0.9421	0.2067
58.91059				//	0.0296	-0.0264	0.3927	-0.1903	0.0151	-0.0709	-0.3153	-0.3041	0.7715	0.1253
68.85023	0.57153	-0.44012	0.03870	//	0.0203	-0.0730	0.0246	-0.1160	-0.0417	0.0577	0.2041	-0.0032	-0.2011	0.9450
64.73482				//	-0.0040	-0.2491	-0.0224	0.0292	-0.0099	0.0416	-0.0654	0.3422	-0.0240	0.9016

STYRENE IRM



ATOMIC COORDINATES

x 1.7320 1.7320 0.8660 0. 0. 0.8660 0.8660 1.7320
y 1.5000 0.5000 0. 0.5000 1.5000 2.0000 3.0000 3.5000
0.2468127 20 0.99996

STYRENE IRM APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1.623040 1.345062 1.196862 1.104256 0.802927 0.733662 0.655821 0.538368
0.396849 0.010799-0.485897-0.330546 0.326878 0.480635-0.016957-0.398611
0.342378-0.326034-0.512646 0.114083 0.085315-0.516655-0.348392 0.324145
0.326692-0.463815-0.027255 0.423713-0.390654 0.036581 0.502074-0.303060
0.340920-0.342318 0.485367 0.175487 0.161937 0.480001-0.375326 0.320502
0.392701-0.015931 0.513048-0.293664 0.273102-0.517253 0.019073-0.391887
0.485418 0.329510 0.027518-0.364785-0.314349 0.037178 0.371946 0.532378
0.297560 0.530737 0.004266 0.320269-0.441170 0.004556-0.495265-0.295375
0.154750 0.413238-0.027932 0.587807 0.582243-0.036945 0.318420 0.131246

STYRENE IRM IRM APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

29.97969 20.03527 12.84571 7.37343-19.16861-28.35165-40.98641-66.96651
0.311502 0.009311-0.444142-0.314556 0.364794-0.561136-0.020938-0.543262
0.268746-0.281120-0.468593 0.108564 0.095211-0.603188-0.430205 0.441774
0.256433-0.399921-0.024913 0.403215-0.435968 0.042708 0.619977-0.413037
0.267601-0.295161 0.443658 0.166997 0.180721 0.560395-0.463464 0.436808
0.308246-0.013737 0.468961-0.279458 0.304780-0.603886 0.023552-0.534099
0.381023 0.284118 0.025154-0.347138-0.350811 0.043404 0.459291 0.725572
0.233566 0.457623 0.003899 0.304776-0.492343 0.005320-0.611569-0.402563
0.121469 0.356311-0.025531 0.559371 0.649780-0.043132 0.393195 0.178874

STYRENE IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8
1	1.00592	0.68747	-0.00435	-0.32450	0.00690	0.60681	0.03176	-0.22970
2	0.68747	0.99868	0.65076	-0.00094	-0.31374	0.00608	-0.07362	-0.00074
3	-0.00435	0.65076	1.00425	0.66255	-0.00546	-0.29913	-0.02674	0.21742
4	-0.32450	-0.00094	0.66255	0.99957	0.67363	0.00407	-0.04393	0.00179
5	0.00690	-0.31374	-0.00546	0.67363	1.00785	0.61323	0.03307	-0.26552
6	0.60681	0.00608	-0.29913	0.00407	0.61323	0.95607	0.40522	-0.00781
7	0.03176	-0.07362	-0.02674	-0.04393	0.03307	0.40522	0.94563	0.90701
8	-0.22970	-0.00074	0.21742	0.00179	-0.26552	-0.00781	0.90701	1.08202

STYRENE IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8
1	0.78666	0.51014	-0.07923	-0.33793	-0.04898	0.43871	-0.04117	-0.24692
2	0.51014	0.76524	0.47358	-0.06975	-0.32678	-0.05389	-0.06923	0.01034
3	-0.07923	0.47358	0.77779	0.48589	-0.07965	-0.31303	-0.00065	0.22967
4	-0.33793	-0.06975	0.48589	0.76690	0.49586	-0.05742	-0.03989	0.01885
5	-0.04898	-0.32678	-0.07965	0.49586	0.78645	0.44470	-0.03527	-0.27149
6	0.43871	-0.05389	-0.31303	-0.05742	0.44470	0.69408	0.22662	-0.09461
7	-0.04117	-0.06923	-0.00065	-0.03989	-0.03527	0.22662	0.71375	0.72362
8	-0.24692	0.01034	0.22967	0.01885	-0.27149	-0.09461	0.72362	0.91052

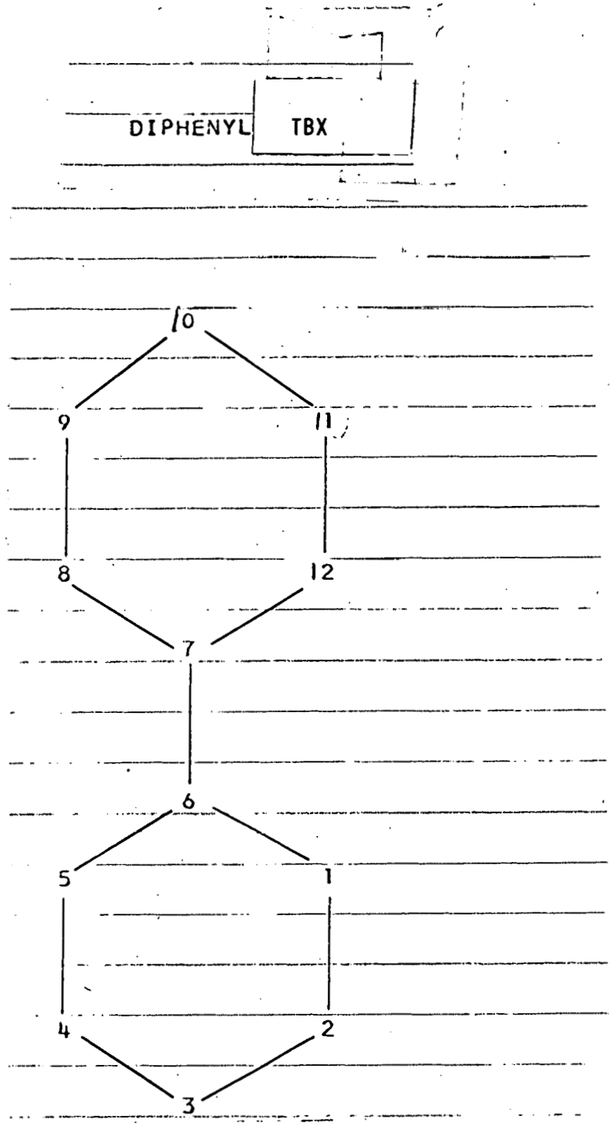
ENERGIES FOR STYRENE , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF NO SYMMETRY

JUMP	4, 5	3, 5	4, 6	2, 5	3, 6	4, 7	2, 6	1, 5	3, 7	1, 6
XMOMNT	0.25935	-0.38648	-0.42056	0.24711	0.05776	0.20105	0.28491	0.07967	0.31722	0.04453
YMOMNT	0.74944	-0.09232	-0.09859	-0.11403	-0.50859	-0.14987	0.00056	0.01489	0.00863	-0.00546
JUMP E	26.5420	32.0143	35.7251	39.2039	41.1974	48.3598	48.3869	49.1483	53.8321	58.3313
DIAG E	39.2849	43.0376	44.3618	53.7392	52.5185	59.6732	59.2600	62.7380	63.5418	69.5692
DIAG E	40.1529	45.4697	42.7973	55.7956	52.5181	57.6507	58.8839	66.2307	63.0836	70.6295
CORRSP	38.3968	36.6786	47.9877	54.0326	51.2991	60.8427	59.3948	63.6099	65.7606	69.7211
CORRSP	38.2148	47.5347	36.4944	56.3457	51.4286	60.1046	59.0590	67.1292	65.9954	70.9054

FINAL EXCITED STATES OF NO SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
38.39682	0.70510	0.14956	0.63989	//	0.9706	0.0926	0.1175	-0.0293	0.1499	-0.0463	-0.0050	-0.1001	0.0026	-0.0103
19.64819				//	0.9422	-0.0150	-0.0252	0.2760	0.1252	0.1367	-0.0099	0.0260	-0.0045	-0.0020
36.67861	0.00045	-0.01609	0.00542	//	0.0096	0.7138	-0.6294	0.0058	-0.0093	-0.0012	0.2147	-0.0192	-0.2170	0.0257
32.34129				//	-0.0005	0.6060	0.5727	0.1866	-0.3961	0.1263	-0.2104	0.0637	-0.2134	-0.0583
47.98773	0.42020	-0.45140	-0.04631	//	-0.0676	0.5895	0.6637	0.2826	-0.3383	0.1080	-0.0181	0.0310	0.0118	0.0005
36.71297				//	0.0129	-0.6409	0.7013	-0.0294	0.0342	-0.0146	-0.2279	0.0122	0.2035	-0.0400
54.03261	0.24257	0.10705	-0.30677	//	-0.0517	0.0137	-0.0091	0.7112	0.4993	-0.4251	-0.0495	0.2413	-0.0039	-0.0238
34.85927				//	-0.3191	0.0326	0.0359	0.6125	0.5677	0.4283	-0.0230	0.1189	-0.0128	-0.0146
51.29912	0.86314	-0.39324	-0.49094	//	-0.1970	0.2941	0.3133	-0.5309	0.6984	-0.0664	0.0105	-0.0404	0.0222	0.0153
31.80520				//	0.0858	0.3493	0.2665	-0.4186	0.7052	-0.2805	-0.0761	-0.1758	-0.1036	-0.0296
60.84267	0.47691	0.24782	-0.35058	//	-0.0170	-0.0540	-0.0381	0.3240	0.3530	0.8428	-0.0260	-0.2130	-0.0901	-0.0359
53.99129				//	0.0134	-0.0199	-0.0051	-0.3148	-0.0532	0.7072	-0.0225	-0.6275	-0.0084	0.0558
59.39481	0.05376	0.14566	-0.00821	//	0.0024	-0.1920	0.1972	0.0262	0.0134	-0.0173	0.8955	0.0532	-0.3323	-0.0887
50.30882				//	0.0096	0.1331	0.1844	0.0206	-0.0202	0.0258	0.6627	-0.0650	0.4259	-0.5674
63.60995	0.01253	0.00971	0.06736	//	0.1020	-0.0033	-0.0047	-0.1570	0.0005	0.2630	-0.1289	0.9114	-0.2128	-0.0559
58.61066				//	0.0493	-0.0216	0.0313	-0.4789	0.0582	0.4423	0.1242	0.7295	-0.1375	-0.0352
65.76057	0.57451	0.45325	-0.00200	//	0.0291	-0.0801	-0.1015	0.0199	0.0280	0.1411	0.3556	0.2154	0.8877	-0.0222
60.76078				//	0.0063	0.2199	-0.2100	-0.0947	0.0059	0.0801	-0.5943	0.1260	0.6937	-0.2046
69.72107	0.02333	0.08832	-0.00839	//	0.0177	-0.0395	0.0258	0.0302	0.0178	0.0372	0.0728	0.0590	-0.0198	0.9928
64.95172				//	0.0101	0.1786	0.1679	-0.0002	0.0031	0.0154	0.2984	0.0637	0.4697	0.7911



ATOMIC COORDINATES

x	1.7630	1.7630	0.8815	0.	0.	0.8815
y	1.5270	0.5090	0.	0.5090	1.5270	2.0360

0.8815	0.	0.	0.8815	1.7630	1.7630
3.0970	3.6060	4.6240	5.1330	4.6240	3.6060

DIPHENYL X — TBX APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 A S	3 S S	4 S A	5 A A	6 A S	7 S S	8 S A	9 A A	10 A S	11 S S	12 A S
1.529817	1.449137	1.305407	1.236577	1.236577	1.172572	0.827427	0.763422	0.763422	0.694592	0.550862	0.470182
0.294041	0.269755	-0.072887	0.353553	0.353553	0.292334	0.292334	-0.353553	-0.353553	-0.072886	0.269755	0.294041
0.218449	0.319421	0.281376	0.353553	0.353554	-0.145180	0.145180	0.353553	0.353553	-0.281376	-0.319421	-0.218449
0.195132	0.336581	0.436026	-0.000000	0.000000	-0.398144	-0.398144	0.000000	0.000000	0.436026	0.336581	0.195132
0.218449	0.319421	0.281377	-0.353553	-0.353553	-0.145180	0.145180	-0.353553	-0.353553	-0.281376	-0.319421	-0.218449
0.294041	0.269755	-0.072886	-0.353553	-0.353553	0.292334	0.292334	0.353553	0.353553	-0.072886	0.269755	0.294041
0.439958	0.192658	-0.375381	-0.000000	-0.000000	0.358341	-0.358342	0.000000	0.000000	0.375381	-0.192659	-0.439958
0.439958	-0.192659	-0.375381	-0.000000	-0.000000	-0.358341	-0.358341	0.000000	0.000000	-0.375381	-0.192659	0.439958
0.294042	-0.269755	-0.072887	-0.353553	0.353553	-0.292334	0.292334	0.353553	-0.353553	0.072887	0.269755	-0.294041
0.218449	-0.319421	0.281376	-0.353553	0.353553	0.145180	0.145180	-0.353553	0.353553	0.281376	-0.319421	0.218449
0.195132	-0.336581	0.436026	0.000000	0.000000	0.398144	-0.398144	0.000000	0.000000	-0.436026	0.336581	-0.195132
0.218449	-0.319421	0.281377	0.353554	-0.353553	0.145180	0.145180	0.353553	-0.353553	0.281376	-0.319421	0.218449
0.294041	-0.269755	-0.072886	0.353553	-0.353553	-0.292334	0.292334	-0.353553	0.353553	0.072887	0.269755	-0.294042

