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Tables of Einstein Functions

Vibrational Contributions to
The Thermodynamic Functions



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Tables of Einstein Functions

Vibrational Contributions to the Thermodynamic Functions

Joseph Hilsenrath and Guy G. Ziegler



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Foreword

This Monograph is one in a series of publications presenting definitive thermodynamic data of interest in pure and applied science and in technology. The tables of Einstein functions should be useful in estimating the thermodynamic properties of polyatomic gases at high and low temperature, as well as the heat conductivity and electrical conductivity of solids.

A. V. ASTIN, *Director*.

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Tables of Einstein Functions

Vibrational Contributions to the Thermodynamic Functions

Joseph Hilsenrath and Guy G. Ziegler

Tables are presented for the contribution of a harmonic oscillator to the free energy function, enthalpy function, entropy, and heat capacity of gases. Dimensionless values of the Planck-Einstein functions are given as a function of $x=hc\nu/kT$ for $x=0.0010(.0001)$ 0.1500(.001) 4.000(.01) 10.00 (.2) 16.0. A second table which gives the contributions in cal/mole °K directly as a function of frequency ν , and temperature T , was computed using the values 1.43880 for the second radiation constant hc/k , and 1.98717 for the universal gas constant R . The arguments for the latter table are spaced at 10 wave number intervals from 100 cm^{-1} to 4000 cm^{-1} .

1. Introduction

Since the publication in 1940 [1]¹ of a short table of harmonic oscillator contributions obtained by interpolation from unpublished calculations of H. L. Johnston, the interest and need for such tables has increased steadily. In 1942 the tables were modified as a result of changes in the physical constants, and published as an appendix to a treatise on physical chemistry [2]. In the same year independent calculations were published by Sherman and Ewell [3].

The advent of punched-card computing equipment stimulated the computation in 1948 of more extensive tables by Krieger [4] and by Johnston, Savedoff, and Belzer [5]. These tables incorporated the then most recent physical constants. The Krieger tables were issued as a Rand report. The extensive tables of Johnston et al.—perhaps the most convenient tabulation for thermodynamic calculations—were published as an ONR

report and have long since been out of print. Other works on this subject include shorter but useful tables by Miller, West, and Bernstein [6], Torkington [7], and Overton and Hancock [8].

The recent acceptance by physicists and chemists of new values for the fundamental constants and the continued demand for expanded and convenient tables prompted the recomputation and preparation of this volume. The authors have tried to incorporate in this work a number of the more desirable features of the above-cited works, particularly with respect to their use in calculations involving: Thermodynamic properties of gases; specific heats, electrical and thermal conductivity of solids; and molecular structure and spectroscopy of diatomic and polyatomic molecules. It is the hope of the authors that the formal character of this publication will insure a more adequate notice and dissemination than was accorded the earlier works, thereby reducing the probability of still further duplication of effort.

¹ Figures in brackets indicate the literature references on p. vii.

2. Harmonic Oscillator Contributions to the Thermodynamic Properties

The application of statistical mechanical methods to the computation of thermodynamic properties of gases from the energy states of atoms or molecules requires, in part, the evaluation of the vibrational and electronic contributions to the partition function. These can be written in terms of sums of exponential functions with suitable weighting factors, provided the partition function is assumed separable. In computing the vibrational contributions to the thermodynamic properties, it is usually the practice to assume a rigid-rotator-harmonic oscillator as a first approximation and then to add corrections for anharmonicities, centrifugal stretching, etc., when suitable experimental data are available. The harmonic oscillator contributions can be written in terms of exponentials of the variable

$x=hc\nu/kT$ as follows:

$$\begin{aligned}-(F^\circ - E_0^\circ)/RT &= -\ln(1 - e^{-x}) \\(H^\circ - E_0^\circ)/RT &= xe^{-x}(1 - e^{-x})^{-1} \\S^\circ/R &= xe^{-x}(1 - e^{-x})^{-1} - \ln(1 - e^{-x}) \\C_p^\circ/R &= x^2e^{-x}(1 - e^{-x})^{-2}\end{aligned}$$

where: ν is the oscillator or vibrational frequency in wave numbers, T is the absolute temperature in °K, $hc/k=1.43880$ cm°K , and $R=1.98717$ cal/mole °K. The value of the universal gas constant, R , is consistent with $T_0=273.15$ °K for the ice point, [9, 10] and with the new scale of atomic weights based on $\text{C}^{12}=12$ [11]. The value used for hc/k in this calculation is very close to the value 1.43879 cm°K of the new least squares adjusted physical constants [12].

3. The Tables and Their Use

Two tables have been generated from the present calculations. The first constitutes a basic mathematical table, independent of any physical constants, tabulated at closely spaced intervals of the argument. The second table is presented primarily for the convenience of those engaged in thermodynamic investigations to facilitate calculations at specific temperatures physically attainable.

Table I gives the contributions to the four thermodynamic functions in dimensionless form for closely spaced values of $x = hc\nu/kT$. The values can easily be converted to any desired set of units by multiplying by the gas constant R , in appropriate units. For properties on a molar basis $R = 1.98717$ cal/mole °K. The use of this table requires the evaluation of a single argument $x = 1.43879\nu/T$ for each frequency at each temperature.

Interpolation, if required, is facilitated by the listing of first differences for each of the four tabulated functions. The spacing of the argument x is as follows: 0.0010(.0001)0.1500(.001)4.000(.01)10.00(.2)16.0. The spacing of table I is such that, except for values on the first two pages, linear interpolation will give values accurate to one unit in the fifth decimal place. For values of x below 0.01 (on the first two pages) the error resulting from linear interpolation is at most one-eighth of the second difference. For such applications where this error is excessive, use may be made of a 3 or 4 point nonlinear interpolation scheme using Lagrangian interpolation coefficients or an equivalent method employing higher order differences.

Table II lists the vibrational contributions to the free energy function, entropy and heat capacity (in cal/mole °K) explicitly as a function of fre-

quency ν in cm^{-1} and temperature T in °K. The tabulated temperatures are 273.15 °K, 298.15 °K, 400 °K and from there on in 100° intervals to 5000 °K. For each temperature the tables start uniformly at $\nu = 100 \text{ cm}^{-1}$ and extend to 4000 cm^{-1} .

The usefulness of table II can be easily extended to temperatures below 400 °K or to values other than those listed by simple inspection. The tabulated contributions to the thermal function depend only on the ratio ν/T . Thus the values listed at 1000 °K are equally applicable to 10 and 100 °K. In the former case the corresponding frequency would be divided by 100 giving a range of 1 to 40 cm^{-1} at easily interpolatable intervals of 0.1 cm^{-1} . In the latter case the frequency would be divided by 10 giving a frequency range of 10 to 400 cm^{-1} at intervals of 1 cm^{-1} . This reduction of the frequency range which accompanies any calculations at lower temperatures is not restrictive in practice. In the examples cited, frequencies greater than 40 cm^{-1} at 10 °K, and 400 cm^{-1} at 100 °K do not contribute appreciably to the thermal functions. In a similar fashion, the present construction of table II permits simple conversion of the tabulated values to a range of intermediate temperatures within the tabulated range. For example, between 500 and 600 °K, one can obtain contributions to the thermal function at 550 °K by doubling the frequencies and reading the values from the 1100 °K table.

Table II is intended for use at the tabulated arguments or at equivalent arguments easily derivable from them. Since it is not recommended for situations involving interpolations (except as outlined above), no differences are given. Where interpolation cannot be avoided, use should be made of table I.

4. Computation of the Tables

The tables were computed on the IBM 704 Computer from a program written in the Fortran language and employing mathematical subroutines obtained from the Fortran Library. These were Bell Laboratory modifications of Fortran versions of Los Alamos programs distributed by SHARE under numbers LA S816 for e^x and LA S820 for $\ln x$. These subroutines, which are now fairly standard, have an error of at most 3 in the 8th significant decimal digit.

The calculations were carried out in single precision to machine accuracy and rounded to the figures tabulated. Accordingly, the tables should be correct to within $\frac{1}{2}$ unit in the last place tabulated. The tables were printed directly from the machine-printed copy, except for the headings,

which were hand typed. Such comparisons as were made between our table I and the corresponding table of Johnston, Savedoff, and Belzer indicate exact agreement over all but the first few entries where the difference is only one in the 5th decimal. The differences between our table II and the earlier works are small and result from the use of different fundamental constants.

The authors acknowledge the assistance rendered by Miss Carla Harms in checking the tables, and by Mrs. Eleanor F. Rozsics in preparing the manuscript. Thanks are also due Dr. David White for stimulating discussions and helpful editorial suggestions.

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Table I.
Harmonic Oscillator Contributions
(in dimensionless form)
to the Thermodynamic Functions
for Values of $X = hc\nu/kT$

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = h\nu/kT$

X	$-(F^0 - E_0^0)/RT$	Δ	$(H^0 - E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0010	6.90827	9526	0.99951	4	7.90778	9530	1.00000
0.0011	6.81301	8697	0.99947	7	7.81248	8704	1.00000
0.0012	6.72604	7999	0.99940	4	7.72544	8003	1.00000
0.0013	6.64605	7407	0.99936	6	7.64541	7412	1.00000
0.0014	6.57198	6894	0.99930	5	7.57129	6899	1.00000
0.0015	6.50304	6449	0.99925	5	7.50230	6455	1.00000
0.0016	6.43855	6057	0.99920	5	7.43775	6062	1.00000
0.0017	6.37798	5710	0.99915	4	7.37713	5714	1.00000
0.0018	6.32088	5402	0.99911	5	7.31999	5408	1.00000
0.0019	6.26686	5124	0.99906	5	7.26591	5129	1.00000
0.0020	6.21562	4875	0.99901	6	7.21432	4880	1.00000
0.0021	6.16687	4647	0.99895	4	7.16582	4651	1.00000
0.0022	6.12040	4440	0.99891	6	7.11931	4446	1.00000
0.0023	6.07600	4251	0.99885	5	7.07485	4256	1.00000
0.0024	6.03349	4078	0.99880	5	7.03229	4082	1.00000
0.0025	5.99271	3916	0.99875	5	6.99147	3922	1.00000
0.0026	5.95355	3769	0.99870	4	6.95225	3773	1.00000
0.0027	5.91586	3632	0.99866	6	6.91452	3638	1.00000
0.0028	5.87954	3504	0.99860	5	6.87814	3509	1.00000
0.0029	5.84450	3386	0.99855	5	6.84305	3390	1.00000
0.0030	5.81064	3273	0.99850	5	6.80915	3279	1.00000
0.0031	5.77791	3171	0.99845	5	6.77636	3175	1.00000
0.0032	5.74620	3072	0.99840	5	6.74461	3077	1.00000
0.0033	5.71548	2980	0.99835	5	6.71384	2986	1.00000
0.0034	5.68568	2894	0.99830	5	6.68398	2898	1.00000
0.0035	5.65674	2811	0.99825	4	6.65500	2817	1.00000
0.0036	5.62863	2736	0.99821	6	6.62683	2740	1.00000
0.0037	5.60127	2661	0.99815	5	6.59943	2667	1.00000
0.0038	5.57466	2593	0.99810	5	6.57276	2598	1.00000
0.0039	5.54873	2527	0.99805	5	6.54678	2531	1.00000
0.0040	5.52346	2464	0.99800	5	6.52147	2470	1.00000
0.0041	5.49882	2405	0.99795	5	6.49677	2409	1.00000
0.0042	5.47477	2348	0.99790	5	6.47268	2354	1.00000
0.0043	5.45129	2294	0.99785	5	6.44914	2299	1.00000
0.0044	5.42835	2242	0.99780	5	6.42615	2247	1.00000
0.0045	5.40593	2193	0.99775	5	6.40368	2198	1.00000
0.0046	5.38400	2145	0.99770	4	6.38170	2150	1.00000
0.0047	5.36255	2101	0.99766	6	6.36020	2106	1.00000
0.0048	5.34154	2057	0.99760	5	6.33914	2062	1.00000
0.0049	5.32097	2015	0.99755	5	6.31852	2020	1.00000
0.0050	5.30082		0.99750		6.29832		1.00000

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0050	5.30082	1976	0.99750	5	6.29832	1980	1.00000
0.0051	5.28106	1937	0.99745	5	6.27852	1942	1.00000
0.0052	5.26170	1899	0.99740	5	6.25910	1905	1.00000
0.0053	5.24270	1864	0.99735	4	6.24005	1869	1.00000
0.0054	5.22406	1830	0.99731	6	6.22136	1835	1.00000
0.0055	5.20576	1797	0.99725	5	6.20301	1802	1.00000
0.0056	5.18779	1765	0.99720	5	6.18499	1770	1.00000
0.0057	5.17014	1734	0.99715	5	6.16729	1739	1.00000
0.0058	5.15280	1705	0.99710	5	6.14990	1710	1.00000
0.0059	5.13575	1675	0.99705	5	6.13280	1680	1.00000
0.0060	5.11900	1649	0.99700	5	6.11600	1653	1.00000
0.0061	5.10251	1620	0.99695	4	6.09947	1626	1.00000
0.0062	5.08631	1595	0.99691	5	6.08321	1600	1.00000
0.0063	5.07036	1570	0.99686	6	6.06721	1575	1.00000
0.0064	5.05466	1546	0.99680	4	6.05146	1550	1.00000
0.0065	5.03920	1522	0.99676	6	6.03596	1527	1.00000
0.0066	5.02398	1498	0.99670	5	6.02069	1504	1.00000
0.0067	5.00900	1477	0.99665	5	6.00565	1481	1.00000
0.0068	4.99423	1455	0.99660	5	5.99084	1460	1.00000
0.0069	4.97968	1434	0.99655	5	5.97624	1439	1.00000
0.0070	4.96534	1413	0.99650	4	5.96185	1419	1.00000
0.0071	4.95121	1394	0.99646	5	5.94766	1398	1.00000
0.0072	4.93727	1374	0.99641	5	5.93368	1380	1.00000
0.0073	4.92353	1356	0.99636	5	5.91988	1360	1.00000
0.0074	4.90997	1337	0.99631	5	5.90628	1342	1.00000
0.0075	4.89660	1319	0.99626	5	5.89286	1325	1.00000
0.0076	4.88341	1303	0.99621	6	5.87961	1307	1.00000
0.0077	4.87038	1285	0.99615	4	5.86654	1290	0.99999
0.0078	4.85753	1269	0.99611	6	5.85354	1275	1.00000
0.0079	4.84484	1253	0.99605	4	5.84089	1257	0.99999
0.0080	4.83231	1237	0.99601	5	5.82832	1242	1.00000
0.0081	4.81994	1222	0.99596	5	5.81590	1227	1.00000
0.0082	4.80772	1207	0.99591	5	5.80363	1212	1.00000
0.0083	4.79565	1193	0.99586	5	5.79151	1198	1.00000
0.0084	4.78372	1178	0.99581	5	5.77953	1184	0.99999
0.0085	4.77194	1165	0.99576	5	5.76769	1169	1.00000
0.0086	4.76029	1151	0.99571	5	5.75600	1156	0.99999
0.0087	4.74878	1138	0.99566	5	5.74444	1143	0.99999
0.0088	4.73740	1125	0.99561	5	5.73301	1130	0.99999
0.0089	4.72615	1112	0.99556	5	5.72171	1117	0.99999
0.0090	4.71503	1100	0.99551	5	5.71054	1105	1.00000
0.0091	4.70403	1088	0.99546	5	5.69949	1093	0.99999
0.0092	4.69315	1076	0.99541	5	5.68856	1081	1.00000
0.0093	4.68239	1065	0.99536	5	5.67775	1070	0.99999
0.0094	4.67174	1053	0.99531	5	5.66705	1058	0.99999
0.0095	4.66121	1042	0.99526	5	5.65647	1047	0.99999
0.0096	4.65079	1031	0.99521	5	5.64600	1036	0.99999
0.0097	4.64048	1021	0.99516	5	5.63564	1026	1.00000
0.0098	4.63027	1010	0.99511	5	5.62538	1015	0.99999
0.0099	4.62017	1000	0.99506	5	5.61523	1005	0.99999
0.0100	4.61017		0.99501		5.60518		0.99999

Table 1 Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0 - E_0^0)/RT$	Δ	$(H^0 - E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0100	4.61017	990	0.99501	5	5.60518	995	0.99999
0.0101	4.60027	981	0.99496	5	5.59523	986	0.99999
0.0102	4.59046	970	0.99491	5	5.58537	975	0.99999
0.0103	4.58076	962	0.99486	5	5.57562	967	0.99999
0.0104	4.57114	951	0.99481	5	5.56595	957	0.99999
0.0105	4.56163	943	0.99476	5	5.55638	947	0.99999
0.0106	4.55220	934	0.99471	5	5.54691	939	0.99999
0.0107	4.54286	925	0.99466	5	5.53752	930	0.99999
0.0108	4.53361	917	0.99461	5	5.52822	922	0.99999
0.0109	4.52444	908	0.99456	5	5.51900	913	0.99999
0.0110	4.51536	901	0.99451	5	5.50987	906	0.99999
0.0111	4.50635	891	0.99446	5	5.50081	896	0.99999
0.0112	4.49744	884	0.99441	5	5.49185	889	0.99999
0.0113	4.48860	876	0.99436	5	5.48296	881	0.99999
0.0114	4.47984	869	0.99431	5	5.47415	873	0.99999
0.0115	4.47115	860	0.99426	5	5.46542	866	0.99999
0.0116	4.46255	854	0.99421	5	5.45676	859	0.99999
0.0117	4.45401	846	0.99416	5	5.44817	851	0.99999
0.0118	4.44555	839	0.99411	5	5.43966	844	0.99999
0.0119	4.43716	832	0.99406	5	5.43122	836	0.99999
0.0120	4.42884	825	0.99401	5	5.42286	830	0.99999
0.0121	4.42059	818	0.99396	5	5.41456	824	0.99999
0.0122	4.41241	811	0.99391	5	5.40632	816	0.99999
0.0123	4.40430	805	0.99386	5	5.39816	809	0.99999
0.0124	4.39625	798	0.99381	5	5.39007	804	0.99999
0.0125	4.38827	792	0.99376	5	5.38203	796	0.99999
0.0126	4.38035	785	0.99371	5	5.37407	791	0.99999
0.0127	4.37250	780	0.99366	5	5.36616	784	0.99999
0.0128	4.36470	773	0.99361	5	5.35832	779	0.99999
0.0129	4.35697	767	0.99356	5	5.35053	772	0.99999
0.0130	4.34930	761	0.99351	5	5.34281	766	0.99999
0.0131	4.34169	756	0.99346	5	5.33515	760	0.99999
0.0132	4.33413	749	0.99341	4	5.32755	755	0.99999
0.0133	4.32664	745	0.99337	5	5.32000	749	0.99999
0.0134	4.31919	738	0.99332	5	5.31251	744	0.99999
0.0135	4.31181	733	0.99327	5	5.30507	738	0.99999
0.0136	4.30448	728	0.99322	5	5.29769	732	0.99999
0.0137	4.29720	722	0.99317	5	5.29037	728	0.99999
0.0138	4.28998	717	0.99312	5	5.28309	721	0.99998
0.0139	4.28281	712	0.99307	5	5.27588	717	0.99999
0.0140	4.27569	707	0.99302	5	5.26871	712	0.99998
0.0141	4.26862	701	0.99297	5	5.26159	707	0.99999
0.0142	4.26161	697	0.99292	5	5.25452	702	0.99999
0.0143	4.25464	692	0.99287	5	5.24750	696	0.99998
0.0144	4.24772	687	0.99282	5	5.24054	692	0.99998
0.0145	4.24085	682	0.99277	5	5.23362	688	0.99998
0.0146	4.23403	678	0.99272	5	5.22674	682	0.99998
0.0147	4.22725	673	0.99267	5	5.21992	678	0.99998
0.0148	4.22052	669	0.99262	5	5.21314	674	0.99998
0.0149	4.21383	663	0.99257	5	5.20640	668	0.99998
0.0150	4.20720		0.99252		5.19972		0.99998

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0150	4.20720	660	0.99252	5	5.19972	665	0.99998
0.0151	4.20060	655	0.99247	5	5.19307	660	0.99998
0.0152	4.19405	651	0.99242	5	5.18647	656	0.99998
0.0153	4.18754	646	0.99237	5	5.17991	651	0.99998
0.0154	4.18108	642	0.99232	5	5.17340	647	0.99998
0.0155	4.17466	639	0.99227	5	5.16693	644	0.99998
0.0156	4.16827	634	0.99222	5	5.16049	638	0.99998
0.0157	4.16193	630	0.99217	5	5.15411	635	0.99998
0.0158	4.15563	625	0.99212	5	5.14776	631	0.99998
0.0159	4.14938	622	0.99207	5	5.14145	627	0.99998
0.0160	4.14316	618	0.99202	5	5.13518	623	0.99998
0.0161	4.13698	615	0.99197	5	5.12895	619	0.99998
0.0162	4.13083	610	0.99192	5	5.12276	616	0.99998
0.0163	4.12473	607	0.99187	5	5.11660	611	0.99998
0.0164	4.11866	603	0.99182	5	5.11049	608	0.99998
0.0165	4.11263	599	0.99177	5	5.10441	605	0.99998
0.0166	4.10664	596	0.99172	5	5.09836	600	0.99998
0.0167	4.10068	591	0.99167	5	5.09236	597	0.99998
0.0168	4.09477	589	0.99162	5	5.08639	593	0.99998
0.0169	4.08888	585	0.99157	5	5.08046	591	0.99998
0.0170	4.08303	581	0.99152	5	5.07455	586	0.99998
0.0171	4.07722	579	0.99147	5	5.06869	583	0.99998
0.0172	4.07143	574	0.99142	4	5.06286	580	0.99998
0.0173	4.06569	572	0.99138	5	5.05706	576	0.99998
0.0174	4.05997	568	0.99133	5	5.05130	573	0.99997
0.0175	4.05429	565	0.99128	5	5.04557	570	0.99997
0.0176	4.04864	561	0.99123	5	5.03987	566	0.99997
0.0177	4.04303	559	0.99118	5	5.03421	564	0.99998
0.0178	4.03744	555	0.99113	5	5.02857	560	0.99998
0.0179	4.03189	552	0.99108	5	5.02297	557	0.99997
0.0180	4.02637	549	0.99103	5	5.01740	554	0.99997
0.0181	4.02088	546	0.99098	5	5.01186	551	0.99997
0.0182	4.01542	543	0.99093	5	5.00635	548	0.99997
0.0183	4.00999	540	0.99088	5	5.00087	545	0.99997
0.0184	4.00459	537	0.99083	5	4.99542	542	0.99997
0.0185	3.99922	534	0.99078	5	4.99000	539	0.99997
0.0186	3.99388	531	0.99073	5	4.98461	536	0.99997
0.0187	3.98857	529	0.99068	5	4.97925	534	0.99997
0.0188	3.98328	525	0.99063	5	4.97391	530	0.99997
0.0189	3.97803	523	0.99058	5	4.96861	528	0.99997
0.0190	3.97280	520	0.99053	5	4.96333	525	0.99997
0.0191	3.96760	517	0.99048	5	4.95808	522	0.99997
0.0192	3.96243	515	0.99043	5	4.95286	519	0.99997
0.0193	3.95728	511	0.99038	5	4.94767	517	0.99997
0.0194	3.95217	509	0.99033	5	4.94250	514	0.99997
0.0195	3.94708	507	0.99028	5	4.93736	512	0.99997
0.0196	3.94201	504	0.99023	5	4.93224	509	0.99997
0.0197	3.93697	501	0.99018	5	4.92715	506	0.99997
0.0198	3.93196	499	0.99013	5	4.92209	504	0.99997
0.0199	3.92697	496	0.99008	5	4.91705	501	0.99997
0.0200	3.92201		0.99003		4.91204		0.99997

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0200	3.92201	494	0.99003	5	4.91204	499	0.99997
0.0201	3.91707	491	0.98998	5	4.90705	496	0.99997
0.0202	3.91216	489	0.98993	4	4.90209	494	0.99997
0.0203	3.90727	487	0.98989	5	4.89715	491	0.99997
0.0204	3.90240	484	0.98984	5	4.89224	489	0.99997
0.0205	3.89756	481	0.98979	5	4.88735	487	0.99997
0.0206	3.89275	480	0.98974	5	4.88248	484	0.99996
0.0207	3.88795	477	0.98969	5	4.87764	482	0.99997
0.0208	3.88318	474	0.98964	5	4.87282	480	0.99996
0.0209	3.87844	473	0.98959	5	4.86802	477	0.99996
0.0210	3.87371	470	0.98954	5	4.86325	475	0.99996
0.0211	3.86901	467	0.98949	5	4.85850	473	0.99996
0.0212	3.86434	466	0.98944	5	4.85377	470	0.99996
0.0213	3.85968	463	0.98939	5	4.84907	469	0.99996
0.0214	3.85505	462	0.98934	5	4.84438	466	0.99996
0.0215	3.85043	459	0.98929	5	4.83972	464	0.99996
0.0216	3.84584	457	0.98924	5	4.83508	462	0.99996
0.0217	3.84127	454	0.98919	5	4.83046	459	0.99996
0.0218	3.83673	453	0.98914	5	4.82587	458	0.99996
0.0219	3.83220	451	0.98909	5	4.82129	456	0.99996
0.0220	3.82769	448	0.98904	5	4.81673	453	0.99996
0.0221	3.82321	447	0.98899	5	4.81220	452	0.99996
0.0222	3.81874	444	0.98894	5	4.80768	449	0.99996
0.0223	3.81430	443	0.98889	5	4.80319	447	0.99996
0.0224	3.80987	440	0.98884	5	4.79872	446	0.99996
0.0225	3.80547	439	0.98879	5	4.79426	443	0.99996
0.0226	3.80108	436	0.98874	5	4.78983	442	0.99996
0.0227	3.79672	435	0.98869	5	4.78541	439	0.99996
0.0228	3.79237	432	0.98864	5	4.78102	438	0.99996
0.0229	3.78805	431	0.98859	5	4.77664	436	0.99996
0.0230	3.78374	429	0.98854	5	4.77228	433	0.99996
0.0231	3.77945	427	0.98849	4	4.76795	432	0.99996
0.0232	3.77518	425	0.98845	5	4.76363	431	0.99996
0.0233	3.77093	423	0.98840	5	4.75932	428	0.99996
0.0234	3.76670	422	0.98835	5	4.75504	426	0.99996
0.0235	3.76248	419	0.98830	5	4.75078	425	0.99995
0.0236	3.75829	418	0.98825	5	4.74653	423	0.99995
0.0237	3.75411	416	0.98820	5	4.74230	421	0.99995
0.0238	3.74995	415	0.98815	5	4.73809	419	0.99995
0.0239	3.74580	412	0.98810	5	4.73390	417	0.99995
0.0240	3.74168	411	0.98805	5	4.72973	416	0.99995
0.0241	3.73757	409	0.98800	5	4.72557	414	0.99995
0.0242	3.73348	408	0.98795	5	4.72143	413	0.99995
0.0243	3.72940	405	0.98790	5	4.71730	410	0.99995
0.0244	3.72535	404	0.98785	5	4.71320	409	0.99995
0.0245	3.72131	403	0.98780	5	4.70911	408	0.99995
0.0246	3.71728	400	0.98775	5	4.70503	405	0.99995
0.0247	3.71328	399	0.98770	5	4.70098	404	0.99995
0.0248	3.70929	398	0.98765	5	4.69694	403	0.99995
0.0249	3.70531	396	0.98760	5	4.69291	400	0.99995
0.0250	3.70135		0.98755		4.68891		0.99995

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F_0 - E_0)/RT$	Δ	$(H_0 - E_0)/RT$	Δ	S_0/R	Δ	C_p^0/R
0.0250	3.70135	394	0.98755	5	4.68891	400	0.99995
0.0251	3.69741	392	0.98750	5	4.58491	397	0.99995
0.0252	3.69349	392	0.98745	5	4.68094	396	0.99995
0.0253	3.68957	389	0.98740	5	4.67698	395	0.99995
0.0254	3.68568	388	0.98735	5	4.67303	393	0.99995
0.0255	3.68180	386	0.98730	5	4.66910	391	0.99995
0.0256	3.67794	385	0.98725	4	4.66519	390	0.99995
0.0257	3.67409	384	0.98721	5	4.66129	388	0.99995
0.0258	3.67025	382	0.98716	5	4.65741	387	0.99994
0.0259	3.66643	380	0.98711	5	4.65354	385	0.99995
0.0260	3.66263	379	0.98706	5	4.64969	384	0.99994
0.0261	3.65884	377	0.98701	5	4.64585	383	0.99994
0.0262	3.65507	376	0.98696	5	4.64202	380	0.99994
0.0263	3.65131	375	0.98691	5	4.63822	380	0.99994
0.0264	3.64756	373	0.98686	5	4.63442	378	0.99994
0.0265	3.64383	371	0.98681	5	4.63064	377	0.99994
0.0266	3.64012	371	0.98676	5	4.62687	375	0.99994
0.0267	3.63641	369	0.98671	5	4.62312	374	0.99994
0.0268	3.63272	367	0.98666	5	4.61938	372	0.99994
0.0269	3.62905	366	0.98661	5	4.61566	371	0.99994
0.0270	3.62539	365	0.98656	5	4.61195	370	0.99994
0.0271	3.62174	363	0.98651	5	4.60825	368	0.99994
0.0272	3.61811	362	0.98646	5	4.60457	367	0.99994
0.0273	3.61449	361	0.98641	5	4.60090	366	0.99994
0.0274	3.61088	359	0.98636	5	4.59724	364	0.99994
0.0275	3.60729	358	0.98631	5	4.59360	363	0.99994
0.0276	3.60371	357	0.98626	5	4.58997	361	0.99994
0.0277	3.60014	355	0.98621	5	4.58636	361	0.99994
0.0278	3.59659	354	0.98616	4	4.58275	359	0.99994
0.0279	3.59305	353	0.98612	5	4.57916	358	0.99994
0.0280	3.58952	352	0.98607	5	4.57558	356	0.99993
0.0281	3.58600	350	0.98602	5	4.57202	355	0.99993
0.0282	3.58250	349	0.98597	5	4.56847	354	0.99994
0.0283	3.57901	348	0.98592	5	4.56493	353	0.99993
0.0284	3.57553	346	0.98587	5	4.56140	351	0.99993
0.0285	3.57207	346	0.98582	5	4.55789	351	0.99993
0.0286	3.56861	344	0.98577	5	4.55438	349	0.99993
0.0287	3.56517	342	0.98572	5	4.55089	347	0.99993
0.0288	3.56175	342	0.98567	5	4.54742	347	0.99993
0.0289	3.55833	341	0.98562	5	4.54395	346	0.99993
0.0290	3.55492	339	0.98557	5	4.54049	344	0.99993
0.0291	3.55153	338	0.98552	5	4.53705	343	0.99993
0.0292	3.54815	337	0.98547	5	4.53362	342	0.99993
0.0293	3.54478	336	0.98542	5	4.53020	340	0.99993
0.0294	3.54142	334	0.98537	5	4.52680	340	0.99993
0.0295	3.53808	334	0.98532	5	4.52340	338	0.99993
0.0296	3.53474	332	0.98527	5	4.52002	337	0.99993
0.0297	3.53142	331	0.98522	5	4.51665	337	0.99993
0.0298	3.52811	330	0.98517	5	4.51328	335	0.99993
0.0299	3.52481	329	0.98512	4	4.50993	333	0.99993
0.0300	3.52152		0.98508		4.50660		0.99993

Table 1 Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0300	3.52152	328	0.98508	5	4.50660	333	0.99993
0.0301	3.51824	326	0.98503	5	4.50327	332	0.99992
0.0302	3.51498	326	0.98498	5	4.49995	330	0.99992
0.0303	3.51172	325	0.98493	5	4.49665	330	0.99992
0.0304	3.50847	323	0.98488	5	4.49335	328	0.99992
0.0305	3.50524	322	0.98483	5	4.49007	328	0.99992
0.0306	3.50202	322	0.98478	5	4.48679	326	0.99992
0.0307	3.49880	320	0.98473	5	4.48353	325	0.99992
0.0308	3.49560	319	0.98468	5	4.48028	324	0.99992
0.0309	3.49241	318	0.98463	5	4.47704	323	0.99992
0.0310	3.48923	317	0.98458	5	4.47381	322	0.99992
0.0311	3.48606	316	0.98453	5	4.47059	321	0.99992
0.0312	3.48290	315	0.98448	5	4.46738	320	0.99992
0.0313	3.47975	314	0.98443	5	4.46418	319	0.99992
0.0314	3.47661	313	0.98438	5	4.46099	318	0.99992
0.0315	3.47348	312	0.98433	5	4.45781	317	0.99992
0.0316	3.47036	311	0.98428	5	4.45464	316	0.99992
0.0317	3.46725	310	0.98423	5	4.45148	315	0.99992
0.0318	3.46415	309	0.98418	4	4.44833	314	0.99992
0.0319	3.46106	308	0.98414	5	4.44519	313	0.99992
0.0320	3.45798	307	0.98409	5	4.44206	312	0.99992
0.0321	3.45491	306	0.98404	5	4.43894	311	0.99991
0.0322	3.45185	306	0.98399	5	4.43583	310	0.99991
0.0323	3.44879	304	0.98394	5	4.43273	309	0.99991
0.0324	3.44575	303	0.98389	5	4.42964	308	0.99991
0.0325	3.44272	302	0.98384	5	4.42656	307	0.99991
0.0326	3.43970	301	0.98379	5	4.42349	306	0.99991
0.0327	3.43669	301	0.98374	5	4.42043	306	0.99991
0.0328	3.43368	299	0.98369	5	4.41737	304	0.99991
0.0329	3.43069	299	0.98364	5	4.41433	304	0.99991
0.0330	3.42770	297	0.98359	5	4.41129	302	0.99991
0.0331	3.42473	297	0.98354	5	4.40827	302	0.99991
0.0332	3.42176	296	0.98349	5	4.40525	301	0.99991
0.0333	3.41880	295	0.98344	5	4.40224	299	0.99991
0.0334	3.41585	294	0.98339	5	4.39925	299	0.99991
0.0335	3.41291	293	0.98334	5	4.39626	298	0.99991
0.0336	3.40998	292	0.98329	5	4.39328	298	0.99991
0.0337	3.40706	291	0.98324	4	4.39030	296	0.99991
0.0338	3.40415	291	0.98320	5	4.38734	295	0.99991
0.0339	3.40124	289	0.98315	5	4.38439	295	0.99990
0.0340	3.39835	289	0.98310	5	4.38144	293	0.99990
0.0341	3.39546	288	0.98305	5	4.37851	293	0.99990
0.0342	3.39258	287	0.98300	5	4.37558	292	0.99990
0.0343	3.38971	286	0.98295	5	4.37266	291	0.99990
0.0344	3.38685	285	0.98290	5	4.36975	290	0.99990
0.0345	3.38400	285	0.98285	5	4.36685	290	0.99990
0.0346	3.38115	283	0.98280	5	4.36395	288	0.99990
0.0347	3.37832	283	0.98275	5	4.36107	288	0.99990
0.0348	3.37549	282	0.98270	5	4.35819	287	0.99990
0.0349	3.37267	281	0.98265	5	4.35532	286	0.99990
0.0350	3.36986		0.98260		4.35246		0.99990

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0350	3.36986	281	0.98260	5	4.35246	285	0.99990
0.0351	3.36705	279	0.98255	5	4.34961	285	0.99990
0.0352	3.36426	279	0.98250	5	4.34676	284	0.99990
0.0353	3.36147	278	0.98245	5	4.34392	282	0.99990
0.0354	3.35869	277	0.98240	4	4.34110	282	0.99990
0.0355	3.35592	276	0.98236	5	4.33828	282	0.99990
0.0356	3.35316	276	0.98231	5	4.33546	280	0.99989
0.0357	3.35040	275	0.98226	5	4.33266	280	0.99989
0.0358	3.34765	274	0.98221	5	4.32986	279	0.99989
0.0359	3.34491	273	0.98216	5	4.32707	278	0.99989
0.0360	3.34218	272	0.98211	5	4.32429	277	0.99989
0.0361	3.33946	272	0.98206	5	4.32152	277	0.99989
0.0362	3.33674	271	0.98201	5	4.31875	276	0.99989
0.0363	3.33403	270	0.98196	5	4.31599	275	0.99989
0.0364	3.33133	269	0.98191	5	4.31324	274	0.99989
0.0365	3.32864	269	0.98186	5	4.31050	274	0.99989
0.0366	3.32595	268	0.98181	5	4.30776	273	0.99989
0.0367	3.32327	267	0.98176	5	4.30503	272	0.99989
0.0368	3.32060	266	0.98171	5	4.30231	271	0.99989
0.0369	3.31794	266	0.98166	5	4.29960	270	0.99989
0.0370	3.31528	265	0.98161	5	4.29690	270	0.99989
0.0371	3.31263	264	0.98156	4	4.29420	270	0.99989
0.0372	3.30999	264	0.98152	5	4.29150	268	0.99989
0.0373	3.30735	262	0.98147	5	4.28882	268	0.99988
0.0374	3.30473	262	0.98142	5	4.28614	267	0.99988
0.0375	3.30211	262	0.98137	5	4.28247	266	0.99988
0.0376	3.29949	260	0.98132	5	4.28081	266	0.99988
0.0377	3.29689	260	0.98127	5	4.27815	264	0.99988
0.0378	3.29429	260	0.98122	5	4.27551	265	0.99988
0.0379	3.29169	258	0.98117	5	4.27286	263	0.99988
0.0380	3.28911	258	0.98112	5	4.27023	263	0.99988
0.0381	3.28653	257	0.98107	5	4.26760	262	0.99988
0.0382	3.28396	257	0.98102	5	4.26498	261	0.99988
0.0383	3.28139	255	0.98097	5	4.26237	261	0.99988
0.0384	3.27884	255	0.98092	5	4.25976	260	0.99988
0.0385	3.27629	255	0.98087	5	4.25716	260	0.99988
0.0386	3.27374	254	0.98082	5	4.25456	258	0.99988
0.0387	3.27120	253	0.98077	4	4.25198	258	0.99988
0.0388	3.26867	252	0.98073	5	4.24940	258	0.99988
0.0389	3.26615	252	0.98068	5	4.24682	256	0.99987
0.0390	3.26363	251	0.98063	5	4.24426	256	0.99987
0.0391	3.26112	251	0.98058	5	4.24170	256	0.99987
0.0392	3.25861	249	0.98053	5	4.23914	254	0.99987
0.0393	3.25612	250	0.98048	5	4.23660	255	0.99987
0.0394	3.25362	248	0.98043	5	4.23405	253	0.99987
0.0395	3.25114	248	0.98038	5	4.23152	253	0.99987
0.0396	3.24866	247	0.98033	5	4.22899	252	0.99987
0.0397	3.24619	247	0.98028	5	4.22647	252	0.99987
0.0398	3.24372	246	0.98023	5	4.22395	250	0.99987
0.0399	3.24126	245	0.98018	5	4.22145	251	0.99987
0.0400	3.23881		0.98013		4.21894		0.99987

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F_0 - E_0)/RT$	Δ	$(H^0 - E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0400	3.23881	245	0.98013	5	4.21894	249	0.99987
0.0401	3.23636	244	0.98008	5	4.21645	249	0.99987
0.0402	3.23392	243	0.98003	4	4.21396	249	0.99987
0.0403	3.23149	243	0.97999	5	4.21147	248	0.99987
0.0404	3.22906	242	0.97994	5	4.20899	247	0.99986
0.0405	3.22664	242	0.97989	5	4.20652	246	0.99986
0.0406	3.22422	241	0.97984	5	4.20406	246	0.99986
0.0407	3.22181	241	0.97979	5	4.20160	246	0.99986
0.0408	3.21940	239	0.97974	5	4.19914	244	0.99986
0.0409	3.21701	240	0.97969	5	4.19670	245	0.99986
0.0410	3.21461	238	0.97964	5	4.19425	243	0.99986
0.0411	3.21223	238	0.97959	5	4.19182	243	0.99986
0.0412	3.20985	238	0.97954	5	4.18939	243	0.99986
0.0413	3.20747	237	0.97949	5	4.18696	241	0.99986
0.0414	3.20510	236	0.97944	5	4.18455	242	0.99986
0.0415	3.20274	236	0.97939	5	4.18213	240	0.99986
0.0416	3.20038	235	0.97934	4	4.17973	240	0.99986
0.0417	3.19803	234	0.97930	5	4.17733	240	0.99986
0.0418	3.19569	234	0.97925	5	4.17493	239	0.99985
0.0419	3.19335	234	0.97920	5	4.17254	238	0.99985
0.0420	3.19101	233	0.97915	5	4.17016	238	0.99985
0.0421	3.18868	232	0.97910	5	4.16778	237	0.99985
0.0422	3.18636	232	0.97905	5	4.16541	237	0.99985
0.0423	3.18404	231	0.97900	5	4.16304	236	0.99985
0.0424	3.18173	230	0.97895	5	4.16068	235	0.99985
0.0425	3.17943	230	0.97890	5	4.15833	235	0.99985
0.0426	3.17713	230	0.97885	5	4.15598	235	0.99985
0.0427	3.17483	229	0.97880	5	4.15363	234	0.99985
0.0428	3.17254	228	0.97875	5	4.15129	233	0.99985
0.0429	3.17026	228	0.97870	5	4.14896	233	0.99985
0.0430	3.16798	228	0.97865	5	4.14663	232	0.99985
0.0431	3.16570	226	0.97860	4	4.14431	232	0.99985
0.0432	3.16344	227	0.97856	5	4.14199	231	0.99984
0.0433	3.16117	225	0.97851	5	4.13968	231	0.99984
0.0434	3.15892	225	0.97846	5	4.13737	230	0.99984
0.0435	3.15667	225	0.97841	5	4.13507	229	0.99984
0.0436	3.15442	224	0.97836	5	4.13278	229	0.99984
0.0437	3.15218	224	0.97831	5	4.13049	229	0.99984
0.0438	3.14994	223	0.97826	5	4.12820	228	0.99984
0.0439	3.14771	223	0.97821	5	4.12592	227	0.99984
0.0440	3.14548	222	0.97816	5	4.12365	227	0.99984
0.0441	3.14326	221	0.97811	5	4.12138	227	0.99984
0.0442	3.14105	221	0.97806	5	4.11911	226	0.99984
0.0443	3.13884	221	0.97801	5	4.11685	225	0.99984
0.0444	3.13663	220	0.97796	4	4.11460	225	0.99984
0.0445	3.13443	219	0.97792	5	4.11235	225	0.99983
0.0446	3.13224	219	0.97787	5	4.11010	224	0.99983
0.0447	3.13005	219	0.97782	5	4.10786	223	0.99983
0.0448	3.12786	218	0.97777	5	4.10563	223	0.99983
0.0449	3.12568	217	0.97772	5	4.10340	222	0.99983
0.0450	3.12351		0.97767		4.10118		0.99983

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0450	3.12351	217	0.97767	5	4.10118	222	0.99983
0.0451	3.12134	217	0.97762	5	4.09896	222	0.99983
0.0452	3.11917	216	0.97757	5	4.09674	221	0.99983
0.0453	3.11701	215	0.97752	5	4.09453	220	0.99983
0.0454	3.11486	215	0.97747	5	4.09233	220	0.99983
0.0455	3.11271	215	0.97742	5	4.09013	220	0.99983
0.0456	3.11056	214	0.97737	5	4.08793	219	0.99983
0.0457	3.10842	214	0.97732	4	4.08574	218	0.99983
0.0458	3.10628	213	0.97728	5	4.08356	218	0.99983
0.0459	3.10415	212	0.97723	5	4.08138	218	0.99982
0.0460	3.10203	213	0.97718	5	4.07920	217	0.99982
0.0461	3.09990	211	0.97713	5	4.07703	217	0.99982
0.0462	3.09779	212	0.97708	5	4.07486	216	0.99982
0.0463	3.09567	210	0.97703	5	4.07270	215	0.99982
0.0464	3.09357	211	0.97698	5	4.07055	216	0.99982
0.0465	3.09146	210	0.97693	5	4.06839	214	0.99982
0.0466	3.08936	209	0.97688	5	4.06625	215	0.99982
0.0467	3.08727	209	0.97683	5	4.06410	214	0.99982
0.0468	3.08518	208	0.97678	5	4.06196	213	0.99982
0.0469	3.08310	208	0.97673	5	4.05983	213	0.99982
0.0470	3.08102	208	0.97668	4	4.05770	213	0.99982
0.0471	3.07894	207	0.97664	5	4.05558	212	0.99982
0.0472	3.07687	207	0.97659	5	4.05345	211	0.99981
0.0473	3.07480	206	0.97654	5	4.05134	211	0.99981
0.0474	3.07274	206	0.97649	5	4.04923	211	0.99981
0.0475	3.07068	205	0.97644	5	4.04712	210	0.99981
0.0476	3.06863	205	0.97639	5	4.04502	210	0.99981
0.0477	3.06658	205	0.97634	5	4.04292	209	0.99981
0.0478	3.06453	204	0.97629	5	4.04083	209	0.99981
0.0479	3.06249	203	0.97624	5	4.03874	209	0.99981
0.0480	3.06046	203	0.97619	5	4.03665	208	0.99981
0.0481	3.05843	203	0.97614	5	4.03457	208	0.99981
0.0482	3.05640	202	0.97609	5	4.03249	207	0.99981
0.0483	3.05438	202	0.97604	4	4.03042	207	0.99981
0.0484	3.05236	202	0.97600	5	4.02835	206	0.99980
0.0485	3.05034	201	0.97595	5	4.02629	206	0.99980
0.0486	3.04833	200	0.97590	5	4.02423	205	0.99980
0.0487	3.04633	200	0.97585	5	4.02218	206	0.99980
0.0488	3.04433	200	0.97580	5	4.02012	204	0.99980
0.0489	3.04233	200	0.97575	5	4.01808	205	0.99980
0.0490	3.04033	198	0.97570	5	4.01603	203	0.99980
0.0491	3.03835	199	0.97565	5	4.01400	204	0.99980
0.0492	3.03636	198	0.97560	5	4.01196	203	0.99980
0.0493	3.03438	198	0.97555	5	4.00993	202	0.99980
0.0494	3.03240	197	0.97550	5	4.00791	203	0.99980
0.0495	3.03043	197	0.97545	4	4.00588	201	0.99980
0.0496	3.02846	196	0.97541	5	4.00387	202	0.99980
0.0497	3.02650	196	0.97536	5	4.00185	201	0.99979
0.0498	3.02454	196	0.97531	5	3.99984	200	0.99979
0.0499	3.02258	195	0.97526	5	3.99784	200	0.99979
0.0500	3.02063		0.97521		3.99584		0.99979

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0500	3.02063	195	0.97521	5	3.99584	200	0.99979
0.0501	3.01868	194	0.97516	5	3.99384	199	0.99979
0.0502	3.01674	195	0.97511	5	3.99185	199	0.99979
0.0503	3.01480	193	0.97506	5	3.98986	199	0.99979
0.0504	3.01286	193	0.97501	5	3.98787	198	0.99979
0.0505	3.01093	193	0.97496	5	3.98589	198	0.99979
0.0506	3.00900	193	0.97491	5	3.98391	197	0.99979
0.0507	3.00707	192	0.97486	4	3.98194	197	0.99979
0.0508	3.00515	192	0.97482	5	3.97997	197	0.99979
0.0509	3.00323	191	0.97477	5	3.97800	196	0.99978
0.0510	3.00132	191	0.97472	5	3.97604	196	0.99978
0.0511	2.99941	190	0.97467	5	3.97408	195	0.99978
0.0512	2.99751	191	0.97462	5	3.97213	196	0.99978
0.0513	2.99560	189	0.97457	5	3.97017	194	0.99978
0.0514	2.99371	190	0.97452	5	3.96823	195	0.99978
0.0515	2.99181	189	0.97447	5	3.96628	194	0.99978
0.0516	2.98992	188	0.97442	5	3.96434	193	0.99978
0.0517	2.98804	189	0.97437	5	3.96241	193	0.99978
0.0518	2.98615	188	0.97432	5	3.96048	193	0.99978
0.0519	2.98427	187	0.97427	4	3.95855	193	0.99978
0.0520	2.98240	187	0.97423	5	3.95662	192	0.99978
0.0521	2.98053	187	0.97418	5	3.95470	191	0.99977
0.0522	2.97866	186	0.97413	5	3.95279	192	0.99977
0.0523	2.97680	187	0.97408	5	3.95087	191	0.99977
0.0524	2.97493	185	0.97403	5	3.94896	190	0.99977
0.0525	2.97308	186	0.97398	5	3.94706	191	0.99977
0.0526	2.97122	185	0.97393	5	3.94515	189	0.99977
0.0527	2.96937	184	0.97388	5	3.94326	190	0.99977
0.0528	2.96753	184	0.97383	5	3.94136	189	0.99977
0.0529	2.96569	184	0.97378	5	3.93947	189	0.99977
0.0530	2.96385	184	0.97373	4	3.93758	188	0.99977
0.0531	2.96201	183	0.97369	5	3.93570	188	0.99977
0.0532	2.96018	183	0.97364	5	3.93382	188	0.99976
0.0533	2.95835	182	0.97359	5	3.93194	188	0.99976
0.0534	2.95653	183	0.97354	5	3.93006	187	0.99976
0.0535	2.95470	181	0.97349	5	3.92819	186	0.99976
0.0536	2.95289	182	0.97344	5	3.92633	187	0.99976
0.0537	2.95107	181	0.97339	5	3.92446	186	0.99976
0.0538	2.94926	181	0.97334	5	3.92260	185	0.99976
0.0539	2.94745	180	0.97329	5	3.92075	186	0.99976
0.0540	2.94565	180	0.97324	5	3.91889	185	0.99976
0.0541	2.94385	180	0.97319	5	3.91704	184	0.99976
0.0542	2.94205	179	0.97314	4	3.91520	185	0.99976
0.0543	2.94026	179	0.97310	5	3.91335	184	0.99975
0.0544	2.93847	179	0.97305	5	3.91151	183	0.99975
0.0545	2.93668	178	0.97300	5	3.90968	183	0.99975
0.0546	2.93490	178	0.97295	5	3.90785	183	0.99975
0.0547	2.93312	178	0.97290	5	3.90602	183	0.99975
0.0548	2.93134	177	0.97285	5	3.90419	182	0.99975
0.0549	2.92957	177	0.97280	5	3.90237	182	0.99975
0.0550	2.92780		0.97275		3.90055		0.99975

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0550	2.92780	177	0.97275	5	3.90055	182	0.99975
0.0551	2.92603	176	0.97270	5	3.89873	181	0.99975
0.0552	2.92427	177	0.97265	5	3.89692	181	0.99975
0.0553	2.92250	175	0.97260	4	3.89511	181	0.99975
0.0554	2.92075	176	0.97256	5	3.89330	180	0.99974
0.0555	2.91899	175	0.97251	5	3.89150	180	0.99974
0.0556	2.91724	174	0.97246	5	3.88970	180	0.99974
0.0557	2.91550	175	0.97241	5	3.88790	179	0.99974
0.0558	2.91375	174	0.97236	5	3.88611	179	0.99974
0.0559	2.91201	174	0.97231	5	3.88432	179	0.99974
0.0560	2.91027	173	0.97226	5	3.88253	178	0.99974
0.0561	2.90854	173	0.97221	5	3.88075	178	0.99974
0.0562	2.90681	173	0.97216	5	3.87897	178	0.99974
0.0563	2.90508	173	0.97211	4	3.87719	177	0.99974
0.0564	2.90335	172	0.97207	5	3.87542	177	0.99974
0.0565	2.90163	172	0.97202	5	3.87365	177	0.99973
0.0566	2.89991	171	0.97197	5	3.87188	176	0.99973
0.0567	2.89820	172	0.97192	5	3.87012	177	0.99973
0.0568	2.89648	170	0.97187	5	3.86835	176	0.99973
0.0569	2.89478	171	0.97182	5	3.86659	175	0.99973
0.0570	2.89307	170	0.97177	5	3.86484	175	0.99973
0.0571	2.89137	170	0.97172	5	3.86309	175	0.99973
0.0572	2.88967	170	0.97167	5	3.86134	175	0.99973
0.0573	2.88797	170	0.97162	5	3.85959	174	0.99973
0.0574	2.88627	169	0.97157	4	3.85785	174	0.99973
0.0575	2.88458	169	0.97153	5	3.85611	174	0.99972
0.0576	2.88289	168	0.97148	5	3.85437	173	0.99972
0.0577	2.88121	168	0.97143	5	3.85264	173	0.99972
0.0578	2.87953	168	0.97138	5	3.85091	173	0.99972
0.0579	2.87785	168	0.97133	5	3.84918	173	0.99972
0.0580	2.87617	167	0.97128	5	3.84745	172	0.99972
0.0581	2.87450	167	0.97123	5	3.84573	172	0.99972
0.0582	2.87283	167	0.97118	5	3.84401	172	0.99972
0.0583	2.87116	166	0.97113	5	3.84229	171	0.99972
0.0584	2.86950	166	0.97108	4	3.84058	171	0.99972
0.0585	2.86784	166	0.97104	5	3.83887	171	0.99971
0.0586	2.86618	166	0.97099	5	3.83716	170	0.99971
0.0587	2.86452	165	0.97094	5	3.83546	170	0.99971
0.0588	2.86287	165	0.97089	5	3.83376	170	0.99971
0.0589	2.86122	165	0.97084	5	3.83206	170	0.99971
0.0590	2.85957	164	0.97079	5	3.83036	169	0.99971
0.0591	2.85793	164	0.97074	5	3.82867	169	0.99971
0.0592	2.85629	164	0.97069	5	3.82698	169	0.99971
0.0593	2.85465	164	0.97064	5	3.82529	168	0.99971
0.0594	2.85301	163	0.97059	4	3.82361	168	0.99971
0.0595	2.85138	163	0.97055	5	3.82193	168	0.99971
0.0596	2.84975	163	0.97050	5	3.82025	168	0.99970
0.0597	2.84812	162	0.97045	5	3.81857	167	0.99970
0.0598	2.84650	162	0.97040	5	3.81690	167	0.99970
0.0599	2.84488	162	0.97035	5	3.81523	167	0.99970
0.0600	2.84326		0.97030		3.81356		0.99970

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0600	2.84326	162	0.97030	5	3.81356	166	0.99970
0.0601	2.84165	161	0.97025	5	3.81190	167	0.99970
0.0602	2.84003	161	0.97020	5	3.81023	166	0.99970
0.0603	2.83842	161	0.97015	5	3.80857	165	0.99970
0.0604	2.83681	160	0.97010	5	3.80692	166	0.99970
0.0605	2.83521	160	0.97005	4	3.80526	165	0.99969
0.0606	2.83361	160	0.97001	5	3.80361	165	0.99969
0.0607	2.83201	160	0.96996	5	3.80196	164	0.99969
0.0608	2.83041	159	0.96991	5	3.80032	164	0.99969
0.0609	2.82882	159	0.96986	5	3.79868	164	0.99969
0.0610	2.82723	159	0.96981	5	3.79704	164	0.99969
0.0611	2.82564	159	0.96976	5	3.79540	164	0.99969
0.0612	2.82405	158	0.96971	5	3.79376	163	0.99969
0.0613	2.82247	158	0.96966	5	3.79213	163	0.99969
0.0614	2.82089	158	0.96961	4	3.79050	162	0.99969
0.0615	2.81931	157	0.96957	5	3.78888	163	0.99969
0.0616	2.81774	158	0.96952	5	3.78725	162	0.99968
0.0617	2.81616	157	0.96947	5	3.78563	162	0.99968
0.0618	2.81459	156	0.96942	5	3.78401	162	0.99968
0.0619	2.81303	157	0.96937	5	3.78239	161	0.99968
0.0620	2.81146	156	0.96932	5	3.78078	161	0.99968
0.0621	2.80990	156	0.96927	5	3.77917	161	0.99968
0.0622	2.80834	156	0.96922	5	3.77756	160	0.99968
0.0623	2.80678	155	0.96917	5	3.77596	161	0.99968
0.0624	2.80523	155	0.96912	4	3.77435	160	0.99968
0.0625	2.80368	155	0.96908	5	3.77275	160	0.99967
0.0626	2.80213	155	0.96903	5	3.77115	159	0.99967
0.0627	2.80058	154	0.96898	5	3.76956	160	0.99967
0.0628	2.79904	155	0.96893	5	3.76796	159	0.99967
0.0629	2.79749	153	0.96888	5	3.76637	158	0.99967
0.0630	2.79596	154	0.96883	5	3.76479	159	0.99967
0.0631	2.79442	154	0.96878	5	3.76320	158	0.99967
0.0632	2.79288	153	0.96873	5	3.76162	158	0.99967
0.0633	2.79135	153	0.96868	4	3.76004	158	0.99967
0.0634	2.78982	152	0.96864	5	3.75846	158	0.99967
0.0635	2.78830	153	0.96859	5	3.75688	157	0.99966
0.0636	2.78677	152	0.96854	5	3.75531	157	0.99966
0.0637	2.78525	152	0.96849	5	3.75374	157	0.99966
0.0638	2.78373	151	0.96844	5	3.75217	156	0.99966
0.0639	2.78222	152	0.96839	5	3.75061	157	0.99966
0.0640	2.78070	151	0.96834	5	3.74904	156	0.99966
0.0641	2.77919	151	0.96829	5	3.74748	156	0.99966
0.0642	2.77768	151	0.96824	5	3.74592	155	0.99966
0.0643	2.77617	150	0.96819	4	3.74437	156	0.99966
0.0644	2.77467	150	0.96815	5	3.74281	155	0.99965
0.0645	2.77317	150	0.96810	5	3.74126	155	0.99965
0.0646	2.77167	150	0.96805	5	3.73971	154	0.99965
0.0647	2.77017	150	0.96800	5	3.73817	155	0.99965
0.0648	2.76867	149	0.96795	5	3.73662	154	0.99965
0.0649	2.76718	149	0.96790	5	3.73508	154	0.99965
0.0650	2.76569		0.96785		3.73354		0.99965

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0650	2.76569	149	0.96785	5	3.73354	153	0.99965
0.0651	2.76420	148	0.96780	5	3.73201	154	0.99965
0.0652	2.76272	148	0.96775	4	3.73047	153	0.99965
0.0653	2.76124	149	0.96771	5	3.72894	153	0.99964
0.0654	2.75975	147	0.96766	5	3.72741	153	0.99964
0.0655	2.75828	148	0.96761	5	3.72588	152	0.99964
0.0656	2.75680	147	0.96756	5	3.72436	152	0.99964
0.0657	2.75533	147	0.96751	5	3.72284	152	0.99964
0.0658	2.75386	147	0.96746	5	3.72132	152	0.99964
0.0659	2.75239	147	0.96741	5	3.71980	152	0.99964
0.0660	2.75092	147	0.96736	5	3.71828	151	0.99964
0.0661	2.74945	146	0.96731	4	3.71677	151	0.99964
0.0662	2.74799	146	0.96727	5	3.71526	151	0.99964
0.0663	2.74653	146	0.96722	5	3.71375	151	0.99963
0.0664	2.74507	145	0.96717	5	3.71224	150	0.99963
0.0665	2.74362	145	0.96712	5	3.71074	150	0.99963
0.0666	2.74217	145	0.96707	5	3.70924	150	0.99963
0.0667	2.74072	145	0.96702	5	3.70774	150	0.99963
0.0668	2.73927	145	0.96697	5	3.70624	150	0.99963
0.0669	2.73782	144	0.96692	5	3.70474	149	0.99963
0.0670	2.73638	145	0.96687	4	3.70325	149	0.99963
0.0671	2.73493	144	0.96683	5	3.70176	149	0.99963
0.0672	2.73349	143	0.96678	5	3.70027	149	0.99962
0.0673	2.73206	144	0.96673	5	3.69878	148	0.99962
0.0674	2.73062	143	0.96668	5	3.69730	148	0.99962
0.0675	2.72919	143	0.96663	5	3.69582	148	0.99962
0.0676	2.72776	143	0.96658	5	3.69434	148	0.99962
0.0677	2.72633	143	0.96653	5	3.69286	148	0.99962
0.0678	2.72490	142	0.96648	5	3.69138	147	0.99962
0.0679	2.72348	143	0.96643	4	3.68991	147	0.99962
0.0680	2.72205	142	0.96639	5	3.68844	147	0.99961
0.0681	2.72063	141	0.96634	5	3.68697	147	0.99961
0.0682	2.71922	142	0.96629	5	3.68550	146	0.99961
0.0683	2.71780	141	0.96624	5	3.68404	146	0.99961
0.0684	2.71639	141	0.96619	5	3.68258	146	0.99961
0.0685	2.71498	141	0.96614	5	3.68112	146	0.99961
0.0686	2.71357	141	0.96609	5	3.67966	146	0.99961
0.0687	2.71216	141	0.96604	5	3.67820	145	0.99961
0.0688	2.71075	140	0.96599	4	3.67675	145	0.99961
0.0689	2.70935	140	0.96595	5	3.67530	145	0.99960
0.0690	2.70795	140	0.96590	5	3.67385	145	0.99960
0.0691	2.70655	140	0.96585	5	3.67240	145	0.99960
0.0692	2.70515	139	0.96580	5	3.67095	144	0.99960
0.0693	2.70376	139	0.96575	5	3.66951	144	0.99960
0.0694	2.70237	139	0.96570	5	3.66807	144	0.99960
0.0695	2.70098	139	0.96565	5	3.66663	144	0.99960
0.0696	2.69959	139	0.96560	4	3.66519	143	0.99960
0.0697	2.69820	138	0.96556	5	3.66376	144	0.99960
0.0698	2.69682	138	0.96551	5	3.66232	143	0.99959
0.0699	2.69544	138	0.96546	5	3.66089	143	0.99959
0.0700	2.69406		0.96541		3.65946		0.99959

Table I | Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0700	2.69406	138	0.96541	5	3.65946	142	0.99959
0.0701	2.69268	138	0.96536	5	3.65804	143	0.99959
0.0702	2.69130	137	0.96531	5	3.65661	142	0.99959
0.0703	2.68993	137	0.96526	5	3.65519	142	0.99959
0.0704	2.68856	137	0.96521	5	3.65377	142	0.99959
0.0705	2.68719	137	0.96516	4	3.65235	142	0.99959
0.0706	2.68582	137	0.96512	5	3.65093	141	0.99959
0.0707	2.68445	136	0.96507	5	3.64952	141	0.99958
0.0708	2.68309	136	0.96502	5	3.64811	142	0.99958
0.0709	2.68173	136	0.96497	5	3.64669	140	0.99958
0.0710	2.68037	136	0.96492	5	3.64529	141	0.99958
0.0711	2.67901	136	0.96487	5	3.64388	141	0.99958
0.0712	2.67765	135	0.96482	5	3.64247	140	0.99958
0.0713	2.67630	135	0.96477	5	3.64107	140	0.99958
0.0714	2.67495	136	0.96472	4	3.63967	140	0.99958
0.0715	2.67359	134	0.96468	5	3.63827	140	0.99957
0.0716	2.67225	135	0.96463	5	3.63687	139	0.99957
0.0717	2.67090	134	0.96458	5	3.63548	139	0.99957
0.0718	2.66956	135	0.96453	5	3.63409	140	0.99957
0.0719	2.66821	134	0.96448	5	3.63269	139	0.99957
0.0720	2.66687	134	0.96443	5	3.63130	138	0.99957
0.0721	2.66553	133	0.96438	5	3.62992	139	0.99957
0.0722	2.66420	134	0.96433	4	3.62853	138	0.99957
0.0723	2.66286	133	0.96429	5	3.62715	138	0.99956
0.0724	2.66153	133	0.96424	5	3.62577	138	0.99956
0.0725	2.66020	133	0.96419	5	3.62439	138	0.99956
0.0726	2.65887	133	0.96414	5	3.62301	138	0.99956
0.0727	2.65754	132	0.96409	5	3.62163	137	0.99956
0.0728	2.65622	132	0.96404	5	3.62026	137	0.99956
0.0729	2.65490	133	0.96399	5	3.61889	137	0.99956
0.0730	2.65357	132	0.96394	4	3.61752	137	0.99956
0.0731	2.65225	131	0.96390	5	3.61615	137	0.99956
0.0732	2.65094	132	0.96385	5	3.61478	136	0.99955
0.0733	2.64962	131	0.96380	5	3.61342	136	0.99955
0.0734	2.64831	132	0.96375	5	3.61206	136	0.99955
0.0735	2.64699	131	0.96370	5	3.61070	136	0.99955
0.0736	2.64568	130	0.96365	5	3.60934	136	0.99955
0.0737	2.64438	131	0.96360	5	3.60798	136	0.99955
0.0738	2.64307	131	0.96355	4	3.60662	135	0.99955
0.0739	2.64176	130	0.96351	5	3.60527	135	0.99955
0.0740	2.64046	130	0.96346	5	3.60392	135	0.99954
0.0741	2.63916	130	0.96341	5	3.60257	135	0.99954
0.0742	2.63786	130	0.96336	5	3.60122	135	0.99954
0.0743	2.63656	129	0.96331	5	3.59987	134	0.99954
0.0744	2.63527	130	0.96326	5	3.59853	134	0.99954
0.0745	2.63397	129	0.96321	5	3.59719	134	0.99954
0.0746	2.63268	129	0.96316	5	3.59585	134	0.99954
0.0747	2.63139	129	0.96311	4	3.59451	134	0.99954
0.0748	2.63010	128	0.96307	5	3.59317	133	0.99953
0.0749	2.62882	129	0.96302	5	3.59184	134	0.99953
0.0750	2.62753		0.96297		3.59050		0.99953

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0750	2.62753	128	0.96297	5	3.59050	133	0.99953
0.0751	2.62625	128	0.96292	5	3.58917	133	0.99953
0.0752	2.62497	128	0.96287	5	3.58784	133	0.99953
0.0753	2.62369	128	0.96282	5	3.58651	133	0.99953
0.0754	2.62241	127	0.96277	5	3.58518	132	0.99953
0.0755	2.62114	128	0.96272	4	3.58386	132	0.99953
0.0756	2.61986	127	0.96268	5	3.58254	132	0.99952
0.0757	2.61859	127	0.96263	5	3.58122	132	0.99952
0.0758	2.61732	127	0.96258	5	3.57990	132	0.99952
0.0759	2.61605	127	0.96253	5	3.57858	132	0.99952
0.0760	2.61478	126	0.96248	5	3.57726	131	0.99952
0.0761	2.61352	127	0.96243	5	3.57595	131	0.99952
0.0762	2.61225	126	0.96238	4	3.57464	132	0.99952
0.0763	2.61099	126	0.96234	5	3.57332	130	0.99952
0.0764	2.60973	126	0.96229	5	3.57202	131	0.99951
0.0765	2.60847	126	0.96224	5	3.57071	131	0.99951
0.0766	2.60721	125	0.96219	5	3.56940	130	0.99951
0.0767	2.60596	126	0.96214	5	3.56810	130	0.99951
0.0768	2.60470	125	0.96209	5	3.56680	130	0.99951
0.0769	2.60345	125	0.96204	5	3.56550	130	0.99951
0.0770	2.60220	125	0.96199	4	3.56420	130	0.99951
0.0771	2.60095	124	0.96195	5	3.56290	130	0.99950
0.0772	2.59971	125	0.96190	5	3.56160	129	0.99950
0.0773	2.59846	124	0.96185	5	3.56031	129	0.99950
0.0774	2.59722	124	0.96180	5	3.55902	129	0.99950
0.0775	2.59598	124	0.96175	5	3.55773	129	0.99950
0.0776	2.59474	124	0.96170	5	3.55644	129	0.99950
0.0777	2.59350	124	0.96165	5	3.55515	128	0.99950
0.0778	2.59226	123	0.96160	4	3.55387	129	0.99950
0.0779	2.59103	124	0.96156	5	3.55258	128	0.99949
0.0780	2.58979	123	0.96151	5	3.55130	128	0.99949
0.0781	2.58856	123	0.96146	5	3.55002	128	0.99949
0.0782	2.58733	123	0.96141	5	3.54874	128	0.99949
0.0783	2.58610	122	0.96136	5	3.54746	127	0.99949
0.0784	2.58488	123	0.96131	5	3.54619	128	0.99949
0.0785	2.58365	122	0.96126	5	3.54491	127	0.99949
0.0786	2.58243	123	0.96121	4	3.54364	127	0.99949
0.0787	2.58120	122	0.96117	5	3.54237	127	0.99948
0.0788	2.57998	122	0.96112	5	3.54110	127	0.99948
0.0789	2.57876	121	0.96107	5	3.53983	126	0.99948
0.0790	2.57755	122	0.96102	5	3.53857	127	0.99948
0.0791	2.57633	121	0.96097	5	3.53730	126	0.99948
0.0792	2.57512	121	0.96092	5	3.53604	126	0.99948
0.0793	2.57391	122	0.96087	4	3.53478	126	0.99948
0.0794	2.57269	121	0.96083	5	3.53352	126	0.99948
0.0795	2.57148	120	0.96078	5	3.53226	125	0.99947
0.0796	2.57028	121	0.96073	5	3.53101	126	0.99947
0.0797	2.56907	120	0.96068	5	3.52975	125	0.99947
0.0798	2.56787	121	0.96063	5	3.52850	125	0.99947
0.0799	2.56666	120	0.96058	5	3.52725	125	0.99947
0.0800	2.56546		0.96053		3.52600		0.99947

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R
0.0800	2.56546	120	0.96053	5	3.52600	125	0.99947
0.0801	2.56426	120	0.96048	4	3.52475	125	0.99947
0.0802	2.56306	119	0.96044	5	3.52350	125	0.99946
0.0803	2.56187	120	0.96039	5	3.52225	124	0.99946
0.0804	2.56067	119	0.96034	5	3.52101	124	0.99946
0.0805	2.55948	119	0.96029	5	3.51977	124	0.99946
0.0806	2.55829	119	0.96024	5	3.51853	124	0.99946
0.0807	2.55710	119	0.96019	5	3.51729	124	0.99946
0.0808	2.55591	119	0.96014	4	3.51605	124	0.99946
0.0809	2.55472	119	0.96010	5	3.51481	123	0.99945
0.0810	2.55353	118	0.96005	5	3.51358	123	0.99945
0.0811	2.55235	118	0.96000	5	3.51235	124	0.99945
0.0812	2.55117	119	0.95995	5	3.51111	123	0.99945
0.0813	2.54998	118	0.95990	5	3.50988	122	0.99945
0.0814	2.54880	117	0.95985	5	3.50866	123	0.99945
0.0815	2.54763	118	0.95980	5	3.50743	123	0.99945
0.0816	2.54645	118	0.95975	4	3.50620	122	0.99945
0.0817	2.54527	117	0.95971	5	3.50498	122	0.99944
0.0818	2.54410	117	0.95966	5	3.50376	122	0.99944
0.0819	2.54293	117	0.95961	5	3.50254	122	0.99944
0.0820	2.54176	117	0.95956	5	3.50132	122	0.99944
0.0821	2.54059	117	0.95951	5	3.50010	122	0.99944
0.0822	2.53942	117	0.95946	5	3.49888	121	0.99944
0.0823	2.53825	116	0.95941	4	3.49767	122	0.99944
0.0824	2.53709	117	0.95937	5	3.49645	121	0.99943
0.0825	2.53592	116	0.95932	5	3.49524	121	0.99943
0.0826	2.53476	116	0.95927	5	3.49403	121	0.99943
0.0827	2.53360	116	0.95922	5	3.49282	121	0.99943
0.0828	2.53244	116	0.95917	5	3.49161	120	0.99943
0.0829	2.53128	115	0.95912	5	3.49041	121	0.99943
0.0830	2.53013	116	0.95907	4	3.48920	120	0.99943
0.0831	2.52897	115	0.95903	5	3.48800	120	0.99942
0.0832	2.52782	115	0.95898	5	3.48680	120	0.99942
0.0833	2.52667	115	0.95893	5	3.48560	120	0.99942
0.0834	2.52552	115	0.95888	5	3.48440	120	0.99942
0.0835	2.52437	115	0.95883	5	3.48320	120	0.99942
0.0836	2.52322	115	0.95878	5	3.48200	119	0.99942
0.0837	2.52207	114	0.95873	4	3.48081	120	0.99942
0.0838	2.52093	114	0.95869	5	3.47961	119	0.99942
0.0839	2.51979	115	0.95864	5	3.47842	119	0.99941
0.0840	2.51864	114	0.95859	5	3.47723	119	0.99941
0.0841	2.51750	114	0.95854	5	3.47604	118	0.99941
0.0842	2.51636	113	0.95849	5	3.47486	119	0.99941
0.0843	2.51523	114	0.95844	5	3.47367	119	0.99941
0.0844	2.51409	113	0.95839	5	3.47248	118	0.99941
0.0845	2.51296	114	0.95834	4	3.47130	118	0.99941
0.0846	2.51182	113	0.95830	5	3.47012	118	0.99940
0.0847	2.51069	113	0.95825	5	3.46894	118	0.99940
0.0848	2.50956	113	0.95820	5	3.46776	118	0.99940
0.0849	2.50843	113	0.95815	5	3.46658	117	0.99940
0.0850	2.50730		0.95810		3.46541		0.99940

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0 - E_0^0)/RT$	Δ	$(H^0 - E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0850	2.50730	112	0.95810	5	3.46541	118	0.99940
0.0851	2.50618	113	0.95805	5	3.46423	117	0.99940
0.0852	2.50505	112	0.95800	4	3.46306	118	0.99940
0.0853	2.50393	112	0.95796	5	3.46188	117	0.99939
0.0854	2.50281	113	0.95791	5	3.46071	117	0.99939
0.0855	2.50168	112	0.95786	5	3.45954	116	0.99939
0.0856	2.50056	111	0.95781	5	3.45838	117	0.99939
0.0857	2.49945	112	0.95776	5	3.45721	117	0.99939
0.0858	2.49833	112	0.95771	5	3.45604	116	0.99939
0.0859	2.49721	111	0.95766	4	3.45488	116	0.99939
0.0860	2.49610	111	0.95762	5	3.45372	117	0.99938
0.0861	2.49499	111	0.95757	5	3.45255	116	0.99938
0.0862	2.49388	111	0.95752	5	3.45139	115	0.99938
0.0863	2.49277	111	0.95747	5	3.45024	116	0.99938
0.0864	2.49166	111	0.95742	5	3.44908	116	0.99938
0.0865	2.49055	111	0.95737	5	3.44792	115	0.99938
0.0866	2.48944	110	0.95732	4	3.44677	116	0.99938
0.0867	2.48834	111	0.95728	5	3.44561	115	0.99937
0.0868	2.48723	110	0.95723	5	3.44446	115	0.99937
0.0869	2.48613	110	0.95718	5	3.44331	115	0.99937
0.0870	2.48503	110	0.95713	5	3.44216	115	0.99937
0.0871	2.48393	110	0.95708	5	3.44101	114	0.99937
0.0872	2.48283	109	0.95703	4	3.43987	115	0.99937
0.0873	2.48174	110	0.95699	5	3.43872	114	0.99937
0.0874	2.48064	109	0.95694	5	3.43758	114	0.99936
0.0875	2.47955	110	0.95689	5	3.43644	115	0.99936
0.0876	2.47845	109	0.95684	5	3.43529	114	0.99936
0.0877	2.47736	109	0.95679	5	3.43415	114	0.99936
0.0878	2.47627	109	0.95674	5	3.43301	113	0.99936
0.0879	2.47518	108	0.95669	4	3.43188	114	0.99936
0.0880	2.47410	109	0.95665	5	3.43074	113	0.99935
0.0881	2.47301	109	0.95660	5	3.42961	114	0.99935
0.0882	2.47192	108	0.95655	5	3.42847	113	0.99935
0.0883	2.47084	108	0.95650	5	3.42734	113	0.99935
0.0884	2.46976	108	0.95645	5	3.42621	113	0.99935
0.0885	2.46868	108	0.95640	5	3.42508	113	0.99935
0.0886	2.46760	108	0.95635	4	3.42395	113	0.99935
0.0887	2.46652	108	0.95631	5	3.42282	112	0.99934
0.0888	2.46544	108	0.95626	5	3.42170	113	0.99934
0.0889	2.46436	107	0.95621	5	3.42057	112	0.99934
0.0890	2.46329	107	0.95616	5	3.41945	112	0.99934
0.0891	2.46222	108	0.95611	5	3.41833	112	0.99934
0.0892	2.46114	107	0.95606	5	3.41721	112	0.99934
0.0893	2.46007	107	0.95601	4	3.41609	112	0.99934
0.0894	2.45900	107	0.95597	5	3.41497	112	0.99933
0.0895	2.45793	106	0.95592	5	3.41385	112	0.99933
0.0896	2.45687	107	0.95587	5	3.41273	111	0.99933
0.0897	2.45580	107	0.95582	5	3.41162	111	0.99933
0.0898	2.45473	106	0.95577	5	3.41051	112	0.99933
0.0899	2.45367	106	0.95572	4	3.40939	111	0.99933
0.0900	2.45261		0.95568		3.40828		0.99933

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0900	2.45261	106	0.95568	5	3.40828	111	0.99933
0.0901	2.45155	106	0.95563	5	3.40717	111	0.99932
0.0902	2.45049	106	0.95558	5	3.40606	110	0.99932
0.0903	2.44943	106	0.95553	5	3.40496	111	0.99932
0.0904	2.44837	106	0.95548	5	3.40385	110	0.99932
0.0905	2.44731	105	0.95543	5	3.40275	111	0.99932
0.0906	2.44626	105	0.95538	4	3.40164	110	0.99932
0.0907	2.44521	106	0.95534	5	3.40054	110	0.99932
0.0908	2.44415	105	0.95529	5	3.39944	110	0.99931
0.0909	2.44310	105	0.95524	5	3.39834	110	0.99931
0.0910	2.44205	105	0.95519	5	3.39724	110	0.99931
0.0911	2.44100	105	0.95514	5	3.39614	109	0.99931
0.0912	2.43995	104	0.95509	5	3.39505	110	0.99931
0.0913	2.43891	105	0.95504	4	3.39395	109	0.99931
0.0914	2.43786	104	0.95500	5	3.39286	109	0.99930
0.0915	2.43682	105	0.95495	5	3.39177	110	0.99930
0.0916	2.43577	104	0.95490	5	3.39067	109	0.99930
0.0917	2.43473	104	0.95485	5	3.38958	109	0.99930
0.0918	2.43369	104	0.95480	5	3.38849	108	0.99930
0.0919	2.43265	104	0.95475	4	3.38741	109	0.99930
0.0920	2.43161	103	0.95471	5	3.38632	109	0.99930
0.0921	2.43058	104	0.95466	5	3.38523	108	0.99929
0.0922	2.42954	103	0.95461	5	3.38415	108	0.99929
0.0923	2.42851	104	0.95456	5	3.38307	109	0.99929
0.0924	2.42747	103	0.95451	5	3.38198	108	0.99929
0.0925	2.42644	103	0.95446	5	3.38090	108	0.99929
0.0926	2.42541	103	0.95441	4	3.37982	108	0.99929
0.0927	2.42438	103	0.95437	5	3.37875	107	0.99928
0.0928	2.42335	103	0.95432	5	3.37767	108	0.99928
0.0929	2.42232	102	0.95427	5	3.37659	107	0.99928
0.0930	2.42130	103	0.95422	5	3.37552	108	0.99928
0.0931	2.42027	102	0.95417	5	3.37444	107	0.99928
0.0932	2.41925	103	0.95412	4	3.37337	107	0.99928
0.0933	2.41822	102	0.95408	5	3.37230	107	0.99927
0.0934	2.41720	102	0.95403	5	3.37123	107	0.99927
0.0935	2.41618	102	0.95398	5	3.37016	107	0.99927
0.0936	2.41516	102	0.95393	5	3.36909	107	0.99927
0.0937	2.41414	102	0.95388	5	3.36802	106	0.99927
0.0938	2.41312	101	0.95383	5	3.36696	107	0.99927
0.0939	2.41211	102	0.95378	4	3.36589	106	0.99927
0.0940	2.41109	101	0.95374	5	3.36483	106	0.99926
0.0941	2.41008	101	0.95369	5	3.36377	107	0.99926
0.0942	2.40907	102	0.95364	5	3.36270	106	0.99926
0.0943	2.40805	101	0.95359	5	3.36164	105	0.99926
0.0944	2.40704	101	0.95354	5	3.36059	106	0.99926
0.0945	2.40603	101	0.95349	4	3.35953	106	0.99926
0.0946	2.40502	100	0.95345	5	3.35847	106	0.99925
0.0947	2.40402	101	0.95340	5	3.35741	105	0.99925
0.0948	2.40301	100	0.95335	5	3.35636	105	0.99925
0.0949	2.40201	101	0.95330	5	3.35531	106	0.99925
0.0950	2.40100		0.95325		3.35425		0.99925