DIPHENYL X — TBX APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 A S	3 S S	4 S A	5 A A	6 A S	7 S S	8 S A	9 A A	10 A S	11 S S	12 A S
26.5782	23.7852	17.9544	14.6822	14.6821	11.2946	-16.0060	-23.7820	-23.7820	-33.7435	-62.5713	-86.4768
0.237733	0.224086	-0.063794	0.317939	0.317939	0.269966	0.321377	-0.404644	-0.404644	-0.087454	0.363453	0.428821
0.176616	0.265344	0.246271	0.317939	0.317940	-0.134072	0.159604	0.404643	0.404643	-0.337616	-0.430370	-0.318579
0.157764	0.279598	0.381627	-0.000000	0.000000	-0.367680	-0.437699	0.000000	0.000000	0.523175	0.453490	0.284574
0.176616	0.265344	0.246272	-0.317939	-0.317939	-0.134072	0.159604	-0.404644	-0.404643	-0.337616	-0.430370	-0.318579
0.237733	0.224086	-0.063793	-0.317939	-0.317940	0.269966	0.321377	0.404643	0.404643	-0.087454	0.363453	0.428821
0.355706	0.160042	-0.328549	-0.000000	-0.000000	0.330923	-0.393942	0.000000	0.000000	0.450410	-0.259578	-0.641620
0.355706	-0.160042	-0.328549	-0.000000	-0.000000	-0.330923	-0.393942	0.000000	0.000000	-0.450410	-0.259577	0.641620
0.237733	-0.224086	-0.063793	-0.317940	0.317939	-0.269966	0.321377	0.404643	-0.404644	0.087455	0.363453	-0.428821
0.176616	-0.265344	0.246272	-0.317939	0.317939	0.134072	0.159604	-0.404643	0.404644	0.337616	-0.430370	0.318579
0.157764	-0.279598	0.381627	0.000000	0.000000	0.367680	-0.437698	0.000000	0.000000	-0.523175	0.453490	-0.284574
0.176616	-0.265344	0.246272	-0.317940	-0.317939	0.134072	0.159604	0.404643	-0.404644	0.337616	-0.430370	0.318579
0.237733	-0.224086	-0.063793	0.317939	-0.317939	-0.269966	0.321377	-0.404643	0.404644	-0.087455	0.363453	-0.428821

DIPHENYL X — TBX TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.00000	0.67490	-0.00000	-0.32510	-0.00000	0.62690	0.00000	-0.13291	0.00000	0.10239	0.00000	-0.13291
2	0.67490	1.00000	0.66125	-0.00000	-0.32510	-0.00000	-0.03806	0.00000	0.00757	0.00000	0.00757	0.00000
3	-0.00000	0.66125	1.00000	0.66125	-0.	-0.31130	-0.00000	0.10239	-0.00000	-0.08722	0.00000	0.10239
4	-0.32510	-0.00000	0.66125	1.00000	0.67490	0.00000	-0.03806	-0.00000	0.00757	0.00000	0.00757	-0.00000
5	-0.00000	-0.32510	-0.	0.67490	1.00000	0.62690	-0.00000	-0.13291	0.00000	0.10239	0.00000	-0.13291
6	0.62690	-0.00000	-0.31130	0.00000	0.62690	1.00000	0.33790	-0.00000	-0.03806	-0.00000	-0.03806	0.00000
7	0.00000	-0.03806	-0.00000	-0.03806	-0.00000	0.33790	1.00000	0.62690	0.00000	-0.31130	0.00000	0.62690
8	-0.13291	0.00000	0.10239	-0.00000	-0.13291	0.00000	0.62690	1.00000	0.67490	0.00000	-0.32510	-0.00000
9	0.00000	0.00757	-0.00000	0.00757	0.00000	-0.03806	0.00000	0.67490	1.00000	0.66125	-0.00000	-0.32510
10	0.10239	0.00000	-0.08722	0.00000	0.10239	-0.00000	-0.31130	0.00000	0.66125	1.00000	0.66125	0.00000
11	0.00000	0.00757	0.00000	0.00757	0.00000	-0.03806	0.00000	-0.32510	-0.00000	0.66125	1.00000	0.67490
12	-0.13291	0.00000	0.10239	-0.00000	-0.13291	0.00000	0.62690	-0.00000	-0.32510	0.00000	0.67490	1.00000

DIPHENYL X — TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.77171	0.50343	-0.04689	-0.30526	-0.03698	0.46145	-0.03936	-0.12502	0.00602	0.09953	0.00602	-0.12502
2	0.50343	0.76479	0.49067	-0.04389	-0.30526	-0.03998	-0.03238	0.00602	0.00692	-0.00328	0.00692	0.00602
3	-0.04689	0.49067	0.76779	0.49067	-0.04689	-0.29238	0.01532	0.09953	-0.00328	-0.08567	-0.00328	0.09953
4	-0.30526	-0.04389	0.49067	0.76479	0.50343	-0.03998	-0.03238	0.00602	0.00692	-0.00328	0.00692	0.00602
5	-0.03698	-0.30526	-0.04689	0.50343	0.77171	0.46145	-0.03936	-0.12502	0.00602	0.09953	0.00602	-0.12502
6	0.46145	-0.03998	-0.29238	-0.03998	0.46145	0.73919	0.19869	-0.03936	-0.03238	0.01532	-0.03238	-0.03936
7	-0.03936	-0.03238	0.01532	-0.03238	-0.03936	0.19869	0.73919	0.46145	-0.03998	-0.29238	-0.03998	0.46145
8	-0.12502	0.00602	0.09953	0.00602	-0.12502	-0.03936	0.46145	0.77171	0.50343	-0.04689	-0.30526	-0.03698
9	0.00602	0.00692	-0.00328	0.00692	0.00602	-0.03238	-0.03998	0.50343	0.76479	0.49067	-0.04389	-0.30526
10	0.09953	-0.00328	-0.08567	-0.00328	0.09953	0.01532	-0.29238	-0.04689	0.49067	0.76779	0.49067	-0.04689
11	0.00602	0.00692	-0.00328	0.00692	0.00602	-0.03238	-0.03998	-0.30526	-0.04389	0.49067	0.76479	0.50343
12	-0.12502	0.00602	0.09953	0.00602	-0.12502	-0.03936	0.46145	-0.03698	-0.30526	-0.04689	0.50343	0.77171

ENERGIES FOR DIPHENYL X TBX APPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	4, 7	6, 9	3, 8	2, 9	5,10	1, 8
XMOMNT	0.55646	-0.55802	0.45762	0.06512	-0.46013	-0.09998
YMOMNT	-0.00000	0.00000	0.00000	-0.00000	-0.00000	-0.00000
JUMP E	30.6881	35.0765	41.7364	47.5672	48.4256	50.3601
DIAG E	42.7221	46.8365	56.2854	65.1197	62.4620	66.0644
DIAG E	42.2330	47.4289	56.9005	65.4298	61.8588	66.7917
CORRSP	35.1486	50.4529	55.4149	60.7024	64.5229	73.2483
CORRSP	35.0840	50.5967	55.9513	61.3786	64.0904	73.5415

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
35.14857	0.00603	0.06350	-0.00000	//	0.7314	-0.5523	-0.3119	-0.0146	-0.2457	0.0466
30.57703				//	0.7858	-0.4632	0.2678	-0.0030	-0.2987	-0.0842
50.45291	1.35942	-0.79600	0.00000	//	-0.6387	0.7555	-0.1182	0.0004	-0.0638	-0.0569
35.49885				//	0.5138	0.7282	-0.4162	-0.0306	-0.1672	0.0598
55.41492	0.17838	0.27513	0.00000	//	0.1807	0.2904	0.8078	0.4600	0.1376	-0.0028
57.06853				//	0.0203	0.4421	0.6741	-0.1263	0.1319	-0.5625
60.70241	0.03017	-0.10810	-0.00000	//	-0.1154	-0.0918	-0.2528	0.5886	-0.1230	0.7435
45.81694				//	-0.0385	0.2178	0.4297	0.7050	-0.1962	0.4805
64.52290	0.90888	-0.57554	-0.00000	//	0.1052	0.1395	-0.2393	0.0076	0.9495	0.1032
61.52223				//	0.3413	-0.0356	-0.0054	0.1656	0.9094	0.1669
73.24827	0.00043	-0.01175	0.00000	//	0.0077	0.1095	0.3392	-0.6646	0.0026	0.6567
73.23753				//	0.0130	0.1048	0.3406	-0.6772	0.0024	0.6436

ENERGIES FOR DIPHENYL X TBX APPROXIMATION

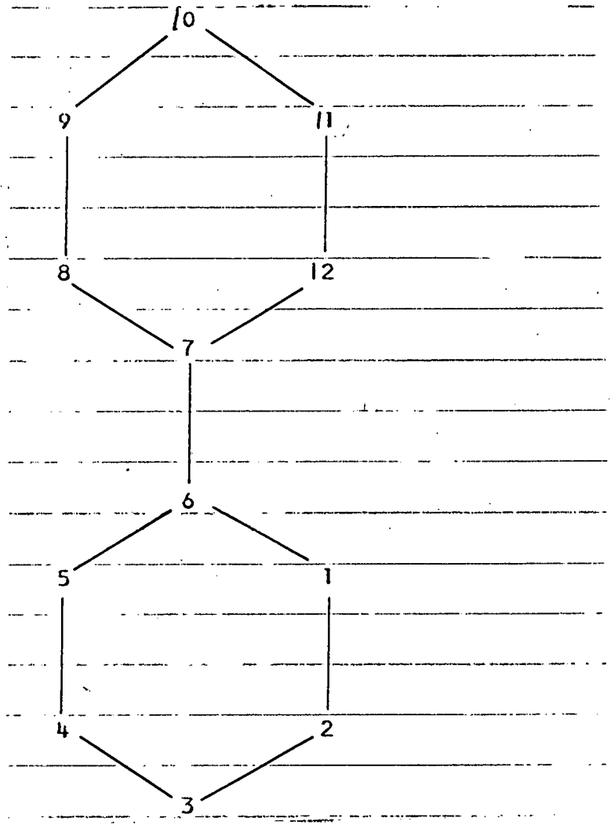
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	6, 7	5, 8	4, 9	2, 7	3,10
XMOMNT	-0.00000	0.00000	-0.00000	0.00000	0.00000
YMOMNT	-0.87239	-0.52387	0.52387	0.05360	-0.20675
JUMP E	27.3005	38.4641	38.4641	39.7912	51.6979
DIAG E	38.3913	53.2935	52.4288	54.8270	67.8811
DIAG E	38.3270	53.4612	52.5964	54.4804	67.7254
CORRSP	37.2649	57.7078	48.2418	54.2985	69.3086
CORRSP	37.2466	57.8710	48.3976	53.9454	69.1298

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION				
37.26491	0.83792	-0.00000	-0.72716	//	0.9697	-0.1378	-0.1241	0.1078	0.1168
22.90460				//	0.8741	-0.2829	-0.2812	0.0269	0.2759
57.70783	0.00138	0.00000	-0.02375	//	0.0094	0.7287	-0.6765	0.1012	-0.0309
57.66699				//	0.0172	0.7180	-0.6948	0.0258	-0.0290
48.24176	1.46105	-0.00000	-0.84391	//	0.1695	0.6424	0.7236	0.1810	-0.0476
31.36941				//	0.3905	0.6337	0.6583	-0.0664	0.0903
54.29855	0.24682	-0.00000	0.32695	//	-0.1091	-0.1918	-0.0560	0.9413	-0.2492
45.59339				//	0.1267	0.0093	0.0634	0.8989	-0.4146
69.30862	0.02113	0.00000	-0.08467	//	-0.1376	0.0223	0.0147	0.2435	0.9597
65.24357				//	-0.2592	0.0529	0.0282	0.4315	0.8620

DIPHENYL IRX



ATOMIC COORDINATES

x	1.7630	1.7630	0.8815	0.	0.	0.8815
y	1.5270	0.5090	0.	0.5090	1.5270	2.0360

0.8815	0.	0.	0.8815	1.7630	1.7630
3.0970	3.6060	4.6240	5.1330	4.6240	3.6060

DIPHENYL X IRX APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 S S	2 A S	3 S S	4 S A	5 A A	6 A S	7 S S	8 S A	9 A A	10 A S	11 S S	12 A S
1.631836	1.507697	1.275942	1.197211	1.185123	1.103222	0.791150	0.751549	0.739461	0.687587	0.590001	0.539214
0.297009	0.267589	0.089554	-0.358317	0.348725	-0.298378	0.282312	0.348726	0.358315	-0.059749	0.272150	-0.292911
0.228877	0.321427	-0.273359	-0.348726	0.358315	0.138153	0.150934	-0.358317	-0.348725	-0.287783	-0.316400	0.211611
0.210328	0.338140	-0.428858	0.000000	-0.000000	0.403964	-0.403523	0.000000	0.000000	0.431444	0.330170	-0.190604
0.228877	0.321427	-0.273359	0.348726	-0.358316	0.138153	0.150934	0.358317	0.348725	-0.287783	-0.316401	0.211611
0.297009	0.267589	0.089554	0.358317	-0.348724	-0.298378	0.282311	-0.348726	-0.358316	-0.059749	0.272151	-0.292911
0.417809	0.189269	0.388061	0.000000	0.000000	-0.347248	-0.363603	-0.000000	0.000000	0.375604	-0.206488	0.450019
0.417809	-0.189269	0.388060	-0.000000	0.000000	0.347248	-0.363603	-0.000000	0.000000	-0.375604	-0.206488	-0.450020
0.297009	-0.267589	0.089553	0.358315	0.348726	0.298378	0.282311	-0.348725	0.358317	0.059749	0.272150	0.292911
0.228877	-0.321427	-0.273359	0.348725	0.358317	-0.138153	0.150934	0.358315	-0.348726	0.287783	-0.316400	-0.211611
0.210328	-0.338140	-0.428858	0.000000	-0.000000	-0.403965	-0.403523	0.000000	0.000000	-0.431444	0.330170	0.190604
0.228877	-0.321427	-0.273359	-0.348725	-0.358317	-0.138153	0.150934	-0.358315	0.348726	0.287783	-0.316400	-0.211611
0.297009	-0.267589	0.089554	-0.358315	-0.348726	0.298378	0.282312	0.348725	-0.358317	0.059749	0.272150	0.292911

DIPHENYL X IRX APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S S	2 A S	3 S S	4 S A	5 A A	6 A S	7 S S	8 S A	9 A A	10 A S	11 S S	12 A S
29.7143	25.8422	16.5968	12.6415	11.9877	7.1804	-20.2588	-25.3701	-27.0394	-34.8691	-53.3297	-65.5807
0.232505	0.217927	0.079281	-0.327478	0.320332	-0.284076	0.317394	0.402259	0.416685	-0.072055	0.354309	-0.398891
0.179169	0.261774	-0.242002	-0.318713	0.329142	0.131531	0.169690	-0.413322	-0.405532	-0.347057	-0.411918	0.288176
0.164649	0.275384	-0.379663	0.000000	-0.000000	0.384602	-0.453669	0.000000	0.000000	0.520308	0.429844	-0.259569
0.179169	0.261773	-0.242001	0.318713	-0.329143	0.131531	0.169690	0.413322	0.405532	-0.347057	-0.411918	0.288176
0.232505	0.217927	0.079281	0.327478	-0.320332	-0.284077	0.317394	-0.402259	-0.416685	-0.072055	0.354310	-0.398891
0.327069	0.154143	0.343546	0.000000	0.000000	-0.330604	-0.408788	-0.000000	0.000000	0.452967	-0.268825	0.612845
0.327069	-0.154143	0.343545	-0.000000	0.000000	0.330604	-0.408788	-0.000000	0.000000	-0.452967	-0.268825	-0.612845
0.232505	-0.217927	0.079280	0.327476	0.320334	0.284077	0.317394	-0.402258	0.416687	0.072055	0.354309	0.398891
0.179169	-0.261773	-0.242001	0.318711	0.329144	-0.131531	0.169690	-0.413321	-0.405534	0.347057	-0.411918	-0.288176
0.164649	-0.275384	-0.379662	-0.000000	-0.000000	-0.384602	-0.453669	0.000000	0.000000	-0.520308	0.429844	0.259569
0.179169	-0.261773	-0.242001	-0.318711	-0.329144	-0.131531	0.169690	-0.413321	0.405534	0.347057	-0.411918	-0.288176
0.232505	-0.217927	0.079281	-0.327476	-0.320334	0.284077	0.317394	0.402257	-0.416687	0.072055	0.354309	0.398891

DIPHENYL X — IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.01373	0.67639	-0.01198	-0.32324	0.01374	0.62621	0.00918	-0.14236	-0.00258	0.10823	-0.00258	-0.11524
2	0.67639	0.99902	0.65973	-0.00098	-0.32324	0.00482	-0.04663	-0.00258	0.02298	0.00175	-0.00415	-0.00258
3	-0.01198	0.65973	1.01136	0.65973	-0.01198	-0.30964	-0.00454	0.10823	0.00175	-0.09874	0.00175	0.10823
4	-0.32324	-0.00098	0.65973	0.99902	0.67639	0.00482	-0.04663	-0.00258	-0.00415	0.00175	0.02298	-0.00258
5	0.01374	-0.32324	-0.01198	0.67639	1.01373	0.62621	0.00918	-0.11524	-0.00258	0.10823	-0.00258	-0.14236
6	0.62621	0.00482	-0.30964	0.00482	0.62621	0.96312	0.33750	0.00918	-0.04663	-0.00454	-0.04663	0.00918
7	0.00918	-0.04663	-0.00454	-0.04663	0.00918	0.33750	0.96312	0.62621	0.00482	-0.30964	0.00482	0.62621
8	-0.14236	-0.00258	0.10823	-0.00258	-0.11524	0.00918	0.62621	1.01373	0.67639	-0.01198	-0.32324	0.01374
9	-0.00258	0.02298	0.00175	-0.00415	-0.00258	-0.04663	0.00482	0.67639	0.99902	0.65973	-0.00098	-0.32324
10	0.10823	0.00175	-0.09874	0.00175	0.10823	-0.00454	-0.30964	-0.01198	0.65973	1.01136	0.65973	-0.01198
11	-0.00258	-0.00415	0.00175	0.02298	-0.00258	-0.04663	0.00482	-0.32324	-0.00098	0.65973	0.99902	0.67639
12	-0.11524	-0.00258	0.10823	-0.00258	-0.14236	0.00918	0.62621	-0.01374	-0.32324	-0.01198	0.67639	1.01373

DIPHENYL X — IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.79678	0.50392	-0.08212	-0.33530	-0.04264	0.46158	-0.04845	-0.14495	0.00771	-0.11485	0.00345	-0.12644
2	0.50392	0.77281	0.48811	-0.06684	-0.33530	-0.05534	-0.04281	0.00771	0.02320	-0.00259	-0.00383	0.00345
3	-0.08212	0.48811	0.79002	0.48811	-0.08212	-0.32256	0.01625	0.11485	-0.00259	-0.10500	-0.00259	0.11485
4	-0.33530	-0.06684	0.48811	0.77281	0.50392	-0.05534	-0.04281	0.00345	-0.00383	-0.00259	0.02320	0.00771
5	-0.04264	-0.33530	-0.08212	0.50392	0.79678	0.46158	-0.04845	-0.12644	0.00345	0.11485	0.00771	-0.14495
6	0.46158	-0.05534	-0.32256	-0.05534	0.46158	0.71611	0.18388	-0.04845	-0.04281	0.01625	-0.04281	-0.04845
7	-0.04845	-0.04281	0.01625	-0.04281	-0.04845	0.18388	0.71611	0.46158	-0.05534	-0.32256	-0.05534	0.46158
8	-0.14495	0.00771	0.11485	0.00345	-0.12644	-0.04845	0.46158	0.79678	0.50392	-0.08212	-0.33530	-0.04264
9	0.00771	0.02320	-0.00259	-0.00383	0.00345	-0.04281	-0.05534	0.50392	0.77281	0.48811	-0.06684	-0.33530
10	0.11485	-0.00259	-0.10500	-0.00259	0.11485	0.01625	-0.32256	-0.08212	0.48811	0.79002	0.48811	-0.08212
11	0.00345	-0.00383	-0.00259	0.02320	0.00771	-0.04281	-0.05534	-0.33530	-0.06684	0.48811	0.77281	0.50392
12	-0.12644	0.00345	0.11485	0.00771	-0.14495	-0.04845	0.46158	-0.04264	-0.33530	-0.08212	0.50392	0.79678

ENERGIES FOR DIPHENYL X IRX APPROXIMATION

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	4, 7	6, 9	3, 8	5,10	2, 9	1, 8
XMOMNT	-0.55394	-0.55783	0.47153	-0.45335	-0.06082	0.08182
YMOMNT	0.00000	-0.00000	-0.00000	0.00000	0.00000	0.00000
JUMP E	32.9003	34.2198	41.9669	46.8567	52.8816	55.0844
DIAG E	44.5431	45.9602	56.4412	60.7748	70.6001	71.6616
DIAG E	44.0158	46.5480	57.0978	60.1555	70.9259	72.3310
CORRSP	50.7678	35.6964	56.4555	62.9938	66.0877	77.9797
CORRSP	50.8545	35.6755	56.9886	62.4950	66.7362	78.3241

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
50.76781	1.33791	-0.78722	0.00000	//	0.6726	0.7369	-0.0259	-0.0076	-0.0027	-0.0620
35.69318				//	0.6657	-0.6174	0.3202	0.2680	-0.0139	-0.0324
35.69638	0.00003	0.00426	-0.00000	//	-0.6766	0.6057	-0.3198	-0.2682	0.0216	-0.0255
31.17951				//	0.6376	0.6219	-0.3530	0.2792	0.0164	-0.0618
56.45550	0.25555	0.32626	-0.00000	//	-0.2586	0.2644	0.8532	0.2048	-0.3037	0.0314
58.52151				//	-0.1866	0.3503	0.6079	0.5008	0.1769	0.4368
62.99377	0.79407	-0.54445	0.00000	//	-0.1369	0.1217	-0.2620	0.9381	0.1243	-0.0486
61.33936				//	-0.3208	-0.1516	-0.2088	0.7314	-0.3359	-0.4274
66.08766	-0.09309	0.18200	-0.00000	//	-0.0649	0.0077	-0.2043	-0.0777	0.6577	0.7179
48.93157				//	-0.1115	-0.2862	-0.5461	0.2539	0.6185	0.4005
77.97972	0.00184	0.02358	0.00000	//	0.0036	-0.0724	-0.2422	-0.0037	-0.6778	0.6905
77.96908				//	0.0102	-0.0659	-0.2478	0.0012	-0.6877	0.6792

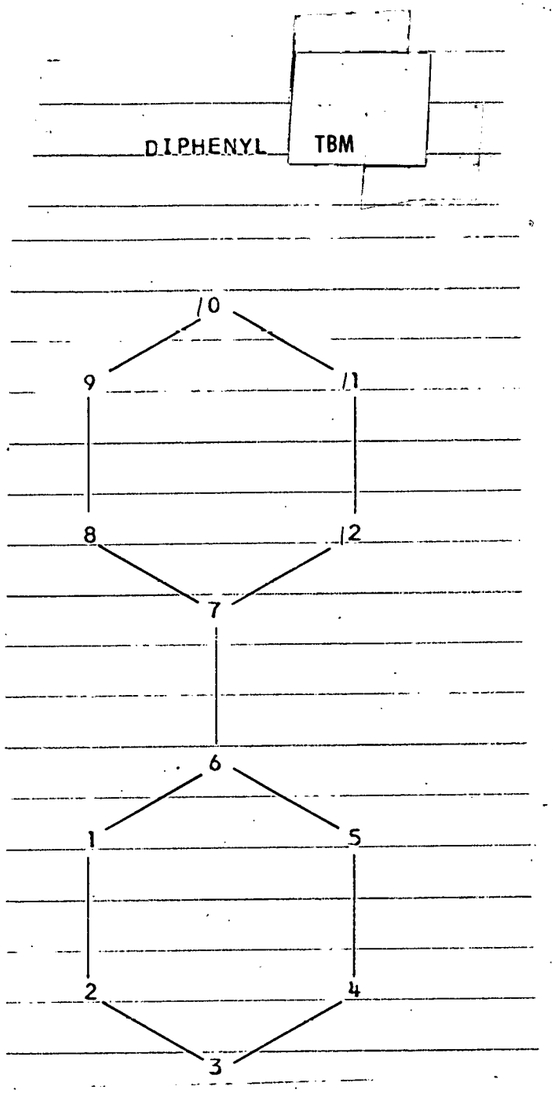
ENERGIES FOR DIPHENYL X IRX APPROXIMATION

ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	6, 7	5, 8	4, 9	2, 7	3,10
XMOMNT	0.00000	0.00000	-0.00000	0.00000	0.00000
YMOMNT	-0.89361	0.56535	-0.48062	0.06317	0.17810
JUMP E	27.4392	37.3578	39.6809	46.1010	51.4659
DIAG E	38.4162	52.1570	53.4806	60.9476	67.4906
DIAG E	38.3038	52.3198	53.6535	60.5732	67.3651
CORRSP	37.2653	48.3184	57.5607	59.9397	69.4079
CORRSP	37.1886	48.4776	57.6888	59.6330	69.2274

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION				
37.26526	0.85266	-0.00000	0.73352	//	0.9682	-0.1677	0.1152	-0.0688	0.1281
22.72202				//	0.8790	-0.2813	0.2618	-0.0044	0.2823
48.31840	1.63910	0.00000	0.89315	//	0.1995	0.7250	-0.6531	-0.0877	-0.0190
31.27999				//	0.3770	0.6698	-0.6327	0.0487	0.0813
57.56069	0.02065	0.00000	0.09184	//	0.0331	0.6604	0.7110	0.2202	0.0938
57.63086				//	0.0115	0.6854	0.7272	-0.0226	-0.0276
59.93972	0.10257	0.00000	0.20060	//	0.0254	-0.0998	-0.2338	0.8943	0.3674
50.41867				//	-0.1733	0.0101	0.0390	0.8315	0.5263
69.40793	0.00124	0.00000	0.02050	//	-0.1448	0.0109	-0.0086	-0.3734	0.9162
66.17625				//	-0.2348	0.0484	-0.0288	-0.5529	0.7975