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.0950	2.40100	100	0.95325	5	3.35425	105	0.99925
0.0951	2.40000	100	0.95320	4	3.35320	105	0.99925
0.0952	2.39900	100	0.95316	5	3.35215	105	0.99925
0.0953	2.39800	100	0.95311	5	3.35110	104	0.99924
0.0954	2.39700	100	0.95306	5	3.35006	105	0.99924
0.0955	2.39600	100	0.95301	5	3.34901	105	0.99924
0.0956	2.39500	99	0.95296	5	3.34796	104	0.99924
0.0957	2.39401	100	0.95291	5	3.34692	105	0.99924
0.0958	2.39301	99	0.95286	4	3.34587	104	0.99924
0.0959	2.39202	100	0.95282	5	3.34483	104	0.99923
0.0960	2.39102	99	0.95277	5	3.34379	104	0.99923
0.0961	2.39003	99	0.95272	5	3.34275	104	0.99923
0.0962	2.38904	99	0.95267	5	3.34171	104	0.99923
0.0963	2.38805	99	0.95262	5	3.34067	103	0.99923
0.0964	2.38706	99	0.95257	4	3.33964	104	0.99923
0.0965	2.38607	98	0.95253	5	3.33860	103	0.99922
0.0966	2.38509	99	0.95248	5	3.33757	104	0.99922
0.0967	2.38410	98	0.95243	5	3.33653	103	0.99922
0.0968	2.38312	99	0.95238	5	3.33550	103	0.99922
0.0969	2.38213	98	0.95233	5	3.33447	103	0.99922
0.0970	2.38115	98	0.95228	4	3.33344	103	0.99922
0.0971	2.38017	98	0.95224	5	3.33241	103	0.99921
0.0972	2.37919	98	0.95219	5	3.33138	103	0.99921
0.0973	2.37821	98	0.95214	5	3.33035	103	0.99921
0.0974	2.37723	97	0.95209	5	3.32932	102	0.99921
0.0975	2.37626	98	0.95204	5	3.32830	103	0.99921
0.0976	2.37528	97	0.95199	4	3.32727	102	0.99921
0.0977	2.37431	98	0.95195	5	3.32625	102	0.99920
0.0978	2.37333	97	0.95190	5	3.32523	102	0.99920
0.0979	2.37236	97	0.95185	5	3.32421	102	0.99920
0.0980	2.37139	97	0.95180	5	3.32319	102	0.99920
0.0981	2.37042	97	0.95175	5	3.32217	102	0.99920
0.0982	2.36945	97	0.95170	4	3.32115	102	0.99920
0.0983	2.36848	97	0.95166	5	3.32013	101	0.99920
0.0984	2.36751	97	0.95161	5	3.31912	102	0.99919
0.0985	2.36654	96	0.95156	5	3.31810	101	0.99919
0.0986	2.36558	97	0.95151	5	3.31709	101	0.99919
0.0987	2.36461	96	0.95146	5	3.31608	102	0.99919
0.0988	2.36365	96	0.95141	5	3.31506	101	0.99919
0.0989	2.36269	96	0.95136	4	3.31405	101	0.99919
0.0990	2.36173	96	0.95132	5	3.31304	101	0.99918
0.0991	2.36077	96	0.95127	5	3.31203	100	0.99918
0.0992	2.35981	96	0.95122	5	3.31103	101	0.99918
0.0993	2.35885	96	0.95117	5	3.31002	101	0.99918
0.0994	2.35789	95	0.95112	4	3.30901	100	0.99918
0.0995	2.35694	96	0.95108	5	3.30801	100	0.99918
0.0996	2.35598	95	0.95103	5	3.30701	101	0.99917
0.0997	2.35503	96	0.95098	5	3.30600	100	0.99917
0.0998	2.35407	95	0.95093	5	3.30500	100	0.99917
0.0999	2.35312	95	0.95088	5	3.30400	100	0.99917
0.1000	2.35217		0.95083		3.30300		0.99917

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1000	2.35217	95	0.95083	5	3.30300	100	0.99917
0.1001	2.35122	95	0.95078	4	3.30200	99	0.99917
0.1002	2.35027	95	0.95074	5	3.30101	100	0.99916
0.1003	2.34932	95	0.95069	5	3.30001	100	0.99916
0.1004	2.34837	94	0.95064	5	3.29901	99	0.99916
0.1005	2.34743	95	0.95059	5	3.29802	100	0.99916
0.1006	2.34648	94	0.95054	5	3.29702	99	0.99916
0.1007	2.34554	95	0.95049	4	3.29603	99	0.99916
0.1008	2.34459	94	0.95045	5	3.29504	99	0.99915
0.1009	2.34365	94	0.95040	5	3.29405	99	0.99915
0.1010	2.34271	94	0.95035	5	3.29306	99	0.99915
0.1011	2.34177	94	0.95030	5	3.29207	99	0.99915
0.1012	2.34083	94	0.95025	4	3.29108	98	0.99915
0.1013	2.33989	94	0.95021	5	3.29010	99	0.99915
0.1014	2.33895	93	0.95016	5	3.28911	98	0.99914
0.1015	2.33802	94	0.95011	5	3.28813	99	0.99914
0.1016	2.33708	93	0.95006	5	3.28714	98	0.99914
0.1017	2.33615	94	0.95001	5	3.28616	98	0.99914
0.1018	2.33521	93	0.94996	4	3.28518	98	0.99914
0.1019	2.33428	93	0.94992	5	3.28420	98	0.99914
0.1020	2.33335	93	0.94987	5	3.28322	98	0.99913
0.1021	2.33242	93	0.94982	5	3.28224	98	0.99913
0.1022	2.33149	93	0.94977	5	3.28126	98	0.99913
0.1023	2.33056	93	0.94972	5	3.28028	97	0.99913
0.1024	2.32963	93	0.94967	4	3.27931	98	0.99913
0.1025	2.32870	92	0.94963	5	3.27833	97	0.99912
0.1026	2.32778	93	0.94958	5	3.27736	98	0.99912
0.1027	2.32685	92	0.94953	5	3.27638	97	0.99912
0.1028	2.32593	92	0.94948	5	3.27541	97	0.99912
0.1029	2.32501	93	0.94943	5	3.27444	97	0.99912
0.1030	2.32408	92	0.94938	4	3.27347	97	0.99912
0.1031	2.32316	92	0.94934	5	3.27250	97	0.99911
0.1032	2.32224	92	0.94929	5	3.27153	97	0.99911
0.1033	2.32132	92	0.94924	5	3.27056	96	0.99911
0.1034	2.32040	91	0.94919	5	3.26960	97	0.99911
0.1035	2.31949	92	0.94914	5	3.26863	97	0.99911
0.1036	2.31857	91	0.94909	4	3.26766	96	0.99911
0.1037	2.31766	92	0.94905	5	3.26670	96	0.99910
0.1038	2.31674	91	0.94900	5	3.26574	96	0.99910
0.1039	2.31583	92	0.94895	5	3.26478	96	0.99910
0.1040	2.31491	91	0.94890	5	3.26382	97	0.99910
0.1041	2.31400	91	0.94885	5	3.26285	95	0.99910
0.1042	2.31309	91	0.94880	4	3.26190	96	0.99910
0.1043	2.31218	91	0.94876	5	3.26094	96	0.99909
0.1044	2.31127	91	0.94871	5	3.25998	96	0.99909
0.1045	2.31036	90	0.94866	5	3.25902	95	0.99909
0.1046	2.30946	91	0.94861	5	3.25807	96	0.99909
0.1047	2.30855	91	0.94856	4	3.25711	95	0.99909
0.1048	2.30764	90	0.94852	5	3.25616	95	0.99909
0.1049	2.30674	90	0.94847	5	3.25521	96	0.99908
0.1050	2.30584		0.94842		3.25425		0.99908

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1050	2.30584	91	0.94842	5	3.25425	95	0.99908
0.1051	2.30493	90	0.94837	5	3.25330	95	0.99908
0.1052	2.30403	90	0.94832	5	3.25235	95	0.99908
0.1053	2.30313	90	0.94827	4	3.25140	94	0.99908
0.1054	2.30223	90	0.94823	5	3.25046	95	0.99907
0.1055	2.30133	90	0.94818	5	3.24951	95	0.99907
0.1056	2.30043	90	0.94813	5	3.24856	94	0.99907
0.1057	2.29953	89	0.94808	5	3.24762	95	0.99907
0.1058	2.29864	90	0.94803	5	3.24667	94	0.99907
0.1059	2.29774	89	0.94798	4	3.24573	95	0.99907
0.1060	2.29685	90	0.94794	5	3.24478	94	0.99906
0.1061	2.29595	89	0.94789	5	3.24384	94	0.99906
0.1062	2.29506	89	0.94784	5	3.24290	94	0.99906
0.1063	2.29417	89	0.94779	5	3.24196	94	0.99906
0.1064	2.29328	89	0.94774	5	3.24102	94	0.99906
0.1065	2.29239	89	0.94769	4	3.24008	93	0.99906
0.1066	2.29150	89	0.94765	5	3.23915	94	0.99905
0.1067	2.29061	89	0.94760	5	3.23821	94	0.99905
0.1068	2.28972	88	0.94755	5	3.23727	93	0.99905
0.1069	2.28884	89	0.94750	5	3.23634	94	0.99905
0.1070	2.28795	89	0.94745	4	3.23540	93	0.99905
0.1071	2.28706	88	0.94741	5	3.23447	93	0.99904
0.1072	2.28618	88	0.94736	5	3.23354	93	0.99904
0.1073	2.28530	89	0.94731	5	3.23261	93	0.99904
0.1074	2.28441	88	0.94726	5	3.23168	93	0.99904
0.1075	2.28353	88	0.94721	5	3.23075	93	0.99904
0.1076	2.28265	88	0.94716	4	3.22982	93	0.99904
0.1077	2.28177	88	0.94712	5	3.22889	93	0.99903
0.1078	2.28089	87	0.94707	5	3.22796	92	0.99903
0.1079	2.28002	88	0.94702	5	3.22704	93	0.99903
0.1080	2.27914	88	0.94697	5	3.22611	92	0.99903
0.1081	2.27826	87	0.94692	4	3.22519	93	0.99903
0.1082	2.27739	88	0.94688	5	3.22426	92	0.99903
0.1083	2.27651	87	0.94683	5	3.22334	92	0.99902
0.1084	2.27564	88	0.94678	5	3.22242	92	0.99902
0.1085	2.27476	87	0.94673	5	3.22150	92	0.99902
0.1086	2.27389	87	0.94668	5	3.22058	92	0.99902
0.1087	2.27302	87	0.94663	4	3.21966	92	0.99902
0.1088	2.27215	87	0.94659	5	3.21874	92	0.99901
0.1089	2.27128	87	0.94654	5	3.21782	92	0.99901
0.1090	2.27041	87	0.94649	5	3.21690	91	0.99901
0.1091	2.26954	86	0.94644	5	3.21599	92	0.99901
0.1092	2.26868	87	0.94639	4	3.21507	91	0.99901
0.1093	2.26781	86	0.94635	5	3.21416	92	0.99901
0.1094	2.26695	87	0.94630	5	3.21324	91	0.99900
0.1095	2.26608	86	0.94625	5	3.21233	91	0.99900
0.1096	2.26522	87	0.94620	5	3.21142	91	0.99900
0.1097	2.26435	86	0.94615	5	3.21051	91	0.99900
0.1098	2.26349	86	0.94610	4	3.20960	91	0.99900
0.1099	2.26263	86	0.94606	5	3.20869	91	0.99899
0.1100	2.26177		0.94601		3.20778		0.99899

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1100	2.26177	86	0.94601	5	3.20778	91	0.99899
0.1101	2.26091	86	0.94596	5	3.20687	91	0.99899
0.1102	2.26005	86	0.94591	5	3.20596	90	0.99899
0.1103	2.25919	85	0.94586	4	3.20506	91	0.99899
0.1104	2.25834	86	0.94582	5	3.20415	90	0.99899
0.1105	2.25748	85	0.94577	5	3.20325	91	0.99898
0.1106	2.25663	86	0.94572	5	3.20234	90	0.99898
0.1107	2.25577	85	0.94567	5	3.20144	90	0.99898
0.1108	2.25492	86	0.94562	5	3.20054	90	0.99898
0.1109	2.25406	85	0.94557	4	3.19964	90	0.99898
0.1110	2.25321	85	0.94553	5	3.19874	90	0.99897
0.1111	2.25236	85	0.94548	5	3.19784	90	0.99897
0.1112	2.25151	85	0.94543	5	3.19694	90	0.99897
0.1113	2.25066	85	0.94538	5	3.19604	89	0.99897
0.1114	2.24981	85	0.94533	4	3.19515	90	0.99897
0.1115	2.24896	84	0.94529	5	3.19425	90	0.99896
0.1116	2.24812	85	0.94524	5	3.19335	89	0.99896
0.1117	2.24727	85	0.94519	5	3.19246	90	0.99896
0.1118	2.24642	84	0.94514	5	3.19156	89	0.99896
0.1119	2.24558	85	0.94509	4	3.19067	89	0.99896
0.1120	2.24473	84	0.94505	5	3.18978	89	0.99896
0.1121	2.24389	84	0.94500	5	3.18889	89	0.99895
0.1122	2.24305	84	0.94495	5	3.18800	89	0.99895
0.1123	2.24221	85	0.94490	5	3.18711	89	0.99895
0.1124	2.24137	84	0.94485	5	3.18622	89	0.99895
0.1125	2.24052	83	0.94480	4	3.18533	89	0.99895
0.1126	2.23969	84	0.94476	5	3.18444	88	0.99894
0.1127	2.23885	84	0.94471	5	3.18356	89	0.99894
0.1128	2.23801	84	0.94466	5	3.18267	89	0.99894
0.1129	2.23717	83	0.94461	5	3.18178	88	0.99894
0.1130	2.23634	84	0.94456	4	3.18090	88	0.99894
0.1131	2.23550	83	0.94452	5	3.18002	89	0.99893
0.1132	2.23467	84	0.94447	5	3.17913	88	0.99893
0.1133	2.23383	83	0.94442	5	3.17825	88	0.99893
0.1134	2.23300	83	0.94437	5	3.17737	88	0.99893
0.1135	2.23217	84	0.94432	4	3.17649	88	0.99893
0.1136	2.23133	83	0.94428	5	3.17561	88	0.99893
0.1137	2.23050	83	0.94423	5	3.17473	88	0.99892
0.1138	2.22967	83	0.94418	5	3.17385	88	0.99892
0.1139	2.22884	82	0.94413	5	3.17297	87	0.99892
0.1140	2.22802	83	0.94408	5	3.17210	88	0.99892
0.1141	2.22719	83	0.94403	4	3.17122	87	0.99892
0.1142	2.22636	83	0.94399	5	3.17035	88	0.99891
0.1143	2.22553	82	0.94394	5	3.16947	87	0.99891
0.1144	2.22471	83	0.94389	5	3.16860	87	0.99891
0.1145	2.22388	82	0.94384	5	3.16773	88	0.99891
0.1146	2.22306	82	0.94379	4	3.16685	87	0.99891
0.1147	2.22224	83	0.94375	5	3.16598	87	0.99890
0.1148	2.22141	82	0.94370	5	3.16511	87	0.99890
0.1149	2.22059	82	0.94365	5	3.16424	87	0.99890
0.1150	2.21977		0.94360		3.16337		0.99890

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1150	2.21977	82	0.94360	5	3.16337	86	0.99890
0.1151	2.21895	82	0.94355	4	3.16251	87	0.99890
0.1152	2.21813	82	0.94351	5	3.16164	87	0.99889
0.1153	2.21731	81	0.94346	5	3.16077	86	0.99889
0.1154	2.21650	82	0.94341	5	3.15991	87	0.99889
0.1155	2.21568	82	0.94336	5	3.15904	86	0.99889
0.1156	2.21486	81	0.94331	4	3.15818	87	0.99889
0.1157	2.21405	82	0.94327	5	3.15731	86	0.99889
0.1158	2.21323	81	0.94322	5	3.15645	86	0.99888
0.1159	2.21242	82	0.94317	5	3.15559	86	0.99888
0.1160	2.21160	81	0.94312	5	3.15473	87	0.99888
0.1161	2.21079	81	0.94307	4	3.15386	85	0.99888
0.1162	2.20998	81	0.94303	5	3.15301	86	0.99888
0.1163	2.20917	81	0.94298	5	3.15215	86	0.99887
0.1164	2.20836	81	0.94293	5	3.15129	86	0.99887
0.1165	2.20755	81	0.94288	5	3.15043	86	0.99887
0.1166	2.20674	81	0.94283	5	3.14957	85	0.99887
0.1167	2.20593	81	0.94278	4	3.14872	86	0.99887
0.1168	2.20512	80	0.94274	5	3.14786	85	0.99886
0.1169	2.20432	81	0.94269	5	3.14701	86	0.99886
0.1170	2.20351	80	0.94264	5	3.14615	85	0.99886
0.1171	2.20271	81	0.94259	5	3.14530	85	0.99886
0.1172	2.20190	80	0.94254	4	3.14445	86	0.99886
0.1173	2.20110	81	0.94250	5	3.14359	85	0.99885
0.1174	2.20029	80	0.94245	5	3.14274	85	0.99885
0.1175	2.19949	80	0.94240	5	3.14189	85	0.99885
0.1176	2.19869	80	0.94235	5	3.14104	85	0.99885
0.1177	2.19789	80	0.94230	4	3.14019	85	0.99885
0.1178	2.19709	80	0.94226	5	3.13934	84	0.99884
0.1179	2.19629	80	0.94221	5	3.13850	85	0.99884
0.1180	2.19549	80	0.94216	5	3.13765	85	0.99884
0.1181	2.19469	79	0.94211	5	3.13680	84	0.99884
0.1182	2.19390	80	0.94206	4	3.13596	85	0.99884
0.1183	2.19310	80	0.94202	5	3.13511	84	0.99883
0.1184	2.19230	79	0.94197	5	3.13427	84	0.99883
0.1185	2.19151	80	0.94192	5	3.13343	85	0.99883
0.1186	2.19071	79	0.94187	5	3.13258	84	0.99883
0.1187	2.18992	79	0.94182	4	3.13174	84	0.99883
0.1188	2.18913	80	0.94178	5	3.13090	84	0.99882
0.1189	2.18833	79	0.94173	5	3.13006	84	0.99882
0.1190	2.18754	79	0.94168	5	3.12922	84	0.99882
0.1191	2.18675	79	0.94163	5	3.12838	84	0.99882
0.1192	2.18596	79	0.94158	4	3.12754	83	0.99882
0.1193	2.18517	79	0.94154	5	3.12671	84	0.99881
0.1194	2.18438	79	0.94149	5	3.12587	84	0.99881
0.1195	2.18359	78	0.94144	5	3.12503	83	0.99881
0.1196	2.18281	79	0.94139	5	3.12420	84	0.99881
0.1197	2.18202	79	0.94134	4	3.12336	83	0.99881
0.1198	2.18123	78	0.94130	5	3.12253	83	0.99881
0.1199	2.18045	79	0.94125	5	3.12170	84	0.99880
0.1200	2.17966		0.94120		3.12086		0.99880

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1200	2.17966	78	0.94120	5	3.12086	83	0.99880
0.1201	2.17888	78	0.94115	5	3.12003	83	0.99880
0.1202	2.17810	79	0.94110	4	3.11920	83	0.99880
0.1203	2.17731	78	0.94106	5	3.11837	83	0.99879
0.1204	2.17653	78	0.94101	5	3.11754	83	0.99879
0.1205	2.17575	78	0.94096	5	3.11671	83	0.99879
0.1206	2.17497	78	0.94091	5	3.11588	83	0.99879
0.1207	2.17419	78	0.94086	4	3.11505	82	0.99879
0.1208	2.17341	78	0.94082	5	3.11423	83	0.99878
0.1209	2.17263	78	0.94077	5	3.11340	83	0.99878
0.1210	2.17185	77	0.94072	5	3.11257	82	0.99878
0.1211	2.17108	78	0.94067	5	3.11175	83	0.99878
0.1212	2.17030	77	0.94062	4	3.11092	82	0.99878
0.1213	2.16953	78	0.94058	5	3.11010	82	0.99877
0.1214	2.16875	77	0.94053	5	3.10928	82	0.99877
0.1215	2.16798	78	0.94048	5	3.10846	83	0.99877
0.1216	2.16720	77	0.94043	5	3.10763	82	0.99877
0.1217	2.16643	77	0.94038	4	3.10681	82	0.99877
0.1218	2.16566	77	0.94034	5	3.10599	82	0.99876
0.1219	2.16489	78	0.94029	5	3.10517	82	0.99876
0.1220	2.16411	77	0.94024	5	3.10435	81	0.99876
0.1221	2.16334	77	0.94019	5	3.10354	82	0.99876
0.1222	2.16257	76	0.94014	4	3.10272	82	0.99876
0.1223	2.16181	77	0.94010	5	3.10190	81	0.99875
0.1224	2.16104	77	0.94005	5	3.10109	82	0.99875
0.1225	2.16027	77	0.94000	5	3.10027	82	0.99875
0.1226	2.15950	76	0.93995	5	3.09945	81	0.99875
0.1227	2.15874	77	0.93990	4	3.09864	81	0.99875
0.1228	2.15797	76	0.93986	5	3.09783	82	0.99874
0.1229	2.15721	77	0.93981	5	3.09701	81	0.99874
0.1230	2.15644	76	0.93976	5	3.09620	81	0.99874
0.1231	2.15568	77	0.93971	5	3.09539	81	0.99874
0.1232	2.15491	76	0.93966	4	3.09458	81	0.99874
0.1233	2.15415	76	0.93962	5	3.09377	81	0.99873
0.1234	2.15339	76	0.93957	5	3.09296	81	0.99873
0.1235	2.15263	76	0.93952	5	3.09215	81	0.99873
0.1236	2.15187	76	0.93947	5	3.09134	81	0.99873
0.1237	2.15111	76	0.93942	4	3.09053	80	0.99873
0.1238	2.15035	76	0.93938	5	3.08973	81	0.99872
0.1239	2.14959	76	0.93933	5	3.08892	81	0.99872
0.1240	2.14883	75	0.93928	5	3.08811	80	0.99872
0.1241	2.14808	76	0.93923	4	3.08731	81	0.99872
0.1242	2.14732	76	0.93919	5	3.08650	80	0.99872
0.1243	2.14656	75	0.93914	5	3.08570	80	0.99871
0.1244	2.14581	76	0.93909	5	3.08490	80	0.99871
0.1245	2.14505	75	0.93904	5	3.08410	81	0.99871
0.1246	2.14430	75	0.93899	4	3.08329	80	0.99871
0.1247	2.14355	76	0.93895	5	3.08249	80	0.99871
0.1248	2.14279	75	0.93890	5	3.08169	80	0.99870
0.1249	2.14204	75	0.93885	5	3.08089	80	0.99870
0.1250	2.14129		0.93880		3.08009		0.99870

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R
0.1250	2.14129	75	0.93880	5	3.08009	80	0.99870
0.1251	2.14054	75	0.93875	4	3.07929	79	0.99870
0.1252	2.13979	75	0.93871	5	3.07850	80	0.99869
0.1253	2.13904	75	0.93866	5	3.07770	80	0.99869
0.1254	2.13829	75	0.93861	5	3.07690	79	0.99869
0.1255	2.13754	74	0.93856	5	3.07611	80	0.99869
0.1256	2.13680	75	0.93851	4	3.07531	79	0.99869
0.1257	2.13605	75	0.93847	5	3.07452	80	0.99868
0.1258	2.13530	74	0.93842	5	3.07372	79	0.99868
0.1259	2.13456	75	0.93837	5	3.07293	80	0.99868
0.1260	2.13381	74	0.93832	5	3.07213	79	0.99868
0.1261	2.13307	75	0.93827	4	3.07134	79	0.99868
0.1262	2.13232	74	0.93823	5	3.07055	79	0.99867
0.1263	2.13158	74	0.93818	5	3.06976	79	0.99867
0.1264	2.13084	74	0.93813	5	3.06897	79	0.99867
0.1265	2.13010	75	0.93808	4	3.06818	79	0.99867
0.1266	2.12936	74	0.93804	5	3.06739	79	0.99867
0.1267	2.12861	74	0.93799	5	3.06660	79	0.99866
0.1268	2.12787	73	0.93794	5	3.06581	78	0.99866
0.1269	2.12714	74	0.93789	5	3.06503	79	0.99866
0.1270	2.12640	74	0.93784	4	3.06424	79	0.99866
0.1271	2.12566	74	0.93780	5	3.06345	78	0.99865
0.1272	2.12492	74	0.93775	5	3.06267	79	0.99865
0.1273	2.12418	73	0.93770	5	3.06188	78	0.99865
0.1274	2.12345	74	0.93765	5	3.06110	78	0.99865
0.1275	2.12271	73	0.93760	4	3.06032	79	0.99865
0.1276	2.12198	74	0.93756	5	3.05953	78	0.99864
0.1277	2.12124	73	0.93751	5	3.05875	78	0.99864
0.1278	2.12051	73	0.93746	5	3.05797	78	0.99864
0.1279	2.11978	74	0.93741	5	3.05719	78	0.99864
0.1280	2.11904	73	0.93736	4	3.05641	78	0.99864
0.1281	2.11831	73	0.93732	5	3.05563	78	0.99863
0.1282	2.11758	73	0.93727	5	3.05485	78	0.99863
0.1283	2.11685	73	0.93722	5	3.05407	78	0.99863
0.1284	2.11612	73	0.93717	4	3.05329	78	0.99863
0.1285	2.11539	73	0.93713	5	3.05251	77	0.99863
0.1286	2.11466	73	0.93708	5	3.05174	78	0.99862
0.1287	2.11393	73	0.93703	5	3.05096	77	0.99862
0.1288	2.11320	72	0.93698	5	3.05019	78	0.99862
0.1289	2.11248	73	0.93693	4	3.04941	77	0.99862
0.1290	2.11175	73	0.93689	5	3.04864	78	0.99861
0.1291	2.11102	72	0.93684	5	3.04786	77	0.99861
0.1292	2.11030	73	0.93679	5	3.04709	77	0.99861
0.1293	2.10957	72	0.93674	5	3.04632	78	0.99861
0.1294	2.10885	72	0.93669	4	3.04554	77	0.99861
0.1295	2.10813	73	0.93665	5	3.04477	77	0.99860
0.1296	2.10740	72	0.93660	5	3.04400	77	0.99860
0.1297	2.10668	72	0.93655	5	3.04323	77	0.99860
0.1298	2.10596	72	0.93650	4	3.04246	77	0.99860
0.1299	2.10524	72	0.93646	5	3.04169	77	0.99860
0.1300	2.10452		0.93641		3.04092		0.99859

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1300	2.10452	72	0.93641	5	3.04092	76	0.99859
0.1301	2.10380	72	0.93636	5	3.04016	77	0.99859
0.1302	2.10308	72	0.93631	5	3.03939	77	0.99859
0.1303	2.10236	72	0.93626	4	3.03862	76	0.99859
0.1304	2.10164	72	0.93622	5	3.03786	77	0.99858
0.1305	2.10092	71	0.93617	5	3.03709	76	0.99858
0.1306	2.10021	72	0.93612	5	3.03633	77	0.99858
0.1307	2.09949	72	0.93607	4	3.03556	76	0.99858
0.1308	2.09877	71	0.93603	5	3.03480	76	0.99858
0.1309	2.09806	72	0.93598	5	3.03404	77	0.99857
0.1310	2.09734	71	0.93593	5	3.03327	76	0.99857
0.1311	2.09663	71	0.93588	5	3.03251	76	0.99857
0.1312	2.09592	72	0.93583	4	3.03175	76	0.99857
0.1313	2.09520	71	0.93579	5	3.03099	76	0.99856
0.1314	2.09449	71	0.93574	5	3.03023	76	0.99856
0.1315	2.09378	71	0.93569	5	3.02947	76	0.99856
0.1316	2.09307	71	0.93564	4	3.02871	76	0.99856
0.1317	2.09236	71	0.93560	5	3.02795	76	0.99856
0.1318	2.09165	71	0.93555	5	3.02719	75	0.99855
0.1319	2.09094	71	0.93550	5	3.02644	76	0.99855
0.1320	2.09023	71	0.93545	5	3.02568	76	0.99855
0.1321	2.08952	71	0.93540	4	3.02492	75	0.99855
0.1322	2.08881	71	0.93536	5	3.02417	76	0.99855
0.1323	2.08810	70	0.93531	5	3.02341	75	0.99854
0.1324	2.08740	71	0.93526	5	3.02266	76	0.99854
0.1325	2.08669	70	0.93521	5	3.02190	75	0.99854
0.1326	2.08599	71	0.93516	4	3.02115	75	0.99854
0.1327	2.08528	70	0.93512	5	3.02040	75	0.99853
0.1328	2.08458	71	0.93507	5	3.01965	76	0.99853
0.1329	2.08387	70	0.93502	5	3.01889	75	0.99853
0.1330	2.08317	70	0.93497	4	3.01814	75	0.99853
0.1331	2.08247	71	0.93493	5	3.01739	75	0.99853
0.1332	2.08176	70	0.93488	5	3.01664	75	0.99852
0.1333	2.08106	70	0.93483	5	3.01589	75	0.99852
0.1334	2.08036	70	0.93478	5	3.01514	74	0.99852
0.1335	2.07966	70	0.93473	4	3.01440	75	0.99852
0.1336	2.07896	70	0.93469	5	3.01365	75	0.99851
0.1337	2.07826	70	0.93464	5	3.01290	75	0.99851
0.1338	2.07756	69	0.93459	5	3.01215	74	0.99851
0.1339	2.07687	70	0.93454	4	3.01141	75	0.99851
0.1340	2.07617	70	0.93450	5	3.01066	74	0.99851
0.1341	2.07547	70	0.93445	5	3.00992	75	0.99850
0.1342	2.07477	69	0.93440	5	3.00917	74	0.99850
0.1343	2.07408	70	0.93435	5	3.00843	74	0.99850
0.1344	2.07338	69	0.93430	4	3.00769	75	0.99850
0.1345	2.07269	70	0.93426	5	3.00694	74	0.99849
0.1346	2.07199	69	0.93421	5	3.00620	74	0.99849
0.1347	2.07130	69	0.93416	5	3.00546	74	0.99849
0.1348	2.07061	70	0.93411	4	3.00472	74	0.99849
0.1349	2.06991	69	0.93407	5	3.00398	74	0.99848
0.1350	2.06922		0.93402		3.00324		0.99848

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1350	2.06922	69	0.93402	5	3.00324	74	0.99848
0.1351	2.06853	69	0.93397	5	3.00250	74	0.99848
0.1352	2.06784	69	0.93392	4	3.00176	74	0.99848
0.1353	2.06715	69	0.93388	5	3.00102	73	0.99848
0.1354	2.06646	69	0.93383	5	3.00029	74	0.99847
0.1355	2.06577	69	0.93378	5	2.99955	74	0.99847
0.1356	2.06508	69	0.93373	5	2.99881	73	0.99847
0.1357	2.06439	69	0.93368	4	2.99808	74	0.99847
0.1358	2.06370	68	0.93364	5	2.99734	73	0.99846
0.1359	2.06302	69	0.93359	5	2.99661	74	0.99846
0.1360	2.06233	69	0.93354	5	2.99587	73	0.99846
0.1361	2.06164	68	0.93349	4	2.99514	74	0.99846
0.1362	2.06096	69	0.93345	5	2.99440	73	0.99846
0.1363	2.06027	68	0.93340	5	2.99367	73	0.99845
0.1364	2.05959	69	0.93335	5	2.99294	73	0.99845
0.1365	2.05890	68	0.93330	5	2.99221	73	0.99845
0.1366	2.05822	68	0.93325	4	2.99148	74	0.99845
0.1367	2.05754	68	0.93321	5	2.99074	73	0.99844
0.1368	2.05686	69	0.93316	5	2.99001	72	0.99844
0.1369	2.05617	68	0.93311	5	2.98929	73	0.99844
0.1370	2.05549	68	0.93306	4	2.98856	73	0.99844
0.1371	2.05481	68	0.93302	5	2.98783	73	0.99844
0.1372	2.05413	68	0.93297	5	2.98710	73	0.99843
0.1373	2.05345	68	0.93292	5	2.98637	72	0.99843
0.1374	2.05277	68	0.93287	4	2.98565	73	0.99843
0.1375	2.05209	67	0.93283	5	2.98492	73	0.99843
0.1376	2.05142	68	0.93278	5	2.98419	72	0.99842
0.1377	2.05074	68	0.93273	5	2.98347	73	0.99842
0.1378	2.05006	68	0.93268	5	2.98274	72	0.99842
0.1379	2.04938	67	0.93263	4	2.98202	73	0.99842
0.1380	2.04871	68	0.93259	5	2.98129	72	0.99841
0.1381	2.04803	67	0.93254	5	2.98057	72	0.99841
0.1382	2.04736	68	0.93249	5	2.97985	72	0.99841
0.1383	2.04668	67	0.93244	4	2.97913	72	0.99841
0.1384	2.04601	67	0.93240	5	2.97841	73	0.99841
0.1385	2.04534	68	0.93235	5	2.97768	72	0.99840
0.1386	2.04466	67	0.93230	5	2.97696	72	0.99840
0.1387	2.04399	67	0.93225	5	2.97624	72	0.99840
0.1388	2.04332	67	0.93220	4	2.97552	72	0.99840
0.1389	2.04265	67	0.93216	5	2.97480	71	0.99839
0.1390	2.04198	67	0.93211	5	2.97409	72	0.99839
0.1391	2.04131	67	0.93206	5	2.97337	72	0.99839
0.1392	2.04064	67	0.93201	4	2.97265	72	0.99839
0.1393	2.03997	67	0.93197	5	2.97193	71	0.99838
0.1394	2.03930	67	0.93192	5	2.97122	72	0.99838
0.1395	2.03863	67	0.93187	5	2.97050	71	0.99838
0.1396	2.03796	67	0.93182	4	2.96979	72	0.99838
0.1397	2.03729	66	0.93178	5	2.96907	71	0.99838
0.1398	2.03663	67	0.93173	5	2.96836	72	0.99837
0.1399	2.03596	66	0.93168	5	2.96764	71	0.99837
0.1400	2.03530		0.93163		2.96693		0.99837

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1400	2.03530	67	0.93163	4	2.96693	71	0.99837
0.1401	2.03463	66	0.93159	5	2.96622	72	0.99837
0.1402	2.03397	67	0.93154	5	2.96550	71	0.99836
0.1403	2.03330	66	0.93149	5	2.96479	71	0.99836
0.1404	2.03264	66	0.93144	5	2.96408	71	0.99836
0.1405	2.03198	67	0.93139	4	2.96337	71	0.99836
0.1406	2.03131	66	0.93135	5	2.96266	71	0.99835
0.1407	2.03065	66	0.93130	5	2.96195	71	0.99835
0.1408	2.02999	66	0.93125	5	2.96124	71	0.99835
0.1409	2.02933	66	0.93120	4	2.96053	71	0.99835
0.1410	2.02867	66	0.93116	5	2.95982	70	0.99835
0.1411	2.02801	66	0.93111	5	2.95912	71	0.99834
0.1412	2.02735	66	0.93106	5	2.95841	71	0.99834
0.1413	2.02669	66	0.93101	4	2.95770	70	0.99834
0.1414	2.02603	66	0.93097	5	2.95700	71	0.99834
0.1415	2.02537	66	0.93092	5	2.95629	71	0.99833
0.1416	2.02471	65	0.93087	5	2.95558	70	0.99833
0.1417	2.02406	66	0.93082	4	2.95488	70	0.99833
0.1418	2.02340	66	0.93078	5	2.95418	71	0.99833
0.1419	2.02274	65	0.93073	5	2.95347	70	0.99832
0.1420	2.02209	66	0.93068	5	2.95277	70	0.99832
0.1421	2.02143	65	0.93063	5	2.95207	71	0.99832
0.1422	2.02078	66	0.93058	4	2.95136	70	0.99832
0.1423	2.02012	65	0.93054	5	2.95066	70	0.99831
0.1424	2.01947	65	0.93049	5	2.94996	70	0.99831
0.1425	2.01882	66	0.93044	5	2.94926	70	0.99831
0.1426	2.01816	65	0.93039	4	2.94856	70	0.99831
0.1427	2.01751	65	0.93035	5	2.94786	70	0.99830
0.1428	2.01686	65	0.93030	5	2.94716	70	0.99830
0.1429	2.01621	65	0.93025	5	2.94646	70	0.99830
0.1430	2.01556	65	0.93020	4	2.94576	70	0.99830
0.1431	2.01491	65	0.93016	5	2.94506	69	0.99830
0.1432	2.01426	65	0.93011	5	2.94437	70	0.99829
0.1433	2.01361	65	0.93006	5	2.94367	70	0.99829
0.1434	2.01296	65	0.93001	4	2.94297	69	0.99829
0.1435	2.01231	65	0.92997	5	2.94228	70	0.99829
0.1436	2.01166	64	0.92992	5	2.94158	69	0.99828
0.1437	2.01102	65	0.92987	5	2.94089	70	0.99828
0.1438	2.01037	65	0.92982	4	2.94019	69	0.99828
0.1439	2.00972	64	0.92978	5	2.93950	69	0.99828
0.1440	2.00908	65	0.92973	5	2.93881	70	0.99827
0.1441	2.00843	64	0.92968	5	2.93811	69	0.99827
0.1442	2.00779	65	0.92963	5	2.93742	69	0.99827
0.1443	2.00714	64	0.92958	4	2.93673	69	0.99827
0.1444	2.00650	64	0.92954	5	2.93604	69	0.99826
0.1445	2.00586	65	0.92949	5	2.93535	70	0.99826
0.1446	2.00521	64	0.92944	5	2.93465	69	0.99826
0.1447	2.00457	64	0.92939	4	2.93396	68	0.99826
0.1448	2.00393	64	0.92935	5	2.93328	69	0.99825
0.1449	2.00329	64	0.92930	5	2.93259	69	0.99825
0.1450	2.00265		0.92925		2.93190		0.99825

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R
0.1450	2.00265	65	0.92925	5	2.93190	69	0.99825
0.1451	2.00200	64	0.92920	4	2.93121	69	0.99825
0.1452	2.00136	63	0.92916	5	2.93052	69	0.99824
0.1453	2.00073	64	0.92911	5	2.92983	68	0.99824
0.1454	2.00009	64	0.92906	5	2.92915	69	0.99824
0.1455	1.99945	64	0.92901	4	2.92846	69	0.99824
0.1456	1.99881	64	0.92897	5	2.92777	68	0.99824
0.1457	1.99817	64	0.92892	5	2.92709	69	0.99823
0.1458	1.99753	63	0.92887	5	2.92640	68	0.99823
0.1459	1.99690	64	0.92882	4	2.92572	68	0.99823
0.1460	1.99626	64	0.92878	5	2.92504	69	0.99823
0.1461	1.99562	63	0.92873	5	2.92435	68	0.99822
0.1462	1.99499	64	0.92868	5	2.92367	68	0.99822
0.1463	1.99435	63	0.92863	4	2.92299	68	0.99822
0.1464	1.99372	63	0.92859	5	2.92231	69	0.99822
0.1465	1.99309	64	0.92854	5	2.92162	68	0.99821
0.1466	1.99245	63	0.92849	5	2.92094	68	0.99821
0.1467	1.99182	63	0.92844	4	2.92026	68	0.99821
0.1468	1.99119	64	0.92840	5	2.91958	68	0.99821
0.1469	1.99055	63	0.92835	5	2.91890	68	0.99820
0.1470	1.98992	63	0.92830	5	2.91822	68	0.99820
0.1471	1.98929	63	0.92825	5	2.91754	67	0.99820
0.1472	1.98866	63	0.92820	4	2.91687	68	0.99820
0.1473	1.98803	63	0.92816	5	2.91619	68	0.99819
0.1474	1.98740	63	0.92811	5	2.91551	68	0.99819
0.1475	1.98677	63	0.92806	5	2.91483	67	0.99819
0.1476	1.98614	63	0.92801	4	2.91416	68	0.99819
0.1477	1.98551	62	0.92797	5	2.91348	68	0.99818
0.1478	1.98489	63	0.92792	5	2.91280	67	0.99818
0.1479	1.98426	63	0.92787	5	2.91213	67	0.99818
0.1480	1.98363	63	0.92782	4	2.91146	68	0.99818
0.1481	1.98300	62	0.92778	5	2.91078	67	0.99817
0.1482	1.98238	63	0.92773	5	2.91011	68	0.99817
0.1483	1.98175	62	0.92768	5	2.90943	67	0.99817
0.1484	1.98113	63	0.92763	4	2.90876	67	0.99817
0.1485	1.98050	62	0.92759	5	2.90809	67	0.99816
0.1486	1.97988	63	0.92754	5	2.90742	67	0.99816
0.1487	1.97925	62	0.92749	5	2.90675	68	0.99816
0.1488	1.97863	62	0.92744	4	2.90607	67	0.99816
0.1489	1.97801	63	0.92740	5	2.90540	67	0.99815
0.1490	1.97738	62	0.92735	5	2.90473	67	0.99815
0.1491	1.97676	62	0.92730	5	2.90406	67	0.99815
0.1492	1.97614	62	0.92725	4	2.90339	66	0.99815
0.1493	1.97552	62	0.92721	5	2.90273	67	0.99814
0.1494	1.97490	62	0.92716	5	2.90206	67	0.99814
0.1495	1.97428	62	0.92711	5	2.90139	67	0.99814
0.1496	1.97366	62	0.92706	4	2.90072	66	0.99814
0.1497	1.97304	62	0.92702	5	2.90006	67	0.99813
0.1498	1.97242	62	0.92697	5	2.89939	67	0.99813
0.1499	1.97180	62	0.92692	5	2.89872	66	0.99813
0.1500	1.97118		0.92687		2.89806		0.99813

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R	Δ
0.150	1.97118	615	0.92687	47	2.89806	664	0.99813	3
0.151	1.96503	612	0.92640	48	2.89142	658	0.99810	2
0.152	1.95891	607	0.92592	47	2.88484	655	0.99808	3
0.153	1.95284	603	0.92545	47	2.87829	650	0.99805	2
0.154	1.94681	598	0.92498	48	2.87179	646	0.99803	3
0.155	1.94083	594	0.92450	47	2.86533	642	0.99800	3
0.156	1.93489	591	0.92403	48	2.85891	637	0.99797	2
0.157	1.92898	586	0.92355	47	2.85254	634	0.99795	3
0.158	1.92312	582	0.92308	47	2.84620	630	0.99792	2
0.159	1.91730	579	0.92261	48	2.83990	625	0.99790	3
0.160	1.91151	574	0.92213	47	2.83365	622	0.99787	3
0.161	1.90577	570	0.92166	47	2.82743	618	0.99784	2
0.162	1.90007	567	0.92119	48	2.82125	614	0.99782	3
0.163	1.89440	563	0.92071	47	2.81511	610	0.99779	3
0.164	1.88877	559	0.92024	47	2.80901	607	0.99776	3
0.165	1.88318	556	0.91977	47	2.80294	603	0.99773	2
0.166	1.87762	552	0.91930	48	2.79691	599	0.99771	3
0.167	1.87210	548	0.91882	47	2.79092	595	0.99768	3
0.168	1.86662	545	0.91835	47	2.78497	592	0.99765	3
0.169	1.86117	542	0.91788	47	2.77905	589	0.99762	2
0.170	1.85575	538	0.91741	47	2.77316	585	0.99760	3
0.171	1.85037	534	0.91694	48	2.76731	582	0.99757	3
0.172	1.84503	531	0.91646	47	2.76149	578	0.99754	3
0.173	1.83972	528	0.91599	47	2.75571	575	0.99751	3
0.174	1.83444	525	0.91552	47	2.74996	572	0.99748	3
0.175	1.82919	521	0.91505	47	2.74424	568	0.99745	3
0.176	1.82398	518	0.91458	47	2.73856	565	0.99742	3
0.177	1.81880	515	0.91411	47	2.73291	562	0.99739	3
0.178	1.81365	512	0.91364	47	2.72729	559	0.99736	3
0.179	1.80853	508	0.91317	47	2.72170	555	0.99733	3
0.180	1.80345	506	0.91270	47	2.71615	553	0.99730	3
0.181	1.79839	502	0.91223	47	2.71062	549	0.99727	3
0.182	1.79337	500	0.91176	47	2.70513	547	0.99724	3
0.183	1.78837	496	0.91129	47	2.69966	543	0.99721	3
0.184	1.78341	494	0.91082	47	2.69423	541	0.99718	3
0.185	1.77847	490	0.91035	47	2.68882	537	0.99715	3
0.186	1.77357	488	0.90988	47	2.68345	535	0.99712	3
0.187	1.76869	485	0.90941	47	2.67810	532	0.99709	3
0.188	1.76384	482	0.90894	46	2.67278	528	0.99706	3
0.189	1.75902	479	0.90848	47	2.66750	527	0.99703	3
0.190	1.75423	477	0.90801	47	2.66223	523	0.99700	3
0.191	1.74946	474	0.90754	47	2.65700	521	0.99697	4
0.192	1.74472	471	0.90707	47	2.65179	517	0.99693	3
0.193	1.74001	468	0.90660	47	2.64662	516	0.99690	3
0.194	1.73533	466	0.90613	46	2.64146	512	0.99687	3
0.195	1.73067	463	0.90567	47	2.63634	510	0.99684	4
0.196	1.72604	460	0.90520	47	2.63124	507	0.99680	3
0.197	1.72144	458	0.90473	47	2.62617	505	0.99677	3
0.198	1.71686	456	0.90426	46	2.62112	502	0.99674	3
0.199	1.71230	453	0.90380	47	2.61610	500	0.99671	4
0.200	1.70777		0.90333		2.61110		0.99667	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.200	1.70777	450	0.90333	47	2.61110	497	0.99667	3
0.201	1.70327	448	0.90286	46	2.60613	494	0.99664	3
0.202	1.69879	446	0.90240	47	2.60119	493	0.99661	4
0.203	1.69433	443	0.90193	46	2.59626	489	0.99657	3
0.204	1.68990	441	0.90147	47	2.59137	488	0.99654	3
0.205	1.68549	438	0.90100	47	2.58649	484	0.99651	4
0.206	1.68111	436	0.90053	46	2.58165	483	0.99647	3
0.207	1.67675	433	0.90007	47	2.57682	480	0.99644	4
0.208	1.67242	432	0.89960	46	2.57202	478	0.99640	3
0.209	1.66810	429	0.89914	47	2.56724	476	0.99637	4
0.210	1.66381	427	0.89867	46	2.56248	473	0.99633	3
0.211	1.65954	424	0.89821	47	2.55775	471	0.99630	4
0.212	1.65530	423	0.89774	46	2.55304	469	0.99626	3
0.213	1.65107	420	0.89728	47	2.54835	466	0.99623	4
0.214	1.64687	418	0.89681	46	2.54369	465	0.99619	3
0.215	1.64269	416	0.89635	47	2.53904	462	0.99616	4
0.216	1.63853	413	0.89588	46	2.53442	460	0.99612	3
0.217	1.63440	412	0.89542	46	2.52982	458	0.99609	4
0.218	1.63028	409	0.89496	47	2.52524	456	0.99605	4
0.219	1.62619	408	0.89449	46	2.52068	454	0.99601	3
0.220	1.62211	405	0.89403	46	2.51614	451	0.99598	4
0.221	1.61806	403	0.89357	47	2.51163	450	0.99594	4
0.222	1.61403	402	0.89310	46	2.50713	448	0.99590	3
0.223	1.61001	399	0.89264	46	2.50265	445	0.99587	4
0.224	1.60602	397	0.89218	46	2.49820	444	0.99583	4
0.225	1.60205	396	0.89172	47	2.49376	441	0.99579	4
0.226	1.59809	393	0.89125	46	2.48935	440	0.99575	3
0.227	1.59416	392	0.89079	46	2.48495	438	0.99572	4
0.228	1.59024	389	0.89033	46	2.48057	435	0.99568	4
0.229	1.58635	388	0.88987	47	2.47622	434	0.99564	4
0.230	1.58247	385	0.88940	46	2.47188	432	0.99560	3
0.231	1.57862	384	0.88894	46	2.46756	430	0.99557	4
0.232	1.57478	382	0.88848	46	2.46326	428	0.99553	4
0.233	1.57096	381	0.88802	46	2.45898	427	0.99549	4
0.234	1.56715	378	0.88756	46	2.45471	424	0.99545	4
0.235	1.56337	377	0.88710	46	2.45047	423	0.99541	4
0.236	1.55960	374	0.88664	46	2.44624	421	0.99537	4
0.237	1.55586	373	0.88618	46	2.44203	419	0.99533	4
0.238	1.55213	372	0.88572	46	2.43784	417	0.99529	4
0.239	1.54841	369	0.88526	46	2.43367	416	0.99525	4
0.240	1.54472	368	0.88480	46	2.42951	414	0.99521	4
0.241	1.54104	366	0.88434	46	2.42537	412	0.99517	4
0.242	1.53738	365	0.88388	46	2.42125	410	0.99513	4
0.243	1.53373	362	0.88342	46	2.41715	409	0.99509	4
0.244	1.53011	361	0.88296	46	2.41306	407	0.99505	4
0.245	1.52650	360	0.88250	46	2.40899	405	0.99501	4
0.246	1.52290	357	0.88204	46	2.40494	403	0.99497	4
0.247	1.51933	356	0.88158	46	2.40091	402	0.99493	4
0.248	1.51577	355	0.88112	46	2.39689	401	0.99489	4
0.249	1.51222	353	0.88066	46	2.39288	399	0.99485	4
0.250	1.50869		0.88020		2.38889		0.99481	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = h\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.250	1.50869	351	0.88020	46	2.38889	397	0.99481	4
0.251	1.50518	350	0.87974	45	2.38492	395	0.99477	5
0.252	1.50168	348	0.87929	46	2.38097	394	0.99472	4
0.253	1.49820	347	0.87883	46	2.37703	393	0.99468	4
0.254	1.49473	345	0.87837	46	2.37310	390	0.99464	4
0.255	1.49128	343	0.87791	45	2.36920	390	0.99460	4
0.256	1.48785	342	0.87746	46	2.36530	387	0.99456	5
0.257	1.48443	341	0.87700	46	2.36143	387	0.99451	4
0.258	1.48102	339	0.87654	46	2.35756	384	0.99447	4
0.259	1.47763	337	0.87608	45	2.35372	383	0.99443	4
0.260	1.47426	336	0.87563	46	2.34989	382	0.99439	5
0.261	1.47090	335	0.87517	46	2.34607	380	0.99434	4
0.262	1.46755	333	0.87471	45	2.34227	379	0.99430	4
0.263	1.46422	332	0.87426	46	2.33848	377	0.99426	5
0.264	1.46090	330	0.87380	45	2.33471	376	0.99421	4
0.265	1.45760	329	0.87335	46	2.33095	375	0.99417	5
0.266	1.45431	327	0.87289	46	2.32720	373	0.99412	4
0.267	1.45104	326	0.87243	45	2.32347	371	0.99408	4
0.268	1.44778	325	0.87198	46	2.31976	371	0.99404	5
0.269	1.44453	323	0.87152	45	2.31605	368	0.99399	4
0.270	1.44130	322	0.87107	46	2.31237	368	0.99395	5
0.271	1.43808	321	0.87061	45	2.30869	366	0.99390	4
0.272	1.43487	319	0.87016	46	2.30503	365	0.99386	5
0.273	1.43168	318	0.86970	45	2.30138	363	0.99381	4
0.274	1.42850	316	0.86925	46	2.29775	362	0.99377	5
0.275	1.42534	316	0.86879	45	2.29413	361	0.99372	4
0.276	1.42218	314	0.86834	45	2.29052	359	0.99368	5
0.277	1.41904	312	0.86789	46	2.28693	358	0.99363	5
0.278	1.41592	312	0.86743	45	2.28335	357	0.99358	4
0.279	1.41280	310	0.86698	46	2.27978	355	0.99354	5
0.280	1.40970	309	0.86652	45	2.27623	355	0.99349	4
0.281	1.40661	307	0.86607	45	2.27268	352	0.99345	5
0.282	1.40354	307	0.86562	45	2.26916	352	0.99340	5
0.283	1.40047	305	0.86517	46	2.26564	351	0.99335	4
0.284	1.39742	304	0.86471	45	2.26213	349	0.99331	5
0.285	1.39438	302	0.86426	45	2.25864	348	0.99326	5
0.286	1.39136	302	0.86381	46	2.25516	346	0.99321	5
0.287	1.38834	300	0.86335	45	2.25170	346	0.99316	4
0.288	1.38534	299	0.86290	45	2.24824	344	0.99312	5
0.289	1.38235	298	0.86245	45	2.24480	343	0.99307	5
0.290	1.37937	296	0.86200	45	2.24137	342	0.99302	5
0.291	1.37641	296	0.86155	45	2.23795	340	0.99297	5
0.292	1.37345	294	0.86110	46	2.23455	340	0.99292	4
0.293	1.37051	293	0.86064	45	2.23115	338	0.99288	5
0.294	1.36758	292	0.86019	45	2.22777	337	0.99283	5
0.295	1.36466	291	0.85974	45	2.22440	336	0.99278	5
0.296	1.36175	290	0.85929	45	2.22104	335	0.99273	5
0.297	1.35885	289	0.85884	45	2.21769	334	0.99268	5
0.298	1.35596	287	0.85839	45	2.21435	332	0.99263	5
0.299	1.35309	286	0.85794	45	2.21103	332	0.99258	5
0.300	1.35023		0.85749		2.20771		0.99253	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.300	1.35023	286	0.85749	45	2.20771	330	0.99253	5
0.301	1.34737	284	0.85704	45	2.20441	329	0.99248	5
0.302	1.34453	283	0.85659	45	2.20112	328	0.99243	5
0.303	1.34170	282	0.85614	45	2.19784	327	0.99238	5
0.304	1.33888	281	0.85569	45	2.19457	326	0.99233	5
0.305	1.33607	280	0.85524	45	2.19131	325	0.99228	5
0.306	1.33327	279	0.85479	45	2.18806	323	0.99223	5
0.307	1.33048	277	0.85434	45	2.18483	323	0.99218	5
0.308	1.32771	277	0.85389	45	2.18160	322	0.99213	5
0.309	1.32494	276	0.85344	44	2.17838	320	0.99208	5
0.310	1.32218	274	0.85300	45	2.17518	320	0.99203	5
0.311	1.31944	274	0.85255	45	2.17198	318	0.99198	5
0.312	1.31670	273	0.85210	45	2.16880	318	0.99193	5
0.313	1.31397	271	0.85165	45	2.16562	316	0.99188	6
0.314	1.31126	271	0.85120	44	2.16246	315	0.99182	5
0.315	1.30855	269	0.85076	45	2.15931	315	0.99177	5
0.316	1.30586	269	0.85031	45	2.15616	313	0.99172	5
0.317	1.30317	268	0.84986	45	2.15303	312	0.99167	5
0.318	1.30049	266	0.84941	44	2.14991	312	0.99162	6
0.319	1.29783	266	0.84897	45	2.14679	310	0.99156	5
0.320	1.29517	265	0.84852	45	2.14369	309	0.99151	5
0.321	1.29252	263	0.84807	44	2.14060	309	0.99146	6
0.322	1.28989	263	0.84763	45	2.13751	307	0.99140	5
0.323	1.28726	262	0.84718	45	2.13444	307	0.99135	5
0.324	1.28464	261	0.84673	44	2.13137	305	0.99130	6
0.325	1.28203	260	0.84629	45	2.12832	305	0.99124	5
0.326	1.27943	259	0.84584	45	2.12527	303	0.99119	5
0.327	1.27684	258	0.84539	44	2.12224	303	0.99114	6
0.328	1.27426	257	0.84495	45	2.11921	301	0.99108	5
0.329	1.27169	256	0.84450	44	2.11620	301	0.99103	6
0.330	1.26913	255	0.84406	45	2.11319	300	0.99097	5
0.331	1.26658	255	0.84361	44	2.11019	299	0.99092	5
0.332	1.26403	253	0.84317	45	2.10720	298	0.99087	6
0.333	1.26150	253	0.84272	44	2.10422	297	0.99081	5
0.334	1.25897	252	0.84228	45	2.10125	296	0.99076	6
0.335	1.25645	251	0.84183	44	2.09829	296	0.99070	6
0.336	1.25394	250	0.84139	44	2.09533	294	0.99064	5
0.337	1.25144	249	0.84095	45	2.09239	293	0.99059	6
0.338	1.24895	248	0.84050	44	2.08946	293	0.99053	5
0.339	1.24647	247	0.84006	45	2.08653	292	0.99048	6
0.340	1.24400	247	0.83961	44	2.08361	291	0.99042	5
0.341	1.24153	245	0.83917	44	2.08070	290	0.99037	6
0.342	1.23908	245	0.83873	45	2.07780	289	0.99031	6
0.343	1.23663	244	0.83828	44	2.07491	288	0.99025	5
0.344	1.23419	243	0.83784	44	2.07203	287	0.99020	6
0.345	1.23176	243	0.83740	44	2.06916	287	0.99014	6
0.346	1.22933	241	0.83696	45	2.06629	286	0.99008	5
0.347	1.22692	241	0.83651	44	2.06343	285	0.99003	6
0.348	1.22451	240	0.83607	44	2.06058	284	0.98997	6
0.349	1.22211	239	0.83563	44	2.05774	283	0.98991	6
0.350	1.21972		0.83519		2.05491		0.98985	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.350	1.21972	238	0.83519	44	2.05491	282	0.98985	5
0.351	1.21734	237	0.83475	45	2.05209	282	0.98980	6
0.352	1.21497	237	0.83430	44	2.04927	281	0.98974	6
0.353	1.21260	236	0.83386	44	2.04646	280	0.98968	6
0.354	1.21024	235	0.83342	44	2.04366	279	0.98962	6
0.355	1.20789	234	0.83298	44	2.04087	278	0.98956	5
0.356	1.20555	234	0.83254	44	2.03809	278	0.98951	6
0.357	1.20321	232	0.83210	44	2.03531	276	0.98945	6
0.358	1.20089	232	0.83166	44	2.03255	276	0.98939	6
0.359	1.19857	231	0.83122	44	2.02979	276	0.98933	6
0.360	1.19626	231	0.83078	44	2.02703	274	0.98927	6
0.361	1.19395	229	0.83034	44	2.02429	274	0.98921	6
0.362	1.19166	229	0.82990	44	2.02155	273	0.98915	6
0.363	1.18937	228	0.82946	44	2.01882	272	0.98909	6
0.364	1.18709	228	0.82902	44	2.01610	271	0.98903	6
0.365	1.18481	226	0.82858	44	2.01339	271	0.98897	6
0.366	1.18255	226	0.82814	44	2.01068	269	0.98891	6
0.367	1.18029	225	0.82770	44	2.00799	269	0.98885	6
0.368	1.17804	225	0.82726	44	2.00530	269	0.98879	6
0.369	1.17579	224	0.82682	44	2.00261	267	0.98873	6
0.370	1.17355	223	0.82638	44	1.99994	267	0.98867	6
0.371	1.17132	222	0.82594	43	1.99727	266	0.98861	6
0.372	1.16910	221	0.82551	44	1.99461	266	0.98855	6
0.373	1.16689	221	0.82507	44	1.99195	264	0.98849	7
0.374	1.16468	220	0.82463	44	1.98931	264	0.98842	6
0.375	1.16248	220	0.82419	44	1.98667	263	0.98836	6
0.376	1.16028	218	0.82375	43	1.98404	263	0.98830	6
0.377	1.15810	219	0.82332	44	1.98141	262	0.98824	6
0.378	1.15591	217	0.82288	44	1.97879	261	0.98818	6
0.379	1.15374	217	0.82244	44	1.97618	260	0.98812	7
0.380	1.15157	216	0.82200	43	1.97358	260	0.98805	6
0.381	1.14941	215	0.82157	44	1.97098	259	0.98799	6
0.382	1.14726	214	0.82113	44	1.96839	258	0.98793	6
0.383	1.14512	214	0.82069	43	1.96581	258	0.98787	7
0.384	1.14298	214	0.82026	44	1.96323	256	0.98780	6
0.385	1.14084	212	0.81982	43	1.96067	257	0.98774	6
0.386	1.13872	212	0.81939	44	1.95810	255	0.98768	7
0.387	1.13660	211	0.81895	44	1.95555	255	0.98761	6
0.388	1.13449	211	0.81851	43	1.95300	254	0.98755	7
0.389	1.13238	210	0.81808	44	1.95046	254	0.98748	6
0.390	1.13028	209	0.81764	43	1.94792	253	0.98742	6
0.391	1.12819	209	0.81721	44	1.94539	252	0.98736	7
0.392	1.12610	208	0.81677	43	1.94287	251	0.98729	6
0.393	1.12402	208	0.81634	44	1.94036	251	0.98723	7
0.394	1.12194	206	0.81590	43	1.93785	250	0.98716	6
0.395	1.11988	206	0.81547	44	1.93535	250	0.98710	7
0.396	1.11782	206	0.81503	43	1.93285	249	0.98703	6
0.397	1.11576	205	0.81460	43	1.93036	248	0.98697	7
0.398	1.11371	204	0.81417	44	1.92788	248	0.98690	6
0.399	1.11167	204	0.81373	43	1.92540	247	0.98684	7
0.400	1.10963		0.81330		1.92293		0.98677	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.400	1.10963	203	0.81330	44	1.92293	246	0.98677	6
0.401	1.10760	202	0.81286	43	1.92047	246	0.98671	7
0.402	1.10558	202	0.81243	43	1.91801	245	0.98664	6
0.403	1.10356	201	0.81200	44	1.91556	245	0.98658	7
0.404	1.10155	201	0.81156	43	1.91311	244	0.98651	7
0.405	1.09954	200	0.81113	43	1.91067	243	0.98644	6
0.406	1.09754	199	0.81070	43	1.90824	242	0.98638	7
0.407	1.09555	199	0.81027	44	1.90582	242	0.98631	7
0.408	1.09356	198	0.80983	43	1.90340	242	0.98624	6
0.409	1.09158	198	0.80940	43	1.90098	241	0.98618	7
0.410	1.08960	197	0.80897	43	1.89857	240	0.98611	7
0.411	1.08763	196	0.80854	43	1.89617	240	0.98604	7
0.412	1.08567	196	0.80811	44	1.89377	239	0.98597	6
0.413	1.08371	195	0.80767	43	1.89138	238	0.98591	7
0.414	1.08176	195	0.80724	43	1.88900	238	0.98584	7
0.415	1.07981	194	0.80681	43	1.88662	237	0.98577	7
0.416	1.07787	194	0.80638	43	1.88425	237	0.98570	7
0.417	1.07593	193	0.80595	43	1.88188	236	0.98563	6
0.418	1.07400	192	0.80552	43	1.87952	235	0.98557	7
0.419	1.07208	192	0.80509	43	1.87717	235	0.98550	7
0.420	1.07016	191	0.80466	43	1.87482	235	0.98543	7
0.421	1.06825	191	0.80423	43	1.87247	233	0.98536	7
0.422	1.06634	190	0.80380	43	1.87014	233	0.98529	7
0.423	1.06444	190	0.80337	43	1.86781	233	0.98522	7
0.424	1.06254	189	0.80294	43	1.86548	232	0.98515	7
0.425	1.06065	188	0.80251	43	1.86316	232	0.98508	7
0.426	1.05877	188	0.80208	43	1.86084	231	0.98501	7
0.427	1.05689	188	0.80165	43	1.85853	230	0.98494	7
0.428	1.05501	187	0.80122	43	1.85623	230	0.98487	7
0.429	1.05314	186	0.80079	43	1.85393	229	0.98480	7
0.430	1.05128	186	0.80036	43	1.85164	229	0.98473	7
0.431	1.04942	185	0.79993	43	1.84935	228	0.98466	7
0.432	1.04757	185	0.79950	42	1.84707	228	0.98459	7
0.433	1.04572	185	0.79908	43	1.84479	227	0.98452	7
0.434	1.04387	183	0.79865	43	1.84252	226	0.98445	7
0.435	1.04204	184	0.79822	43	1.84026	226	0.98438	7
0.436	1.04020	182	0.79779	43	1.83800	226	0.98431	7
0.437	1.03838	182	0.79736	42	1.83574	225	0.98424	7
0.438	1.03656	182	0.79694	43	1.83349	224	0.98417	8
0.439	1.03474	181	0.79651	43	1.83125	224	0.98409	7
0.440	1.03293	181	0.79608	43	1.82901	224	0.98402	7
0.441	1.03112	180	0.79565	42	1.82677	222	0.98395	7
0.442	1.02932	180	0.79523	43	1.82455	223	0.98388	7
0.443	1.02752	179	0.79480	43	1.82232	222	0.98381	8
0.444	1.02573	179	0.79437	42	1.82010	221	0.98373	7
0.445	1.02394	178	0.79395	43	1.81789	221	0.98366	7
0.446	1.02216	177	0.79352	42	1.81568	220	0.98359	8
0.447	1.02039	178	0.79310	43	1.81348	220	0.98351	7
0.448	1.01861	176	0.79267	43	1.81128	219	0.98344	7
0.449	1.01685	177	0.79224	42	1.80909	219	0.98337	8
0.450	1.01508		0.79182		1.80690		0.98329	

Table I / Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.450	1.01508	175	0.79182	43	1.80690	218	0.98329	7
0.451	1.01333	176	0.79139	42	1.80472	218	0.98322	7
0.452	1.01157	174	0.79097	43	1.80254	217	0.98315	8
0.453	1.00983	175	0.79054	42	1.80037	217	0.98307	7
0.454	1.00808	173	0.79012	43	1.79820	216	0.98300	7
0.455	1.00635	174	0.78969	42	1.79604	216	0.98293	8
0.456	1.00461	173	0.78927	43	1.79388	215	0.98285	7
0.457	1.00288	172	0.78884	42	1.79173	215	0.98278	8
0.458	1.00116	172	0.78842	42	1.78958	214	0.98270	7
0.459	0.99944	171	0.78800	43	1.78744	214	0.98263	8
0.460	0.99773	171	0.78757	42	1.78530	213	0.98255	7
0.461	0.99602	171	0.78715	43	1.78317	213	0.98248	8
0.462	0.99431	170	0.78672	42	1.78104	213	0.98240	7
0.463	0.99261	169	0.78630	42	1.77891	212	0.98233	8
0.464	0.99092	170	0.78588	43	1.77679	211	0.98225	8
0.465	0.98922	168	0.78545	42	1.77468	211	0.98217	7
0.466	0.98754	168	0.78503	42	1.77257	211	0.98210	8
0.467	0.98586	168	0.78461	42	1.77046	210	0.98202	7
0.468	0.98418	168	0.78419	43	1.76836	209	0.98195	8
0.469	0.98250	166	0.78376	42	1.76627	209	0.98187	8
0.470	0.98084	167	0.78334	42	1.76418	209	0.98179	7
0.471	0.97917	166	0.78292	42	1.76209	208	0.98172	8
0.472	0.97751	165	0.78250	43	1.76001	208	0.98164	8
0.473	0.97586	166	0.78207	42	1.75793	207	0.98156	7
0.474	0.97420	164	0.78165	42	1.75586	207	0.98149	8
0.475	0.97256	165	0.78123	42	1.75379	207	0.98141	8
0.476	0.97091	163	0.78081	42	1.75172	205	0.98133	8
0.477	0.96928	164	0.78039	42	1.74967	206	0.98125	7
0.478	0.96764	163	0.77997	42	1.74761	205	0.98118	8
0.479	0.96601	162	0.77955	42	1.74556	205	0.98110	8
0.480	0.96439	162	0.77913	42	1.74351	204	0.98102	8
0.481	0.96277	162	0.77871	42	1.74147	203	0.98094	8
0.482	0.96115	161	0.77829	42	1.73944	204	0.98086	8
0.483	0.95954	161	0.77787	42	1.73740	203	0.98078	7
0.484	0.95793	161	0.77745	42	1.73537	202	0.98071	8
0.485	0.95632	160	0.77703	42	1.73335	202	0.98063	8
0.486	0.95472	159	0.77661	42	1.73133	202	0.98055	8
0.487	0.95313	159	0.77619	42	1.72931	201	0.98047	8
0.488	0.95154	159	0.77577	42	1.72730	200	0.98039	8
0.489	0.94995	158	0.77535	42	1.72530	201	0.98031	8
0.490	0.94837	158	0.77493	42	1.72329	199	0.98023	8
0.491	0.94679	158	0.77451	42	1.72130	200	0.98015	8
0.492	0.94521	157	0.77409	42	1.71930	199	0.98007	8
0.493	0.94364	157	0.77367	42	1.71731	198	0.97999	8
0.494	0.94207	156	0.77325	41	1.71533	199	0.97991	8
0.495	0.94051	156	0.77284	42	1.71334	197	0.97983	8
0.496	0.93895	156	0.77242	42	1.71137	198	0.97975	8
0.497	0.93739	155	0.77200	42	1.70939	197	0.97967	8
0.498	0.93584	154	0.77158	42	1.70742	196	0.97959	8
0.499	0.93430	155	0.77116	41	1.70546	196	0.97951	9
0.500	0.93275		0.77075		1.70350		0.97942	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.500	0.93275	154	0.77075	42	1.70350	196	0.97942	8
0.501	0.93121	153	0.77033	42	1.70154	195	0.97934	8
0.502	0.92968	153	0.76991	41	1.69959	195	0.97926	8
0.503	0.92815	153	0.76950	42	1.69764	194	0.97918	8
0.504	0.92662	153	0.76908	42	1.69570	194	0.97910	8
0.505	0.92509	152	0.76866	41	1.69376	194	0.97902	9
0.506	0.92357	151	0.76825	42	1.69182	193	0.97893	8
0.507	0.92206	152	0.76783	42	1.68989	193	0.97885	8
0.508	0.92054	150	0.76741	41	1.68796	193	0.97877	8
0.509	0.91904	151	0.76700	42	1.68603	192	0.97869	9
0.510	0.91753	150	0.76658	41	1.68411	191	0.97860	8
0.511	0.91603	150	0.76617	42	1.68220	192	0.97852	8
0.512	0.91453	149	0.76575	41	1.68028	191	0.97844	9
0.513	0.91304	149	0.76534	42	1.67837	190	0.97835	8
0.514	0.91155	149	0.76492	42	1.67647	190	0.97827	8
0.515	0.91006	148	0.76450	41	1.67457	190	0.97819	9
0.516	0.90858	148	0.76409	41	1.67267	189	0.97810	8
0.517	0.90710	148	0.76368	42	1.67078	189	0.97802	8
0.518	0.90562	147	0.76326	41	1.66889	189	0.97794	9
0.519	0.90415	146	0.76285	42	1.66700	188	0.97785	8
0.520	0.90269	147	0.76243	41	1.66512	188	0.97777	9
0.521	0.90122	146	0.76202	42	1.66324	188	0.97768	8
0.522	0.89976	146	0.76160	41	1.66136	187	0.97760	9
0.523	0.89830	145	0.76119	41	1.65949	186	0.97751	8
0.524	0.89685	145	0.76078	42	1.65763	187	0.97743	9
0.525	0.89540	145	0.76036	41	1.65576	186	0.97734	8
0.526	0.89395	144	0.75995	41	1.65390	185	0.97726	9
0.527	0.89251	144	0.75954	42	1.65205	186	0.97717	8
0.528	0.89107	144	0.75912	41	1.65019	184	0.97709	9
0.529	0.88963	143	0.75871	41	1.64835	185	0.97700	8
0.530	0.88820	143	0.75830	41	1.64650	184	0.97692	9
0.531	0.88677	142	0.75789	42	1.64466	184	0.97683	9
0.532	0.88535	143	0.75747	41	1.64282	183	0.97674	8
0.533	0.88392	141	0.75706	41	1.64099	183	0.97666	9
0.534	0.88251	142	0.75665	41	1.63916	183	0.97657	8
0.535	0.88109	141	0.75624	41	1.63733	182	0.97649	9
0.536	0.87968	141	0.75583	41	1.63551	182	0.97640	9
0.537	0.87827	140	0.75542	42	1.63369	182	0.97631	9
0.538	0.87687	141	0.75500	41	1.63187	181	0.97622	8
0.539	0.87546	139	0.75459	41	1.63006	181	0.97614	9
0.540	0.87407	140	0.75418	41	1.62825	181	0.97605	9
0.541	0.87267	139	0.75377	41	1.62644	180	0.97596	8
0.542	0.87128	139	0.75336	41	1.62464	180	0.97588	9
0.543	0.86989	138	0.75295	41	1.62284	179	0.97579	9
0.544	0.86851	139	0.75254	41	1.62105	180	0.97570	9
0.545	0.86712	137	0.75213	41	1.61925	178	0.97561	9
0.546	0.86575	138	0.75172	41	1.61747	179	0.97552	9
0.547	0.86437	137	0.75131	41	1.61568	178	0.97543	8
0.548	0.86300	137	0.75090	41	1.61390	178	0.97535	9
0.549	0.86163	137	0.75049	41	1.61212	177	0.97526	9
0.550	0.86026		0.75008		1.61035		0.97517	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.550	0.86026	136	0.75008	41	1.61035	177	0.97517	9
0.551	0.85890	136	0.74967	41	1.60858	177	0.97508	9
0.552	0.85754	135	0.74926	40	1.60681	177	0.97499	9
0.553	0.85619	136	0.74886	41	1.60504	176	0.97490	9
0.554	0.85483	134	0.74845	41	1.60328	176	0.97481	9
0.555	0.85349	135	0.74804	41	1.60152	175	0.97472	9
0.556	0.85214	134	0.74763	41	1.59977	175	0.97463	9
0.557	0.85080	134	0.74722	41	1.59802	175	0.97454	9
0.558	0.84946	134	0.74681	40	1.59627	175	0.97445	9
0.559	0.84812	133	0.74641	41	1.59452	174	0.97436	9
0.560	0.84679	133	0.74600	41	1.59278	173	0.97427	9
0.561	0.84546	133	0.74559	41	1.59105	174	0.97418	9
0.562	0.84413	133	0.74518	40	1.58931	173	0.97409	9
0.563	0.84280	132	0.74478	41	1.58758	173	0.97400	9
0.564	0.84148	132	0.74437	41	1.58585	172	0.97391	9
0.565	0.84016	131	0.74396	41	1.58413	173	0.97382	9
0.566	0.83885	131	0.74355	40	1.58240	172	0.97373	10
0.567	0.83754	131	0.74315	41	1.58068	171	0.97363	9
0.568	0.83623	131	0.74274	40	1.57897	171	0.97354	9
0.569	0.83492	130	0.74234	41	1.57726	171	0.97345	9
0.570	0.83362	130	0.74193	41	1.57555	171	0.97336	9
0.571	0.83232	130	0.74152	40	1.57384	170	0.97327	10
0.572	0.83102	129	0.74112	41	1.57214	170	0.97317	9
0.573	0.82973	129	0.74071	40	1.57044	170	0.97308	9
0.574	0.82844	129	0.74031	41	1.56874	169	0.97299	9
0.575	0.82715	129	0.73990	40	1.56705	169	0.97290	10
0.576	0.82586	128	0.73950	41	1.56536	169	0.97280	9
0.577	0.82458	128	0.73909	40	1.56367	168	0.97271	9
0.578	0.82330	128	0.73869	41	1.56199	168	0.97262	9
0.579	0.82202	127	0.73828	40	1.56031	168	0.97253	10
0.580	0.82075	127	0.73788	41	1.55863	168	0.97243	9
0.581	0.81948	127	0.73747	40	1.55695	167	0.97234	10
0.582	0.81821	126	0.73707	41	1.55528	167	0.97224	9
0.583	0.81695	127	0.73666	40	1.55361	167	0.97215	9
0.584	0.81568	126	0.73626	40	1.55194	166	0.97206	10
0.585	0.81442	125	0.73586	41	1.55028	166	0.97196	9
0.586	0.81317	126	0.73545	40	1.54862	166	0.97187	10
0.587	0.81191	125	0.73505	40	1.54696	165	0.97177	9
0.588	0.81066	124	0.73465	41	1.54531	165	0.97168	10
0.589	0.80942	125	0.73424	40	1.54366	165	0.97158	9
0.590	0.80817	124	0.73384	40	1.54201	164	0.97149	10
0.591	0.80693	124	0.73344	40	1.54037	165	0.97139	9
0.592	0.80569	124	0.73304	41	1.53872	163	0.97130	10
0.593	0.80445	123	0.73263	40	1.53709	164	0.97120	9
0.594	0.80322	123	0.73223	40	1.53545	163	0.97111	10
0.595	0.80199	123	0.73183	40	1.53382	163	0.97101	9
0.596	0.80076	123	0.73143	40	1.53219	163	0.97092	10
0.597	0.79953	122	0.73103	41	1.53056	163	0.97082	10
0.598	0.79831	122	0.73062	40	1.52893	162	0.97072	9
0.599	0.79709	122	0.73022	40	1.52731	162	0.97063	10
0.600	0.79587		0.72982		1.52569		0.97053	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.600	0.79587	121	0.72982	40	1.52569	161	0.97053	9
0.601	0.79466	122	0.72942	40	1.52408	162	0.97044	10
0.602	0.79344	121	0.72902	40	1.52246	161	0.97034	10
0.603	0.79223	120	0.72862	40	1.52085	161	0.97024	9
0.604	0.79103	121	0.72822	40	1.51924	160	0.97015	10
0.605	0.78982	120	0.72782	40	1.51764	160	0.97005	10
0.606	0.78862	120	0.72742	40	1.51604	160	0.96995	10
0.607	0.78742	120	0.72702	40	1.51444	160	0.96985	9
0.608	0.78622	119	0.72662	40	1.51284	159	0.96976	10
0.609	0.78503	119	0.72622	40	1.51125	159	0.96966	10
0.610	0.78384	119	0.72582	40	1.50966	159	0.96956	10
0.611	0.78265	118	0.72542	40	1.50807	159	0.96946	10
0.612	0.78147	119	0.72502	40	1.50648	158	0.96936	9
0.613	0.78028	118	0.72462	40	1.50490	158	0.96927	10
0.614	0.77910	118	0.72422	40	1.50332	158	0.96917	10
0.615	0.77792	117	0.72382	40	1.50174	157	0.96907	10
0.616	0.77675	118	0.72342	40	1.50017	157	0.96897	10
0.617	0.77557	117	0.72302	39	1.49860	157	0.96887	10
0.618	0.77440	116	0.72263	40	1.49703	157	0.96877	10
0.619	0.77324	117	0.72223	40	1.49546	156	0.96867	10
0.620	0.77207	116	0.72183	40	1.49390	156	0.96857	10
0.621	0.77091	116	0.72143	40	1.49234	156	0.96847	10
0.622	0.76975	116	0.72103	39	1.49078	155	0.96837	10
0.623	0.76859	116	0.72064	40	1.48923	156	0.96827	10
0.624	0.76743	115	0.72024	40	1.48767	155	0.96817	10
0.625	0.76628	115	0.71984	40	1.48612	155	0.96807	10
0.626	0.76513	115	0.71944	39	1.48457	154	0.96797	10
0.627	0.76398	114	0.71905	40	1.48303	154	0.96787	10
0.628	0.76284	115	0.71865	40	1.48149	154	0.96777	10
0.629	0.76169	114	0.71825	39	1.47995	154	0.96767	10
0.630	0.76055	114	0.71786	40	1.47841	153	0.96757	10
0.631	0.75941	113	0.71746	39	1.47688	154	0.96747	10
0.632	0.75828	114	0.71707	40	1.47534	153	0.96737	10
0.633	0.75714	113	0.71667	40	1.47381	152	0.96727	10
0.634	0.75601	112	0.71627	39	1.47229	153	0.96717	11
0.635	0.75489	113	0.71588	40	1.47076	152	0.96706	10
0.636	0.75376	112	0.71548	39	1.46924	152	0.96696	10
0.637	0.75264	113	0.71509	40	1.46772	151	0.96686	10
0.638	0.75151	112	0.71469	39	1.46621	152	0.96676	10
0.639	0.75039	111	0.71430	40	1.46469	151	0.96666	11
0.640	0.74928	112	0.71390	39	1.46318	151	0.96655	10
0.641	0.74816	111	0.71351	40	1.46167	150	0.96645	10
0.642	0.74705	111	0.71311	39	1.46017	151	0.96635	10
0.643	0.74594	110	0.71272	40	1.45866	150	0.96625	11
0.644	0.74484	111	0.71232	39	1.45716	150	0.96614	10
0.645	0.74373	110	0.71193	39	1.45566	150	0.96604	10
0.646	0.74263	110	0.71154	40	1.45416	149	0.96594	11
0.647	0.74153	110	0.71114	39	1.45267	149	0.96583	10
0.648	0.74043	110	0.71075	39	1.45118	149	0.96573	10
0.649	0.73933	109	0.71036	40	1.44969	149	0.96563	11
0.650	0.73824		0.70996		1.44820		0.96552	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.650	0.73824	109	0.70996	39	1.44820	148	0.96552	10
0.651	0.73715	109	0.70957	39	1.44672	148	0.96542	10
0.652	0.73606	109	0.70918	40	1.44524	148	0.96532	11
0.653	0.73497	108	0.70878	39	1.44376	148	0.96521	10
0.654	0.73389	108	0.70839	39	1.44228	147	0.96511	11
0.655	0.73281	108	0.70800	39	1.44081	148	0.96500	10
0.656	0.73173	108	0.70761	40	1.43933	147	0.96490	11
0.657	0.73065	108	0.70721	39	1.43786	146	0.96479	10
0.658	0.72957	107	0.70682	39	1.43640	147	0.96469	11
0.659	0.72850	107	0.70643	39	1.43493	146	0.96458	10
0.660	0.72743	107	0.70604	39	1.43347	146	0.96448	11
0.661	0.72636	106	0.70565	39	1.43201	146	0.96437	10
0.662	0.72530	107	0.70526	39	1.43055	145	0.96427	11
0.663	0.72423	106	0.70487	40	1.42910	146	0.96416	11
0.664	0.72317	106	0.70447	39	1.42764	145	0.96405	10
0.665	0.72211	106	0.70408	39	1.42619	145	0.96395	11
0.666	0.72105	105	0.70369	39	1.42474	144	0.96384	10
0.667	0.72000	106	0.70330	39	1.42330	145	0.96374	11
0.668	0.71894	105	0.70291	39	1.42185	144	0.96363	11
0.669	0.71789	105	0.70252	39	1.42041	144	0.96352	10
0.670	0.71684	104	0.70213	39	1.41897	143	0.96342	11
0.671	0.71580	105	0.70174	39	1.41754	144	0.96331	11
0.672	0.71475	104	0.70135	39	1.41610	143	0.96320	10
0.673	0.71371	104	0.70096	39	1.41467	143	0.96310	11
0.674	0.71267	104	0.70057	39	1.41324	143	0.96299	11
0.675	0.71163	104	0.70018	39	1.41181	142	0.96288	11
0.676	0.71059	103	0.69979	38	1.41039	143	0.96277	10
0.677	0.70956	103	0.69941	39	1.40896	142	0.96267	11
0.678	0.70853	103	0.69902	39	1.40754	141	0.96256	11
0.679	0.70750	103	0.69863	39	1.40613	142	0.96245	11
0.680	0.70647	103	0.69824	39	1.40471	142	0.96234	11
0.681	0.70544	102	0.69785	39	1.40329	141	0.96223	11
0.682	0.70442	102	0.69746	38	1.40188	141	0.96212	10
0.683	0.70340	102	0.69708	39	1.40047	140	0.96202	11
0.684	0.70238	102	0.69669	39	1.39907	141	0.96191	11
0.685	0.70136	101	0.69630	39	1.39766	140	0.96180	11
0.686	0.70035	102	0.69591	39	1.39626	140	0.96169	11
0.687	0.69933	101	0.69552	38	1.39486	140	0.96158	11
0.688	0.69832	101	0.69514	39	1.39346	140	0.96147	11
0.689	0.69731	101	0.69475	39	1.39206	139	0.96136	11
0.690	0.69630	100	0.69436	38	1.39067	139	0.96125	11
0.691	0.69530	100	0.69398	39	1.38928	139	0.96114	11
0.692	0.69430	101	0.69359	39	1.38789	139	0.96103	11
0.693	0.69329	99	0.69320	38	1.38650	139	0.96092	11
0.694	0.69230	100	0.69282	39	1.38511	138	0.96081	11
0.695	0.69130	100	0.69243	38	1.38373	138	0.96070	11
0.696	0.69030	99	0.69205	39	1.38235	138	0.96059	11
0.697	0.68931	99	0.69166	39	1.38097	138	0.96048	11
0.698	0.68832	99	0.69127	38	1.37959	137	0.96037	11
0.699	0.68733	99	0.69089	39	1.37822	138	0.96026	11
0.700	0.68634		0.69050		1.37684		0.96015	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.700	0.68634	98	0.69050	38	1.37684	137	0.96015	11
0.701	0.68536	99	0.69012	39	1.37547	136	0.96004	11
0.702	0.68437	98	0.68973	38	1.37411	137	0.95993	12
0.703	0.68339	98	0.68935	39	1.37274	137	0.95981	11
0.704	0.68241	98	0.68896	38	1.37137	136	0.95970	11
0.705	0.68143	97	0.68858	38	1.37001	136	0.95959	11
0.706	0.68046	98	0.68820	39	1.36865	136	0.95948	11
0.707	0.67948	97	0.68781	38	1.36729	135	0.95937	12
0.708	0.67851	97	0.68743	39	1.36594	135	0.95925	11
0.709	0.67754	97	0.68704	38	1.36459	136	0.95914	11
0.710	0.67657	96	0.68666	38	1.36323	135	0.95903	11
0.711	0.67561	97	0.68628	39	1.36188	134	0.95892	12
0.712	0.67464	96	0.68589	38	1.36054	135	0.95880	11
0.713	0.67368	96	0.68551	38	1.35919	134	0.95869	11
0.714	0.67272	96	0.68513	39	1.35785	134	0.95858	11
0.715	0.67176	96	0.68474	38	1.35651	134	0.95847	12
0.716	0.67080	95	0.68436	38	1.35517	134	0.95835	11
0.717	0.66985	95	0.68398	38	1.35383	134	0.95824	12
0.718	0.66890	95	0.68360	39	1.35249	133	0.95812	11
0.719	0.66795	95	0.68321	38	1.35116	133	0.95801	11
0.720	0.66700	95	0.68283	38	1.34983	133	0.95790	12
0.721	0.66605	95	0.68245	38	1.34850	133	0.95778	11
0.722	0.66510	94	0.68207	38	1.34717	132	0.95767	12
0.723	0.66416	94	0.68169	39	1.34585	133	0.95755	11
0.724	0.66322	94	0.68130	38	1.34452	132	0.95744	11
0.725	0.66228	94	0.68092	38	1.34320	132	0.95733	12
0.726	0.66134	94	0.68054	38	1.34188	132	0.95721	11
0.727	0.66040	93	0.68016	38	1.34056	131	0.95710	12
0.728	0.65947	93	0.67978	38	1.33925	132	0.95698	11
0.729	0.65854	94	0.67940	38	1.33793	131	0.95687	12
0.730	0.65760	92	0.67902	38	1.33662	131	0.95675	12
0.731	0.65668	93	0.67864	38	1.33531	130	0.95663	11
0.732	0.65575	93	0.67826	38	1.33401	131	0.95652	12
0.733	0.65482	92	0.67788	38	1.33270	130	0.95640	11
0.734	0.65390	92	0.67750	38	1.33140	131	0.95629	12
0.735	0.65298	92	0.67712	38	1.33009	130	0.95617	11
0.736	0.65206	92	0.67674	38	1.32879	129	0.95606	12
0.737	0.65114	92	0.67636	38	1.32750	130	0.95594	12
0.738	0.65022	92	0.67598	38	1.32620	129	0.95582	11
0.739	0.64930	91	0.67560	38	1.32491	130	0.95571	12
0.740	0.64839	91	0.67522	38	1.32361	129	0.95559	12
0.741	0.64748	91	0.67484	38	1.32232	129	0.95547	11
0.742	0.64657	91	0.67446	37	1.32103	128	0.95536	12
0.743	0.64566	90	0.67409	38	1.31975	129	0.95524	12
0.744	0.64476	91	0.67371	38	1.31846	128	0.95512	12
0.745	0.64385	90	0.67333	38	1.31718	128	0.95500	11
0.746	0.64295	90	0.67295	38	1.31590	128	0.95489	12
0.747	0.64205	90	0.67257	37	1.31462	128	0.95477	12
0.748	0.64115	90	0.67220	38	1.31334	127	0.95465	12
0.749	0.64025	90	0.67182	38	1.31207	128	0.95453	12
0.750	0.63935		0.67144		1.31079		0.95441	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.750	0.63935	89	0.67144	38	1.31079	127	0.95441	11
0.751	0.63846	89	0.67106	37	1.30952	127	0.95430	12
0.752	0.63757	89	0.67069	38	1.30825	126	0.95418	12
0.753	0.63668	89	0.67031	38	1.30699	127	0.95406	12
0.754	0.63579	89	0.66993	37	1.30572	126	0.95394	12
0.755	0.63490	89	0.66956	38	1.30446	127	0.95382	12
0.756	0.63401	88	0.66918	38	1.30319	126	0.95370	12
0.757	0.63313	88	0.66880	37	1.30193	126	0.95358	12
0.758	0.63225	89	0.66843	38	1.30067	125	0.95346	11
0.759	0.63136	88	0.66805	37	1.29942	126	0.95335	12
0.760	0.63048	87	0.66768	38	1.29816	125	0.95323	12
0.761	0.62961	88	0.66730	37	1.29691	125	0.95311	12
0.762	0.62873	87	0.66693	38	1.29566	125	0.95299	12
0.763	0.62786	88	0.66655	38	1.29441	125	0.95287	12
0.764	0.62698	87	0.66617	37	1.29316	125	0.95275	12
0.765	0.62611	87	0.66580	38	1.29191	124	0.95263	12
0.766	0.62524	86	0.66542	37	1.29067	124	0.95251	13
0.767	0.62438	87	0.66505	37	1.28943	125	0.95238	12
0.768	0.62351	87	0.66468	38	1.28818	123	0.95226	12
0.769	0.62264	86	0.66430	37	1.28695	124	0.95214	12
0.770	0.62178	86	0.66393	38	1.28571	124	0.95202	12
0.771	0.62092	86	0.66355	37	1.28447	123	0.95190	12
0.772	0.62006	86	0.66318	37	1.28324	123	0.95178	12
0.773	0.61920	85	0.66281	38	1.28201	123	0.95166	12
0.774	0.61835	86	0.66243	37	1.28078	123	0.95154	12
0.775	0.61749	85	0.66206	38	1.27955	123	0.95142	13
0.776	0.61664	86	0.66168	37	1.27832	122	0.95129	12
0.777	0.61578	85	0.66131	37	1.27710	123	0.95117	12
0.778	0.61493	84	0.66094	37	1.27587	122	0.95105	12
0.779	0.61409	85	0.66057	38	1.27465	122	0.95093	12
0.780	0.61324	85	0.66019	37	1.27343	122	0.95081	13
0.781	0.61239	84	0.65982	37	1.27221	121	0.95068	12
0.782	0.61155	84	0.65945	37	1.27100	122	0.95056	12
0.783	0.61071	84	0.65908	38	1.26978	121	0.95044	12
0.784	0.60987	84	0.65870	37	1.26857	121	0.95032	13
0.785	0.60903	84	0.65833	37	1.26736	121	0.95019	12
0.786	0.60819	84	0.65796	37	1.26615	121	0.95007	12
0.787	0.60735	83	0.65759	37	1.26494	121	0.94995	13
0.788	0.60652	84	0.65722	37	1.26373	120	0.94982	12
0.789	0.60568	83	0.65685	37	1.26253	120	0.94970	12
0.790	0.60485	83	0.65648	38	1.26133	120	0.94958	13
0.791	0.60402	83	0.65610	37	1.26013	120	0.94945	12
0.792	0.60319	82	0.65573	37	1.25893	120	0.94933	13
0.793	0.60237	83	0.65536	37	1.25773	120	0.94920	12
0.794	0.60154	82	0.65499	37	1.25653	119	0.94908	13
0.795	0.60072	83	0.65462	37	1.25534	119	0.94895	12
0.796	0.59989	82	0.65425	37	1.25415	120	0.94883	12
0.797	0.59907	82	0.65388	37	1.25295	119	0.94871	13
0.798	0.59825	82	0.65351	37	1.25176	118	0.94858	12
0.799	0.59743	81	0.65314	37	1.25058	119	0.94846	13
0.800	0.59662		0.65277		1.24939		0.94833	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R	Δ
0.800	0.59662	82	0.65277	37	1.24939	118	0.94833	12
0.801	0.59580	81	0.65240	37	1.24821	119	0.94821	13
0.802	0.59499	81	0.65203	36	1.24702	118	0.94808	12
0.803	0.59418	81	0.65167	37	1.24584	118	0.94796	13
0.804	0.59337	81	0.65130	37	1.24466	118	0.94783	13
0.805	0.59256	81	0.65093	37	1.24348	117	0.94770	12
0.806	0.59175	81	0.65056	37	1.24231	118	0.94758	13
0.807	0.59094	80	0.65019	37	1.24113	117	0.94745	12
0.808	0.59014	81	0.64982	37	1.23996	117	0.94733	13
0.809	0.58933	80	0.64945	36	1.23879	117	0.94720	13
0.810	0.58853	80	0.64909	37	1.23762	117	0.94707	12
0.811	0.58773	80	0.64872	37	1.23645	117	0.94695	13
0.812	0.58693	80	0.64835	37	1.23528	116	0.94682	13
0.813	0.58613	79	0.64798	36	1.23412	117	0.94669	12
0.814	0.58534	80	0.64762	37	1.23295	116	0.94657	13
0.815	0.58454	79	0.64725	37	1.23179	116	0.94644	13
0.816	0.58375	79	0.64688	37	1.23063	116	0.94631	13
0.817	0.58296	79	0.64651	36	1.22947	116	0.94618	12
0.818	0.58217	79	0.64615	37	1.22831	115	0.94606	13
0.819	0.58138	79	0.64578	36	1.22716	116	0.94593	13
0.820	0.58059	79	0.64542	37	1.22600	115	0.94580	13
0.821	0.57980	78	0.64505	37	1.22485	115	0.94567	12
0.822	0.57902	79	0.64468	36	1.22370	115	0.94555	13
0.823	0.57823	78	0.64432	37	1.22255	115	0.94542	13
0.824	0.57745	78	0.64395	36	1.22140	114	0.94529	13
0.825	0.57667	78	0.64359	37	1.22026	115	0.94516	13
0.826	0.57589	78	0.64322	37	1.21911	114	0.94503	13
0.827	0.57511	77	0.64285	36	1.21797	114	0.94490	13
0.828	0.57434	78	0.64249	37	1.21683	114	0.94477	12
0.829	0.57356	77	0.64212	36	1.21569	114	0.94465	13
0.830	0.57279	77	0.64176	36	1.21455	114	0.94452	13
0.831	0.57202	78	0.64140	37	1.21341	113	0.94439	13
0.832	0.57124	77	0.64103	36	1.21228	114	0.94426	13
0.833	0.57047	76	0.64067	37	1.21114	113	0.94413	13
0.834	0.56971	77	0.64030	36	1.21001	113	0.94400	13
0.835	0.56894	77	0.63994	37	1.20888	113	0.94387	13
0.836	0.56817	76	0.63957	36	1.20775	113	0.94374	13
0.837	0.56741	76	0.63921	36	1.20662	113	0.94361	13
0.838	0.56665	77	0.63885	37	1.20549	112	0.94348	13
0.839	0.56588	76	0.63848	36	1.20437	113	0.94335	13
0.840	0.56512	75	0.63812	36	1.20324	112	0.94322	13
0.841	0.56437	76	0.63776	37	1.20212	112	0.94309	13
0.842	0.56361	76	0.63739	36	1.20100	112	0.94296	13
0.843	0.56285	75	0.63703	36	1.19988	112	0.94283	14
0.844	0.56210	76	0.63667	36	1.19876	111	0.94269	13
0.845	0.56134	75	0.63631	37	1.19765	112	0.94256	13
0.846	0.56059	75	0.63594	36	1.19653	111	0.94243	13
0.847	0.55984	75	0.63558	36	1.19542	111	0.94230	13
0.848	0.55909	75	0.63522	36	1.19431	111	0.94217	13
0.849	0.55834	75	0.63486	36	1.19320	111	0.94204	13
0.850	0.55759		0.63450		1.19209		0.94191	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.850	0.55759	74	0.63450	37	1.19209	111	0.94191	14
0.851	0.55685	75	0.63413	36	1.19098	110	0.94177	13
0.852	0.55610	74	0.63377	36	1.18988	111	0.94164	13
0.853	0.55536	74	0.63341	36	1.18877	110	0.94151	13
0.854	0.55462	74	0.63305	36	1.18767	110	0.94138	14
0.855	0.55388	74	0.63269	36	1.18657	110	0.94124	13
0.856	0.55314	74	0.63233	36	1.18547	110	0.94111	13
0.857	0.55240	74	0.63197	36	1.18437	110	0.94098	13
0.858	0.55166	73	0.63161	36	1.18327	109	0.94085	14
0.859	0.55093	74	0.63125	36	1.18218	110	0.94071	13
0.860	0.55019	73	0.63089	36	1.18108	109	0.94058	13
0.861	0.54946	73	0.63053	36	1.17999	109	0.94045	14
0.862	0.54873	73	0.63017	36	1.17890	109	0.94031	13
0.863	0.54800	73	0.62981	36	1.17781	109	0.94018	13
0.864	0.54727	73	0.62945	36	1.17672	109	0.94005	14
0.865	0.54654	72	0.62909	36	1.17563	109	0.93991	13
0.866	0.54582	73	0.62873	36	1.17454	108	0.93978	13
0.867	0.54509	72	0.62837	36	1.17346	108	0.93965	14
0.868	0.54437	73	0.62801	36	1.17238	109	0.93951	13
0.869	0.54364	72	0.62765	36	1.17129	108	0.93938	14
0.870	0.54292	72	0.62729	36	1.17021	107	0.93924	13
0.871	0.54220	72	0.62693	35	1.16914	108	0.93911	14
0.872	0.54148	72	0.62658	36	1.16806	108	0.93897	13
0.873	0.54076	71	0.62622	36	1.16698	107	0.93884	14
0.874	0.54005	72	0.62586	36	1.16591	108	0.93870	13
0.875	0.53933	71	0.62550	36	1.16483	107	0.93857	14
0.876	0.53862	72	0.62514	35	1.16376	107	0.93843	13
0.877	0.53790	71	0.62479	36	1.16269	107	0.93830	14
0.878	0.53719	71	0.62443	36	1.16162	107	0.93816	13
0.879	0.53648	71	0.62407	35	1.16055	106	0.93803	14
0.880	0.53577	71	0.62372	36	1.15949	107	0.93789	14
0.881	0.53506	70	0.62336	36	1.15842	106	0.93775	13
0.882	0.53436	71	0.62300	35	1.15736	106	0.93762	14
0.883	0.53365	70	0.62265	36	1.15630	106	0.93748	13
0.884	0.53295	71	0.62229	36	1.15524	106	0.93735	14
0.885	0.53224	70	0.62193	35	1.15418	106	0.93721	14
0.886	0.53154	70	0.62158	36	1.15312	106	0.93707	13
0.887	0.53084	70	0.62122	36	1.15206	105	0.93694	14
0.888	0.53014	70	0.62086	35	1.15101	106	0.93680	14
0.889	0.52944	70	0.62051	36	1.14995	105	0.93666	13
0.890	0.52874	69	0.62015	35	1.14890	105	0.93653	14
0.891	0.52805	70	0.61980	36	1.14785	105	0.93639	14
0.892	0.52735	69	0.61944	35	1.14680	105	0.93625	14
0.893	0.52666	69	0.61909	36	1.14575	105	0.93611	13
0.894	0.52597	69	0.61873	35	1.14470	105	0.93598	14
0.895	0.52528	69	0.61838	36	1.14365	104	0.93584	14
0.896	0.52459	69	0.61802	35	1.14261	105	0.93570	14
0.897	0.52390	69	0.61767	36	1.14156	104	0.93556	14
0.898	0.52321	69	0.61731	35	1.14052	104	0.93542	13
0.899	0.52252	68	0.61696	35	1.13948	104	0.93529	14
0.900	0.52184		0.61661		1.13844		0.93515	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.900	0.52184	69	0.61661	36	1.13844	104	0.93515	14
0.901	0.52115	68	0.61625	35	1.13740	103	0.93501	14
0.902	0.52047	68	0.61590	36	1.13637	104	0.93487	14
0.903	0.51979	69	0.61554	35	1.13533	103	0.93473	14
0.904	0.51910	68	0.61519	35	1.13430	104	0.93459	14
0.905	0.51842	67	0.61484	35	1.13326	103	0.93445	13
0.906	0.51775	68	0.61449	36	1.13223	103	0.93432	14
0.907	0.51707	68	0.61413	35	1.13120	103	0.93418	14
0.908	0.51639	67	0.61378	35	1.13017	103	0.93404	14
0.909	0.51572	68	0.61343	36	1.12914	102	0.93390	14
0.910	0.51504	67	0.61307	35	1.12812	103	0.93376	14
0.911	0.51437	67	0.61272	35	1.12709	102	0.93362	14
0.912	0.51370	67	0.61237	35	1.12607	103	0.93348	14
0.913	0.51303	67	0.61202	35	1.12504	102	0.93334	14
0.914	0.51236	67	0.61167	36	1.12402	102	0.93320	14
0.915	0.51169	67	0.61131	35	1.12300	102	0.93306	14
0.916	0.51102	67	0.61096	35	1.12198	102	0.93292	14
0.917	0.51035	66	0.61061	35	1.12096	101	0.93278	14
0.918	0.50969	67	0.61026	35	1.11995	102	0.93264	14
0.919	0.50902	66	0.60991	35	1.11893	101	0.93250	15
0.920	0.50836	66	0.60956	35	1.11792	101	0.93235	14
0.921	0.50770	66	0.60921	35	1.11691	102	0.93221	14
0.922	0.50704	66	0.60886	35	1.11589	101	0.93207	14
0.923	0.50638	66	0.60851	35	1.11488	101	0.93193	14
0.924	0.50572	66	0.60816	35	1.11387	100	0.93179	14
0.925	0.50506	66	0.60781	35	1.11287	101	0.93165	14
0.926	0.50440	65	0.60746	35	1.11186	101	0.93151	15
0.927	0.50375	66	0.60711	35	1.11085	100	0.93136	14
0.928	0.50309	65	0.60676	35	1.10985	100	0.93122	14
0.929	0.50244	65	0.60641	35	1.10885	100	0.93108	14
0.930	0.50179	65	0.60606	35	1.10785	100	0.93094	14
0.931	0.50114	65	0.60571	35	1.10685	100	0.93080	15
0.932	0.50049	65	0.60536	35	1.10585	100	0.93065	14
0.933	0.49984	65	0.60501	35	1.10485	100	0.93051	14
0.934	0.49919	65	0.60466	35	1.10385	99	0.93037	14
0.935	0.49854	64	0.60431	35	1.10286	100	0.93023	15
0.936	0.49790	65	0.60396	34	1.10186	99	0.93008	14
0.937	0.49725	64	0.60362	35	1.10087	99	0.92994	14
0.938	0.49661	64	0.60327	35	1.09988	99	0.92980	15
0.939	0.49597	64	0.60292	35	1.09889	99	0.92965	14
0.940	0.49533	64	0.60257	35	1.09790	99	0.92951	14
0.941	0.49469	64	0.60222	34	1.09691	99	0.92937	15
0.942	0.49405	64	0.60188	35	1.09592	98	0.92922	14
0.943	0.49341	64	0.60153	35	1.09494	99	0.92908	15
0.944	0.49277	64	0.60118	35	1.09395	98	0.92893	14
0.945	0.49213	63	0.60083	34	1.09297	98	0.92879	14
0.946	0.49150	64	0.60049	35	1.09199	99	0.92865	15
0.947	0.49086	63	0.60014	35	1.09100	98	0.92850	14
0.948	0.49023	63	0.59979	34	1.09002	97	0.92836	15
0.949	0.48960	63	0.59945	35	1.08905	98	0.92821	14
0.950	0.48897		0.59910		1.08807		0.92807	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
0.950	0.48897	63	0.59910	35	1.08807	98	0.92807	15
0.951	0.48834	63	0.59875	34	1.08709	97	0.92792	14
0.952	0.48771	63	0.59841	35	1.08612	98	0.92778	15
0.953	0.48708	63	0.59806	34	1.08514	97	0.92763	14
0.954	0.48645	62	0.59772	35	1.08417	97	0.92749	15
0.955	0.48583	63	0.59737	34	1.08320	97	0.92734	14
0.956	0.48520	62	0.59703	35	1.08223	97	0.92720	15
0.957	0.48458	62	0.59668	34	1.08126	97	0.92705	14
0.958	0.48396	63	0.59634	35	1.08029	97	0.92691	15
0.959	0.48333	62	0.59599	34	1.07932	96	0.92676	15
0.960	0.48271	62	0.59565	35	1.07836	97	0.92661	14
0.961	0.48209	62	0.59530	34	1.07739	96	0.92647	15
0.962	0.48147	61	0.59496	35	1.07643	96	0.92632	15
0.963	0.48086	62	0.59461	34	1.07547	96	0.92617	14
0.964	0.48024	62	0.59427	35	1.07451	96	0.92603	15
0.965	0.47962	61	0.59392	34	1.07355	96	0.92588	14
0.966	0.47901	62	0.59358	34	1.07259	96	0.92574	15
0.967	0.47839	61	0.59324	35	1.07163	96	0.92559	15
0.968	0.47778	61	0.59289	34	1.07067	95	0.92544	15
0.969	0.47717	61	0.59255	34	1.06972	96	0.92529	14
0.970	0.47656	61	0.59221	35	1.06876	95	0.92515	15
0.971	0.47595	61	0.59186	34	1.06781	95	0.92500	15
0.972	0.47534	61	0.59152	34	1.06686	95	0.92485	15
0.973	0.47473	61	0.59118	35	1.06591	95	0.92470	14
0.974	0.47412	60	0.59083	34	1.06496	95	0.92456	15
0.975	0.47352	61	0.59049	34	1.06401	95	0.92441	15
0.976	0.47291	60	0.59015	34	1.06306	95	0.92426	15
0.977	0.47231	60	0.58981	35	1.06211	94	0.92411	15
0.978	0.47171	61	0.58946	34	1.06117	94	0.92396	14
0.979	0.47110	60	0.58912	34	1.06023	95	0.92382	15
0.980	0.47050	60	0.58878	34	1.05928	94	0.92367	15
0.981	0.46990	60	0.58844	34	1.05834	94	0.92352	15
0.982	0.46930	60	0.58810	34	1.05740	94	0.92337	15
0.983	0.46870	59	0.58776	34	1.05646	94	0.92322	15
0.984	0.46811	60	0.58742	35	1.05552	94	0.92307	15
0.985	0.46751	60	0.58707	34	1.05458	93	0.92292	15
0.986	0.46691	59	0.58673	34	1.05365	94	0.92277	14
0.987	0.46632	59	0.58639	34	1.05271	93	0.92263	15
0.988	0.46573	60	0.58605	34	1.05178	94	0.92248	15
0.989	0.46513	59	0.58571	34	1.05084	93	0.92233	15
0.990	0.46454	59	0.58537	34	1.04991	93	0.92218	15
0.991	0.46395	59	0.58503	34	1.04898	93	0.92203	15
0.992	0.46336	59	0.58469	34	1.04805	93	0.92188	15
0.993	0.46277	59	0.58435	34	1.04712	92	0.92173	15
0.994	0.46218	58	0.58401	34	1.04620	93	0.92158	15
0.995	0.46160	59	0.58367	34	1.04527	93	0.92143	15
0.996	0.46101	58	0.58333	34	1.04434	92	0.92128	15
0.997	0.46043	59	0.58299	34	1.04342	92	0.92113	15
0.998	0.45984	58	0.58265	33	1.04250	93	0.92098	16
0.999	0.45926	58	0.58232	34	1.04157	92	0.92082	15
1.000	0.45868		0.58198		1.04065		0.92067	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.000	0.45868	59	0.58198	34	1.04065	92	0.92067	15
1.001	0.45809	58	0.58164	34	1.03973	92	0.92052	15
1.002	0.45751	58	0.58130	34	1.03881	92	0.92037	15
1.003	0.45693	58	0.58096	34	1.03789	91	0.92022	15
1.004	0.45635	57	0.58062	33	1.03698	92	0.92007	15
1.005	0.45578	58	0.58029	34	1.03606	91	0.91992	15
1.006	0.45520	58	0.57995	34	1.03515	92	0.91977	16
1.007	0.45462	57	0.57961	34	1.03423	91	0.91961	15
1.008	0.45405	58	0.57927	34	1.03332	91	0.91946	15
1.009	0.45347	57	0.57893	33	1.03241	91	0.91931	15
1.010	0.45290	57	0.57860	34	1.03150	91	0.91916	15
1.011	0.45233	57	0.57826	34	1.03059	91	0.91901	16
1.012	0.45176	57	0.57792	33	1.02968	91	0.91885	15
1.013	0.45119	57	0.57759	34	1.02877	90	0.91870	15
1.014	0.45062	57	0.57725	34	1.02787	91	0.91855	15
1.015	0.45005	57	0.57691	33	1.02696	90	0.91840	16
1.016	0.44948	57	0.57658	34	1.02606	91	0.91824	15
1.017	0.44891	56	0.57624	34	1.02515	90	0.91809	15
1.018	0.44835	57	0.57590	33	1.02425	90	0.91794	16
1.019	0.44778	56	0.57557	34	1.02335	90	0.91778	15
1.020	0.44722	57	0.57523	33	1.02245	90	0.91763	15
1.021	0.44665	56	0.57490	34	1.02155	90	0.91748	16
1.022	0.44609	56	0.57456	33	1.02065	89	0.91732	15
1.023	0.44553	56	0.57423	34	1.01976	90	0.91717	15
1.024	0.44497	56	0.57389	33	1.01886	90	0.91702	16
1.025	0.44441	56	0.57356	34	1.01796	89	0.91686	15
1.026	0.44385	56	0.57322	33	1.01707	89	0.91671	16
1.027	0.44329	56	0.57289	34	1.01618	89	0.91655	15
1.028	0.44273	55	0.57255	33	1.01529	90	0.91640	15
1.029	0.44218	56	0.57222	34	1.01439	89	0.91625	16
1.030	0.44162	55	0.57188	33	1.01350	88	0.91609	15
1.031	0.44107	56	0.57155	33	1.01262	89	0.91594	16
1.032	0.44051	55	0.57122	34	1.01173	89	0.91578	15
1.033	0.43996	55	0.57088	33	1.01084	88	0.91563	16
1.034	0.43941	55	0.57055	34	1.00996	89	0.91547	15
1.035	0.43886	55	0.57021	33	1.00907	88	0.91532	16
1.036	0.43831	55	0.56988	33	1.00819	89	0.91516	15
1.037	0.43776	55	0.56955	34	1.00730	88	0.91501	16
1.038	0.43721	55	0.56921	33	1.00642	88	0.91485	15
1.039	0.43666	55	0.56888	33	1.00554	88	0.91470	16
1.040	0.43611	54	0.56855	33	1.00466	88	0.91454	16
1.041	0.43557	55	0.56822	34	1.00378	88	0.91438	15
1.042	0.43502	54	0.56788	33	1.00290	87	0.91423	16
1.043	0.43448	55	0.56755	33	1.00203	88	0.91407	15
1.044	0.43393	54	0.56722	33	1.00115	87	0.91392	16
1.045	0.43339	54	0.56689	33	1.00028	88	0.91376	16
1.046	0.43285	54	0.56656	34	0.99940	87	0.91360	15
1.047	0.43231	54	0.56622	33	0.99853	87	0.91345	16
1.048	0.43177	54	0.56589	33	0.99766	87	0.91329	16
1.049	0.43123	54	0.56556	33	0.99679	87	0.91313	15
1.050	0.43069		0.56523		0.99592		0.91298	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.050	0.43069	54	0.56523	33	0.99592	87	0.91298	16
1.051	0.43015	54	0.56490	33	0.99505	87	0.91282	16
1.052	0.42961	53	0.56457	33	0.99418	87	0.91266	15
1.053	0.42908	54	0.56424	33	0.99331	86	0.91251	16
1.054	0.42854	53	0.56391	33	0.99245	87	0.91235	16
1.055	0.42801	54	0.56358	33	0.99158	86	0.91219	16
1.056	0.42747	53	0.56325	33	0.99072	87	0.91203	15
1.057	0.42694	53	0.56292	33	0.98985	86	0.91188	16
1.058	0.42641	53	0.56259	33	0.98899	86	0.91172	16
1.059	0.42588	53	0.56226	33	0.98813	86	0.91156	16
1.060	0.42535	53	0.56193	33	0.98727	86	0.91140	16
1.061	0.42482	53	0.56160	33	0.98641	86	0.91124	16
1.062	0.42429	53	0.56127	33	0.98555	85	0.91108	15
1.063	0.42376	53	0.56094	33	0.98470	86	0.91093	16
1.064	0.42323	53	0.56061	33	0.98384	86	0.91077	16
1.065	0.42270	52	0.56028	33	0.98298	85	0.91061	16
1.066	0.42218	53	0.55995	33	0.98213	85	0.91045	16
1.067	0.42165	52	0.55962	33	0.98128	86	0.91029	16
1.068	0.42113	52	0.55929	33	0.98042	85	0.91013	16
1.069	0.42061	53	0.55896	32	0.97957	85	0.90997	16
1.070	0.42008	52	0.55864	33	0.97872	85	0.90981	15
1.071	0.41956	52	0.55831	33	0.97787	85	0.90966	16
1.072	0.41904	52	0.55798	33	0.97702	85	0.90950	16
1.073	0.41852	52	0.55765	33	0.97617	84	0.90934	16
1.074	0.41800	52	0.55732	32	0.97533	85	0.90918	16
1.075	0.41748	51	0.55700	33	0.97448	84	0.90902	16
1.076	0.41697	52	0.55667	33	0.97364	85	0.90886	16
1.077	0.41645	52	0.55634	32	0.97279	84	0.90870	16
1.078	0.41593	51	0.55602	33	0.97195	84	0.90854	16
1.079	0.41542	52	0.55569	33	0.97111	85	0.90838	16
1.080	0.41490	51	0.55536	33	0.97026	84	0.90822	16
1.081	0.41439	51	0.55503	32	0.96942	84	0.90806	16
1.082	0.41388	52	0.55471	33	0.96858	83	0.90790	17
1.083	0.41336	51	0.55438	32	0.96775	84	0.90773	16
1.084	0.41285	51	0.55406	33	0.96691	84	0.90757	16
1.085	0.41234	51	0.55373	33	0.96607	83	0.90741	16
1.086	0.41183	51	0.55340	32	0.96524	84	0.90725	16
1.087	0.41132	51	0.55308	33	0.96440	83	0.90709	16
1.088	0.41081	50	0.55275	32	0.96357	84	0.90693	16
1.089	0.41031	51	0.55243	33	0.96273	83	0.90677	16
1.090	0.40980	51	0.55210	32	0.96190	83	0.90661	16
1.091	0.40929	50	0.55178	33	0.96107	83	0.90645	17
1.092	0.40879	51	0.55145	32	0.96024	83	0.90628	16
1.093	0.40828	50	0.55113	33	0.95941	83	0.90612	16
1.094	0.40778	50	0.55080	32	0.95858	83	0.90596	16
1.095	0.40728	51	0.55048	33	0.95775	82	0.90580	16
1.096	0.40677	50	0.55015	32	0.95693	83	0.90564	17
1.097	0.40627	50	0.54983	33	0.95610	82	0.90547	16
1.098	0.40577	50	0.54950	32	0.95528	83	0.90531	16
1.099	0.40527	50	0.54918	32	0.95445	82	0.90515	16
1.100	0.40477		0.54886		0.95363		0.90499	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.100	0.40477	50	0.54886	33	0.95363	82	0.90499	17
1.101	0.40427	49	0.54853	32	0.95281	82	0.90482	16
1.102	0.40378	50	0.54821	32	0.95199	83	0.90466	16
1.103	0.40328	50	0.54789	33	0.95116	82	0.90450	17
1.104	0.40278	49	0.54756	32	0.95034	81	0.90433	16
1.105	0.40229	50	0.54724	32	0.94953	82	0.90417	16
1.106	0.40179	49	0.54692	33	0.94871	82	0.90401	17
1.107	0.40130	50	0.54659	32	0.94789	81	0.90384	16
1.108	0.40080	49	0.54627	32	0.94708	82	0.90368	16
1.109	0.40031	49	0.54595	32	0.94626	81	0.90352	17
1.110	0.39982	49	0.54563	33	0.94545	82	0.90335	16
1.111	0.39933	49	0.54530	32	0.94463	81	0.90319	16
1.112	0.39884	49	0.54498	32	0.94382	81	0.90303	17
1.113	0.39835	49	0.54466	32	0.94301	81	0.90286	16
1.114	0.39786	49	0.54434	32	0.94220	81	0.90270	17
1.115	0.39737	49	0.54402	32	0.94139	81	0.90253	16
1.116	0.39688	48	0.54370	33	0.94058	81	0.90237	17
1.117	0.39640	49	0.54337	32	0.93977	81	0.90220	16
1.118	0.39591	48	0.54305	32	0.93896	80	0.90204	16
1.119	0.39543	49	0.54273	32	0.93816	81	0.90188	17
1.120	0.39494	48	0.54241	32	0.93735	80	0.90171	16
1.121	0.39446	49	0.54209	32	0.93655	81	0.90155	17
1.122	0.39397	48	0.54177	32	0.93574	80	0.90138	16
1.123	0.39349	48	0.54145	32	0.93494	80	0.90122	17
1.124	0.39301	48	0.54113	32	0.93414	80	0.90105	17
1.125	0.39253	48	0.54081	32	0.93334	80	0.90088	16
1.126	0.39205	48	0.54049	32	0.93254	80	0.90072	17
1.127	0.39157	48	0.54017	32	0.93174	80	0.90055	16
1.128	0.39109	48	0.53985	32	0.93094	80	0.90039	17
1.129	0.39061	48	0.53953	32	0.93014	80	0.90022	16
1.130	0.39013	47	0.53921	32	0.92934	79	0.90006	17
1.131	0.38966	48	0.53889	32	0.92855	80	0.89989	17
1.132	0.38918	48	0.53857	32	0.92775	79	0.89972	16
1.133	0.38870	47	0.53825	32	0.92696	80	0.89956	17
1.134	0.38823	47	0.53793	31	0.92616	79	0.89939	17
1.135	0.38776	48	0.53762	32	0.92537	79	0.89922	16
1.136	0.38728	47	0.53730	32	0.92458	79	0.89906	17
1.137	0.38681	47	0.53698	32	0.92379	79	0.89889	17
1.138	0.38634	47	0.53666	32	0.92300	79	0.89872	16
1.139	0.38587	47	0.53634	32	0.92221	79	0.89856	17
1.140	0.38540	47	0.53602	31	0.92142	79	0.89839	17
1.141	0.38493	47	0.53571	32	0.92063	78	0.89822	16
1.142	0.38446	47	0.53539	32	0.91985	79	0.89806	17
1.143	0.38399	47	0.53507	32	0.91906	78	0.89789	17
1.144	0.38352	47	0.53475	31	0.91828	79	0.89772	17
1.145	0.38305	46	0.53444	32	0.91749	78	0.89755	16
1.146	0.38259	47	0.53412	32	0.91671	79	0.89739	17
1.147	0.38212	46	0.53380	31	0.91592	78	0.89722	17
1.148	0.38166	47	0.53349	32	0.91514	78	0.89705	17
1.149	0.38119	46	0.53317	32	0.91436	78	0.89688	17
1.150	0.38073		0.53285		0.91358		0.89671	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.150	0.38073	46	0.53285	31	0.91358	78	0.89671	16
1.151	0.38027	47	0.53254	32	0.91280	78	0.89655	17
1.152	0.37980	46	0.53222	32	0.91202	77	0.89638	17
1.153	0.37934	46	0.53190	31	0.91125	78	0.89621	17
1.154	0.37888	46	0.53159	32	0.91047	78	0.89604	17
1.155	0.37842	46	0.53127	31	0.90969	77	0.89587	17
1.156	0.37796	46	0.53096	32	0.90892	78	0.89570	17
1.157	0.37750	46	0.53064	31	0.90814	77	0.89553	17
1.158	0.37704	45	0.53033	32	0.90737	77	0.89536	16
1.159	0.37659	46	0.53001	31	0.90660	77	0.89520	17
1.160	0.37613	46	0.52970	32	0.90583	78	0.89503	17
1.161	0.37567	45	0.52938	31	0.90505	77	0.89486	17
1.162	0.37522	46	0.52907	32	0.90428	77	0.89469	17
1.163	0.37476	45	0.52875	31	0.90351	76	0.89452	17
1.164	0.37431	46	0.52844	32	0.90275	77	0.89435	17
1.165	0.37385	45	0.52812	31	0.90198	77	0.89418	17
1.166	0.37340	45	0.52781	31	0.90121	77	0.89401	17
1.167	0.37295	45	0.52750	32	0.90044	76	0.89384	17
1.168	0.37250	45	0.52718	31	0.89968	77	0.89367	17
1.169	0.37205	45	0.52687	32	0.89891	76	0.89350	17
1.170	0.37160	45	0.52655	31	0.89815	76	0.89333	17
1.171	0.37115	45	0.52624	31	0.89739	77	0.89316	17
1.172	0.37070	45	0.52593	32	0.89662	76	0.89299	17
1.173	0.37025	45	0.52561	31	0.89586	76	0.89282	17
1.174	0.36980	45	0.52530	31	0.89510	76	0.89265	17
1.175	0.36935	44	0.52499	31	0.89434	76	0.89248	18
1.176	0.36891	45	0.52468	32	0.89358	76	0.89230	17
1.177	0.36846	44	0.52436	31	0.89282	75	0.89213	17
1.178	0.36802	45	0.52405	31	0.89207	76	0.89196	17
1.179	0.36757	44	0.52374	31	0.89131	76	0.89179	17
1.180	0.36713	45	0.52343	32	0.89055	75	0.89162	17
1.181	0.36668	44	0.52311	31	0.88980	76	0.89145	17
1.182	0.36624	44	0.52280	31	0.88904	75	0.89128	18
1.183	0.36580	44	0.52249	31	0.88829	75	0.89110	17
1.184	0.36536	44	0.52218	31	0.88754	75	0.89093	17
1.185	0.36492	44	0.52187	31	0.88679	76	0.89076	17
1.186	0.36448	44	0.52156	31	0.88603	75	0.89059	17
1.187	0.36404	44	0.52125	31	0.88528	75	0.89042	18
1.188	0.36360	44	0.52094	32	0.88453	74	0.89024	17
1.189	0.36316	44	0.52062	31	0.88379	75	0.89007	17
1.190	0.36272	43	0.52031	31	0.88304	75	0.88990	17
1.191	0.36229	44	0.52000	31	0.88229	75	0.88973	18
1.192	0.36185	44	0.51969	31	0.88154	74	0.88955	17
1.193	0.36141	43	0.51938	31	0.88080	75	0.88938	17
1.194	0.36098	43	0.51907	31	0.88005	74	0.88921	17
1.195	0.36055	44	0.51876	31	0.87931	75	0.88904	18
1.196	0.36011	43	0.51845	31	0.87856	74	0.88886	17
1.197	0.35968	43	0.51814	31	0.87782	74	0.88869	17
1.198	0.35925	44	0.51783	31	0.87708	74	0.88852	18
1.199	0.35881	43	0.51752	30	0.87634	74	0.88834	17
1.200	0.35838		0.51722		0.87560		0.88817	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.200	0.35838	43	0.51722	31	0.87560	74	0.88817	17
1.201	0.35795	43	0.51691	31	0.87486	74	0.88800	18
1.202	0.35752	43	0.51660	31	0.87412	74	0.88782	17
1.203	0.35709	43	0.51629	31	0.87338	74	0.88765	17
1.204	0.35666	42	0.51598	31	0.87264	73	0.88748	18
1.205	0.35624	43	0.51567	31	0.87191	74	0.88730	17
1.206	0.35581	43	0.51536	31	0.87117	73	0.88713	18
1.207	0.35538	43	0.51505	30	0.87044	74	0.88695	17
1.208	0.35495	42	0.51475	31	0.86970	73	0.88678	18
1.209	0.35453	43	0.51444	31	0.86897	74	0.88660	17
1.210	0.35410	42	0.51413	31	0.86823	73	0.88643	17
1.211	0.35368	43	0.51382	30	0.86750	73	0.88626	18
1.212	0.35325	42	0.51352	31	0.86677	73	0.88608	17
1.213	0.35283	42	0.51321	31	0.86604	73	0.88591	18
1.214	0.35241	42	0.51290	31	0.86531	73	0.88573	17
1.215	0.35199	43	0.51259	30	0.86458	73	0.88556	18
1.216	0.35156	42	0.51229	31	0.86385	73	0.88538	17
1.217	0.35114	42	0.51198	31	0.86312	72	0.88521	18
1.218	0.35072	42	0.51167	30	0.86240	73	0.88503	18
1.219	0.35030	42	0.51137	31	0.86167	72	0.88485	17
1.220	0.34988	41	0.51106	30	0.86095	73	0.88468	18
1.221	0.34947	42	0.51076	31	0.86022	72	0.88450	17
1.222	0.34905	42	0.51045	31	0.85950	73	0.88433	18
1.223	0.34863	42	0.51014	30	0.85877	72	0.88415	17
1.224	0.34821	41	0.50984	31	0.85805	72	0.88398	18
1.225	0.34780	42	0.50953	30	0.85733	72	0.88380	18
1.226	0.34738	41	0.50923	31	0.85661	72	0.88362	17
1.227	0.34697	42	0.50892	30	0.85589	72	0.88345	18
1.228	0.34655	41	0.50862	31	0.85517	72	0.88327	18
1.229	0.34614	42	0.50831	30	0.85445	72	0.88309	17
1.230	0.34572	41	0.50801	31	0.85373	72	0.88292	18
1.231	0.34531	41	0.50770	30	0.85301	71	0.88274	18
1.232	0.34490	41	0.50740	31	0.85230	72	0.88256	17
1.233	0.34449	41	0.50709	30	0.85158	71	0.88239	18
1.234	0.34408	41	0.50679	31	0.85087	72	0.88221	18
1.235	0.34367	41	0.50648	30	0.85015	71	0.88203	17
1.236	0.34326	41	0.50618	30	0.84944	72	0.88186	18
1.237	0.34285	41	0.50588	31	0.84872	71	0.88168	18
1.238	0.34244	41	0.50557	30	0.84801	71	0.88150	18
1.239	0.34203	41	0.50527	30	0.84730	71	0.88132	17
1.240	0.34162	40	0.50497	31	0.84659	71	0.88115	18
1.241	0.34122	41	0.50466	30	0.84588	71	0.88097	18
1.242	0.34081	41	0.50436	30	0.84517	71	0.88079	18
1.243	0.34040	40	0.50406	31	0.84446	71	0.88061	17
1.244	0.34000	41	0.50375	30	0.84375	71	0.88044	18
1.245	0.33959	40	0.50345	30	0.84304	70	0.88026	18
1.246	0.33919	40	0.50315	30	0.84234	71	0.88008	18
1.247	0.33879	41	0.50285	31	0.84163	70	0.87990	18
1.248	0.33838	40	0.50254	30	0.84093	71	0.87972	18
1.249	0.33798	40	0.50224	30	0.84022	70	0.87954	17
1.250	0.33758		0.50194		0.83952		0.87937	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.250	0.33758	40	0.50194	30	0.83952	70	0.87937	18
1.251	0.33718	40	0.50164	30	0.83882	71	0.87919	18
1.252	0.33678	40	0.50134	31	0.83811	70	0.87901	18
1.253	0.33638	40	0.50103	30	0.83741	70	0.87883	18
1.254	0.33598	40	0.50073	30	0.83671	70	0.87865	18
1.255	0.33558	40	0.50043	30	0.83601	70	0.87847	18
1.256	0.33518	40	0.50013	30	0.83531	70	0.87829	18
1.257	0.33478	39	0.49983	30	0.83461	70	0.87811	18
1.258	0.33439	40	0.49953	30	0.83391	69	0.87793	18
1.259	0.33399	40	0.49923	30	0.83322	70	0.87775	17
1.260	0.33359	39	0.49893	30	0.83252	70	0.87758	18
1.261	0.33320	40	0.49863	30	0.83182	69	0.87740	18
1.262	0.33280	39	0.49833	30	0.83113	70	0.87722	18
1.263	0.33241	40	0.49803	30	0.83043	69	0.87704	18
1.264	0.33201	39	0.49773	30	0.82974	70	0.87686	18
1.265	0.33162	39	0.49743	30	0.82904	69	0.87668	18
1.266	0.33123	40	0.49713	30	0.82835	69	0.87650	18
1.267	0.33083	39	0.49683	30	0.82766	69	0.87632	18
1.268	0.33044	39	0.49653	30	0.82697	69	0.87614	19
1.269	0.33005	39	0.49623	30	0.82628	69	0.87595	18
1.270	0.32966	39	0.49593	30	0.82559	69	0.87577	18
1.271	0.32927	39	0.49563	30	0.82490	69	0.87559	18
1.272	0.32888	39	0.49533	30	0.82421	69	0.87541	18
1.273	0.32849	39	0.49503	30	0.82352	68	0.87523	18
1.274	0.32810	39	0.49473	30	0.82284	69	0.87505	18
1.275	0.32771	38	0.49443	29	0.82215	69	0.87487	18
1.276	0.32733	39	0.49414	30	0.82146	68	0.87469	18
1.277	0.32694	39	0.49384	30	0.82078	69	0.87451	18
1.278	0.32655	38	0.49354	30	0.82009	68	0.87433	18
1.279	0.32617	39	0.49324	30	0.81941	68	0.87415	19
1.280	0.32578	38	0.49294	29	0.81873	69	0.87396	18
1.281	0.32540	39	0.49265	30	0.81804	68	0.87378	18
1.282	0.32501	38	0.49235	30	0.81736	68	0.87360	18
1.283	0.32463	38	0.49205	29	0.81668	68	0.87342	18
1.284	0.32425	39	0.49176	30	0.81600	68	0.87324	19
1.285	0.32386	38	0.49146	30	0.81532	68	0.87305	18
1.286	0.32348	38	0.49116	30	0.81464	68	0.87287	18
1.287	0.32310	38	0.49086	29	0.81396	67	0.87269	18
1.288	0.32272	38	0.49057	30	0.81329	68	0.87251	18
1.289	0.32234	38	0.49027	29	0.81261	68	0.87233	19
1.290	0.32196	38	0.48998	30	0.81193	67	0.87214	18
1.291	0.32158	38	0.48968	30	0.81126	68	0.87196	18
1.292	0.32120	38	0.48938	29	0.81058	67	0.87178	18
1.293	0.32082	38	0.48909	30	0.80991	68	0.87160	19
1.294	0.32044	38	0.48879	29	0.80923	67	0.87141	18
1.295	0.32006	37	0.48850	30	0.80856	67	0.87123	18
1.296	0.31969	38	0.48820	30	0.80789	67	0.87105	19
1.297	0.31931	37	0.48790	29	0.80722	68	0.87086	18
1.298	0.31894	38	0.48761	30	0.80654	67	0.87068	18
1.299	0.31856	38	0.48731	29	0.80587	67	0.87050	19
1.300	0.31818		0.48702		0.80520		0.87031	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.300	0.31818	37	0.48702	30	0.80520	66	0.87031	18
1.301	0.31781	37	0.48672	29	0.80454	67	0.87013	18
1.302	0.31744	38	0.48643	29	0.80387	67	0.86995	19
1.303	0.31706	37	0.48614	30	0.80320	67	0.86976	18
1.304	0.31669	37	0.48584	29	0.80253	66	0.86958	18
1.305	0.31632	37	0.48555	30	0.80187	67	0.86940	19
1.306	0.31595	37	0.48525	29	0.80120	67	0.86921	18
1.307	0.31558	38	0.48496	29	0.80053	66	0.86903	19
1.308	0.31520	37	0.48467	30	0.79987	66	0.86884	18
1.309	0.31483	37	0.48437	29	0.79921	67	0.86866	19
1.310	0.31446	37	0.48408	30	0.79854	66	0.86847	18
1.311	0.31409	36	0.48378	29	0.79788	66	0.86829	18
1.312	0.31373	37	0.48349	29	0.79722	66	0.86811	19
1.313	0.31336	37	0.48320	29	0.79656	66	0.86792	18
1.314	0.31299	37	0.48291	30	0.79590	66	0.86774	19
1.315	0.31262	36	0.48261	29	0.79524	66	0.86755	18
1.316	0.31226	37	0.48232	29	0.79458	66	0.86737	19
1.317	0.31189	37	0.48203	29	0.79392	66	0.86718	18
1.318	0.31152	36	0.48174	30	0.79326	66	0.86700	19
1.319	0.31116	37	0.48144	29	0.79260	65	0.86681	18
1.320	0.31079	36	0.48115	29	0.79195	66	0.86663	19
1.321	0.31043	36	0.48086	29	0.79129	66	0.86644	19
1.322	0.31007	37	0.48057	29	0.79063	65	0.86625	18
1.323	0.30970	36	0.48028	30	0.78998	66	0.86607	19
1.324	0.30934	36	0.47998	29	0.78932	65	0.86588	18
1.325	0.30898	36	0.47969	29	0.78867	65	0.86570	19
1.326	0.30862	37	0.47940	29	0.78802	66	0.86551	18
1.327	0.30825	36	0.47911	29	0.78736	65	0.86533	19
1.328	0.30789	36	0.47882	29	0.78671	65	0.86514	19
1.329	0.30753	36	0.47853	29	0.78606	65	0.86495	18
1.330	0.30717	36	0.47824	29	0.78541	65	0.86477	19
1.331	0.30681	35	0.47795	29	0.78476	65	0.86458	19
1.332	0.30646	36	0.47766	29	0.78411	65	0.86439	18
1.333	0.30610	36	0.47737	29	0.78346	64	0.86421	19
1.334	0.30574	36	0.47708	29	0.78282	65	0.86402	18
1.335	0.30538	35	0.47679	29	0.78217	65	0.86384	19
1.336	0.30503	36	0.47650	29	0.78152	64	0.86365	19
1.337	0.30467	36	0.47621	29	0.78088	65	0.86346	19
1.338	0.30431	35	0.47592	29	0.78023	64	0.86327	18
1.339	0.30396	36	0.47563	29	0.77959	65	0.86309	19
1.340	0.30360	35	0.47534	29	0.77894	64	0.86290	19
1.341	0.30325	36	0.47505	29	0.77830	65	0.86271	18
1.342	0.30289	35	0.47476	29	0.77765	64	0.86253	19
1.343	0.30254	35	0.47447	29	0.77701	64	0.86234	19
1.344	0.30219	36	0.47418	29	0.77637	64	0.86215	19
1.345	0.30183	35	0.47389	28	0.77573	64	0.86196	18
1.346	0.30148	35	0.47361	29	0.77509	64	0.86178	19
1.347	0.30113	35	0.47332	29	0.77445	64	0.86159	19
1.348	0.30078	35	0.47303	29	0.77381	64	0.86140	19
1.349	0.30043	35	0.47274	29	0.77317	64	0.86121	19
1.350	0.30008		0.47245		0.77253		0.86102	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.350	0.30008	35	0.47245	28	0.77253	64	0.86102	18
1.351	0.29973	35	0.47217	29	0.77189	63	0.86084	19
1.352	0.29938	35	0.47188	29	0.77126	64	0.86065	19
1.353	0.29903	35	0.47159	29	0.77062	63	0.86046	19
1.354	0.29868	35	0.47130	28	0.76999	64	0.86027	19
1.355	0.29833	34	0.47102	29	0.76935	63	0.86008	19
1.356	0.29799	35	0.47073	29	0.76872	64	0.85989	18
1.357	0.29764	35	0.47044	28	0.76808	63	0.85971	19
1.358	0.29729	34	0.47016	29	0.76745	63	0.85952	19
1.359	0.29695	35	0.46987	29	0.76682	64	0.85933	19
1.360	0.29660	34	0.46958	28	0.76618	63	0.85914	19
1.361	0.29626	35	0.46930	29	0.76555	63	0.85895	19
1.362	0.29591	34	0.46901	29	0.76492	63	0.85876	19
1.363	0.29557	34	0.46872	28	0.76429	63	0.85857	19
1.364	0.29523	35	0.46844	29	0.76366	63	0.85838	19
1.365	0.29488	34	0.46815	28	0.76303	62	0.85819	19
1.366	0.29454	34	0.46787	29	0.76241	63	0.85800	19
1.367	0.29420	34	0.46758	29	0.76178	63	0.85781	19
1.368	0.29386	35	0.46729	28	0.76115	63	0.85762	19
1.369	0.29351	34	0.46701	29	0.76052	62	0.85743	19
1.370	0.29317	34	0.46672	28	0.75990	63	0.85724	19
1.371	0.29283	34	0.46644	29	0.75927	62	0.85705	19
1.372	0.29249	34	0.46615	28	0.75865	63	0.85686	19
1.373	0.29215	34	0.46587	28	0.75802	62	0.85667	19
1.374	0.29181	33	0.46559	29	0.75740	62	0.85648	19
1.375	0.29148	34	0.46530	28	0.75678	63	0.85629	19
1.376	0.29114	34	0.46502	29	0.75615	62	0.85610	19
1.377	0.29080	34	0.46473	28	0.75553	62	0.85591	19
1.378	0.29046	33	0.46445	29	0.75491	62	0.85572	19
1.379	0.29013	34	0.46416	28	0.75429	62	0.85553	19
1.380	0.28979	34	0.46388	28	0.75367	62	0.85534	19
1.381	0.28945	33	0.46360	29	0.75305	62	0.85515	19
1.382	0.28912	34	0.46331	28	0.75243	62	0.85496	19
1.383	0.28878	33	0.46303	28	0.75181	61	0.85477	19
1.384	0.28845	34	0.46275	29	0.75120	62	0.85458	19
1.385	0.28811	33	0.46246	28	0.75058	62	0.85439	20
1.386	0.28778	33	0.46218	28	0.74996	61	0.85419	19
1.387	0.28745	34	0.46190	28	0.74935	62	0.85400	19
1.388	0.28711	33	0.46162	29	0.74873	61	0.85381	19
1.389	0.28678	33	0.46133	28	0.74812	62	0.85362	19
1.390	0.28645	33	0.46105	28	0.74750	61	0.85343	19
1.391	0.28612	33	0.46077	28	0.74689	62	0.85324	19
1.392	0.28579	33	0.46049	29	0.74627	61	0.85305	20
1.393	0.28546	33	0.46020	28	0.74566	61	0.85285	19
1.394	0.28513	33	0.45992	28	0.74505	61	0.85266	19
1.395	0.28480	33	0.45964	28	0.74444	61	0.85247	19
1.396	0.28447	33	0.45936	28	0.74383	61	0.85228	19
1.397	0.28414	33	0.45908	28	0.74322	61	0.85209	20
1.398	0.28381	33	0.45880	28	0.74261	61	0.85189	19
1.399	0.28348	33	0.45852	28	0.74200	61	0.85170	19
1.400	0.28315		0.45824		0.74139		0.85151	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.400	0.28315	32	0.45824	29	0.74139	61	0.85151	19
1.401	0.28283	33	0.45795	28	0.74078	61	0.85132	20
1.402	0.28250	33	0.45767	28	0.74017	60	0.85112	19
1.403	0.28217	32	0.45739	28	0.73957	61	0.85093	19
1.404	0.28185	33	0.45711	28	0.73896	60	0.85074	19
1.405	0.28152	32	0.45683	28	0.73836	61	0.85055	20
1.406	0.28120	33	0.45655	28	0.73775	60	0.85035	19
1.407	0.28087	32	0.45627	28	0.73715	61	0.85016	19
1.408	0.28055	32	0.45599	28	0.73654	60	0.84997	20
1.409	0.28023	33	0.45571	28	0.73594	60	0.84977	19
1.410	0.27990	32	0.45543	28	0.73534	61	0.84958	19
1.411	0.27958	32	0.45515	28	0.73473	60	0.84939	20
1.412	0.27926	32	0.45487	28	0.73413	60	0.84919	19
1.413	0.27894	33	0.45459	27	0.73353	60	0.84900	19
1.414	0.27861	32	0.45432	28	0.73293	60	0.84881	20
1.415	0.27829	32	0.45404	28	0.73233	60	0.84861	19
1.416	0.27797	32	0.45376	28	0.73173	60	0.84842	20
1.417	0.27765	32	0.45348	28	0.73113	60	0.84822	19
1.418	0.27733	32	0.45320	28	0.73053	59	0.84803	19
1.419	0.27701	32	0.45292	28	0.72994	60	0.84784	20
1.420	0.27669	31	0.45264	27	0.72934	60	0.84764	19
1.421	0.27638	32	0.45237	28	0.72874	59	0.84745	20
1.422	0.27606	32	0.45209	28	0.72815	60	0.84725	19
1.423	0.27574	32	0.45181	28	0.72755	59	0.84706	20
1.424	0.27542	31	0.45153	27	0.72696	60	0.84686	19
1.425	0.27511	32	0.45126	28	0.72636	59	0.84667	19
1.426	0.27479	32	0.45098	28	0.72577	60	0.84648	20
1.427	0.27447	31	0.45070	28	0.72517	59	0.84628	19
1.428	0.27416	32	0.45042	27	0.72458	59	0.84609	20
1.429	0.27384	31	0.45015	28	0.72399	59	0.84589	19
1.430	0.27353	32	0.44987	28	0.72340	59	0.84570	20
1.431	0.27321	31	0.44959	27	0.72281	59	0.84550	19
1.432	0.27290	31	0.44932	28	0.72222	59	0.84531	20
1.433	0.27259	32	0.44904	28	0.72163	59	0.84511	19
1.434	0.27227	31	0.44876	27	0.72104	59	0.84492	20
1.435	0.27196	31	0.44849	28	0.72045	59	0.84472	20
1.436	0.27165	31	0.44821	27	0.71986	59	0.84452	19
1.437	0.27134	32	0.44794	28	0.71927	59	0.84433	20
1.438	0.27102	31	0.44766	28	0.71868	58	0.84413	19
1.439	0.27071	31	0.44738	27	0.71810	59	0.84394	20
1.440	0.27040	31	0.44711	28	0.71751	58	0.84374	19
1.441	0.27009	31	0.44683	27	0.71693	59	0.84355	20
1.442	0.26978	31	0.44656	28	0.71634	58	0.84335	20
1.443	0.26947	31	0.44628	27	0.71576	59	0.84315	19
1.444	0.26916	30	0.44601	28	0.71517	58	0.84296	20
1.445	0.26886	31	0.44573	27	0.71459	58	0.84276	19
1.446	0.26855	31	0.44546	28	0.71401	59	0.84257	20
1.447	0.26824	31	0.44518	27	0.71342	58	0.84237	20
1.448	0.26793	31	0.44491	28	0.71284	58	0.84217	19
1.449	0.26762	30	0.44463	27	0.71226	58	0.84198	20
1.450	0.26732		0.44436		0.71168		0.84178	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.450	0.26732	31	0.44436	27	0.71168	58	0.84178	20
1.451	0.26701	30	0.44409	28	0.71110	58	0.84158	19
1.452	0.26671	31	0.44381	27	0.71052	58	0.84139	20
1.453	0.26640	30	0.44354	27	0.70994	58	0.84119	20
1.454	0.26610	31	0.44327	28	0.70936	58	0.84099	19
1.455	0.26579	30	0.44299	27	0.70878	57	0.84080	20
1.456	0.26549	31	0.44272	27	0.70821	58	0.84060	20
1.457	0.26518	30	0.44245	28	0.70763	58	0.84040	20
1.458	0.26488	30	0.44217	27	0.70705	57	0.84020	19
1.459	0.26458	31	0.44190	27	0.70648	58	0.84001	20
1.460	0.26427	30	0.44163	28	0.70590	58	0.83981	20
1.461	0.26397	30	0.44135	27	0.70532	57	0.83961	20
1.462	0.26367	30	0.44108	27	0.70475	57	0.83941	19
1.463	0.26337	30	0.44081	27	0.70418	58	0.83922	20
1.464	0.26307	30	0.44054	28	0.70360	57	0.83902	20
1.465	0.26277	30	0.44026	27	0.70303	57	0.83882	20
1.466	0.26247	30	0.43999	27	0.70246	57	0.83862	19
1.467	0.26217	30	0.43972	27	0.70189	57	0.83843	20
1.468	0.26187	30	0.43945	27	0.70132	58	0.83823	20
1.469	0.26157	30	0.43918	27	0.70074	57	0.83803	20
1.470	0.26127	30	0.43891	28	0.70017	57	0.83783	20
1.471	0.26097	30	0.43863	27	0.69960	56	0.83763	20
1.472	0.26067	30	0.43836	27	0.69904	57	0.83743	19
1.473	0.26037	29	0.43809	27	0.69847	57	0.83724	20
1.474	0.26008	30	0.43782	27	0.69790	57	0.83704	20
1.475	0.25978	30	0.43755	27	0.69733	57	0.83684	20
1.476	0.25948	29	0.43728	27	0.69676	56	0.83664	20
1.477	0.25919	30	0.43701	27	0.69620	57	0.83644	20
1.478	0.25889	29	0.43674	27	0.69563	56	0.83624	20
1.479	0.25860	30	0.43647	27	0.69507	57	0.83604	20
1.480	0.25830	29	0.43620	27	0.69450	56	0.83584	19
1.481	0.25801	30	0.43593	27	0.69394	57	0.83565	20
1.482	0.25771	29	0.43566	27	0.69337	56	0.83545	20
1.483	0.25742	29	0.43539	27	0.69281	56	0.83525	20
1.484	0.25713	30	0.43512	27	0.69225	57	0.83505	20
1.485	0.25683	29	0.43485	27	0.69168	56	0.83485	20
1.486	0.25654	29	0.43458	27	0.69112	56	0.83465	20
1.487	0.25625	29	0.43431	27	0.69056	56	0.83445	20
1.488	0.25596	30	0.43404	27	0.69000	56	0.83425	20
1.489	0.25566	29	0.43377	26	0.68944	56	0.83405	20
1.490	0.25537	29	0.43351	27	0.68888	56	0.83385	20
1.491	0.25508	29	0.43324	27	0.68832	56	0.83365	20
1.492	0.25479	29	0.43297	27	0.68776	56	0.83345	20
1.493	0.25450	29	0.43270	27	0.68720	56	0.83325	20
1.494	0.25421	29	0.43243	27	0.68664	55	0.83305	20
1.495	0.25392	29	0.43216	26	0.68609	56	0.83285	20
1.496	0.25363	28	0.43190	27	0.68553	56	0.83265	20
1.497	0.25335	29	0.43163	27	0.68497	55	0.83245	20
1.498	0.25306	29	0.43136	27	0.68442	56	0.83225	20
1.499	0.25277	29	0.43109	26	0.68386	55	0.83205	20
1.500	0.25248		0.43083		0.68331		0.83185	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F_0 - E_0)/RT$	Δ	$(H_0 - E_0)/RT$	Δ	S_0/R	Δ	C_p^0/R	Δ
1.500	0.25248	28	0.43083	27	0.68331	56	0.83185	20
1.501	0.25220	29	0.43056	27	0.68275	55	0.83165	20
1.502	0.25191	29	0.43029	27	0.68220	55	0.83145	20
1.503	0.25162	28	0.43002	26	0.68165	56	0.83125	20
1.504	0.25134	29	0.42976	27	0.68109	55	0.83105	21
1.505	0.25105	28	0.42949	27	0.68054	55	0.83084	20
1.506	0.25077	29	0.42922	26	0.67999	55	0.83064	20
1.507	0.25048	28	0.42896	27	0.67944	55	0.83044	20
1.508	0.25020	29	0.42869	27	0.67889	55	0.83024	20
1.509	0.24991	28	0.42842	26	0.67834	55	0.83004	20
1.510	0.24963	28	0.42816	27	0.67779	55	0.82984	20
1.511	0.24935	29	0.42789	26	0.67724	55	0.82964	20
1.512	0.24906	28	0.42763	27	0.67669	55	0.82944	21
1.513	0.24878	28	0.42736	26	0.67614	55	0.82923	20
1.514	0.24850	28	0.42710	27	0.67559	54	0.82903	20
1.515	0.24822	29	0.42683	27	0.67505	55	0.82883	20
1.516	0.24793	28	0.42656	26	0.67450	55	0.82863	20
1.517	0.24765	28	0.42630	27	0.67395	54	0.82843	20
1.518	0.24737	28	0.42603	26	0.67341	55	0.82823	21
1.519	0.24709	28	0.42577	26	0.67286	54	0.82802	20
1.520	0.24681	28	0.42551	27	0.67232	55	0.82782	20
1.521	0.24653	28	0.42524	26	0.67177	54	0.82762	20
1.522	0.24625	28	0.42498	27	0.67123	55	0.82742	20
1.523	0.24597	28	0.42471	26	0.67068	54	0.82722	21
1.524	0.24569	27	0.42445	27	0.67014	54	0.82701	20
1.525	0.24542	28	0.42418	26	0.66960	54	0.82681	20
1.526	0.24514	28	0.42392	26	0.66906	54	0.82661	20
1.527	0.24486	28	0.42366	27	0.66852	54	0.82641	21
1.528	0.24458	27	0.42339	26	0.66798	55	0.82620	20
1.529	0.24431	28	0.42313	27	0.66743	54	0.82600	20
1.530	0.24403	28	0.42286	26	0.66689	53	0.82580	20
1.531	0.24375	27	0.42260	26	0.66636	54	0.82560	21
1.532	0.24348	28	0.42234	26	0.66582	54	0.82539	20
1.533	0.24320	27	0.42208	27	0.66528	54	0.82519	20
1.534	0.24293	28	0.42181	26	0.66474	54	0.82499	21
1.535	0.24265	27	0.42155	26	0.66420	54	0.82478	20
1.536	0.24238	28	0.42129	27	0.66366	53	0.82458	20
1.537	0.24210	27	0.42102	26	0.66313	54	0.82438	21
1.538	0.24183	27	0.42076	26	0.66259	53	0.82417	20
1.539	0.24156	28	0.42050	26	0.66206	54	0.82397	20
1.540	0.24128	27	0.42024	26	0.66152	53	0.82377	21
1.541	0.24101	27	0.41998	27	0.66099	54	0.82356	20
1.542	0.24074	27	0.41971	26	0.66045	53	0.82336	20
1.543	0.24047	28	0.41945	26	0.65992	53	0.82316	21
1.544	0.24019	27	0.41919	26	0.65939	54	0.82295	20
1.545	0.23992	27	0.41893	26	0.65885	53	0.82275	21
1.546	0.23965	27	0.41867	26	0.65832	53	0.82254	20
1.547	0.23938	27	0.41841	26	0.65779	53	0.82234	20
1.548	0.23911	27	0.41815	26	0.65726	53	0.82214	21
1.549	0.23884	27	0.41789	27	0.65673	53	0.82193	20
1.550	0.23857		0.41762		0.65620		0.82173	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.550	0.23857	27	0.41762	26	0.65620	53	0.82173	21
1.551	0.23830	27	0.41736	26	0.65567	53	0.82152	20
1.552	0.23803	26	0.41710	26	0.65514	53	0.82132	21
1.553	0.23777	27	0.41684	26	0.65461	53	0.82111	20
1.554	0.23750	27	0.41658	26	0.65408	53	0.82091	20
1.555	0.23723	27	0.41632	26	0.65355	53	0.82071	21
1.556	0.23696	27	0.41606	26	0.65302	52	0.82050	20
1.557	0.23669	26	0.41580	26	0.65250	53	0.82030	21
1.558	0.23643	27	0.41554	26	0.65197	53	0.82009	20
1.559	0.23616	27	0.41528	26	0.65144	52	0.81989	21
1.560	0.23589	26	0.41502	26	0.65092	53	0.81968	20
1.561	0.23563	27	0.41476	25	0.65039	52	0.81948	21
1.562	0.23536	26	0.41451	26	0.64987	53	0.81927	20
1.563	0.23510	27	0.41425	26	0.64934	52	0.81907	21
1.564	0.23483	26	0.41399	26	0.64882	52	0.81886	20
1.565	0.23457	27	0.41373	26	0.64830	53	0.81866	21
1.566	0.23430	26	0.41347	26	0.64777	52	0.81845	20
1.567	0.23404	26	0.41321	26	0.64725	52	0.81825	21
1.568	0.23378	27	0.41295	26	0.64673	52	0.81804	21
1.569	0.23351	26	0.41269	25	0.64621	52	0.81783	20
1.570	0.23325	26	0.41244	26	0.64569	52	0.81763	21
1.571	0.23299	26	0.41218	26	0.64517	52	0.81742	20
1.572	0.23273	27	0.41192	26	0.64465	52	0.81722	21
1.573	0.23246	26	0.41166	25	0.64413	52	0.81701	20
1.574	0.23220	26	0.41141	26	0.64361	52	0.81681	21
1.575	0.23194	26	0.41115	26	0.64309	52	0.81660	21
1.576	0.23168	26	0.41089	26	0.64257	52	0.81639	20
1.577	0.23142	26	0.41063	25	0.64205	51	0.81619	21
1.578	0.23116	26	0.41038	26	0.64154	52	0.81598	20
1.579	0.23090	26	0.41012	26	0.64102	52	0.81578	21
1.580	0.23064	26	0.40986	25	0.64050	51	0.81557	21
1.581	0.23038	26	0.40961	26	0.63999	52	0.81536	20
1.582	0.23012	26	0.40935	26	0.63947	51	0.81516	21
1.583	0.22986	25	0.40909	25	0.63896	52	0.81495	21
1.584	0.22961	26	0.40884	26	0.63844	51	0.81474	20
1.585	0.22935	26	0.40858	26	0.63793	52	0.81454	21
1.586	0.22909	26	0.40832	25	0.63741	51	0.81433	21
1.587	0.22883	25	0.40807	26	0.63690	51	0.81412	20
1.588	0.22858	26	0.40781	25	0.63639	51	0.81392	21
1.589	0.22832	26	0.40756	26	0.63588	52	0.81371	21
1.590	0.22806	25	0.40730	25	0.63536	51	0.81350	20
1.591	0.22781	26	0.40705	26	0.63485	51	0.81330	21
1.592	0.22755	25	0.40679	26	0.63434	51	0.81309	21
1.593	0.22730	26	0.40653	25	0.63383	51	0.81288	21
1.594	0.22704	25	0.40628	25	0.63332	51	0.81267	20
1.595	0.22679	26	0.40603	26	0.63281	51	0.81247	21
1.596	0.22653	25	0.40577	25	0.63230	51	0.81226	21
1.597	0.22628	26	0.40552	26	0.63179	51	0.81205	21
1.598	0.22602	25	0.40526	25	0.63128	50	0.81184	20
1.599	0.22577	25	0.40501	26	0.63078	51	0.81164	21
1.600	0.22552		0.40475		0.63027		0.81143	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.600	0.22552	26	0.40475	25	0.63027	51	0.81143	21
1.601	0.22526	25	0.40450	26	0.62976	50	0.81122	21
1.602	0.22501	25	0.40424	25	0.62926	51	0.81101	20
1.603	0.22476	25	0.40399	25	0.62875	51	0.81081	21
1.604	0.22451	25	0.40374	26	0.62824	50	0.81060	21
1.605	0.22426	26	0.40348	25	0.62774	51	0.81039	21
1.606	0.22400	25	0.40323	25	0.62723	50	0.81018	21
1.607	0.22375	25	0.40298	26	0.62673	50	0.80997	20
1.608	0.22350	25	0.40272	25	0.62623	51	0.80977	21
1.609	0.22325	25	0.40247	25	0.62572	50	0.80956	21
1.610	0.22300	25	0.40222	26	0.62522	50	0.80935	21
1.611	0.22275	25	0.40196	25	0.62472	50	0.80914	21
1.612	0.22250	25	0.40171	25	0.62422	51	0.80893	21
1.613	0.22225	24	0.40146	25	0.62371	50	0.80872	21
1.614	0.22201	25	0.40121	26	0.62321	50	0.80851	20
1.615	0.22176	25	0.40095	25	0.62271	50	0.80831	21
1.616	0.22151	25	0.40070	25	0.62221	50	0.80810	21
1.617	0.22126	25	0.40045	25	0.62171	50	0.80789	21
1.618	0.22101	24	0.40020	25	0.62121	50	0.80768	21
1.619	0.22077	25	0.39995	25	0.62071	49	0.80747	21
1.620	0.22052	25	0.39970	26	0.62022	50	0.80726	21
1.621	0.22027	24	0.39944	25	0.61972	50	0.80705	21
1.622	0.22003	25	0.39919	25	0.61922	50	0.80684	21
1.623	0.21978	24	0.39894	25	0.61872	49	0.80663	20
1.624	0.21954	25	0.39869	25	0.61823	50	0.80643	21
1.625	0.21929	24	0.39844	25	0.61773	50	0.80622	21
1.626	0.21905	25	0.39819	25	0.61723	49	0.80601	21
1.627	0.21880	24	0.39794	25	0.61674	50	0.80580	21
1.628	0.21856	25	0.39769	25	0.61624	49	0.80559	21
1.629	0.21831	24	0.39744	25	0.61575	50	0.80538	21
1.630	0.21807	25	0.39719	25	0.61525	49	0.80517	21
1.631	0.21782	24	0.39694	25	0.61476	49	0.80496	21
1.632	0.21758	24	0.39669	25	0.61427	50	0.80475	21
1.633	0.21734	24	0.39644	25	0.61377	49	0.80454	21
1.634	0.21710	25	0.39619	25	0.61328	49	0.80433	21
1.635	0.21685	24	0.39594	25	0.61279	49	0.80412	21
1.636	0.21661	24	0.39569	25	0.61230	49	0.80391	21
1.637	0.21637	24	0.39544	25	0.61181	49	0.80370	21
1.638	0.21613	24	0.39519	25	0.61132	49	0.80349	21
1.639	0.21589	24	0.39494	25	0.61083	49	0.80328	21
1.640	0.21565	24	0.39469	25	0.61034	49	0.80307	21
1.641	0.21541	24	0.39444	25	0.60985	49	0.80286	21
1.642	0.21517	24	0.39419	25	0.60936	49	0.80265	21
1.643	0.21493	24	0.39394	25	0.60887	49	0.80244	21
1.644	0.21469	24	0.39369	24	0.60838	49	0.80223	21
1.645	0.21445	24	0.39345	25	0.60789	48	0.80202	21
1.646	0.21421	24	0.39320	25	0.60741	49	0.80181	21
1.647	0.21397	24	0.39295	25	0.60692	49	0.80160	21
1.648	0.21373	24	0.39270	25	0.60643	48	0.80139	22
1.649	0.21349	24	0.39245	24	0.60595	49	0.80117	21
1.650	0.21325		0.39221		0.60546		0.80096	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.650	0.21325	23	0.39221	25	0.60546	48	0.80096	21
1.651	0.21302	24	0.39196	25	0.60498	49	0.80075	21
1.652	0.21278	24	0.39171	25	0.60449	48	0.80054	21
1.653	0.21254	23	0.39146	24	0.60401	49	0.80033	21
1.654	0.21231	24	0.39122	25	0.60352	48	0.80012	21
1.655	0.21207	24	0.39097	25	0.60304	48	0.79991	21
1.656	0.21183	23	0.39072	25	0.60256	49	0.79970	21
1.657	0.21160	24	0.39047	24	0.60207	48	0.79949	22
1.658	0.21136	23	0.39023	25	0.60159	48	0.79927	21
1.659	0.21113	24	0.38998	25	0.60111	48	0.79906	21
1.660	0.21089	23	0.38973	24	0.60063	48	0.79885	21
1.661	0.21066	24	0.38949	25	0.60015	48	0.79864	21
1.662	0.21042	23	0.38924	24	0.59967	48	0.79843	21
1.663	0.21019	23	0.38900	25	0.59919	48	0.79822	21
1.664	0.20996	24	0.38875	25	0.59871	48	0.79801	22
1.665	0.20972	23	0.38850	24	0.59823	48	0.79779	21
1.666	0.20949	23	0.38826	25	0.59775	48	0.79758	21
1.667	0.20926	24	0.38801	24	0.59727	48	0.79737	21
1.668	0.20902	23	0.38777	25	0.59679	48	0.79716	21
1.669	0.20879	23	0.38752	24	0.59631	47	0.79695	22
1.670	0.20856	23	0.38728	25	0.59584	48	0.79673	21
1.671	0.20833	23	0.38703	24	0.59536	48	0.79652	21
1.672	0.20810	24	0.38679	25	0.59488	47	0.79631	21
1.673	0.20786	23	0.38654	24	0.59441	48	0.79610	21
1.674	0.20763	23	0.38630	25	0.59393	47	0.79589	22
1.675	0.20740	23	0.38605	24	0.59346	48	0.79567	21
1.676	0.20717	23	0.38581	25	0.59298	47	0.79546	21
1.677	0.20694	23	0.38556	24	0.59251	48	0.79525	21
1.678	0.20671	23	0.38532	25	0.59203	47	0.79504	22
1.679	0.20648	23	0.38507	24	0.59156	47	0.79482	21
1.680	0.20625	22	0.38483	24	0.59109	48	0.79461	21
1.681	0.20603	23	0.38459	25	0.59061	47	0.79440	22
1.682	0.20580	23	0.38434	24	0.59014	47	0.79418	21
1.683	0.20557	23	0.38410	24	0.58967	47	0.79397	21
1.684	0.20534	23	0.38386	25	0.58920	47	0.79376	21
1.685	0.20511	22	0.38361	24	0.58873	48	0.79355	22
1.686	0.20489	23	0.38337	24	0.58825	47	0.79333	21
1.687	0.20466	23	0.38313	25	0.58778	47	0.79312	21
1.688	0.20443	23	0.38288	24	0.58731	47	0.79291	22
1.689	0.20420	22	0.38264	24	0.58684	46	0.79269	21
1.690	0.20398	23	0.38240	24	0.58638	47	0.79248	21
1.691	0.20375	22	0.38216	25	0.58591	47	0.79227	22
1.692	0.20353	23	0.38191	24	0.58544	47	0.79205	21
1.693	0.20330	23	0.38167	24	0.58497	47	0.79184	21
1.694	0.20307	22	0.38143	24	0.58450	46	0.79163	22
1.695	0.20285	22	0.38119	25	0.58404	47	0.79141	21
1.696	0.20263	23	0.38094	24	0.58357	47	0.79120	21
1.697	0.20240	22	0.38070	24	0.58310	46	0.79099	22
1.698	0.20218	23	0.38046	24	0.58264	47	0.79077	21
1.699	0.20195	22	0.38022	24	0.58217	46	0.79056	22
1.700	0.20173		0.37998		0.58171		0.79034	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.700	0.20173	22	0.37998	24	0.58171	47	0.79034	21
1.701	0.20151	23	0.37974	24	0.58124	46	0.79013	21
1.702	0.20128	22	0.37950	25	0.58078	47	0.78992	22
1.703	0.20106	22	0.37925	24	0.58031	46	0.78970	21
1.704	0.20084	23	0.37901	24	0.57985	46	0.78949	21
1.705	0.20061	22	0.37877	24	0.57939	47	0.78928	22
1.706	0.20039	22	0.37853	24	0.57892	46	0.78906	21
1.707	0.20017	22	0.37829	24	0.57846	46	0.78885	22
1.708	0.19995	22	0.37805	24	0.57800	46	0.78863	21
1.709	0.19973	22	0.37781	24	0.57754	46	0.78842	22
1.710	0.19951	22	0.37757	24	0.57708	46	0.78820	21
1.711	0.19929	22	0.37733	24	0.57662	46	0.78799	22
1.712	0.19907	22	0.37709	24	0.57616	46	0.78777	21
1.713	0.19885	22	0.37685	24	0.57570	46	0.78756	21
1.714	0.19863	22	0.37661	24	0.57524	46	0.78735	22
1.715	0.19841	22	0.37637	24	0.57478	46	0.78713	21
1.716	0.19819	22	0.37613	24	0.57432	46	0.78692	22
1.717	0.19797	22	0.37589	24	0.57386	46	0.78670	21
1.718	0.19775	22	0.37565	24	0.57340	46	0.78649	22
1.719	0.19753	22	0.37541	24	0.57294	45	0.78627	21
1.720	0.19731	22	0.37517	23	0.57249	46	0.78606	22
1.721	0.19709	21	0.37494	24	0.57203	46	0.78584	21
1.722	0.19688	22	0.37470	24	0.57157	45	0.78563	22
1.723	0.19666	22	0.37446	24	0.57112	46	0.78541	21
1.724	0.19644	21	0.37422	24	0.57066	45	0.78520	22
1.725	0.19623	22	0.37398	24	0.57021	46	0.78498	21
1.726	0.19601	22	0.37374	23	0.56975	45	0.78477	22
1.727	0.19579	21	0.37351	24	0.56930	46	0.78455	21
1.728	0.19558	22	0.37327	24	0.56884	45	0.78434	22
1.729	0.19536	22	0.37303	24	0.56839	45	0.78412	22
1.730	0.19514	21	0.37279	24	0.56794	46	0.78390	21
1.731	0.19493	22	0.37255	23	0.56748	45	0.78369	22
1.732	0.19471	21	0.37232	24	0.56703	45	0.78347	21
1.733	0.19450	22	0.37208	24	0.56658	45	0.78326	22
1.734	0.19428	21	0.37184	23	0.56613	45	0.78304	21
1.735	0.19407	21	0.37161	24	0.56568	45	0.78283	22
1.736	0.19386	22	0.37137	24	0.56523	46	0.78261	22
1.737	0.19364	21	0.37113	23	0.56477	45	0.78239	21
1.738	0.19343	21	0.37090	24	0.56432	45	0.78218	22
1.739	0.19322	22	0.37066	24	0.56387	44	0.78196	21
1.740	0.19300	21	0.37042	23	0.56343	45	0.78175	22
1.741	0.19279	21	0.37019	24	0.56298	45	0.78153	22
1.742	0.19258	21	0.36995	24	0.56253	45	0.78131	21
1.743	0.19237	22	0.36971	23	0.56208	45	0.78110	22
1.744	0.19215	21	0.36948	24	0.56163	45	0.78088	21
1.745	0.19194	21	0.36924	23	0.56118	44	0.78067	22
1.746	0.19173	21	0.36901	24	0.56074	45	0.78045	22
1.747	0.19152	21	0.36877	24	0.56029	45	0.78023	21
1.748	0.19131	21	0.36853	23	0.55984	44	0.78002	22
1.749	0.19110	21	0.36830	24	0.55940	45	0.77980	22
1.750	0.19089		0.36806		0.55895		0.77958	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^\circ - E_0)/RT$	Δ	$(H^\circ - E_0)/RT$	Δ	S°/R	Δ	C_p°/R	Δ
1.750	0.19089	21	0.36806	23	0.55895	44	0.77958	21
1.751	0.19068	21	0.36783	24	0.55851	45	0.77937	22
1.752	0.19047	21	0.36759	23	0.55806	44	0.77915	22
1.753	0.19026	21	0.36736	24	0.55762	45	0.77893	21
1.754	0.19005	21	0.36712	23	0.55717	44	0.77872	22
1.755	0.18984	21	0.36689	23	0.55673	44	0.77850	22
1.756	0.18963	21	0.36666	24	0.55629	45	0.77828	21
1.757	0.18942	21	0.36642	23	0.55584	44	0.77807	22
1.758	0.18921	21	0.36619	24	0.55540	44	0.77785	22
1.759	0.18900	20	0.36595	23	0.55496	44	0.77763	21
1.760	0.18880	21	0.36572	23	0.55452	45	0.77742	22
1.761	0.18859	21	0.36549	24	0.55407	44	0.77720	22
1.762	0.18838	21	0.36525	23	0.55363	44	0.77698	22
1.763	0.18817	20	0.36502	24	0.55319	44	0.77676	21
1.764	0.18797	21	0.36478	23	0.55275	44	0.77655	22
1.765	0.18776	21	0.36455	23	0.55231	44	0.77633	22
1.766	0.18755	20	0.36432	24	0.55187	44	0.77611	21
1.767	0.18735	21	0.36408	23	0.55143	44	0.77590	22
1.768	0.18714	20	0.36385	23	0.55099	43	0.77568	22
1.769	0.18694	21	0.36362	23	0.55056	44	0.77546	22
1.770	0.18673	20	0.36339	24	0.55012	44	0.77524	21
1.771	0.18653	21	0.36315	23	0.54968	44	0.77503	22
1.772	0.18632	20	0.36292	23	0.54924	44	0.77481	22
1.773	0.18612	21	0.36269	23	0.54880	43	0.77459	22
1.774	0.18591	20	0.36246	24	0.54837	44	0.77437	22
1.775	0.18571	21	0.36222	23	0.54793	43	0.77415	21
1.776	0.18550	20	0.36199	23	0.54750	44	0.77394	22
1.777	0.18530	20	0.36176	23	0.54706	44	0.77372	22
1.778	0.18510	21	0.36153	23	0.54662	43	0.77350	22
1.779	0.18489	20	0.36130	23	0.54619	43	0.77328	22
1.780	0.18469	20	0.36107	24	0.54576	44	0.77306	21
1.781	0.18449	21	0.36083	23	0.54532	43	0.77285	22
1.782	0.18428	20	0.36060	23	0.54489	44	0.77263	22
1.783	0.18408	20	0.36037	23	0.54445	43	0.77241	22
1.784	0.18388	20	0.36014	23	0.54402	43	0.77219	22
1.785	0.18368	20	0.35991	23	0.54359	43	0.77197	22
1.786	0.18348	20	0.35968	23	0.54316	44	0.77175	21
1.787	0.18328	20	0.35945	23	0.54272	43	0.77154	22
1.788	0.18308	21	0.35922	23	0.54229	43	0.77132	22
1.789	0.18287	20	0.35899	23	0.54186	43	0.77110	22
1.790	0.18267	20	0.35876	23	0.54143	43	0.77088	22
1.791	0.18247	20	0.35853	23	0.54100	43	0.77066	22
1.792	0.18227	20	0.35830	23	0.54057	43	0.77044	21
1.793	0.18207	20	0.35807	23	0.54014	43	0.77023	22
1.794	0.18187	20	0.35784	23	0.53971	43	0.77001	22
1.795	0.18167	19	0.35761	23	0.53928	43	0.76979	22
1.796	0.18148	20	0.35738	23	0.53885	43	0.76957	22
1.797	0.18128	20	0.35715	23	0.53842	42	0.76935	22
1.798	0.18108	20	0.35692	23	0.53800	43	0.76913	22
1.799	0.18088	20	0.35669	23	0.53757	43	0.76891	22
1.800	0.18068		0.35646		0.53714		0.76869	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.800	0.18068	20	0.35646	23	0.53714	42	0.76869	22
1.801	0.18048	19	0.35623	23	0.53672	43	0.76847	22
1.802	0.18029	20	0.35600	23	0.53629	43	0.76825	21
1.803	0.18009	20	0.35577	22	0.53586	42	0.76804	22
1.804	0.17989	20	0.35555	23	0.53544	43	0.76782	22
1.805	0.17969	19	0.35532	23	0.53501	42	0.76760	22
1.806	0.17950	20	0.35509	23	0.53459	43	0.76738	22
1.807	0.17930	20	0.35486	23	0.53416	42	0.76716	22
1.808	0.17910	19	0.35463	23	0.53374	43	0.76694	22
1.809	0.17891	20	0.35440	22	0.53331	42	0.76672	22
1.810	0.17871	19	0.35418	23	0.53289	42	0.76650	22
1.811	0.17852	20	0.35395	23	0.53247	43	0.76628	22
1.812	0.17832	19	0.35372	23	0.53204	42	0.76606	22
1.813	0.17813	20	0.35349	22	0.53162	42	0.76584	22
1.814	0.17793	19	0.35327	23	0.53120	42	0.76562	22
1.815	0.17774	20	0.35304	23	0.53078	43	0.76540	22
1.816	0.17754	19	0.35281	23	0.53035	42	0.76518	22
1.817	0.17735	19	0.35258	22	0.52993	42	0.76496	22
1.818	0.17716	20	0.35236	23	0.52951	42	0.76474	22
1.819	0.17696	19	0.35213	23	0.52909	42	0.76452	22
1.820	0.17677	20	0.35190	22	0.52867	42	0.76430	22
1.821	0.17657	19	0.35168	23	0.52825	42	0.76408	22
1.822	0.17638	19	0.35145	22	0.52783	42	0.76386	22
1.823	0.17619	19	0.35123	23	0.52741	41	0.76364	22
1.824	0.17600	20	0.35100	23	0.52700	42	0.76342	22
1.825	0.17580	19	0.35077	22	0.52658	42	0.76320	22
1.826	0.17561	19	0.35055	23	0.52616	42	0.76298	22
1.827	0.17542	19	0.35032	22	0.52574	42	0.76276	22
1.828	0.17523	19	0.35010	23	0.52532	41	0.76254	22
1.829	0.17504	19	0.34987	23	0.52491	42	0.76232	22
1.830	0.17485	20	0.34964	22	0.52449	42	0.76210	22
1.831	0.17465	19	0.34942	23	0.52407	41	0.76188	22
1.832	0.17446	19	0.34919	22	0.52366	42	0.76166	22
1.833	0.17427	19	0.34897	23	0.52324	41	0.76144	22
1.834	0.17408	19	0.34874	22	0.52283	42	0.76122	22
1.835	0.17389	19	0.34852	23	0.52241	41	0.76100	22
1.836	0.17370	19	0.34829	22	0.52200	42	0.76078	22
1.837	0.17351	19	0.34807	22	0.52158	41	0.76056	22
1.838	0.17332	18	0.34785	23	0.52117	41	0.76034	22
1.839	0.17314	19	0.34762	22	0.52076	42	0.76012	23
1.840	0.17295	19	0.34740	23	0.52034	41	0.75989	22
1.841	0.17276	19	0.34717	22	0.51993	41	0.75967	22
1.842	0.17257	19	0.34695	23	0.51952	41	0.75945	22
1.843	0.17238	19	0.34672	22	0.51911	42	0.75923	22
1.844	0.17219	18	0.34650	22	0.51869	41	0.75901	22
1.845	0.17201	19	0.34628	23	0.51828	41	0.75879	22
1.846	0.17182	19	0.34605	22	0.51787	41	0.75857	22
1.847	0.17163	19	0.34583	22	0.51746	41	0.75835	22
1.848	0.17144	18	0.34561	23	0.51705	41	0.75813	23
1.849	0.17126	19	0.34538	22	0.51664	41	0.75790	22
1.850	0.17107		0.34516		0.51623		0.75768	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.850	0.17107	19	0.34516	22	0.51623	41	0.75768	22
1.851	0.17088	18	0.34494	22	0.51582	41	0.75746	22
1.852	0.17070	19	0.34472	23	0.51541	41	0.75724	22
1.853	0.17051	18	0.34449	22	0.51500	40	0.75702	22
1.854	0.17033	19	0.34427	22	0.51460	41	0.75680	22
1.855	0.17014	19	0.34405	22	0.51419	41	0.75658	22
1.856	0.16995	18	0.34383	23	0.51378	41	0.75636	23
1.857	0.16977	19	0.34360	22	0.51337	41	0.75613	22
1.858	0.16958	18	0.34338	22	0.51296	40	0.75591	22
1.859	0.16940	19	0.34316	22	0.51256	41	0.75569	22
1.860	0.16921	18	0.34294	22	0.51215	40	0.75547	22
1.861	0.16903	18	0.34272	23	0.51175	41	0.75525	22
1.862	0.16885	19	0.34249	22	0.51134	40	0.75503	23
1.863	0.16866	18	0.34227	22	0.51094	41	0.75480	22
1.864	0.16848	18	0.34205	22	0.51053	40	0.75458	22
1.865	0.16830	19	0.34183	22	0.51013	41	0.75436	22
1.866	0.16811	18	0.34161	22	0.50972	40	0.75414	22
1.867	0.16793	18	0.34139	22	0.50932	41	0.75392	23
1.868	0.16775	19	0.34117	22	0.50891	40	0.75369	22
1.869	0.16756	18	0.34095	22	0.50851	40	0.75347	22
1.870	0.16738	18	0.34073	23	0.50811	41	0.75325	22
1.871	0.16720	18	0.34050	22	0.50770	40	0.75303	22
1.872	0.16702	18	0.34028	22	0.50730	40	0.75281	23
1.873	0.16684	18	0.34006	22	0.50690	40	0.75258	22
1.874	0.16666	19	0.33984	22	0.50650	40	0.75236	22
1.875	0.16647	18	0.33962	22	0.50610	40	0.75214	22
1.876	0.16629	18	0.33940	22	0.50570	40	0.75192	23
1.877	0.16611	18	0.33918	22	0.50530	40	0.75169	22
1.878	0.16593	18	0.33896	22	0.50490	40	0.75147	22
1.879	0.16575	18	0.33874	22	0.50450	40	0.75125	22
1.880	0.16557	18	0.33852	21	0.50410	40	0.75103	23
1.881	0.16539	18	0.33831	22	0.50370	40	0.75080	22
1.882	0.16521	18	0.33809	22	0.50330	40	0.75058	22
1.883	0.16503	18	0.33787	22	0.50290	40	0.75036	22
1.884	0.16485	18	0.33765	22	0.50250	40	0.75014	23
1.885	0.16467	18	0.33743	22	0.50210	40	0.74991	22
1.886	0.16449	17	0.33721	22	0.50170	39	0.74969	22
1.887	0.16432	18	0.33699	22	0.50131	40	0.74947	23
1.888	0.16414	18	0.33677	22	0.50091	40	0.74924	22
1.889	0.16396	18	0.33655	21	0.50051	39	0.74902	22
1.890	0.16378	18	0.33634	22	0.50012	40	0.74880	22
1.891	0.16360	17	0.33612	22	0.49972	39	0.74858	23
1.892	0.16343	18	0.33590	22	0.49933	40	0.74835	22
1.893	0.16325	18	0.33568	22	0.49893	39	0.74813	22
1.894	0.16307	18	0.33546	21	0.49854	40	0.74791	23
1.895	0.16289	17	0.33525	22	0.49814	39	0.74768	22
1.896	0.16272	18	0.33503	22	0.49775	40	0.74746	22
1.897	0.16254	18	0.33481	22	0.49735	39	0.74724	23
1.898	0.16236	17	0.33459	21	0.49696	40	0.74701	22
1.899	0.16219	18	0.33438	22	0.49656	39	0.74679	22
1.900	0.16201		0.33416		0.49617		0.74657	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.900	0.16201	17	0.33416	22	0.49617	39	0.74657	23
1.901	0.16184	18	0.33394	21	0.49578	39	0.74634	22
1.902	0.16166	18	0.33373	22	0.49539	40	0.74612	22
1.903	0.16148	17	0.33351	22	0.49499	39	0.74590	23
1.904	0.16131	18	0.33329	21	0.49460	39	0.74567	22
1.905	0.16113	17	0.33308	22	0.49421	39	0.74545	22
1.906	0.16096	17	0.33286	22	0.49382	39	0.74523	23
1.907	0.16079	18	0.33264	21	0.49343	39	0.74500	22
1.908	0.16061	17	0.33243	22	0.49304	39	0.74478	22
1.909	0.16044	18	0.33221	21	0.49265	39	0.74456	23
1.910	0.16026	17	0.33200	22	0.49226	39	0.74433	22
1.911	0.16009	17	0.33178	22	0.49187	39	0.74411	22
1.912	0.15992	18	0.33156	21	0.49148	39	0.74389	23
1.913	0.15974	17	0.33135	22	0.49109	39	0.74366	22
1.914	0.15957	17	0.33113	21	0.49070	39	0.74344	23
1.915	0.15940	18	0.33092	22	0.49031	38	0.74321	22
1.916	0.15922	17	0.33070	21	0.48993	39	0.74299	22
1.917	0.15905	17	0.33049	22	0.48954	39	0.74277	23
1.918	0.15888	17	0.33027	21	0.48915	39	0.74254	22
1.919	0.15871	17	0.33006	22	0.48876	38	0.74232	23
1.920	0.15854	18	0.32984	21	0.48838	39	0.74209	22
1.921	0.15836	17	0.32963	22	0.48799	38	0.74187	22
1.922	0.15819	17	0.32941	21	0.48761	39	0.74165	23
1.923	0.15802	17	0.32920	22	0.48722	39	0.74142	22
1.924	0.15785	17	0.32898	21	0.48683	38	0.74120	23
1.925	0.15768	17	0.32877	21	0.48645	39	0.74097	22
1.926	0.15751	17	0.32856	22	0.48606	38	0.74075	23
1.927	0.15734	17	0.32834	21	0.48568	38	0.74052	22
1.928	0.15717	17	0.32813	22	0.48530	39	0.74030	22
1.929	0.15700	17	0.32791	21	0.48491	38	0.74008	23
1.930	0.15683	17	0.32770	21	0.48453	38	0.73985	22
1.931	0.15666	17	0.32749	22	0.48415	39	0.73963	23
1.932	0.15649	17	0.32727	21	0.48376	38	0.73940	22
1.933	0.15632	17	0.32706	21	0.48338	38	0.73918	23
1.934	0.15615	17	0.32685	22	0.48300	38	0.73895	22
1.935	0.15598	17	0.32663	21	0.48262	39	0.73873	23
1.936	0.15581	17	0.32642	21	0.48223	38	0.73850	22
1.937	0.15564	16	0.32621	21	0.48185	38	0.73828	22
1.938	0.15548	17	0.32600	22	0.48147	38	0.73806	23
1.939	0.15531	17	0.32578	21	0.48109	38	0.73783	22
1.940	0.15514	17	0.32557	21	0.48071	38	0.73761	23
1.941	0.15497	17	0.32536	21	0.48033	38	0.73738	22
1.942	0.15480	16	0.32515	22	0.47995	38	0.73716	23
1.943	0.15464	17	0.32493	21	0.47957	38	0.73693	22
1.944	0.15447	17	0.32472	21	0.47919	38	0.73671	23
1.945	0.15430	16	0.32451	21	0.47881	37	0.73648	22
1.946	0.15414	17	0.32430	21	0.47844	38	0.73626	23
1.947	0.15397	17	0.32409	21	0.47806	38	0.73603	22
1.948	0.15380	16	0.32388	22	0.47768	38	0.73581	23
1.949	0.15364	17	0.32366	21	0.47730	38	0.73558	22
1.950	0.15347		0.32345		0.47692		0.73536	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
1.950	0.15347	17	0.32345	21	0.47692	37	0.73536	23
1.951	0.15330	16	0.32324	21	0.47655	38	0.73513	22
1.952	0.15314	17	0.32303	21	0.47617	38	0.73491	23
1.953	0.15297	16	0.32282	21	0.47579	37	0.73468	22
1.954	0.15281	17	0.32261	21	0.47542	38	0.73446	23
1.955	0.15264	16	0.32240	21	0.47504	37	0.73423	22
1.956	0.15248	17	0.32219	21	0.47467	38	0.73401	23
1.957	0.15231	16	0.32198	21	0.47429	37	0.73378	23
1.958	0.15215	16	0.32177	21	0.47392	38	0.73355	22
1.959	0.15199	17	0.32156	21	0.47354	37	0.73333	23
1.960	0.15182	16	0.32135	21	0.47317	38	0.73310	22
1.961	0.15166	17	0.32114	21	0.47279	37	0.73288	23
1.962	0.15149	16	0.32093	21	0.47242	37	0.73265	22
1.963	0.15133	16	0.32072	21	0.47205	38	0.73243	23
1.964	0.15117	17	0.32051	21	0.47167	37	0.73220	22
1.965	0.15100	16	0.32030	21	0.47130	37	0.73198	23
1.966	0.15084	16	0.32009	21	0.47093	37	0.73175	22
1.967	0.15068	16	0.31988	21	0.47056	37	0.73153	23
1.968	0.15052	17	0.31967	21	0.47019	38	0.73130	23
1.969	0.15035	16	0.31946	21	0.46981	37	0.73107	22
1.970	0.15019	16	0.31925	21	0.46944	37	0.73085	23
1.971	0.15003	16	0.31904	21	0.46907	37	0.73062	22
1.972	0.14987	16	0.31883	20	0.46870	37	0.73040	23
1.973	0.14971	17	0.31863	21	0.46833	37	0.73017	23
1.974	0.14954	16	0.31842	21	0.46796	37	0.72994	22
1.975	0.14938	16	0.31821	21	0.46759	37	0.72972	23
1.976	0.14922	16	0.31800	21	0.46722	37	0.72949	22
1.977	0.14906	16	0.31779	21	0.46685	36	0.72927	23
1.978	0.14890	16	0.31758	20	0.46649	37	0.72904	23
1.979	0.14874	16	0.31738	21	0.46612	37	0.72881	22
1.980	0.14858	16	0.31717	21	0.46575	37	0.72859	23
1.981	0.14842	16	0.31696	21	0.46538	37	0.72836	22
1.982	0.14826	16	0.31675	20	0.46501	36	0.72814	23
1.983	0.14810	16	0.31655	21	0.46465	37	0.72791	23
1.984	0.14794	16	0.31634	21	0.46428	37	0.72768	22
1.985	0.14778	16	0.31613	21	0.46391	36	0.72746	23
1.986	0.14762	16	0.31592	20	0.46355	37	0.72723	22
1.987	0.14746	16	0.31572	21	0.46318	37	0.72701	23
1.988	0.14730	15	0.31551	21	0.46281	36	0.72678	23
1.989	0.14715	16	0.31530	20	0.46245	37	0.72655	22
1.990	0.14699	16	0.31510	21	0.46208	36	0.72633	23
1.991	0.14683	16	0.31489	21	0.46172	37	0.72610	23
1.992	0.14667	16	0.31468	20	0.46135	36	0.72587	22
1.993	0.14651	15	0.31448	21	0.46099	36	0.72565	23
1.994	0.14636	16	0.31427	21	0.46063	37	0.72542	23
1.995	0.14620	16	0.31406	20	0.46026	36	0.72519	22
1.996	0.14604	16	0.31386	21	0.45990	36	0.72497	23
1.997	0.14588	15	0.31365	20	0.45954	37	0.72474	23
1.998	0.14573	16	0.31345	21	0.45917	36	0.72451	22
1.999	0.14557	16	0.31324	20	0.45881	36	0.72429	23
2.000	0.14541		0.31304		0.45845		0.72406	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.000	0.14541	15	0.31304	21	0.45845	36	0.72406	23
2.001	0.14526	16	0.31283	21	0.45809	36	0.72383	22
2.002	0.14510	16	0.31262	20	0.45773	37	0.72361	23
2.003	0.14494	15	0.31242	21	0.45736	36	0.72338	23
2.004	0.14479	16	0.31221	20	0.45700	36	0.72315	22
2.005	0.14463	15	0.31201	21	0.45664	36	0.72293	23
2.006	0.14448	16	0.31180	20	0.45628	36	0.72270	23
2.007	0.14432	15	0.31160	21	0.45592	36	0.72247	22
2.008	0.14417	16	0.31139	20	0.45556	36	0.72225	23
2.009	0.14401	15	0.31119	20	0.45520	36	0.72202	23
2.010	0.14386	16	0.31099	21	0.45484	36	0.72179	22
2.011	0.14370	15	0.31078	20	0.45448	35	0.72157	23
2.012	0.14355	16	0.31058	21	0.45413	36	0.72134	23
2.013	0.14339	15	0.31037	20	0.45377	36	0.72111	22
2.014	0.14324	15	0.31017	20	0.45341	36	0.72089	23
2.015	0.14309	16	0.30997	21	0.45305	36	0.72066	23
2.016	0.14293	15	0.30976	20	0.45269	35	0.72043	23
2.017	0.14278	15	0.30956	21	0.45234	36	0.72020	22
2.018	0.14263	16	0.30935	20	0.45198	36	0.71998	23
2.019	0.14247	15	0.30915	20	0.45162	35	0.71975	23
2.020	0.14232	15	0.30895	21	0.45127	36	0.71952	22
2.021	0.14217	16	0.30874	20	0.45091	36	0.71930	23
2.022	0.14201	15	0.30854	20	0.45055	35	0.71907	23
2.023	0.14186	15	0.30834	20	0.45020	36	0.71884	23
2.024	0.14171	15	0.30814	21	0.44984	35	0.71861	22
2.025	0.14156	16	0.30793	20	0.44949	36	0.71839	23
2.026	0.14140	15	0.30773	20	0.44913	35	0.71816	23
2.027	0.14125	15	0.30753	20	0.44878	35	0.71793	23
2.028	0.14110	15	0.30733	21	0.44843	36	0.71770	22
2.029	0.14095	15	0.30712	20	0.44807	35	0.71748	23
2.030	0.14080	15	0.30692	20	0.44772	35	0.71725	23
2.031	0.14065	15	0.30672	20	0.44737	36	0.71702	23
2.032	0.14050	15	0.30652	21	0.44701	35	0.71679	22
2.033	0.14035	16	0.30631	20	0.44666	35	0.71657	23
2.034	0.14019	15	0.30611	20	0.44631	35	0.71634	23
2.035	0.14004	15	0.30591	20	0.44596	36	0.71611	23
2.036	0.13989	15	0.30571	20	0.44560	35	0.71588	22
2.037	0.13974	15	0.30551	20	0.44525	35	0.71566	23
2.038	0.13959	15	0.30531	20	0.44490	35	0.71543	23
2.039	0.13944	14	0.30511	21	0.44455	35	0.71520	23
2.040	0.13930	15	0.30490	20	0.44420	35	0.71497	22
2.041	0.13915	15	0.30470	20	0.44385	35	0.71475	23
2.042	0.13900	15	0.30450	20	0.44350	35	0.71452	23
2.043	0.13885	15	0.30430	20	0.44315	35	0.71429	23
2.044	0.13870	15	0.30410	20	0.44280	35	0.71406	23
2.045	0.13855	15	0.30390	20	0.44245	35	0.71383	22
2.046	0.13840	15	0.30370	20	0.44210	35	0.71361	23
2.047	0.13825	15	0.30350	20	0.44175	34	0.71338	23
2.048	0.13810	14	0.30330	20	0.44141	35	0.71315	23
2.049	0.13796	15	0.30310	20	0.44106	35	0.71292	23
2.050	0.13781		0.30290		0.44071		0.71269	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0)/RT$	Δ	$(H^{\circ}-E_0)/RT$	Δ	S°/R	Δ	C_p°/R	Δ
2.050	0.13781	15	0.30290	20	0.44071	35	0.71269	22
2.051	0.13766	15	0.30270	20	0.44036	35	0.71247	23
2.052	0.13751	14	0.30250	20	0.44001	34	0.71224	23
2.053	0.13737	15	0.30230	20	0.43967	35	0.71201	23
2.054	0.13722	15	0.30210	20	0.43932	35	0.71178	23
2.055	0.13707	14	0.30190	20	0.43897	34	0.71155	22
2.056	0.13693	15	0.30170	20	0.43863	35	0.71133	23
2.057	0.13678	15	0.30150	20	0.43828	34	0.71110	23
2.058	0.13663	14	0.30130	19	0.43794	35	0.71087	23
2.059	0.13649	15	0.30111	20	0.43759	34	0.71064	23
2.060	0.13634	15	0.30091	20	0.43725	35	0.71041	22
2.061	0.13619	14	0.30071	20	0.43690	34	0.71019	23
2.062	0.13605	15	0.30051	20	0.43656	35	0.70996	23
2.063	0.13590	14	0.30031	20	0.43621	34	0.70973	23
2.064	0.13576	15	0.30011	20	0.43587	34	0.70950	23
2.065	0.13561	14	0.29991	19	0.43553	35	0.70927	23
2.066	0.13547	15	0.29972	20	0.43518	34	0.70904	22
2.067	0.13532	14	0.29952	20	0.43484	34	0.70882	23
2.068	0.13518	15	0.29932	20	0.43450	35	0.70859	23
2.069	0.13503	14	0.29912	20	0.43415	34	0.70836	23
2.070	0.13489	15	0.29892	19	0.43381	34	0.70813	23
2.071	0.13474	14	0.29873	20	0.43347	34	0.70790	23
2.072	0.13460	14	0.29853	20	0.43313	34	0.70767	23
2.073	0.13446	15	0.29833	20	0.43279	34	0.70744	22
2.074	0.13431	14	0.29813	19	0.43245	34	0.70722	23
2.075	0.13417	15	0.29794	20	0.43211	35	0.70699	23
2.076	0.13402	14	0.29774	20	0.43176	34	0.70676	23
2.077	0.13388	14	0.29754	19	0.43142	34	0.70653	23
2.078	0.13374	15	0.29735	20	0.43108	34	0.70630	23
2.079	0.13359	14	0.29715	20	0.43074	34	0.70607	23
2.080	0.13345	14	0.29695	19	0.43040	33	0.70584	22
2.081	0.13331	14	0.29676	20	0.43007	34	0.70562	23
2.082	0.13317	15	0.29656	20	0.42973	34	0.70539	23
2.083	0.13302	14	0.29636	19	0.42939	34	0.70516	23
2.084	0.13288	14	0.29617	20	0.42905	34	0.70493	23
2.085	0.13274	14	0.29597	19	0.42871	34	0.70470	23
2.086	0.13260	14	0.29578	20	0.42837	33	0.70447	23
2.087	0.13246	15	0.29558	20	0.42804	34	0.70424	23
2.088	0.13231	14	0.29538	19	0.42770	34	0.70401	23
2.089	0.13217	14	0.29519	20	0.42736	33	0.70378	22
2.090	0.13203	14	0.29499	19	0.42703	34	0.70356	23
2.091	0.13189	14	0.29480	20	0.42669	34	0.70333	23
2.092	0.13175	14	0.29460	19	0.42635	33	0.70310	23
2.093	0.13161	14	0.29441	20	0.42602	34	0.70287	23
2.094	0.13147	14	0.29421	19	0.42568	33	0.70264	23
2.095	0.13133	14	0.29402	20	0.42535	34	0.70241	23
2.096	0.13119	14	0.29382	19	0.42501	33	0.70218	23
2.097	0.13105	14	0.29363	20	0.42468	34	0.70195	23
2.098	0.13091	14	0.29343	19	0.42434	33	0.70172	22
2.099	0.13077	14	0.29324	20	0.42401	34	0.70150	23
2.100	0.13063		0.29304		0.42367		0.70127	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0 - E_0^0)/RT$	Δ	$(H^0 - E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.100	0.13063	14	0.29304	19	0.42367	33	0.70127	23
2.101	0.13049	14	0.29285	20	0.42334	34	0.70104	23
2.102	0.13035	14	0.29265	19	0.42300	33	0.70081	23
2.103	0.13021	14	0.29246	19	0.42267	33	0.70058	23
2.104	0.13007	14	0.29227	20	0.42234	33	0.70035	23
2.105	0.12993	14	0.29207	19	0.42201	34	0.70012	23
2.106	0.12979	13	0.29188	19	0.42167	33	0.69989	23
2.107	0.12966	14	0.29169	20	0.42134	33	0.69966	23
2.108	0.12952	14	0.29149	19	0.42101	33	0.69943	23
2.109	0.12938	14	0.29130	19	0.42068	33	0.69920	23
2.110	0.12924	14	0.29111	20	0.42035	33	0.69897	23
2.111	0.12910	13	0.29091	19	0.42002	34	0.69874	22
2.112	0.12897	14	0.29072	19	0.41968	33	0.69852	23
2.113	0.12883	14	0.29053	20	0.41935	33	0.69829	23
2.114	0.12869	14	0.29033	19	0.41902	33	0.69806	23
2.115	0.12855	13	0.29014	19	0.41869	33	0.69783	23
2.116	0.12842	14	0.28995	20	0.41836	33	0.69760	23
2.117	0.12828	14	0.28975	19	0.41803	33	0.69737	23
2.118	0.12814	13	0.28956	19	0.41770	32	0.69714	23
2.119	0.12801	14	0.28937	19	0.41738	33	0.69691	23
2.120	0.12787	14	0.28918	19	0.41705	33	0.69668	23
2.121	0.12773	13	0.28899	20	0.41672	33	0.69645	23
2.122	0.12760	14	0.28879	19	0.41639	33	0.69622	23
2.123	0.12746	14	0.28860	19	0.41606	33	0.69599	23
2.124	0.12732	13	0.28841	19	0.41573	32	0.69576	23
2.125	0.12719	14	0.28822	19	0.41541	33	0.69553	23
2.126	0.12705	13	0.28803	20	0.41508	33	0.69530	23
2.127	0.12692	14	0.28783	19	0.41475	32	0.69507	23
2.128	0.12678	13	0.28764	19	0.41443	33	0.69484	23
2.129	0.12665	14	0.28745	19	0.41410	33	0.69461	23
2.130	0.12651	13	0.28726	19	0.41377	32	0.69438	23
2.131	0.12638	14	0.28707	19	0.41345	33	0.69415	23
2.132	0.12624	13	0.28688	19	0.41312	32	0.69392	23
2.133	0.12611	14	0.28669	19	0.41280	33	0.69369	22
2.134	0.12597	13	0.28650	19	0.41247	32	0.69347	23
2.135	0.12584	13	0.28631	19	0.41215	33	0.69324	23
2.136	0.12571	14	0.28612	19	0.41182	32	0.69301	23
2.137	0.12557	13	0.28593	19	0.41150	33	0.69278	23
2.138	0.12544	13	0.28574	20	0.41117	32	0.69255	23
2.139	0.12531	14	0.28554	19	0.41085	32	0.69232	23
2.140	0.12517	13	0.28535	19	0.41053	33	0.69209	23
2.141	0.12504	13	0.28516	19	0.41020	32	0.69186	23
2.142	0.12491	14	0.28497	18	0.40988	32	0.69163	23
2.143	0.12477	13	0.28479	19	0.40956	32	0.69140	23
2.144	0.12464	13	0.28460	19	0.40924	33	0.69117	23
2.145	0.12451	14	0.28441	19	0.40891	32	0.69094	23
2.146	0.12437	13	0.28422	19	0.40859	32	0.69071	23
2.147	0.12424	13	0.28403	19	0.40827	32	0.69048	23
2.148	0.12411	13	0.28384	19	0.40795	32	0.69025	23
2.149	0.12398	13	0.28365	19	0.40763	32	0.69002	23
2.150	0.12385		0.28346		0.40731		0.68979	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R	Δ
2.150	0.12385	14	0.28346	19	0.40731	33	0.68979	23
2.151	0.12371	13	0.28327	19	0.40698	32	0.68956	23
2.152	0.12358	13	0.28308	19	0.40666	32	0.68933	23
2.153	0.12345	13	0.28289	19	0.40634	32	0.68910	23
2.154	0.12332	13	0.28270	18	0.40602	32	0.68887	23
2.155	0.12319	13	0.28252	19	0.40570	31	0.68864	23
2.156	0.12306	13	0.28233	19	0.40539	32	0.68841	23
2.157	0.12293	13	0.28214	19	0.40507	32	0.68818	23
2.158	0.12280	13	0.28195	19	0.40475	32	0.68795	23
2.159	0.12267	13	0.28176	19	0.40443	32	0.68772	23
2.160	0.12254	14	0.28157	18	0.40411	32	0.68749	23
2.161	0.12240	13	0.28139	19	0.40379	32	0.68726	23
2.162	0.12227	13	0.28120	19	0.40347	31	0.68703	23
2.163	0.12214	13	0.28101	19	0.40316	32	0.68680	23
2.164	0.12201	12	0.28082	18	0.40284	32	0.68657	23
2.165	0.12189	13	0.28064	19	0.40252	32	0.68634	23
2.166	0.12176	13	0.28045	19	0.40220	31	0.68611	24
2.167	0.12163	13	0.28026	19	0.40189	32	0.68587	23
2.168	0.12150	13	0.28007	18	0.40157	31	0.68564	23
2.169	0.12137	13	0.27989	19	0.40126	32	0.68541	23
2.170	0.12124	13	0.27970	19	0.40094	32	0.68518	23
2.171	0.12111	13	0.27951	18	0.40062	31	0.68495	23
2.172	0.12098	13	0.27933	19	0.40031	32	0.68472	23
2.173	0.12085	13	0.27914	19	0.39999	31	0.68449	23
2.174	0.12072	12	0.27895	18	0.39968	32	0.68426	23
2.175	0.12060	13	0.27877	19	0.39936	31	0.68403	23
2.176	0.12047	13	0.27858	18	0.39905	31	0.68380	23
2.177	0.12034	13	0.27840	19	0.39874	32	0.68357	23
2.178	0.12021	13	0.27821	19	0.39842	31	0.68334	23
2.179	0.12008	12	0.27802	18	0.39811	32	0.68311	23
2.180	0.11996	13	0.27784	19	0.39779	31	0.68288	23
2.181	0.11983	13	0.27765	18	0.39748	31	0.68265	23
2.182	0.11970	12	0.27747	19	0.39717	31	0.68242	23
2.183	0.11958	13	0.27728	18	0.39686	32	0.68219	23
2.184	0.11945	13	0.27710	19	0.39654	31	0.68196	23
2.185	0.11932	12	0.27691	19	0.39623	31	0.68173	23
2.186	0.11920	13	0.27672	18	0.39592	31	0.68150	23
2.187	0.11907	13	0.27654	19	0.39561	31	0.68127	23
2.188	0.11894	12	0.27635	18	0.39530	31	0.68104	23
2.189	0.11882	13	0.27617	18	0.39499	32	0.68081	24
2.190	0.11869	13	0.27599	19	0.39467	31	0.68057	23
2.191	0.11856	12	0.27580	18	0.39436	31	0.68034	23
2.192	0.11844	13	0.27562	19	0.39405	31	0.68011	23
2.193	0.11831	12	0.27543	18	0.39374	31	0.67988	23
2.194	0.11819	13	0.27525	19	0.39343	31	0.67965	23
2.195	0.11806	12	0.27506	18	0.39312	31	0.67942	23
2.196	0.11794	13	0.27488	19	0.39281	30	0.67919	23
2.197	0.11781	12	0.27469	18	0.39251	31	0.67896	23
2.198	0.11769	13	0.27451	18	0.39220	31	0.67873	23
2.199	0.11756	12	0.27433	19	0.39189	31	0.67850	23
2.200	0.11744		0.27414		0.39158		0.67827	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.200	0.11744	13	0.27414	18	0.39158	31	0.67827	23
2.201	0.11731	12	0.27396	18	0.39127	31	0.67804	23
2.202	0.11719	13	0.27378	19	0.39096	30	0.67781	23
2.203	0.11706	12	0.27359	18	0.39066	31	0.67758	23
2.204	0.11694	12	0.27341	18	0.39035	31	0.67735	24
2.205	0.11682	13	0.27323	19	0.39004	31	0.67711	23
2.206	0.11669	12	0.27304	18	0.38973	30	0.67688	23
2.207	0.11657	13	0.27286	18	0.38943	31	0.67665	23
2.208	0.11644	12	0.27268	19	0.38912	31	0.67642	23
2.209	0.11632	12	0.27249	18	0.38881	30	0.67619	23
2.210	0.11620	13	0.27231	18	0.38851	31	0.67596	23
2.211	0.11607	12	0.27213	18	0.38820	30	0.67573	23
2.212	0.11595	12	0.27195	19	0.38790	31	0.67550	23
2.213	0.11583	12	0.27176	18	0.38759	30	0.67527	23
2.214	0.11571	13	0.27158	18	0.38729	31	0.67504	23
2.215	0.11558	12	0.27140	18	0.38698	30	0.67481	23
2.216	0.11546	12	0.27122	18	0.38668	31	0.67458	23
2.217	0.11534	12	0.27104	19	0.38637	30	0.67435	24
2.218	0.11522	13	0.27085	18	0.38607	30	0.67411	23
2.219	0.11509	12	0.27067	18	0.38577	31	0.67388	23
2.220	0.11497	12	0.27049	18	0.38546	30	0.67365	23
2.221	0.11485	12	0.27031	18	0.38516	30	0.67342	23
2.222	0.11473	12	0.27013	18	0.38486	31	0.67319	23
2.223	0.11461	12	0.26995	19	0.38455	30	0.67296	23
2.224	0.11449	13	0.26976	18	0.38425	30	0.67273	23
2.225	0.11436	12	0.26958	18	0.38395	30	0.67250	23
2.226	0.11424	12	0.26940	18	0.38365	31	0.67227	23
2.227	0.11412	12	0.26922	18	0.38334	30	0.67204	24
2.228	0.11400	12	0.26904	18	0.38304	30	0.67180	23
2.229	0.11388	12	0.26886	18	0.38274	30	0.67157	23
2.230	0.11376	12	0.26868	18	0.38244	30	0.67134	23
2.231	0.11364	12	0.26850	18	0.38214	30	0.67111	23
2.232	0.11352	12	0.26832	18	0.38184	30	0.67088	23
2.233	0.11340	12	0.26814	18	0.38154	30	0.67065	23
2.234	0.11328	12	0.26796	18	0.38124	30	0.67042	23
2.235	0.11316	12	0.26778	18	0.38094	30	0.67019	23
2.236	0.11304	12	0.26760	18	0.38064	30	0.66996	23
2.237	0.11292	12	0.26742	18	0.38034	30	0.66973	24
2.238	0.11280	12	0.26724	18	0.38004	30	0.66949	23
2.239	0.11268	12	0.26706	18	0.37974	30	0.66926	23
2.240	0.11256	12	0.26688	18	0.37944	30	0.66903	23
2.241	0.11244	12	0.26670	18	0.37914	30	0.66880	23
2.242	0.11232	11	0.26652	18	0.37884	29	0.66857	23
2.243	0.11221	12	0.26634	18	0.37855	30	0.66834	23
2.244	0.11209	12	0.26616	18	0.37825	30	0.66811	23
2.245	0.11197	12	0.26598	18	0.37795	30	0.66788	23
2.246	0.11185	12	0.26580	18	0.37765	29	0.66765	24
2.247	0.11173	12	0.26562	17	0.37736	30	0.66741	23
2.248	0.11161	11	0.26545	18	0.37706	30	0.66718	23
2.249	0.11150	12	0.26527	18	0.37676	29	0.66695	23
2.250	0.11138		0.26509		0.37647		0.66672	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.250	0.11138	12	0.26509	18	0.37647	30	0.66672	23
2.251	0.11126	12	0.26491	18	0.37617	30	0.66649	23
2.252	0.11114	12	0.26473	18	0.37587	29	0.66626	23
2.253	0.11102	11	0.26455	17	0.37558	30	0.66603	23
2.254	0.11091	12	0.26438	18	0.37528	29	0.66580	24
2.255	0.11079	12	0.26420	18	0.37499	30	0.66556	23
2.256	0.11067	11	0.26402	18	0.37469	29	0.66533	23
2.257	0.11056	12	0.26384	18	0.37440	30	0.66510	23
2.258	0.11044	12	0.26366	17	0.37410	29	0.66487	23
2.259	0.11032	11	0.26349	18	0.37381	30	0.66464	23
2.260	0.11021	12	0.26331	18	0.37351	29	0.66441	23
2.261	0.11009	12	0.26313	18	0.37322	29	0.66418	23
2.262	0.10997	11	0.26295	17	0.37293	30	0.66395	24
2.263	0.10986	12	0.26278	18	0.37263	29	0.66371	23
2.264	0.10974	11	0.26260	18	0.37234	29	0.66348	23
2.265	0.10963	12	0.26242	17	0.37205	30	0.66325	23
2.266	0.10951	12	0.26225	18	0.37175	29	0.66302	23
2.267	0.10939	11	0.26207	18	0.37146	29	0.66279	23
2.268	0.10928	12	0.26189	17	0.37117	29	0.66256	23
2.269	0.10916	11	0.26172	18	0.37088	29	0.66233	23
2.270	0.10905	12	0.26154	18	0.37059	30	0.66210	24
2.271	0.10893	11	0.26136	17	0.37029	29	0.66186	23
2.272	0.10882	12	0.26119	18	0.37000	29	0.66163	23
2.273	0.10870	11	0.26101	18	0.36971	29	0.66140	23
2.274	0.10859	12	0.26083	17	0.36942	29	0.66117	23
2.275	0.10847	11	0.26066	18	0.36913	29	0.66094	23
2.276	0.10836	12	0.26048	17	0.36884	29	0.66071	23
2.277	0.10824	11	0.26031	18	0.36855	29	0.66048	24
2.278	0.10813	11	0.26013	18	0.36826	29	0.66024	23
2.279	0.10802	12	0.25995	17	0.36797	29	0.66001	23
2.280	0.10790	11	0.25978	18	0.36768	29	0.65978	23
2.281	0.10779	12	0.25960	17	0.36739	29	0.65955	23
2.282	0.10767	11	0.25943	18	0.36710	29	0.65932	23
2.283	0.10756	11	0.25925	17	0.36681	28	0.65909	23
2.284	0.10745	12	0.25908	18	0.36653	29	0.65886	23
2.285	0.10733	11	0.25890	17	0.36624	29	0.65863	24
2.286	0.10722	11	0.25873	18	0.36595	29	0.65839	23
2.287	0.10711	12	0.25855	17	0.36566	29	0.65816	23
2.288	0.10699	11	0.25838	18	0.36537	28	0.65793	23
2.289	0.10688	11	0.25820	17	0.36509	29	0.65770	23
2.290	0.10677	11	0.25803	17	0.36480	29	0.65747	23
2.291	0.10666	12	0.25786	18	0.36451	29	0.65724	23
2.292	0.10654	11	0.25768	17	0.36422	28	0.65701	24
2.293	0.10643	11	0.25751	18	0.36394	29	0.65677	23
2.294	0.10632	11	0.25733	17	0.36365	28	0.65654	23
2.295	0.10621	12	0.25716	17	0.36337	29	0.65631	23
2.296	0.10609	11	0.25699	18	0.36308	29	0.65608	23
2.297	0.10598	11	0.25681	17	0.36279	28	0.65585	23
2.298	0.10587	11	0.25664	18	0.36251	29	0.65562	23
2.299	0.10576	11	0.25646	17	0.36222	28	0.65539	24
2.300	0.10565		0.25629		0.36194		0.65515	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.300	0.10565	11	0.25629	17	0.36194	29	0.65515	23
2.301	0.10554	11	0.25612	18	0.36165	28	0.65492	23
2.302	0.10543	12	0.25594	17	0.36137	28	0.65469	23
2.303	0.10531	11	0.25577	17	0.36109	29	0.65446	23
2.304	0.10520	11	0.25560	18	0.36080	28	0.65423	23
2.305	0.10509	11	0.25542	17	0.36052	29	0.65400	24
2.306	0.10498	11	0.25525	17	0.36023	28	0.65376	23
2.307	0.10487	11	0.25508	17	0.35995	28	0.65353	23
2.308	0.10476	11	0.25491	18	0.35967	29	0.65330	23
2.309	0.10465	11	0.25473	17	0.35938	28	0.65307	23
2.310	0.10454	11	0.25456	17	0.35910	28	0.65284	23
2.311	0.10443	11	0.25439	17	0.35882	28	0.65261	23
2.312	0.10432	11	0.25422	18	0.35854	29	0.65238	24
2.313	0.10421	11	0.25404	17	0.35825	28	0.65214	23
2.314	0.10410	11	0.25387	17	0.35797	28	0.65191	23
2.315	0.10399	11	0.25370	17	0.35769	28	0.65168	23
2.316	0.10388	11	0.25353	17	0.35741	28	0.65145	23
2.317	0.10377	11	0.25336	17	0.35713	28	0.65122	23
2.318	0.10366	11	0.25319	18	0.35685	28	0.65099	23
2.319	0.10355	11	0.25301	17	0.35657	28	0.65076	24
2.320	0.10344	10	0.25284	17	0.35629	28	0.65052	23
2.321	0.10334	11	0.25267	17	0.35601	28	0.65029	23
2.322	0.10323	11	0.25250	17	0.35573	28	0.65006	23
2.323	0.10312	11	0.25233	17	0.35545	28	0.64983	23
2.324	0.10301	11	0.25216	17	0.35517	28	0.64960	23
2.325	0.10290	11	0.25199	17	0.35489	28	0.64937	24
2.326	0.10279	11	0.25182	18	0.35461	28	0.64913	23
2.327	0.10268	10	0.25164	17	0.35433	28	0.64890	23
2.328	0.10258	11	0.25147	17	0.35405	28	0.64867	23
2.329	0.10247	11	0.25130	17	0.35377	28	0.64844	23
2.330	0.10236	11	0.25113	17	0.35349	27	0.64821	23
2.331	0.10225	11	0.25096	17	0.35322	28	0.64798	23
2.332	0.10214	10	0.25079	17	0.35294	28	0.64775	24
2.333	0.10204	11	0.25062	17	0.35266	28	0.64751	23
2.334	0.10193	11	0.25045	17	0.35238	27	0.64728	23
2.335	0.10182	10	0.25028	17	0.35211	28	0.64705	23
2.336	0.10172	11	0.25011	17	0.35183	28	0.64682	23
2.337	0.10161	11	0.24994	17	0.35155	28	0.64659	23
2.338	0.10150	10	0.24977	17	0.35127	27	0.64636	24
2.339	0.10140	11	0.24960	17	0.35100	28	0.64612	23
2.340	0.10129	11	0.24943	17	0.35072	27	0.64589	23
2.341	0.10118	10	0.24926	16	0.35045	28	0.64566	23
2.342	0.10108	11	0.24910	17	0.35017	27	0.64543	23
2.343	0.10097	11	0.24893	17	0.34990	28	0.64520	23
2.344	0.10086	10	0.24876	17	0.34962	27	0.64497	23
2.345	0.10076	11	0.24859	17	0.34935	28	0.64474	24
2.346	0.10065	10	0.24842	17	0.34907	27	0.64450	23
2.347	0.10055	11	0.24825	17	0.34880	28	0.64427	23
2.348	0.10044	11	0.24808	17	0.34852	27	0.64404	23
2.349	0.10033	10	0.24791	17	0.34825	28	0.64381	23
2.350	0.10023		0.24774		0.34797		0.64358	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.350	0.10023	11	0.24774	16	0.34797	27	0.64358	23
2.351	0.10012	10	0.24758	17	0.34770	27	0.64335	24
2.352	0.10002	11	0.24741	17	0.34743	28	0.64311	23
2.353	0.09991	10	0.24724	17	0.34715	27	0.64288	23
2.354	0.09981	11	0.24707	17	0.34688	27	0.64265	23
2.355	0.09970	10	0.24690	16	0.34661	28	0.64242	23
2.356	0.09960	11	0.24674	17	0.34633	27	0.64219	23
2.357	0.09949	10	0.24657	17	0.34606	27	0.64196	23
2.358	0.09939	11	0.24640	17	0.34579	27	0.64173	24
2.359	0.09928	10	0.24623	16	0.34552	27	0.64149	23
2.360	0.09918	10	0.24607	17	0.34525	28	0.64126	23
2.361	0.09908	11	0.24590	17	0.34497	27	0.64103	23
2.362	0.09897	10	0.24573	17	0.34470	27	0.64080	23
2.363	0.09887	11	0.24556	16	0.34443	27	0.64057	23
2.364	0.09876	10	0.24540	17	0.34416	27	0.64034	24
2.365	0.09866	10	0.24523	17	0.34389	27	0.64010	23
2.366	0.09856	11	0.24506	16	0.34362	27	0.63987	23
2.367	0.09845	10	0.24490	17	0.34335	27	0.63964	23
2.368	0.09835	10	0.24473	17	0.34308	27	0.63941	23
2.369	0.09825	11	0.24456	16	0.34281	27	0.63918	23
2.370	0.09814	10	0.24440	17	0.34254	27	0.63895	23
2.371	0.09804	10	0.24423	17	0.34227	27	0.63872	24
2.372	0.09794	11	0.24406	16	0.34200	27	0.63848	23
2.373	0.09783	10	0.24390	17	0.34173	27	0.63825	23
2.374	0.09773	10	0.24373	17	0.34146	27	0.63802	23
2.375	0.09763	10	0.24356	16	0.34119	27	0.63779	23
2.376	0.09753	11	0.24340	17	0.34092	26	0.63756	23
2.377	0.09742	10	0.24323	16	0.34066	27	0.63733	24
2.378	0.09732	10	0.24307	17	0.34039	27	0.63709	23
2.379	0.09722	10	0.24290	16	0.34012	27	0.63686	23
2.380	0.09712	10	0.24274	17	0.33985	26	0.63663	23
2.381	0.09702	11	0.24257	17	0.33959	27	0.63640	23
2.382	0.09691	10	0.24240	16	0.33932	27	0.63617	23
2.383	0.09681	10	0.24224	17	0.33905	27	0.63594	23
2.384	0.09671	10	0.24207	16	0.33878	26	0.63571	24
2.385	0.09661	10	0.24191	17	0.33852	27	0.63547	23
2.386	0.09651	10	0.24174	16	0.33825	26	0.63524	23
2.387	0.09641	10	0.24158	17	0.33799	27	0.63501	23
2.388	0.09631	11	0.24141	16	0.33772	27	0.63478	23
2.389	0.09620	10	0.24125	16	0.33745	26	0.63455	23
2.390	0.09610	10	0.24109	17	0.33719	27	0.63432	23
2.391	0.09600	10	0.24092	16	0.33692	26	0.63409	24
2.392	0.09590	10	0.24076	17	0.33666	27	0.63385	23
2.393	0.09580	10	0.24059	16	0.33639	26	0.63362	23
2.394	0.09570	10	0.24043	17	0.33613	27	0.63339	23
2.395	0.09560	10	0.24026	16	0.33586	26	0.63316	23
2.396	0.09550	10	0.24010	16	0.33560	26	0.63293	23
2.397	0.09540	10	0.23994	17	0.33534	27	0.63270	24
2.398	0.09530	10	0.23977	16	0.33507	26	0.63246	23
2.399	0.09520	10	0.23961	16	0.33481	26	0.63223	23
2.400	0.09510		0.23945		0.33455		0.63200	

**Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$**

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R	Δ
2.400	0.09510	10	0.23945	17	0.33455	27	0.63200	23
2.401	0.09500	10	0.23928	16	0.33428	26	0.63177	23
2.402	0.09490	10	0.23912	17	0.33402	26	0.63154	23
2.403	0.09480	10	0.23895	16	0.33376	27	0.63131	23
2.404	0.09470	10	0.23879	16	0.33349	26	0.63108	24
2.405	0.09460	10	0.23863	16	0.33323	26	0.63084	23
2.406	0.09450	10	0.23847	17	0.33297	26	0.63061	23
2.407	0.09440	9	0.23830	16	0.33271	27	0.63038	23
2.408	0.09431	10	0.23814	16	0.33244	26	0.63015	23
2.409	0.09421	10	0.23798	17	0.33218	26	0.62992	23
2.410	0.09411	10	0.23781	16	0.33192	26	0.62969	23
2.411	0.09401	10	0.23765	16	0.33166	26	0.62946	23
2.412	0.09391	10	0.23749	16	0.33140	26	0.62923	24
2.413	0.09381	10	0.23733	17	0.33114	26	0.62899	23
2.414	0.09371	9	0.23716	16	0.33088	26	0.62876	23
2.415	0.09362	10	0.23700	16	0.33062	26	0.62853	23
2.416	0.09352	10	0.23684	16	0.33036	26	0.62830	23
2.417	0.09342	10	0.23668	16	0.33010	26	0.62807	23
2.418	0.09332	10	0.23652	17	0.32984	26	0.62784	23
2.419	0.09322	9	0.23635	16	0.32958	26	0.62761	24
2.420	0.09313	10	0.23619	16	0.32932	26	0.62737	23
2.421	0.09303	10	0.23603	16	0.32906	26	0.62714	23
2.422	0.09293	10	0.23587	16	0.32880	26	0.62691	23
2.423	0.09283	9	0.23571	16	0.32854	26	0.62668	23
2.424	0.09274	10	0.23555	16	0.32828	25	0.62645	23
2.425	0.09264	10	0.23539	17	0.32803	26	0.62622	23
2.426	0.09254	9	0.23522	16	0.32777	26	0.62599	24
2.427	0.09245	10	0.23506	16	0.32751	26	0.62575	23
2.428	0.09235	10	0.23490	16	0.32725	26	0.62552	23
2.429	0.09225	9	0.23474	16	0.32699	25	0.62529	23
2.430	0.09216	10	0.23458	16	0.32674	26	0.62506	23
2.431	0.09206	10	0.23442	16	0.32648	26	0.62483	23
2.432	0.09196	9	0.23426	16	0.32622	25	0.62460	23
2.433	0.09187	10	0.23410	16	0.32597	26	0.62437	23
2.434	0.09177	10	0.23394	16	0.32571	26	0.62414	24
2.435	0.09167	9	0.23378	16	0.32545	25	0.62390	23
2.436	0.09158	10	0.23362	16	0.32520	26	0.62367	23
2.437	0.09148	9	0.23346	16	0.32494	25	0.62344	23
2.438	0.09139	10	0.23330	16	0.32469	26	0.62321	23
2.439	0.09129	9	0.23314	16	0.32443	26	0.62298	23
2.440	0.09120	10	0.23298	16	0.32417	25	0.62275	23
2.441	0.09110	10	0.23282	16	0.32392	26	0.62252	23
2.442	0.09100	9	0.23266	16	0.32366	25	0.62229	24
2.443	0.09091	10	0.23250	16	0.32341	25	0.62205	23
2.444	0.09081	9	0.23234	16	0.32316	26	0.62182	23
2.445	0.09072	10	0.23218	16	0.32290	25	0.62159	23
2.446	0.09062	9	0.23202	16	0.32265	26	0.62136	23
2.447	0.09053	9	0.23186	16	0.32239	25	0.62113	23
2.448	0.09044	10	0.23170	15	0.32214	25	0.62090	23
2.449	0.09034	9	0.23155	16	0.32189	26	0.62067	23
2.450	0.09025		0.23139		0.32163		0.62044	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.450	0.09025	10	0.23139	16	0.32163	25	0.62044	23
2.451	0.09015	9	0.23123	16	0.32138	25	0.62021	24
2.452	0.09006	10	0.23107	16	0.32113	26	0.61997	23
2.453	0.08996	9	0.23091	16	0.32087	25	0.61974	23
2.454	0.08987	9	0.23075	16	0.32062	25	0.61951	23
2.455	0.08978	10	0.23059	15	0.32037	25	0.61928	23
2.456	0.08968	9	0.23044	16	0.32012	26	0.61905	23
2.457	0.08959	10	0.23028	16	0.31986	25	0.61882	23
2.458	0.08949	9	0.23012	16	0.31961	25	0.61859	23
2.459	0.08940	9	0.22996	16	0.31936	25	0.61836	23
2.460	0.08931	10	0.22980	15	0.31911	25	0.61813	24
2.461	0.08921	9	0.22965	16	0.31886	25	0.61789	23
2.462	0.08912	9	0.22949	16	0.31861	25	0.61766	23
2.463	0.08903	10	0.22933	16	0.31836	25	0.61743	23
2.464	0.08893	9	0.22917	15	0.31811	25	0.61720	23
2.465	0.08884	9	0.22902	16	0.31786	25	0.61697	23
2.466	0.08875	9	0.22886	16	0.31761	25	0.61674	23
2.467	0.08866	10	0.22870	16	0.31736	25	0.61651	23
2.468	0.08856	9	0.22854	15	0.31711	25	0.61628	23
2.469	0.08847	9	0.22839	16	0.31686	25	0.61605	23
2.470	0.08838	9	0.22823	16	0.31661	25	0.61582	24
2.471	0.08829	10	0.22807	15	0.31636	25	0.61558	23
2.472	0.08819	9	0.22792	16	0.31611	25	0.61535	23
2.473	0.08810	9	0.22776	16	0.31586	25	0.61512	23
2.474	0.08801	9	0.22760	15	0.31561	25	0.61489	23
2.475	0.08792	9	0.22745	16	0.31536	25	0.61466	23
2.476	0.08783	10	0.22729	16	0.31511	24	0.61443	23
2.477	0.08773	9	0.22713	15	0.31487	25	0.61420	23
2.478	0.08764	9	0.22698	16	0.31462	25	0.61397	23
2.479	0.08755	9	0.22682	16	0.31437	25	0.61374	23
2.480	0.08746	9	0.22666	15	0.31412	24	0.61351	24
2.481	0.08737	9	0.22651	16	0.31388	25	0.61327	23
2.482	0.08728	10	0.22635	15	0.31363	25	0.61304	23
2.483	0.08718	9	0.22620	16	0.31338	24	0.61281	23
2.484	0.08709	9	0.22604	15	0.31314	25	0.61258	23
2.485	0.08700	9	0.22589	16	0.31289	25	0.61235	23
2.486	0.08691	9	0.22573	15	0.31264	24	0.61212	23
2.487	0.08682	9	0.22558	16	0.31240	25	0.61189	23
2.488	0.08673	9	0.22542	16	0.31215	25	0.61166	23
2.489	0.08664	9	0.22526	15	0.31190	24	0.61143	23
2.490	0.08655	9	0.22511	16	0.31166	25	0.61120	23
2.491	0.08646	9	0.22495	15	0.31141	24	0.61097	23
2.492	0.08637	9	0.22480	16	0.31117	25	0.61074	23
2.493	0.08628	9	0.22464	15	0.31092	24	0.61051	24
2.494	0.08619	9	0.22449	15	0.31068	25	0.61027	23
2.495	0.08610	9	0.22434	16	0.31043	24	0.61004	23
2.496	0.08601	9	0.22418	15	0.31019	24	0.60981	23
2.497	0.08592	9	0.22403	16	0.30995	25	0.60958	23
2.498	0.08583	9	0.22387	15	0.30970	24	0.60935	23
2.499	0.08574	9	0.22372	16	0.30946	25	0.60912	23
2.500	0.08565		0.22356		0.30921		0.60889	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.500	0.08565	9	0.22356	15	0.30921	24	0.60889	23
2.501	0.08556	9	0.22341	15	0.30897	24	0.60866	23
2.502	0.08547	9	0.22326	16	0.30873	25	0.60843	23
2.503	0.08538	9	0.22310	15	0.30848	24	0.60820	23
2.504	0.08529	9	0.22295	16	0.30824	24	0.60797	23
2.505	0.08520	8	0.22279	15	0.30800	24	0.60774	23
2.506	0.08512	9	0.22264	15	0.30776	25	0.60751	23
2.507	0.08503	9	0.22249	16	0.30751	24	0.60728	24
2.508	0.08494	9	0.22233	15	0.30727	24	0.60704	23
2.509	0.08485	9	0.22218	15	0.30703	24	0.60681	23
2.510	0.08476	9	0.22203	16	0.30679	24	0.60658	23
2.511	0.08467	9	0.22187	15	0.30655	24	0.60635	23
2.512	0.08458	8	0.22172	15	0.30631	25	0.60612	23
2.513	0.08450	9	0.22157	16	0.30606	24	0.60589	23
2.514	0.08441	9	0.22141	15	0.30582	24	0.60566	23
2.515	0.08432	9	0.22126	15	0.30558	24	0.60543	23
2.516	0.08423	9	0.22111	15	0.30534	24	0.60520	23
2.517	0.08414	8	0.22096	16	0.30510	24	0.60497	23
2.518	0.08406	9	0.22080	15	0.30486	24	0.60474	23
2.519	0.08397	9	0.22065	15	0.30462	24	0.60451	23
2.520	0.08388	9	0.22050	15	0.30438	24	0.60428	23
2.521	0.08379	8	0.22035	15	0.30414	24	0.60405	23
2.522	0.08371	9	0.22020	16	0.30390	24	0.60382	23
2.523	0.08362	9	0.22004	15	0.30366	24	0.60359	23
2.524	0.08353	9	0.21989	15	0.30342	24	0.60336	23
2.525	0.08344	8	0.21974	15	0.30318	23	0.60313	23
2.526	0.08336	9	0.21959	15	0.30295	24	0.60290	23
2.527	0.08327	9	0.21944	16	0.30271	24	0.60267	23
2.528	0.08318	8	0.21928	15	0.30247	24	0.60244	23
2.529	0.08310	9	0.21913	15	0.30223	24	0.60221	23
2.530	0.08301	9	0.21898	15	0.30199	24	0.60198	24
2.531	0.08292	8	0.21883	15	0.30175	23	0.60174	23
2.532	0.08284	9	0.21868	15	0.30152	24	0.60151	23
2.533	0.08275	8	0.21853	15	0.30128	24	0.60128	23
2.534	0.08267	9	0.21838	15	0.30104	24	0.60105	23
2.535	0.08258	9	0.21823	16	0.30080	23	0.60082	23
2.536	0.08249	8	0.21807	15	0.30057	24	0.60059	23
2.537	0.08241	9	0.21792	15	0.30033	24	0.60036	23
2.538	0.08232	8	0.21777	15	0.30009	23	0.60013	23
2.539	0.08224	9	0.21762	15	0.29986	24	0.59990	23
2.540	0.08215	9	0.21747	15	0.29962	23	0.59967	23
2.541	0.08206	8	0.21732	15	0.29939	24	0.59944	23
2.542	0.08198	9	0.21717	15	0.29915	24	0.59921	23
2.543	0.08189	8	0.21702	15	0.29891	23	0.59898	23
2.544	0.08181	9	0.21687	15	0.29868	24	0.59875	23
2.545	0.08172	8	0.21672	15	0.29844	23	0.59852	23
2.546	0.08164	9	0.21657	15	0.29821	24	0.59829	23
2.547	0.08155	8	0.21642	15	0.29797	23	0.59806	23
2.548	0.08147	9	0.21627	15	0.29774	24	0.59783	23
2.549	0.08138	8	0.21612	15	0.29750	23	0.59760	23
2.550	0.08130		0.21597		0.29727		0.59737	

**Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$**

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.550	0.08130	9	0.21597	15	0.29727	23	0.59737	23
2.551	0.08121	8	0.21582	15	0.29704	24	0.59714	23
2.552	0.08113	9	0.21567	15	0.29680	23	0.59691	23
2.553	0.08104	8	0.21552	15	0.29657	24	0.59668	23
2.554	0.08096	8	0.21537	15	0.29633	23	0.59645	23
2.555	0.08088	9	0.21522	14	0.29610	23	0.59622	23
2.556	0.08079	8	0.21508	15	0.29587	24	0.59599	23
2.557	0.08071	9	0.21493	15	0.29563	23	0.59576	23
2.558	0.08062	8	0.21478	15	0.29540	23	0.59553	23
2.559	0.08054	8	0.21463	15	0.29517	23	0.59530	23
2.560	0.08046	9	0.21448	15	0.29494	24	0.59507	23
2.561	0.08037	8	0.21433	15	0.29470	23	0.59484	23
2.562	0.08029	8	0.21418	15	0.29447	23	0.59461	23
2.563	0.08021	9	0.21403	14	0.29424	23	0.59438	23
2.564	0.08012	8	0.21389	15	0.29401	23	0.59415	23
2.565	0.08004	8	0.21374	15	0.29378	23	0.59392	23
2.566	0.07996	9	0.21359	15	0.29355	24	0.59369	23
2.567	0.07987	8	0.21344	15	0.29331	23	0.59346	23
2.568	0.07979	8	0.21329	14	0.29308	23	0.59323	23
2.569	0.07971	9	0.21315	15	0.29285	23	0.59300	23
2.570	0.07962	8	0.21300	15	0.29262	23	0.59277	23
2.571	0.07954	8	0.21285	15	0.29239	23	0.59254	23
2.572	0.07946	9	0.21270	14	0.29216	23	0.59231	23
2.573	0.07937	8	0.21256	15	0.29193	23	0.59208	22
2.574	0.07929	8	0.21241	15	0.29170	23	0.59186	23
2.575	0.07921	8	0.21226	15	0.29147	23	0.59163	23
2.576	0.07913	8	0.21211	14	0.29124	23	0.59140	23
2.577	0.07905	9	0.21197	15	0.29101	23	0.59117	23
2.578	0.07896	8	0.21182	15	0.29078	23	0.59094	23
2.579	0.07888	8	0.21167	14	0.29055	23	0.59071	23
2.580	0.07880	8	0.21153	15	0.29032	23	0.59048	23
2.581	0.07872	9	0.21138	15	0.29009	22	0.59025	23
2.582	0.07863	8	0.21123	15	0.28987	23	0.59002	23
2.583	0.07855	8	0.21108	14	0.28964	23	0.58979	23
2.584	0.07847	8	0.21094	15	0.28941	23	0.58956	23
2.585	0.07839	8	0.21079	14	0.28918	23	0.58933	23
2.586	0.07831	8	0.21065	15	0.28895	22	0.58910	23
2.587	0.07823	8	0.21050	15	0.28873	23	0.58887	23
2.588	0.07815	9	0.21035	14	0.28850	23	0.58864	23
2.589	0.07806	8	0.21021	15	0.28827	23	0.58841	23
2.590	0.07798	8	0.21006	15	0.28804	22	0.58818	23
2.591	0.07790	8	0.20991	14	0.28782	23	0.58795	23
2.592	0.07782	8	0.20977	15	0.28759	23	0.58772	23
2.593	0.07774	8	0.20962	14	0.28736	22	0.58749	22
2.594	0.07766	8	0.20948	15	0.28714	23	0.58727	23
2.595	0.07758	8	0.20933	14	0.28691	23	0.58704	23
2.596	0.07750	8	0.20919	15	0.28668	22	0.58681	23
2.597	0.07742	8	0.20904	14	0.28646	23	0.58658	23
2.598	0.07734	8	0.20890	15	0.28623	22	0.58635	23
2.599	0.07726	8	0.20875	14	0.28601	23	0.58612	23
2.600	0.07718		0.20861		0.28578		0.58589	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.600	0.07718	8	0.20861	15	0.28578	22	0.58589	23
2.601	0.07710	8	0.20846	14	0.28556	23	0.58566	23
2.602	0.07702	8	0.20832	15	0.28533	22	0.58543	23
2.603	0.07694	8	0.20817	14	0.28511	23	0.58520	23
2.604	0.07686	8	0.20803	15	0.28488	22	0.58497	23
2.605	0.07678	8	0.20788	14	0.28466	23	0.58474	23
2.606	0.07670	8	0.20774	15	0.28443	22	0.58451	22
2.607	0.07662	8	0.20759	14	0.28421	23	0.58429	23
2.608	0.07654	8	0.20745	15	0.28398	22	0.58406	23
2.609	0.07646	8	0.20730	14	0.28376	22	0.58383	23
2.610	0.07638	8	0.20716	15	0.28354	23	0.58360	23
2.611	0.07630	8	0.20701	14	0.28331	22	0.58337	23
2.612	0.07622	8	0.20687	14	0.28309	22	0.58314	23
2.613	0.07614	8	0.20673	15	0.28287	23	0.58291	23
2.614	0.07606	8	0.20658	14	0.28264	22	0.58268	23
2.615	0.07598	8	0.20644	15	0.28242	22	0.58245	23
2.616	0.07590	7	0.20629	14	0.28220	22	0.58222	22
2.617	0.07583	8	0.20615	14	0.28198	23	0.58200	23
2.618	0.07575	8	0.20601	15	0.28175	22	0.58177	23
2.619	0.07567	8	0.20586	14	0.28153	22	0.58154	23
2.620	0.07559	8	0.20572	14	0.28131	22	0.58131	23
2.621	0.07551	8	0.20558	15	0.28109	22	0.58108	23
2.622	0.07543	8	0.20543	14	0.28087	23	0.58085	23
2.623	0.07535	7	0.20529	14	0.28064	22	0.58062	23
2.624	0.07528	8	0.20515	15	0.28042	22	0.58039	23
2.625	0.07520	8	0.20500	14	0.28020	22	0.58016	22
2.626	0.07512	8	0.20486	14	0.27998	22	0.57994	23
2.627	0.07504	8	0.20472	14	0.27976	22	0.57971	23
2.628	0.07496	7	0.20458	15	0.27954	22	0.57948	23
2.629	0.07489	8	0.20443	14	0.27932	22	0.57925	23
2.630	0.07481	8	0.20429	14	0.27910	22	0.57902	23
2.631	0.07473	8	0.20415	14	0.27888	22	0.57879	23
2.632	0.07465	7	0.20401	15	0.27866	22	0.57856	22
2.633	0.07458	8	0.20386	14	0.27844	22	0.57834	23
2.634	0.07450	8	0.20372	14	0.27822	22	0.57811	23
2.635	0.07442	8	0.20358	14	0.27800	22	0.57788	23
2.636	0.07434	7	0.20344	14	0.27778	22	0.57765	23
2.637	0.07427	8	0.20330	15	0.27756	22	0.57742	23
2.638	0.07419	8	0.20315	14	0.27734	22	0.57719	23
2.639	0.07411	7	0.20301	14	0.27712	21	0.57696	22
2.640	0.07404	8	0.20287	14	0.27691	22	0.57674	23
2.641	0.07396	8	0.20273	14	0.27669	22	0.57651	23
2.642	0.07388	7	0.20259	14	0.27647	22	0.57628	23
2.643	0.07381	8	0.20245	14	0.27625	22	0.57605	23
2.644	0.07373	8	0.20231	15	0.27603	21	0.57582	23
2.645	0.07365	7	0.20216	14	0.27582	22	0.57559	22
2.646	0.07358	8	0.20202	14	0.27560	22	0.57537	23
2.647	0.07350	8	0.20188	14	0.27538	22	0.57514	23
2.648	0.07342	7	0.20174	14	0.27516	21	0.57491	23
2.649	0.07335	8	0.20160	14	0.27495	22	0.57468	23
2.650	0.07327		0.20146		0.27473		0.57445	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the

Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R	Δ
2.650	0.07327	7	0.20146	14	0.27473	22	0.57445	23
2.651	0.07320	8	0.20132	14	0.27451	21	0.57422	22
2.652	0.07312	8	0.20118	14	0.27430	22	0.57400	23
2.653	0.07304	7	0.20104	14	0.27408	22	0.57377	23
2.654	0.07297	8	0.20090	14	0.27386	21	0.57354	23
2.655	0.07289	7	0.20076	14	0.27365	22	0.57331	23
2.656	0.07282	8	0.20062	14	0.27343	21	0.57308	23
2.657	0.07274	7	0.20048	14	0.27322	22	0.57285	22
2.658	0.07267	8	0.20034	14	0.27300	21	0.57263	23
2.659	0.07259	7	0.20020	14	0.27279	22	0.57240	23
2.660	0.07252	8	0.20006	14	0.27257	21	0.57217	23
2.661	0.07244	8	0.19992	14	0.27236	22	0.57194	23
2.662	0.07236	7	0.19978	14	0.27214	21	0.57171	22
2.663	0.07229	8	0.19964	14	0.27193	22	0.57149	23
2.664	0.07221	7	0.19950	14	0.27171	21	0.57126	23
2.665	0.07214	7	0.19936	14	0.27150	22	0.57103	23
2.666	0.07207	8	0.19922	14	0.27128	21	0.57080	22
2.667	0.07199	7	0.19908	14	0.27107	21	0.57058	23
2.668	0.07192	8	0.19894	14	0.27086	22	0.57035	23
2.669	0.07184	7	0.19880	14	0.27064	21	0.57012	23
2.670	0.07177	8	0.19866	14	0.27043	22	0.56989	23
2.671	0.07169	7	0.19852	14	0.27021	21	0.56966	22
2.672	0.07162	8	0.19838	14	0.27000	21	0.56944	23
2.673	0.07154	7	0.19824	13	0.26979	21	0.56921	23
2.674	0.07147	7	0.19811	14	0.26958	22	0.56898	23
2.675	0.07140	8	0.19797	14	0.26936	21	0.56875	22
2.676	0.07132	7	0.19783	14	0.26915	21	0.56853	23
2.677	0.07125	8	0.19769	14	0.26894	21	0.56830	23
2.678	0.07117	7	0.19755	14	0.26873	22	0.56807	23
2.679	0.07110	7	0.19741	13	0.26851	21	0.56784	23
2.680	0.07103	8	0.19728	14	0.26830	21	0.56761	22
2.681	0.07095	7	0.19714	14	0.26809	21	0.56739	23
2.682	0.07088	7	0.19700	14	0.26788	21	0.56716	23
2.683	0.07081	8	0.19686	14	0.26767	21	0.56693	23
2.684	0.07073	7	0.19672	13	0.26746	22	0.56670	22
2.685	0.07066	7	0.19659	14	0.26724	21	0.56648	23
2.686	0.07059	8	0.19645	14	0.26703	21	0.56625	23
2.687	0.07051	7	0.19631	14	0.26682	21	0.56602	23
2.688	0.07044	7	0.19617	14	0.26661	21	0.56579	22
2.689	0.07037	8	0.19603	13	0.26640	21	0.56557	23
2.690	0.07029	7	0.19590	14	0.26619	21	0.56534	23
2.691	0.07022	7	0.19576	14	0.26598	21	0.56511	22
2.692	0.07015	7	0.19562	13	0.26577	21	0.56489	23
2.693	0.07008	8	0.19549	14	0.26556	21	0.56466	23
2.694	0.07000	7	0.19535	14	0.26535	21	0.56443	23
2.695	0.06993	7	0.19521	14	0.26514	21	0.56420	22
2.696	0.06986	7	0.19507	13	0.26493	21	0.56398	23
2.697	0.06979	8	0.19494	14	0.26472	20	0.56375	23
2.698	0.06971	7	0.19480	14	0.26452	21	0.56352	23
2.699	0.06964	7	0.19466	13	0.26431	21	0.56329	22
2.700	0.06957		0.19453		0.26410		0.56307	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.700	0.06957	7	0.19453	14	0.26410	21	0.56307	23
2.701	0.06950	7	0.19439	13	0.26389	21	0.56284	23
2.702	0.06943	8	0.19426	14	0.26368	21	0.56261	22
2.703	0.06935	7	0.19412	14	0.26347	20	0.56239	23
2.704	0.06928	7	0.19398	13	0.26327	21	0.56216	23
2.705	0.06921	7	0.19385	14	0.26306	21	0.56193	22
2.706	0.06914	7	0.19371	14	0.26285	21	0.56171	23
2.707	0.06907	7	0.19357	13	0.26264	20	0.56148	23
2.708	0.06900	7	0.19344	14	0.26244	21	0.56125	23
2.709	0.06893	8	0.19330	13	0.26223	21	0.56102	22
2.710	0.06885	7	0.19317	14	0.26202	21	0.56080	23
2.711	0.06878	7	0.19303	13	0.26181	20	0.56057	23
2.712	0.06871	7	0.19290	14	0.26161	21	0.56034	22
2.713	0.06864	7	0.19276	13	0.26140	21	0.56012	23
2.714	0.06857	7	0.19263	14	0.26119	20	0.55989	23
2.715	0.06850	7	0.19249	13	0.26099	21	0.55966	22
2.716	0.06843	7	0.19236	14	0.26078	20	0.55944	23
2.717	0.06836	7	0.19222	14	0.26058	21	0.55921	23
2.718	0.06829	7	0.19208	13	0.26037	20	0.55898	22
2.719	0.06822	8	0.19195	13	0.26017	21	0.55876	23
2.720	0.06814	7	0.19182	14	0.25996	21	0.55853	23
2.721	0.06807	7	0.19168	13	0.25975	20	0.55830	22
2.722	0.06800	7	0.19155	14	0.25955	21	0.55808	23
2.723	0.06793	7	0.19141	13	0.25934	20	0.55785	23
2.724	0.06786	7	0.19128	14	0.25914	20	0.55762	22
2.725	0.06779	7	0.19114	13	0.25894	21	0.55740	23
2.726	0.06772	7	0.19101	14	0.25873	20	0.55717	23
2.727	0.06765	7	0.19087	13	0.25853	21	0.55694	22
2.728	0.06758	7	0.19074	13	0.25832	20	0.55672	23
2.729	0.06751	7	0.19061	14	0.25812	21	0.55649	22
2.730	0.06744	7	0.19047	13	0.25791	20	0.55627	23
2.731	0.06737	7	0.19034	14	0.25771	20	0.55604	23
2.732	0.06730	7	0.19020	13	0.25751	21	0.55581	22
2.733	0.06723	7	0.19007	13	0.25730	20	0.55559	23
2.734	0.06716	6	0.18994	14	0.25710	20	0.55536	23
2.735	0.06710	7	0.18980	13	0.25690	21	0.55513	22
2.736	0.06703	7	0.18967	13	0.25669	20	0.55491	23
2.737	0.06696	7	0.18954	14	0.25649	20	0.55468	22
2.738	0.06689	7	0.18940	13	0.25629	20	0.55446	23
2.739	0.06682	7	0.18927	13	0.25609	21	0.55423	23
2.740	0.06675	7	0.18914	14	0.25588	20	0.55400	22
2.741	0.06668	7	0.18900	13	0.25568	20	0.55378	23
2.742	0.06661	7	0.18887	13	0.25548	20	0.55355	23
2.743	0.06654	7	0.18874	14	0.25528	20	0.55332	22
2.744	0.06647	6	0.18860	13	0.25508	20	0.55310	23
2.745	0.06641	7	0.18847	13	0.25488	21	0.55287	22
2.746	0.06634	7	0.18834	13	0.25467	20	0.55265	23
2.747	0.06627	7	0.18821	14	0.25447	20	0.55242	23
2.748	0.06620	7	0.18807	13	0.25427	20	0.55219	22
2.749	0.06613	7	0.18794	13	0.25407	20	0.55197	23
2.750	0.06606		0.18781		0.25387		0.55174	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.750	0.06606	7	0.18781	13	0.25387	20	0.55174	22
2.751	0.06599	6	0.18768	14	0.25367	20	0.55152	23
2.752	0.06593	7	0.18754	13	0.25347	20	0.55129	22
2.753	0.06586	7	0.18741	13	0.25327	20	0.55107	23
2.754	0.06579	7	0.18728	13	0.25307	20	0.55084	23
2.755	0.06572	7	0.18715	13	0.25287	20	0.55061	22
2.756	0.06565	6	0.18702	14	0.25267	20	0.55039	23
2.757	0.06559	7	0.18688	13	0.25247	20	0.55016	22
2.758	0.06552	7	0.18675	13	0.25227	20	0.54994	23
2.759	0.06545	7	0.18662	13	0.25207	20	0.54971	22
2.760	0.06538	6	0.18649	13	0.25187	20	0.54949	23
2.761	0.06532	7	0.18636	13	0.25167	20	0.54926	22
2.762	0.06525	7	0.18623	14	0.25147	19	0.54904	23
2.763	0.06518	7	0.18609	13	0.25128	20	0.54881	23
2.764	0.06511	6	0.18596	13	0.25108	20	0.54858	22
2.765	0.06505	7	0.18583	13	0.25088	20	0.54836	23
2.766	0.06498	7	0.18570	13	0.25068	20	0.54813	22
2.767	0.06491	6	0.18557	13	0.25048	20	0.54791	23
2.768	0.06485	7	0.18544	13	0.25028	19	0.54768	22
2.769	0.06478	7	0.18531	13	0.25009	20	0.54746	23
2.770	0.06471	7	0.18518	13	0.24989	20	0.54723	22
2.771	0.06464	6	0.18505	13	0.24969	20	0.54701	23
2.772	0.06458	7	0.18492	13	0.24949	19	0.54678	22
2.773	0.06451	7	0.18479	13	0.24930	20	0.54656	23
2.774	0.06444	6	0.18466	14	0.24910	20	0.54633	22
2.775	0.06438	7	0.18452	13	0.24890	19	0.54611	23
2.776	0.06431	6	0.18439	13	0.24871	20	0.54588	22
2.777	0.06425	7	0.18426	13	0.24851	20	0.54566	23
2.778	0.06418	7	0.18413	13	0.24831	19	0.54543	22
2.779	0.06411	6	0.18400	13	0.24812	20	0.54521	23
2.780	0.06405	7	0.18387	13	0.24792	20	0.54498	22
2.781	0.06398	7	0.18374	13	0.24772	19	0.54476	23
2.782	0.06391	6	0.18361	12	0.24753	20	0.54453	22
2.783	0.06385	7	0.18349	13	0.24733	19	0.54431	23
2.784	0.06378	6	0.18336	13	0.24714	20	0.54408	22
2.785	0.06372	7	0.18323	13	0.24694	19	0.54386	23
2.786	0.06365	6	0.18310	13	0.24675	20	0.54363	22
2.787	0.06359	7	0.18297	13	0.24655	19	0.54341	23
2.788	0.06352	7	0.18284	13	0.24636	20	0.54318	22
2.789	0.06345	6	0.18271	13	0.24616	19	0.54296	23
2.790	0.06339	7	0.18258	13	0.24597	20	0.54273	22
2.791	0.06332	6	0.18245	13	0.24577	19	0.54251	23
2.792	0.06326	7	0.18232	13	0.24558	20	0.54228	22
2.793	0.06319	6	0.18219	13	0.24538	19	0.54206	23
2.794	0.06313	7	0.18206	12	0.24519	19	0.54183	22
2.795	0.06306	6	0.18194	13	0.24500	20	0.54161	23
2.796	0.06300	7	0.18181	13	0.24480	19	0.54138	22
2.797	0.06293	6	0.18168	13	0.24461	19	0.54116	22
2.798	0.06287	7	0.18155	13	0.24442	20	0.54094	23
2.799	0.06280	6	0.18142	13	0.24422	19	0.54071	22
2.800	0.06274		0.18129		0.24403		0.54049	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.800	0.06274	7	0.18129	13	0.24403	19	0.54049	23
2.801	0.06267	6	0.18116	12	0.24384	20	0.54026	22
2.802	0.06261	7	0.18104	13	0.24364	19	0.54004	23
2.803	0.06254	6	0.18091	13	0.24345	19	0.53981	22
2.804	0.06248	7	0.18078	13	0.24326	19	0.53959	23
2.805	0.06241	6	0.18065	13	0.24307	20	0.53936	22
2.806	0.06235	6	0.18052	12	0.24287	19	0.53914	22
2.807	0.06229	7	0.18040	13	0.24268	19	0.53892	23
2.808	0.06222	6	0.18027	13	0.24249	19	0.53869	22
2.809	0.06216	7	0.18014	13	0.24230	19	0.53847	23
2.810	0.06209	6	0.18001	12	0.24211	19	0.53824	22
2.811	0.06203	6	0.17989	13	0.24192	20	0.53802	22
2.812	0.06197	7	0.17976	13	0.24172	19	0.53780	23
2.813	0.06190	6	0.17963	13	0.24153	19	0.53757	22
2.814	0.06184	7	0.17950	12	0.24134	19	0.53735	23
2.815	0.06177	6	0.17938	13	0.24115	19	0.53712	22
2.816	0.06171	6	0.17925	13	0.24096	19	0.53690	22
2.817	0.06165	7	0.17912	12	0.24077	19	0.53668	23
2.818	0.06158	6	0.17900	13	0.24058	19	0.53645	22
2.819	0.06152	6	0.17887	13	0.24039	19	0.53623	23
2.820	0.06146	7	0.17874	12	0.24020	19	0.53600	22
2.821	0.06139	6	0.17862	13	0.24001	19	0.53578	22
2.822	0.06133	6	0.17849	13	0.23982	19	0.53556	23
2.823	0.06127	7	0.17836	12	0.23963	19	0.53533	22
2.824	0.06120	6	0.17824	13	0.23944	19	0.53511	22
2.825	0.06114	6	0.17811	13	0.23925	19	0.53489	23
2.826	0.06108	7	0.17798	12	0.23906	19	0.53466	22
2.827	0.06101	6	0.17786	13	0.23887	19	0.53444	23
2.828	0.06095	6	0.17773	12	0.23868	19	0.53421	22
2.829	0.06089	6	0.17761	13	0.23849	18	0.53399	22
2.830	0.06083	7	0.17748	13	0.23831	19	0.53377	23
2.831	0.06076	6	0.17735	12	0.23812	19	0.53354	22
2.832	0.06070	6	0.17723	13	0.23793	19	0.53332	22
2.833	0.06064	6	0.17710	12	0.23774	19	0.53310	23
2.834	0.06058	7	0.17698	13	0.23755	19	0.53287	22
2.835	0.06051	6	0.17685	12	0.23736	18	0.53265	22
2.836	0.06045	6	0.17673	13	0.23718	19	0.53243	23
2.837	0.06039	6	0.17660	12	0.23699	19	0.53220	22
2.838	0.06033	7	0.17648	13	0.23680	19	0.53198	22
2.839	0.06026	6	0.17635	13	0.23661	18	0.53176	23
2.840	0.06020	6	0.17622	12	0.23643	19	0.53153	22
2.841	0.06014	6	0.17610	13	0.23624	19	0.53131	22
2.842	0.06008	6	0.17597	12	0.23605	18	0.53109	23
2.843	0.06002	7	0.17585	12	0.23587	19	0.53086	22
2.844	0.05995	6	0.17573	13	0.23568	19	0.53064	22
2.845	0.05989	6	0.17560	12	0.23549	18	0.53042	22
2.846	0.05983	6	0.17548	13	0.23531	19	0.53020	23
2.847	0.05977	6	0.17535	12	0.23512	19	0.52997	22
2.848	0.05971	6	0.17523	13	0.23493	18	0.52975	22
2.849	0.05965	7	0.17510	12	0.23475	19	0.52953	23
2.850	0.05958		0.17498		0.23456		0.52930	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.850	0.05958	6	0.17498	13	0.23456	18	0.52930	22
2.851	0.05952	6	0.17485	12	0.23438	19	0.52908	22
2.852	0.05946	6	0.17473	12	0.23419	18	0.52886	22
2.853	0.05940	6	0.17461	13	0.23401	19	0.52864	23
2.854	0.05934	6	0.17448	12	0.23382	18	0.52841	22
2.855	0.05928	6	0.17436	13	0.23364	19	0.52819	22
2.856	0.05922	6	0.17423	12	0.23345	18	0.52797	23
2.857	0.05916	6	0.17411	12	0.23327	19	0.52774	22
2.858	0.05910	7	0.17399	13	0.23308	18	0.52752	22
2.859	0.05903	6	0.17386	12	0.23290	19	0.52730	22
2.860	0.05897	6	0.17374	13	0.23271	18	0.52708	23
2.861	0.05891	6	0.17361	12	0.23253	19	0.52685	22
2.862	0.05885	6	0.17349	12	0.23234	18	0.52663	22
2.863	0.05879	6	0.17337	13	0.23216	18	0.52641	22
2.864	0.05873	6	0.17324	12	0.23198	19	0.52619	23
2.865	0.05867	6	0.17312	12	0.23179	18	0.52596	22
2.866	0.05861	6	0.17300	12	0.23161	18	0.52574	22
2.867	0.05855	6	0.17288	13	0.23143	19	0.52552	22
2.868	0.05849	6	0.17275	12	0.23124	18	0.52530	22
2.869	0.05843	6	0.17263	12	0.23106	18	0.52508	23
2.870	0.05837	6	0.17251	13	0.23088	19	0.52485	22
2.871	0.05831	6	0.17238	12	0.23069	18	0.52463	22
2.872	0.05825	6	0.17226	12	0.23051	18	0.52441	22
2.873	0.05819	6	0.17214	12	0.23033	18	0.52419	23
2.874	0.05813	6	0.17202	13	0.23015	19	0.52396	22
2.875	0.05807	6	0.17189	12	0.22996	18	0.52374	22
2.876	0.05801	6	0.17177	12	0.22978	18	0.52352	22
2.877	0.05795	6	0.17165	12	0.22960	18	0.52330	22
2.878	0.05789	6	0.17153	12	0.22942	18	0.52308	23
2.879	0.05783	6	0.17141	13	0.22924	19	0.52285	22
2.880	0.05777	6	0.17128	12	0.22905	18	0.52263	22
2.881	0.05771	6	0.17116	12	0.22887	18	0.52241	22
2.882	0.05765	6	0.17104	12	0.22869	18	0.52219	22
2.883	0.05759	6	0.17092	12	0.22851	18	0.52197	22
2.884	0.05753	5	0.17080	13	0.22833	18	0.52175	23
2.885	0.05748	6	0.17067	12	0.22815	18	0.52152	22
2.886	0.05742	6	0.17055	12	0.22797	18	0.52130	22
2.887	0.05736	6	0.17043	12	0.22779	18	0.52108	22
2.888	0.05730	6	0.17031	12	0.22761	18	0.52086	22
2.889	0.05724	6	0.17019	12	0.22743	18	0.52064	22
2.890	0.05718	6	0.17007	12	0.22725	18	0.52042	23
2.891	0.05712	6	0.16995	13	0.22707	18	0.52019	22
2.892	0.05706	6	0.16982	12	0.22689	18	0.51997	22
2.893	0.05700	5	0.16970	12	0.22671	18	0.51975	22
2.894	0.05695	6	0.16958	12	0.22653	18	0.51953	22
2.895	0.05689	6	0.16946	12	0.22635	18	0.51931	22
2.896	0.05683	6	0.16934	12	0.22617	18	0.51909	22
2.897	0.05677	6	0.16922	12	0.22599	18	0.51887	22
2.898	0.05671	6	0.16910	12	0.22581	18	0.51865	23
2.899	0.05665	6	0.16898	12	0.22563	18	0.51842	22
2.900	0.05659		0.16886		0.22545		0.51820	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.900	0.05659	5	0.16886	12	0.22545	18	0.51820	22
2.901	0.05654	6	0.16874	12	0.22527	17	0.51798	22
2.902	0.05648	6	0.16862	12	0.22510	18	0.51776	22
2.903	0.05642	6	0.16850	12	0.22492	18	0.51754	22
2.904	0.05636	6	0.16838	12	0.22474	18	0.51732	22
2.905	0.05630	5	0.16826	12	0.22456	18	0.51710	22
2.906	0.05625	6	0.16814	12	0.22438	17	0.51688	22
2.907	0.05619	6	0.16802	12	0.22421	18	0.51666	23
2.908	0.05613	6	0.16790	12	0.22403	18	0.51643	22
2.909	0.05607	5	0.16778	12	0.22385	18	0.51621	22
2.910	0.05602	6	0.16766	12	0.22367	17	0.51599	22
2.911	0.05596	6	0.16754	12	0.22350	18	0.51577	22
2.912	0.05590	6	0.16742	12	0.22332	18	0.51555	22
2.913	0.05584	5	0.16730	12	0.22314	17	0.51533	22
2.914	0.05579	6	0.16718	12	0.22297	18	0.51511	22
2.915	0.05573	6	0.16706	12	0.22279	18	0.51489	22
2.916	0.05567	6	0.16694	12	0.22261	17	0.51467	22
2.917	0.05561	5	0.16682	12	0.22244	18	0.51445	22
2.918	0.05556	6	0.16670	12	0.22226	18	0.51423	22
2.919	0.05550	6	0.16658	12	0.22208	17	0.51401	22
2.920	0.05544	5	0.16646	11	0.22191	18	0.51379	22
2.921	0.05539	6	0.16635	12	0.22173	17	0.51357	22
2.922	0.05533	6	0.16623	12	0.22156	18	0.51335	22
2.923	0.05527	5	0.16611	12	0.22138	18	0.51313	23
2.924	0.05522	6	0.16599	12	0.22120	17	0.51290	22
2.925	0.05516	6	0.16587	12	0.22103	18	0.51268	22
2.926	0.05510	5	0.16575	12	0.22085	17	0.51246	22
2.927	0.05505	6	0.16563	11	0.22068	18	0.51224	22
2.928	0.05499	6	0.16552	12	0.22050	17	0.51202	22
2.929	0.05493	5	0.16540	12	0.22033	18	0.51180	22
2.930	0.05488	6	0.16528	12	0.22015	17	0.51158	22
2.931	0.05482	6	0.16516	12	0.21998	17	0.51136	22
2.932	0.05476	5	0.16504	12	0.21981	18	0.51114	22
2.933	0.05471	6	0.16492	11	0.21963	17	0.51092	22
2.934	0.05465	6	0.16481	12	0.21946	18	0.51070	22
2.935	0.05459	5	0.16469	12	0.21928	17	0.51048	22
2.936	0.05454	6	0.16457	12	0.21911	17	0.51026	22
2.937	0.05448	5	0.16445	11	0.21894	18	0.51004	22
2.938	0.05443	6	0.16434	12	0.21876	17	0.50982	22
2.939	0.05437	6	0.16422	12	0.21859	18	0.50960	22
2.940	0.05431	5	0.16410	12	0.21841	17	0.50938	22
2.941	0.05426	6	0.16398	11	0.21824	17	0.50916	21
2.942	0.05420	5	0.16387	12	0.21807	17	0.50895	22
2.943	0.05415	6	0.16375	12	0.21790	18	0.50873	22
2.944	0.05409	5	0.16363	12	0.21772	17	0.50851	22
2.945	0.05404	6	0.16351	11	0.21755	17	0.50829	22
2.946	0.05398	5	0.16340	12	0.21738	17	0.50807	22
2.947	0.05393	6	0.16328	12	0.21721	18	0.50785	22
2.948	0.05387	6	0.16316	11	0.21703	17	0.50763	22
2.949	0.05381	5	0.16305	12	0.21686	17	0.50741	22
2.950	0.05376		0.16293		0.21669		0.50719	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
2.950	0.05376	6	0.16293	12	0.21669	17	0.50719	22
2.951	0.05370	5	0.16281	11	0.21652	17	0.50697	22
2.952	0.05365	6	0.16270	12	0.21635	18	0.50675	22
2.953	0.05359	5	0.16258	12	0.21617	17	0.50653	22
2.954	0.05354	6	0.16246	11	0.21600	17	0.50631	22
2.955	0.05348	5	0.16235	12	0.21583	17	0.50609	22
2.956	0.05343	6	0.16223	12	0.21566	17	0.50587	22
2.957	0.05337	5	0.16211	11	0.21549	17	0.50565	21
2.958	0.05332	6	0.16200	12	0.21532	17	0.50544	22
2.959	0.05326	5	0.16188	11	0.21515	17	0.50522	22
2.960	0.05321	5	0.16177	12	0.21498	17	0.50500	22
2.961	0.05316	6	0.16165	12	0.21481	17	0.50478	22
2.962	0.05310	5	0.16153	11	0.21464	17	0.50456	22
2.963	0.05305	6	0.16142	12	0.21447	18	0.50434	22
2.964	0.05299	5	0.16130	11	0.21429	17	0.50412	22
2.965	0.05294	6	0.16119	12	0.21412	16	0.50390	22
2.966	0.05288	5	0.16107	11	0.21396	17	0.50368	21
2.967	0.05283	6	0.16096	12	0.21379	17	0.50347	22
2.968	0.05277	5	0.16084	11	0.21362	17	0.50325	22
2.969	0.05272	5	0.16073	12	0.21345	17	0.50303	22
2.970	0.05267	6	0.16061	11	0.21328	17	0.50281	22
2.971	0.05261	5	0.16050	12	0.21311	17	0.50259	22
2.972	0.05256	6	0.16038	11	0.21294	17	0.50237	22
2.973	0.05250	5	0.16027	12	0.21277	17	0.50215	21
2.974	0.05245	5	0.16015	11	0.21260	17	0.50194	22
2.975	0.05240	6	0.16004	12	0.21243	17	0.50172	22
2.976	0.05234	5	0.15992	11	0.21226	17	0.50150	22
2.977	0.05229	5	0.15981	12	0.21209	16	0.50128	22
2.978	0.05224	6	0.15969	11	0.21193	17	0.50106	22
2.979	0.05218	5	0.15958	12	0.21176	17	0.50084	21
2.980	0.05213	6	0.15946	11	0.21159	17	0.50063	22
2.981	0.05207	5	0.15935	12	0.21142	17	0.50041	22
2.982	0.05202	5	0.15923	11	0.21125	16	0.50019	22
2.983	0.05197	6	0.15912	12	0.21109	17	0.49997	22
2.984	0.05191	5	0.15900	11	0.21092	17	0.49975	22
2.985	0.05186	5	0.15889	11	0.21075	17	0.49953	21
2.986	0.05181	6	0.15878	12	0.21058	16	0.49932	22
2.987	0.05175	5	0.15866	11	0.21042	17	0.49910	22
2.988	0.05170	5	0.15855	12	0.21025	17	0.49888	22
2.989	0.05165	5	0.15843	11	0.21008	16	0.49866	21
2.990	0.05160	6	0.15832	11	0.20992	17	0.49845	22
2.991	0.05154	5	0.15821	12	0.20975	17	0.49823	22
2.992	0.05149	5	0.15809	11	0.20958	16	0.49801	22
2.993	0.05144	6	0.15798	11	0.20942	17	0.49779	22
2.994	0.05138	5	0.15787	12	0.20925	17	0.49757	21
2.995	0.05133	5	0.15775	11	0.20908	16	0.49736	22
2.996	0.05128	5	0.15764	11	0.20892	17	0.49714	22
2.997	0.05123	6	0.15753	12	0.20875	16	0.49692	22
2.998	0.05117	5	0.15741	11	0.20859	17	0.49670	21
2.999	0.05112	5	0.15730	11	0.20842	16	0.49649	22
3.000	0.05107		0.15719		0.20826		0.49627	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.000	0.05107	5	0.15719	12	0.20826	17	0.49627	22
3.001	0.05102	6	0.15707	11	0.20809	16	0.49605	22
3.002	0.05096	5	0.15696	11	0.20793	17	0.49583	21
3.003	0.05091	5	0.15685	11	0.20776	16	0.49562	22
3.004	0.05086	5	0.15674	12	0.20760	17	0.49540	22
3.005	0.05081	5	0.15662	11	0.20743	16	0.49518	21
3.006	0.05076	6	0.15651	11	0.20727	17	0.49497	22
3.007	0.05070	5	0.15640	11	0.20710	16	0.49475	22
3.008	0.05065	5	0.15629	12	0.20694	17	0.49453	22
3.009	0.05060	5	0.15617	11	0.20677	16	0.49431	21
3.010	0.05055	5	0.15606	11	0.20661	17	0.49410	22
3.011	0.05050	6	0.15595	11	0.20644	16	0.49388	22
3.012	0.05044	5	0.15584	12	0.20628	16	0.49366	21
3.013	0.05039	5	0.15572	11	0.20612	17	0.49345	22
3.014	0.05034	5	0.15561	11	0.20595	16	0.49323	22
3.015	0.05029	5	0.15550	11	0.20579	16	0.49301	21
3.016	0.05024	5	0.15539	11	0.20563	17	0.49280	22
3.017	0.05019	6	0.15528	12	0.20546	16	0.49258	22
3.018	0.05013	5	0.15516	11	0.20530	16	0.49236	21
3.019	0.05008	5	0.15505	11	0.20514	17	0.49215	22
3.020	0.05003	5	0.15494	11	0.20497	16	0.49193	22
3.021	0.04998	5	0.15483	11	0.20481	16	0.49171	21
3.022	0.04993	5	0.15472	11	0.20465	16	0.49150	22
3.023	0.04988	5	0.15461	11	0.20449	17	0.49128	22
3.024	0.04983	5	0.15450	12	0.20432	16	0.49106	21
3.025	0.04978	5	0.15438	11	0.20416	16	0.49085	22
3.026	0.04973	6	0.15427	11	0.20400	16	0.49063	22
3.027	0.04967	5	0.15416	11	0.20384	17	0.49041	21
3.028	0.04962	5	0.15405	11	0.20367	16	0.49020	22
3.029	0.04957	5	0.15394	11	0.20351	16	0.48998	22
3.030	0.04952	5	0.15383	11	0.20335	16	0.48976	21
3.031	0.04947	5	0.15372	11	0.20319	16	0.48955	22
3.032	0.04942	5	0.15361	11	0.20303	16	0.48933	21
3.033	0.04937	5	0.15350	11	0.20287	17	0.48912	22
3.034	0.04932	5	0.15339	11	0.20270	16	0.48890	22
3.035	0.04927	5	0.15328	12	0.20254	16	0.48868	21
3.036	0.04922	5	0.15316	11	0.20238	16	0.48847	22
3.037	0.04917	5	0.15305	11	0.20222	16	0.48825	21
3.038	0.04912	5	0.15294	11	0.20206	16	0.48804	22
3.039	0.04907	5	0.15283	11	0.20190	16	0.48782	22
3.040	0.04902	5	0.15272	11	0.20174	16	0.48760	21
3.041	0.04897	5	0.15261	11	0.20158	16	0.48739	22
3.042	0.04892	5	0.15250	11	0.20142	16	0.48717	21
3.043	0.04887	5	0.15239	11	0.20126	16	0.48696	22
3.044	0.04882	5	0.15228	11	0.20110	16	0.48674	21
3.045	0.04877	5	0.15217	11	0.20094	16	0.48653	22
3.046	0.04872	5	0.15206	11	0.20078	16	0.48631	22
3.047	0.04867	5	0.15195	11	0.20062	16	0.48609	21
3.048	0.04862	5	0.15184	10	0.20046	16	0.48588	22
3.049	0.04857	5	0.15174	11	0.20030	16	0.48566	21
3.050	0.04852		0.15163		0.20014		0.48545	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.050	0.04852	5	0.15163	11	0.20014	16	0.48545	22
3.051	0.04847	5	0.15152	11	0.19998	16	0.48523	21
3.052	0.04842	5	0.15141	11	0.19982	15	0.48502	22
3.053	0.04837	5	0.15130	11	0.19967	16	0.48480	21
3.054	0.04832	5	0.15119	11	0.19951	16	0.48459	22
3.055	0.04827	5	0.15108	11	0.19935	16	0.48437	21
3.056	0.04822	5	0.15097	11	0.19919	16	0.48416	22
3.057	0.04817	5	0.15086	11	0.19903	16	0.48394	21
3.058	0.04812	5	0.15075	11	0.19887	15	0.48373	22
3.059	0.04807	5	0.15064	11	0.19872	16	0.48351	21
3.060	0.04802	5	0.15053	10	0.19856	16	0.48330	22
3.061	0.04797	5	0.15043	11	0.19840	16	0.48308	21
3.062	0.04792	4	0.15032	11	0.19824	16	0.48287	22
3.063	0.04788	5	0.15021	11	0.19808	15	0.48265	21
3.064	0.04783	5	0.15010	11	0.19793	16	0.48244	22
3.065	0.04778	5	0.14999	11	0.19777	16	0.48222	21
3.066	0.04773	5	0.14988	10	0.19761	16	0.48201	22
3.067	0.04768	5	0.14978	11	0.19745	15	0.48179	21
3.068	0.04763	5	0.14967	11	0.19730	16	0.48158	22
3.069	0.04758	5	0.14956	11	0.19714	16	0.48136	21
3.070	0.04753	5	0.14945	11	0.19698	15	0.48115	22
3.071	0.04748	4	0.14934	11	0.19683	16	0.48093	21
3.072	0.04744	5	0.14923	10	0.19667	16	0.48072	21
3.073	0.04739	5	0.14913	11	0.19651	15	0.48051	22
3.074	0.04734	5	0.14902	11	0.19636	16	0.48029	21
3.075	0.04729	5	0.14891	11	0.19620	15	0.48008	22
3.076	0.04724	5	0.14880	10	0.19605	16	0.47986	21
3.077	0.04719	4	0.14870	11	0.19589	16	0.47965	22
3.078	0.04715	5	0.14859	11	0.19573	15	0.47943	21
3.079	0.04710	5	0.14848	11	0.19558	16	0.47922	21
3.080	0.04705	5	0.14837	10	0.19542	15	0.47901	22
3.081	0.04700	5	0.14827	11	0.19527	16	0.47879	21
3.082	0.04695	5	0.14816	11	0.19511	15	0.47858	22
3.083	0.04690	4	0.14805	11	0.19496	16	0.47836	21
3.084	0.04686	5	0.14794	10	0.19480	15	0.47815	21
3.085	0.04681	5	0.14784	11	0.19465	16	0.47794	22
3.086	0.04676	5	0.14773	11	0.19449	15	0.47772	21
3.087	0.04671	4	0.14762	10	0.19434	16	0.47751	22
3.088	0.04667	5	0.14752	11	0.19418	15	0.47729	21
3.089	0.04662	5	0.14741	11	0.19403	16	0.47708	21
3.090	0.04657	5	0.14730	10	0.19387	15	0.47687	22
3.091	0.04652	5	0.14720	11	0.19372	16	0.47665	21
3.092	0.04647	4	0.14709	11	0.19356	15	0.47644	21
3.093	0.04643	5	0.14698	10	0.19341	15	0.47623	22
3.094	0.04638	5	0.14688	11	0.19326	16	0.47601	21
3.095	0.04633	5	0.14677	11	0.19310	15	0.47580	21
3.096	0.04628	4	0.14666	10	0.19295	15	0.47559	22
3.097	0.04624	5	0.14656	11	0.19280	16	0.47537	21
3.098	0.04619	5	0.14645	10	0.19264	15	0.47516	21
3.099	0.04614	4	0.14635	11	0.19249	15	0.47495	22
3.100	0.04610		0.14624		0.19234		0.47473	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_P^0/R	Δ
3.100	0.04610	5	0.14624	11	0.19234	16	0.47473	21
3.101	0.04605	5	0.14613	10	0.19218	15	0.47452	21
3.102	0.04600	5	0.14603	11	0.19203	15	0.47431	22
3.103	0.04595	4	0.14592	10	0.19188	16	0.47409	21
3.104	0.04591	5	0.14582	11	0.19172	15	0.47388	21
3.105	0.04586	5	0.14571	10	0.19157	15	0.47367	22
3.106	0.04581	4	0.14561	11	0.19142	15	0.47345	21
3.107	0.04577	5	0.14550	10	0.19127	16	0.47324	21
3.108	0.04572	5	0.14540	11	0.19111	15	0.47303	22
3.109	0.04567	4	0.14529	11	0.19096	15	0.47281	21
3.110	0.04563	5	0.14518	10	0.19081	15	0.47260	21
3.111	0.04558	5	0.14508	11	0.19066	15	0.47239	21
3.112	0.04553	4	0.14497	10	0.19051	15	0.47218	22
3.113	0.04549	5	0.14487	11	0.19036	16	0.47196	21
3.114	0.04544	5	0.14476	10	0.19020	15	0.47175	21
3.115	0.04539	4	0.14466	11	0.19005	15	0.47154	21
3.116	0.04535	5	0.14455	10	0.18990	15	0.47133	22
3.117	0.04530	5	0.14445	11	0.18975	15	0.47111	21
3.118	0.04525	4	0.14434	10	0.18960	15	0.47090	21
3.119	0.04521	5	0.14424	11	0.18945	15	0.47069	21
3.120	0.04516	4	0.14413	10	0.18930	15	0.47048	22
3.121	0.04512	5	0.14403	10	0.18915	15	0.47026	21
3.122	0.04507	5	0.14393	11	0.18900	16	0.47005	21
3.123	0.04502	4	0.14382	10	0.18884	15	0.46984	21
3.124	0.04498	5	0.14372	11	0.18869	15	0.46963	22
3.125	0.04493	4	0.14361	10	0.18854	15	0.46941	21
3.126	0.04489	5	0.14351	11	0.18839	15	0.46920	21
3.127	0.04484	5	0.14340	10	0.18824	15	0.46899	21
3.128	0.04479	4	0.14330	10	0.18809	15	0.46878	21
3.129	0.04475	5	0.14320	11	0.18794	15	0.46857	22
3.130	0.04470	4	0.14309	10	0.18779	14	0.46835	21
3.131	0.04466	5	0.14299	11	0.18765	15	0.46814	21
3.132	0.04461	4	0.14288	10	0.18750	15	0.46793	21
3.133	0.04457	5	0.14278	10	0.18735	15	0.46772	21
3.134	0.04452	5	0.14268	11	0.18720	15	0.46751	21
3.135	0.04447	4	0.14257	10	0.18705	15	0.46730	22
3.136	0.04443	5	0.14247	10	0.18690	15	0.46708	21
3.137	0.04438	4	0.14237	11	0.18675	15	0.46687	21
3.138	0.04434	5	0.14226	10	0.18660	15	0.46666	21
3.139	0.04429	4	0.14216	10	0.18645	15	0.46645	21
3.140	0.04425	5	0.14206	11	0.18630	14	0.46624	21
3.141	0.04420	4	0.14195	10	0.18616	15	0.46603	22
3.142	0.04416	5	0.14185	10	0.18601	15	0.46581	21
3.143	0.04411	4	0.14175	11	0.18586	15	0.46560	21
3.144	0.04407	5	0.14164	10	0.18571	15	0.46539	21
3.145	0.04402	4	0.14154	10	0.18556	14	0.46518	21
3.146	0.04398	5	0.14144	10	0.18542	15	0.46497	21
3.147	0.04393	4	0.14134	11	0.18527	15	0.46476	21
3.148	0.04389	5	0.14123	10	0.18512	15	0.46455	21
3.149	0.04384	4	0.14113	10	0.18497	15	0.46434	21
3.150	0.04380		0.14103		0.18482		0.46413	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.150	0.04380	5	0.14103	11	0.18482	14	0.46413	22
3.151	0.04375	4	0.14092	10	0.18468	15	0.46391	21
3.152	0.04371	5	0.14082	10	0.18453	15	0.46370	21
3.153	0.04366	4	0.14072	10	0.18438	14	0.46349	21
3.154	0.04362	5	0.14062	10	0.18424	15	0.46328	21
3.155	0.04357	4	0.14052	11	0.18409	15	0.46307	21
3.156	0.04353	4	0.14041	10	0.18394	14	0.46286	21
3.157	0.04349	5	0.14031	10	0.18380	15	0.46265	21
3.158	0.04344	4	0.14021	10	0.18365	15	0.46244	21
3.159	0.04340	5	0.14011	10	0.18350	14	0.46223	21
3.160	0.04335	4	0.14001	11	0.18336	15	0.46202	21
3.161	0.04331	5	0.13990	10	0.18321	15	0.46181	21
3.162	0.04326	4	0.13980	10	0.18306	14	0.46160	21
3.163	0.04322	4	0.13970	10	0.18292	15	0.46139	21
3.164	0.04318	5	0.13960	10	0.18277	14	0.46118	21
3.165	0.04313	4	0.13950	11	0.18263	15	0.46097	21
3.166	0.04309	5	0.13939	10	0.18248	14	0.46076	21
3.167	0.04304	4	0.13929	10	0.18234	15	0.46055	22
3.168	0.04300	4	0.13919	10	0.18219	14	0.46033	21
3.169	0.04296	5	0.13909	10	0.18205	15	0.46012	21
3.170	0.04291	4	0.13899	10	0.18190	14	0.45991	21
3.171	0.04287	5	0.13889	10	0.18176	15	0.45970	21
3.172	0.04282	4	0.13879	10	0.18161	14	0.45949	21
3.173	0.04278	4	0.13869	10	0.18147	15	0.45928	21
3.174	0.04274	5	0.13859	11	0.18132	14	0.45907	21
3.175	0.04269	4	0.13848	10	0.18118	15	0.45886	20
3.176	0.04265	4	0.13838	10	0.18103	14	0.45866	21
3.177	0.04261	5	0.13828	10	0.18089	15	0.45845	21
3.178	0.04256	4	0.13818	10	0.18074	14	0.45824	21
3.179	0.04252	4	0.13808	10	0.18060	14	0.45803	21
3.180	0.04248	5	0.13798	10	0.18046	15	0.45782	21
3.181	0.04243	4	0.13788	10	0.18031	14	0.45761	21
3.182	0.04239	4	0.13778	10	0.18017	15	0.45740	21
3.183	0.04235	5	0.13768	10	0.18002	14	0.45719	21
3.184	0.04230	4	0.13758	10	0.17988	14	0.45698	21
3.185	0.04226	4	0.13748	10	0.17974	15	0.45677	21
3.186	0.04222	5	0.13738	10	0.17959	14	0.45656	21
3.187	0.04217	4	0.13728	10	0.17945	14	0.45635	21
3.188	0.04213	4	0.13718	10	0.17931	15	0.45614	21
3.189	0.04209	5	0.13708	10	0.17916	14	0.45593	21
3.190	0.04204	4	0.13698	10	0.17902	14	0.45572	21
3.191	0.04200	4	0.13688	10	0.17888	14	0.45551	21
3.192	0.04196	5	0.13678	10	0.17874	15	0.45530	20
3.193	0.04191	4	0.13668	10	0.17859	14	0.45510	21
3.194	0.04187	4	0.13658	10	0.17845	14	0.45489	21
3.195	0.04183	4	0.13648	10	0.17831	14	0.45468	21
3.196	0.04179	5	0.13638	10	0.17817	15	0.45447	21
3.197	0.04174	4	0.13628	10	0.17802	14	0.45426	21
3.198	0.04170	4	0.13618	10	0.17788	14	0.45405	21
3.199	0.04166	4	0.13608	10	0.17774	14	0.45384	21
3.200	0.04162		0.13598		0.17760		0.45363	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.200	0.04162	5	0.13598	10	0.17760	14	0.45363	21
3.201	0.04157	4	0.13588	10	0.17746	15	0.45342	20
3.202	0.04153	4	0.13578	10	0.17731	14	0.45322	21
3.203	0.04149	4	0.13568	9	0.17717	14	0.45301	21
3.204	0.04145	5	0.13559	10	0.17703	14	0.45280	21
3.205	0.04140	4	0.13549	10	0.17689	14	0.45259	21
3.206	0.04136	4	0.13539	10	0.17675	14	0.45238	21
3.207	0.04132	4	0.13529	10	0.17661	14	0.45217	20
3.208	0.04128	4	0.13519	10	0.17647	14	0.45197	21
3.209	0.04124	5	0.13509	10	0.17633	14	0.45176	21
3.210	0.04119	4	0.13499	10	0.17619	14	0.45155	21
3.211	0.04115	4	0.13489	9	0.17605	15	0.45134	21
3.212	0.04111	4	0.13480	10	0.17590	14	0.45113	21
3.213	0.04107	4	0.13470	10	0.17576	14	0.45092	20
3.214	0.04103	5	0.13460	10	0.17562	14	0.45072	21
3.215	0.04098	4	0.13450	10	0.17548	14	0.45051	21
3.216	0.04094	4	0.13440	10	0.17534	14	0.45030	21
3.217	0.04090	4	0.13430	9	0.17520	14	0.45009	20
3.218	0.04086	4	0.13421	10	0.17506	14	0.44989	21
3.219	0.04082	4	0.13411	10	0.17492	14	0.44968	21
3.220	0.04078	5	0.13401	10	0.17478	13	0.44947	21
3.221	0.04073	4	0.13391	10	0.17465	14	0.44926	21
3.222	0.04069	4	0.13381	9	0.17451	14	0.44905	20
3.223	0.04065	4	0.13372	10	0.17437	14	0.44885	21
3.224	0.04061	4	0.13362	10	0.17423	14	0.44864	21
3.225	0.04057	4	0.13352	10	0.17409	14	0.44843	21
3.226	0.04053	5	0.13342	9	0.17395	14	0.44822	20
3.227	0.04048	4	0.13333	10	0.17381	14	0.44802	21
3.228	0.04044	4	0.13323	10	0.17367	14	0.44781	21
3.229	0.04040	4	0.13313	10	0.17353	14	0.44760	21
3.230	0.04036	4	0.13303	9	0.17339	13	0.44739	20
3.231	0.04032	4	0.13294	10	0.17326	14	0.44719	21
3.232	0.04028	4	0.13284	10	0.17312	14	0.44698	21
3.233	0.04024	4	0.13274	10	0.17298	14	0.44677	20
3.234	0.04020	4	0.13264	9	0.17284	14	0.44657	21
3.235	0.04016	5	0.13255	10	0.17270	13	0.44636	21
3.236	0.04011	4	0.13245	10	0.17257	14	0.44615	20
3.237	0.04007	4	0.13235	9	0.17243	14	0.44595	21
3.238	0.04003	4	0.13226	10	0.17229	14	0.44574	21
3.239	0.03999	4	0.13216	10	0.17215	14	0.44553	20
3.240	0.03995	4	0.13206	9	0.17201	13	0.44533	21
3.241	0.03991	4	0.13197	10	0.17188	14	0.44512	21
3.242	0.03987	4	0.13187	10	0.17174	14	0.44491	20
3.243	0.03983	4	0.13177	9	0.17160	13	0.44471	21
3.244	0.03979	4	0.13168	10	0.17147	14	0.44450	21
3.245	0.03975	4	0.13158	10	0.17133	14	0.44429	20
3.246	0.03971	4	0.13148	9	0.17119	13	0.44409	21
3.247	0.03967	4	0.13139	10	0.17106	14	0.44388	21
3.248	0.03963	4	0.13129	9	0.17092	14	0.44367	20
3.249	0.03959	4	0.13120	10	0.17078	13	0.44347	21
3.250	0.03955		0.13110		0.17065		0.44326	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_P^0/R	Δ
3.250	0.03955	4	0.13110	10	0.17065	14	0.44326	21
3.251	0.03951	4	0.13100	9	0.17051	14	0.44305	20
3.252	0.03947	4	0.13091	10	0.17037	13	0.44285	21
3.253	0.03943	5	0.13081	9	0.17024	14	0.44264	20
3.254	0.03938	4	0.13072	10	0.17010	14	0.44244	21
3.255	0.03934	4	0.13062	10	0.16996	13	0.44223	21
3.256	0.03930	4	0.13052	9	0.16983	14	0.44202	20
3.257	0.03926	4	0.13043	10	0.16969	13	0.44182	21
3.258	0.03922	4	0.13033	9	0.16956	14	0.44161	20
3.259	0.03918	4	0.13024	10	0.16942	13	0.44141	21
3.260	0.03914	4	0.13014	9	0.16929	14	0.44120	21
3.261	0.03910	4	0.13005	10	0.16915	13	0.44099	20
3.262	0.03906	3	0.12995	9	0.16902	14	0.44079	21
3.263	0.03903	4	0.12986	10	0.16888	13	0.44058	20
3.264	0.03899	4	0.12976	9	0.16875	14	0.44038	21
3.265	0.03895	4	0.12967	10	0.16861	13	0.44017	20
3.266	0.03891	4	0.12957	9	0.16848	14	0.43997	21
3.267	0.03887	4	0.12948	10	0.16834	13	0.43976	20
3.268	0.03883	4	0.12938	9	0.16821	14	0.43956	21
3.269	0.03879	4	0.12929	10	0.16807	13	0.43935	20
3.270	0.03875	4	0.12919	9	0.16794	14	0.43915	21
3.271	0.03871	4	0.12910	10	0.16780	13	0.43894	21
3.272	0.03867	4	0.12900	9	0.16767	13	0.43873	20
3.273	0.03863	4	0.12891	10	0.16754	14	0.43853	21
3.274	0.03859	4	0.12881	9	0.16740	13	0.43832	20
3.275	0.03855	4	0.12872	10	0.16727	14	0.43812	21
3.276	0.03851	4	0.12862	9	0.16713	13	0.43791	20
3.277	0.03847	4	0.12853	10	0.16700	13	0.43771	21
3.278	0.03843	4	0.12843	9	0.16687	14	0.43750	20
3.279	0.03839	4	0.12834	9	0.16673	13	0.43730	20
3.280	0.03835	3	0.12825	10	0.16660	13	0.43710	21
3.281	0.03832	4	0.12815	9	0.16647	14	0.43689	20
3.282	0.03828	4	0.12806	10	0.16633	13	0.43669	21
3.283	0.03824	4	0.12796	9	0.16620	13	0.43648	20
3.284	0.03820	4	0.12787	9	0.16607	13	0.43628	21
3.285	0.03816	4	0.12778	10	0.16594	14	0.43607	20
3.286	0.03812	4	0.12768	9	0.16580	13	0.43587	21
3.287	0.03808	4	0.12759	9	0.16567	13	0.43566	20
3.288	0.03804	4	0.12750	10	0.16554	13	0.43546	21
3.289	0.03800	3	0.12740	9	0.16541	14	0.43525	20
3.290	0.03797	4	0.12731	10	0.16527	13	0.43505	20
3.291	0.03793	4	0.12721	9	0.16514	13	0.43485	21
3.292	0.03789	4	0.12712	9	0.16501	13	0.43464	20
3.293	0.03785	4	0.12703	10	0.16488	13	0.43444	21
3.294	0.03781	4	0.12693	9	0.16475	14	0.43423	20
3.295	0.03777	4	0.12684	9	0.16461	13	0.43403	20
3.296	0.03773	3	0.12675	10	0.16448	13	0.43383	21
3.297	0.03770	4	0.12665	9	0.16435	13	0.43362	20
3.298	0.03766	4	0.12656	9	0.16422	13	0.43342	21
3.299	0.03762	4	0.12647	9	0.16409	13	0.43321	20
3.300	0.03758		0.12638		0.16396		0.43301	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_P^0/R	Δ
3.300	0.03758	4	0.12638	10	0.16396	14	0.43301	20
3.301	0.03754	4	0.12628	9	0.16382	13	0.43281	21
3.302	0.03750	3	0.12619	9	0.16369	13	0.43260	20
3.303	0.03747	4	0.12610	10	0.16356	13	0.43240	20
3.304	0.03743	4	0.12600	9	0.16343	13	0.43220	21
3.305	0.03739	4	0.12591	9	0.16330	13	0.43199	20
3.306	0.03735	4	0.12582	9	0.16317	13	0.43179	20
3.307	0.03731	3	0.12573	10	0.16304	13	0.43159	21
3.308	0.03728	4	0.12563	9	0.16291	13	0.43138	20
3.309	0.03724	4	0.12554	9	0.16278	13	0.43118	20
3.310	0.03720	4	0.12545	9	0.16265	13	0.43098	21
3.311	0.03716	4	0.12536	10	0.16252	13	0.43077	20
3.312	0.03712	3	0.12526	9	0.16239	13	0.43057	20
3.313	0.03709	4	0.12517	9	0.16226	13	0.43037	21
3.314	0.03705	4	0.12508	9	0.16213	13	0.43016	20
3.315	0.03701	4	0.12499	9	0.16200	13	0.42996	20
3.316	0.03697	3	0.12490	10	0.16187	13	0.42976	21
3.317	0.03694	4	0.12480	9	0.16174	13	0.42955	20
3.318	0.03690	4	0.12471	9	0.16161	13	0.42935	20
3.319	0.03686	4	0.12462	9	0.16148	13	0.42915	20
3.320	0.03682	3	0.12453	9	0.16135	13	0.42895	21
3.321	0.03679	4	0.12444	9	0.16122	13	0.42874	20
3.322	0.03675	4	0.12435	10	0.16109	13	0.42854	20
3.323	0.03671	4	0.12425	9	0.16096	12	0.42834	20
3.324	0.03667	3	0.12416	9	0.16084	13	0.42814	21
3.325	0.03664	4	0.12407	9	0.16071	13	0.42793	20
3.326	0.03660	4	0.12398	9	0.16058	13	0.42773	20
3.327	0.03656	4	0.12389	9	0.16045	13	0.42753	20
3.328	0.03652	3	0.12380	9	0.16032	13	0.42733	21
3.329	0.03649	4	0.12371	9	0.16019	13	0.42712	20
3.330	0.03645	4	0.12362	10	0.16006	12	0.42692	20
3.331	0.03641	3	0.12352	9	0.15994	13	0.42672	20
3.332	0.03638	4	0.12343	9	0.15981	13	0.42652	21
3.333	0.03634	4	0.12334	9	0.15968	13	0.42631	20
3.334	0.03630	4	0.12325	9	0.15955	12	0.42611	20
3.335	0.03626	3	0.12316	9	0.15943	13	0.42591	20
3.336	0.03623	4	0.12307	9	0.15930	13	0.42571	20
3.337	0.03619	4	0.12298	9	0.15917	13	0.42551	21
3.338	0.03615	3	0.12289	9	0.15904	12	0.42530	20
3.339	0.03612	4	0.12280	9	0.15892	13	0.42510	20
3.340	0.03608	4	0.12271	9	0.15879	13	0.42490	20
3.341	0.03604	3	0.12262	9	0.15866	13	0.42470	20
3.342	0.03601	4	0.12253	9	0.15853	12	0.42450	20
3.343	0.03597	4	0.12244	9	0.15841	13	0.42430	20
3.344	0.03593	3	0.12235	9	0.15828	13	0.42410	21
3.345	0.03590	4	0.12226	9	0.15815	12	0.42389	20
3.346	0.03586	4	0.12217	9	0.15803	13	0.42369	20
3.347	0.03582	3	0.12208	9	0.15790	13	0.42349	20
3.348	0.03579	4	0.12199	9	0.15777	12	0.42329	20
3.349	0.03575	4	0.12190	9	0.15765	13	0.42309	20
3.350	0.03571		0.12181		0.15752		0.42289	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	G_p^0/R	Δ
3.350	0.03571	3	0.12181	9	0.15752	13	0.42289	20
3.351	0.03568	4	0.12172	9	0.15739	12	0.42269	21
3.352	0.03564	3	0.12163	9	0.15727	13	0.42248	20
3.353	0.03561	4	0.12154	9	0.15714	12	0.42228	20
3.354	0.03557	4	0.12145	9	0.15702	13	0.42208	20
3.355	0.03553	3	0.12136	9	0.15689	13	0.42188	20
3.356	0.03550	4	0.12127	9	0.15676	12	0.42168	20
3.357	0.03546	4	0.12118	9	0.15664	13	0.42148	20
3.358	0.03542	3	0.12109	9	0.15651	12	0.42128	20
3.359	0.03539	4	0.12100	9	0.15639	13	0.42108	20
3.360	0.03535	3	0.12091	9	0.15626	12	0.42088	20
3.361	0.03532	4	0.12082	9	0.15614	13	0.42068	20
3.362	0.03528	3	0.12073	9	0.15601	12	0.42048	20
3.363	0.03525	4	0.12064	9	0.15589	13	0.42028	20
3.364	0.03521	4	0.12055	9	0.15576	12	0.42008	20
3.365	0.03517	3	0.12046	8	0.15564	13	0.41988	20
3.366	0.03514	4	0.12038	9	0.15551	12	0.41968	21
3.367	0.03510	3	0.12029	9	0.15539	13	0.41947	20
3.368	0.03507	4	0.12020	9	0.15526	12	0.41927	20
3.369	0.03503	4	0.12011	9	0.15514	12	0.41907	20
3.370	0.03499	3	0.12002	9	0.15502	13	0.41887	20
3.371	0.03496	4	0.11993	9	0.15489	12	0.41867	20
3.372	0.03492	3	0.11984	9	0.15477	13	0.41847	20
3.373	0.03489	4	0.11975	8	0.15464	12	0.41827	20
3.374	0.03485	3	0.11967	9	0.15452	12	0.41807	20
3.375	0.03482	4	0.11958	9	0.15440	13	0.41787	20
3.376	0.03478	3	0.11949	9	0.15427	12	0.41767	20
3.377	0.03475	4	0.11940	9	0.15415	13	0.41747	20
3.378	0.03471	3	0.11931	9	0.15402	12	0.41727	19
3.379	0.03468	4	0.11922	8	0.15390	12	0.41708	20
3.380	0.03464	3	0.11914	9	0.15378	13	0.41688	20
3.381	0.03461	4	0.11905	9	0.15365	12	0.41668	20
3.382	0.03457	4	0.11896	9	0.15353	12	0.41648	20
3.383	0.03453	3	0.11887	9	0.15341	13	0.41628	20
3.384	0.03450	4	0.11878	8	0.15328	12	0.41608	20
3.385	0.03446	3	0.11870	9	0.15316	12	0.41588	20
3.386	0.03443	4	0.11861	9	0.15304	12	0.41568	20
3.387	0.03439	3	0.11852	9	0.15292	13	0.41548	20
3.388	0.03436	4	0.11843	8	0.15279	12	0.41528	20
3.389	0.03432	3	0.11835	9	0.15267	12	0.41508	20
3.390	0.03429	3	0.11826	9	0.15255	12	0.41488	20
3.391	0.03426	4	0.11817	9	0.15243	13	0.41468	20
3.392	0.03422	3	0.11808	8	0.15230	12	0.41448	19
3.393	0.03419	4	0.11800	9	0.15218	12	0.41429	20
3.394	0.03415	3	0.11791	9	0.15206	12	0.41409	20
3.395	0.03412	4	0.11782	9	0.15194	12	0.41389	20
3.396	0.03408	3	0.11773	8	0.15182	13	0.41369	20
3.397	0.03405	4	0.11765	9	0.15169	12	0.41349	20
3.398	0.03401	3	0.11756	9	0.15157	12	0.41329	20
3.399	0.03398	4	0.11747	8	0.15145	12	0.41309	20
3.400	0.03394		0.11739		0.15133		0.41289	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.400	0.03394	3	0.11739	9	0.15133	12	0.41289	19
3.401	0.03391	4	0.11730	9	0.15121	12	0.41270	20
3.402	0.03387	3	0.11721	8	0.15109	12	0.41250	20
3.403	0.03384	3	0.11713	9	0.15097	13	0.41230	20
3.404	0.03381	4	0.11704	9	0.15084	12	0.41210	20
3.405	0.03377	3	0.11695	8	0.15072	12	0.41190	20
3.406	0.03374	4	0.11687	9	0.15060	12	0.41170	19
3.407	0.03370	3	0.11678	9	0.15048	12	0.41151	20
3.408	0.03367	4	0.11669	8	0.15036	12	0.41131	20
3.409	0.03363	3	0.11661	9	0.15024	12	0.41111	20
3.410	0.03360	3	0.11652	9	0.15012	12	0.41091	20
3.411	0.03357	4	0.11643	8	0.15000	12	0.41071	19
3.412	0.03353	3	0.11635	9	0.14988	12	0.41052	20
3.413	0.03350	4	0.11626	8	0.14976	12	0.41032	20
3.414	0.03346	3	0.11618	9	0.14964	12	0.41012	20
3.415	0.03343	4	0.11609	9	0.14952	12	0.40992	20
3.416	0.03339	3	0.11600	8	0.14940	12	0.40972	19
3.417	0.03336	3	0.11592	9	0.14928	12	0.40953	20
3.418	0.03333	4	0.11583	8	0.14916	12	0.40933	20
3.419	0.03329	3	0.11575	9	0.14904	12	0.40913	20
3.420	0.03326	3	0.11566	9	0.14892	12	0.40893	19
3.421	0.03323	4	0.11557	8	0.14880	12	0.40874	20
3.422	0.03319	3	0.11549	9	0.14868	12	0.40854	20
3.423	0.03316	4	0.11540	8	0.14856	12	0.40834	19
3.424	0.03312	3	0.11532	9	0.14844	12	0.40815	20
3.425	0.03309	3	0.11523	8	0.14832	12	0.40795	20
3.426	0.03306	4	0.11515	9	0.14820	12	0.40775	20
3.427	0.03302	3	0.11506	8	0.14808	11	0.40755	19
3.428	0.03299	3	0.11498	9	0.14797	12	0.40736	20
3.429	0.03296	4	0.11489	8	0.14785	12	0.40716	20
3.430	0.03292	3	0.11481	9	0.14773	12	0.40696	19
3.431	0.03289	3	0.11472	8	0.14761	12	0.40677	20
3.432	0.03286	4	0.11464	9	0.14749	12	0.40657	20
3.433	0.03282	3	0.11455	8	0.14737	12	0.40637	19
3.434	0.03279	3	0.11447	9	0.14725	11	0.40618	20
3.435	0.03276	4	0.11438	8	0.14714	12	0.40598	20
3.436	0.03272	3	0.11430	9	0.14702	12	0.40578	19
3.437	0.03269	3	0.11421	8	0.14690	12	0.40559	20
3.438	0.03266	4	0.11413	9	0.14678	12	0.40539	20
3.439	0.03262	3	0.11404	8	0.14666	11	0.40519	19
3.440	0.03259	3	0.11396	9	0.14655	12	0.40500	20
3.441	0.03256	4	0.11387	8	0.14643	12	0.40480	20
3.442	0.03252	3	0.11379	9	0.14631	12	0.40460	19
3.443	0.03249	3	0.11370	8	0.14619	11	0.40441	20
3.444	0.03246	4	0.11362	9	0.14608	12	0.40421	19
3.445	0.03242	3	0.11353	8	0.14596	12	0.40402	20
3.446	0.03239	3	0.11345	8	0.14584	12	0.40382	20
3.447	0.03236	3	0.11337	9	0.14572	11	0.40362	19
3.448	0.03233	4	0.11328	8	0.14561	12	0.40343	20
3.449	0.03229	3	0.11320	9	0.14549	12	0.40323	19
3.450	0.03226		0.11311		0.14537		0.40304	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.450	0.03226	3	0.11311	8	0.14537	11	0.40304	20
3.451	0.03223	4	0.11303	8	0.14526	12	0.40284	20
3.452	0.03219	3	0.11295	9	0.14514	12	0.40264	19
3.453	0.03216	3	0.11286	8	0.14502	11	0.40245	20
3.454	0.03213	3	0.11278	9	0.14491	12	0.40225	19
3.455	0.03210	4	0.11269	8	0.14479	12	0.40206	20
3.456	0.03206	3	0.11261	8	0.14467	11	0.40186	19
3.457	0.03203	3	0.11253	9	0.14456	12	0.40167	20
3.458	0.03200	3	0.11244	8	0.14444	11	0.40147	19
3.459	0.03197	4	0.11236	8	0.14433	12	0.40128	20
3.460	0.03193	3	0.11228	9	0.14421	12	0.40108	20
3.461	0.03190	3	0.11219	8	0.14409	11	0.40088	19
3.462	0.03187	3	0.11211	8	0.14398	12	0.40069	20
3.463	0.03184	4	0.11203	9	0.14386	11	0.40049	19
3.464	0.03180	3	0.11194	8	0.14375	12	0.40030	20
3.465	0.03177	3	0.11186	8	0.14363	11	0.40010	19
3.466	0.03174	3	0.11178	9	0.14352	12	0.39991	20
3.467	0.03171	3	0.11169	8	0.14340	11	0.39971	19
3.468	0.03168	4	0.11161	8	0.14329	12	0.39952	20
3.469	0.03164	3	0.11153	9	0.14317	11	0.39932	19
3.470	0.03161	3	0.11144	8	0.14306	12	0.39913	19
3.471	0.03158	3	0.11136	8	0.14294	11	0.39894	20
3.472	0.03155	3	0.11128	8	0.14283	12	0.39874	19
3.473	0.03152	4	0.11120	9	0.14271	11	0.39855	20
3.474	0.03148	3	0.11111	8	0.14260	12	0.39835	19
3.475	0.03145	3	0.11103	8	0.14248	11	0.39816	20
3.476	0.03142	3	0.11095	9	0.14237	12	0.39796	19
3.477	0.03139	3	0.11086	8	0.14225	11	0.39777	20
3.478	0.03136	4	0.11078	8	0.14214	12	0.39757	19
3.479	0.03132	3	0.11070	8	0.14202	11	0.39738	19
3.480	0.03129	3	0.11062	8	0.14191	11	0.39719	20
3.481	0.03126	3	0.11054	9	0.14180	12	0.39699	19
3.482	0.03123	3	0.11045	8	0.14168	11	0.39680	20
3.483	0.03120	3	0.11037	8	0.14157	12	0.39660	19
3.484	0.03117	4	0.11029	8	0.14145	11	0.39641	19
3.485	0.03113	3	0.11021	9	0.14134	11	0.39622	20
3.486	0.03110	3	0.11012	8	0.14123	12	0.39602	19
3.487	0.03107	3	0.11004	8	0.14111	11	0.39583	20
3.488	0.03104	3	0.10996	8	0.14100	11	0.39563	19
3.489	0.03101	3	0.10988	8	0.14089	12	0.39544	19
3.490	0.03098	4	0.10980	8	0.14077	11	0.39525	20
3.491	0.03094	3	0.10972	9	0.14066	11	0.39505	19
3.492	0.03091	3	0.10963	8	0.14055	12	0.39486	19
3.493	0.03088	3	0.10955	8	0.14043	11	0.39467	20
3.494	0.03085	3	0.10947	8	0.14032	11	0.39447	19
3.495	0.03082	3	0.10939	8	0.14021	12	0.39428	19
3.496	0.03079	3	0.10931	8	0.14009	11	0.39409	20
3.497	0.03076	3	0.10923	9	0.13998	11	0.39389	19
3.498	0.03073	4	0.10914	8	0.13987	11	0.39370	19
3.499	0.03069	3	0.10906	8	0.13976	12	0.39351	20
3.500	0.03066		0.10898		0.13964		0.39331	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.500	0.03066	3	0.10898	8	0.13964	11	0.39331	19
3.501	0.03063	3	0.10890	8	0.13953	11	0.39312	19
3.502	0.03060	3	0.10882	8	0.13942	11	0.39293	20
3.503	0.03057	3	0.10874	8	0.13931	11	0.39273	19
3.504	0.03054	3	0.10866	8	0.13920	12	0.39254	19
3.505	0.03051	3	0.10858	8	0.13908	11	0.39235	19
3.506	0.03048	3	0.10850	9	0.13897	11	0.39216	20
3.507	0.03045	4	0.10841	8	0.13886	11	0.39196	19
3.508	0.03041	3	0.10833	8	0.13875	11	0.39177	19
3.509	0.03038	3	0.10825	8	0.13864	11	0.39158	19
3.510	0.03035	3	0.10817	8	0.13853	12	0.39139	20
3.511	0.03032	3	0.10809	8	0.13841	11	0.39119	19
3.512	0.03029	3	0.10801	8	0.13830	11	0.39100	19
3.513	0.03026	3	0.10793	8	0.13819	11	0.39081	19
3.514	0.03023	3	0.10785	8	0.13808	11	0.39062	20
3.515	0.03020	3	0.10777	8	0.13797	11	0.39042	19
3.516	0.03017	3	0.10769	8	0.13786	11	0.39023	19
3.517	0.03014	3	0.10761	8	0.13775	11	0.39004	19
3.518	0.03011	3	0.10753	8	0.13764	11	0.38985	19
3.519	0.03008	3	0.10745	8	0.13753	12	0.38966	20
3.520	0.03005	3	0.10737	8	0.13741	11	0.38946	19
3.521	0.03002	3	0.10729	8	0.13730	11	0.38927	19
3.522	0.02999	4	0.10721	8	0.13719	11	0.38908	19
3.523	0.02995	3	0.10713	8	0.13708	11	0.38889	19
3.524	0.02992	3	0.10705	8	0.13697	11	0.38870	20
3.525	0.02989	3	0.10697	8	0.13686	11	0.38850	19
3.526	0.02986	3	0.10689	8	0.13675	11	0.38831	19
3.527	0.02983	3	0.10681	8	0.13664	11	0.38812	19
3.528	0.02980	3	0.10673	8	0.13653	11	0.38793	19
3.529	0.02977	3	0.10665	8	0.13642	11	0.38774	19
3.530	0.02974	3	0.10657	8	0.13631	11	0.38755	19
3.531	0.02971	3	0.10649	8	0.13620	11	0.38736	20
3.532	0.02968	3	0.10641	8	0.13609	11	0.38716	19
3.533	0.02965	3	0.10633	8	0.13598	11	0.38697	19
3.534	0.02962	3	0.10625	8	0.13587	11	0.38678	19
3.535	0.02959	3	0.10617	8	0.13576	10	0.38659	19
3.536	0.02956	3	0.10609	8	0.13566	11	0.38640	19
3.537	0.02953	3	0.10601	8	0.13555	11	0.38621	19
3.538	0.02950	3	0.10593	7	0.13544	11	0.38602	19
3.539	0.02947	3	0.10586	8	0.13533	11	0.38583	19
3.540	0.02944	3	0.10578	8	0.13522	11	0.38564	19
3.541	0.02941	3	0.10570	8	0.13511	11	0.38545	20
3.542	0.02938	3	0.10562	8	0.13500	11	0.38525	19
3.543	0.02935	3	0.10554	8	0.13489	11	0.38506	19
3.544	0.02932	3	0.10546	8	0.13478	11	0.38487	19
3.545	0.02929	3	0.10538	8	0.13467	10	0.38468	19
3.546	0.02926	3	0.10530	8	0.13457	11	0.38449	19
3.547	0.02923	3	0.10522	7	0.13446	11	0.38430	19
3.548	0.02920	3	0.10515	8	0.13435	11	0.38411	19
3.549	0.02917	2	0.10507	8	0.13424	11	0.38392	19
3.550	0.02915		0.10499		0.13413		0.38373	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.550	0.02915	3	0.10499	8	0.13413	10	0.38373	19
3.551	0.02912	3	0.10491	8	0.13403	11	0.38354	19
3.552	0.02909	3	0.10483	8	0.13392	11	0.38335	19
3.553	0.02906	3	0.10475	8	0.13381	11	0.38316	19
3.554	0.02903	3	0.10467	7	0.13370	11	0.38297	19
3.555	0.02900	3	0.10460	8	0.13359	10	0.38278	19
3.556	0.02897	3	0.10452	8	0.13349	11	0.38259	19
3.557	0.02894	3	0.10444	8	0.13338	11	0.38240	19
3.558	0.02891	3	0.10436	8	0.13327	11	0.38221	19
3.559	0.02888	3	0.10428	7	0.13316	10	0.38202	19
3.560	0.02885	3	0.10421	8	0.13306	11	0.38183	19
3.561	0.02882	3	0.10413	8	0.13295	11	0.38164	19
3.562	0.02879	3	0.10405	8	0.13284	10	0.38145	19
3.563	0.02876	3	0.10397	8	0.13274	11	0.38126	19
3.564	0.02873	2	0.10389	7	0.13263	11	0.38107	19
3.565	0.02871	3	0.10382	8	0.13252	11	0.38088	19
3.566	0.02868	3	0.10374	8	0.13241	10	0.38069	19
3.567	0.02865	3	0.10366	8	0.13231	11	0.38050	18
3.568	0.02862	3	0.10358	7	0.13220	11	0.38032	19
3.569	0.02859	3	0.10351	8	0.13209	10	0.38013	19
3.570	0.02856	3	0.10343	8	0.13199	11	0.37994	19
3.571	0.02853	3	0.10335	8	0.13188	10	0.37975	19
3.572	0.02850	3	0.10327	7	0.13178	11	0.37956	19
3.573	0.02847	3	0.10320	8	0.13167	11	0.37937	19
3.574	0.02844	2	0.10312	8	0.13156	10	0.37918	19
3.575	0.02842	3	0.10304	8	0.13146	11	0.37899	19
3.576	0.02839	3	0.10296	7	0.13135	10	0.37880	19
3.577	0.02836	3	0.10289	8	0.13125	11	0.37861	18
3.578	0.02833	3	0.10281	8	0.13114	11	0.37843	19
3.579	0.02830	3	0.10273	7	0.13103	10	0.37824	19
3.580	0.02827	3	0.10266	8	0.13093	11	0.37805	19
3.581	0.02824	3	0.10258	8	0.13082	10	0.37786	19
3.582	0.02821	2	0.10250	7	0.13072	11	0.37767	19
3.583	0.02819	3	0.10243	8	0.13061	10	0.37748	18
3.584	0.02816	3	0.10235	8	0.13051	11	0.37730	19
3.585	0.02813	3	0.10227	7	0.13040	10	0.37711	19
3.586	0.02810	3	0.10220	8	0.13030	11	0.37692	19
3.587	0.02807	3	0.10212	8	0.13019	10	0.37673	19
3.588	0.02804	3	0.10204	7	0.13009	11	0.37654	19
3.589	0.02801	2	0.10197	8	0.12998	10	0.37635	18
3.590	0.02799	3	0.10189	8	0.12988	11	0.37617	19
3.591	0.02796	3	0.10181	7	0.12977	10	0.37598	19
3.592	0.02793	3	0.10174	8	0.12967	11	0.37579	19
3.593	0.02790	3	0.10166	8	0.12956	10	0.37560	18
3.594	0.02787	3	0.10158	7	0.12946	11	0.37542	19
3.595	0.02784	2	0.10151	8	0.12935	10	0.37523	19
3.596	0.02782	3	0.10143	7	0.12925	11	0.37504	19
3.597	0.02779	3	0.10136	8	0.12914	10	0.37485	19
3.598	0.02776	3	0.10128	8	0.12904	10	0.37466	18
3.599	0.02773	3	0.10120	7	0.12894	11	0.37448	19
3.600	0.02770		0.10113		0.12883		0.37429	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.600	0.02770	2	0.10113	8	0.12883	10	0.37429	19
3.601	0.02768	3	0.10105	7	0.12873	11	0.37410	18
3.602	0.02765	3	0.10098	8	0.12862	10	0.37392	19
3.603	0.02762	3	0.10090	7	0.12852	10	0.37373	19
3.604	0.02759	3	0.10083	8	0.12842	11	0.37354	19
3.605	0.02756	2	0.10075	8	0.12831	10	0.37335	18
3.606	0.02754	3	0.10067	7	0.12821	10	0.37317	19
3.607	0.02751	3	0.10060	8	0.12811	11	0.37298	19
3.608	0.02748	3	0.10052	7	0.12800	10	0.37279	18
3.609	0.02745	3	0.10045	8	0.12790	10	0.37261	19
3.610	0.02742	2	0.10037	7	0.12780	11	0.37242	19
3.611	0.02740	3	0.10030	8	0.12769	10	0.37223	18
3.612	0.02737	3	0.10022	7	0.12759	10	0.37205	19
3.613	0.02734	3	0.10015	8	0.12749	11	0.37186	19
3.614	0.02731	2	0.10007	7	0.12738	10	0.37167	18
3.615	0.02729	3	0.10000	8	0.12728	10	0.37149	19
3.616	0.02726	3	0.09992	7	0.12718	10	0.37130	19
3.617	0.02723	3	0.09985	8	0.12708	11	0.37111	18
3.618	0.02720	2	0.09977	7	0.12697	10	0.37093	19
3.619	0.02718	3	0.09970	8	0.12687	10	0.37074	19
3.620	0.02715	3	0.09962	7	0.12677	10	0.37055	18
3.621	0.02712	3	0.09955	8	0.12667	11	0.37037	19
3.622	0.02709	2	0.09947	7	0.12656	10	0.37018	18
3.623	0.02707	3	0.09940	8	0.12646	10	0.37000	19
3.624	0.02704	3	0.09932	7	0.12636	10	0.36981	19
3.625	0.02701	3	0.09925	8	0.12626	10	0.36962	18
3.626	0.02698	2	0.09917	7	0.12616	11	0.36944	19
3.627	0.02696	3	0.09910	8	0.12605	10	0.36925	18
3.628	0.02693	3	0.09902	7	0.12595	10	0.36907	19
3.629	0.02690	3	0.09895	7	0.12585	10	0.36888	19
3.630	0.02687	2	0.09888	8	0.12575	10	0.36869	18
3.631	0.02685	3	0.09880	7	0.12565	10	0.36851	19
3.632	0.02682	3	0.09873	8	0.12555	10	0.36832	18
3.633	0.02679	2	0.09865	7	0.12545	11	0.36814	19
3.634	0.02677	3	0.09858	8	0.12534	10	0.36795	18
3.635	0.02674	3	0.09850	7	0.12524	10	0.36777	19
3.636	0.02671	3	0.09843	7	0.12514	10	0.36758	18
3.637	0.02668	2	0.09836	8	0.12504	10	0.36740	19
3.638	0.02666	3	0.09828	7	0.12494	10	0.36721	18
3.639	0.02663	3	0.09821	8	0.12484	10	0.36703	19
3.640	0.02660	2	0.09813	7	0.12474	10	0.36684	18
3.641	0.02658	3	0.09806	7	0.12464	10	0.36666	19
3.642	0.02655	3	0.09799	8	0.12454	10	0.36647	18
3.643	0.02652	2	0.09791	7	0.12444	10	0.36629	19
3.644	0.02650	3	0.09784	7	0.12434	11	0.36610	18
3.645	0.02647	3	0.09777	8	0.12423	10	0.36592	19
3.646	0.02644	2	0.09769	7	0.12413	10	0.36573	18
3.647	0.02642	3	0.09762	7	0.12403	10	0.36555	19
3.648	0.02639	3	0.09755	8	0.12393	10	0.36536	18
3.649	0.02636	3	0.09747	7	0.12383	10	0.36518	19
3.650	0.02633		0.09740		0.12373		0.36499	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R	Δ
3.650	0.02633	2	0.09740	7	0.12373	10	0.36499	18
3.651	0.02631	3	0.09733	8	0.12363	10	0.36481	19
3.652	0.02628	3	0.09725	7	0.12353	10	0.36462	18
3.653	0.02625	2	0.09718	7	0.12343	10	0.36444	18
3.654	0.02623	3	0.09711	8	0.12333	10	0.36426	19
3.655	0.02620	2	0.09703	7	0.12323	9	0.36407	18
3.656	0.02618	3	0.09696	7	0.12314	10	0.36389	19
3.657	0.02615	3	0.09689	8	0.12304	10	0.36370	18
3.658	0.02612	2	0.09681	7	0.12294	10	0.36352	18
3.659	0.02610	3	0.09674	7	0.12284	10	0.36334	19
3.660	0.02607	3	0.09667	7	0.12274	10	0.36315	18
3.661	0.02604	2	0.09660	8	0.12264	10	0.36297	19
3.662	0.02602	3	0.09652	7	0.12254	10	0.36278	18
3.663	0.02599	3	0.09645	7	0.12244	10	0.36260	18
3.664	0.02596	2	0.09638	7	0.12234	10	0.36242	19
3.665	0.02594	3	0.09631	8	0.12224	10	0.36223	18
3.666	0.02591	2	0.09623	7	0.12214	9	0.36205	18
3.667	0.02589	3	0.09616	7	0.12205	10	0.36187	19
3.668	0.02586	3	0.09609	7	0.12195	10	0.36168	18
3.669	0.02583	2	0.09602	8	0.12185	10	0.36150	18
3.670	0.02581	3	0.09594	7	0.12175	10	0.36132	19
3.671	0.02578	3	0.09587	7	0.12165	10	0.36113	18
3.672	0.02575	2	0.09580	7	0.12155	10	0.36095	18
3.673	0.02573	3	0.09573	8	0.12145	9	0.36077	19
3.674	0.02570	2	0.09565	7	0.12136	10	0.36058	18
3.675	0.02568	3	0.09558	7	0.12126	10	0.36040	18
3.676	0.02565	3	0.09551	7	0.12116	10	0.36022	19
3.677	0.02562	2	0.09544	7	0.12106	10	0.36003	18
3.678	0.02560	3	0.09537	8	0.12096	9	0.35985	18
3.679	0.02557	2	0.09529	7	0.12087	10	0.35967	18
3.680	0.02555	3	0.09522	7	0.12077	10	0.35949	19
3.681	0.02552	3	0.09515	7	0.12067	10	0.35930	18
3.682	0.02549	2	0.09508	7	0.12057	9	0.35912	18
3.683	0.02547	3	0.09501	7	0.12048	10	0.35894	18
3.684	0.02544	2	0.09494	8	0.12038	10	0.35876	19
3.685	0.02542	3	0.09486	7	0.12028	10	0.35857	18
3.686	0.02539	2	0.09479	7	0.12018	9	0.35839	18
3.687	0.02537	3	0.09472	7	0.12009	10	0.35821	18
3.688	0.02534	3	0.09465	7	0.11999	10	0.35803	19
3.689	0.02531	2	0.09458	7	0.11989	9	0.35784	18
3.690	0.02529	3	0.09451	7	0.11980	10	0.35766	18
3.691	0.02526	2	0.09444	8	0.11970	10	0.35748	18
3.692	0.02524	3	0.09436	7	0.11960	9	0.35730	18
3.693	0.02521	2	0.09429	7	0.11951	10	0.35712	19
3.694	0.02519	3	0.09422	7	0.11941	10	0.35693	18
3.695	0.02516	2	0.09415	7	0.11931	9	0.35675	18
3.696	0.02514	3	0.09408	7	0.11922	10	0.35657	18
3.697	0.02511	2	0.09401	7	0.11912	10	0.35639	18
3.698	0.02509	3	0.09394	7	0.11902	9	0.35621	19
3.699	0.02506	3	0.09387	7	0.11893	10	0.35602	18
3.700	0.02503		0.09380		0.11883		0.35584	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.700	0.02503	2	0.09380	7	0.11883	10	0.35584	18
3.701	0.02501	3	0.09373	8	0.11873	9	0.35566	18
3.702	0.02498	2	0.09365	7	0.11864	10	0.35548	18
3.703	0.02496	3	0.09358	7	0.11854	9	0.35530	18
3.704	0.02493	2	0.09351	7	0.11845	10	0.35512	18
3.705	0.02491	3	0.09344	7	0.11835	10	0.35494	19
3.706	0.02488	2	0.09337	7	0.11825	9	0.35475	18
3.707	0.02486	3	0.09330	7	0.11816	10	0.35457	18
3.708	0.02483	2	0.09323	7	0.11806	9	0.35439	18
3.709	0.02481	3	0.09316	7	0.11797	10	0.35421	18
3.710	0.02478	2	0.09309	7	0.11787	9	0.35403	18
3.711	0.02476	3	0.09302	7	0.11778	10	0.35385	18
3.712	0.02473	2	0.09295	7	0.11768	9	0.35367	18
3.713	0.02471	3	0.09288	7	0.11759	10	0.35349	18
3.714	0.02468	2	0.09281	7	0.11749	9	0.35331	18
3.715	0.02466	3	0.09274	7	0.11740	10	0.35313	18
3.716	0.02463	2	0.09267	7	0.11730	9	0.35295	18
3.717	0.02461	3	0.09260	7	0.11721	10	0.35277	19
3.718	0.02458	2	0.09253	7	0.11711	9	0.35258	18
3.719	0.02456	3	0.09246	7	0.11702	10	0.35240	18
3.720	0.02453	2	0.09239	7	0.11692	9	0.35222	18
3.721	0.02451	3	0.09232	7	0.11683	10	0.35204	18
3.722	0.02448	2	0.09225	7	0.11673	9	0.35186	18
3.723	0.02446	3	0.09218	7	0.11664	10	0.35168	18
3.724	0.02443	2	0.09211	7	0.11654	9	0.35150	18
3.725	0.02441	3	0.09204	7	0.11645	10	0.35132	18
3.726	0.02438	2	0.09197	7	0.11635	9	0.35114	18
3.727	0.02436	3	0.09190	7	0.11626	9	0.35096	18
3.728	0.02433	2	0.09183	7	0.11617	10	0.35078	18
3.729	0.02431	2	0.09176	7	0.11607	9	0.35060	18
3.730	0.02429	3	0.09169	7	0.11598	10	0.35042	18
3.731	0.02426	2	0.09162	7	0.11588	9	0.35024	18
3.732	0.02424	3	0.09155	6	0.11579	9	0.35006	18
3.733	0.02421	2	0.09149	7	0.11570	10	0.34988	18
3.734	0.02419	3	0.09142	7	0.11560	9	0.34970	17
3.735	0.02416	2	0.09135	7	0.11551	9	0.34953	18
3.736	0.02414	3	0.09128	7	0.11542	10	0.34935	18
3.737	0.02411	2	0.09121	7	0.11532	9	0.34917	18
3.738	0.02409	2	0.09114	7	0.11523	9	0.34899	18
3.739	0.02407	3	0.09107	7	0.11514	10	0.34881	18
3.740	0.02404	2	0.09100	7	0.11504	9	0.34863	18
3.741	0.02402	3	0.09093	7	0.11495	9	0.34845	18
3.742	0.02399	2	0.09086	6	0.11486	10	0.34827	18
3.743	0.02397	3	0.09080	7	0.11476	9	0.34809	18
3.744	0.02394	2	0.09073	7	0.11467	9	0.34791	18
3.745	0.02392	2	0.09066	7	0.11458	10	0.34773	17
3.746	0.02390	3	0.09059	7	0.11448	9	0.34756	18
3.747	0.02387	2	0.09052	7	0.11439	9	0.34738	18
3.748	0.02385	3	0.09045	7	0.11430	9	0.34720	18
3.749	0.02382	2	0.09038	6	0.11421	10	0.34702	18
3.750	0.02380		0.09032		0.11411		0.34684	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0)/RT$	Δ	$(H^0-E_0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.750	0.02380	3	0.09032	7	0.11411	9	0.34684	18
3.751	0.02377	2	0.09025	7	0.11402	9	0.34666	18
3.752	0.02375	2	0.09018	7	0.11393	9	0.34648	18
3.753	0.02373	3	0.09011	7	0.11384	10	0.34630	17
3.754	0.02370	2	0.09004	7	0.11374	9	0.34613	18
3.755	0.02368	3	0.08997	6	0.11365	9	0.34595	18
3.756	0.02365	2	0.08991	7	0.11356	9	0.34577	18
3.757	0.02363	2	0.08984	7	0.11347	9	0.34559	18
3.758	0.02361	3	0.08977	7	0.11338	10	0.34541	17
3.759	0.02358	2	0.08970	7	0.11328	9	0.34524	18
3.760	0.02356	2	0.08963	6	0.11319	9	0.34506	18
3.761	0.02354	3	0.08957	7	0.11310	9	0.34488	18
3.762	0.02351	2	0.08950	7	0.11301	9	0.34470	18
3.763	0.02349	3	0.08943	7	0.11292	9	0.34452	17
3.764	0.02346	2	0.08936	7	0.11283	10	0.34435	18
3.765	0.02344	2	0.08929	6	0.11273	9	0.34417	18
3.766	0.02342	3	0.08923	7	0.11264	9	0.34399	18
3.767	0.02339	2	0.08916	7	0.11255	9	0.34381	17
3.768	0.02337	2	0.08909	7	0.11246	9	0.34364	18
3.769	0.02335	3	0.08902	6	0.11237	9	0.34346	18
3.770	0.02332	2	0.08896	7	0.11228	9	0.34328	18
3.771	0.02330	3	0.08889	7	0.11219	9	0.34310	17
3.772	0.02327	2	0.08882	7	0.11210	9	0.34293	18
3.773	0.02325	2	0.08875	6	0.11201	9	0.34275	18
3.774	0.02323	3	0.08869	7	0.11192	10	0.34257	18
3.775	0.02320	2	0.08862	7	0.11182	9	0.34239	17
3.776	0.02318	2	0.08855	6	0.11173	9	0.34222	18
3.777	0.02316	3	0.08849	7	0.11164	9	0.34204	18
3.778	0.02313	2	0.08842	7	0.11155	9	0.34186	17
3.779	0.02311	2	0.08835	7	0.11146	9	0.34169	18
3.780	0.02309	3	0.08828	6	0.11137	9	0.34151	18
3.781	0.02306	2	0.08822	7	0.11128	9	0.34133	17
3.782	0.02304	2	0.08815	7	0.11119	9	0.34116	18
3.783	0.02302	3	0.08808	6	0.11110	9	0.34098	18
3.784	0.02299	2	0.08802	7	0.11101	9	0.34080	17
3.785	0.02297	2	0.08795	7	0.11092	9	0.34063	18
3.786	0.02295	3	0.08788	6	0.11083	9	0.34045	18
3.787	0.02292	2	0.08782	7	0.11074	9	0.34027	17
3.788	0.02290	2	0.08775	7	0.11065	9	0.34010	18
3.789	0.02288	3	0.08768	6	0.11056	9	0.33992	17
3.790	0.02285	2	0.08762	7	0.11047	9	0.33975	18
3.791	0.02283	2	0.08755	7	0.11038	9	0.33957	18
3.792	0.02281	2	0.08748	6	0.11029	9	0.33939	17
3.793	0.02279	3	0.08742	7	0.11020	9	0.33922	18
3.794	0.02276	2	0.08735	6	0.11011	9	0.33904	17
3.795	0.02274	2	0.08729	7	0.11002	8	0.33887	18
3.796	0.02272	3	0.08722	7	0.10994	9	0.33869	18
3.797	0.02269	2	0.08715	6	0.10985	9	0.33851	17
3.798	0.02267	2	0.08709	7	0.10976	9	0.33834	18
3.799	0.02265	3	0.08702	7	0.10967	9	0.33816	17
3.800	0.02262		0.08695		0.10958		0.33799	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.800	0.02262	2	0.08695	6	0.10958	9	0.33799	18
3.801	0.02260	2	0.08689	7	0.10949	9	0.33781	17
3.802	0.02258	2	0.08682	6	0.10940	9	0.33764	18
3.803	0.02256	3	0.08676	7	0.10931	9	0.33746	17
3.804	0.02253	2	0.08669	7	0.10922	8	0.33729	18
3.805	0.02251	2	0.08662	6	0.10914	9	0.33711	18
3.806	0.02249	2	0.08656	7	0.10905	9	0.33693	17
3.807	0.02247	3	0.08649	6	0.10896	9	0.33676	18
3.808	0.02244	2	0.08643	7	0.10887	9	0.33658	17
3.809	0.02242	2	0.08636	6	0.10878	9	0.33641	18
3.810	0.02240	3	0.08630	7	0.10869	9	0.33623	17
3.811	0.02237	2	0.08623	7	0.10860	8	0.33606	18
3.812	0.02235	2	0.08616	6	0.10852	9	0.33588	17
3.813	0.02233	2	0.08610	7	0.10843	9	0.33571	18
3.814	0.02231	3	0.08603	6	0.10834	9	0.33553	17
3.815	0.02228	2	0.08597	7	0.10825	9	0.33536	17
3.816	0.02226	2	0.08590	6	0.10816	8	0.33519	18
3.817	0.02224	2	0.08584	7	0.10808	9	0.33501	17
3.818	0.02222	3	0.08577	6	0.10799	9	0.33484	18
3.819	0.02219	2	0.08571	7	0.10790	9	0.33466	17
3.820	0.02217	2	0.08564	6	0.10781	8	0.33449	18
3.821	0.02215	2	0.08558	7	0.10773	9	0.33431	17
3.822	0.02213	3	0.08551	6	0.10764	9	0.33414	18
3.823	0.02210	2	0.08545	7	0.10755	9	0.33396	17
3.824	0.02208	2	0.08538	6	0.10746	8	0.33379	17
3.825	0.02206	2	0.08532	7	0.10738	9	0.33362	18
3.826	0.02204	2	0.08525	6	0.10729	9	0.33344	17
3.827	0.02202	3	0.08519	7	0.10720	8	0.33327	18
3.828	0.02199	2	0.08512	6	0.10712	9	0.33309	17
3.829	0.02197	2	0.08506	7	0.10703	9	0.33292	17
3.830	0.02195	2	0.08499	6	0.10694	9	0.33275	18
3.831	0.02193	3	0.08493	7	0.10685	8	0.33257	17
3.832	0.02190	2	0.08486	6	0.10677	9	0.33240	17
3.833	0.02188	2	0.08480	7	0.10668	9	0.33223	18
3.834	0.02186	2	0.08473	6	0.10659	8	0.33205	17
3.835	0.02184	2	0.08467	6	0.10651	9	0.33188	17
3.836	0.02182	3	0.08461	7	0.10642	8	0.33171	18
3.837	0.02179	2	0.08454	6	0.10634	9	0.33153	17
3.838	0.02177	2	0.08448	7	0.10625	9	0.33136	17
3.839	0.02175	2	0.08441	6	0.10616	8	0.33119	18
3.840	0.02173	2	0.08435	7	0.10608	9	0.33101	17
3.841	0.02171	3	0.08428	6	0.10599	9	0.33084	17
3.842	0.02168	2	0.08422	6	0.10590	8	0.33067	18
3.843	0.02166	2	0.08416	7	0.10582	9	0.33049	17
3.844	0.02164	2	0.08409	6	0.10573	8	0.33032	17
3.845	0.02162	2	0.08403	7	0.10565	9	0.33015	18
3.846	0.02160	3	0.08396	6	0.10556	9	0.32997	17
3.847	0.02157	2	0.08390	6	0.10547	8	0.32980	17
3.848	0.02155	2	0.08384	7	0.10539	9	0.32963	17
3.849	0.02153	2	0.08377	6	0.10530	8	0.32946	18
3.850	0.02151		0.08371		0.10522		0.32928	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.850	0.02151	2	0.08371	7	0.10522	9	0.32928	17
3.851	0.02149	2	0.08364	6	0.10513	8	0.32911	17
3.852	0.02147	3	0.08358	6	0.10505	9	0.32894	17
3.853	0.02144	2	0.08352	7	0.10496	8	0.32877	18
3.854	0.02142	2	0.08345	6	0.10488	9	0.32859	17
3.855	0.02140	2	0.08339	6	0.10479	8	0.32842	17
3.856	0.02138	2	0.08333	7	0.10471	9	0.32825	17
3.857	0.02136	2	0.08326	6	0.10462	8	0.32808	17
3.858	0.02134	3	0.08320	6	0.10454	9	0.32791	18
3.859	0.02131	2	0.08314	7	0.10445	8	0.32773	17
3.860	0.02129	2	0.08307	6	0.10437	9	0.32756	17
3.861	0.02127	2	0.08301	6	0.10428	8	0.32739	17
3.862	0.02125	2	0.08295	7	0.10420	9	0.32722	17
3.863	0.02123	2	0.08288	6	0.10411	8	0.32705	18
3.864	0.02121	2	0.08282	6	0.10403	9	0.32687	17
3.865	0.02119	3	0.08276	7	0.10394	8	0.32670	17
3.866	0.02116	2	0.08269	6	0.10386	9	0.32653	17
3.867	0.02114	2	0.08263	6	0.10377	8	0.32636	17
3.868	0.02112	2	0.08257	7	0.10369	9	0.32619	17
3.869	0.02110	2	0.08250	6	0.10360	8	0.32602	17
3.870	0.02108	2	0.08244	6	0.10352	8	0.32585	18
3.871	0.02106	2	0.08238	6	0.10344	9	0.32567	17
3.872	0.02104	2	0.08232	7	0.10335	8	0.32550	17
3.873	0.02102	3	0.08225	6	0.10327	9	0.32533	17
3.874	0.02099	2	0.08219	6	0.10318	8	0.32516	17
3.875	0.02097	2	0.08213	7	0.10310	8	0.32499	17
3.876	0.02095	2	0.08206	6	0.10302	9	0.32482	17
3.877	0.02093	2	0.08200	6	0.10293	8	0.32465	17
3.878	0.02091	2	0.08194	6	0.10285	8	0.32448	17
3.879	0.02089	2	0.08188	7	0.10277	9	0.32431	18
3.880	0.02087	2	0.08181	6	0.10268	8	0.32413	17
3.881	0.02085	3	0.08175	6	0.10260	9	0.32396	17
3.882	0.02082	2	0.08169	6	0.10251	8	0.32379	17
3.883	0.02080	2	0.08163	6	0.10243	8	0.32362	17
3.884	0.02078	2	0.08157	7	0.10235	9	0.32345	17
3.885	0.02076	2	0.08150	6	0.10226	8	0.32328	17
3.886	0.02074	2	0.08144	6	0.10218	8	0.32311	17
3.887	0.02072	2	0.08138	6	0.10210	8	0.32294	17
3.888	0.02070	2	0.08132	7	0.10202	9	0.32277	17
3.889	0.02068	2	0.08125	6	0.10193	8	0.32260	17
3.890	0.02066	2	0.08119	6	0.10185	8	0.32243	17
3.891	0.02064	2	0.08113	6	0.10177	9	0.32226	17
3.892	0.02062	3	0.08107	6	0.10168	8	0.32209	17
3.893	0.02059	2	0.08101	7	0.10160	8	0.32192	17
3.894	0.02057	2	0.08094	6	0.10152	8	0.32175	17
3.895	0.02055	2	0.08088	6	0.10144	9	0.32158	17
3.896	0.02053	2	0.08082	6	0.10135	8	0.32141	17
3.897	0.02051	2	0.08076	6	0.10127	8	0.32124	17
3.898	0.02049	2	0.08070	6	0.10119	8	0.32107	17
3.899	0.02047	2	0.08064	7	0.10111	9	0.32090	17
3.900	0.02045		0.08057		0.10102		0.32073	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.900	0.02045	2	0.08057	6	0.10102	8	0.32073	17
3.901	0.02043	2	0.08051	6	0.10094	8	0.32056	17
3.902	0.02041	2	0.08045	6	0.10086	8	0.32039	17
3.903	0.02039	2	0.08039	6	0.10078	8	0.32022	17
3.904	0.02037	2	0.08033	6	0.10070	9	0.32005	16
3.905	0.02035	2	0.08027	6	0.10061	8	0.31989	17
3.906	0.02033	2	0.08021	7	0.10053	8	0.31972	17
3.907	0.02031	3	0.08014	6	0.10045	8	0.31955	17
3.908	0.02028	2	0.08008	6	0.10037	8	0.31938	17
3.909	0.02026	2	0.08002	6	0.10029	9	0.31921	17
3.910	0.02024	2	0.07996	6	0.10020	8	0.31904	17
3.911	0.02022	2	0.07990	6	0.10012	8	0.31887	17
3.912	0.02020	2	0.07984	6	0.10004	8	0.31870	17
3.913	0.02018	2	0.07978	6	0.09996	8	0.31853	16
3.914	0.02016	2	0.07972	6	0.09988	8	0.31837	17
3.915	0.02014	2	0.07966	7	0.09980	8	0.31820	17
3.916	0.02012	2	0.07959	6	0.09972	8	0.31803	17
3.917	0.02010	2	0.07953	6	0.09964	9	0.31786	17
3.918	0.02008	2	0.07947	6	0.09955	8	0.31769	17
3.919	0.02006	2	0.07941	6	0.09947	8	0.31752	17
3.920	0.02004	2	0.07935	6	0.09939	8	0.31735	16
3.921	0.02002	2	0.07929	6	0.09931	8	0.31719	17
3.922	0.02000	2	0.07923	6	0.09923	8	0.31702	17
3.923	0.01998	2	0.07917	6	0.09915	8	0.31685	17
3.924	0.01996	2	0.07911	6	0.09907	8	0.31668	17
3.925	0.01994	2	0.07905	6	0.09899	8	0.31651	16
3.926	0.01992	2	0.07899	6	0.09891	8	0.31635	17
3.927	0.01990	2	0.07893	6	0.09883	8	0.31618	17
3.928	0.01988	2	0.07887	6	0.09875	8	0.31601	17
3.929	0.01986	2	0.07881	6	0.09867	8	0.31584	17
3.930	0.01984	2	0.07875	6	0.09859	8	0.31567	16
3.931	0.01982	2	0.07869	6	0.09851	8	0.31551	17
3.932	0.01980	2	0.07863	6	0.09843	9	0.31534	17
3.933	0.01978	2	0.07857	6	0.09834	8	0.31517	17
3.934	0.01976	2	0.07851	6	0.09826	8	0.31500	16
3.935	0.01974	2	0.07845	6	0.09818	8	0.31484	17
3.936	0.01972	2	0.07839	6	0.09810	8	0.31467	17
3.937	0.01970	2	0.07833	6	0.09802	7	0.31450	16
3.938	0.01968	2	0.07827	6	0.09795	8	0.31434	17
3.939	0.01966	2	0.07821	6	0.09787	8	0.31417	17
3.940	0.01964	2	0.07815	6	0.09779	8	0.31400	17
3.941	0.01962	2	0.07809	6	0.09771	8	0.31383	16
3.942	0.01960	2	0.07803	6	0.09763	8	0.31367	17
3.943	0.01958	2	0.07797	6	0.09755	8	0.31350	17
3.944	0.01956	2	0.07791	6	0.09747	8	0.31333	16
3.945	0.01954	2	0.07785	6	0.09739	8	0.31317	17
3.946	0.01952	2	0.07779	6	0.09731	8	0.31300	17
3.947	0.01950	2	0.07773	6	0.09723	8	0.31283	16
3.948	0.01948	2	0.07767	6	0.09715	8	0.31267	17
3.949	0.01946	2	0.07761	6	0.09707	8	0.31250	17
3.950	0.01944		0.07755		0.09699		0.31233	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
3.950	0.01944	2	0.07755	6	0.09699	8	0.31233	16
3.951	0.01942	2	0.07749	6	0.09691	8	0.31217	17
3.952	0.01940	2	0.07743	6	0.09683	8	0.31200	17
3.953	0.01938	2	0.07737	6	0.09675	7	0.31183	16
3.954	0.01936	2	0.07731	6	0.09668	8	0.31167	17
3.955	0.01934	1	0.07725	6	0.09660	8	0.31150	16
3.956	0.01933	2	0.07719	6	0.09652	8	0.31134	17
3.957	0.01931	2	0.07713	5	0.09644	8	0.31117	17
3.958	0.01929	2	0.07708	6	0.09636	8	0.31100	16
3.959	0.01927	2	0.07702	6	0.09628	8	0.31084	17
3.960	0.01925	2	0.07696	6	0.09620	7	0.31067	16
3.961	0.01923	2	0.07690	6	0.09613	8	0.31051	17
3.962	0.01921	2	0.07684	6	0.09605	8	0.31034	17
3.963	0.01919	2	0.07678	6	0.09597	8	0.31017	16
3.964	0.01917	2	0.07672	6	0.09589	8	0.31001	17
3.965	0.01915	2	0.07666	6	0.09581	8	0.30984	16
3.966	0.01913	2	0.07660	6	0.09573	7	0.30968	17
3.967	0.01911	2	0.07654	5	0.09566	8	0.30951	16
3.968	0.01909	2	0.07649	6	0.09558	8	0.30935	17
3.969	0.01907	2	0.07643	6	0.09550	8	0.30918	16
3.970	0.01905	2	0.07637	6	0.09542	8	0.30902	17
3.971	0.01903	1	0.07631	6	0.09534	7	0.30885	16
3.972	0.01902	2	0.07625	6	0.09527	8	0.30869	17
3.973	0.01900	2	0.07619	6	0.09519	8	0.30852	16
3.974	0.01898	2	0.07613	5	0.09511	8	0.30836	17
3.975	0.01896	2	0.07608	6	0.09503	7	0.30819	16
3.976	0.01894	2	0.07602	6	0.09496	8	0.30803	17
3.977	0.01892	2	0.07596	6	0.09488	8	0.30786	16
3.978	0.01890	2	0.07590	6	0.09480	8	0.30770	17
3.979	0.01888	2	0.07584	6	0.09472	7	0.30753	16
3.980	0.01886	2	0.07578	5	0.09465	8	0.30737	17
3.981	0.01884	2	0.07573	6	0.09457	8	0.30720	16
3.982	0.01882	1	0.07567	6	0.09449	7	0.30704	17
3.983	0.01881	2	0.07561	6	0.09442	8	0.30687	16
3.984	0.01879	2	0.07555	6	0.09434	8	0.30671	16
3.985	0.01877	2	0.07549	5	0.09426	7	0.30655	17
3.986	0.01875	2	0.07544	6	0.09419	8	0.30638	16
3.987	0.01873	2	0.07538	6	0.09411	8	0.30622	17
3.988	0.01871	2	0.07532	6	0.09403	8	0.30605	16
3.989	0.01869	2	0.07526	5	0.09395	7	0.30589	17
3.990	0.01867	2	0.07521	6	0.09388	8	0.30572	16
3.991	0.01865	1	0.07515	6	0.09380	8	0.30556	16
3.992	0.01864	2	0.07509	6	0.09372	7	0.30540	17
3.993	0.01862	2	0.07503	6	0.09365	8	0.30523	16
3.994	0.01860	2	0.07497	5	0.09357	7	0.30507	16
3.995	0.01858	2	0.07492	6	0.09350	8	0.30491	17
3.996	0.01856	2	0.07486	6	0.09342	8	0.30474	16
3.997	0.01854	2	0.07480	6	0.09334	7	0.30458	17
3.998	0.01852	2	0.07474	5	0.09327	8	0.30441	16
3.999	0.01850	1	0.07469	6	0.09319	8	0.30425	
4.000	0.01849		0.07463		0.09311		0.30409	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
4.00	0.01849	19	0.07463	57	0.09311	75	0.3040969591	
4.01	0.01830	18	0.07406	57	0.09236	75	1.00000	0
4.02	0.01812	19	0.07349	56	0.09161	75	1.00000	0
4.03	0.01793	18	0.07293	56	0.09086	74	1.00000	0
4.04	0.01775	17	0.07237	56	0.09012	73	1.00000	0
4.05	0.01758	18	0.07181	55	0.08939	73	1.00000	0
4.06	0.01740	18	0.07126	55	0.08866	72	1.00000	0
4.07	0.01722	17	0.07071	54	0.08794	72	1.0000070879	
4.08	0.01705	17	0.07017	54	0.08722	71	0.29121	158
4.09	0.01688	17	0.06963	54	0.08651	71	0.28963	157
4.10	0.01671	17	0.06909	53	0.08580	70	0.28806	157
4.11	0.01654	16	0.06856	53	0.08510	69	0.28649	157
4.12	0.01638	17	0.06803	52	0.08441	69	0.28492	155
4.13	0.01621	16	0.06751	52	0.08372	68	0.28337	156
4.14	0.01605	16	0.06699	52	0.08304	68	0.28181	154
4.15	0.01589	16	0.06647	51	0.08236	67	0.28027	154
4.16	0.01573	16	0.06596	51	0.08169	67	0.27873	153
4.17	0.01557	15	0.06545	51	0.08102	66	0.27720	153
4.18	0.01542	16	0.06494	50	0.08036	66	0.27567	152
4.19	0.01526	15	0.06444	50	0.07970	65	0.27415	151
4.20	0.01511	15	0.06394	49	0.07905	65	0.27264	151
4.21	0.01496	15	0.06345	50	0.07840	64	0.27113	150
4.22	0.01481	15	0.06295	48	0.07776	64	0.26963	150
4.23	0.01466	15	0.06247	49	0.07712	63	0.26813	149
4.24	0.01451	14	0.06198	48	0.07649	62	0.26664	148
4.25	0.01437	15	0.06150	48	0.07587	62	0.26516	148
4.26	0.01422	14	0.06102	47	0.07525	62	0.26368	147
4.27	0.01408	14	0.06055	47	0.07463	61	0.26221	147
4.28	0.01394	14	0.06008	47	0.07402	61	0.26074	145
4.29	0.01380	14	0.05961	46	0.07341	60	0.25929	146
4.30	0.01366	14	0.05915	46	0.07281	60	0.25783	144
4.31	0.01352	13	0.05869	46	0.07221	59	0.25639	145
4.32	0.01339	13	0.05823	45	0.07162	59	0.25494	143
4.33	0.01326	14	0.05778	45	0.07103	58	0.25351	143
4.34	0.01312	13	0.05733	45	0.07045	58	0.25208	142
4.35	0.01299	13	0.05688	45	0.06987	57	0.25066	142
4.36	0.01286	13	0.05643	44	0.06930	57	0.24924	141
4.37	0.01273	13	0.05599	43	0.06873	57	0.24783	140
4.38	0.01260	12	0.05556	44	0.06816	56	0.24643	140
4.39	0.01248	13	0.05512	43	0.06760	55	0.24503	140
4.40	0.01235	12	0.05469	43	0.06705	56	0.24363	138
4.41	0.01223	12	0.05426	42	0.06649	54	0.24225	138
4.42	0.01211	12	0.05384	42	0.06595	55	0.24087	138
4.43	0.01199	12	0.05342	42	0.06540	53	0.23949	136
4.44	0.01187	12	0.05300	42	0.06487	54	0.23813	137
4.45	0.01175	12	0.05258	41	0.06433	53	0.23676	135
4.46	0.01163	12	0.05217	41	0.06380	52	0.23541	135
4.47	0.01151	11	0.05176	40	0.06328	53	0.23406	135
4.48	0.01140	12	0.05136	41	0.06275	51	0.23271	134
4.49	0.01128	11	0.05095	40	0.06224	52	0.23137	133
4.50	0.01117		0.05055		0.06172		0.23004	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
4.50	0.01117	11	0.05055	40	0.06172	51	0.23004	133
4.51	0.01106	11	0.05015	39	0.06121	50	0.22871	132
4.52	0.01095	11	0.04976	39	0.06071	50	0.22739	131
4.53	0.01084	11	0.04937	39	0.06021	50	0.22608	131
4.54	0.01073	11	0.04898	39	0.05971	49	0.22477	130
4.55	0.01062	10	0.04859	38	0.05922	49	0.22347	130
4.56	0.01052	11	0.04821	38	0.05873	49	0.22217	129
4.57	0.01041	10	0.04783	38	0.05824	48	0.22088	129
4.58	0.01031	11	0.04745	37	0.05776	48	0.21959	128
4.59	0.01020	10	0.04708	37	0.05728	47	0.21831	127
4.60	0.01010	10	0.04671	37	0.05681	47	0.21704	127
4.61	0.01000	10	0.04634	37	0.05634	47	0.21577	126
4.62	0.00990	10	0.04597	36	0.05587	46	0.21451	126
4.63	0.00980	10	0.04561	36	0.05541	46	0.21325	125
4.64	0.00970	9	0.04525	36	0.05495	45	0.21200	124
4.65	0.00961	10	0.04489	35	0.05450	45	0.21076	124
4.66	0.00951	9	0.04454	36	0.05405	45	0.20952	124
4.67	0.00942	10	0.04418	35	0.05360	45	0.20828	122
4.68	0.00932	9	0.04383	34	0.05315	44	0.20706	122
4.69	0.00923	9	0.04349	35	0.05271	43	0.20584	122
4.70	0.00914	9	0.04314	34	0.05228	44	0.20462	121
4.71	0.00905	9	0.04280	34	0.05184	43	0.20341	120
4.72	0.00896	9	0.04246	34	0.05141	42	0.20221	120
4.73	0.00887	9	0.04212	33	0.05099	43	0.20101	120
4.74	0.00878	9	0.04179	34	0.05056	42	0.19981	118
4.75	0.00869	9	0.04145	33	0.05014	41	0.19863	119
4.76	0.00860	8	0.04112	32	0.04973	42	0.19744	117
4.77	0.00852	9	0.04080	33	0.04931	41	0.19627	117
4.78	0.00843	8	0.04047	32	0.04890	40	0.19510	117
4.79	0.00835	9	0.04015	32	0.04850	41	0.19393	116
4.80	0.00826	8	0.03983	32	0.04809	40	0.19277	115
4.81	0.00818	8	0.03951	31	0.04769	39	0.19162	115
4.82	0.00810	8	0.03920	31	0.04730	40	0.19047	114
4.83	0.00802	8	0.03889	31	0.04690	39	0.18933	114
4.84	0.00794	8	0.03858	31	0.04651	38	0.18819	113
4.85	0.00786	8	0.03827	31	0.04613	39	0.18706	113
4.86	0.00778	8	0.03796	30	0.04574	38	0.18593	112
4.87	0.00770	7	0.03766	30	0.04536	38	0.18481	111
4.88	0.00763	8	0.03736	30	0.04498	37	0.18370	111
4.89	0.00755	8	0.03706	30	0.04461	37	0.18259	110
4.90	0.00747	7	0.03676	29	0.04424	37	0.18149	110
4.91	0.00740	7	0.03647	29	0.04387	37	0.18039	110
4.92	0.00733	8	0.03618	29	0.04350	36	0.17929	108
4.93	0.00725	7	0.03589	29	0.04314	36	0.17821	109
4.94	0.00718	7	0.03560	29	0.04278	36	0.17712	107
4.95	0.00711	7	0.03531	28	0.04242	35	0.17605	108
4.96	0.00704	7	0.03503	28	0.04207	35	0.17497	106
4.97	0.00697	7	0.03475	28	0.04172	35	0.17391	106
4.98	0.00690	7	0.03447	28	0.04137	35	0.17285	106
4.99	0.00683	7	0.03419	27	0.04102	34	0.17179	105
5.00	0.00676		0.03392		0.04068		0.17074	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
5.00	0.00676	7	0.03392	27	0.04068	34	0.17074	104
5.01	0.00669	6	0.03365	27	0.04034	34	0.16970	104
5.02	0.00663	7	0.03338	27	0.04000	33	0.16866	104
5.03	0.00656	7	0.03311	27	0.03967	33	0.16762	103
5.04	0.00649	6	0.03284	26	0.03934	33	0.16659	102
5.05	0.00643	6	0.03258	27	0.03901	33	0.16557	102
5.06	0.00637	7	0.03231	26	0.03868	32	0.16455	101
5.07	0.00630	6	0.03205	26	0.03836	33	0.16354	101
5.08	0.00624	6	0.03179	25	0.03803	31	0.16253	100
5.09	0.00618	6	0.03154	26	0.03772	32	0.16153	100
5.10	0.00612	7	0.03128	25	0.03740	31	0.16053	100
5.11	0.00605	6	0.03103	25	0.03709	31	0.15953	98
5.12	0.00599	6	0.03078	25	0.03678	31	0.15855	99
5.13	0.00593	6	0.03053	24	0.03647	31	0.15756	97
5.14	0.00587	5	0.03029	25	0.03616	30	0.15659	98
5.15	0.00582	6	0.03004	24	0.03586	30	0.15561	96
5.16	0.00576	6	0.02980	24	0.03556	30	0.15465	97
5.17	0.00570	6	0.02956	24	0.03526	30	0.15368	95
5.18	0.00564	5	0.02932	24	0.03496	29	0.15273	96
5.19	0.00559	6	0.02908	23	0.03467	29	0.15177	94
5.20	0.00553	5	0.02885	24	0.03438	29	0.15083	95
5.21	0.00548	6	0.02861	23	0.03409	29	0.14988	93
5.22	0.00542	5	0.02838	23	0.03380	28	0.14895	93
5.23	0.00537	6	0.02815	23	0.03352	28	0.14801	93
5.24	0.00531	5	0.02792	23	0.03324	28	0.14709	93
5.25	0.00526	5	0.02769	22	0.03296	28	0.14616	91
5.26	0.00521	5	0.02747	22	0.03268	28	0.14525	92
5.27	0.00516	5	0.02725	22	0.03240	27	0.14433	90
5.28	0.00511	6	0.02703	22	0.03213	27	0.14343	91
5.29	0.00505	5	0.02681	22	0.03186	27	0.14252	90
5.30	0.00500	5	0.02659	22	0.03159	26	0.14162	89
5.31	0.00495	5	0.02637	21	0.03133	27	0.14073	89
5.32	0.00490	4	0.02616	22	0.03106	26	0.13984	88
5.33	0.00486	5	0.02594	21	0.03080	26	0.13896	88
5.34	0.00481	5	0.02573	21	0.03054	26	0.13808	88
5.35	0.00476	5	0.02552	20	0.03028	25	0.13720	87
5.36	0.00471	4	0.02532	21	0.03003	26	0.13633	86
5.37	0.00467	5	0.02511	21	0.02977	25	0.13547	86
5.38	0.00462	5	0.02490	20	0.02952	25	0.13461	86
5.39	0.00457	4	0.02470	20	0.02927	24	0.13375	85
5.40	0.00453	5	0.02450	20	0.02903	25	0.13290	85
5.41	0.00448	4	0.02430	20	0.02878	24	0.13205	84
5.42	0.00444	5	0.02410	20	0.02854	24	0.13121	83
5.43	0.00439	4	0.02390	19	0.02830	24	0.13038	84
5.44	0.00435	4	0.02371	19	0.02806	24	0.12954	83
5.45	0.00431	5	0.02352	20	0.02782	23	0.12871	82
5.46	0.00426	4	0.02332	19	0.02759	24	0.12789	82
5.47	0.00422	4	0.02313	19	0.02735	23	0.12707	81
5.48	0.00418	4	0.02294	18	0.02712	23	0.12626	81
5.49	0.00414	4	0.02276	19	0.02689	23	0.12545	81
5.50	0.00410		0.02257		0.02666		0.12464	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
5.50	0.00410	5	0.02257	19	0.02666	22	0.12464	80
5.51	0.00405	4	0.02238	18	0.02644	22	0.12384	80
5.52	0.00401	4	0.02220	18	0.02622	23	0.12304	79
5.53	0.00397	4	0.02202	18	0.02599	22	0.12225	79
5.54	0.00393	3	0.02184	18	0.02577	22	0.12146	78
5.55	0.00390	4	0.02166	18	0.02555	21	0.12068	78
5.56	0.00386	4	0.02148	17	0.02534	22	0.11990	77
5.57	0.00382	4	0.02131	18	0.02512	21	0.11913	77
5.58	0.00378	4	0.02113	17	0.02491	21	0.11836	77
5.59	0.00374	4	0.02096	18	0.02470	21	0.11759	76
5.60	0.00370	3	0.02078	17	0.02449	21	0.11683	76
5.61	0.00367	4	0.02061	17	0.02428	20	0.11607	75
5.62	0.00363	3	0.02044	16	0.02408	21	0.11532	75
5.63	0.00360	4	0.02028	17	0.02387	20	0.11457	75
5.64	0.00356	4	0.02011	17	0.02367	20	0.11382	74
5.65	0.00352	3	0.01994	16	0.02347	20	0.11308	73
5.66	0.00349	4	0.01978	16	0.02327	20	0.11235	74
5.67	0.00345	3	0.01962	16	0.02307	20	0.11161	72
5.68	0.00342	3	0.01946	16	0.02287	19	0.11089	73
5.69	0.00339	4	0.01930	16	0.02268	19	0.11016	72
5.70	0.00335	3	0.01914	16	0.02249	19	0.10944	71
5.71	0.00332	3	0.01898	16	0.02230	19	0.10873	72
5.72	0.00329	4	0.01882	15	0.02211	19	0.10801	70
5.73	0.00325	3	0.01867	16	0.02192	19	0.10731	71
5.74	0.00322	3	0.01851	15	0.02173	18	0.10660	70
5.75	0.00319	3	0.01836	15	0.02155	19	0.10590	69
5.76	0.00316	4	0.01821	15	0.02136	18	0.10521	69
5.77	0.00312	3	0.01806	15	0.02118	18	0.10452	69
5.78	0.00309	3	0.01791	15	0.02100	18	0.10383	68
5.79	0.00306	3	0.01776	15	0.02082	17	0.10315	68
5.80	0.00303	3	0.01761	14	0.02065	18	0.10247	68
5.81	0.00300	3	0.01747	15	0.02047	18	0.10179	67
5.82	0.00297	3	0.01732	14	0.02029	17	0.10112	67
5.83	0.00294	3	0.01718	14	0.02012	17	0.10045	66
5.84	0.00291	3	0.01704	14	0.01995	17	0.09979	66
5.85	0.00288	2	0.01690	14	0.01978	17	0.09913	66
5.86	0.00286	3	0.01676	14	0.01961	17	0.09847	65
5.87	0.00283	3	0.01662	14	0.01944	16	0.09782	65
5.88	0.00280	3	0.01648	14	0.01928	17	0.09717	64
5.89	0.00277	3	0.01634	13	0.01911	16	0.09653	65
5.90	0.00274	2	0.01621	14	0.01895	16	0.09588	63
5.91	0.00272	3	0.01607	13	0.01879	16	0.09525	64
5.92	0.00269	3	0.01594	13	0.01863	16	0.09461	63
5.93	0.00266	2	0.01581	13	0.01847	16	0.09398	62
5.94	0.00264	3	0.01568	13	0.01831	16	0.09336	62
5.95	0.00261	3	0.01555	13	0.01815	15	0.09274	62
5.96	0.00258	2	0.01542	13	0.01800	15	0.09212	62
5.97	0.00256	3	0.01529	13	0.01785	16	0.09150	61
5.98	0.00253	2	0.01516	13	0.01769	15	0.09089	61
5.99	0.00251	3	0.01503	12	0.01754	15	0.09028	60
6.00	0.00248		0.01491		0.01739		0.08968	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
6.00	0.00248	2	0.01491	12	0.01739	15	0.08968	60
6.01	0.00246	3	0.01479	13	0.01724	15	0.08908	60
6.02	0.00243	2	0.01466	12	0.01709	14	0.08848	59
6.03	0.00241	3	0.01454	12	0.01695	15	0.08789	59
6.04	0.00238	2	0.01442	12	0.01680	14	0.08730	59
6.05	0.00236	2	0.01430	12	0.01666	14	0.08671	58
6.06	0.00234	3	0.01418	12	0.01652	14	0.08613	58
6.07	0.00231	2	0.01406	12	0.01638	15	0.08555	58
6.08	0.00229	2	0.01394	11	0.01623	13	0.08497	57
6.09	0.00227	2	0.01383	12	0.01610	14	0.08440	57
6.10	0.00225	3	0.01371	11	0.01596	14	0.08383	56
6.11	0.00222	2	0.01360	12	0.01582	13	0.08327	56
6.12	0.00220	2	0.01348	11	0.01569	14	0.08271	56
6.13	0.00218	2	0.01337	11	0.01555	13	0.08215	56
6.14	0.00216	2	0.01326	11	0.01542	14	0.08159	55
6.15	0.00214	3	0.01315	11	0.01528	13	0.08104	55
6.16	0.00211	2	0.01304	11	0.01515	13	0.08049	54
6.17	0.00209	2	0.01293	11	0.01502	13	0.07995	55
6.18	0.00207	2	0.01282	11	0.01489	12	0.07940	54
6.19	0.00205	2	0.01271	10	0.01477	13	0.07886	53
6.20	0.00203	2	0.01261	11	0.01464	13	0.07833	53
6.21	0.00201	2	0.01250	10	0.01451	12	0.07780	53
6.22	0.00199	2	0.01240	11	0.01439	12	0.07727	53
6.23	0.00197	2	0.01229	10	0.01427	13	0.07674	52
6.24	0.00195	2	0.01219	10	0.01414	12	0.07622	52
6.25	0.00193	2	0.01209	10	0.01402	12	0.07570	52
6.26	0.00191	2	0.01199	10	0.01390	12	0.07518	51
6.27	0.00189	1	0.01189	10	0.01378	12	0.07467	51
6.28	0.00188	2	0.01179	10	0.01366	12	0.07416	51
6.29	0.00186	2	0.01169	10	0.01354	11	0.07365	50
6.30	0.00184	2	0.01159	10	0.01343	12	0.07315	50
6.31	0.00182	2	0.01149	9	0.01331	11	0.07265	50
6.32	0.00180	2	0.01140	10	0.01320	12	0.07215	49
6.33	0.00178	1	0.01130	9	0.01308	11	0.07166	49
6.34	0.00177	2	0.01121	10	0.01297	11	0.07117	49
6.35	0.00175	2	0.01111	9	0.01286	11	0.07068	49
6.36	0.00173	2	0.01102	9	0.01275	11	0.07019	48
6.37	0.00171	1	0.01093	10	0.01264	11	0.06971	48
6.38	0.00170	2	0.01083	9	0.01253	11	0.06923	47
6.39	0.00168	2	0.01074	9	0.01242	11	0.06876	48
6.40	0.00166	1	0.01065	9	0.01231	10	0.06828	47
6.41	0.00165	2	0.01056	9	0.01221	11	0.06781	46
6.42	0.00163	2	0.01047	9	0.01210	10	0.06735	47
6.43	0.00161	1	0.01038	8	0.01200	10	0.06688	46
6.44	0.00160	2	0.01030	9	0.01190	11	0.06642	46
6.45	0.00158	1	0.01021	9	0.01179	10	0.06596	45
6.46	0.00157	2	0.01012	8	0.01169	10	0.06551	46
6.47	0.00155	1	0.01004	9	0.01159	10	0.06505	45
6.48	0.00154	2	0.00995	8	0.01149	10	0.06460	44
6.49	0.00152	2	0.00987	8	0.01139	10	0.06416	45
6.50	0.00150		0.00979		0.01129		0.06371	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
6.50	0.00150	1	0.00979	9	0.01129	10	0.06371	44
6.51	0.00149	2	0.00970	8	0.01119	9	0.06327	44
6.52	0.00147	1	0.00962	8	0.01110	10	0.06283	43
6.53	0.00146	1	0.00954	8	0.01100	9	0.06240	44
6.54	0.00145	2	0.00946	8	0.01091	10	0.06196	43
6.55	0.00143	1	0.00938	8	0.01081	9	0.06153	43
6.56	0.00142	2	0.00930	8	0.01072	9	0.06110	42
6.57	0.00140	1	0.00922	8	0.01063	10	0.06068	42
6.58	0.00139	1	0.00914	7	0.01053	9	0.06026	42
6.59	0.00138	2	0.00907	8	0.01044	9	0.05984	42
6.60	0.00136	1	0.00899	8	0.01035	9	0.05942	42
6.61	0.00135	2	0.00891	7	0.01026	9	0.05900	41
6.62	0.00133	1	0.00884	8	0.01017	8	0.05859	41
6.63	0.00132	1	0.00876	7	0.01009	9	0.05818	40
6.64	0.00131	2	0.00869	7	0.01000	9	0.05778	41
6.65	0.00129	1	0.00862	8	0.00991	8	0.05737	40
6.66	0.00128	1	0.00854	7	0.00983	9	0.05697	40
6.67	0.00127	1	0.00847	7	0.00974	8	0.05657	39
6.68	0.00126	2	0.00840	7	0.00966	9	0.05618	40
6.69	0.00124	1	0.00833	7	0.00957	8	0.05578	39
6.70	0.00123	1	0.00826	7	0.00949	8	0.05539	39
6.71	0.00122	1	0.00819	7	0.00941	8	0.05500	38
6.72	0.00121	1	0.00812	7	0.00933	9	0.05462	39
6.73	0.00120	2	0.00805	7	0.00924	8	0.05423	38
6.74	0.00118	1	0.00798	7	0.00916	8	0.05385	38
6.75	0.00117	1	0.00791	6	0.00908	7	0.05347	37
6.76	0.00116	1	0.00785	7	0.00901	8	0.05310	38
6.77	0.00115	1	0.00778	7	0.00893	8	0.05272	37
6.78	0.00114	1	0.00771	6	0.00885	8	0.05235	37
6.79	0.00113	2	0.00765	7	0.00877	7	0.05198	36
6.80	0.00111	1	0.00758	6	0.00870	8	0.05162	37
6.81	0.00110	1	0.00752	7	0.00862	7	0.05125	36
6.82	0.00109	1	0.00745	6	0.00855	8	0.05089	36
6.83	0.00108	1	0.00739	6	0.00847	7	0.05053	36
6.84	0.00107	1	0.00733	7	0.00840	8	0.05017	35
6.85	0.00106	1	0.00726	6	0.00832	7	0.04982	35
6.86	0.00105	1	0.00720	6	0.00825	7	0.04947	36
6.87	0.00104	1	0.00714	6	0.00818	7	0.04911	34
6.88	0.00103	1	0.00708	6	0.00811	7	0.04877	35
6.89	0.00102	1	0.00702	6	0.00804	7	0.04842	34
6.90	0.00101	1	0.00696	6	0.00797	7	0.04808	34
6.91	0.00100	1	0.00690	6	0.00790	7	0.04774	34
6.92	0.00099	1	0.00684	6	0.00783	7	0.04740	34
6.93	0.00098	1	0.00678	5	0.00776	6	0.04706	33
6.94	0.00097	1	0.00673	6	0.00770	7	0.04673	34
6.95	0.00096	1	0.00667	6	0.00763	7	0.04639	33
6.96	0.00095	1	0.00661	5	0.00756	6	0.04606	32
6.97	0.00094	1	0.00656	6	0.00750	7	0.04574	33
6.98	0.00093	1	0.00650	6	0.00743	6	0.04541	32
6.99	0.00092	1	0.00644	5	0.00737	7	0.04509	33
7.00	0.00091		0.00639		0.00730		0.04476	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^\circ - E_0^\circ)/RT$	Δ	$(H^\circ - E_0^\circ)/RT$	Δ	S°/R	Δ	C_p°/R	Δ
7.00	0.00091	1	0.00639	6	0.00730	6	0.04476	32
7.01	0.00090	1	0.00633	5	0.00724	7	0.04444	31
7.02	0.00089	0	0.00628	5	0.00717	6	0.04413	32
7.03	0.00089	1	0.00623	6	0.00711	6	0.04381	31
7.04	0.00088	1	0.00617	5	0.00705	6	0.04350	31
7.05	0.00087	1	0.00612	5	0.00699	6	0.04319	31
7.06	0.00086	1	0.00607	5	0.00693	6	0.04288	31
7.07	0.00085	1	0.00602	6	0.00687	6	0.04257	30
7.08	0.00084	1	0.00596	5	0.00681	6	0.04227	31
7.09	0.00083	0	0.00591	5	0.00675	6	0.04196	30
7.10	0.00083	1	0.00586	5	0.00669	6	0.04166	30
7.11	0.00082	1	0.00581	5	0.00663	6	0.04136	29
7.12	0.00081	1	0.00576	5	0.00657	6	0.04107	30
7.13	0.00080	1	0.00571	5	0.00651	5	0.04077	29
7.14	0.00079	0	0.00566	4	0.00646	6	0.04048	29
7.15	0.00079	1	0.00562	5	0.00640	5	0.04019	29
7.16	0.00078	1	0.00557	5	0.00635	6	0.03990	29
7.17	0.00077	1	0.00552	5	0.00629	6	0.03961	28
7.18	0.00076	1	0.00547	4	0.00623	5	0.03933	29
7.19	0.00075	0	0.00543	5	0.00618	5	0.03904	28
7.20	0.00075	1	0.00538	5	0.00613	6	0.03876	28
7.21	0.00074	1	0.00533	4	0.00607	5	0.03848	28
7.22	0.00073	1	0.00529	5	0.00602	5	0.03820	27
7.23	0.00072	0	0.00524	4	0.00597	6	0.03793	28
7.24	0.00072	1	0.00520	5	0.00591	5	0.03765	27
7.25	0.00071	1	0.00515	4	0.00586	5	0.03738	27
7.26	0.00070	0	0.00511	5	0.00581	5	0.03711	27
7.27	0.00070	1	0.00506	4	0.00576	5	0.03684	26
7.28	0.00069	1	0.00502	4	0.00571	5	0.03658	27
7.29	0.00068	0	0.00498	5	0.00566	5	0.03631	26
7.30	0.00068	1	0.00493	4	0.00561	5	0.03605	26
7.31	0.00067	1	0.00489	4	0.00556	5	0.03579	26
7.32	0.00066	0	0.00485	4	0.00551	5	0.03553	26
7.33	0.00066	1	0.00481	4	0.00546	4	0.03527	26
7.34	0.00065	1	0.00477	4	0.00542	5	0.03501	25
7.35	0.00064	0	0.00473	4	0.00537	5	0.03476	25
7.36	0.00064	1	0.00469	4	0.00532	4	0.03451	25
7.37	0.00063	1	0.00465	4	0.00528	5	0.03426	25
7.38	0.00062	0	0.00461	4	0.00523	5	0.03401	25
7.39	0.00062	1	0.00457	4	0.00518	4	0.03376	25
7.40	0.00061	0	0.00453	4	0.00514	5	0.03351	24
7.41	0.00061	1	0.00449	4	0.00509	4	0.03327	24
7.42	0.00060	1	0.00445	4	0.00505	5	0.03303	24
7.43	0.00059	0	0.00441	4	0.00500	4	0.03279	24
7.44	0.00059	1	0.00437	4	0.00496	4	0.03255	24
7.45	0.00058	0	0.00433	3	0.00492	5	0.03231	24
7.46	0.00058	1	0.00430	4	0.00487	4	0.03207	23
7.47	0.00057	1	0.00426	4	0.00483	4	0.03184	23
7.48	0.00056	0	0.00422	3	0.00479	4	0.03161	24
7.49	0.00056	1	0.00419	4	0.00475	5	0.03137	22
7.50	0.00055		0.00415		0.00470		0.03115	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R	Δ
7.50	0.00055	0	0.00415	4	0.00470	4	0.03115	23
7.51	0.00055	1	0.00411	3	0.00466	4	0.03092	23
7.52	0.00054	0	0.00408	4	0.00462	4	0.03069	22
7.53	0.00054	1	0.00404	3	0.00458	4	0.03047	23
7.54	0.00053	0	0.00401	4	0.00454	4	0.03024	22
7.55	0.00053	1	0.00397	3	0.00450	4	0.03002	22
7.56	0.00052	0	0.00394	3	0.00446	4	0.02980	22
7.57	0.00052	1	0.00391	4	0.00442	4	0.02958	22
7.58	0.00051	0	0.00387	3	0.00438	4	0.02936	21
7.59	0.00051	1	0.00384	3	0.00434	3	0.02915	21
7.60	0.00050	0	0.00381	4	0.00431	4	0.02894	22
7.61	0.00050	1	0.00377	3	0.00427	4	0.02872	21
7.62	0.00049	0	0.00374	3	0.00423	4	0.02851	21
7.63	0.00049	1	0.00371	3	0.00419	3	0.02830	21
7.64	0.00048	0	0.00368	4	0.00416	4	0.02809	20
7.65	0.00048	1	0.00364	3	0.00412	4	0.02789	21
7.66	0.00047	0	0.00361	3	0.00408	3	0.02768	20
7.67	0.00047	1	0.00358	3	0.00405	4	0.02748	21
7.68	0.00046	0	0.00355	3	0.00401	3	0.02727	20
7.69	0.00046	1	0.00352	3	0.00398	4	0.02707	20
7.70	0.00045	0	0.00349	3	0.00394	3	0.02687	20
7.71	0.00045	1	0.00346	3	0.00391	4	0.02667	19
7.72	0.00044	0	0.00343	3	0.00387	3	0.02648	20
7.73	0.00044	0	0.00340	3	0.00384	4	0.02628	19
7.74	0.00044	1	0.00337	3	0.00380	3	0.02609	20
7.75	0.00043	0	0.00334	3	0.00377	3	0.02589	19
7.76	0.00043	1	0.00331	3	0.00374	4	0.02570	19
7.77	0.00042	0	0.00328	3	0.00370	3	0.02551	19
7.78	0.00042	1	0.00325	2	0.00367	3	0.02532	18
7.79	0.00041	0	0.00323	3	0.00364	3	0.02514	19
7.80	0.00041	0	0.00320	3	0.00361	3	0.02495	19
7.81	0.00041	1	0.00317	3	0.00358	4	0.02476	18
7.82	0.00040	0	0.00314	3	0.00354	3	0.02458	18
7.83	0.00040	1	0.00311	2	0.00351	3	0.02440	18
7.84	0.00039	0	0.00309	3	0.00348	3	0.02422	18
7.85	0.00039	0	0.00306	3	0.00345	3	0.02404	18
7.86	0.00039	1	0.00303	2	0.00342	3	0.02386	18
7.87	0.00038	0	0.00301	3	0.00339	3	0.02368	18
7.88	0.00038	1	0.00298	2	0.00336	3	0.02350	17
7.89	0.00037	0	0.00296	3	0.00333	3	0.02333	17
7.90	0.00037	0	0.00293	3	0.00330	3	0.02316	18
7.91	0.00037	1	0.00290	2	0.00327	3	0.02298	17
7.92	0.00036	0	0.00288	3	0.00324	3	0.02281	17
7.93	0.00036	0	0.00285	2	0.00321	2	0.02264	17
7.94	0.00036	1	0.00283	3	0.00319	3	0.02247	17
7.95	0.00035	0	0.00280	2	0.00316	3	0.02230	16
7.96	0.00035	0	0.00278	2	0.00313	3	0.02214	17
7.97	0.00035	1	0.00276	3	0.00310	3	0.02197	16
7.98	0.00034	0	0.00273	2	0.00307	2	0.02181	16
7.99	0.00034	0	0.00271	3	0.00305	3	0.02165	17
8.00	0.00034		0.00268		0.00302		0.02148	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^{\circ}-E_0^{\circ})/RT$	Δ	$(H^{\circ}-E_0^{\circ})/RT$	Δ	S°/R	Δ	C_p°/R	Δ
8.00	0.00034	1	0.00268	2	0.00302	3	0.02148	16
8.01	0.00033	0	0.00266	2	0.00299	2	0.02132	16
8.02	0.00033	0	0.00264	2	0.00297	3	0.02116	15
8.03	0.00033	1	0.00261	3	0.00294	3	0.02101	16
8.04	0.00032	0	0.00259	2	0.00291	2	0.02085	16
8.05	0.00032	0	0.00257	2	0.00289	3	0.02069	15
8.06	0.00032	1	0.00255	3	0.00286	2	0.02054	16
8.07	0.00031	0	0.00252	2	0.00284	3	0.02038	15
8.08	0.00031	0	0.00250	2	0.00281	2	0.02023	15
8.09	0.00031	1	0.00248	2	0.00279	3	0.02008	15
8.10	0.00030	0	0.00246	2	0.00276	2	0.01993	15
8.11	0.00030	0	0.00244	2	0.00274	3	0.01978	15
8.12	0.00030	1	0.00242	2	0.00271	2	0.01963	15
8.13	0.00029	0	0.00240	3	0.00269	2	0.01948	14
8.14	0.00029	0	0.00237	2	0.00267	3	0.01934	15
8.15	0.00029	0	0.00235	2	0.00264	2	0.01919	14
8.16	0.00029	1	0.00233	2	0.00262	2	0.01905	15
8.17	0.00028	0	0.00231	2	0.00260	3	0.01890	14
8.18	0.00028	0	0.00229	2	0.00257	2	0.01876	14
8.19	0.00028	1	0.00227	2	0.00255	2	0.01862	14
8.20	0.00027	0	0.00225	2	0.00253	2	0.01848	14
8.21	0.00027	0	0.00223	2	0.00251	3	0.01834	14
8.22	0.00027	0	0.00221	2	0.00248	2	0.01820	14
8.23	0.00027	1	0.00219	2	0.00246	2	0.01806	13
8.24	0.00026	0	0.00217	1	0.00244	2	0.01793	14
8.25	0.00026	0	0.00216	2	0.00242	2	0.01779	13
8.26	0.00026	0	0.00214	2	0.00240	3	0.01766	14
8.27	0.00026	1	0.00212	2	0.00237	2	0.01752	13
8.28	0.00025	0	0.00210	2	0.00235	2	0.01739	13
8.29	0.00025	0	0.00208	2	0.00233	2	0.01726	13
8.30	0.00025	0	0.00206	1	0.00231	2	0.01713	13
8.31	0.00025	1	0.00205	2	0.00229	2	0.01700	13
8.32	0.00024	0	0.00203	2	0.00227	2	0.01687	13
8.33	0.00024	0	0.00201	2	0.00225	2	0.01674	12
8.34	0.00024	0	0.00199	2	0.00223	2	0.01662	13
8.35	0.00024	1	0.00197	1	0.00221	2	0.01649	13
8.36	0.00023	0	0.00196	2	0.00219	2	0.01636	12
8.37	0.00023	0	0.00194	2	0.00217	2	0.01624	12
8.38	0.00023	0	0.00192	1	0.00215	2	0.01612	12
8.39	0.00023	1	0.00191	2	0.00213	2	0.01600	13
8.40	0.00022	0	0.00189	2	0.00211	1	0.01587	12
8.41	0.00022	0	0.00187	1	0.00210	2	0.01575	12
8.42	0.00022	0	0.00186	2	0.00208	2	0.01563	12
8.43	0.00022	0	0.00184	2	0.00206	2	0.01551	11
8.44	0.00022	1	0.00182	1	0.00204	2	0.01540	12
8.45	0.00021	0	0.00181	2	0.00202	2	0.01528	12
8.46	0.00021	0	0.00179	1	0.00200	1	0.01516	11
8.47	0.00021	0	0.00178	2	0.00199	2	0.01505	12
8.48	0.00021	0	0.00176	1	0.00197	2	0.01493	11
8.49	0.00021	1	0.00175	2	0.00195	2	0.01482	11
8.50	0.00020		0.00173		0.00193		0.01471	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
8.50	0.00020	0	0.00173	2	0.00193	1	0.01471	12
8.51	0.00020	0	0.00171	1	0.00192	2	0.01459	11
8.52	0.00020	0	0.00170	2	0.00190	2	0.01448	11
8.53	0.00020	0	0.00168	1	0.00188	1	0.01437	11
8.54	0.00020	1	0.00167	1	0.00187	2	0.01426	11
8.55	0.00019	0	0.00166	2	0.00185	2	0.01415	10
8.56	0.00019	0	0.00164	1	0.00183	1	0.01405	11
8.57	0.00019	0	0.00163	2	0.00182	2	0.01394	11
8.58	0.00019	0	0.00161	1	0.00180	2	0.01383	10
8.59	0.00019	1	0.00160	2	0.00178	1	0.01373	11
8.60	0.00018	0	0.00158	1	0.00177	2	0.01362	10
8.61	0.00018	0	0.00157	1	0.00175	1	0.01352	11
8.62	0.00018	0	0.00156	2	0.00174	2	0.01341	10
8.63	0.00018	0	0.00154	1	0.00172	1	0.01331	10
8.64	0.00018	0	0.00153	1	0.00171	2	0.01321	10
8.65	0.00018	1	0.00152	2	0.00169	1	0.01311	10
8.66	0.00017	0	0.00150	1	0.00168	2	0.01301	10
8.67	0.00017	0	0.00149	1	0.00166	1	0.01291	10
8.68	0.00017	0	0.00148	2	0.00165	2	0.01281	10
8.69	0.00017	0	0.00146	1	0.00163	1	0.01271	10
8.70	0.00017	1	0.00145	1	0.00162	2	0.01261	9
8.71	0.00016	0	0.00144	2	0.00160	1	0.01252	10
8.72	0.00016	0	0.00142	1	0.00159	2	0.01242	10
8.73	0.00016	0	0.00141	1	0.00157	1	0.01232	9
8.74	0.00016	0	0.00140	1	0.00156	1	0.01223	9
8.75	0.00016	0	0.00139	2	0.00155	2	0.01214	10
8.76	0.00016	0	0.00137	1	0.00153	1	0.01204	9
8.77	0.00016	1	0.00136	1	0.00152	2	0.01195	9
8.78	0.00015	0	0.00135	1	0.00150	1	0.01186	9
8.79	0.00015	0	0.00134	1	0.00149	1	0.01177	9
8.80	0.00015	0	0.00133	2	0.00148	2	0.01168	9
8.81	0.00015	0	0.00131	1	0.00146	1	0.01159	9
8.82	0.00015	0	0.00130	1	0.00145	1	0.01150	9
8.83	0.00015	1	0.00129	1	0.00144	1	0.01141	9
8.84	0.00014	0	0.00128	1	0.00143	2	0.01132	9
8.85	0.00014	0	0.00127	1	0.00141	1	0.01123	8
8.86	0.00014	0	0.00126	1	0.00140	1	0.01115	9
8.87	0.00014	0	0.00125	1	0.00139	2	0.01106	8
8.88	0.00014	0	0.00124	2	0.00137	1	0.01098	9
8.89	0.00014	0	0.00122	1	0.00136	1	0.01089	8
8.90	0.00014	0	0.00121	1	0.00135	1	0.01081	9
8.91	0.00014	1	0.00120	1	0.00134	1	0.01072	8
8.92	0.00013	0	0.00119	1	0.00133	2	0.01064	8
8.93	0.00013	0	0.00118	1	0.00131	1	0.01056	8
8.94	0.00013	0	0.00117	1	0.00130	1	0.01048	9
8.95	0.00013	0	0.00116	1	0.00129	1	0.01039	8
8.96	0.00013	0	0.00115	1	0.00128	1	0.01031	8
8.97	0.00013	0	0.00114	1	0.00127	1	0.01023	7
8.98	0.00013	1	0.00113	1	0.00126	1	0.01016	8
8.99	0.00012	0	0.00112	1	0.00125	2	0.01008	8
9.00	0.00012		0.00111		0.00123		0.01000	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^\circ - E_0)/RT$	Δ	$(H^\circ - E_0)/RT$	Δ	S°/R	Δ	C_p°/R	Δ
9.00	0.00012	0	0.00111	1	0.00123	1	0.01000	8
9.01	0.00012	0	0.00110	1	0.00122	1	0.00992	8
9.02	0.00012	0	0.00109	1	0.00121	1	0.00984	7
9.03	0.00012	0	0.00108	1	0.00120	1	0.00977	8
9.04	0.00012	0	0.00107	1	0.00119	1	0.00969	7
9.05	0.00012	0	0.00106	1	0.00118	1	0.00962	8
9.06	0.00012	0	0.00105	1	0.00117	1	0.00954	7
9.07	0.00012	1	0.00104	1	0.00116	1	0.00947	8
9.08	0.00011	0	0.00103	0	0.00115	1	0.00939	7
9.09	0.00011	0	0.00103	1	0.00114	1	0.00932	7
9.10	0.00011	0	0.00102	1	0.00113	1	0.00925	7
9.11	0.00011	0	0.00101	1	0.00112	1	0.00918	7
9.12	0.00011	0	0.00100	1	0.00111	1	0.00911	8
9.13	0.00011	0	0.00099	1	0.00110	1	0.00903	7
9.14	0.00011	0	0.00098	1	0.00109	1	0.00896	7
9.15	0.00011	0	0.00097	1	0.00108	1	0.00889	6
9.16	0.00011	1	0.00096	1	0.00107	1	0.00883	7
9.17	0.00010	0	0.00095	0	0.00106	1	0.00876	7
9.18	0.00010	0	0.00095	1	0.00105	1	0.00869	7
9.19	0.00010	0	0.00094	1	0.00104	1	0.00862	7
9.20	0.00010	0	0.00093	1	0.00103	1	0.00855	6
9.21	0.00010	0	0.00092	1	0.00102	1	0.00849	7
9.22	0.00010	0	0.00091	0	0.00101	1	0.00842	6
9.23	0.00010	0	0.00091	1	0.00100	1	0.00836	7
9.24	0.00010	0	0.00090	1	0.00099	0	0.00829	6
9.25	0.00010	0	0.00089	1	0.00099	1	0.00823	7
9.26	0.00010	1	0.00088	1	0.00098	1	0.00816	6
9.27	0.00009	0	0.00087	0	0.00097	1	0.00810	7
9.28	0.00009	0	0.00087	1	0.00096	1	0.00803	6
9.29	0.00009	0	0.00086	1	0.00095	1	0.00797	6
9.30	0.00009	0	0.00085	1	0.00094	1	0.00791	6
9.31	0.00009	0	0.00084	0	0.00093	1	0.00785	6
9.32	0.00009	0	0.00084	1	0.00092	0	0.00779	7
9.33	0.00009	0	0.00083	1	0.00092	1	0.00772	6
9.34	0.00009	0	0.00082	1	0.00091	1	0.00766	6
9.35	0.00009	0	0.00081	0	0.00090	1	0.00760	6
9.36	0.00009	0	0.00081	1	0.00089	1	0.00754	5
9.37	0.00009	1	0.00080	1	0.00088	0	0.00749	6
9.38	0.00008	0	0.00079	1	0.00088	1	0.00743	6
9.39	0.00008	0	0.00078	0	0.00087	1	0.00737	6
9.40	0.00008	0	0.00078	1	0.00086	1	0.00731	6
9.41	0.00008	0	0.00077	1	0.00085	0	0.00725	5
9.42	0.00008	0	0.00076	0	0.00085	1	0.00720	6
9.43	0.00008	0	0.00076	1	0.00084	1	0.00714	6
9.44	0.00008	0	0.00075	1	0.00083	1	0.00708	5
9.45	0.00008	0	0.00074	0	0.00082	1	0.00703	6
9.46	0.00008	0	0.00074	1	0.00081	0	0.00697	5
9.47	0.00008	0	0.00073	1	0.00081	1	0.00692	6
9.48	0.00008	0	0.00072	0	0.00080	1	0.00686	5
9.49	0.00008	1	0.00072	1	0.00079	0	0.00681	5
9.50	0.00007		0.00071		0.00079		0.00676	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
9.50	0.00007	0	0.00071	1	0.00079	1	0.00676	6
9.51	0.00007	0	0.00070	0	0.00078	1	0.00670	5
9.52	0.00007	0	0.00070	1	0.00077	1	0.00665	5
9.53	0.00007	0	0.00069	0	0.00076	0	0.00660	5
9.54	0.00007	0	0.00069	1	0.00076	1	0.00655	6
9.55	0.00007	0	0.00068	1	0.00075	1	0.00649	5
9.56	0.00007	0	0.00067	0	0.00074	0	0.00644	5
9.57	0.00007	0	0.00067	1	0.00074	1	0.00639	5
9.58	0.00007	0	0.00066	0	0.00073	1	0.00634	5
9.59	0.00007	0	0.00066	1	0.00072	0	0.00629	5
9.60	0.00007	0	0.00065	1	0.00072	1	0.00624	5
9.61	0.00007	0	0.00064	0	0.00071	0	0.00619	5
9.62	0.00007	0	0.00064	1	0.00071	1	0.00614	4
9.63	0.00007	0	0.00063	0	0.00070	1	0.00610	5
9.64	0.00007	1	0.00063	1	0.00069	0	0.00605	5
9.65	0.00006	0	0.00062	0	0.00069	1	0.00600	5
9.66	0.00006	0	0.00062	1	0.00068	1	0.00595	4
9.67	0.00006	0	0.00061	0	0.00067	0	0.00591	5
9.68	0.00006	0	0.00061	1	0.00067	1	0.00586	5
9.69	0.00006	0	0.00060	1	0.00066	0	0.00581	4
9.70	0.00006	0	0.00059	0	0.00066	1	0.00577	5
9.71	0.00006	0	0.00059	1	0.00065	1	0.00572	4
9.72	0.00006	0	0.00058	0	0.00064	0	0.00568	5
9.73	0.00006	0	0.00058	1	0.00064	1	0.00563	4
9.74	0.00006	0	0.00057	0	0.00063	0	0.00559	5
9.75	0.00006	0	0.00057	1	0.00063	1	0.00554	4
9.76	0.00006	0	0.00056	0	0.00062	0	0.00550	5
9.77	0.00006	0	0.00056	1	0.00062	1	0.00545	4
9.78	0.00006	0	0.00055	0	0.00061	1	0.00541	4
9.79	0.00006	0	0.00055	1	0.00060	0	0.00537	4
9.80	0.00006	1	0.00054	0	0.00060	1	0.00533	5
9.81	0.00005	0	0.00054	1	0.00059	0	0.00528	4
9.82	0.00005	0	0.00053	0	0.00059	1	0.00524	4
9.83	0.00005	0	0.00053	1	0.00058	0	0.00520	4
9.84	0.00005	0	0.00052	0	0.00058	1	0.00516	4
9.85	0.00005	0	0.00052	1	0.00057	0	0.00512	4
9.86	0.00005	0	0.00051	0	0.00057	1	0.00508	4
9.87	0.00005	0	0.00051	0	0.00056	0	0.00504	4
9.88	0.00005	0	0.00051	1	0.00056	1	0.00500	4
9.89	0.00005	0	0.00050	0	0.00055	0	0.00496	4
9.90	0.00005	0	0.00050	1	0.00055	1	0.00492	4
9.91	0.00005	0	0.00049	0	0.00054	0	0.00488	4
9.92	0.00005	0	0.00049	1	0.00054	1	0.00484	4
9.93	0.00005	0	0.00048	0	0.00053	0	0.00480	4
9.94	0.00005	0	0.00048	1	0.00053	1	0.00476	3
9.95	0.00005	0	0.00047	0	0.00052	0	0.00473	4
9.96	0.00005	0	0.00047	0	0.00052	1	0.00469	4
9.97	0.00005	0	0.00047	1	0.00051	0	0.00465	4
9.98	0.00005	0	0.00046	0	0.00051	1	0.00461	3
9.99	0.00005	0	0.00046	1	0.00050	0	0.00458	4
10.00	0.00005		0.00045		0.00050		0.00454	