ATOMIC COORDINATES

x	0.	0.	0.8660	1.7321	1.7321	0.8660
y	1.5000	0.5000	0.	0.5000	1.5000	2.0000

0.8660	0.	0.	0.8660	1.7321	1.7321
3.0000	3.5000	4.5000	5.0000	4.5000	3.5000

DIPHENYL TBM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SS	4 SA	5 AA	6 AS	7 SS	8 SA	9 AA	10 AS	11 SS	12 AS
1.562295	1.466736	1.325126	1.246799	1.246799	1.173885	0.826114	0.753200	0.753200	0.674872	0.533262	0.437704
0.292138	0.267962	-0.058007	0.499902	-0.006876	-0.299228	0.299228	0.015198	0.499718	-0.058007	0.267962	-0.292138
0.208580	-0.321410	0.289094	0.499902	-0.006876	0.140232	0.140232	-0.015197	-0.499718	-0.289094	-0.321410	0.208580
0.183070	0.339858	0.438829	-0.000000	0.000000	0.398009	-0.398009	-0.000000	0.000000	0.438829	0.339857	-0.183070
0.208538	0.321345	0.289035	-0.500003	0.006877	0.140203	0.140204	0.015201	0.499819	-0.289035	-0.321345	0.208538
0.292079	0.267908	-0.057996	-0.500003	0.006877	-0.299167	0.299167	-0.015200	-0.499819	-0.057995	0.267908	-0.292079
0.456987	0.185339	-0.365492	0.000000	-0.000000	-0.351038	-0.351038	-0.000000	0.000000	0.365492	-0.185339	0.456987
0.456987	-0.185339	-0.365492	-0.000000	0.000000	0.351038	-0.351038	0.000000	0.000000	-0.365492	-0.185339	-0.456987
0.292138	-0.267962	-0.058007	0.006876	0.499902	0.299228	0.299228	0.499718	-0.015198	0.058007	0.267962	0.292138
0.208580	-0.321410	0.289094	0.006876	0.499902	-0.140232	0.140232	-0.499718	0.015197	0.289094	-0.321410	-0.208580
0.183070	-0.339857	0.438829	-0.000000	-0.000000	-0.398009	-0.398009	0.000000	0.000000	-0.438829	0.339858	0.183070
0.208538	-0.321345	0.289035	-0.006877	-0.500003	-0.140203	0.140203	0.499819	-0.015201	0.289035	-0.321345	-0.208538
0.292078	-0.267908	-0.057995	-0.006877	-0.500003	0.299168	0.299167	-0.499819	0.015201	0.057995	0.267908	0.292079

DIPHENYL TBM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SS	4 SA	5 AA	6 AS	7 SS	8 SA	9 AA	10 AS	11 SS	12 AS
27.62100	24.42070	18.82927	15.19098	15.19097	11.36774	-16.15336	-25.14630	-25.14630	-36.97181	-67.16925	-98.58765
0.233726	0.221257	-0.050391	-0.316601	0.316601	-0.276178	0.329217	-0.407339	-0.407339	-0.070611	0.366947	-0.441568
0.166875	0.265390	0.251137	-0.316601	0.316601	0.129430	0.154286	0.407339	0.407339	-0.351907	-0.440139	0.315270
0.146466	0.280621	0.381212	-0.000000	-0.000000	0.367350	-0.437898	0.000000	-0.000000	0.534176	0.465400	-0.276711
0.166841	0.265336	0.251086	0.316665	-0.316666	0.129403	0.154255	-0.407421	-0.407421	-0.351836	-0.440049	0.315206
0.233678	0.221213	-0.050381	0.316666	-0.316665	-0.276122	0.329150	0.407421	0.407421	-0.070596	0.366873	-0.441478
0.365614	0.153035	-0.317504	0.000000	0.000000	-0.323997	-0.386220	0.000000	-0.000000	0.444905	-0.253803	0.690738
0.365614	-0.153035	-0.317504	-0.000000	-0.000000	0.323997	-0.386219	-0.000000	0.000000	-0.444905	-0.253803	-0.690738
0.233725	-0.221257	-0.050391	-0.316601	-0.316601	0.276178	0.329217	-0.407339	0.407339	0.070611	0.366947	0.441568
0.166875	-0.265390	0.251137	-0.316601	-0.316601	-0.129430	0.154286	0.407339	-0.407339	0.351907	-0.440139	-0.315270
0.146466	-0.280621	0.381212	0.000000	0.000000	-0.367350	-0.437898	-0.000000	0.000000	-0.534176	0.465400	0.276711
0.166841	-0.265336	0.251086	0.316665	0.316665	-0.129403	0.154255	-0.407421	0.407421	0.351836	-0.440050	-0.315206
0.233678	-0.221213	-0.050381	0.316665	0.316665	0.276123	0.329150	0.407421	-0.407421	0.070596	0.366873	0.441478

DIPHENYL — TBM TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.00000	0.67656	-0.00000	-0.32338	-0.00000	0.61882	-0.00000	-0.14526	0.00000	0.11211	0.00000	-0.14523
2	0.67656	1.00000	0.66019	-0.00000	-0.32338	-0.00000	-0.04137	-0.00000	0.00822	0.00000	0.00822	0.00000
3	-0.00000	0.66019	1.00000	0.66006	-0.00000	-0.30691	0.00000	0.11211	-0.00000	-0.09566	-0.00000	0.11208
4	-0.32338	-0.00000	0.66006	1.00000	0.67669	0.00000	-0.04136	-0.00000	0.00822	0.00000	0.00822	-0.00000
5	-0.00000	-0.32338	-0.00000	0.67669	1.00000	0.61869	-0.00000	-0.14523	-0.00000	0.11208	0.00000	-0.14521
6	0.61882	-0.00000	-0.30691	0.00000	0.61869	1.00000	0.36969	0.00000	-0.04137	-0.00000	-0.04136	0.00000
7	-0.00000	-0.04137	0.00000	-0.04136	-0.00000	0.36969	1.00000	0.61882	0.00000	-0.30691	-0.	0.61869
8	-0.14526	-0.00000	0.11211	-0.00000	-0.14523	0.00000	0.61882	1.00000	0.67656	0.00000	-0.32338	-0.00000
9	0.00000	0.00822	-0.00000	0.00822	-0.00000	-0.04137	0.00000	0.67656	1.00000	0.66019	0.00000	-0.32338
10	-0.11211	0.00000	-0.09566	0.00000	0.11208	-0.00000	-0.30691	0.00000	0.66019	1.00000	0.66006	0.00000
11	-0.00000	0.00822	-0.00000	0.00822	0.00000	-0.04136	-0.	-0.32338	0.00000	0.66006	1.00000	0.67669
12	-0.14523	0.00000	0.11208	-0.00000	-0.14521	0.00000	0.61869	-0.00000	-0.32338	0.00000	0.67669	1.00000

DIPHENYL — TBM DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.76574	0.49959	-0.04868	-0.30240	-0.03631	0.44959	-0.04378	-0.13612	0.00675	0.10878	0.00675	-0.13610
2	0.49959	0.75715	0.48440	-0.04490	-0.30240	-0.04009	-0.03481	0.00675	0.00747	-0.00368	0.00746	0.00675
3	-0.04868	0.48440	0.76094	0.48430	-0.04867	-0.28712	0.01718	0.10878	-0.00368	-0.09384	-0.00368	0.10875
4	-0.30240	-0.04490	0.48430	0.75716	0.49971	-0.04008	-0.03480	0.00675	0.00746	-0.00368	0.00746	0.00675
5	-0.03631	-0.30240	-0.04867	0.49971	0.76575	0.44950	-0.04377	-0.13610	0.00675	0.10875	0.00675	-0.13607
6	0.44959	-0.04009	-0.28712	-0.04008	0.44950	0.72575	0.21218	-0.04378	-0.03481	0.01718	-0.03480	-0.04377
7	-0.04378	-0.03481	0.01718	-0.03480	-0.04377	0.21218	0.72575	0.44959	-0.04009	-0.28712	-0.04008	0.44950
8	-0.13612	0.00675	0.10878	0.00675	-0.13610	-0.04378	0.44959	0.76574	0.49959	-0.04868	-0.30240	-0.03631
9	0.00675	0.00747	-0.00368	0.00746	0.00675	-0.03481	-0.04009	0.49959	0.75715	0.48440	-0.04490	-0.30240
10	0.10878	-0.00368	-0.09384	-0.00368	0.10875	0.01718	-0.28712	-0.04868	0.48440	0.76094	0.48430	-0.04867
11	0.00675	0.00746	-0.00368	0.00746	0.00675	-0.03480	-0.04008	-0.30240	-0.04490	0.48430	0.75716	0.49971
12	-0.13610	0.00675	0.10875	0.00675	-0.13607	-0.04377	0.44950	-0.03631	-0.30240	-0.04867	0.49971	0.76575

ENERGIES FOR DIPHENYL , TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	4, 7	6, 9	3, 8	2, 9	5,10	1, 8
XMOMNT	-0.54962	-0.55149	-0.44215	-0.06912	0.44526	0.10921
YMOMNT	-0.00000	0.00000	-0.00000	-0.00000	0.00000	-0.00000
JUMP E	31.3443	36.5140	43.9756	49.5670	52.1628	52.7673
DIAG E	42.9893	47.8417	58.4977	66.8401	66.0835	67.8895
DIAG E	42.5272	48.4221	59.0939	67.1501	65.5164	68.6560
CORRSP	36.0889	51.2934	57.1367	62.8359	67.8906	74.8962
CORRSP	36.0100	51.4810	57.6627	63.5700	67.4428	75.1991

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
36.08887	0.01041	0.08237	-0.00000	//	0.7587	0.5419	0.2853	0.0125	0.2166	-0.0480
31.56971				//	0.8336	-0.4199	-0.2193	0.0113	0.2704	0.0866
51.29339	1.31133	-0.77536	0.00000	//	-0.6119	0.7790	0.1051	-0.0081	0.0686	0.0542
36.71309				//	0.4627	0.7731	0.4082	0.0276	0.1266	-0.0700
57.13671	0.20795	-0.29255	-0.00000	//	-0.1739	-0.2525	0.8174	0.4688	0.1334	-0.0170
59.05168				//	-0.0088	-0.4101	0.6563	-0.1558	0.1216	-0.6016
62.83591	0.04300	0.12686	-0.00000	//	0.1052	0.0797	-0.2580	0.5862	-0.0956	0.7505
47.50252				//	0.0242	-0.2172	0.4741	0.7012	-0.1989	0.4430
67.89065	0.88600	0.55397	0.00000	//	-0.0928	-0.1350	-0.2107	-0.0099	0.9599	0.0849
64.59591				//	-0.3005	0.0242	0.0239	0.1640	0.9255	0.1586
74.89615	0.00048	0.01230	-0.00000	//	-0.0068	-0.1057	0.3584	-0.6605	-0.0013	0.6512
74.88171				//	-0.0129	-0.1004	0.3595	-0.6755	-0.0001	0.6358

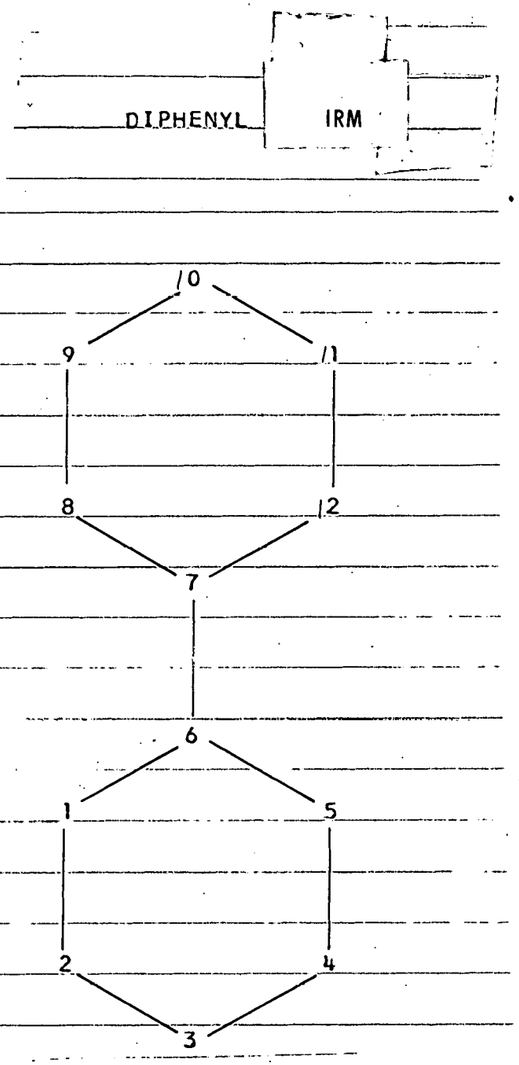
ENERGIES FOR DIPHENYL ,TBM APPROXIMATION 1.7

ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	6, 7	5, 8	4, 9	2, 7	3,10
XMOMNT	0.00000	0.00000	0.00000	0.00000	-0.00000
YMOMNT	0.88307	-0.51596	0.51596	0.06273	-0.18427
JUMP E	27.5211	40.3373	40.3373	40.5741	55.8011
DIAG E	38.3185	54.9556	53.9949	55.1455	72.0516
DIAG E	38.2611	55.1314	54.1707	54.8177	71.9050
CORRSP	37.3122	59.1707	49.9423	54.8449	73.1960
CORRSP	37.2981	59.3433	50.0997	54.5099	73.0348