Table I Harmonic Oscillator Contributions (in dimensionless form) to the
Thermodynamic Functions for Values of $X = hc\nu/kT$

X	$-(F^0-E_0^0)/RT$	Δ	$(H^0-E_0^0)/RT$	Δ	S^0/R	Δ	C_p^0/R	Δ
10.0	0.00005	1	0.00045	7	0.00050	8	0.00454	67
10.2	0.00004	1	0.00038	6	0.00042	7	0.00387	58
10.4	0.00003	1	0.00032	4	0.00035	6	0.00329	49
10.6	0.00002	0	0.00026	4	0.00029	5	0.00280	42
10.8	0.00002	0	0.00022	4	0.00024	4	0.00238	36
11.0	0.00002	0	0.00018	3	0.00020	3	0.00202	30
11.2	0.00001	1	0.00015	2	0.00017	3	0.00172	27
11.4	0.00001	0	0.00013	2	0.00014	2	0.00145	22
11.6	0.00001	0	0.00011	2	0.00012	2	0.00123	19
11.8	0.00001	0	0.00009	2	0.00010	2	0.00104	16
12.0	0.00001	0	0.00007	1	0.00008	1	0.00088	13
12.2	0.00001	1	0.00006	1	0.00007	1	0.00075	12
12.4	0.00000	0	0.00005	1	0.00006	1	0.00063	9
12.6	0.00000	0	0.00004	0	0.00005	1	0.00054	9
12.8	0.00000	0	0.00004	0	0.00004	1	0.00045	7
13.0	0.00000	0	0.00003	1	0.00003	0	0.00038	6
13.2	0.00000	0	0.00002	0	0.00003	1	0.00032	5
13.4	0.00000	0	0.00002	0	0.00002	0	0.00027	4
13.6	0.00000	0	0.00002	1	0.00002	1	0.00023	4
13.8	0.00000	0	0.00001	0	0.00001	0	0.00019	3
14.0	0.00000	0	0.00001	0	0.00001	0	0.00016	2
14.2	0.00000	0	0.00001	0	0.00001	0	0.00014	2
14.4	0.00000	0	0.00001	0	0.00001	0	0.00012	2
14.6	0.00000	0	0.00001	0	0.00001	0	0.00010	2
14.8	0.00000	0	0.00001	0	0.00001	0	0.00008	1
15.0	0.00000	0	0.00001	1	0.00001	0	0.00007	1
15.2	0.00000	0	0.00000	0	0.00000	1	0.00006	1
15.4	0.00000	0	0.00000	0	0.00000	0	0.00005	1
15.6	0.00000	0	0.00000	0	0.00000	0	0.00004	1
15.8	0.00000		0.00000		0.00000		0.00003	
16.0	0.00000		0.00000		0.00000		0.00002	

Table II.
Harmonic Oscillator Contributions
to the Thermodynamic Functions
(in units of calories, moles, °K)