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION				
37.31223	0.89680	0.00000	0.75180	//	0.9752	0.1239	-0.1097	-0.1097	-0.0979
23.23737				//	0.9069	0.2439	-0.2409	-0.0342	-0.2424
59.17073	0.00283	0.00000	-0.03355	//	-0.0103	0.7360	0.6710	0.0865	-0.0200
59.13181				//	-0.0149	0.7197	0.6931	0.0294	-0.0245
49.94233	1.37805	0.00000	0.80552	//	0.1428	-0.6338	0.7269	-0.2171	0.0490
33.00513				//	0.3413	-0.6478	0.6749	0.0733	-0.0560
54.84489	0.29942	0.00000	0.35830	//	0.1227	-0.2021	-0.0956	0.9459	-0.2007
46.26041				//	-0.0899	0.0157	-0.0706	0.9177	-0.3801
73.19596	0.02046	0.00000	-0.08108	//	0.1160	0.0178	-0.0141	0.1967	0.9733
68.48813				//	0.2295	0.0522	-0.0342	0.3878	-0.8905



ATOMIC COORDINATES

x	0.	0.	0.8660	1.7321	1.7321	0.8660
y	1.5000	0.5000	0.	0.5000	1.5000	2.0000

0.8660	0.	0.	0.8660	1.7321	1.7321
3.0000	3.5000	4.5000	5.0000	4.5000	3.5000

DIPHENYL IRM APPROXIMATION

OVERLAP EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SS	4 SA	5 AA	6 AS	7 SS	8 SA*	9 AA	10 AS	11 SS	12 AS
1.677828	1.529210	1.294085	1.204513	1.189065	1.094215	0.784531	0.741549	0.726100	0.667946	0.575187	0.515763
0.296709	-0.265001	-0.078367	0.359367	-0.347570	-0.306884	0.287235	-0.347565	0.359362	-0.040156	0.270872	-0.289892
0.221524	-0.323966	0.279708	0.347578	-0.359377	0.130990	0.147243	0.359361	-0.347560	-0.297412	-0.317897	0.198705
0.201477	-0.342147	0.430882	0.000020	-0.000020	0.404995	-0.404047	0.000010	-0.000012	0.433515	0.332405	-0.176006
0.221491	-0.323919	0.279672	-0.347629	0.359432	0.130980	0.147203	-0.359448	0.347647	-0.297334	-0.317816	0.198652
0.296663	-0.264965	-0.078334	-0.359439	0.347641	-0.306810	0.287172	0.347645	-0.359444	-0.040154	0.270802	-0.289818
0.430384	-0.180624	-0.381588	0.000002	-0.000002	-0.336681	-0.358365	-0.000004	0.000004	0.363287	-0.201829	0.471214
0.430384	0.180624	-0.381588	0.000001	0.000002	0.336681	-0.358364	-0.000005	-0.000004	-0.363288	-0.201829	-0.471214
0.296709	0.265001	-0.078367	0.359369	0.347568	0.306885	0.287235	-0.347564	-0.359364	0.040157	0.270872	0.289893
0.221524	0.323966	0.279708	0.347580	-0.359376	-0.130990	0.147243	0.359360	0.347562	0.297412	-0.317897	-0.198705
0.201477	0.342147	0.430882	0.000020	0.000020	-0.404995	-0.404046	0.000010	0.000012	-0.433515	0.332406	0.176006
0.221491	0.323919	0.279672	-0.347631	-0.359430	-0.130980	0.147203	-0.359446	-0.347649	0.297334	-0.317816	-0.198652
0.296663	0.264965	-0.078333	-0.359440	-0.347639	0.306810	0.287172	0.347643	0.359445	0.040154	0.270802	0.289818

DIPHENYL IRM APPROXIMATION

ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 SS	2 AS	3 SS	4 SA	5 AA	6 AS	7 SS	8 SA	9 AA	10 AS	11 SS	12 AS
31.00350	26.55825	17.44007	13.03011	12.20234	6.60776	-21.07722	-26.74711	-28.94897	-38.15096	-56.67973	-72.05214
0.229064	-0.214296	-0.068889	0.327441	-0.318742	-0.293375	0.324289	-0.403614	0.421730	-0.049134	0.357157	-0.403657
0.171020	-0.261979	0.245880	0.316699	-0.329570	0.125224	0.166238	0.417312	-0.407879	-0.363905	-0.419163	0.276684
0.155544	-0.276681	0.378772	0.000018	-0.000019	0.387167	-0.456170	0.000012	-0.000014	0.530437	0.438292	-0.245077
0.170995	-0.261941	0.245849	-0.316746	0.329620	0.125214	0.166193	-0.417413	0.407981	-0.363810	-0.419056	0.276611
0.229028	-0.214267	-0.068860	-0.327506	0.318807	-0.293304	0.324218	0.403707	-0.421825	-0.049132	0.357066	-0.403553
0.332263	-0.146063	-0.335439	0.000002	-0.000002	-0.321860	-0.404595	-0.000005	0.000005	0.444508	-0.266121	0.656136
0.332263	0.146064	-0.335439	0.000001	0.000002	0.321860	-0.404594	-0.000005	-0.000005	-0.444508	-0.266121	-0.656136
0.229064	0.214296	-0.068889	0.327442	0.318741	0.293375	0.324289	-0.403612	-0.421731	0.049134	0.357157	0.403657
0.171020	0.261979	0.245881	0.316700	0.329569	-0.125224	0.166238	0.417311	0.407881	0.363904	-0.419163	-0.276684
0.155544	0.276681	0.378772	0.000019	0.000019	-0.387167	-0.456169	0.000011	0.000014	-0.530437	0.438292	0.245077
0.170995	0.261941	0.245849	-0.316747	-0.329619	-0.125214	0.166193	-0.417411	-0.407983	0.363810	-0.419056	-0.276611
0.229028	0.214267	-0.068860	-0.327507	-0.318806	0.293304	0.324217	0.403705	0.421827	0.049132	0.357066	0.403553

DIPHENYL IRM AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.01706	0.67856	-0.01518	-0.32082	0.01707	0.61758	0.01283	-0.12377	-0.00369	0.11926	-0.00368	-0.15710
2	0.67856	0.99877	0.65812	-0.00122	-0.32082	0.00604	-0.05161	-0.00369	-0.00629	0.00252	0.02708	-0.00369
3	-0.01518	0.65812	1.01468	0.65798	-0.01519	-0.30452	-0.00631	0.11926	0.00252	-0.10967	0.00251	0.11924
4	-0.32082	-0.00122	0.65798	0.99878	0.67869	0.00603	-0.05160	-0.00368	0.02708	0.00251	-0.00630	-0.00368
5	0.01707	-0.32082	-0.01519	0.67869	1.01707	0.61745	0.01283	-0.15710	-0.00369	0.11924	-0.00368	-0.12370
6	0.61758	0.00604	-0.30452	0.00603	0.61745	0.95364	0.36972	0.01283	-0.05161	-0.00631	-0.05160	0.01283
7	0.01283	-0.05161	-0.00631	-0.05160	0.01283	0.36972	0.95364	0.61758	0.00604	-0.30452	0.00603	0.61745
8	-0.12377	-0.00369	0.11926	-0.00368	-0.15710	0.01283	0.61758	1.01706	0.67856	-0.01518	-0.32082	0.01707
9	-0.00369	-0.00629	0.00252	-0.02708	-0.00369	-0.05161	0.00604	0.67856	0.99877	0.65812	-0.00122	-0.32082
10	0.11926	0.00252	-0.10967	0.00251	0.11924	-0.00631	-0.30452	-0.01518	0.65812	1.01468	0.65798	-0.01519
11	0.00368	0.02708	0.00251	-0.00630	-0.00368	-0.05160	0.00603	-0.32082	-0.00122	0.65798	0.99878	0.67869
12	-0.15710	-0.00369	0.11924	-0.00368	-0.12370	0.01283	0.61745	0.01707	-0.32082	-0.01519	0.67869	1.01707

DIPHENYL IRM AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.79604	0.50077	-0.08949	-0.33430	-0.03937	0.44989	-0.05302	-0.13831	0.00297	0.12766	0.00836	-0.16076
2	0.50077	0.76587	0.48143	-0.06990	-0.33430	-0.05538	-0.04723	0.00297	-0.00585	-0.00247	0.02742	0.00836
3	-0.08949	0.48143	0.78823	0.48132	-0.08949	-0.31915	0.01765	0.12766	-0.00247	-0.11758	-0.00247	0.12763
4	-0.33430	-0.06990	0.48132	0.76590	0.50091	-0.05539	-0.04722	0.00836	0.02742	-0.00247	-0.00586	0.00297
5	-0.03937	-0.33430	-0.08949	0.50091	0.79606	0.44979	-0.05301	-0.16076	0.00836	0.12763	0.00297	-0.13824
6	0.44989	-0.05538	-0.31915	-0.05539	0.44979	0.69569	0.19598	-0.05302	-0.04723	0.01765	-0.04722	-0.05301
7	-0.05302	-0.04723	0.01765	-0.04722	-0.05301	0.19598	0.69569	0.44989	-0.05538	-0.31915	-0.05539	0.44979
8	-0.13831	0.00297	0.12766	0.00836	-0.16076	-0.05302	0.44989	0.79604	0.50077	-0.08949	-0.33430	-0.03937
9	0.00297	-0.00585	-0.00247	0.02742	0.00836	-0.04723	-0.05538	0.50077	0.76587	0.48143	-0.06990	-0.33430
10	0.12766	-0.00247	-0.11758	-0.00247	0.12763	0.01765	-0.31915	-0.08949	0.48143	0.78823	0.48132	-0.08949
11	0.00836	0.02742	-0.00247	-0.00586	0.00297	-0.04722	-0.05539	-0.33430	-0.06990	0.48132	0.76590	0.50091
12	-0.16076	0.00836	0.12763	0.00297	-0.13824	-0.05301	0.44979	-0.03937	-0.33430	-0.08949	0.50091	0.79606

ENERGIES FOR DIPHENYL , IRM APPROXIMATION 5.8

ONE ELECTRON EXCITATIONS OF SA SYMMETRY

JUMP	4, 7	6, 9	3, 8	5,10	2, 9	1, 8
XMOMNT	-0.54720	0.55115	-0.45984	-0.43612	-0.06439	0.08836
YMOMNT	-0.00000	0.00000	-0.00000	-0.00000	-0.00000	-0.00000
JUMP E	34.1073	35.5567	44.1872	50.3533	55.5072	57.7506
DIAG E	45.2918	46.8584	58.6092	64.2087	72.9416	73.9707
DIAG E	44.7835	47.4291	59.2534	63.6351	73.2692	74.6654
CORRSP	51.6911	36.9259	58.3235	66.1624	68.7401	80.0374
CORRSP	36.9021	51.7930	58.8604	65.6817	69.4030	80.3953

FINAL EXCITED STATES OF SA SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION					
51.69105	1.29646	-0.76798	-0.00000	//	0.6640	-0.7450	0.0113	-0.0126	-0.0032	0.0619
36.92313				//	0.6752	0.6295	-0.2998	0.2383	-0.0136	0.0324
36.92587	0.00006	-0.00642	-0.00000	//	0.6927	0.6109	-0.2975	0.2396	-0.0216	0.0248
32.55910				//	-0.6522	0.6330	-0.3288	-0.2475	-0.0123	0.0664
58.32353	0.29490	-0.34482	-0.00000	//	0.2459	0.2316	0.8684	-0.1925	0.3059	-0.0320
60.93150				//	0.1564	0.3230	0.5963	-0.4944	-0.2182	-0.4728
66.16242	0.76860	-0.52266	-0.00000	//	-0.1218	-0.1172	0.2346	0.9480	0.1224	0.0514
64.27887				//	-0.2911	0.1227	0.1718	0.7552	-0.3436	-0.4269
68.74009	0.09987	0.18484	-0.00000	//	-0.0636	-0.0013	-0.2036	0.0815	0.6542	0.7210
50.60278				//	-0.0972	0.2832	0.5941	0.2592	0.5985	0.3634
80.03737	0.00250	-0.02712	-0.00000	//	0.0024	0.0660	0.2463	-0.0018	-0.6804	0.6871
80.02552				//	0.0095	0.0588	0.2530	0.0047	-0.6897	0.6758

ENERGIES FOR DIPHENYL , IRM APPROXIMATION 5.8

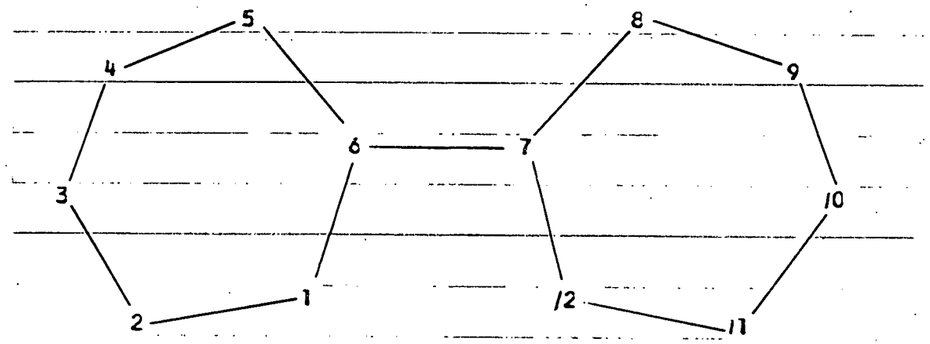
ONE ELECTRON EXCITATIONS OF AS SYMMETRY

JUMP	6, 7	5, 8	4, 9	2, 7	3,10
XMOMNT	-0.00000	-0.00000	-0.00000	0.00000	0.00000
YMOMNT	0.90819	0.56545	0.46443	-0.07393	-0.15042
JUMP E	27.6850	38.9494	41.9791	47.6355	55.5910
DIAG E	38.3309	53.5600	55.4530	61.9278	71.7053
DIAG E	38.2104	53.7297	55.6359	61.5641	71.6061
CORRSP	37.3034	50.0880	59.1014	61.3306	73.1535
CORRSP	37.2152	50.2556	59.2177	61.0374	73.0202

FINAL EXCITED STATES OF AS SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION				
37.30341	0.92225	-0.00000	0.76248	//	0.9744	-0.1571	-0.0972	0.0665	-0.1091
23.00998				//	0.9123	-0.2408	-0.2194	0.0059	-0.2482
50.08800	1.61677	-0.00000	0.87123	//	0.1796	0.7479	0.6330	0.0865	0.0154
32.96780				//	0.3249	0.6941	0.6388	-0.0498	-0.0450
59.10137	0.02204	-0.00000	-0.09365	//	-0.0388	-0.6318	0.7174	0.2759	0.0929
59.17696				//	-0.0074	-0.6767	0.7355	-0.0260	-0.0215
61.33062	0.10118	0.00000	-0.19696	//	-0.0378	0.1298	-0.2739	0.9116	0.2751
51.89572				//	0.1335	-0.0063	0.0403	0.8650	0.4819
73.15351	0.00109	0.00000	-0.01873	//	0.1237	-0.0060	-0.0122	-0.2846	0.9505
69.30413				//	0.2104	-0.0478	-0.0349	-0.4986	0.8388

FLUORENE TBX



ATOMIC COORDINATES

x	1.6487	0.6352	0.	0.3244	1.3059	1.9538
y	0.6360	0.4480	1.2070	2.1440	2.3740	1.6000

	3.0204	3.6683	4.6498	4.9742	4.3390	3.3255
	1.6000	2.3740	2.1440	1.2070	0.4480	0.6360

TBX APPROXIMATION

FLUORENE X
OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 S	9 A	10 A	11 S	12 A
1.538469	1.464446	1.320840	1.235825	1.235792	1.184180	0.815819	0.764207	0.764174	0.679159	0.535552	0.461530
0.285167	0.251671	-0.094713	-0.354421	0.346738	0.317064	-0.317064	-0.346738	0.354421	0.094713	0.251670	-0.285167
0.221391	0.314854	0.271613	-0.358741	0.364247	-0.129262	-0.129261	0.364247	-0.358741	0.271613	-0.314853	0.221391
0.212673	0.349975	0.430730	-0.012824	0.024983	-0.382061	0.382060	-0.024983	0.012824	-0.430730	0.349975	-0.212673
0.232624	0.329566	0.276256	0.348268	-0.342403	-0.149747	-0.149748	-0.342403	0.348267	0.276256	-0.329566	0.232624
0.296203	0.268309	-0.081695	0.352434	-0.359408	0.283224	-0.283224	0.359409	-0.352434	0.081695	0.268309	-0.296203
0.427301	0.185587	-0.385662	-0.005122	-0.007621	0.366267	0.366267	-0.007621	-0.005122	-0.385662	-0.185587	0.427301
0.427301	-0.185587	-0.385663	-0.005122	0.007620	-0.366267	0.366267	-0.007621	0.005122	0.385663	-0.185587	-0.427301
0.296203	-0.268309	-0.081695	0.352434	0.359408	-0.283224	-0.283224	0.359409	0.352434	-0.081695	0.268309	0.296203
0.232624	-0.329566	0.276256	0.348267	0.342404	0.149748	-0.149747	-0.342403	-0.348267	-0.276256	-0.329566	-0.232624
0.212673	-0.349975	0.430730	-0.012825	-0.024983	0.382060	0.382060	-0.024983	-0.012824	0.430730	0.349975	0.212673
0.221391	-0.314853	0.271613	-0.358741	-0.364247	0.129261	-0.129261	0.364247	0.358741	-0.271613	-0.314853	-0.221391
0.285167	-0.251670	-0.094713	-0.354421	-0.346738	-0.317064	-0.317064	-0.346738	-0.354421	-0.094713	0.251670	0.285167

TBX APPROXIMATION

FLUORENE X
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 S	9 A	10 A	11 S	12 A
26.3860	23.9091	18.3122	14.3858	14.3842	11.7253	-17.0197	-23.2606	-23.2649	-35.6139	-65.3786	-87.9555
0.229908	0.207968	-0.082411	-0.318817	0.311910	0.291365	-0.351035	-0.396639	0.405437	0.114928	0.343899	-0.419758
0.178491	0.260179	0.236334	-0.322703	0.327660	-0.118785	-0.143110	0.416668	-0.410379	0.329583	-0.430237	0.325882
0.171462	0.289202	0.374783	-0.011536	0.022474	-0.351094	0.422995	-0.028579	0.014670	-0.522660	0.478230	-0.313049
0.187547	0.272337	0.240374	0.313281	-0.308010	-0.137610	-0.165792	-0.391681	0.398398	0.335217	-0.450341	0.342416
0.238806	0.221717	-0.071084	0.317029	-0.323307	0.260269	-0.313569	0.411134	-0.403164	0.099131	0.366636	-0.436003
0.344500	0.153360	-0.335569	-0.004608	-0.006855	0.336580	0.405509	-0.008718	-0.005859	-0.467974	-0.253599	0.628976
0.344500	-0.153359	-0.335569	-0.004607	0.006855	-0.336580	0.405509	-0.008717	0.005859	0.467974	-0.253599	-0.628976
0.238806	-0.221717	-0.071084	0.317029	0.323307	-0.260268	-0.313569	0.411134	0.403164	-0.099131	0.366636	0.436003
0.187547	-0.272337	0.240373	0.313281	0.308011	0.137610	-0.165792	-0.391681	-0.398398	-0.335217	-0.450341	-0.342416
0.171462	-0.289202	0.374783	-0.011536	-0.022473	0.351094	0.422995	-0.028579	-0.014670	0.522661	0.478230	0.313049
0.178491	-0.260178	0.236334	-0.322703	-0.327660	-0.118784	-0.143110	0.416668	0.410379	-0.329583	-0.430237	-0.325882
0.229908	-0.207967	-0.082411	-0.318816	-0.311910	-0.291366	-0.351035	-0.396639	-0.405437	-0.114928	0.343899	0.419758

FLUORENE X — TBX TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.00000	0.65821	-0.00000	-0.33305	0.00000	0.64078	-0.00000	-0.13082	0.00000	0.09759	0.00000	-0.13638
2	0.65821	1.00000	0.67471	-0.00000	-0.33218	0.00000	-0.03325	-0.00000	0.00639	0.00000	0.00593	0.00000
3	-0.00000	0.67471	1.00000	0.65599	-0.00000	-0.30070	0.00000	0.09314	-0.00000	-0.07631	-0.00000	0.09759
4	-0.33305	-0.00000	0.65599	1.00000	0.67631	0.00000	-0.03570	-0.00000	0.00689	0.00000	0.00639	-0.00000
5	0.00000	-0.33218	-0.00000	0.67631	1.00000	0.62508	-0.00000	-0.12552	0.00000	0.09314	-0.00000	-0.13082
6	0.64078	0.00000	-0.30070	0.00000	0.62508	1.00000	0.32539	0.00000	-0.03570	-0.00000	-0.03325	0.00000
7	-0.00000	-0.03325	0.00000	-0.03570	-0.00000	0.32539	1.00000	0.62508	0.00000	-0.30070	0.00000	0.64078
8	-0.13082	-0.00000	0.09314	-0.00000	-0.12552	0.00000	0.62508	1.00000	0.67631	0.00000	-0.33218	-0.00000
9	0.00000	0.00639	-0.00000	0.00689	0.00000	-0.03570	-0.00000	0.67631	1.00000	0.65599	0.00000	-0.33305
10	0.09759	0.00000	-0.07631	0.00000	0.09314	-0.00000	-0.30070	0.00000	0.65599	1.00000	0.67471	0.00000
11	0.00000	0.00593	-0.00000	0.00639	0.00000	-0.03325	0.00000	-0.33218	0.00000	0.67471	1.00000	0.65821
12	-0.13638	0.00000	0.09759	-0.00000	-0.13082	0.00000	0.64078	-0.00000	-0.33305	0.00000	0.65821	1.00000

FLUORENE X — TBX DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.77345	0.49228	-0.04586	-0.31220	-0.03842	0.47230	-0.03899	-0.12283	0.00592	0.09471	0.00549	-0.12828
2	0.49228	0.76203	0.49443	-0.04907	-0.31129	-0.03731	-0.02801	0.00537	0.00582	-0.00282	0.00537	0.00549
3	-0.04586	0.49443	0.75481	0.47757	-0.04775	-0.28124	0.01466	0.09034	-0.00304	-0.07483	-0.00282	0.09471
4	-0.31220	-0.04907	0.47757	0.75815	0.50234	-0.03987	-0.03011	0.00574	0.00625	-0.00304	0.00582	0.00592
5	-0.03842	-0.31129	-0.04775	0.50234	0.76803	0.45696	-0.03832	-0.11767	0.00574	0.09034	0.00537	-0.12283
6	0.47230	-0.03731	-0.28124	-0.03987	0.45696	0.73632	0.18891	-0.03832	-0.03011	0.01466	-0.02801	-0.03899
7	-0.03899	-0.02801	0.01466	-0.03011	-0.03832	0.18891	0.73632	0.45696	-0.03987	-0.28124	-0.03731	0.47230
8	-0.12283	0.00537	0.09034	0.00574	-0.11767	-0.03832	0.45696	0.76803	0.50234	-0.04775	-0.31129	-0.03842
9	0.00592	0.00582	-0.00304	0.00625	0.00574	-0.03011	-0.03987	0.50234	0.75815	0.47757	-0.04907	-0.31220
10	0.09471	-0.00282	-0.07483	-0.00304	0.09034	0.01466	-0.28124	-0.04775	0.47757	0.75481	0.49443	-0.04586
11	0.00549	0.00537	-0.00282	0.00582	0.00537	-0.02801	-0.03731	-0.31129	-0.04907	0.49443	0.76203	0.49228
12	-0.12828	0.00549	0.09471	0.00592	-0.12283	-0.03899	0.47230	-0.03842	-0.31220	-0.04586	0.49228	0.77345

ENERGIES FOR FLUORENE X TBX APPROXIMATION

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	4, 7	6, 9	3, 7	4, 8	5, 9	4, 9	3, 8	3, 9	1, 7	2, 9	6,10	1, 8	1, 9	5,10	4,10
XMOMNT	-0.00000	-0.00000	0.00000	0.00000	-0.00000	-0.51088	0.00000	-0.10021	0.00000	0.00000	-0.00000	-0.00000	0.01025	-0.00000	-0.10093
YMOMNT	-0.54239	-0.54369	-0.11892	0.13400	0.13400	0.00000	-0.44741	-0.00000	0.00906	0.06661	-0.12004	0.09254	-0.00000	-0.45063	0.00000
JUMP E	31.4055	34.9902	35.3319	37.6464	37.6490	37.6807	41.5728	41.5770	43.4057	47.1740	47.3393	49.6466	49.6508	49.9981	49.9997
DIAG E	43.3660	46.7646	49.3651	53.4904	53.4976	51.4529	55.8030	54.4972	56.7449	64.4141	60.5806	65.1833	64.2766	63.5594	62.4369
DIAG E	42.8982	47.2106	49.0033	53.6008	53.5624	51.3351	56.0194	54.8854	56.6639	64.4407	60.8641	65.6805	64.3457	63.4617	62.3567
CORRSP	35.4965	50.8321	45.4629	56.2224	52.4720	51.1500	54.6310	52.7572	57.7025	59.8495	61.9771	72.5562	65.7503	65.5665	66.0061
CORRSP	35.3923	50.8398	45.4161	56.1139	52.5678	51.3051	55.0437	53.1378	57.3695	60.3992	62.2117	72.5165	65.8011	65.5349	63.0788