Table II Harmonic Oscillator Contributions to the Thermodynamic
 Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
	T=273.15			T=298.15			T=400.			
100	1.77430	3.28384	1.94185	1.90812	3.45423	1.94905	2.37854	4.02970	1.96588	100
110	1.63244	3.09920	1.93250	1.76264	3.26883	1.94116	2.22264	3.84254	1.96145	110
120	1.50662	2.93148	1.92231	1.63327	3.10029	1.93256	2.08302	3.67207	1.95660	120
130	1.39420	2.77804	1.91131	1.51737	2.94596	1.92326	1.95703	3.51567	1.95135	130
140	1.29312	2.63682	1.89951	1.41288	2.80380	1.91328	1.84262	3.37126	1.94570	140
150	1.20175	2.50620	1.88694	1.31818	2.67215	1.90263	1.73817	3.23722	1.93966	150
160	1.11880	2.38484	1.87361	1.23196	2.54972	1.89132	1.64235	3.11224	1.93322	160
170	1.04317	2.27167	1.85954	1.15314	2.43541	1.87937	1.55411	2.99525	1.92639	170
180	0.97400	2.16580	1.84476	1.08083	2.32834	1.86680	1.47254	2.88534	1.91918	180
190	0.91053	2.06647	1.82929	1.01430	2.22776	1.85362	1.39690	2.78178	1.91160	190
200	0.85213	1.97304	1.81315	0.95291	2.13303	1.83984	1.32657	2.68392	1.90364	200
210	0.79827	1.88498	1.79637	0.89612	2.04361	1.82549	1.26100	2.59125	1.89532	210
220	0.74849	1.80182	1.77896	0.84348	1.95903	1.81059	1.19973	2.50327	1.88664	220
230	0.70239	1.72313	1.76096	0.79458	1.87888	1.79514	1.14237	2.41961	1.87760	230
240	0.65962	1.64858	1.74240	0.74908	1.80282	1.77918	1.08856	2.33989	1.86822	240
250	0.61988	1.57783	1.72329	0.70668	1.73052	1.76272	1.03800	2.26383	1.85850	250
260	0.58290	1.51063	1.70367	0.66709	1.66171	1.74578	0.99041	2.19113	1.84845	260
270	0.54844	1.44670	1.68356	0.63009	1.59615	1.72838	0.94556	2.12156	1.83808	270
280	0.51630	1.38585	1.66299	0.59547	1.53362	1.71055	0.90323	2.05491	1.82738	280
290	0.48627	1.32786	1.64199	0.56302	1.47391	1.69230	0.86324	1.99097	1.81638	290
300	0.45820	1.27255	1.62058	0.53259	1.41685	1.67365	0.82540	1.92958	1.80507	300
310	0.43193	1.21977	1.59880	0.50402	1.36228	1.65462	0.78958	1.87059	1.79346	310
320	0.40733	1.16936	1.57667	0.47718	1.31005	1.63525	0.75562	1.81383	1.78157	320
330	0.38427	1.12118	1.55421	0.45193	1.26004	1.61554	0.72340	1.75920	1.76941	330
340	0.36263	1.07512	1.53147	0.42816	1.21210	1.59552	0.69280	1.70656	1.75697	340
350	0.34233	1.03106	1.50846	0.40578	1.16615	1.57521	0.66373	1.65581	1.74427	350
360	0.32325	0.98889	1.48521	0.38469	1.12206	1.55463	0.63608	1.60685	1.73131	360
370	0.30532	0.94852	1.46175	0.36479	1.07975	1.53381	0.60977	1.55960	1.71811	370
380	0.28846	0.90985	1.43810	0.34601	1.03912	1.51276	0.58471	1.51396	1.70467	380
390	0.27259	0.87280	1.41430	0.32829	1.00010	1.49151	0.56084	1.46985	1.69101	390
400	0.25766	0.83729	1.39036	0.31154	0.96261	1.47008	0.53808	1.42721	1.67713	400
410	0.24359	0.80326	1.36631	0.29571	0.92657	1.44848	0.51636	1.38597	1.66303	410
420	0.23034	0.77062	1.34218	0.28075	0.89193	1.42673	0.49564	1.34607	1.64874	420
430	0.21784	0.73932	1.31800	0.26659	0.85861	1.40487	0.47585	1.30744	1.63425	430
440	0.20607	0.70930	1.29377	0.25320	0.82657	1.38290	0.45694	1.27004	1.61957	440
450	0.19496	0.68050	1.26954	0.24051	0.79574	1.36085	0.43887	1.23381	1.60473	450
460	0.18447	0.65286	1.24531	0.22851	0.76607	1.33873	0.42160	1.19870	1.58971	460
470	0.17458	0.62634	1.22112	0.21713	0.73752	1.31657	0.40507	1.16468	1.57454	470
480	0.16524	0.60088	1.19697	0.20635	0.71003	1.29437	0.38926	1.13169	1.55922	480
490	0.15642	0.57645	1.17290	0.19613	0.68357	1.27217	0.37413	1.09970	1.54377	490
500	0.14808	0.55299	1.14892	0.18644	0.65809	1.24997	0.35964	1.06867	1.52818	500
510	0.14021	0.53048	1.12506	0.17726	0.63356	1.22780	0.34576	1.03856	1.51247	510
520	0.13277	0.50886	1.10132	0.16854	0.60993	1.20566	0.33246	1.00934	1.49664	520
530	0.12574	0.48811	1.07772	0.16027	0.58717	1.18358	0.31971	0.98099	1.48071	530
540	0.11909	0.46818	1.05429	0.15242	0.56526	1.16157	0.30750	0.95346	1.46468	540
550	0.11280	0.44905	1.03104	0.14497	0.54414	1.13964	0.29578	0.92673	1.44857	550
560	0.10685	0.43068	1.00797	0.13790	0.52380	1.11782	0.28454	0.90077	1.43238	560
570	0.10123	0.41304	0.98512	0.13119	0.50421	1.09610	0.27376	0.87556	1.41611	570
580	0.09591	0.39610	0.96248	0.12481	0.48534	1.07451	0.26342	0.85108	1.39979	580
590	0.09087	0.37984	0.94008	0.11875	0.46715	1.05306	0.25349	0.82729	1.38340	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	ν cm ⁻¹
	T=273.15			T=298.15			T=400.			
600	0.08611	0.36423	0.91791	0.11299	0.44963	1.03176	0.24396	0.80417	1.36698	600
610	0.08160	0.34924	0.89601	0.10752	0.43275	1.01061	0.23482	0.78172	1.35051	610
620	0.07733	0.33484	0.87437	0.10232	0.41649	0.98964	0.22603	0.75989	1.33401	620
630	0.07329	0.32102	0.85300	0.09738	0.40082	0.96885	0.21759	0.73868	1.31748	630
640	0.06946	0.30776	0.83191	0.09269	0.38572	0.94826	0.20948	0.71806	1.30094	640
650	0.06584	0.29502	0.81112	0.08822	0.37118	0.92786	0.20169	0.69802	1.28440	650
660	0.06240	0.28279	0.79062	0.08398	0.35717	0.90768	0.19420	0.67853	1.26785	660
670	0.05915	0.27105	0.77043	0.07994	0.34367	0.88771	0.18701	0.65959	1.25130	670
680	0.05607	0.25979	0.75055	0.07610	0.33066	0.86797	0.18009	0.64117	1.23477	680
690	0.05316	0.24897	0.73099	0.07245	0.31813	0.84846	0.17345	0.62327	1.21825	690
700	0.05040	0.23859	0.71175	0.06897	0.30606	0.82918	0.16705	0.60586	1.20177	700
710	0.04778	0.22863	0.69283	0.06567	0.29444	0.81016	0.16090	0.58893	1.18531	710
720	0.04530	0.21907	0.67424	0.06253	0.28324	0.79138	0.15499	0.57246	1.16889	720
730	0.04295	0.20990	0.65598	0.05954	0.27245	0.77286	0.14930	0.55645	1.15252	730
740	0.04072	0.20109	0.63806	0.05669	0.26206	0.75460	0.14383	0.54088	1.13619	740
750	0.03861	0.19265	0.62047	0.05398	0.25205	0.73661	0.13857	0.52574	1.11993	750
760	0.03661	0.18454	0.60322	0.05141	0.24241	0.71888	0.13351	0.51102	1.10372	760
770	0.03472	0.17677	0.58631	0.04896	0.23313	0.70142	0.12863	0.49669	1.08758	770
780	0.03292	0.16931	0.56973	0.04662	0.22419	0.68424	0.12394	0.48276	1.07151	780
790	0.03122	0.16216	0.55350	0.04440	0.21558	0.66734	0.11943	0.46921	1.05553	790
800	0.02961	0.15530	0.53760	0.04229	0.20729	0.65071	0.11509	0.45604	1.03962	800
810	0.02808	0.14871	0.52204	0.04027	0.19931	0.63437	0.11090	0.44322	1.02380	810
820	0.02663	0.14240	0.50682	0.03836	0.19162	0.61831	0.10688	0.43076	1.00807	820
830	0.02525	0.13635	0.49193	0.03653	0.18422	0.60253	0.10300	0.41863	0.99244	830
840	0.02395	0.13054	0.47738	0.03480	0.17710	0.58703	0.09927	0.40684	0.97691	840
850	0.02271	0.12498	0.46315	0.03315	0.17024	0.57182	0.09568	0.39537	0.96148	850
860	0.02154	0.11964	0.44926	0.03157	0.16364	0.55690	0.09222	0.38421	0.94616	860
870	0.02043	0.11453	0.43569	0.03007	0.15729	0.54225	0.08889	0.37336	0.93096	870
880	0.01938	0.10963	0.42244	0.02865	0.15117	0.52790	0.08568	0.36281	0.91587	880
890	0.01838	0.10493	0.40951	0.02729	0.14529	0.51382	0.08259	0.35254	0.90090	890
900	0.01743	0.10042	0.39690	0.02599	0.13963	0.50003	0.07961	0.34256	0.88605	900
910	0.01653	0.09610	0.38460	0.02476	0.13418	0.48651	0.07674	0.33285	0.87132	910
920	0.01568	0.09196	0.37261	0.02359	0.12893	0.47328	0.07398	0.32341	0.85673	920
930	0.01487	0.08800	0.36092	0.02247	0.12388	0.46032	0.07132	0.31422	0.84226	930
940	0.01411	0.08420	0.34954	0.02141	0.11903	0.44764	0.06875	0.30529	0.82793	940
950	0.01338	0.08056	0.33845	0.02039	0.11436	0.43523	0.06628	0.29661	0.81374	950
960	0.01269	0.07707	0.32765	0.01943	0.10986	0.42309	0.06390	0.28816	0.79969	960
970	0.01204	0.07373	0.31714	0.01851	0.10554	0.41122	0.06161	0.27994	0.78577	970
980	0.01142	0.07053	0.30691	0.01763	0.10138	0.39961	0.05940	0.27196	0.77200	980
990	0.01083	0.06747	0.29696	0.01680	0.09738	0.38827	0.05727	0.26419	0.75838	990
1000	0.01027	0.06453	0.28728	0.01600	0.09354	0.37719	0.05522	0.25663	0.74490	1000
1010	0.00975	0.06172	0.27787	0.01525	0.08984	0.36637	0.05324	0.24929	0.73156	1010
1020	0.00924	0.05903	0.26872	0.01452	0.08628	0.35579	0.05134	0.24214	0.71838	1020
1030	0.00877	0.05645	0.25983	0.01384	0.08286	0.34547	0.04950	0.23520	0.70535	1030
1040	0.00832	0.05398	0.25120	0.01318	0.07957	0.33540	0.04773	0.22845	0.69247	1040
1050	0.00789	0.05162	0.24281	0.01256	0.07641	0.32557	0.04602	0.22188	0.67975	1050
1060	0.00748	0.04935	0.23466	0.01197	0.07337	0.31598	0.04438	0.21550	0.66717	1060
1070	0.00710	0.04719	0.22675	0.01140	0.07045	0.30663	0.04280	0.20929	0.65476	1070
1080	0.00674	0.04511	0.21908	0.01086	0.06764	0.29751	0.04127	0.20326	0.64250	1080
1090	0.00639	0.04313	0.21163	0.01035	0.06493	0.28862	0.03979	0.19739	0.63039	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=273.15			T=298.15			T=400.				
1100	0.00606	0.04123	0.20440	0.00986	0.06234	0.27995	0.03838	0.19169	0.61845	1100
1110	0.00575	0.03941	0.19740	0.00940	0.05984	0.27151	0.03701	0.18615	0.60666	1110
1120	0.00545	0.03767	0.19060	0.00895	0.05744	0.26328	0.03569	0.18076	0.59502	1120
1130	0.00517	0.03601	0.18401	0.00853	0.05514	0.25527	0.03442	0.17552	0.58355	1130
1140	0.00491	0.03441	0.17762	0.00813	0.05293	0.24747	0.03319	0.17043	0.57223	1140
1150	0.00466	0.03289	0.17144	0.00774	0.05080	0.23987	0.03201	0.16548	0.56108	1150
1160	0.00442	0.03143	0.16544	0.00738	0.04875	0.23248	0.03087	0.16067	0.55007	1160
1170	0.00419	0.03004	0.15963	0.00703	0.04679	0.22528	0.02977	0.15599	0.53923	1170
1180	0.00397	0.02870	0.15401	0.00670	0.04490	0.21828	0.02871	0.15145	0.52855	1180
1190	0.00377	0.02743	0.14856	0.00638	0.04309	0.21147	0.02769	0.14703	0.51802	1190
1200	0.00358	0.02621	0.14329	0.00608	0.04135	0.20485	0.02670	0.14274	0.50765	1200
1210	0.00339	0.02504	0.13819	0.00579	0.03967	0.19840	0.02575	0.13857	0.49743	1210
1220	0.00322	0.02392	0.13325	0.00552	0.03807	0.19214	0.02484	0.13452	0.48737	1220
1230	0.00305	0.02285	0.12847	0.00526	0.03652	0.18605	0.02396	0.13058	0.47747	1230
1240	0.00290	0.02183	0.12385	0.00501	0.03504	0.18014	0.02310	0.12675	0.46772	1240
1250	0.00275	0.02085	0.11938	0.00478	0.03362	0.17439	0.02228	0.12304	0.45812	1250
1260	0.00261	0.01992	0.11506	0.00455	0.03225	0.16881	0.02149	0.11942	0.44868	1260
1270	0.00247	0.01903	0.11088	0.00434	0.03094	0.16338	0.02073	0.11591	0.43938	1270
1280	0.00235	0.01817	0.10684	0.00413	0.02968	0.15811	0.01999	0.11250	0.43024	1280
1290	0.00223	0.01736	0.10293	0.00394	0.02846	0.15300	0.01928	0.10919	0.42125	1290
1300	0.00211	0.01658	0.09916	0.00375	0.02730	0.14803	0.01860	0.10597	0.41241	1300
1310	0.00200	0.01583	0.09552	0.00357	0.02619	0.14321	0.01794	0.10284	0.40371	1310
1320	0.00190	0.01512	0.09199	0.00341	0.02512	0.13853	0.01730	0.09981	0.39517	1320
1330	0.00180	0.01444	0.08859	0.00324	0.02409	0.13399	0.01669	0.09686	0.38676	1330
1340	0.00171	0.01379	0.08531	0.00309	0.02310	0.12958	0.01610	0.09399	0.37850	1340
1350	0.00162	0.01316	0.08213	0.00295	0.02215	0.12531	0.01552	0.09121	0.37039	1350
1360	0.00154	0.01257	0.07907	0.00281	0.02124	0.12117	0.01497	0.08850	0.36241	1360
1370	0.00146	0.01200	0.07612	0.00267	0.02037	0.11715	0.01444	0.08588	0.35458	1370
1380	0.00139	0.01146	0.07326	0.00255	0.01953	0.11325	0.01393	0.08332	0.34689	1380
1390	0.00131	0.01094	0.07051	0.00243	0.01873	0.10947	0.01344	0.08085	0.33933	1390
1400	0.00125	0.01044	0.06785	0.00231	0.01796	0.10581	0.01296	0.07844	0.33191	1400
1410	0.00118	0.00997	0.06529	0.00220	0.01722	0.10226	0.01250	0.07611	0.32462	1410
1420	0.00112	0.00952	0.06282	0.00210	0.01651	0.09882	0.01206	0.07384	0.31747	1420
1430	0.00106	0.00908	0.06043	0.00200	0.01582	0.09548	0.01163	0.07163	0.31045	1430
1440	0.00101	0.00867	0.05813	0.00191	0.01517	0.09225	0.01122	0.06949	0.30356	1440
1450	0.00096	0.00828	0.05592	0.00182	0.01454	0.08912	0.01082	0.06742	0.29679	1450
1460	0.00091	0.00790	0.05378	0.00173	0.01394	0.08609	0.01044	0.06540	0.29016	1460
1470	0.00086	0.00754	0.05172	0.00165	0.01336	0.08316	0.01007	0.06344	0.28365	1470
1480	0.00082	0.00719	0.04973	0.00157	0.01281	0.08031	0.00971	0.06154	0.27726	1480
1490	0.00078	0.00687	0.04782	0.00150	0.01228	0.07756	0.00937	0.05969	0.27100	1490
1500	0.00074	0.00655	0.04597	0.00143	0.01177	0.07490	0.00904	0.05790	0.26486	1500
1510	0.00070	0.00625	0.04420	0.00136	0.01128	0.07232	0.00872	0.05616	0.25883	1510
1520	0.00066	0.00597	0.04248	0.00130	0.01081	0.06982	0.00841	0.05447	0.25293	1520
1530	0.00063	0.00569	0.04084	0.00124	0.01036	0.06741	0.00811	0.05283	0.24714	1530
1540	0.00060	0.00543	0.03925	0.00118	0.00993	0.06507	0.00782	0.05124	0.24147	1540
1550	0.00057	0.00518	0.03772	0.00112	0.00951	0.06281	0.00755	0.04970	0.23590	1550
1560	0.00054	0.00495	0.03624	0.00107	0.00912	0.06062	0.00728	0.04820	0.23045	1560
1570	0.00051	0.00472	0.03483	0.00102	0.00874	0.05851	0.00702	0.04674	0.22511	1570
1580	0.00048	0.00450	0.03346	0.00097	0.00837	0.05646	0.00677	0.04533	0.21988	1580
1590	0.00046	0.00430	0.03215	0.00092	0.00802	0.05448	0.00653	0.04396	0.21475	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
T=273.15			T=298.15			T=400.				
1600	0.00043	0.00410	0.03088	0.00088	0.00769	0.05257	0.00630	0.04263	0.20973	1600
1610	0.00041	0.00391	0.02966	0.00084	0.00736	0.05072	0.00608	0.04134	0.20481	1610
1620	0.00039	0.00373	0.02849	0.00080	0.00706	0.04893	0.00586	0.04008	0.19999	1620
1630	0.00037	0.00356	0.02736	0.00076	0.00676	0.04720	0.00566	0.03887	0.19528	1630
1640	0.00035	0.00339	0.02628	0.00073	0.00648	0.04553	0.00546	0.03769	0.19066	1640
1650	0.00033	0.00324	0.02523	0.00069	0.00620	0.04391	0.00526	0.03654	0.18613	1650
1660	0.00032	0.00309	0.02423	0.00066	0.00594	0.04235	0.00508	0.03543	0.18171	1660
1670	0.00030	0.00294	0.02326	0.00063	0.00569	0.04084	0.00490	0.03435	0.17737	1670
1680	0.00029	0.00281	0.02233	0.00060	0.00546	0.03938	0.00472	0.03331	0.17313	1680
1690	0.00027	0.00268	0.02144	0.00057	0.00523	0.03797	0.00456	0.03229	0.16898	1690
1700	0.00026	0.00255	0.02058	0.00054	0.00501	0.03661	0.00440	0.03131	0.16492	1700
1710	0.00024	0.00244	0.01976	0.00052	0.00479	0.03530	0.00424	0.03035	0.16094	1710
1720	0.00023	0.00232	0.01896	0.00049	0.00459	0.03403	0.00409	0.02942	0.15705	1720
1730	0.00022	0.00222	0.01820	0.00047	0.00440	0.03280	0.00395	0.02852	0.15325	1730
1740	0.00021	0.00211	0.01746	0.00045	0.00421	0.03162	0.00381	0.02765	0.14953	1740
1750	0.00020	0.00202	0.01676	0.00043	0.00404	0.03048	0.00367	0.02681	0.14589	1750
1760	0.00019	0.00192	0.01608	0.00041	0.00386	0.02937	0.00354	0.02598	0.14233	1760
1770	0.00018	0.00183	0.01543	0.00039	0.00370	0.02831	0.00342	0.02519	0.13885	1770
1780	0.00017	0.00175	0.01480	0.00037	0.00354	0.02728	0.00330	0.02441	0.13544	1780
1790	0.00016	0.00167	0.01420	0.00035	0.00339	0.02629	0.00318	0.02367	0.13211	1790
1800	0.00015	0.00159	0.01362	0.00034	0.00325	0.02533	0.00307	0.02294	0.12886	1800
1810	0.00014	0.00151	0.01307	0.00032	0.00311	0.02440	0.00296	0.02223	0.12568	1810
1820	0.00014	0.00144	0.01254	0.00030	0.00298	0.02351	0.00285	0.02155	0.12257	1820
1830	0.00013	0.00138	0.01202	0.00029	0.00285	0.02265	0.00275	0.02089	0.11953	1830
1840	0.00012	0.00131	0.01153	0.00028	0.00273	0.02182	0.00266	0.02024	0.11656	1840
1850	0.00012	0.00125	0.01106	0.00026	0.00262	0.02102	0.00256	0.01962	0.11365	1850
1860	0.00011	0.00119	0.01061	0.00025	0.00251	0.02024	0.00247	0.01901	0.11082	1860
1870	0.00010	0.00114	0.01017	0.00024	0.00240	0.01950	0.00238	0.01843	0.10805	1870
1880	0.00010	0.00108	0.00975	0.00023	0.00230	0.01878	0.00230	0.01786	0.10534	1880
1890	0.00009	0.00103	0.00935	0.00022	0.00220	0.01809	0.00222	0.01731	0.10269	1890
1900	0.00009	0.00099	0.00896	0.00021	0.00211	0.01742	0.00214	0.01677	0.10011	1900
1910	0.00008	0.00094	0.00859	0.00020	0.00202	0.01677	0.00206	0.01625	0.09758	1910
1920	0.00008	0.00090	0.00824	0.00019	0.00193	0.01615	0.00199	0.01575	0.09511	1920
1930	0.00008	0.00085	0.00790	0.00018	0.00185	0.01555	0.00192	0.01526	0.09271	1930
1940	0.00007	0.00081	0.00757	0.00017	0.00177	0.01497	0.00185	0.01479	0.09035	1940
1950	0.00007	0.00078	0.00726	0.00016	0.00169	0.01441	0.00179	0.01433	0.08806	1950
1960	0.00007	0.00074	0.00695	0.00016	0.00162	0.01387	0.00172	0.01389	0.08581	1960
1970	0.00006	0.00070	0.00666	0.00015	0.00155	0.01335	0.00166	0.01345	0.08362	1970
1980	0.00006	0.00067	0.00639	0.00014	0.00149	0.01286	0.00160	0.01304	0.08148	1980
1990	0.00006	0.00064	0.00612	0.00013	0.00142	0.01237	0.00155	0.01263	0.07940	1990
2000	0.00005	0.00061	0.00587	0.00013	0.00136	0.01191	0.00149	0.01224	0.07736	2000
2010	0.00005	0.00058	0.00562	0.00012	0.00130	0.01146	0.00144	0.01186	0.07537	2010
2020	0.00005	0.00055	0.00538	0.00012	0.00125	0.01103	0.00139	0.01149	0.07343	2020
2030	0.00005	0.00053	0.00516	0.00011	0.00119	0.01062	0.00134	0.01113	0.07153	2030
2040	0.00004	0.00050	0.00494	0.00011	0.00114	0.01022	0.00129	0.01078	0.06969	2040
2050	0.00004	0.00048	0.00474	0.00010	0.00109	0.00983	0.00125	0.01045	0.06788	2050
2060	0.00004	0.00046	0.00454	0.00010	0.00105	0.00946	0.00120	0.01012	0.06612	2060
2070	0.00004	0.00044	0.00435	0.00009	0.00100	0.00910	0.00116	0.00981	0.06440	2070
2080	0.00003	0.00041	0.00416	0.00009	0.00096	0.00876	0.00112	0.00950	0.06273	2080
2090	0.00003	0.00040	0.00399	0.00008	0.00092	0.00842	0.00108	0.00920	0.06109	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	ν cm ⁻¹	
T=273.15			T=298.15			T=400.					
2100	0.00003	0.00038	0.00382	0.00008	0.00088	0.00810	0.00104	0.00891	0.05949	2100	
2110	0.00003	0.00036	0.00366	0.00008	0.00084	0.00780	0.00101	0.00864	0.05794	2110	
2120	0.00003	0.00034	0.00350	0.00007	0.00080	0.00750	0.00097	0.00836	0.05642	2120	
2130	0.00003	0.00033	0.00335	0.00007	0.00077	0.00721	0.00094	0.00810	0.05494	2130	
2140	0.00003	0.00031	0.00321	0.00007	0.00074	0.00694	0.00090	0.00785	0.05350	2140	
2150	0.00002	0.00030	0.00308	0.00006	0.00071	0.00667	0.00087	0.00760	0.05209	2150	
2160	0.00002	0.00028	0.00295	0.00006	0.00067	0.00642	0.00084	0.00736	0.05071	2160	
2170	0.00002	0.00027	0.00282	0.00006	0.00065	0.00617	0.00081	0.00713	0.04938	2170	
2180	0.00002	0.00026	0.00270	0.00005	0.00062	0.00594	0.00078	0.00691	0.04807	2180	
2190	0.00002	0.00024	0.00258	0.00005	0.00059	0.00571	0.00075	0.00669	0.04680	2190	
2200	0.00002	0.00023	0.00247	0.00005	0.00057	0.00549	0.00073	0.00648	0.04555	2200	
2210	0.00002	0.00022	0.00237	0.00005	0.00054	0.00528	0.00070	0.00628	0.04434	2210	
2220	0.00002	0.00021	0.00227	0.00004	0.00052	0.00507	0.00068	0.00608	0.04316	2220	
2230	0.00002	0.00020	0.00217	0.00004	0.00050	0.00488	0.00065	0.00589	0.04201	2230	
2240	0.00001	0.00019	0.00208	0.00004	0.00047	0.00469	0.00063	0.00570	0.04089	2240	
2250	0.00001	0.00018	0.00199	0.00004	0.00045	0.00451	0.00061	0.00552	0.03980	2250	
2260	0.00001	0.00017	0.00190	0.00004	0.00043	0.00434	0.00059	0.00535	0.03874	2260	
2270	0.00001	0.00017	0.00182	0.00003	0.00042	0.00417	0.00057	0.00518	0.03770	2270	
2280	0.00001	0.00016	0.00174	0.00003	0.00040	0.00401	0.00055	0.00502	0.03669	2280	
2290	0.00001	0.00015	0.00167	0.00003	0.00038	0.00385	0.00053	0.00486	0.03570	2290	
2300	0.00001	0.00014	0.00160	0.00003	0.00036	0.00370	0.00051	0.00471	0.03474	2300	
2310	0.00001	0.00014	0.00153	0.00003	0.00035	0.00356	0.00049	0.00456	0.03380	2310	
2320	0.00001	0.00013	0.00146	0.00003	0.00033	0.00342	0.00047	0.00441	0.03289	2320	
2330	0.00001	0.00012	0.00140	0.00003	0.00032	0.00329	0.00046	0.00427	0.03200	2330	
2340	0.00001	0.00012	0.00134	0.00002	0.00030	0.00316	0.00044	0.00414	0.03114	2340	
2350	0.00001	0.00011	0.00128	0.00002	0.00029	0.00304	0.00042	0.00401	0.03029	2350	
2360	0.00001	0.00011	0.00123	0.00002	0.00028	0.00292	0.00041	0.00388	0.02947	2360	
2370	0.00001	0.00010	0.00117	0.00002	0.00027	0.00280	0.00039	0.00376	0.02867	2370	
2380	0.00001	0.00010	0.00112	0.00002	0.00026	0.00269	0.00038	0.00364	0.02789	2380	
2390	0.00001	0.00009	0.00107	0.00002	0.00024	0.00259	0.00037	0.00352	0.02713	2390	
2400	0.00001	0.00009	0.00103	0.00002	0.00023	0.00249	0.00035	0.00341	0.02639	2400	
2410	0.00001	0.00008	0.00098	0.00002	0.00022	0.00239	0.00034	0.00330	0.02567	2410	
2420	0.00001	0.00008	0.00094	0.00002	0.00021	0.00230	0.00033	0.00320	0.02497	2420	
2430	0.00001	0.00008	0.00090	0.00002	0.00020	0.00221	0.00032	0.00310	0.02429	2430	
2440	0.00001	0.00007	0.00086	0.00002	0.00020	0.00212	0.00031	0.00300	0.02362	2440	
2450	0.00000	0.00007	0.00082	0.00001	0.00019	0.00204	0.00030	0.00290	0.02298	2450	
2460	0.00000	0.00007	0.00079	0.00001	0.00018	0.00196	0.00029	0.00281	0.02235	2460	
2470	0.00000	0.00006	0.00075	0.00001	0.00017	0.00188	0.00028	0.00272	0.02173	2470	
2480	0.00000	0.00006	0.00072	0.00001	0.00016	0.00181	0.00027	0.00263	0.02113	2480	
2490	0.00000	0.00006	0.00069	0.00001	0.00016	0.00173	0.00026	0.00255	0.02055	2490	
2500	0.00000	0.00005	0.00066	0.00001	0.00015	0.00167	0.00025	0.00247	0.01999	2500	
2510	0.00000	0.00005	0.00063	0.00001	0.00014	0.00160	0.00024	0.00239	0.01943	2510	
2520	0.00000	0.00005	0.00060	0.00001	0.00014	0.00154	0.00023	0.00231	0.01890	2520	
2530	0.00000	0.00005	0.00058	0.00001	0.00013	0.00148	0.00022	0.00224	0.01837	2530	
2540	0.00000	0.00004	0.00055	0.00001	0.00013	0.00142	0.00021	0.00217	0.01786	2540	
2550	0.00000	0.00004	0.00053	0.00001	0.00012	0.00136	0.00021	0.00210	0.01737	2550	
2560	0.00000	0.00004	0.00050	0.00001	0.00011	0.00131	0.00020	0.00203	0.01689	2560	
2570	0.00000	0.00004	0.00048	0.00001	0.00011	0.00126	0.00019	0.00197	0.01642	2570	
2580	0.00000	0.00004	0.00046	0.00001	0.00010	0.00121	0.00019	0.00191	0.01596	2580	
2590	0.00000	0.00003	0.00044	0.00001	0.00010	0.00116	0.00018	0.00184	0.01552	2590	

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
T=273.15			T=298.15			T=400.				
2600	0.00000	0.00003	0.00042	0.00001	0.00010	0.00111	0.00017	0.00179	0.01508	2600
2610	0.00000	0.00003	0.00040	0.00001	0.00009	0.00107	0.00017	0.00173	0.01466	2610
2620	0.00000	0.00003	0.00038	0.00001	0.00009	0.00103	0.00016	0.00167	0.01425	2620
2630	0.00000	0.00003	0.00037	0.00001	0.00008	0.00098	0.00015	0.00162	0.01386	2630
2640	0.00000	0.00003	0.00035	0.00001	0.00008	0.00095	0.00015	0.00157	0.01347	2640
2650	0.00000	0.00003	0.00034	0.00001	0.00008	0.00091	0.00014	0.00152	0.01309	2650
2660	0.00000	0.00002	0.00032	0.00001	0.00007	0.00087	0.00014	0.00147	0.01272	2660
2670	0.00000	0.00002	0.00031	0.00001	0.00007	0.00084	0.00013	0.00142	0.01237	2670
2680	0.00000	0.00002	0.00029	0.00000	0.00007	0.00080	0.00013	0.00138	0.01202	2680
2690	0.00000	0.00002	0.00028	0.00000	0.00006	0.00077	0.00012	0.00133	0.01168	2690
2700	0.00000	0.00002	0.00027	0.00000	0.00006	0.00074	0.00012	0.00129	0.01135	2700
2710	0.00000	0.00002	0.00026	0.00000	0.00006	0.00071	0.00012	0.00125	0.01103	2710
2720	0.00000	0.00002	0.00024	0.00000	0.00006	0.00068	0.00011	0.00121	0.01072	2720
2730	0.00000	0.00002	0.00023	0.00000	0.00005	0.00065	0.00011	0.00117	0.01042	2730
2740	0.00000	0.00002	0.00022	0.00000	0.00005	0.00063	0.00010	0.00113	0.01012	2740
2750	0.00000	0.00002	0.00021	0.00000	0.00005	0.00060	0.00010	0.00110	0.00984	2750
2760	0.00000	0.00002	0.00020	0.00000	0.00005	0.00058	0.00010	0.00106	0.00956	2760
2770	0.00000	0.00001	0.00019	0.00000	0.00004	0.00056	0.00009	0.00103	0.00929	2770
2780	0.00000	0.00001	0.00019	0.00000	0.00004	0.00053	0.00009	0.00099	0.00903	2780
2790	0.00000	0.00001	0.00018	0.00000	0.00004	0.00051	0.00009	0.00096	0.00877	2790
2800	0.00000	0.00001	0.00017	0.00000	0.00004	0.00049	0.00008	0.00093	0.00852	2800
2810	0.00000	0.00001	0.00016	0.00000	0.00004	0.00047	0.00008	0.00090	0.00828	2810
2820	0.00000	0.00001	0.00016	0.00000	0.00004	0.00045	0.00008	0.00087	0.00804	2820
2830	0.00000	0.00001	0.00015	0.00000	0.00003	0.00043	0.00008	0.00084	0.00781	2830
2840	0.00000	0.00001	0.00014	0.00000	0.00003	0.00042	0.00007	0.00082	0.00759	2840
2850	0.00000	0.00001	0.00014	0.00000	0.00003	0.00040	0.00007	0.00079	0.00737	2850
2860	0.00000	0.00001	0.00013	0.00000	0.00003	0.00038	0.00007	0.00076	0.00716	2860
2870	0.00000	0.00001	0.00012	0.00000	0.00003	0.00037	0.00007	0.00074	0.00696	2870
2880	0.00000	0.00001	0.00012	0.00000	0.00003	0.00035	0.00006	0.00072	0.00676	2880
2890	0.00000	0.00001	0.00011	0.00000	0.00003	0.00034	0.00006	0.00069	0.00657	2890
2900	0.00000	0.00001	0.00011	0.00000	0.00002	0.00033	0.00006	0.00067	0.00638	2900
2910	0.00000	0.00001	0.00010	0.00000	0.00002	0.00031	0.00006	0.00065	0.00620	2910
2920	0.00000	0.00001	0.00010	0.00000	0.00002	0.00030	0.00005	0.00063	0.00602	2920
2930	0.00000	0.00001	0.00009	0.00000	0.00002	0.00029	0.00005	0.00061	0.00584	2930
2940	0.00000	0.00001	0.00009	0.00000	0.00002	0.00028	0.00005	0.00059	0.00568	2940
2950	0.00000	0.00001	0.00009	0.00000	0.00002	0.00026	0.00005	0.00057	0.00551	2950
2960	0.00000	0.00001	0.00008	0.00000	0.00002	0.00025	0.00005	0.00055	0.00535	2960
2970	0.00000	0.00001	0.00008	0.00000	0.00002	0.00024	0.00005	0.00053	0.00520	2970
2980	0.00000	0.00001	0.00007	0.00000	0.00002	0.00023	0.00004	0.00052	0.00505	2980
2990	0.00000	0.00000	0.00007	0.00000	0.00002	0.00022	0.00004	0.00050	0.00490	2990
3000	0.00000	0.00000	0.00007	0.00000	0.00002	0.00021	0.00004	0.00048	0.00476	3000
3010	0.00000	0.00000	0.00006	0.00000	0.00002	0.00021	0.00004	0.00047	0.00463	3010
3020	0.00000	0.00000	0.00006	0.00000	0.00001	0.00020	0.00004	0.00045	0.00449	3020
3030	0.00000	0.00000	0.00006	0.00000	0.00001	0.00019	0.00004	0.00044	0.00436	3030
3040	0.00000	0.00000	0.00006	0.00000	0.00001	0.00018	0.00004	0.00042	0.00424	3040
3050	0.00000	0.00000	0.00005	0.00000	0.00001	0.00017	0.00003	0.00041	0.00411	3050
3060	0.00000	0.00000	0.00005	0.00000	0.00001	0.00017	0.00003	0.00040	0.00399	3060
3070	0.00000	0.00000	0.00005	0.00000	0.00001	0.00016	0.00003	0.00038	0.00388	3070
3080	0.00000	0.00000	0.00005	0.00000	0.00001	0.00015	0.00003	0.00037	0.00377	3080
3090	0.00000	0.00000	0.00004	0.00000	0.00001	0.00015	0.00003	0.00036	0.00366	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic
 Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ - E_0^\circ)/T$	S [°]	C _p [°]	$-(F^\circ - E_0^\circ)/T$	S [°]	C _p [°]	$-(F^\circ - E_0^\circ)/T$	S [°]	C _p [°]	ν cm ⁻¹
T=273.15			T=298.15			T=400.				
3100	0.00000	0.00000	0.00004	0.00000	0.00001	0.00014	0.00003	0.00035	0.00355	3100
3110	0.00000	0.00000	0.00004	0.00000	0.00001	0.00014	0.00003	0.00034	0.00345	3110
3120	0.00000	0.00000	0.00004	0.00000	0.00001	0.00013	0.00003	0.00032	0.00335	3120
3130	0.00000	0.00000	0.00004	0.00000	0.00001	0.00012	0.00003	0.00031	0.00325	3130
3140	0.00000	0.00000	0.00004	0.00000	0.00001	0.00012	0.00002	0.00030	0.00315	3140
3150	0.00000	0.00000	0.00003	0.00000	0.00001	0.00011	0.00002	0.00029	0.00306	3150
3160	0.00000	0.00000	0.00003	0.00000	0.00001	0.00011	0.00002	0.00028	0.00297	3160
3170	0.00000	0.00000	0.00003	0.00000	0.00001	0.00011	0.00002	0.00028	0.00289	3170
3180	0.00000	0.00000	0.00003	0.00000	0.00001	0.00010	0.00002	0.00027	0.00280	3180
3190	0.00000	0.00000	0.00003	0.00000	0.00001	0.00010	0.00002	0.00026	0.00272	3190
3200	0.00000	0.00000	0.00003	0.00000	0.00001	0.00009	0.00002	0.00025	0.00264	3200
3210	0.00000	0.00000	0.00003	0.00000	0.00001	0.00009	0.00002	0.00024	0.00256	3210
3220	0.00000	0.00000	0.00002	0.00000	0.00001	0.00009	0.00002	0.00023	0.00249	3220
3230	0.00000	0.00000	0.00002	0.00000	0.00001	0.00008	0.00002	0.00023	0.00241	3230
3240	0.00000	0.00000	0.00002	0.00000	0.00001	0.00008	0.00002	0.00022	0.00234	3240
3250	0.00000	0.00000	0.00002	0.00000	0.00001	0.00008	0.00002	0.00021	0.00227	3250
3260	0.00000	0.00000	0.00002	0.00000	0.00000	0.00007	0.00002	0.00020	0.00221	3260
3270	0.00000	0.00000	0.00002	0.00000	0.00000	0.00007	0.00002	0.00020	0.00214	3270
3280	0.00000	0.00000	0.00002	0.00000	0.00000	0.00007	0.00002	0.00019	0.00208	3280
3290	0.00000	0.00000	0.00002	0.00000	0.00000	0.00006	0.00001	0.00019	0.00202	3290
3300	0.00000	0.00000	0.00002	0.00000	0.00000	0.00006	0.00001	0.00018	0.00196	3300
3310	0.00000	0.00000	0.00002	0.00000	0.00000	0.00006	0.00001	0.00017	0.00190	3310
3320	0.00000	0.00000	0.00002	0.00000	0.00000	0.00006	0.00001	0.00017	0.00185	3320
3330	0.00000	0.00000	0.00001	0.00000	0.00000	0.00005	0.00001	0.00016	0.00179	3330
3340	0.00000	0.00000	0.00001	0.00000	0.00000	0.00005	0.00001	0.00016	0.00174	3340
3350	0.00000	0.00000	0.00001	0.00000	0.00000	0.00005	0.00001	0.00015	0.00169	3350
3360	0.00000	0.00000	0.00001	0.00000	0.00000	0.00005	0.00001	0.00015	0.00164	3360
3370	0.00000	0.00000	0.00001	0.00000	0.00000	0.00005	0.00001	0.00014	0.00159	3370
3380	0.00000	0.00000	0.00001	0.00000	0.00000	0.00004	0.00001	0.00014	0.00154	3380
3390	0.00000	0.00000	0.00001	0.00000	0.00000	0.00004	0.00001	0.00013	0.00150	3390
3400	0.00000	0.00000	0.00001	0.00000	0.00000	0.00004	0.00001	0.00013	0.00145	3400
3410	0.00000	0.00000	0.00001	0.00000	0.00000	0.00004	0.00001	0.00012	0.00141	3410
3420	0.00000	0.00000	0.00001	0.00000	0.00000	0.00004	0.00001	0.00012	0.00137	3420
3430	0.00000	0.00000	0.00001	0.00000	0.00000	0.00004	0.00001	0.00012	0.00133	3430
3440	0.00000	0.00000	0.00001	0.00000	0.00000	0.00003	0.00001	0.00011	0.00129	3440
3450	0.00000	0.00000	0.00001	0.00000	0.00000	0.00003	0.00001	0.00011	0.00125	3450
3460	0.00000	0.00000	0.00001	0.00000	0.00000	0.00003	0.00001	0.00011	0.00121	3460
3470	0.00000	0.00000	0.00001	0.00000	0.00000	0.00003	0.00001	0.00010	0.00118	3470
3480	0.00000	0.00000	0.00001	0.00000	0.00000	0.00003	0.00001	0.00010	0.00114	3480
3490	0.00000	0.00000	0.00001	0.00000	0.00000	0.00003	0.00001	0.00010	0.00111	3490
3500	0.00000	0.00000	0.00001	0.00000	0.00000	0.00003	0.00001	0.00009	0.00107	3500
3510	0.00000	0.00000	0.00001	0.00000	0.00000	0.00003	0.00001	0.00009	0.00104	3510
3520	0.00000	0.00000	0.00001	0.00000	0.00000	0.00002	0.00001	0.00009	0.00101	3520
3530	0.00000	0.00000	0.00001	0.00000	0.00000	0.00002	0.00001	0.00008	0.00098	3530
3540	0.00000	0.00000	0.00001	0.00000	0.00000	0.00002	0.00001	0.00008	0.00095	3540
3550	0.00000	0.00000	0.00001	0.00000	0.00000	0.00002	0.00001	0.00008	0.00092	3550
3560	0.00000	0.00000	0.00001	0.00000	0.00000	0.00002	0.00001	0.00008	0.00089	3560
3570	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00001	0.00007	0.00087	3570
3580	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00001	0.00007	0.00084	3580
3590	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00000	0.00007	0.00082	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic
 Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=273.15			T=298.15			T=400.			ν cm ⁻¹
	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	
3600	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00000	0.00007	0.00079	3600
3610	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00000	0.00006	0.00077	3610
3620	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00000	0.00006	0.00075	3620
3630	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00000	0.00006	0.00072	3630
3640	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00006	0.00070	3640
3650	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00006	0.00068	3650
3660	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00005	0.00066	3660
3670	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00005	0.00064	3670
3680	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00005	0.00062	3680
3690	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00005	0.00060	3690
3700	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00005	0.00058	3700
3710	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00005	0.00057	3710
3720	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00004	0.00055	3720
3730	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00004	0.00053	3730
3740	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00004	0.00052	3740
3750	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00004	0.00050	3750
3760	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00004	0.00049	3760
3770	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00004	0.00047	3770
3780	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00004	0.00046	3780
3790	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00044	3790
3800	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00043	3800
3810	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00042	3810
3820	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00040	3820
3830	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00039	3830
3840	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00038	3840
3850	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00037	3850
3860	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00036	3860
3870	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00035	3870
3880	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00003	0.00034	3880
3890	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00003	0.00033	3890
3900	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00032	3900
3910	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00031	3910
3920	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00030	3920
3930	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00029	3930
3940	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00028	3940
3950	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00027	3950
3960	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00026	3960
3970	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00025	3970
3980	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00025	3980
3990	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00024	3990
4000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00023	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
T= 500.			T= 600.			T= 700.				
100	2.75434	4.46929	1.97351	3.07108	4.82950	1.97767	3.34463	5.13457	1.98019	100
110	2.59209	4.28132	1.97066	2.90451	4.64110	1.97569	3.17492	4.94590	1.97873	110
120	2.44621	4.10999	1.96754	2.75434	4.46929	1.97351	3.02163	4.77380	1.97713	120
130	2.31403	3.95263	1.96416	2.61792	4.31141	1.97115	2.88212	4.61561	1.97539	130
140	2.19351	3.80720	1.96051	2.49319	4.16543	1.96861	2.75434	4.46929	1.97351	140
150	2.08302	3.67207	1.95660	2.37854	4.02970	1.96588	2.63665	4.33320	1.97150	150
160	1.98124	3.54593	1.95243	2.27265	3.90292	1.96297	2.52774	4.20603	1.96936	160
170	1.88711	3.42769	1.94801	2.17443	3.78400	1.95988	2.42654	4.08670	1.96707	170
180	1.79972	3.31648	1.94333	2.08302	3.67207	1.95660	2.33215	3.97434	1.96466	180
190	1.71835	3.21154	1.93840	1.99765	3.56638	1.95315	2.24384	3.86818	1.96211	190
200	1.64235	3.11224	1.93322	1.91769	3.46628	1.94951	2.16098	3.76761	1.95942	200
210	1.57119	3.01805	1.92779	1.84262	3.37126	1.94570	2.08302	3.67207	1.95660	210
220	1.50441	2.92850	1.92211	1.77197	3.28084	1.94172	2.00950	3.58112	1.95365	220
230	1.44161	2.84319	1.91619	1.70533	3.19461	1.93755	1.94002	3.49434	1.95057	230
240	1.38243	2.76177	1.91003	1.64235	3.11224	1.93322	1.87423	3.41139	1.94736	240
250	1.32657	2.68392	1.90364	1.58274	3.03342	1.92871	1.81182	3.33197	1.94402	250
260	1.27375	2.60939	1.89701	1.52621	2.95786	1.92403	1.75253	3.25579	1.94054	260
270	1.22375	2.53792	1.89015	1.47254	2.88534	1.91918	1.69611	3.18262	1.93694	270
280	1.17634	2.46931	1.88307	1.42149	2.81563	1.91417	1.64235	3.11224	1.93322	280
290	1.13134	2.40336	1.87576	1.37290	2.74855	1.90899	1.59106	3.04447	1.92936	290
300	1.08856	2.33989	1.86822	1.32657	2.68392	1.90364	1.54206	2.97913	1.92538	300
310	1.04786	2.27876	1.86048	1.28236	2.62159	1.89813	1.49521	2.91606	1.92128	310
320	1.00910	2.21982	1.85251	1.24012	2.56142	1.89246	1.45035	2.85513	1.91705	320
330	0.97215	2.16294	1.84434	1.19973	2.50327	1.88664	1.40737	2.79621	1.91270	330
340	0.93690	2.10800	1.83596	1.16108	2.44704	1.88065	1.36614	2.73917	1.90823	340
350	0.90323	2.05491	1.82738	1.12406	2.39261	1.87452	1.32657	2.68392	1.90364	350
360	0.87106	2.00355	1.81860	1.08856	2.33989	1.86822	1.28855	2.63036	1.89893	360
370	0.84029	1.95384	1.80963	1.05451	2.28879	1.86178	1.25199	2.57840	1.89410	370
380	0.81084	1.90571	1.80046	1.02182	2.23923	1.85519	1.21682	2.52795	1.88915	380
390	0.78264	1.85906	1.79111	0.99041	2.19113	1.84845	1.18296	2.47895	1.88409	390
400	0.75562	1.81383	1.78157	0.96022	2.14442	1.84157	1.15034	2.43131	1.87892	400
410	0.72971	1.76996	1.77186	0.93118	2.09903	1.83455	1.11889	2.38498	1.87363	410
420	0.70485	1.72738	1.76197	0.90323	2.05491	1.82738	1.08856	2.33989	1.86822	420
430	0.68100	1.68604	1.75192	0.87632	2.01199	1.82008	1.05929	2.29600	1.86271	430
440	0.65809	1.64588	1.74169	0.85039	1.97024	1.81264	1.03102	2.25324	1.85709	440
450	0.63608	1.60685	1.73131	0.82540	1.92958	1.80507	1.00372	2.21157	1.85136	450
460	0.61493	1.56892	1.72077	0.80130	1.89000	1.79736	0.97733	2.17094	1.84552	460
470	0.59459	1.53202	1.71008	0.77805	1.85142	1.78953	0.95181	2.13132	1.83958	470
480	0.57503	1.49613	1.69923	0.75562	1.81383	1.78157	0.92712	2.09265	1.83353	480
490	0.55620	1.46121	1.68825	0.73395	1.77718	1.77349	0.90323	2.05491	1.82738	490
500	0.53808	1.42721	1.67713	0.71302	1.74143	1.76529	0.88010	2.01805	1.82113	500
510	0.52062	1.39411	1.66587	0.69280	1.70656	1.75697	0.85770	1.98205	1.81478	510
520	0.50381	1.36188	1.65448	0.67326	1.67252	1.74853	0.83600	1.94687	1.80833	520
530	0.48761	1.33047	1.64296	0.65436	1.63930	1.73998	0.81497	1.91249	1.80178	530
540	0.47200	1.29987	1.63133	0.63608	1.60685	1.73131	0.79458	1.87887	1.79514	540
550	0.45694	1.27004	1.61957	0.61840	1.57517	1.72254	0.77480	1.84600	1.78840	550
560	0.44242	1.24097	1.60771	0.60128	1.54421	1.71366	0.75562	1.81383	1.78157	560
570	0.42842	1.21262	1.59574	0.58471	1.51396	1.70467	0.73700	1.78236	1.77465	570
580	0.41490	1.18497	1.58366	0.56867	1.48439	1.69559	0.71893	1.75156	1.76765	580
590	0.40186	1.15800	1.57149	0.55313	1.45548	1.68641	0.70138	1.72140	1.76055	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T= 500.			T= 600.			T= 700.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
600	0.38926	1.13169	1.55922	0.53808	1.42721	1.67713	0.68435	1.69187	1.75336	600
610	0.37710	1.10602	1.54687	0.52349	1.39957	1.66775	0.66779	1.66295	1.74610	610
620	0.36536	1.08097	1.53443	0.50935	1.37253	1.65829	0.65171	1.63461	1.73874	620
630	0.35401	1.05651	1.52191	0.49564	1.34607	1.64874	0.63608	1.60685	1.73131	630
640	0.34305	1.03265	1.50931	0.48234	1.32018	1.63910	0.62089	1.57965	1.72380	640
650	0.33246	1.00934	1.49664	0.46945	1.29484	1.62938	0.60612	1.55298	1.71621	650
660	0.32222	0.98659	1.48390	0.45694	1.27004	1.61957	0.59175	1.52684	1.70854	660
670	0.31232	0.96437	1.47111	0.44481	1.24576	1.60970	0.57778	1.50120	1.70079	670
680	0.30275	0.94267	1.45825	0.43303	1.22199	1.59974	0.56418	1.47606	1.69297	680
690	0.29350	0.92148	1.44534	0.42160	1.19870	1.58971	0.55095	1.45140	1.68509	690
700	0.28454	0.90077	1.43238	0.41050	1.17590	1.57962	0.53808	1.42721	1.67713	700
710	0.27589	0.88055	1.41937	0.39973	1.15357	1.56945	0.52554	1.40348	1.66910	710
720	0.26751	0.86079	1.40632	0.38926	1.13169	1.55922	0.51334	1.38019	1.66100	720
730	0.25940	0.84148	1.39324	0.37910	1.11025	1.54893	0.50146	1.35734	1.65284	730
740	0.25156	0.82261	1.38012	0.36923	1.08925	1.53858	0.48989	1.33491	1.64462	740
750	0.24396	0.80417	1.36698	0.35964	1.06867	1.52818	0.47862	1.31289	1.63633	750
760	0.23662	0.78616	1.35380	0.35032	1.04849	1.51772	0.46764	1.29127	1.62798	760
770	0.22950	0.76854	1.34061	0.34126	1.02872	1.50720	0.45694	1.27004	1.61957	770
780	0.22261	0.75133	1.32740	0.33246	1.00934	1.49664	0.44652	1.24920	1.61111	780
790	0.21594	0.73451	1.31418	0.32390	0.99034	1.48603	0.43636	1.22873	1.60259	790
800	0.20948	0.71806	1.30094	0.31558	0.97172	1.47538	0.42646	1.20862	1.59402	800
810	0.20322	0.70198	1.28771	0.30750	0.95346	1.46468	0.41680	1.18887	1.58540	810
820	0.19716	0.68626	1.27447	0.29963	0.93555	1.45395	0.40739	1.16947	1.57672	820
830	0.19129	0.67089	1.26123	0.29198	0.91799	1.44318	0.39821	1.15042	1.56800	830
840	0.18560	0.65587	1.24799	0.28454	0.90077	1.43238	0.38926	1.13169	1.55922	840
850	0.18009	0.64117	1.23477	0.27731	0.88389	1.42154	0.38053	1.11329	1.55041	850
860	0.17475	0.62681	1.22156	0.27027	0.86732	1.41068	0.37202	1.09521	1.54155	860
870	0.16958	0.61276	1.20836	0.26342	0.85108	1.39979	0.36371	1.07744	1.53264	870
880	0.16456	0.59903	1.19518	0.25676	0.83514	1.38887	0.35561	1.05997	1.52370	880
890	0.15970	0.58560	1.18202	0.25027	0.81951	1.37793	0.34770	1.04281	1.51472	890
900	0.15499	0.57246	1.16889	0.24396	0.80417	1.36698	0.33999	1.02593	1.50570	900
910	0.15042	0.55962	1.15579	0.23782	0.78913	1.35600	0.33246	1.00934	1.49664	910
920	0.14600	0.54706	1.14272	0.23185	0.77437	1.34501	0.32511	0.99304	1.48755	920
930	0.14170	0.53478	1.12968	0.22603	0.75989	1.33401	0.31794	0.97700	1.47843	930
940	0.13754	0.52276	1.11668	0.22036	0.74568	1.32299	0.31093	0.96124	1.46927	940
950	0.13351	0.51102	1.10372	0.21485	0.73174	1.31197	0.30410	0.94574	1.46009	950
960	0.12959	0.49953	1.09080	0.20948	0.71806	1.30094	0.29742	0.93050	1.45088	960
970	0.12580	0.48829	1.07793	0.20425	0.70463	1.28991	0.29091	0.91551	1.44164	970
980	0.12212	0.47730	1.06511	0.19916	0.69146	1.27888	0.28454	0.90077	1.43238	980
990	0.11855	0.46655	1.05234	0.19420	0.67853	1.26785	0.27833	0.88628	1.42309	990
1000	0.11509	0.45604	1.03962	0.18938	0.66585	1.25682	0.27226	0.87202	1.41378	1000
1010	0.11173	0.44576	1.02696	0.18467	0.65339	1.24579	0.26633	0.85800	1.40446	1010
1020	0.10847	0.43570	1.01435	0.18009	0.64117	1.23477	0.26054	0.84421	1.39511	1020
1030	0.10531	0.42586	1.00181	0.17563	0.62918	1.22376	0.25489	0.83064	1.38575	1030
1040	0.10225	0.41625	0.98933	0.17129	0.61741	1.21276	0.24936	0.81730	1.37637	1040
1050	0.09927	0.40684	0.97691	0.16705	0.60586	1.20177	0.24396	0.80417	1.36698	1050
1060	0.09639	0.39764	0.96456	0.16293	0.59452	1.19079	0.23869	0.79126	1.35757	1060
1070	0.09359	0.38864	0.95228	0.15891	0.58339	1.17983	0.23354	0.77856	1.34815	1070
1080	0.09087	0.37984	0.94007	0.15499	0.57246	1.16889	0.22850	0.76606	1.33872	1080
1090	0.08823	0.37123	0.92793	0.15118	0.56174	1.15797	0.22358	0.75377	1.32929	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T= 500.			T= 600.			T= 700.				
1100	0.08568	0.36281	0.91587	0.14746	0.55122	1.14707	0.21877	0.74167	1.31985	1100
1110	0.08320	0.35457	0.90388	0.14383	0.54088	1.13619	0.21407	0.72977	1.31040	1110
1120	0.08079	0.34652	0.89197	0.14030	0.53074	1.12534	0.20948	0.71806	1.30095	1120
1130	0.07845	0.33864	0.88014	0.13686	0.52079	1.11452	0.20499	0.70654	1.29149	1130
1140	0.07618	0.33094	0.86839	0.13351	0.51102	1.10372	0.20060	0.69520	1.28203	1140
1150	0.07398	0.32341	0.85673	0.13024	0.50142	1.09295	0.19631	0.68404	1.27257	1150
1160	0.07184	0.31604	0.84515	0.12705	0.49201	1.08222	0.19212	0.67307	1.26312	1160
1170	0.06977	0.30884	0.83365	0.12394	0.48276	1.07151	0.18802	0.66226	1.25366	1170
1180	0.06775	0.30179	0.82224	0.12092	0.47369	1.06085	0.18401	0.65163	1.24421	1180
1190	0.06580	0.29490	0.81092	0.11796	0.46478	1.05021	0.18009	0.64117	1.23477	1190
1200	0.06390	0.28816	0.79969	0.11509	0.45604	1.03962	0.17626	0.63088	1.22533	1200
1210	0.06206	0.28157	0.78854	0.11228	0.44745	1.02906	0.17252	0.62075	1.21590	1210
1220	0.06028	0.27512	0.77749	0.10955	0.43903	1.01855	0.16885	0.61078	1.20647	1220
1230	0.05854	0.26882	0.76653	0.10688	0.43076	1.00807	0.16527	0.60097	1.19706	1230
1240	0.05686	0.26266	0.75567	0.10428	0.42263	0.99764	0.16177	0.59132	1.18766	1240
1250	0.05522	0.25663	0.74490	0.10174	0.41466	0.98725	0.15834	0.58182	1.17827	1250
1260	0.05363	0.25074	0.73422	0.09927	0.40684	0.97691	0.15499	0.57246	1.16889	1260
1270	0.05209	0.24498	0.72364	0.09686	0.39916	0.96661	0.15171	0.56326	1.15953	1270
1280	0.05059	0.23934	0.71315	0.09451	0.39161	0.95636	0.14851	0.55420	1.15018	1280
1290	0.04914	0.23383	0.70276	0.09222	0.38421	0.94616	0.14538	0.54529	1.14085	1290
1300	0.04773	0.22845	0.69247	0.08998	0.37694	0.93601	0.14231	0.53651	1.13154	1300
1310	0.04636	0.22318	0.68228	0.08780	0.36981	0.92591	0.13931	0.52788	1.12225	1310
1320	0.04503	0.21803	0.67218	0.08568	0.36281	0.91587	0.13638	0.51938	1.11297	1320
1330	0.04374	0.21299	0.66219	0.08360	0.35593	0.90587	0.13351	0.51102	1.10372	1330
1340	0.04249	0.20807	0.65229	0.08158	0.34918	0.89593	0.13070	0.50278	1.09449	1340
1350	0.04127	0.20326	0.64250	0.07961	0.34256	0.88605	0.12795	0.49468	1.08528	1350
1360	0.04008	0.19855	0.63280	0.07769	0.33606	0.87622	0.12527	0.48670	1.07610	1360
1370	0.03894	0.19395	0.62321	0.07581	0.32967	0.86644	0.12264	0.47885	1.06694	1370
1380	0.03782	0.18945	0.61371	0.07398	0.32341	0.85673	0.12007	0.47113	1.05781	1380
1390	0.03674	0.18506	0.60432	0.07219	0.31726	0.84707	0.11755	0.46352	1.04870	1390
1400	0.03569	0.18076	0.59502	0.07045	0.31122	0.83747	0.11509	0.45604	1.03962	1400
1410	0.03467	0.17655	0.58583	0.06875	0.30529	0.82793	0.11268	0.44867	1.03057	1410
1420	0.03367	0.17245	0.57674	0.06710	0.29947	0.81846	0.11032	0.44142	1.02155	1420
1430	0.03271	0.16843	0.56775	0.06548	0.29376	0.80904	0.10801	0.43428	1.01256	1430
1440	0.03178	0.16451	0.55886	0.06390	0.28816	0.79969	0.10576	0.42726	1.00360	1440
1450	0.03087	0.16067	0.55007	0.06237	0.28266	0.79039	0.10355	0.42034	0.99467	1450
1460	0.02999	0.15692	0.54139	0.06087	0.27726	0.78117	0.10139	0.41354	0.98577	1460
1470	0.02913	0.15325	0.53280	0.05940	0.27196	0.77200	0.09927	0.40684	0.97691	1470
1480	0.02830	0.14967	0.52432	0.05797	0.26675	0.76290	0.09720	0.40024	0.96808	1480
1490	0.02749	0.14617	0.51593	0.05658	0.26165	0.75387	0.09518	0.39376	0.95929	1490
1500	0.02670	0.14274	0.50765	0.05522	0.25663	0.74490	0.09319	0.38737	0.95053	1500
1510	0.02594	0.13940	0.49946	0.05389	0.25171	0.73599	0.09125	0.38108	0.94181	1510
1520	0.02520	0.13613	0.49138	0.05260	0.24688	0.72715	0.08935	0.37489	0.93312	1520
1530	0.02448	0.13293	0.48339	0.05134	0.24214	0.71838	0.08750	0.36880	0.92448	1530
1540	0.02378	0.12981	0.47550	0.05011	0.23749	0.70968	0.08568	0.36281	0.91587	1540
1550	0.02310	0.12675	0.46772	0.04890	0.23293	0.70104	0.08390	0.35691	0.90730	1550
1560	0.02244	0.12377	0.46003	0.04773	0.22845	0.69247	0.08215	0.35110	0.89877	1560
1570	0.02180	0.12086	0.45244	0.04659	0.22405	0.68397	0.08045	0.34538	0.89028	1570
1580	0.02118	0.11801	0.44494	0.04547	0.21973	0.67554	0.07878	0.33976	0.88183	1580
1590	0.02058	0.11522	0.43754	0.04438	0.21550	0.66717	0.07714	0.33422	0.87342	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	T= 500.			T= 600.			T= 700.			ν cm^{-1}
	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	
1600	0.01999	0.11250	0.43024	0.04332	0.21134	0.65888	0.07555	0.32877	0.86505	1600
1610	0.01942	0.10984	0.42304	0.04228	0.20726	0.65065	0.07398	0.32341	0.85673	1610
1620	0.01887	0.10725	0.41593	0.04127	0.20326	0.64250	0.07245	0.31813	0.84845	1620
1630	0.01833	0.10471	0.40891	0.04028	0.19933	0.63441	0.07095	0.31293	0.84021	1630
1640	0.01781	0.10223	0.40199	0.03932	0.19547	0.62639	0.06948	0.30782	0.83202	1640
1650	0.01730	0.09981	0.39517	0.03838	0.19169	0.61845	0.06804	0.30279	0.82387	1650
1660	0.01681	0.09744	0.38843	0.03746	0.18798	0.61057	0.06663	0.29783	0.81576	1660
1670	0.01633	0.09513	0.38179	0.03656	0.18433	0.60276	0.06525	0.29296	0.80770	1670
1680	0.01586	0.09287	0.37524	0.03569	0.18076	0.59502	0.06390	0.28816	0.79969	1680
1690	0.01541	0.09066	0.36878	0.03483	0.17725	0.58736	0.06258	0.28344	0.79172	1690
1700	0.01497	0.08850	0.36241	0.03400	0.17381	0.57976	0.06129	0.27879	0.78380	1700
1710	0.01455	0.08639	0.35614	0.03319	0.17043	0.57223	0.06002	0.27422	0.77592	1710
1720	0.01413	0.08434	0.34995	0.03240	0.16711	0.56478	0.05878	0.26971	0.76809	1720
1730	0.01373	0.08233	0.34385	0.03162	0.16386	0.55739	0.05757	0.26528	0.76031	1730
1740	0.01334	0.08036	0.33783	0.03087	0.16067	0.55007	0.05638	0.26092	0.75258	1740
1750	0.01296	0.07844	0.33191	0.03013	0.15754	0.54283	0.05522	0.25663	0.74490	1750
1760	0.01259	0.07657	0.32607	0.02941	0.15446	0.53565	0.05408	0.25241	0.73726	1760
1770	0.01223	0.07474	0.32031	0.02871	0.15145	0.52855	0.05297	0.24825	0.72967	1770
1780	0.01189	0.07295	0.31464	0.02802	0.14849	0.52151	0.05187	0.24416	0.72213	1780
1790	0.01155	0.07120	0.30906	0.02736	0.14559	0.51454	0.05081	0.24014	0.71464	1790
1800	0.01122	0.06949	0.30356	0.02670	0.14274	0.50765	0.04976	0.23618	0.70720	1800
1810	0.01090	0.06783	0.29814	0.02607	0.13995	0.50082	0.04873	0.23228	0.69981	1810
1820	0.01059	0.06620	0.29280	0.02544	0.13721	0.49406	0.04773	0.22845	0.69247	1820
1830	0.01029	0.06461	0.28754	0.02484	0.13452	0.48737	0.04675	0.22467	0.68518	1830
1840	0.01000	0.06306	0.28236	0.02425	0.13188	0.48075	0.04579	0.22096	0.67794	1840
1850	0.00971	0.06154	0.27726	0.02367	0.12929	0.47420	0.04484	0.21730	0.67075	1850
1860	0.00944	0.06006	0.27224	0.02310	0.12675	0.46772	0.04392	0.21371	0.66361	1860
1870	0.00917	0.05861	0.26730	0.02255	0.12426	0.46130	0.04302	0.21017	0.65652	1870
1880	0.00891	0.05720	0.26243	0.02202	0.12182	0.45495	0.04213	0.20668	0.64948	1880
1890	0.00865	0.05582	0.25764	0.02149	0.11942	0.44868	0.04127	0.20326	0.64250	1890
1900	0.00841	0.05447	0.25293	0.02098	0.11707	0.44246	0.04042	0.19989	0.63556	1900
1910	0.00817	0.05316	0.24829	0.02048	0.11477	0.43632	0.03959	0.19657	0.62868	1910
1920	0.00794	0.05187	0.24372	0.01999	0.11250	0.43024	0.03878	0.19330	0.62184	1920
1930	0.00771	0.05062	0.23923	0.01952	0.11028	0.42423	0.03798	0.19009	0.61506	1930
1940	0.00749	0.04939	0.23480	0.01905	0.10811	0.41829	0.03720	0.18693	0.60833	1940
1950	0.00728	0.04820	0.23045	0.01860	0.10597	0.41241	0.03644	0.18382	0.60165	1950
1960	0.00707	0.04703	0.22617	0.01816	0.10388	0.40660	0.03569	0.18076	0.59502	1960
1970	0.00687	0.04589	0.22196	0.01772	0.10182	0.40085	0.03495	0.17775	0.58845	1970
1980	0.00668	0.04478	0.21781	0.01730	0.09981	0.39517	0.03424	0.17478	0.58192	1980
1990	0.00649	0.04369	0.21374	0.01689	0.09783	0.38955	0.03354	0.17187	0.57545	1990
2000	0.00630	0.04263	0.20973	0.01649	0.09589	0.38399	0.03285	0.16900	0.56903	2000
2010	0.00612	0.04159	0.20579	0.01610	0.09399	0.37850	0.03217	0.16618	0.56266	2010
2020	0.00595	0.04058	0.20191	0.01571	0.09213	0.37308	0.03151	0.16340	0.55634	2020
2030	0.00578	0.03959	0.19809	0.01534	0.09030	0.36771	0.03087	0.16067	0.55007	2030
2040	0.00562	0.03863	0.19434	0.01497	0.08850	0.36241	0.03023	0.15798	0.54386	2040
2050	0.00546	0.03769	0.19066	0.01462	0.08674	0.35718	0.02961	0.15534	0.53770	2050
2060	0.00530	0.03677	0.18703	0.01427	0.08502	0.35200	0.02901	0.15273	0.53158	2060
2070	0.00515	0.03587	0.18347	0.01393	0.08332	0.34689	0.02841	0.15017	0.52552	2070
2080	0.00500	0.03500	0.17996	0.01360	0.08167	0.34183	0.02783	0.14766	0.51951	2080
2090	0.00486	0.03414	0.17652	0.01328	0.08004	0.33684	0.02726	0.14518	0.51355	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T = 500.			T = 600.			T = 700.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
2100	0.00472	0.03331	0.17313	0.01296	0.07844	0.33191	0.02670	0.14274	0.50765	2100
2110	0.00459	0.03249	0.16980	0.01265	0.07688	0.32704	0.02616	0.14034	0.50179	2110
2120	0.00446	0.03170	0.16653	0.01235	0.07534	0.32222	0.02562	0.13799	0.49598	2120
2130	0.00433	0.03092	0.16332	0.01206	0.07384	0.31747	0.02510	0.13567	0.49023	2130
2140	0.00421	0.03016	0.16016	0.01177	0.07236	0.31277	0.02458	0.13338	0.48453	2140
2150	0.00409	0.02942	0.15705	0.01149	0.07091	0.30814	0.02408	0.13114	0.47887	2150
2160	0.00397	0.02870	0.15400	0.01122	0.06949	0.30356	0.02359	0.12893	0.47327	2160
2170	0.00386	0.02800	0.15101	0.01095	0.06810	0.29903	0.02310	0.12675	0.46772	2170
2180	0.00375	0.02731	0.14806	0.01069	0.06674	0.29457	0.02263	0.12462	0.46221	2180
2190	0.00365	0.02664	0.14517	0.01044	0.06540	0.29016	0.02217	0.12251	0.45676	2190
2200	0.00354	0.02598	0.14233	0.01019	0.06409	0.28580	0.02171	0.12044	0.45136	2200
2210	0.00344	0.02534	0.13954	0.00995	0.06280	0.28151	0.02127	0.11841	0.44601	2210
2220	0.00334	0.02472	0.13680	0.00971	0.06154	0.27726	0.02084	0.11641	0.44070	2220
2230	0.00325	0.02411	0.13410	0.00948	0.06030	0.27307	0.02041	0.11444	0.43545	2230
2240	0.00316	0.02352	0.13146	0.00926	0.05909	0.26894	0.01999	0.11250	0.43024	2240
2250	0.00307	0.02294	0.12886	0.00904	0.05790	0.26486	0.01958	0.11060	0.42509	2250
2260	0.00298	0.02237	0.12631	0.00882	0.05674	0.26083	0.01918	0.10872	0.41998	2260
2270	0.00290	0.02182	0.12380	0.00861	0.05559	0.25685	0.01879	0.10688	0.41492	2270
2280	0.00281	0.02128	0.12134	0.00841	0.05447	0.25293	0.01841	0.10507	0.40991	2280
2290	0.00273	0.02076	0.11893	0.00821	0.05337	0.24906	0.01803	0.10329	0.40495	2290
2300	0.00266	0.02024	0.11656	0.00801	0.05230	0.24524	0.01766	0.10153	0.40003	2300
2310	0.00258	0.01974	0.11423	0.00782	0.05124	0.24147	0.01730	0.09981	0.39517	2310
2320	0.00251	0.01925	0.11194	0.00764	0.05021	0.23774	0.01695	0.09811	0.39035	2320
2330	0.00244	0.01878	0.10970	0.00746	0.04919	0.23407	0.01660	0.09644	0.38557	2330
2340	0.00237	0.01831	0.10750	0.00728	0.04820	0.23045	0.01626	0.09480	0.38085	2340
2350	0.00230	0.01786	0.10534	0.00711	0.04722	0.22688	0.01593	0.09319	0.37617	2350
2360	0.00223	0.01742	0.10322	0.00694	0.04627	0.22335	0.01560	0.09160	0.37154	2360
2370	0.00217	0.01698	0.10113	0.00677	0.04533	0.21988	0.01529	0.09004	0.36695	2370
2380	0.00211	0.01656	0.09909	0.00661	0.04441	0.21645	0.01497	0.08850	0.36241	2380
2390	0.00205	0.01615	0.09708	0.00646	0.04351	0.21307	0.01467	0.08699	0.35792	2390
2400	0.00199	0.01575	0.09511	0.00630	0.04263	0.20973	0.01437	0.08551	0.35347	2400
2410	0.00193	0.01536	0.09318	0.00615	0.04176	0.20644	0.01408	0.08405	0.34907	2410
2420	0.00188	0.01498	0.09129	0.00601	0.04091	0.20319	0.01379	0.08261	0.34471	2420
2430	0.00183	0.01460	0.08943	0.00586	0.04008	0.19999	0.01351	0.08120	0.34040	2430
2440	0.00177	0.01424	0.08760	0.00572	0.03927	0.19684	0.01323	0.07981	0.33613	2440
2450	0.00172	0.01389	0.08581	0.00559	0.03847	0.19372	0.01296	0.07844	0.33191	2450
2460	0.00168	0.01354	0.08406	0.00546	0.03769	0.19066	0.01270	0.07710	0.32773	2460
2470	0.00163	0.01320	0.08233	0.00533	0.03692	0.18763	0.01244	0.07578	0.32359	2470
2480	0.00158	0.01287	0.08064	0.00520	0.03617	0.18465	0.01218	0.07448	0.31950	2480
2490	0.00154	0.01255	0.07899	0.00508	0.03543	0.18171	0.01193	0.07320	0.31545	2490
2500	0.00149	0.01224	0.07736	0.00496	0.03471	0.17881	0.01169	0.07194	0.31144	2500
2510	0.00145	0.01193	0.07576	0.00484	0.03400	0.17595	0.01145	0.07071	0.30748	2510
2520	0.00141	0.01163	0.07420	0.00472	0.03331	0.17313	0.01122	0.06949	0.30356	2520
2530	0.00137	0.01134	0.07267	0.00461	0.03263	0.17035	0.01099	0.06830	0.29968	2530
2540	0.00133	0.01106	0.07116	0.00450	0.03196	0.16762	0.01077	0.06713	0.29584	2540
2550	0.00129	0.01078	0.06969	0.00440	0.03131	0.16492	0.01055	0.06597	0.29204	2550
2560	0.00126	0.01051	0.06824	0.00429	0.03067	0.16226	0.01033	0.06483	0.28829	2560
2570	0.00122	0.01025	0.06682	0.00419	0.03004	0.15964	0.01012	0.06372	0.28457	2570
2580	0.00119	0.00999	0.06543	0.00409	0.02942	0.15705	0.00991	0.06262	0.28090	2580
2590	0.00115	0.00974	0.06406	0.00399	0.02882	0.15451	0.00971	0.06154	0.27726	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	T= 500.			T= 600.			T= 700.			ν cm^{-1}
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
2600	0.00112	0.00950	0.06273	0.00390	0.02823	0.15200	0.00951	0.06048	0.27367	2600
2610	0.00109	0.00926	0.06141	0.00381	0.02765	0.14953	0.00932	0.05943	0.27011	2610
2620	0.00106	0.00903	0.06013	0.00372	0.02708	0.14709	0.00913	0.05841	0.26660	2620
2630	0.00103	0.00880	0.05887	0.00363	0.02653	0.14469	0.00894	0.05740	0.26312	2630
2640	0.00100	0.00858	0.05763	0.00354	0.02598	0.14233	0.00876	0.05641	0.25969	2640
2650	0.00097	0.00836	0.05642	0.00346	0.02545	0.14000	0.00858	0.05543	0.25629	2650
2660	0.00094	0.00815	0.05523	0.00338	0.02493	0.13770	0.00841	0.05447	0.25293	2660
2670	0.00092	0.00795	0.05407	0.00330	0.02441	0.13544	0.00824	0.05353	0.24961	2670
2680	0.00089	0.00775	0.05293	0.00322	0.02391	0.13322	0.00807	0.05260	0.24632	2680
2690	0.00086	0.00755	0.05181	0.00314	0.02342	0.13102	0.00790	0.05169	0.24307	2690
2700	0.00084	0.00736	0.05071	0.00307	0.02294	0.12886	0.00774	0.05080	0.23986	2700
2710	0.00082	0.00718	0.04964	0.00299	0.02247	0.12673	0.00758	0.04992	0.23669	2710
2720	0.00079	0.00700	0.04859	0.00292	0.02200	0.12463	0.00743	0.04905	0.23355	2720
2730	0.00077	0.00682	0.04756	0.00285	0.02155	0.12257	0.00728	0.04820	0.23045	2730
2740	0.00075	0.00665	0.04655	0.00279	0.02111	0.12053	0.00713	0.04736	0.22739	2740
2750	0.00073	0.00648	0.04555	0.00272	0.02067	0.11853	0.00699	0.04654	0.22436	2750
2760	0.00071	0.00632	0.04458	0.00266	0.02024	0.11656	0.00684	0.04573	0.22136	2760
2770	0.00069	0.00616	0.04363	0.00259	0.01983	0.11462	0.00670	0.04493	0.21840	2770
2780	0.00067	0.00600	0.04270	0.00253	0.01942	0.11270	0.00657	0.04415	0.21548	2780
2790	0.00065	0.00585	0.04179	0.00247	0.01901	0.11082	0.00643	0.04338	0.21259	2790
2800	0.00063	0.00570	0.04089	0.00241	0.01862	0.10896	0.00630	0.04263	0.20973	2800
2810	0.00061	0.00556	0.04002	0.00236	0.01824	0.10714	0.00617	0.04189	0.20691	2810
2820	0.00059	0.00542	0.03916	0.00230	0.01786	0.10534	0.00605	0.04116	0.20412	2820
2830	0.00058	0.00528	0.03832	0.00225	0.01749	0.10357	0.00592	0.04044	0.20136	2830
2840	0.00056	0.00515	0.03749	0.00219	0.01713	0.10182	0.00580	0.03973	0.19863	2840
2850	0.00055	0.00502	0.03669	0.00214	0.01677	0.10011	0.00569	0.03904	0.19594	2850
2860	0.00053	0.00489	0.03590	0.00209	0.01642	0.09842	0.00557	0.03836	0.19328	2860
2870	0.00051	0.00477	0.03512	0.00204	0.01608	0.09675	0.00546	0.03769	0.19066	2870
2880	0.00050	0.00465	0.03436	0.00199	0.01575	0.09511	0.00535	0.03703	0.18806	2880
2890	0.00049	0.00453	0.03362	0.00194	0.01542	0.09350	0.00524	0.03638	0.18550	2890
2900	0.00047	0.00441	0.03289	0.00190	0.01510	0.09192	0.00513	0.03574	0.18296	2900
2910	0.00046	0.00430	0.03218	0.00185	0.01479	0.09035	0.00503	0.03512	0.18046	2910
2920	0.00045	0.00419	0.03148	0.00181	0.01448	0.08882	0.00492	0.03450	0.17799	2920
2930	0.00043	0.00409	0.03080	0.00177	0.01418	0.08730	0.00482	0.03390	0.17554	2930
2940	0.00042	0.00398	0.03013	0.00172	0.01389	0.08581	0.00472	0.03331	0.17313	2940
2950	0.00041	0.00388	0.02947	0.00168	0.01360	0.08435	0.00463	0.03272	0.17075	2950
2960	0.00040	0.00378	0.02883	0.00164	0.01331	0.08290	0.00453	0.03215	0.16839	2960
2970	0.00039	0.00369	0.02820	0.00160	0.01304	0.08148	0.00444	0.03158	0.16607	2970
2980	0.00038	0.00359	0.02759	0.00157	0.01276	0.08009	0.00435	0.03103	0.16377	2980
2990	0.00036	0.00350	0.02698	0.00153	0.01250	0.07871	0.00426	0.03049	0.16151	2990
3000	0.00035	0.00341	0.02639	0.00149	0.01224	0.07736	0.00418	0.02995	0.15927	3000
3010	0.00034	0.00332	0.02582	0.00146	0.01198	0.07603	0.00409	0.02942	0.15705	3010
3020	0.00033	0.00324	0.02525	0.00142	0.01173	0.07472	0.00401	0.02891	0.15487	3020
3030	0.00032	0.00316	0.02470	0.00139	0.01149	0.07343	0.00393	0.02840	0.15271	3030
3040	0.00032	0.00308	0.02416	0.00136	0.01125	0.07216	0.00385	0.02790	0.15058	3040
3050	0.00031	0.00300	0.02362	0.00132	0.01101	0.07091	0.00377	0.02741	0.14848	3050
3060	0.00030	0.00292	0.02311	0.00129	0.01078	0.06969	0.00369	0.02692	0.14640	3060
3070	0.00029	0.00285	0.02260	0.00126	0.01056	0.06848	0.00362	0.02645	0.14435	3070
3080	0.00028	0.00277	0.02210	0.00123	0.01034	0.06729	0.00354	0.02598	0.14233	3080
3090	0.00027	0.00270	0.02161	0.00120	0.01012	0.06612	0.00347	0.02553	0.14033	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	ν cm ⁻¹
	T= 500.			T= 600.			T= 700.			
3100	0.00027	0.00263	0.02113	0.00117	0.00991	0.06497	0.00340	0.02508	0.13836	3100
3110	0.00026	0.00257	0.02067	0.00115	0.00970	0.06384	0.00333	0.02463	0.13641	3110
3120	0.00025	0.00250	0.02021	0.00112	0.00950	0.06273	0.00326	0.02420	0.13448	3120
3130	0.00024	0.00244	0.01976	0.00109	0.00930	0.06163	0.00320	0.02377	0.13259	3130
3140	0.00024	0.00238	0.01933	0.00107	0.00910	0.06055	0.00313	0.02335	0.13071	3140
3150	0.00023	0.00231	0.01890	0.00104	0.00891	0.05949	0.00307	0.02294	0.12886	3150
3160	0.00022	0.00226	0.01848	0.00102	0.00873	0.05845	0.00300	0.02253	0.12703	3160
3170	0.00022	0.00220	0.01807	0.00099	0.00854	0.05743	0.00294	0.02213	0.12523	3170
3180	0.00021	0.00214	0.01767	0.00097	0.00836	0.05642	0.00288	0.02174	0.12345	3180
3190	0.00021	0.00209	0.01727	0.00095	0.00819	0.05543	0.00282	0.02136	0.12169	3190
3200	0.00020	0.00203	0.01689	0.00092	0.00802	0.05445	0.00277	0.02098	0.11996	3200
3210	0.00019	0.00198	0.01651	0.00090	0.00785	0.05350	0.00271	0.02061	0.11825	3210
3220	0.00019	0.00193	0.01614	0.00088	0.00768	0.05255	0.00266	0.02024	0.11656	3220
3230	0.00018	0.00188	0.01578	0.00086	0.00752	0.05163	0.00260	0.01988	0.11489	3230
3240	0.00018	0.00183	0.01543	0.00084	0.00736	0.05071	0.00255	0.01953	0.11325	3240
3250	0.00017	0.00179	0.01508	0.00082	0.00721	0.04982	0.00250	0.01919	0.11162	3250
3260	0.00017	0.00174	0.01475	0.00080	0.00706	0.04894	0.00245	0.01884	0.11002	3260
3270	0.00016	0.00169	0.01442	0.00078	0.00691	0.04807	0.00240	0.01851	0.10844	3270
3280	0.00016	0.00165	0.01409	0.00076	0.00676	0.04722	0.00235	0.01818	0.10688	3280
3290	0.00015	0.00161	0.01378	0.00074	0.00662	0.04638	0.00230	0.01786	0.10534	3290
3300	0.00015	0.00157	0.01347	0.00073	0.00648	0.04555	0.00225	0.01754	0.10382	3300
3310	0.00015	0.00153	0.01317	0.00071	0.00635	0.04474	0.00221	0.01723	0.10232	3310
3320	0.00014	0.00149	0.01287	0.00069	0.00621	0.04395	0.00216	0.01692	0.10084	3320
3330	0.00014	0.00145	0.01258	0.00068	0.00608	0.04316	0.00212	0.01662	0.09938	3330
3340	0.00013	0.00141	0.01230	0.00066	0.00595	0.04239	0.00207	0.01633	0.09794	3340
3350	0.00013	0.00138	0.01202	0.00064	0.00583	0.04164	0.00203	0.01604	0.09652	3350
3360	0.00013	0.00134	0.01175	0.00063	0.00570	0.04089	0.00199	0.01575	0.09511	3360
3370	0.00012	0.00131	0.01148	0.00061	0.00558	0.04016	0.00195	0.01547	0.09373	3370
3380	0.00012	0.00127	0.01122	0.00060	0.00547	0.03944	0.00191	0.01519	0.09237	3380
3390	0.00012	0.00124	0.01097	0.00059	0.00535	0.03874	0.00187	0.01492	0.09102	3390
3400	0.00011	0.00121	0.01072	0.00057	0.00524	0.03804	0.00183	0.01466	0.08969	3400
3410	0.00011	0.00118	0.01048	0.00056	0.00513	0.03736	0.00180	0.01439	0.08838	3410
3420	0.00011	0.00115	0.01024	0.00055	0.00502	0.03669	0.00176	0.01414	0.08709	3420
3430	0.00010	0.00112	0.01001	0.00053	0.00491	0.03603	0.00172	0.01389	0.08581	3430
3440	0.00010	0.00109	0.00978	0.00052	0.00481	0.03538	0.00169	0.01364	0.08456	3440
3450	0.00010	0.00106	0.00956	0.00051	0.00471	0.03474	0.00165	0.01339	0.08331	3450
3460	0.00009	0.00103	0.00934	0.00050	0.00461	0.03411	0.00162	0.01315	0.08209	3460
3470	0.00009	0.00101	0.00913	0.00048	0.00451	0.03350	0.00159	0.01292	0.08088	3470
3480	0.00009	0.00098	0.00892	0.00047	0.00441	0.03289	0.00156	0.01269	0.07969	3480
3490	0.00009	0.00095	0.00872	0.00046	0.00432	0.03230	0.00152	0.01246	0.07852	3490
3500	0.00008	0.00093	0.00852	0.00045	0.00423	0.03171	0.00149	0.01224	0.07736	3500
3510	0.00008	0.00091	0.00833	0.00044	0.00414	0.03114	0.00146	0.01202	0.07622	3510
3520	0.00008	0.00088	0.00814	0.00043	0.00405	0.03057	0.00143	0.01180	0.07509	3520
3530	0.00008	0.00086	0.00795	0.00042	0.00396	0.03002	0.00140	0.01159	0.07398	3530
3540	0.00007	0.00084	0.00777	0.00041	0.00388	0.02947	0.00138	0.01138	0.07288	3540
3550	0.00007	0.00082	0.00759	0.00040	0.00380	0.02894	0.00135	0.01118	0.07180	3550
3560	0.00007	0.00079	0.00742	0.00039	0.00372	0.02841	0.00132	0.01098	0.07074	3560
3570	0.00007	0.00077	0.00725	0.00038	0.00364	0.02789	0.00129	0.01078	0.06969	3570
3580	0.00007	0.00075	0.00708	0.00037	0.00356	0.02739	0.00127	0.01059	0.06865	3580
3590	0.00006	0.00073	0.00692	0.00036	0.00349	0.02689	0.00124	0.01040	0.06763	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ-E_0^\circ)/T$	S°	C _P ^o	$-(F^\circ-E_0^\circ)/T$	S°	C _P ^o	$-(F^\circ-E_0^\circ)/T$	S°	C _P ^o	ν cm ⁻¹
	T= 500.			T= 600.			T= 700.			
3600	0.00006	0.00072	0.00676	0.00035	0.00341	0.02639	0.00122	0.01021	0.06662	3600
3610	0.00006	0.00070	0.00660	0.00035	0.00334	0.02591	0.00119	0.01003	0.06562	3610
3620	0.00006	0.00068	0.00645	0.00034	0.00327	0.02544	0.00117	0.00985	0.06464	3620
3630	0.00006	0.00066	0.00630	0.00033	0.00320	0.02497	0.00114	0.00967	0.06368	3630
3640	0.00006	0.00064	0.00616	0.00032	0.00313	0.02452	0.00112	0.00950	0.06273	3640
3650	0.00005	0.00063	0.00602	0.00031	0.00306	0.02407	0.00110	0.00933	0.06179	3650
3660	0.00005	0.00061	0.00588	0.00031	0.00300	0.02362	0.00107	0.00916	0.06086	3660
3670	0.00005	0.00060	0.00574	0.00030	0.00293	0.02319	0.00105	0.00900	0.05995	3670
3680	0.00005	0.00058	0.00561	0.00029	0.00287	0.02276	0.00103	0.00883	0.05905	3680
3690	0.00005	0.00056	0.00548	0.00029	0.00281	0.02235	0.00101	0.00867	0.05816	3690
3700	0.00005	0.00055	0.00535	0.00028	0.00275	0.02193	0.00099	0.00852	0.05728	3700
3710	0.00005	0.00054	0.00523	0.00027	0.00269	0.02153	0.00097	0.00836	0.05642	3710
3720	0.00004	0.00052	0.00511	0.00027	0.00263	0.02113	0.00095	0.00821	0.05557	3720
3730	0.00004	0.00051	0.00499	0.00026	0.00258	0.02074	0.00093	0.00807	0.05473	3730
3740	0.00004	0.00050	0.00488	0.00025	0.00252	0.02036	0.00091	0.00792	0.05390	3740
3750	0.00004	0.00048	0.00476	0.00025	0.00247	0.01999	0.00089	0.00778	0.05309	3750
3760	0.00004	0.00047	0.00465	0.00024	0.00242	0.01962	0.00087	0.00764	0.05229	3760
3770	0.00004	0.00046	0.00454	0.00024	0.00236	0.01925	0.00086	0.00750	0.05149	3770
3780	0.00004	0.00045	0.00444	0.00023	0.00231	0.01890	0.00084	0.00736	0.05071	3780
3790	0.00004	0.00043	0.00434	0.00022	0.00226	0.01855	0.00082	0.00723	0.04994	3790
3800	0.00004	0.00042	0.00424	0.00022	0.00222	0.01820	0.00081	0.00710	0.04919	3800
3810	0.00003	0.00041	0.00414	0.00021	0.00217	0.01786	0.00079	0.00697	0.04844	3810
3820	0.00003	0.00040	0.00404	0.00021	0.00212	0.01753	0.00077	0.00685	0.04770	3820
3830	0.00003	0.00039	0.00395	0.00020	0.00208	0.01721	0.00076	0.00672	0.04698	3830
3840	0.00003	0.00038	0.00386	0.00020	0.00203	0.01689	0.00074	0.00660	0.04626	3840
3850	0.00003	0.00037	0.00377	0.00019	0.00199	0.01657	0.00073	0.00648	0.04555	3850
3860	0.00003	0.00036	0.00368	0.00019	0.00195	0.01626	0.00071	0.00636	0.04486	3860
3870	0.00003	0.00035	0.00359	0.00019	0.00191	0.01596	0.00070	0.00625	0.04417	3870
3880	0.00003	0.00034	0.00351	0.00018	0.00186	0.01566	0.00068	0.00614	0.04350	3880
3890	0.00003	0.00033	0.00343	0.00018	0.00182	0.01537	0.00067	0.00602	0.04283	3890
3900	0.00003	0.00032	0.00335	0.00017	0.00179	0.01508	0.00066	0.00592	0.04218	3900
3910	0.00003	0.00032	0.00327	0.00017	0.00175	0.01480	0.00064	0.00581	0.04153	3910
3920	0.00003	0.00031	0.00319	0.00016	0.00171	0.01453	0.00063	0.00570	0.04089	3920
3930	0.00002	0.00030	0.00312	0.00016	0.00167	0.01425	0.00062	0.00560	0.04027	3930
3940	0.00002	0.00029	0.00304	0.00016	0.00164	0.01399	0.00060	0.00550	0.03965	3940
3950	0.00002	0.00028	0.00297	0.00015	0.00160	0.01373	0.00059	0.00540	0.03904	3950
3960	0.00002	0.00028	0.00290	0.00015	0.00157	0.01347	0.00058	0.00530	0.03844	3960
3970	0.00002	0.00027	0.00283	0.00015	0.00153	0.01322	0.00057	0.00520	0.03784	3970
3980	0.00002	0.00026	0.00277	0.00014	0.00150	0.01297	0.00056	0.00511	0.03726	3980
3990	0.00002	0.00026	0.00270	0.00014	0.00147	0.01272	0.00055	0.00502	0.03669	3990
4000	0.00002	0.00025	0.00264	0.00014	0.00144	0.01248	0.00053	0.00493	0.03612	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T= 800.			T= 900.			T=1000.				
100	3.58527	5.39910	1.98182	3.80003	5.63259	1.98294	3.99392	5.84156	1.98375	100
110	3.41318	5.21026	1.98070	3.62608	5.44364	1.98206	3.81846	5.65252	1.98303	110
120	3.25753	5.03797	1.97947	3.46857	5.27122	1.98109	3.65945	5.48001	1.98224	120
130	3.11567	4.87958	1.97814	3.32486	5.11269	1.98003	3.51426	5.32138	1.98139	130
140	2.98555	4.73304	1.97670	3.19291	4.96599	1.97890	3.38083	5.17458	1.98046	140
150	2.86555	4.59671	1.97516	3.07108	4.82950	1.97767	3.25753	5.03797	1.97947	150
160	2.75434	4.46929	1.97351	2.95806	4.70191	1.97637	3.14304	4.91025	1.97842	160
170	2.65085	4.34970	1.97176	2.85278	4.58213	1.97498	3.03630	4.79034	1.97729	170
180	2.55420	4.23705	1.96991	2.75434	4.46929	1.97351	2.93642	4.67736	1.97610	180
190	2.46364	4.13059	1.96795	2.66200	4.36263	1.97196	2.84264	4.57055	1.97484	190
200	2.37854	4.02970	1.96588	2.57513	4.26152	1.97033	2.75434	4.46929	1.97351	200
210	2.29836	3.93384	1.96372	2.49319	4.16543	1.96861	2.67098	4.37303	1.97212	210
220	2.22264	3.84254	1.96145	2.41573	4.07389	1.96681	2.59209	4.28132	1.97066	220
230	2.15097	3.75540	1.95908	2.34233	3.98650	1.96493	2.51729	4.19376	1.96913	230
240	2.08302	3.67207	1.95660	2.27265	3.90292	1.96297	2.44621	4.10999	1.96754	240
250	2.01846	3.59225	1.95403	2.20638	3.82283	1.96093	2.37854	4.02970	1.96588	250
260	1.95703	3.51567	1.95135	2.14325	3.74596	1.95881	2.31403	3.95263	1.96416	260
270	1.89849	3.44207	1.94858	2.08302	3.67207	1.95660	2.25242	3.87854	1.96237	270
280	1.84262	3.37126	1.94570	2.02547	3.60096	1.95432	2.19351	3.80720	1.96051	280
290	1.78924	3.30303	1.94273	1.97042	3.53242	1.95196	2.13710	3.73844	1.95859	290
300	1.73817	3.23722	1.93966	1.91769	3.46628	1.94951	2.08302	3.67207	1.95660	300
310	1.68925	3.17367	1.93648	1.86713	3.40240	1.94699	2.03111	3.60795	1.95455	310
320	1.64235	3.11224	1.93322	1.81860	3.34063	1.94439	1.98124	3.54593	1.95243	320
330	1.59734	3.05281	1.92985	1.77197	3.28084	1.94172	1.93328	3.48588	1.95025	330
340	1.55411	2.99525	1.92639	1.72712	3.22291	1.93896	1.88711	3.42769	1.94801	340
350	1.51254	2.93946	1.92283	1.68394	3.16675	1.93613	1.84262	3.37126	1.94570	350
360	1.47254	2.88534	1.91918	1.64235	3.11224	1.93322	1.79972	3.31648	1.94333	360
370	1.43402	2.83281	1.91544	1.60225	3.05932	1.93023	1.75833	3.26327	1.94090	370
380	1.39690	2.78178	1.91160	1.56357	3.00788	1.92717	1.71835	3.21154	1.93840	380
390	1.36111	2.73217	1.90766	1.52621	2.95786	1.92403	1.67971	3.16122	1.93584	390
400	1.32657	2.68392	1.90364	1.49013	2.90919	1.92082	1.64235	3.11224	1.93322	400
410	1.29322	2.63697	1.89952	1.45524	2.86180	1.91753	1.60620	3.06454	1.93053	410
420	1.26100	2.59125	1.89532	1.42149	2.81563	1.91417	1.57119	3.01805	1.92779	420
430	1.22985	2.54670	1.89102	1.38883	2.77063	1.91073	1.53728	2.97272	1.92498	430
440	1.19973	2.50327	1.88664	1.35721	2.72675	1.90722	1.50441	2.92850	1.92211	440
450	1.17059	2.46093	1.88216	1.32657	2.68392	1.90364	1.47254	2.88534	1.91918	450
460	1.14237	2.41961	1.87760	1.29687	2.64212	1.89999	1.44161	2.84319	1.91619	460
470	1.11504	2.37928	1.87296	1.26806	2.60130	1.89626	1.41158	2.80201	1.91314	470
480	1.08856	2.33989	1.86822	1.24012	2.56142	1.89246	1.38243	2.76177	1.91003	480
490	1.06289	2.30142	1.86341	1.21300	2.52244	1.88860	1.35410	2.72242	1.90687	490
500	1.03800	2.26383	1.85850	1.18666	2.48432	1.88466	1.32657	2.68392	1.90364	500
510	1.01385	2.22707	1.85352	1.16108	2.44704	1.88065	1.29980	2.64626	1.90035	510
520	0.99041	2.19113	1.84845	1.13622	2.41056	1.87658	1.27375	2.60939	1.89701	520
530	0.96766	2.15597	1.84330	1.11206	2.37486	1.87244	1.24842	2.57329	1.89361	530
540	0.94556	2.12156	1.83808	1.08856	2.33989	1.86822	1.22375	2.53792	1.89015	540
550	0.92409	2.08788	1.83277	1.06570	2.30565	1.86395	1.19973	2.50327	1.88664	550
560	0.90323	2.05491	1.82738	1.04346	2.27211	1.85960	1.17634	2.46931	1.88307	560
570	0.88295	2.02261	1.82192	1.02182	2.23923	1.85519	1.15355	2.43601	1.87944	570
580	0.86324	1.99097	1.81638	1.00074	2.20701	1.85072	1.13134	2.40336	1.87576	580
590	0.84406	1.95997	1.81076	0.98021	2.17541	1.84617	1.10968	2.37133	1.87202	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T= 800.			T= 900.			T=1000.			ν cm ⁻¹
	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	
600	0.82540	1.92958	1.80507	0.96022	2.14442	1.84157	1.08856	2.33989	1.86822	600
610	0.80725	1.89980	1.79930	0.94074	2.11401	1.83690	1.06796	2.30905	1.86438	610
620	0.78958	1.87059	1.79346	0.92175	2.08418	1.83217	1.04786	2.27876	1.86048	620
630	0.77237	1.84194	1.78756	0.90323	2.05491	1.82738	1.02825	2.24902	1.85652	630
640	0.75562	1.81383	1.78157	0.88518	2.02617	1.82253	1.00910	2.21982	1.85251	640
650	0.73930	1.78626	1.77552	0.86757	1.99795	1.81761	0.99041	2.19113	1.84845	650
660	0.72340	1.75920	1.76941	0.85039	1.97024	1.81264	0.97215	2.16294	1.84434	660
670	0.70790	1.73263	1.76322	0.83363	1.94301	1.80761	0.95432	2.13524	1.84018	670
680	0.69280	1.70656	1.75697	0.81727	1.91627	1.80251	0.93690	2.10800	1.83596	680
690	0.67808	1.68095	1.75065	0.80130	1.89000	1.79736	0.91987	2.08123	1.83170	690
700	0.66373	1.65581	1.74427	0.78571	1.86417	1.79216	0.90323	2.05491	1.82738	700
710	0.64973	1.63111	1.73782	0.77049	1.83879	1.78689	0.88696	2.02902	1.82302	710
720	0.63608	1.60685	1.73131	0.75562	1.81383	1.78157	0.87106	2.00355	1.81860	720
730	0.62277	1.58302	1.72474	0.74109	1.78930	1.77620	0.85550	1.97850	1.81414	730
740	0.60977	1.55960	1.71811	0.72689	1.76517	1.77077	0.84029	1.95384	1.80963	740
750	0.59709	1.53658	1.71142	0.71302	1.74143	1.76529	0.82540	1.92958	1.80507	750
760	0.58471	1.51396	1.70467	0.69947	1.71809	1.75975	0.81084	1.90571	1.80046	760
770	0.57263	1.49172	1.69787	0.68622	1.69512	1.75417	0.79659	1.88220	1.79581	770
780	0.56084	1.46985	1.69101	0.67326	1.67252	1.74853	0.78264	1.85906	1.79111	780
790	0.54932	1.44835	1.68409	0.66059	1.65028	1.74284	0.76898	1.83627	1.78636	790
800	0.53808	1.42721	1.67713	0.64820	1.62840	1.73710	0.75562	1.81383	1.78157	800
810	0.52709	1.40642	1.67010	0.63608	1.60685	1.73131	0.74253	1.79173	1.77674	810
820	0.51636	1.38597	1.66303	0.62423	1.58565	1.72547	0.72971	1.76996	1.77186	820
830	0.50588	1.36586	1.65591	0.61263	1.56477	1.71959	0.71715	1.74851	1.76694	830
840	0.49564	1.34607	1.64874	0.60128	1.54421	1.71366	0.70485	1.72738	1.76197	840
850	0.48563	1.32660	1.64151	0.59018	1.52396	1.70768	0.69280	1.70656	1.75697	850
860	0.47585	1.30744	1.63425	0.57931	1.50402	1.70166	0.68100	1.68604	1.75192	860
870	0.46629	1.28859	1.62693	0.56867	1.48439	1.69559	0.66943	1.66581	1.74683	870
880	0.45694	1.27004	1.61957	0.55826	1.46504	1.68948	0.65809	1.64588	1.74169	880
890	0.44781	1.25178	1.61217	0.54806	1.44599	1.68332	0.64698	1.62623	1.73652	890
900	0.43887	1.23381	1.60473	0.53808	1.42721	1.67713	0.63608	1.60685	1.73131	900
910	0.43014	1.21612	1.59724	0.52830	1.40872	1.67089	0.62540	1.58775	1.72606	910
920	0.42160	1.19870	1.58971	0.51873	1.39049	1.66461	0.61493	1.56892	1.72077	920
930	0.41324	1.18156	1.58215	0.50935	1.37253	1.65829	0.60466	1.55034	1.71544	930
940	0.40507	1.16468	1.57454	0.50016	1.35483	1.65193	0.59459	1.53202	1.71008	940
950	0.39708	1.14806	1.56690	0.49116	1.33738	1.64553	0.58471	1.51396	1.70467	950
960	0.38926	1.13169	1.55922	0.48234	1.32018	1.63910	0.57503	1.49613	1.69923	960
970	0.38161	1.11557	1.55151	0.47370	1.30323	1.63263	0.56552	1.47855	1.69376	970
980	0.37413	1.09970	1.54377	0.46524	1.28652	1.62612	0.55620	1.46121	1.68825	980
990	0.36680	1.08406	1.53599	0.45694	1.27004	1.61957	0.54705	1.44410	1.68270	990
1000	0.35964	1.06867	1.52818	0.44881	1.25380	1.61300	0.53808	1.42721	1.67713	1000
1010	0.35262	1.05350	1.52034	0.44084	1.23778	1.60639	0.52927	1.41055	1.67151	1010
1020	0.34576	1.03856	1.51247	0.43303	1.22199	1.59974	0.52062	1.39411	1.66587	1020
1030	0.33904	1.02384	1.50457	0.42537	1.20641	1.59306	0.51214	1.37789	1.66019	1030
1040	0.33246	1.00934	1.49664	0.41786	1.19105	1.58636	0.50381	1.36188	1.65448	1040
1050	0.32602	0.99506	1.48869	0.41050	1.17590	1.57962	0.49564	1.34607	1.64874	1050
1060	0.31971	0.98099	1.48071	0.40328	1.16096	1.57285	0.48761	1.33047	1.64296	1060
1070	0.31354	0.96712	1.47271	0.39620	1.14623	1.56605	0.47973	1.31507	1.63716	1070
1080	0.30750	0.95346	1.46468	0.38926	1.13169	1.55922	0.47200	1.29987	1.63133	1080
1090	0.30158	0.93999	1.45664	0.38245	1.11735	1.55237	0.46440	1.28486	1.62547	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	T= 800.			T= 900.			T=1000.			ν cm^{-1}
	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	
1100	0.29578	0.92673	1.44857	0.37578	1.10320	1.54549	0.45694	1.27004	1.61957	1100
1110	0.29010	0.91366	1.44048	0.36923	1.08925	1.53858	0.44962	1.25541	1.61366	1110
1120	0.28454	0.90077	1.43238	0.36280	1.07548	1.53165	0.44242	1.24097	1.60771	1120
1130	0.27910	0.88808	1.42425	0.35650	1.06190	1.52470	0.43536	1.22670	1.60174	1130
1140	0.27376	0.87556	1.41611	0.35032	1.04849	1.51772	0.42842	1.21262	1.59574	1140
1150	0.26854	0.86323	1.40796	0.34425	1.03527	1.51071	0.42160	1.19870	1.58971	1150
1160	0.26342	0.85108	1.39979	0.33830	1.02222	1.50369	0.41490	1.18497	1.58366	1160
1170	0.25841	0.83910	1.39160	0.33246	1.00934	1.49664	0.40832	1.17140	1.57759	1170
1180	0.25349	0.82729	1.38340	0.32673	0.99664	1.48957	0.40186	1.15800	1.57149	1180
1190	0.24868	0.81565	1.37520	0.32110	0.98410	1.48249	0.39550	1.14476	1.56537	1190
1200	0.24396	0.80417	1.36698	0.31558	0.97172	1.47538	0.38926	1.13169	1.55922	1200
1210	0.23934	0.79286	1.35875	0.31017	0.95950	1.46825	0.38313	1.11878	1.55306	1210
1220	0.23482	0.78172	1.35051	0.30485	0.94745	1.46111	0.37710	1.10602	1.54687	1220
1230	0.23038	0.77072	1.34226	0.29963	0.93555	1.45395	0.37118	1.09342	1.54066	1230
1240	0.22603	0.75989	1.33401	0.29451	0.92381	1.44678	0.36536	1.08097	1.53443	1240
1250	0.22177	0.74921	1.32575	0.28948	0.91222	1.43958	0.35964	1.06867	1.52818	1250
1260	0.21759	0.73868	1.31748	0.28454	0.90077	1.43238	0.35401	1.05651	1.52191	1260
1270	0.21349	0.72829	1.30922	0.27970	0.88948	1.42516	0.34848	1.04451	1.51562	1270
1280	0.20948	0.71806	1.30094	0.27494	0.87833	1.41792	0.34305	1.03265	1.50931	1280
1290	0.20555	0.70797	1.29267	0.27027	0.86732	1.41068	0.33771	1.02092	1.50298	1290
1300	0.20169	0.69802	1.28440	0.26568	0.85646	1.40342	0.33246	1.00934	1.49664	1300
1310	0.19791	0.68821	1.27612	0.26118	0.84573	1.39615	0.32729	0.99790	1.49028	1310
1320	0.19420	0.67853	1.26785	0.25676	0.83514	1.38887	0.32222	0.98659	1.48390	1320
1330	0.19057	0.66899	1.25957	0.25242	0.82469	1.38158	0.31723	0.97541	1.47751	1330
1340	0.18701	0.65959	1.25130	0.24815	0.81437	1.37428	0.31232	0.96437	1.47111	1340
1350	0.18352	0.65032	1.24303	0.24396	0.80417	1.36698	0.30750	0.95346	1.46468	1350
1360	0.18009	0.64117	1.23477	0.23985	0.79411	1.35966	0.30275	0.94267	1.45825	1360
1370	0.17674	0.63216	1.22651	0.23581	0.78418	1.35234	0.29808	0.93201	1.45180	1370
1380	0.17345	0.62327	1.21825	0.23185	0.77437	1.34501	0.29350	0.92148	1.44534	1380
1390	0.17022	0.61450	1.21001	0.22795	0.76469	1.33768	0.28898	0.91106	1.43886	1390
1400	0.16705	0.60586	1.20177	0.22412	0.75512	1.33034	0.28454	0.90077	1.43238	1400
1410	0.16395	0.59733	1.19353	0.22036	0.74568	1.32299	0.28018	0.89060	1.42588	1410
1420	0.16090	0.58893	1.18531	0.21667	0.73636	1.31565	0.27589	0.88055	1.41937	1420
1430	0.15792	0.58064	1.17710	0.21304	0.72715	1.30830	0.27166	0.87061	1.41285	1430
1440	0.15499	0.57246	1.16889	0.20948	0.71806	1.30094	0.26751	0.86079	1.40632	1440
1450	0.15212	0.56440	1.16070	0.20598	0.70908	1.29359	0.26342	0.85108	1.39979	1450
1460	0.14930	0.55645	1.15252	0.20254	0.70021	1.28624	0.25940	0.84148	1.39324	1460
1470	0.14654	0.54861	1.14435	0.19916	0.69146	1.27888	0.25545	0.83199	1.38668	1470
1480	0.14383	0.54088	1.13619	0.19584	0.68281	1.27152	0.25156	0.82261	1.38012	1480
1490	0.14118	0.53326	1.12805	0.19258	0.67428	1.26417	0.24773	0.81334	1.37355	1490
1500	0.13857	0.52574	1.11993	0.18938	0.66585	1.25682	0.24396	0.80417	1.36698	1500
1510	0.13601	0.51833	1.11182	0.18623	0.65752	1.24946	0.24026	0.79511	1.36039	1510
1520	0.13351	0.51102	1.10372	0.18313	0.64930	1.24211	0.23662	0.78616	1.35380	1520
1530	0.13105	0.50380	1.09564	0.18009	0.64117	1.23477	0.23303	0.77730	1.34721	1530
1540	0.12863	0.49669	1.08758	0.17711	0.63315	1.22743	0.22950	0.76854	1.34061	1540
1550	0.12627	0.48968	1.07954	0.17417	0.62523	1.22009	0.22603	0.75989	1.33401	1550
1560	0.12394	0.48276	1.07151	0.17129	0.61741	1.21276	0.22261	0.75133	1.32740	1560
1570	0.12167	0.47594	1.06351	0.16845	0.60968	1.20543	0.21925	0.74287	1.32079	1570
1580	0.11943	0.46921	1.05553	0.16566	0.60205	1.19811	0.21594	0.73451	1.31418	1580
1590	0.11724	0.46258	1.04756	0.16293	0.59452	1.19079	0.21269	0.72623	1.30756	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
	T= 800.			T= 900.			T=1000.			
1600	0.11509	0.45604	1.03962	0.16024	0.58708	1.18348	0.20948	0.71806	1.30094	1600
1610	0.11298	0.44958	1.03170	0.15759	0.57972	1.17618	0.20633	0.70997	1.29433	1610
1620	0.11090	0.44322	1.02380	0.15499	0.57246	1.16889	0.20322	0.70198	1.28771	1620
1630	0.10887	0.43694	1.01592	0.15244	0.56529	1.16161	0.20017	0.69407	1.28109	1630
1640	0.10688	0.43076	1.00807	0.14993	0.55821	1.15433	0.19716	0.68626	1.27447	1640
1650	0.10492	0.42465	1.00024	0.14746	0.55122	1.14707	0.19420	0.67853	1.26785	1650
1660	0.10300	0.41863	0.99244	0.14503	0.54431	1.13982	0.19129	0.67089	1.26123	1660
1670	0.10112	0.41269	0.98466	0.14265	0.53748	1.13257	0.18843	0.66334	1.25461	1670
1680	0.09927	0.40684	0.97691	0.14030	0.53074	1.12534	0.18560	0.65587	1.24799	1680
1690	0.09746	0.40106	0.96918	0.13800	0.52409	1.11812	0.18283	0.64848	1.24138	1690
1700	0.09568	0.39537	0.96148	0.13573	0.51751	1.11092	0.18009	0.64117	1.23477	1700
1710	0.09393	0.38975	0.95381	0.13351	0.51102	1.10372	0.17740	0.63395	1.22816	1710
1720	0.09222	0.38421	0.94616	0.13132	0.50460	1.09654	0.17475	0.62681	1.22156	1720
1730	0.09054	0.37875	0.93855	0.12917	0.49826	1.08937	0.17215	0.61975	1.21495	1730
1740	0.08889	0.37336	0.93096	0.12705	0.49201	1.08222	0.16958	0.61276	1.20836	1740
1750	0.08727	0.36805	0.92340	0.12497	0.48583	1.07508	0.16705	0.60586	1.20177	1750
1760	0.08568	0.36281	0.91587	0.12293	0.47972	1.06795	0.16456	0.59903	1.19518	1760
1770	0.08412	0.35764	0.90837	0.12092	0.47369	1.06085	0.16211	0.59228	1.18860	1770
1780	0.08259	0.35254	0.90090	0.11894	0.46773	1.05375	0.15970	0.58560	1.18202	1780
1790	0.08108	0.34752	0.89346	0.11700	0.46185	1.04668	0.15733	0.57899	1.17545	1790
1800	0.07961	0.34256	0.88605	0.11509	0.45604	1.03962	0.15499	0.57246	1.16889	1800
1810	0.07816	0.33767	0.87867	0.11321	0.45030	1.03258	0.15269	0.56601	1.16234	1810
1820	0.07674	0.33285	0.87132	0.11136	0.44463	1.02555	0.15042	0.55962	1.15579	1820
1830	0.07535	0.32810	0.86401	0.10955	0.43903	1.01855	0.14819	0.55331	1.14925	1830
1840	0.07398	0.32341	0.85673	0.10776	0.43350	1.01156	0.14600	0.54706	1.14272	1840
1850	0.07264	0.31878	0.84948	0.10601	0.42803	1.00459	0.14383	0.54088	1.13619	1850
1860	0.07132	0.31422	0.84226	0.10428	0.42263	0.99764	0.14170	0.53478	1.12968	1860
1870	0.07002	0.30973	0.83508	0.10258	0.41730	0.99071	0.13961	0.52874	1.12318	1870
1880	0.06875	0.30529	0.82793	0.10091	0.41204	0.98380	0.13754	0.52276	1.11668	1880
1890	0.06751	0.30092	0.82082	0.09927	0.40684	0.97691	0.13551	0.51686	1.11020	1890
1900	0.06628	0.29661	0.81374	0.09766	0.40170	0.97004	0.13351	0.51102	1.10372	1900
1910	0.06508	0.29235	0.80670	0.09607	0.39663	0.96319	0.13153	0.50524	1.09726	1910
1920	0.06390	0.28816	0.79969	0.09451	0.39161	0.95636	0.12959	0.49953	1.09080	1920
1930	0.06275	0.28402	0.79271	0.09298	0.38666	0.94956	0.12768	0.49388	1.08436	1930
1940	0.06161	0.27994	0.78577	0.09147	0.38177	0.94277	0.12580	0.48829	1.07793	1940
1950	0.06050	0.27592	0.77887	0.08998	0.37694	0.93601	0.12394	0.48276	1.07151	1950
1960	0.05940	0.27196	0.77200	0.08852	0.37217	0.92927	0.12212	0.47730	1.06511	1960
1970	0.05833	0.26804	0.76517	0.08709	0.36746	0.92256	0.12032	0.47189	1.05872	1970
1980	0.05727	0.26419	0.75838	0.08568	0.36281	0.91587	0.11855	0.46655	1.05234	1980
1990	0.05624	0.26038	0.75162	0.08429	0.35821	0.90920	0.11680	0.46126	1.04597	1990
2000	0.05522	0.25663	0.74490	0.08292	0.35367	0.90255	0.11509	0.45604	1.03962	2000
2010	0.05422	0.25293	0.73821	0.08158	0.34918	0.89593	0.11339	0.45087	1.03328	2010
2020	0.05324	0.24929	0.73156	0.08026	0.34475	0.88934	0.11173	0.44576	1.02696	2020
2030	0.05228	0.24569	0.72495	0.07896	0.34038	0.88276	0.11009	0.44070	1.02065	2030
2040	0.05134	0.24214	0.71838	0.07769	0.33606	0.87622	0.10847	0.43570	1.01435	2040
2050	0.05041	0.23865	0.71185	0.07643	0.33179	0.86970	0.10688	0.43076	1.00807	2050
2060	0.04950	0.23520	0.70535	0.07519	0.32757	0.86320	0.10531	0.42586	1.00181	2060
2070	0.04861	0.23180	0.69889	0.07398	0.32341	0.85673	0.10377	0.42103	0.99556	2070
2080	0.04773	0.22845	0.69247	0.07278	0.31929	0.85028	0.10225	0.41625	0.98933	2080
2090	0.04687	0.22514	0.68609	0.07161	0.31523	0.84387	0.10075	0.41152	0.98311	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	T= 800.			T= 900.			T=1000.			ν cm^{-1}
	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	
2100	0.04602	0.22188	0.67975	0.07045	0.31122	0.83747	0.09927	0.40684	0.97691	2100
2110	0.04519	0.21867	0.67344	0.06932	0.30726	0.83111	0.09782	0.40221	0.97073	2110
2120	0.04438	0.21550	0.66717	0.06820	0.30334	0.82477	0.09639	0.39764	0.96456	2120
2130	0.04358	0.21237	0.66095	0.06710	0.29947	0.81846	0.09498	0.39311	0.95841	2130
2140	0.04280	0.20929	0.65476	0.06602	0.29566	0.81217	0.09359	0.38864	0.95228	2140
2150	0.04202	0.20625	0.64861	0.06495	0.29188	0.80592	0.09222	0.38421	0.94616	2150
2160	0.04127	0.20326	0.64250	0.06390	0.28816	0.79969	0.09087	0.37984	0.94007	2160
2170	0.04052	0.20030	0.63643	0.06287	0.28448	0.79349	0.08954	0.37551	0.93399	2170
2180	0.03979	0.19739	0.63039	0.06186	0.28085	0.78731	0.08823	0.37123	0.92793	2180
2190	0.03908	0.19452	0.62440	0.06087	0.27726	0.78117	0.08695	0.36699	0.92189	2190
2200	0.03838	0.19169	0.61845	0.05989	0.27371	0.77505	0.08568	0.36281	0.91587	2200
2210	0.03768	0.18890	0.61253	0.05892	0.27021	0.76896	0.08443	0.35867	0.90986	2210
2220	0.03701	0.18615	0.60666	0.05797	0.26675	0.76290	0.08320	0.35457	0.90388	2220
2230	0.03634	0.18343	0.60082	0.05704	0.26334	0.75687	0.08198	0.35052	0.89792	2230
2240	0.03569	0.18076	0.59502	0.05612	0.25996	0.75087	0.08079	0.34652	0.89197	2240
2250	0.03505	0.17812	0.58927	0.05522	0.25663	0.74490	0.07961	0.34256	0.88605	2250
2260	0.03442	0.17552	0.58355	0.05433	0.25334	0.73895	0.07845	0.33864	0.88014	2260
2270	0.03380	0.17295	0.57787	0.05346	0.25009	0.73304	0.07731	0.33477	0.87426	2270
2280	0.03319	0.17043	0.57223	0.05260	0.24688	0.72715	0.07618	0.33094	0.86839	2280
2290	0.03259	0.16794	0.56663	0.05175	0.24371	0.72130	0.07507	0.32715	0.86255	2290
2300	0.03201	0.16548	0.56108	0.05092	0.24058	0.71547	0.07398	0.32341	0.85673	2300
2310	0.03143	0.16306	0.55556	0.05011	0.23749	0.70968	0.07290	0.31970	0.85093	2310
2320	0.03087	0.16067	0.55007	0.04930	0.23444	0.70391	0.07184	0.31604	0.84515	2320
2330	0.03031	0.15831	0.54463	0.04851	0.23142	0.69818	0.07080	0.31242	0.83939	2330
2340	0.02977	0.15599	0.53923	0.04773	0.22845	0.69247	0.06977	0.30884	0.83365	2340
2350	0.02923	0.15371	0.53387	0.04696	0.22551	0.68680	0.06875	0.30529	0.82793	2350
2360	0.02871	0.15145	0.52855	0.04621	0.22260	0.68115	0.06775	0.30179	0.82224	2360
2370	0.02819	0.14923	0.52326	0.04547	0.21973	0.67554	0.06677	0.29832	0.81657	2370
2380	0.02769	0.14703	0.51802	0.04474	0.21690	0.66995	0.06580	0.29490	0.81092	2380
2390	0.02719	0.14487	0.51281	0.04402	0.21410	0.66440	0.06485	0.29151	0.80529	2390
2400	0.02670	0.14274	0.50765	0.04332	0.21134	0.65888	0.06390	0.28816	0.79969	2400
2410	0.02622	0.14064	0.50252	0.04262	0.20861	0.65339	0.06298	0.28485	0.79410	2410
2420	0.02575	0.13857	0.49743	0.04194	0.20592	0.64793	0.06206	0.28157	0.78854	2420
2430	0.02529	0.13653	0.49238	0.04127	0.20326	0.64250	0.06116	0.27833	0.78301	2430
2440	0.02484	0.13452	0.48737	0.04061	0.20063	0.63710	0.06028	0.27512	0.77749	2440
2450	0.02439	0.13254	0.48240	0.03996	0.19804	0.63173	0.05940	0.27196	0.77200	2450
2460	0.02396	0.13058	0.47747	0.03932	0.19547	0.62639	0.05854	0.26882	0.76653	2460
2470	0.02353	0.12865	0.47257	0.03869	0.19294	0.62109	0.05769	0.26572	0.76109	2470
2480	0.02310	0.12675	0.46772	0.03807	0.19044	0.61581	0.05686	0.26266	0.75567	2480
2490	0.02269	0.12488	0.46290	0.03746	0.18798	0.61057	0.05603	0.25963	0.75027	2490
2500	0.02228	0.12304	0.45812	0.03686	0.18554	0.60536	0.05522	0.25663	0.74490	2500
2510	0.02188	0.12122	0.45338	0.03627	0.18313	0.60017	0.05442	0.25367	0.73954	2510
2520	0.02149	0.11942	0.44868	0.03569	0.18076	0.59502	0.05363	0.25074	0.73422	2520
2530	0.02111	0.11766	0.44401	0.03512	0.17841	0.58991	0.05286	0.24784	0.72892	2530
2540	0.02073	0.11591	0.43938	0.03455	0.17609	0.58482	0.05209	0.24498	0.72364	2540
2550	0.02036	0.11420	0.43479	0.03400	0.17381	0.57976	0.05134	0.24214	0.71838	2550
2560	0.01999	0.11250	0.43024	0.03346	0.17155	0.57473	0.05059	0.23934	0.71315	2560
2570	0.01963	0.11083	0.42573	0.03292	0.16932	0.56974	0.04986	0.23657	0.70794	2570
2580	0.01928	0.10919	0.42125	0.03240	0.16711	0.56478	0.04914	0.23383	0.70276	2580
2590	0.01894	0.10757	0.41681	0.03188	0.16494	0.55985	0.04843	0.23112	0.69760	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	ν cm ⁻¹
	T= 800.			T= 900.			T=1000.			
2600	0.01860	0.10597	0.41241	0.03137	0.16279	0.55494	0.04773	0.22845	0.69247	2600
2610	0.01826	0.10440	0.40804	0.03087	0.16067	0.55007	0.04704	0.22580	0.68736	2610
2620	0.01794	0.10284	0.40371	0.03037	0.15857	0.54524	0.04636	0.22318	0.68228	2620
2630	0.01762	0.10131	0.39942	0.02989	0.15651	0.54043	0.04569	0.22059	0.67722	2630
2640	0.01730	0.09981	0.39517	0.02941	0.15446	0.53565	0.04503	0.21803	0.67218	2640
2650	0.01699	0.09832	0.39095	0.02894	0.15245	0.53091	0.04438	0.21550	0.66717	2650
2660	0.01669	0.09686	0.38676	0.02848	0.15046	0.52619	0.04374	0.21299	0.66219	2660
2670	0.01639	0.09541	0.38261	0.02802	0.14849	0.52151	0.04311	0.21052	0.65723	2670
2680	0.01610	0.09399	0.37850	0.02758	0.14655	0.51686	0.04249	0.20807	0.65229	2680
2690	0.01581	0.09259	0.37443	0.02714	0.14463	0.51224	0.04187	0.20565	0.64738	2690
2700	0.01552	0.09121	0.37039	0.02670	0.14274	0.50765	0.04127	0.20326	0.64250	2700
2710	0.01525	0.08984	0.36638	0.02628	0.14087	0.50309	0.04067	0.20089	0.63764	2710
2720	0.01497	0.08850	0.36241	0.02586	0.13903	0.49856	0.04008	0.19855	0.63280	2720
2730	0.01471	0.08718	0.35848	0.02544	0.13721	0.49406	0.03951	0.19624	0.62799	2730
2740	0.01444	0.08588	0.35458	0.02504	0.13541	0.48959	0.03894	0.19395	0.62321	2740
2750	0.01418	0.08459	0.35072	0.02464	0.13363	0.48516	0.03838	0.19169	0.61845	2750
2760	0.01393	0.08332	0.34689	0.02425	0.13188	0.48075	0.03782	0.18945	0.61371	2760
2770	0.01368	0.08208	0.34309	0.02386	0.13015	0.47638	0.03728	0.18724	0.60900	2770
2780	0.01344	0.08085	0.33933	0.02348	0.12844	0.47203	0.03674	0.18506	0.60432	2780
2790	0.01320	0.07964	0.33560	0.02310	0.12675	0.46772	0.03621	0.18289	0.59966	2790
2800	0.01296	0.07844	0.33191	0.02274	0.12509	0.46343	0.03569	0.18076	0.59502	2800
2810	0.01273	0.07727	0.32825	0.02237	0.12344	0.45918	0.03517	0.17864	0.59042	2810
2820	0.01250	0.07611	0.32462	0.02202	0.12182	0.45495	0.03467	0.17655	0.58583	2820
2830	0.01228	0.07496	0.32103	0.02166	0.12022	0.45076	0.03417	0.17449	0.58127	2830
2840	0.01206	0.07384	0.31747	0.02132	0.11863	0.44660	0.03367	0.17245	0.57674	2840
2850	0.01184	0.07273	0.31394	0.02098	0.11707	0.44246	0.03319	0.17043	0.57223	2850
2860	0.01163	0.07163	0.31045	0.02064	0.11553	0.43836	0.03271	0.16843	0.56775	2860
2870	0.01142	0.07056	0.30698	0.02032	0.11401	0.43429	0.03224	0.16646	0.56329	2870
2880	0.01122	0.06949	0.30356	0.01999	0.11250	0.43024	0.03178	0.16451	0.55886	2880
2890	0.01102	0.06845	0.30016	0.01967	0.11102	0.42623	0.03132	0.16258	0.55446	2890
2900	0.01082	0.06742	0.29679	0.01936	0.10955	0.42224	0.03087	0.16067	0.55007	2900
2910	0.01063	0.06640	0.29346	0.01905	0.10811	0.41829	0.03042	0.15878	0.54572	2910
2920	0.01044	0.06540	0.29016	0.01875	0.10668	0.41436	0.02999	0.15692	0.54139	2920
2930	0.01025	0.06441	0.28689	0.01845	0.10527	0.41046	0.02955	0.15507	0.53708	2930
2940	0.01007	0.06344	0.28365	0.01816	0.10388	0.40660	0.02913	0.15325	0.53280	2940
2950	0.00989	0.06248	0.28044	0.01787	0.10250	0.40276	0.02871	0.15145	0.52855	2950
2960	0.00971	0.06154	0.27726	0.01758	0.10115	0.39895	0.02830	0.14967	0.52432	2960
2970	0.00954	0.06061	0.27412	0.01730	0.09981	0.39517	0.02789	0.14791	0.52011	2970
2980	0.00937	0.05969	0.27100	0.01703	0.09848	0.39141	0.02749	0.14617	0.51593	2980
2990	0.00920	0.05879	0.26791	0.01675	0.09718	0.38769	0.02709	0.14444	0.51178	2990
3000	0.00904	0.05790	0.26486	0.01649	0.09589	0.38399	0.02670	0.14274	0.50765	3000
3010	0.00887	0.05703	0.26183	0.01623	0.09462	0.38033	0.02632	0.14106	0.50354	3010
3020	0.00872	0.05616	0.25883	0.01597	0.09336	0.37669	0.02594	0.13940	0.49946	3020
3030	0.00856	0.05531	0.25587	0.01571	0.09213	0.37308	0.02557	0.13775	0.49541	3030
3040	0.00841	0.05447	0.25293	0.01546	0.09090	0.36950	0.02520	0.13613	0.49138	3040
3050	0.00826	0.05365	0.25002	0.01522	0.08969	0.36594	0.02484	0.13452	0.48737	3050
3060	0.00811	0.05283	0.24714	0.01497	0.08850	0.36241	0.02448	0.13293	0.48339	3060
3070	0.00797	0.05203	0.24429	0.01474	0.08733	0.35892	0.02413	0.13136	0.47944	3070
3080	0.00782	0.05124	0.24147	0.01450	0.08616	0.35544	0.02378	0.12981	0.47550	3080
3090	0.00768	0.05046	0.23867	0.01427	0.08502	0.35200	0.02344	0.12827	0.47160	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	T= 800.			T= 900.			T=1000.			ν cm^{-1}
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
3100	0.00755	0.04970	0.23590	0.01404	0.08389	0.34858	0.02310	0.12675	0.46772	3100
3110	0.00741	0.04894	0.23316	0.01382	0.08277	0.34519	0.02277	0.12525	0.46386	3110
3120	0.00728	0.04820	0.23045	0.01360	0.08167	0.34183	0.02244	0.12377	0.46003	3120
3130	0.00715	0.04746	0.22777	0.01338	0.08058	0.33850	0.02212	0.12231	0.45622	3130
3140	0.00702	0.04674	0.22511	0.01317	0.07950	0.33519	0.02180	0.12086	0.45244	3140
3150	0.00690	0.04603	0.22248	0.01296	0.07844	0.33191	0.02149	0.11942	0.44868	3150
3160	0.00677	0.04533	0.21988	0.01275	0.07740	0.32865	0.02118	0.11801	0.44494	3160
3170	0.00665	0.04464	0.21730	0.01255	0.07636	0.32542	0.02088	0.11661	0.44123	3170
3180	0.00653	0.04396	0.21475	0.01235	0.07534	0.32222	0.02058	0.11522	0.43754	3180
3190	0.00642	0.04329	0.21223	0.01216	0.07434	0.31905	0.02028	0.11386	0.43388	3190
3200	0.00630	0.04263	0.20973	0.01196	0.07334	0.31590	0.01999	0.11250	0.43024	3200
3210	0.00619	0.04198	0.20726	0.01177	0.07236	0.31277	0.01971	0.11117	0.42663	3210
3220	0.00608	0.04134	0.20481	0.01158	0.07139	0.30967	0.01942	0.10984	0.42304	3220
3230	0.00597	0.04071	0.20239	0.01140	0.07044	0.30660	0.01914	0.10854	0.41947	3230
3240	0.00586	0.04008	0.19999	0.01122	0.06949	0.30356	0.01887	0.10725	0.41593	3240
3250	0.00576	0.03947	0.19762	0.01104	0.06856	0.30053	0.01860	0.10597	0.41241	3250
3260	0.00566	0.03887	0.19528	0.01087	0.06764	0.29754	0.01833	0.10471	0.40891	3260
3270	0.00556	0.03827	0.19295	0.01069	0.06674	0.29457	0.01807	0.10346	0.40544	3270
3280	0.00546	0.03769	0.19066	0.01052	0.06584	0.29162	0.01781	0.10223	0.40199	3280
3290	0.00536	0.03711	0.18838	0.01035	0.06496	0.28870	0.01755	0.10101	0.39857	3290
3300	0.00526	0.03654	0.18613	0.01019	0.06409	0.28580	0.01730	0.09981	0.39517	3300
3310	0.00517	0.03598	0.18391	0.01003	0.06323	0.28293	0.01705	0.09862	0.39179	3310
3320	0.00508	0.03543	0.18171	0.00987	0.06238	0.28009	0.01681	0.09744	0.38843	3320
3330	0.00499	0.03489	0.17953	0.00971	0.06154	0.27726	0.01657	0.09628	0.38510	3330
3340	0.00490	0.03435	0.17737	0.00956	0.06071	0.27446	0.01633	0.09513	0.38179	3340
3350	0.00481	0.03383	0.17524	0.00941	0.05990	0.27169	0.01610	0.09399	0.37850	3350
3360	0.00472	0.03331	0.17313	0.00926	0.05909	0.26894	0.01586	0.09287	0.37524	3360
3370	0.00464	0.03279	0.17104	0.00911	0.05830	0.26621	0.01564	0.09176	0.37200	3370
3380	0.00456	0.03229	0.16898	0.00896	0.05751	0.26351	0.01541	0.09066	0.36878	3380
3390	0.00448	0.03179	0.16694	0.00882	0.05674	0.26083	0.01519	0.08957	0.36559	3390
3400	0.00440	0.03131	0.16492	0.00868	0.05597	0.25817	0.01497	0.08850	0.36241	3400
3410	0.00432	0.03082	0.16292	0.00854	0.05522	0.25554	0.01476	0.08744	0.35926	3410
3420	0.00424	0.03035	0.16094	0.00841	0.05447	0.25293	0.01455	0.08639	0.35614	3420
3430	0.00416	0.02988	0.15899	0.00827	0.05374	0.25034	0.01434	0.08536	0.35303	3430
3440	0.00409	0.02942	0.15705	0.00814	0.05301	0.24778	0.01413	0.08434	0.34995	3440
3450	0.00402	0.02897	0.15514	0.00801	0.05230	0.24524	0.01393	0.08332	0.34689	3450
3460	0.00395	0.02852	0.15325	0.00789	0.05159	0.24272	0.01373	0.08233	0.34385	3460
3470	0.00388	0.02808	0.15138	0.00776	0.05090	0.24022	0.01353	0.08134	0.34083	3470
3480	0.00381	0.02765	0.14953	0.00764	0.05021	0.23774	0.01334	0.08036	0.33783	3480
3490	0.00374	0.02723	0.14770	0.00752	0.04953	0.23529	0.01315	0.07940	0.33486	3490
3500	0.00367	0.02681	0.14589	0.00740	0.04886	0.23286	0.01296	0.07844	0.33191	3500
3510	0.00361	0.02639	0.14410	0.00728	0.04820	0.23045	0.01278	0.07750	0.32898	3510
3520	0.00354	0.02598	0.14233	0.00716	0.04755	0.22807	0.01259	0.07657	0.32607	3520
3530	0.00348	0.02558	0.14058	0.00705	0.04690	0.22570	0.01241	0.07565	0.32318	3530
3540	0.00342	0.02519	0.13885	0.00694	0.04627	0.22335	0.01223	0.07474	0.32031	3540
3550	0.00336	0.02480	0.13714	0.00683	0.04564	0.22103	0.01206	0.07384	0.31747	3550
3560	0.00330	0.02441	0.13544	0.00672	0.04502	0.21873	0.01189	0.07295	0.31464	3560
3570	0.00324	0.02404	0.13377	0.00661	0.04441	0.21645	0.01172	0.07207	0.31184	3570
3580	0.00318	0.02367	0.13211	0.00651	0.04381	0.21419	0.01155	0.07120	0.30906	3580
3590	0.00312	0.02330	0.13048	0.00640	0.04321	0.21195	0.01138	0.07034	0.30630	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm ⁻¹
	T= 800.			T= 900.			T=1000.			
3600	0.00307	0.02294	0.12886	0.00630	0.04263	0.20973	0.01122	0.06949	0.30356	3600
3610	0.00301	0.02258	0.12726	0.00620	0.04205	0.20753	0.01106	0.06866	0.30084	3610
3620	0.00296	0.02223	0.12568	0.00610	0.04148	0.20535	0.01090	0.06783	0.29814	3620
3630	0.00291	0.02189	0.12411	0.00601	0.04091	0.20319	0.01074	0.06701	0.29546	3630
3640	0.00285	0.02155	0.12257	0.00591	0.04036	0.20105	0.01059	0.06620	0.29280	3640
3650	0.00280	0.02122	0.12104	0.00582	0.03981	0.19894	0.01044	0.06540	0.29016	3650
3660	0.00275	0.02089	0.11953	0.00572	0.03927	0.19684	0.01029	0.06461	0.28754	3660
3670	0.00270	0.02056	0.11804	0.00563	0.03873	0.19476	0.01014	0.06383	0.28494	3670
3680	0.00266	0.02024	0.11656	0.00554	0.03821	0.19270	0.01000	0.06306	0.28236	3680
3690	0.00261	0.01993	0.11510	0.00546	0.03769	0.19066	0.00985	0.06229	0.27980	3690
3700	0.00256	0.01962	0.11365	0.00537	0.03717	0.18863	0.00971	0.06154	0.27726	3700
3710	0.00252	0.01931	0.11223	0.00528	0.03667	0.18663	0.00957	0.06080	0.27474	3710
3720	0.00247	0.01901	0.11082	0.00520	0.03617	0.18465	0.00944	0.06006	0.27224	3720
3730	0.00243	0.01872	0.10942	0.00512	0.03567	0.18268	0.00930	0.05933	0.26976	3730
3740	0.00238	0.01843	0.10805	0.00504	0.03519	0.18074	0.00917	0.05861	0.26730	3740
3750	0.00234	0.01814	0.10668	0.00496	0.03471	0.17881	0.00904	0.05790	0.26486	3750
3760	0.00230	0.01786	0.10534	0.00488	0.03423	0.17690	0.00891	0.05720	0.26243	3760
3770	0.00226	0.01758	0.10401	0.00480	0.03377	0.17501	0.00878	0.05651	0.26003	3770
3780	0.00222	0.01731	0.10269	0.00472	0.03331	0.17313	0.00865	0.05582	0.25764	3780
3790	0.00218	0.01704	0.10139	0.00465	0.03285	0.17128	0.00853	0.05514	0.25528	3790
3800	0.00214	0.01677	0.10011	0.00458	0.03240	0.16944	0.00841	0.05447	0.25293	3800
3810	0.00210	0.01651	0.09884	0.00450	0.03196	0.16762	0.00829	0.05381	0.25060	3810
3820	0.00206	0.01625	0.09758	0.00443	0.03152	0.16581	0.00817	0.05316	0.24829	3820
3830	0.00203	0.01600	0.09634	0.00436	0.03109	0.16403	0.00805	0.05251	0.24600	3830
3840	0.00199	0.01575	0.09511	0.00429	0.03067	0.16226	0.00794	0.05187	0.24372	3840
3850	0.00196	0.01550	0.09390	0.00422	0.03025	0.16051	0.00782	0.05124	0.24147	3850
3860	0.00192	0.01526	0.09271	0.00416	0.02983	0.15877	0.00771	0.05062	0.23923	3860
3870	0.00189	0.01502	0.09152	0.00409	0.02942	0.15705	0.00760	0.05000	0.23701	3870
3880	0.00185	0.01479	0.09035	0.00403	0.02902	0.15535	0.00749	0.04939	0.23480	3880
3890	0.00182	0.01456	0.08920	0.00396	0.02862	0.15367	0.00738	0.04879	0.23262	3890
3900	0.00179	0.01433	0.08806	0.00390	0.02823	0.15200	0.00728	0.04820	0.23045	3900
3910	0.00176	0.01411	0.08693	0.00384	0.02784	0.15035	0.00717	0.04761	0.22830	3910
3920	0.00172	0.01389	0.08581	0.00378	0.02746	0.14871	0.00707	0.04703	0.22617	3920
3930	0.00169	0.01367	0.08471	0.00372	0.02708	0.14709	0.00697	0.04646	0.22406	3930
3940	0.00166	0.01345	0.08362	0.00366	0.02671	0.14549	0.00687	0.04589	0.22196	3940
3950	0.00163	0.01324	0.08255	0.00360	0.02635	0.14390	0.00677	0.04533	0.21988	3950
3960	0.00160	0.01304	0.08148	0.00354	0.02598	0.14233	0.00668	0.04478	0.21781	3960
3970	0.00158	0.01283	0.08043	0.00349	0.02563	0.14077	0.00658	0.04423	0.21577	3970
3980	0.00155	0.01263	0.07940	0.00343	0.02527	0.13923	0.00649	0.04369	0.21374	3980
3990	0.00152	0.01243	0.07837	0.00338	0.02493	0.13770	0.00639	0.04316	0.21173	3990
4000	0.00149	0.01224	0.07736	0.00332	0.02458	0.13619	0.00630	0.04263	0.20973	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=1100.			T=1200.			T=1300.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
100	4.17062	6.03066	1.98434	4.33292	6.20334	1.98479	4.48299	6.36222	1.98514	100
110	3.99392	5.84156	1.98375	4.15519	6.01419	1.98429	4.30438	6.17304	1.98472	110
120	3.83368	5.66898	1.98310	3.99392	5.84156	1.98375	4.14224	6.00037	1.98425	120
130	3.68727	5.51027	1.98239	3.84648	5.68280	1.98315	3.99392	5.84156	1.98375	130
140	3.55262	5.36339	1.98163	3.71080	5.53585	1.98251	3.85738	5.69457	1.98320	140
150	3.42810	5.22670	1.98081	3.58527	5.39910	1.98182	3.73098	5.55776	1.98261	150
160	3.31241	5.09889	1.97993	3.46857	5.27122	1.98109	3.61341	5.42983	1.98199	160
170	3.20447	4.97888	1.97900	3.35962	5.15114	1.98030	3.50360	5.30969	1.98132	170
180	3.10338	4.86580	1.97802	3.25753	5.03797	1.97947	3.40066	5.19646	1.98061	180
190	3.00842	4.75888	1.97697	3.16156	4.93097	1.97860	3.30384	5.08939	1.97986	190
200	2.91893	4.65750	1.97588	3.07108	4.82950	1.97767	3.21252	4.98786	1.97908	200
210	2.83439	4.56112	1.97472	2.98555	4.73304	1.97670	3.12614	4.89132	1.97825	210
220	2.75434	4.46929	1.97351	2.90451	4.64110	1.97569	3.04426	4.79931	1.97738	220
230	2.67836	4.38159	1.97225	2.82756	4.55330	1.97462	2.96647	4.71143	1.97647	230
240	2.60612	4.29768	1.97093	2.75434	4.46929	1.97351	2.89242	4.62734	1.97553	240
250	2.53731	4.21725	1.96956	2.68455	4.38875	1.97236	2.82180	4.54671	1.97454	250
260	2.47164	4.14003	1.96813	2.61792	4.31141	1.97115	2.75434	4.46929	1.97351	260
270	2.40889	4.06578	1.96664	2.55420	4.23705	1.96991	2.68980	4.39483	1.97245	270
280	2.34884	3.99428	1.96511	2.49319	4.16543	1.96861	2.62797	4.32311	1.97134	280
290	2.29130	3.92535	1.96351	2.43470	4.09637	1.96727	2.56866	4.25396	1.97020	290
300	2.23609	3.85882	1.96187	2.37854	4.02970	1.96588	2.51169	4.18718	1.96901	300
310	2.18307	3.79451	1.96017	2.32457	3.96526	1.96445	2.45691	4.12264	1.96779	310
320	2.13209	3.73231	1.95841	2.27265	3.90292	1.96297	2.40418	4.06018	1.96653	320
330	2.08302	3.67207	1.95660	2.22264	3.84254	1.96145	2.35337	3.99969	1.96523	330
340	2.03574	3.61369	1.95474	2.17443	3.78400	1.95988	2.30437	3.94104	1.96389	340
350	1.99016	3.55705	1.95282	2.12793	3.72722	1.95826	2.25706	3.88413	1.96251	350
360	1.94618	3.50207	1.95086	2.08302	3.67207	1.95660	2.21136	3.82887	1.96109	360
370	1.90369	3.44864	1.94883	2.03962	3.61849	1.95490	2.16717	3.77516	1.95963	370
380	1.86264	3.39670	1.94676	1.99765	3.56638	1.95315	2.12442	3.72292	1.95814	380
390	1.82293	3.34616	1.94463	1.95703	3.51567	1.95135	2.08302	3.67207	1.95660	390
400	1.78450	3.29695	1.94245	1.91769	3.46628	1.94951	2.04290	3.62256	1.95503	400
410	1.74729	3.24902	1.94022	1.87958	3.41817	1.94763	2.00401	3.57430	1.95342	410
420	1.71123	3.20229	1.93794	1.84262	3.37126	1.94570	1.96628	3.52725	1.95177	420
430	1.67627	3.15672	1.93560	1.80677	3.32550	1.94373	1.92966	3.48134	1.95008	430
440	1.64235	3.11224	1.93322	1.77197	3.28084	1.94172	1.89410	3.43653	1.94836	440
450	1.60944	3.06883	1.93078	1.73817	3.23722	1.93966	1.85954	3.39276	1.94660	450
460	1.57748	3.02642	1.92829	1.70533	3.19461	1.93755	1.82594	3.35000	1.94480	460
470	1.54643	2.98497	1.92575	1.67340	3.15297	1.93541	1.79326	3.30819	1.94296	470
480	1.51625	2.94446	1.92316	1.64235	3.11224	1.93322	1.76146	3.26731	1.94109	480
490	1.48691	2.90483	1.92052	1.61214	3.07241	1.93098	1.73050	3.22730	1.93917	490
500	1.45836	2.86606	1.91783	1.58274	3.03342	1.92871	1.70036	3.18815	1.93723	500
510	1.43059	2.82811	1.91509	1.55411	2.99525	1.92639	1.67098	3.14980	1.93524	510
520	1.40355	2.79095	1.91230	1.52621	2.95786	1.92403	1.64235	3.11224	1.93322	520
530	1.37722	2.75455	1.90946	1.49903	2.92124	1.92163	1.61444	3.07544	1.93116	530
540	1.35156	2.71888	1.90658	1.47254	2.88534	1.91918	1.58721	3.03936	1.92906	540
550	1.32657	2.68392	1.90364	1.44670	2.85015	1.91670	1.56065	3.00398	1.92693	550
560	1.30220	2.64965	1.90066	1.42149	2.81563	1.91417	1.53472	2.96928	1.92476	560
570	1.27844	2.61604	1.89762	1.39690	2.78178	1.91160	1.50940	2.93523	1.92256	570
580	1.25526	2.58306	1.89454	1.37290	2.74855	1.90899	1.48468	2.90182	1.92032	580
590	1.23264	2.55070	1.89142	1.34946	2.71594	1.90633	1.46053	2.86901	1.91804	590