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
35.49651	0.00228	-0.00000	-0.03887	//	0.7189	-0.5686	0.0023	-0.0001	-0.0007	0.0000	-0.3199	-0.0000	-0.0144	0.0206
					-0.0008	0.0401	0.0000	0.2350	-0.0000					
30.83397				//	0.7436	0.5167	0.0042	-0.0545	-0.0606	-0.0000	0.2976	0.0000	-0.0199	0.0069
					-0.0005	-0.0953	-0.0000	0.2746	-0.0000					
50.83214	1.23293	-0.00000	-0.75523	//	0.6401	0.7547	0.0699	-0.0223	-0.0102	0.0000	0.0574	0.0000	-0.0243	0.0059
					-0.0145	0.0779	-0.0000	-0.0700	-0.0000					
35.64194				//	-0.5751	0.6874	0.0386	-0.0035	-0.0048	-0.0000	0.3976	0.0000	0.0044	-0.0434
					0.0223	-0.0404	-0.0000	-0.1820	0.0000					
45.46294	0.00393	0.00000	0.04508	//	-0.0240	-0.0314	0.7343	0.4500	0.4409	0.0000	0.0009	-0.0000	-0.1768	-0.0058
					0.1752	-0.0068	0.0000	-0.0155	-0.0000					
33.83536				//	-0.0012	-0.0447	0.7839	-0.2688	-0.2732	0.0000	-0.0350	0.0000	-0.1962	0.0132
					0.4432	-0.0040	-0.0000	-0.0156	-0.0000					
56.22244	0.05276	0.00000	0.14855	//	-0.0772	0.1119	-0.0819	0.6255	-0.5885	-0.0000	-0.3473	0.0000	-0.2374	0.2254
					-0.0056	-0.0963	-0.0000	0.0159	-0.0000					
28.21901				//	0.0629	0.0373	0.3049	0.6504	0.6463	0.0000	0.0043	-0.0000	-0.1610	0.0049
					0.1865	-0.0104	0.0000	0.0067	-0.0000					
52.47202	0.05257	-0.00000	0.15349	//	0.0118	0.0900	-0.5576	0.4323	0.5168	0.0000	-0.1266	-0.0000	0.3420	0.0769
					0.2949	0.0003	0.0000	0.0315	0.0000					
55.56396				//	-0.0086	0.2896	-0.0127	-0.5318	0.5159	-0.0000	0.4339	-0.0000	-0.0986	-0.0625
					-0.0222	0.3958	0.0000	0.0889	0.0000					
54.63101	0.14395	-0.00000	-0.20892	//	0.2046	-0.2128	-0.1488	0.3870	-0.1966	-0.0000	0.7165	-0.0000	-0.0479	-0.4105
					0.0364	-0.0194	0.0000	-0.1278	0.0000					
56.69457				//	-0.0075	-0.3031	0.2246	-0.4147	0.4371	0.0000	0.4713	-0.0000	0.0589	0.1053
					-0.3542	-0.3623	-0.0000	-0.0343	-0.0000					
57.70246	0.02788	0.00000	-0.10660	//	0.0045	-0.0016	0.3405	0.0705	-0.3233	-0.0000	0.0095	0.0000	0.8736	0.0098
					0.0908	-0.0243	-0.0000	0.0484	-0.0000					
50.88394				//	0.0125	0.0196	0.1034	-0.0166	0.1144	0.0000	-0.0246	0.0000	0.9398	-0.0083
					0.2961	-0.0280	0.0000	0.0547	-0.0000					

ENERGIES FOR FLUORENE X TBXAPPROXIMATION

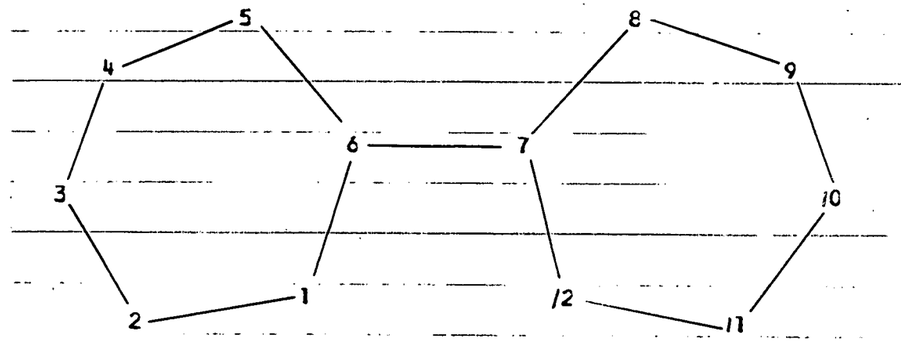
ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	6, 7	5, 7	6, 8	5, 8	4, 9	2, 7	3, 9	2, 8	1, 9	4, 10	3, 10
XMOMNT	0.79580	-0.15123	-0.15159	-0.50289	-0.51085	-0.06267	-0.10021	0.02827	0.01025	-0.10093	0.20238
YMOMNT	-0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
JUMP E	28.7450	31.4039	34.9859	37.6448	37.6507	40.9288	41.5770	47.1697	49.6508	49.9997	53.9261
DIAG E	39.3050	41.8600	45.2420	52.1919	51.2529	56.0160	54.6972	64.8189	64.2766	62.4369	69.7363
DIAG E	39.2009	41.3748	45.7161	52.2849	51.3351	55.4926	54.8854	64.8737	64.7457	62.3567	69.7620
CORRSP	38.1717	36.0684	46.5510	56.3864	47.5348	55.3870	54.7284	72.5496	59.0715	64.3534	71.0312
CORRSP	38.1617	35.8644	46.7400	56.3269	47.6261	54.7268	55.3004	72.5383	59.5042	64.2732	70.9657

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
38.17170	0.61531	0.61568	-0.00000	//	0.9622	0.0156	0.0886	0.1541	0.1347	0.1085	0.0341	0.0029	-0.0025	-0.0085
					0.1054									
23.99249				//	0.8082	0.0242	0.0191	0.3763	0.3761	0.0484	0.0035	0.0098	-0.0087	0.0041
					0.2455									
36.06842	0.00028	0.01344	-0.00000	//	0.0482	0.7330	-0.5329	0.0097	-0.0004	0.0106	-0.3314	0.0438	0.0542	0.2480
					0.0026									
30.81598				//	0.1764	0.6725	0.4985	-0.2334	-0.2373	0.0028	0.2897	0.0207	-0.0792	0.2570
					0.0231									
46.55103	0.16010	-0.28438	0.00000	//	-0.0821	0.6236	0.7396	0.0121	-0.0490	0.0492	0.2023	0.0845	-0.0482	0.0256
					-0.0371									
36.19420				//	-0.0001	-0.5932	0.6566	-0.0028	0.0070	-0.0016	0.4151	-0.0686	-0.0473	-0.1942
					-0.0001									
56.38644	0.00633	0.05137	-0.00000	//	0.0188	0.0412	-0.0813	0.6190	-0.6153	-0.3825	0.1954	-0.1440	0.1060	-0.0467
					0.1046									
56.65281				//	-0.0207	0.0284	-0.3099	0.5324	-0.5101	-0.0121	0.4734	0.0859	-0.3419	-0.0955
					0.0367									
47.53484	1.43474	-0.84248	0.00000	//	-0.1938	0.0186	0.0042	0.6360	0.7329	-0.1354	0.0275	-0.0143	-0.0105	0.0151
					0.0284									
31.08989				//	-0.4888	0.2766	0.2029	0.5334	0.5627	0.0539	0.1112	-0.0006	-0.0296	0.0986
					-0.1283									
55.38696	0.16014	-0.26075	-0.00000	//	-0.1022	-0.0120	-0.1101	0.3461	-0.1611	0.8735	0.1223	-0.0611	0.0119	-0.0587
					-0.2150									
47.21260				//	0.1029	-0.0108	-0.0073	0.0063	-0.0762	0.9034	-0.0166	-0.0217	0.0293	-0.0370
					-0.4054									
54.72837	0.00009	-0.00608	-0.00000	//	0.0169	0.1890	-0.3155	-0.2445	0.1686	-0.0445	0.7912	-0.3654	-0.0818	-0.0883
					0.0158									
55.44373				//	0.0094	-0.0006	-0.3404	-0.4795	0.4646	0.0551	0.4748	0.0814	-0.4493	-0.0304
					-0.0170									
72.54964	0.00000	0.00013	-0.00000	//	0.0098	-0.0176	-0.1110	-0.0274	0.0369	-0.0233	0.3266	0.6903	0.6276	-0.0077
					-0.0867									
45.60429				//	-0.0127	-0.0054	0.2355	0.0128	-0.0199	0.0169	-0.4110	0.6947	-0.5063	-0.1889
					-0.0053									
59.07154	0.00084	-0.01832	-0.00000	//	-0.0059	0.0304	0.1492	-0.0852	0.0860	0.0357	-0.1906	-0.5841	0.7592	-0.0836
					-0.0094									
72.53159				//	0.0043	-0.0131	-0.1047	-0.0289	0.0369	-0.0071	0.3345	0.6934	0.6271	0.0050
					-0.0259									

FLUORENE IRX



ATOMIC COORDINATES

x	1.6487	0.6352	0.	0.3244	1.3059	1.9538
y	0.6360	0.4480	1.2070	2.1440	2.3740	1.6000

3.0204	3.6683	4.6498	4.9742	4.3390	3.3255
1.6000	2.3740	2.1440	1.2070	0.4480	0.6360

FLUORENE X — IRX APPROXIMATION
OVERLAP EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 S	9 A	10 A	11 S	12 A
1.652652	1.524205	1.290052	1.199407	1.179789	1.100915	0.779576	0.755684	0.733520	0.672506	0.578982	0.532704
0.307665	0.237583	-0.139058	0.350406	0.286479	-0.363807	0.344885	0.296065	-0.375102	-0.071520	-0.237952	-0.288637
0.232558	0.314562	0.249513	0.357639	0.392608	0.044654	0.079702	-0.394801	0.341504	-0.283598	0.305834	0.218776
0.219815	0.350709	0.425318	0.035231	0.092606	0.377471	-0.373688	0.083075	0.010614	0.424252	-0.350714	-0.214104
0.232819	0.335731	0.290569	-0.326600	-0.310909	0.207731	0.194539	0.323602	-0.349714	-0.270915	0.334864	0.227536
0.284476	0.273727	-0.064284	-0.373918	-0.392662	-0.237033	0.234470	-0.378862	0.346775	-0.087086	-0.276792	-0.294732
0.409645	0.184301	-0.385937	-0.039825	-0.066063	-0.351894	-0.377144	0.036376	0.002492	0.391776	0.195182	0.429354
0.409645	-0.184301	-0.385937	-0.039825	0.066063	0.351894	-0.377144	0.036376	-0.002492	-0.391776	0.195182	-0.429354
0.284476	-0.273727	-0.064284	-0.373918	0.392663	0.237032	0.234470	-0.378861	-0.346777	0.087087	-0.276792	0.294733
0.232819	-0.335731	0.290569	-0.326600	0.310909	-0.207731	0.194539	0.323600	0.349716	0.270915	-0.334864	-0.227536
0.219815	-0.350709	0.425318	0.035231	-0.092606	-0.377472	-0.373688	0.083075	-0.010614	-0.424252	0.350714	0.214104
0.232558	-0.314562	0.249513	0.357639	-0.392608	-0.044654	0.079702	-0.394800	-0.341505	0.283598	0.305834	-0.218776
0.307664	-0.237583	-0.139058	0.350406	-0.286480	0.363807	0.344885	0.296063	0.375103	0.071520	-0.237952	0.288638

FLUORENE X — IRX APPROXIMATION
ZEROTH HAMILTONIAN EIGNVALUES AND EIGNVECTORS

1 S	2 A	3 S	4 S	5 A	6 A	7 S	8 S	9 A	10 A	11 S	12 A
29.7715	25.9274	16.9500	12.5336	11.4884	6.9104	-21.3158	-24.3732	-27.3875	-36.7120	-54.8196	-66.1314
0.239324	0.192439	-0.122431	0.319955	0.263749	-0.346732	0.390612	0.340578	-0.437969	-0.087212	-0.312721	-0.395467
0.180901	0.254791	0.219680	0.326559	0.361457	0.042558	0.090269	-0.454159	0.398739	-0.345824	0.401933	0.299748
0.170988	0.284070	0.374464	0.032169	0.085258	0.359755	-0.423233	0.095565	0.012393	0.517339	-0.460915	-0.293347
0.181104	0.271938	0.255827	-0.298218	-0.286240	0.197981	0.220332	0.372255	-0.408326	-0.330358	0.440084	0.311751
0.221286	0.221716	-0.056598	-0.341424	-0.361507	-0.225908	0.265557	-0.435824	0.404895	-0.106195	-0.363765	-0.403818
0.318653	0.149281	-0.339792	-0.036364	-0.060821	-0.335378	-0.427148	0.041845	0.002910	0.477738	0.256512	0.588265
0.318652	-0.149282	-0.339792	-0.036364	0.060821	0.335378	-0.427148	0.041845	-0.002910	-0.477738	0.256511	-0.588265
0.221286	-0.221716	-0.056598	-0.341423	0.361507	0.225908	0.265557	-0.435823	-0.404896	0.106195	-0.363764	0.403818
0.181104	-0.271938	0.255827	-0.298217	0.286241	-0.197981	0.220332	0.372254	0.408328	0.330358	0.440084	-0.311751
0.170988	-0.284070	0.374464	0.032169	-0.085258	-0.359755	-0.423233	0.095565	-0.012393	-0.517339	-0.460915	0.293347
0.180901	-0.254791	0.219680	0.326559	-0.361457	-0.042558	0.090269	-0.454158	-0.398741	0.345824	0.401932	-0.299748
0.239324	-0.192439	-0.122431	0.319955	-0.263749	0.346732	0.390612	0.340576	0.437970	0.087213	-0.312721	0.395467

FLUORENE X | IRX AUGMENTED TOPOLOGICAL BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.01530	0.66627	-0.01329	-0.33620	0.00843	0.63726	0.02573	-0.14668	0.00332	0.09661	-0.01758	-0.06818
2	0.66627	0.99866	0.66675	0.00532	-0.32451	0.00210	-0.06319	-0.00993	0.03404	0.01262	-0.02168	-0.01758
3	-0.01329	0.66675	1.00903	0.66124	-0.01564	-0.29963	-0.00238	0.10371	-0.00822	-0.08720	0.01262	0.09661
4	-0.33620	0.00532	0.66124	0.99567	0.66883	0.01111	-0.02615	0.00986	-0.01446	-0.00822	0.03404	0.00332
5	0.00843	-0.32451	-0.01564	0.66883	1.02034	0.63207	-0.00713	-0.12084	0.00986	0.10371	-0.00993	-0.14668
6	0.63726	0.00210	-0.29963	0.01111	0.63207	0.96101	0.31237	-0.00713	-0.02615	-0.00238	-0.06319	0.02573
7	0.02573	-0.06319	-0.00238	-0.02615	-0.00713	0.31237	0.96101	0.63207	0.01111	-0.29963	0.00210	0.63726
8	-0.14668	-0.00993	0.10371	0.00986	-0.12084	-0.00713	0.63207	1.02034	0.66883	-0.01564	-0.32451	0.00843
9	0.00332	0.03404	-0.00822	-0.01446	0.00986	-0.02615	0.01111	0.66883	0.99567	0.66124	0.00532	-0.33620
10	0.09661	0.01262	-0.08720	-0.00822	0.10371	-0.00238	-0.29963	-0.01564	0.66124	1.00903	0.66675	-0.01329
11	-0.01758	-0.02168	0.01262	0.03404	-0.00993	-0.06319	0.00210	-0.32451	0.00532	0.66675	0.99866	0.66627
12	-0.06818	-0.01758	0.09661	0.00332	-0.14668	0.02573	0.63726	0.00843	-0.33620	-0.01329	0.66627	1.01530

FLUORENE X | IRX AUGMENTED DENSITY BOND ORDERS

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.80291	0.50098	-0.08444	-0.35041	-0.04741	0.47040	-0.04549	-0.15000	0.01683	0.10591	-0.01745	-0.10437
2	0.50098	0.77001	0.48441	-0.06835	-0.33538	-0.05420	-0.06131	-0.00021	0.03465	0.01039	-0.01951	-0.01745
3	-0.08444	0.48441	0.77577	0.48248	-0.08690	-0.31471	0.01902	0.10954	-0.01380	-0.09379	0.01039	0.10591
4	-0.35041	-0.06835	0.48248	0.76452	0.49292	-0.05354	-0.01996	0.01674	-0.01580	-0.01380	0.03465	0.01683
5	-0.04741	-0.33538	-0.08690	0.49292	0.79924	0.46602	-0.05738	-0.12428	0.01674	0.10954	-0.00021	-0.15000
6	0.47040	-0.05420	-0.31471	-0.05354	0.46602	0.71357	0.15972	-0.05738	-0.01996	0.01902	-0.06131	-0.04549
7	-0.04549	-0.06131	0.01902	-0.01996	-0.05738	0.15972	0.71357	0.46602	-0.05354	-0.31471	-0.05420	0.47040
8	-0.15000	-0.00021	0.10954	0.01674	-0.12428	-0.05738	0.46602	0.79924	0.49292	-0.08690	-0.33538	-0.04741
9	0.01683	0.03465	-0.01380	-0.01580	0.01674	-0.01996	-0.05354	0.49292	0.76452	0.48248	-0.06835	-0.35041
10	0.10591	0.01039	-0.09379	-0.01380	0.10954	0.01902	-0.31471	-0.08690	0.48248	0.77577	0.48441	-0.08443
11	-0.01745	-0.01951	0.01039	0.03465	-0.00021	-0.06131	-0.05420	-0.33538	-0.06835	0.48441	0.77001	0.50098
12	-0.10437	-0.01745	0.10591	0.01683	-0.15000	-0.04549	0.47040	-0.04741	-0.35041	-0.08443	0.50098	0.80291

ENERGIES FOR -FLUORENE X IRX APPROXIMATION

ONE ELECTRON EXCITATIONS OF S SYMMETRY

JUMP	4, 7	6, 9	4, 8	3, 7	5, 9	4, 9	3, 8	6,10	3, 9	5,10	4,10	1, 7	2, 9	3,10	1, 8
XMOMNT	-0.00000	-0.00000	0.00000	0.00000	0.00000	-0.43424	-0.00000	0.00000	0.07042	0.00000	-0.10387	0.00000	-0.00000	-1.17236	0.00000
YMOMNT	-0.50466	-0.51817	0.23340	0.21643	-0.20052	0.00000	0.43362	-0.18151	0.00000	0.42602	0.00000	-0.03234	-0.06343	0.00000	-0.06821
JUMP E	33.8494	34.2979	36.9068	38.2658	38.8760	39.9211	41.3232	43.6224	44.3375	48.2004	49.2456	51.0874	53.3150	53.6820	54.1447
DIAG E	45.4862	46.2043	52.5046	52.1200	54.3337	53.8948	55.5768	56.4776	57.4877	61.4693	61.5017	64.9608	70.7734	69.2589	70.2008
DIAG E	44.8581	46.6726	52.7756	51.6384	54.2028	53.2053	55.9945	56.8520	57.6348	61.2445	61.4083	64.7069	70.7146	69.8121	70.8461
CORRSP	51.3881	36.1752	55.0921	46.5131	53.7595	53.2568	56.7915	58.6779	56.0165	63.5206	62.9767	65.2139	77.3908	69.2841	65.5846
CORRSP	51.3239	36.0826	56.9425	46.5071	53.6412	53.2257	55.4249	58.8850	56.1431	63.2947	62.9414	64.8712	66.1350	69.3402	77.3978

FINAL EXCITED STATES OF S SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
51.38806	0.97906	-0.00000	-0.66934	//	0.6408	0.7423	-0.0760	0.1209	0.0358	0.0000	0.0769	0.0541	-0.0000	0.0137
					-0.0000	-0.0463	-0.0303	0.0000	-0.0681					
36.25578				//	0.6969	-0.5424	-0.0755	-0.1125	-0.0597	-0.0000	0.3157	0.1716	0.0000	-0.2584
					-0.0000	0.0344	-0.0257	-0.0000	-0.0195					
36.17519	0.00079	-0.00000	-0.02266	//	-0.6587	0.6110	0.0462	-0.0260	0.0888	-0.0000	-0.3327	-0.0710	-0.0000	0.2550
					-0.0000	-0.0092	0.0246	0.0000	0.0262					
31.50829				//	0.5357	0.6119	-0.2703	-0.0365	0.2344	-0.0000	-0.3715	0.0001	-0.0000	-0.2586
					0.0000	0.0044	-0.0137	0.0000	0.0647					
55.09208	0.10032	-0.00000	-0.20694	//	0.3116	-0.1757	0.5006	0.1271	0.3618	0.0000	-0.6317	-0.0679	0.0000	0.1540
					0.0000	-0.0005	0.2121	-0.0000	0.0444					
28.30438				//	0.1896	0.2877	0.6442	-0.2566	-0.5925	0.0000	-0.0714	0.1768	-0.0000	0.0106
					-0.0000	0.1104	-0.0010	-0.0000	0.0269					
46.51310	0.00205	0.00000	-0.03221	//	-0.0499	-0.1038	-0.5952	0.5480	0.4771	-0.0000	-0.0664	-0.3050	-0.0000	-0.0561
					0.0000	-0.0628	-0.0059	0.0000	0.0036					
34.64070				//	0.2065	-0.0449	0.2089	0.7260	-0.2246	0.0000	-0.0558	-0.5482	0.0000	-0.1227
					-0.0000	-0.1235	-0.0114	-0.0000	0.0117					
53.75947	0.25651	0.00000	-0.33497	//	0.1547	0.0003	-0.3160	-0.7689	0.2368	-0.0000	-0.1159	-0.4310	-0.0000	0.0248
					-0.0000	0.1462	0.0817	0.0000	-0.0331					
55.96579				//	0.1283	-0.1161	0.6244	0.1393	0.6858	0.0000	-0.1247	0.1741	0.0000	0.1510
					0.0000	0.0356	-0.0498	-0.0000	0.1345					
56.79149	0.15911	-0.00000	0.25668	//	-0.1204	0.0823	-0.4802	-0.0250	0.5863	0.0000	0.5664	-0.1918	-0.0000	-0.0951
					0.0000	0.0786	-0.1755	-0.0000	-0.0143					
48.63689				//	0.0698	0.3156	-0.0662	0.0779	0.0262	-0.0000	0.5715	-0.0347	0.0000	0.2194
					0.0000	0.0697	-0.5939	-0.0000	0.3884					
58.67788	0.25674	0.00000	-0.32076	//	-0.0413	-0.0324	-0.2208	-0.2248	0.4813	0.0000	-0.0339	0.8136	-0.0000	0.0001
					0.0000	-0.0451	0.0313	0.0000	-0.0172					
54.17340				//	-0.0547	0.1341	-0.0735	0.4952	-0.1177	-0.0000	0.0904	0.7326	0.0000	-0.0506
					-0.0000	-0.3956	0.0556	0.0000	-0.0861					

ENERGIES FOR FLUORENE X IRX APPROXIMATION

ONE ELECTRON EXCITATIONS OF A SYMMETRY

JUMP	6, 7	6, 8	5, 7	5, 8	4, 9	3, 9	2, 7	4,10	2, 8	3,10	1, 9
XMOMNT	0.72445	-0.40643	0.35050	0.49186	-0.43424	0.07042	0.06515	-0.10387	-0.03715	-0.17236	0.00627
YMOMNT	-0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000	0.00000	-0.00000
JUMP E	28.2262	31.2836	32.8043	35.8616	39.9211	44.3375	47.2432	49.2456	50.3006	53.6620	57.1591
DIAG E	38.0012	41.4531	42.6877	50.3815	53.2948	57.4877	62.0926	61.5017	68.0106	69.2589	72.6037
DIAG E	37.8410	42.1921	41.9282	50.5212	53.2953	57.6348	61.4053	61.4083	68.2224	69.3121	72.9784
CORRSP	36.9270	35.1810	45.1565	47.4935	56.3885	57.2603	61.0489	63.4875	64.8826	71.1056	77.8420
CORRSP	36.8349	45.1995	35.1267	47.6117	56.4174	57.3998	60.5510	63.4703	65.2005	71.0482	77.8787

FINAL EXCITED STATES OF A SYMMETRY

ENERGY	F	XMOMNT	YMOMNT	//	STATE COMPOSITION									
36.92699	0.44415	0.53183	-0.00000	//	0.9662	0.1129	-0.0339	-0.1650	0.0910	-0.0241	-0.0782	0.0071	-0.0124	-0.1008
					-0.0025									
23.31260				//	0.8414	0.0601	-0.0140	-0.3500	0.3175	-0.0609	-0.0319	-0.0004	-0.0092	-0.2443
					0.0212									
35.18098	0.00859	-0.07579	0.00000	//	-0.0534	0.6895	0.6153	0.0240	-0.0390	-0.2882	0.0004	-0.2354	0.0307	0.0263
					0.0310									
30.16987				//	-0.0924	0.7540	-0.5074	0.0218	0.1079	-0.3220	-0.0176	0.1911	0.0067	0.0928
					0.0649									
45.15649	0.60810	0.56274	-0.00000	//	0.0851	-0.6569	0.7276	-0.0898	0.0003	0.0479	0.0201	-0.1066	0.0777	-0.0612
					-0.0048									
35.41673				//	-0.0190	0.5078	0.7784	0.0017	-0.0545	-0.2188	0.0045	-0.2894	0.0309	-0.0031
					0.0190									
47.49350	1.30009	0.80232	-0.00000	//	0.1916	-0.0547	0.0318	0.7794	-0.5864	0.0272	-0.0782	0.0218	-0.0195	0.0178
					-0.0022									
30.80337				//	0.4564	0.0358	-0.0429	0.6708	-0.5591	-0.0902	0.0326	0.0963	-0.0028	-0.0859
					0.0046									
56.38850	0.00051	0.01463	0.00000	//	0.0380	-0.0587	0.0111	0.5879	0.7687	-0.1736	0.1442	-0.0003	0.0644	-0.0523
					0.0243									
56.17006				//	-0.0100	-0.0804	0.1050	0.6358	0.7441	-0.0180	-0.0322	0.0173	-0.0850	0.0184
					0.1232									
57.26028	0.00001	-0.00165	0.00000	//	-0.0096	0.2328	0.2352	0.0898	0.1709	0.8310	-0.0450	0.2134	-0.3376	-0.0100
					-0.0285									
59.07951				//	0.0490	0.3144	0.1291	0.0643	0.0762	0.6770	0.0572	0.3644	0.2323	0.0189
					-0.4727									
61.04891	0.07828	0.17365	-0.00000	//	0.0383	0.0527	0.0041	-0.0313	-0.1590	0.0144	0.9068	0.1087	-0.0518	-0.3589
					-0.0601									
52.09157				//	-0.1344	0.0616	-0.0287	0.0026	0.0211	0.0460	0.8044	-0.0009	-0.2201	-0.5255
					0.0562									
63.48751	0.02090	-0.08798	-0.00000	//	-0.0221	0.0077	0.1754	-0.0414	-0.0185	-0.3239	-0.0954	0.8920	-0.1302	0.0143
					0.1993									
61.86644				//	-0.0437	-0.0801	0.3182	-0.1263	-0.0506	-0.1512	-0.0677	0.8303	-0.2694	0.0069
					0.2870									
64.88256	0.01801	-0.08080	0.00000	//	0.0067	0.1068	0.0525	0.0062	0.0028	0.1567	-0.0105	0.2818	0.7259	0.0747
					-0.5909									
48.88662				//	-0.0450	-0.2209	0.0627	0.0061	0.0895	-0.5316	0.2069	0.2183	0.6517	-0.0568
					-0.3691									