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=1100.			T=1200.			T=1300.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
600	1.21057	2.51894	1.88824	1.32657	2.68392	1.90364	1.43693	2.83679	1.91573	600
610	1.18902	2.48775	1.88502	1.30421	2.65248	1.90091	1.41386	2.80515	1.91338	610
620	1.16798	2.45713	1.88175	1.28236	2.62159	1.89813	1.39131	2.77405	1.91100	620
630	1.14743	2.42705	1.87844	1.26100	2.59125	1.89532	1.36925	2.74350	1.90858	630
640	1.12736	2.39749	1.87508	1.24012	2.56142	1.89246	1.34768	2.71346	1.90613	640
650	1.10774	2.36844	1.87167	1.21970	2.53210	1.88957	1.32657	2.68392	1.90364	650
660	1.08856	2.33989	1.86822	1.19973	2.50327	1.88664	1.30591	2.65488	1.90112	660
670	1.06981	2.31183	1.86473	1.18020	2.47493	1.88367	1.28568	2.62631	1.89856	670
680	1.05148	2.28423	1.86119	1.16108	2.44704	1.88065	1.26588	2.59820	1.89597	680
690	1.03355	2.25708	1.85760	1.14237	2.41961	1.87760	1.24649	2.57054	1.89335	690
700	1.01601	2.23038	1.85398	1.12406	2.39261	1.87452	1.22750	2.54332	1.89069	700
710	0.99885	2.20411	1.85031	1.10612	2.36605	1.87139	1.20890	2.51652	1.88800	710
720	0.98206	2.17825	1.84659	1.08856	2.33989	1.86822	1.19066	2.49013	1.88527	720
730	0.96562	2.15281	1.84283	1.07136	2.31415	1.86502	1.17280	2.46415	1.88251	730
740	0.94953	2.12776	1.83903	1.05451	2.28879	1.86178	1.15528	2.43855	1.87972	740
750	0.93377	2.10310	1.83519	1.03800	2.26383	1.85850	1.13811	2.41334	1.87689	750
760	0.91834	2.07882	1.83131	1.02182	2.23923	1.85519	1.12127	2.38850	1.87404	760
770	0.90323	2.05491	1.82738	1.00596	2.21500	1.85184	1.10476	2.36402	1.87115	770
780	0.88843	2.03135	1.82341	0.99041	2.19113	1.84845	1.08856	2.33989	1.86822	780
790	0.87392	2.00815	1.81941	0.97517	2.16760	1.84503	1.07267	2.31611	1.86527	790
800	0.85971	1.98529	1.81536	0.96022	2.14442	1.84157	1.05708	2.29267	1.86228	800
810	0.84578	1.96276	1.81127	0.94556	2.12156	1.83808	1.04178	2.26955	1.85926	810
820	0.83213	1.94056	1.80715	0.93118	2.09903	1.83455	1.02676	2.24676	1.85621	820
830	0.81874	1.91868	1.80298	0.91707	2.07681	1.83098	1.01202	2.22428	1.85313	830
840	0.80562	1.89712	1.79877	0.90323	2.05491	1.82738	0.99755	2.20210	1.85002	840
850	0.79275	1.87585	1.79453	0.88965	2.03330	1.82375	0.98334	2.18023	1.84688	850
860	0.78013	1.85489	1.79025	0.87632	2.01199	1.82008	0.96938	2.15865	1.84370	860
870	0.76776	1.83422	1.78593	0.86324	1.99097	1.81638	0.95568	2.13735	1.84050	870
880	0.75562	1.81383	1.78157	0.85039	1.97024	1.81264	0.94222	2.11633	1.83726	880
890	0.74370	1.79373	1.77718	0.83778	1.94977	1.80887	0.92899	2.09559	1.83400	890
900	0.73202	1.77389	1.77275	0.82540	1.92958	1.80507	0.91600	2.07512	1.83071	900
910	0.72055	1.75433	1.76829	0.81324	1.90966	1.80123	0.90323	2.05491	1.82738	910
920	0.70930	1.73503	1.76379	0.80130	1.89000	1.79736	0.89069	2.03495	1.82403	920
930	0.69825	1.71598	1.75925	0.78958	1.87059	1.79346	0.87835	2.01525	1.82064	930
940	0.68741	1.69719	1.75468	0.77805	1.85142	1.78953	0.86623	1.99580	1.81723	940
950	0.67676	1.67865	1.75007	0.76674	1.83251	1.78557	0.85432	1.97659	1.81379	950
960	0.66631	1.66035	1.74543	0.75562	1.81383	1.78157	0.84261	1.95761	1.81032	960
970	0.65605	1.64228	1.74076	0.74469	1.79539	1.77755	0.83109	1.93887	1.80683	970
980	0.64598	1.62445	1.73605	0.73395	1.77718	1.77349	0.81976	1.92036	1.80330	980
990	0.63608	1.60685	1.73131	0.72340	1.75920	1.76941	0.80863	1.90207	1.79975	990
1000	0.62636	1.58948	1.72654	0.71302	1.74143	1.76529	0.79767	1.88400	1.79617	1000
1010	0.61682	1.57232	1.72173	0.70283	1.72389	1.76114	0.78690	1.86614	1.79256	1010
1020	0.60744	1.55538	1.71690	0.69280	1.70656	1.75697	0.77630	1.84850	1.78893	1020
1030	0.59823	1.53866	1.71203	0.68295	1.68944	1.75276	0.76587	1.83106	1.78526	1030
1040	0.58918	1.52214	1.70713	0.67326	1.67252	1.74853	0.75562	1.81383	1.78157	1040
1050	0.58029	1.50582	1.70221	0.66373	1.65581	1.74427	0.74552	1.79680	1.77786	1050
1060	0.57155	1.48971	1.69725	0.65436	1.63930	1.73998	0.73559	1.77997	1.77412	1060
1070	0.56296	1.47380	1.69226	0.64515	1.62298	1.73566	0.72582	1.76333	1.77035	1070
1080	0.55452	1.45808	1.68724	0.63608	1.60685	1.73131	0.71620	1.74688	1.76656	1080
1090	0.54623	1.44255	1.68220	0.62717	1.59092	1.72694	0.70673	1.73061	1.76274	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
T=1100.			T=1200.			T=1300.				
1100	0.53808	1.42721	1.67713	0.61840	1.57517	1.72254	0.69741	1.71453	1.75890	1100
1110	0.53006	1.41206	1.67202	0.60977	1.55960	1.71811	0.68823	1.69863	1.75503	1110
1120	0.52218	1.39709	1.66690	0.60128	1.54421	1.71366	0.67920	1.68291	1.75114	1120
1130	0.51444	1.38229	1.66174	0.59293	1.52899	1.70918	0.67031	1.66736	1.74722	1130
1140	0.50682	1.36767	1.65656	0.58471	1.51396	1.70467	0.66155	1.65198	1.74328	1140
1150	0.49933	1.35323	1.65135	0.57663	1.49909	1.70014	0.65293	1.63677	1.73931	1150
1160	0.49197	1.33895	1.64612	0.56867	1.48439	1.69559	0.64444	1.62173	1.73532	1160
1170	0.48473	1.32485	1.64086	0.56084	1.46985	1.69101	0.63608	1.60685	1.73131	1170
1180	0.47761	1.31090	1.63557	0.55313	1.45548	1.68641	0.62785	1.59214	1.72728	1180
1190	0.47061	1.29712	1.63026	0.54554	1.44127	1.68178	0.61974	1.57758	1.72322	1190
1200	0.46372	1.28350	1.62493	0.53808	1.42721	1.67713	0.61175	1.56317	1.71913	1200
1210	0.45694	1.27004	1.61957	0.53073	1.41332	1.67245	0.60388	1.54892	1.71503	1210
1220	0.45028	1.25673	1.61420	0.52349	1.39957	1.66775	0.59613	1.53483	1.71090	1220
1230	0.44372	1.24358	1.60879	0.51636	1.38597	1.66303	0.58849	1.52088	1.70676	1230
1240	0.43727	1.23057	1.60337	0.50935	1.37253	1.65829	0.58097	1.50707	1.70259	1240
1250	0.43093	1.21772	1.59792	0.50244	1.35923	1.65352	0.57355	1.49341	1.69839	1250
1260	0.42468	1.20501	1.59246	0.49564	1.34607	1.64874	0.56625	1.47990	1.69418	1260
1270	0.41854	1.19244	1.58697	0.48894	1.33306	1.64393	0.55905	1.46652	1.68995	1270
1280	0.41249	1.18001	1.58146	0.48234	1.32018	1.63910	0.55196	1.45328	1.68569	1280
1290	0.40655	1.16773	1.57593	0.47585	1.30744	1.63425	0.54497	1.44018	1.68142	1290
1300	0.40069	1.15558	1.57038	0.46945	1.29484	1.62938	0.53808	1.42721	1.67713	1300
1310	0.39493	1.14357	1.56481	0.46315	1.28238	1.62449	0.53129	1.41438	1.67281	1310
1320	0.38926	1.13169	1.55922	0.45694	1.27004	1.61957	0.52459	1.40167	1.66848	1320
1330	0.38368	1.11994	1.55362	0.45083	1.25784	1.61464	0.51800	1.38910	1.66412	1330
1340	0.37819	1.10833	1.54800	0.44481	1.24576	1.60970	0.51149	1.37665	1.65975	1340
1350	0.37278	1.09684	1.54235	0.43887	1.23381	1.60473	0.50508	1.36433	1.65536	1350
1360	0.36746	1.08548	1.53670	0.43303	1.22199	1.59974	0.49876	1.35213	1.65095	1360
1370	0.36222	1.07424	1.53102	0.42727	1.21028	1.59474	0.49253	1.34005	1.64652	1370
1380	0.35707	1.06312	1.52533	0.42160	1.19870	1.58971	0.48639	1.32809	1.64207	1380
1390	0.35199	1.05213	1.51962	0.41601	1.18724	1.58467	0.48033	1.31625	1.63761	1390
1400	0.34699	1.04126	1.51390	0.41050	1.17590	1.57962	0.47436	1.30452	1.63312	1400
1410	0.34207	1.03050	1.50816	0.40507	1.16468	1.57454	0.46847	1.29292	1.62863	1410
1420	0.33723	1.01987	1.50241	0.39973	1.15357	1.56945	0.46267	1.28142	1.62411	1420
1430	0.33246	1.00934	1.49664	0.39446	1.14257	1.56435	0.45694	1.27004	1.61957	1430
1440	0.32776	0.99893	1.49086	0.38926	1.13169	1.55922	0.45130	1.25877	1.61502	1440
1450	0.32314	0.98864	1.48506	0.38414	1.12092	1.55409	0.44573	1.24761	1.61046	1450
1460	0.31858	0.97845	1.47926	0.37910	1.11025	1.54893	0.44024	1.23656	1.60588	1460
1470	0.31410	0.96837	1.47344	0.37413	1.09970	1.54377	0.43482	1.22561	1.60128	1470
1480	0.30968	0.95840	1.46761	0.36923	1.08925	1.53858	0.42948	1.21477	1.59666	1480
1490	0.30533	0.94854	1.46176	0.36440	1.07891	1.53339	0.42421	1.20403	1.59203	1490
1500	0.30104	0.93878	1.45591	0.35964	1.06867	1.52818	0.41901	1.19340	1.58739	1500
1510	0.29683	0.92913	1.45004	0.35494	1.05853	1.52295	0.41388	1.18287	1.58273	1510
1520	0.29267	0.91957	1.44416	0.35032	1.04849	1.51772	0.40882	1.17244	1.57806	1520
1530	0.28858	0.91012	1.43828	0.34576	1.03856	1.51247	0.40383	1.16210	1.57337	1530
1540	0.28454	0.90077	1.43238	0.34126	1.02872	1.50720	0.39891	1.15187	1.56867	1540
1550	0.28057	0.89152	1.42647	0.33683	1.01898	1.50193	0.39405	1.14173	1.56395	1550
1560	0.27666	0.88237	1.42056	0.33246	1.00934	1.49664	0.38926	1.13169	1.55922	1560
1570	0.27281	0.87331	1.41463	0.32815	0.99980	1.49134	0.38453	1.12174	1.55448	1570
1580	0.26901	0.86435	1.40870	0.32390	0.99034	1.48603	0.37987	1.11189	1.54973	1580
1590	0.26527	0.85548	1.40276	0.31971	0.98099	1.48071	0.37527	1.10212	1.54496	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=1100.			T=1200.			T=1300.				
1600	0.26159	0.84670	1.39681	0.31558	0.97172	1.47538	0.37073	1.09245	1.54018	1600
1610	0.25796	0.83802	1.39086	0.31151	0.96254	1.47004	0.36625	1.08287	1.53539	1610
1620	0.25438	0.82942	1.38490	0.30750	0.95346	1.46468	0.36182	1.07338	1.53058	1620
1630	0.25086	0.82092	1.37893	0.30354	0.94446	1.45932	0.35746	1.06398	1.52577	1630
1640	0.24739	0.81250	1.37295	0.29963	0.93555	1.45395	0.35316	1.05466	1.52094	1640
1650	0.24396	0.80417	1.36698	0.29578	0.92673	1.44857	0.34891	1.04543	1.51610	1650
1660	0.24059	0.79593	1.36099	0.29198	0.91799	1.44318	0.34471	1.03628	1.51125	1660
1670	0.23727	0.78778	1.35500	0.28824	0.90934	1.43778	0.34057	1.02722	1.50639	1670
1680	0.23400	0.77971	1.34901	0.28454	0.90077	1.43238	0.33649	1.01824	1.50152	1680
1690	0.23078	0.77172	1.34301	0.28090	0.89229	1.42696	0.33246	1.00934	1.49664	1690
1700	0.22760	0.76381	1.33701	0.27731	0.88389	1.42154	0.32848	1.00053	1.49175	1700
1710	0.22447	0.75599	1.33101	0.27376	0.87556	1.41611	0.32455	0.99179	1.48685	1710
1720	0.22138	0.74824	1.32500	0.27027	0.86732	1.41068	0.32067	0.98314	1.48194	1720
1730	0.21834	0.74058	1.31899	0.26682	0.85916	1.40524	0.31685	0.97456	1.47702	1730
1740	0.21535	0.73299	1.31298	0.26342	0.85108	1.39979	0.31307	0.96606	1.47209	1740
1750	0.21239	0.72549	1.30696	0.26007	0.84307	1.39433	0.30934	0.95764	1.46716	1750
1760	0.20948	0.71806	1.30095	0.25676	0.83514	1.38887	0.30566	0.94929	1.46221	1760
1770	0.20661	0.71070	1.29493	0.25349	0.82729	1.38340	0.30203	0.94102	1.45726	1770
1780	0.20378	0.70343	1.28891	0.25027	0.81951	1.37793	0.29844	0.93283	1.45230	1780
1790	0.20100	0.69622	1.28289	0.24710	0.81181	1.37246	0.29490	0.92471	1.44733	1790
1800	0.19825	0.68909	1.27687	0.24396	0.80417	1.36698	0.29140	0.91666	1.44235	1800
1810	0.19554	0.68203	1.27086	0.24087	0.79662	1.36149	0.28795	0.90868	1.43737	1810
1820	0.19288	0.67505	1.26484	0.23782	0.78913	1.35600	0.28454	0.90077	1.43238	1820
1830	0.19025	0.66813	1.25882	0.23482	0.78172	1.35051	0.28118	0.89294	1.42738	1830
1840	0.18765	0.66129	1.25281	0.23185	0.77437	1.34501	0.27786	0.88517	1.42238	1840
1850	0.18510	0.65452	1.24679	0.22892	0.76710	1.33951	0.27458	0.87748	1.41737	1850
1860	0.18258	0.64781	1.24078	0.22603	0.75989	1.33401	0.27134	0.86985	1.41235	1860
1870	0.18009	0.64117	1.23477	0.22318	0.75275	1.32850	0.26814	0.86229	1.40733	1870
1880	0.17765	0.63461	1.22876	0.22036	0.74568	1.32299	0.26499	0.85480	1.40230	1880
1890	0.17523	0.62810	1.22276	0.21759	0.73868	1.31748	0.26187	0.84737	1.39727	1890
1900	0.17285	0.62167	1.21675	0.21485	0.73174	1.31197	0.25879	0.84001	1.39223	1900
1910	0.17051	0.61529	1.21076	0.21215	0.72487	1.30646	0.25575	0.83272	1.38719	1910
1920	0.16820	0.60899	1.20476	0.20948	0.71806	1.30094	0.25275	0.82549	1.38214	1920
1930	0.16592	0.60274	1.19877	0.20685	0.71131	1.29543	0.24978	0.81832	1.37709	1930
1940	0.16367	0.59656	1.19279	0.20425	0.70463	1.28991	0.24686	0.81122	1.37203	1940
1950	0.16145	0.59045	1.18680	0.20169	0.69802	1.28440	0.24396	0.80417	1.36698	1950
1960	0.15927	0.58439	1.18083	0.19916	0.69146	1.27888	0.24111	0.79720	1.36191	1960
1970	0.15712	0.57840	1.17486	0.19667	0.68497	1.27336	0.23829	0.79028	1.35685	1970
1980	0.15499	0.57246	1.16889	0.19420	0.67853	1.26785	0.23551	0.78342	1.35178	1980
1990	0.15290	0.56659	1.16293	0.19177	0.67216	1.26233	0.23276	0.77662	1.34670	1990
2000	0.15083	0.56078	1.15698	0.18938	0.66585	1.25682	0.23004	0.76989	1.34163	2000
2010	0.14880	0.55502	1.15103	0.18701	0.65959	1.25130	0.22736	0.76321	1.33655	2010
2020	0.14679	0.54932	1.14509	0.18467	0.65339	1.24579	0.22471	0.75659	1.33147	2020
2030	0.14481	0.54368	1.13916	0.18237	0.64726	1.24028	0.22209	0.75002	1.32638	2030
2040	0.14286	0.53810	1.13323	0.18009	0.64117	1.23477	0.21951	0.74352	1.32130	2040
2050	0.14094	0.53257	1.12731	0.17785	0.63515	1.22926	0.21695	0.73707	1.31621	2050
2060	0.13904	0.52710	1.12140	0.17563	0.62918	1.22376	0.21443	0.73068	1.31112	2060
2070	0.13717	0.52169	1.11550	0.17345	0.62327	1.21825	0.21194	0.72434	1.30604	2070
2080	0.13533	0.51632	1.10961	0.17129	0.61741	1.21276	0.20948	0.71806	1.30094	2080
2090	0.13351	0.51102	1.10372	0.16916	0.61161	1.20726	0.20705	0.71183	1.29585	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=1100.			T=1200.			T=1300.				
2100	0.13171	0.50576	1.09784	0.16705	0.60586	1.20177	0.20465	0.70566	1.29076	2100
2110	0.12994	0.50056	1.09198	0.16498	0.60016	1.19628	0.20228	0.69954	1.28567	2110
2120	0.12820	0.49541	1.08612	0.16293	0.59452	1.19079	0.19994	0.69347	1.28058	2120
2130	0.12648	0.49031	1.08027	0.16090	0.58893	1.18531	0.19762	0.68746	1.27548	2130
2140	0.12478	0.48527	1.07443	0.15891	0.58339	1.17983	0.19534	0.68149	1.27039	2140
2150	0.12311	0.48027	1.06860	0.15694	0.57790	1.17436	0.19308	0.67558	1.26530	2150
2160	0.12146	0.47533	1.06278	0.15499	0.57246	1.16889	0.19085	0.66972	1.26021	2160
2170	0.11983	0.47043	1.05698	0.15307	0.56708	1.16343	0.18865	0.66391	1.25512	2170
2180	0.11823	0.46558	1.05118	0.15118	0.56174	1.15797	0.18647	0.65816	1.25003	2180
2190	0.11665	0.46079	1.04539	0.14930	0.55645	1.15252	0.18432	0.65245	1.24494	2190
2200	0.11509	0.45604	1.03962	0.14746	0.55122	1.14707	0.18219	0.64679	1.23985	2200
2210	0.11355	0.45134	1.03386	0.14563	0.54603	1.14163	0.18009	0.64117	1.23477	2210
2220	0.11203	0.44668	1.02810	0.14383	0.54088	1.13619	0.17802	0.63561	1.22969	2220
2230	0.11053	0.44207	1.02237	0.14206	0.53579	1.13077	0.17597	0.63010	1.22460	2230
2240	0.10906	0.43751	1.01664	0.14030	0.53074	1.12534	0.17395	0.62463	1.21952	2240
2250	0.10760	0.43300	1.01092	0.13857	0.52574	1.11993	0.17195	0.61921	1.21445	2250
2260	0.10616	0.42853	1.00522	0.13686	0.52079	1.11452	0.16997	0.61383	1.20937	2260
2270	0.10475	0.42410	0.99953	0.13517	0.51588	1.10912	0.16802	0.60850	1.20430	2270
2280	0.10335	0.41972	0.99386	0.13351	0.51102	1.10372	0.16609	0.60322	1.19923	2280
2290	0.10197	0.41538	0.98819	0.13186	0.50620	1.09833	0.16418	0.59799	1.19417	2290
2300	0.10061	0.41109	0.98254	0.13024	0.50142	1.09295	0.16230	0.59279	1.18910	2300
2310	0.09927	0.40684	0.97691	0.12863	0.49669	1.08758	0.16044	0.58765	1.18405	2310
2320	0.09795	0.40263	0.97129	0.12705	0.49201	1.08222	0.15860	0.58254	1.17899	2320
2330	0.09665	0.39846	0.96568	0.12549	0.48736	1.07686	0.15679	0.57748	1.17394	2330
2340	0.09536	0.39434	0.96008	0.12394	0.48276	1.07151	0.15499	0.57246	1.16889	2340
2350	0.09409	0.39026	0.95451	0.12242	0.47821	1.06618	0.15322	0.56749	1.16385	2350
2360	0.09284	0.38622	0.94894	0.12092	0.47369	1.06085	0.15147	0.56256	1.15881	2360
2370	0.09160	0.38222	0.94339	0.11943	0.46921	1.05553	0.14973	0.55767	1.15378	2370
2380	0.09039	0.37826	0.93785	0.11796	0.46478	1.05021	0.14802	0.55282	1.14875	2380
2390	0.08918	0.37434	0.93233	0.11652	0.46039	1.04491	0.14633	0.54802	1.14372	2390
2400	0.08800	0.37045	0.92683	0.11509	0.45604	1.03962	0.14466	0.54325	1.13870	2400
2410	0.08683	0.36661	0.92134	0.11367	0.45173	1.03434	0.14301	0.53853	1.13369	2410
2420	0.08568	0.36281	0.91587	0.11228	0.44745	1.02906	0.14138	0.53384	1.12868	2420
2430	0.08454	0.35904	0.91041	0.11090	0.44322	1.02380	0.13977	0.52920	1.12368	2430
2440	0.08342	0.35531	0.90497	0.10955	0.43903	1.01855	0.13817	0.52459	1.11868	2440
2450	0.08231	0.35162	0.89954	0.10820	0.43487	1.01330	0.13660	0.52003	1.11369	2450
2460	0.08122	0.34797	0.89413	0.10688	0.43076	1.00807	0.13504	0.51550	1.10870	2460
2470	0.08014	0.34435	0.88874	0.10557	0.42668	1.00285	0.13351	0.51102	1.10372	2470
2480	0.07908	0.34077	0.88336	0.10428	0.42263	0.99764	0.13199	0.50657	1.09875	2480
2490	0.07803	0.33723	0.87800	0.10300	0.41863	0.99244	0.13049	0.50215	1.09378	2490
2500	0.07700	0.33372	0.87266	0.10174	0.41466	0.98725	0.12900	0.49778	1.08882	2500
2510	0.07598	0.33025	0.86733	0.10050	0.41073	0.98207	0.12754	0.49344	1.08387	2510
2520	0.07497	0.32681	0.86202	0.09927	0.40684	0.97691	0.12609	0.48914	1.07892	2520
2530	0.07398	0.32341	0.85673	0.09806	0.40298	0.97175	0.12465	0.48488	1.07398	2530
2540	0.07300	0.32004	0.85145	0.09686	0.39916	0.96661	0.12324	0.48065	1.06905	2540
2550	0.07203	0.31670	0.84620	0.09568	0.39537	0.96148	0.12184	0.47646	1.06413	2550
2560	0.07108	0.31340	0.84096	0.09451	0.39161	0.95636	0.12046	0.47231	1.05921	2560
2570	0.07014	0.31013	0.83573	0.09336	0.38790	0.95126	0.11909	0.46819	1.05430	2570
2580	0.06921	0.30690	0.83053	0.09222	0.38421	0.94616	0.11774	0.46410	1.04940	2580
2590	0.06830	0.30370	0.82534	0.09109	0.38056	0.94108	0.11641	0.46005	1.04450	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	ν cm ⁻¹
	T=1100.			T=1200.			T=1300.			
2600	0.06740	0.30052	0.82018	0.08998	0.37694	0.93601	0.11509	0.45604	1.03962	2600
2610	0.06650	0.29739	0.81503	0.08889	0.37336	0.93096	0.11378	0.45206	1.03474	2610
2620	0.06563	0.29428	0.80989	0.08780	0.36981	0.92591	0.11249	0.44811	1.02987	2620
2630	0.06476	0.29120	0.80478	0.08673	0.36629	0.92088	0.11122	0.44419	1.02501	2630
2640	0.06390	0.28816	0.79969	0.08568	0.36281	0.91587	0.10996	0.44031	1.02016	2640
2650	0.06306	0.28515	0.79461	0.08463	0.35935	0.91086	0.10872	0.43647	1.01532	2650
2660	0.06223	0.28216	0.78955	0.08360	0.35593	0.90587	0.10749	0.43265	1.01049	2660
2670	0.06141	0.27921	0.78451	0.08259	0.35254	0.90090	0.10627	0.42887	1.00566	2670
2680	0.06060	0.27629	0.77950	0.08158	0.34918	0.89593	0.10507	0.42512	1.00084	2680
2690	0.05980	0.27339	0.77449	0.08059	0.34586	0.89098	0.10388	0.42140	0.99604	2690
2700	0.05901	0.27053	0.76951	0.07961	0.34256	0.88605	0.10271	0.41771	0.99124	2700
2710	0.05823	0.26769	0.76455	0.07864	0.33929	0.88112	0.10155	0.41406	0.98645	2710
2720	0.05746	0.26488	0.75961	0.07769	0.33606	0.87622	0.10040	0.41043	0.98168	2720
2730	0.05670	0.26211	0.75468	0.07674	0.33285	0.87132	0.09927	0.40684	0.97691	2730
2740	0.05596	0.25936	0.74978	0.07581	0.32967	0.86644	0.09815	0.40327	0.97215	2740
2750	0.05522	0.25663	0.74490	0.07489	0.32653	0.86158	0.09704	0.39974	0.96740	2750
2760	0.05449	0.25394	0.74003	0.07398	0.32341	0.85673	0.09595	0.39624	0.96266	2760
2770	0.05377	0.25127	0.73518	0.07308	0.32032	0.85189	0.09487	0.39277	0.95794	2770
2780	0.05307	0.24863	0.73036	0.07219	0.31726	0.84707	0.09380	0.38932	0.95322	2780
2790	0.05237	0.24602	0.72555	0.07132	0.31422	0.84226	0.09274	0.38591	0.94851	2790
2800	0.05168	0.24343	0.72077	0.07045	0.31122	0.83747	0.09170	0.38252	0.94382	2800
2810	0.05100	0.24087	0.71600	0.06960	0.30824	0.83270	0.09066	0.37917	0.93913	2810
2820	0.05033	0.23833	0.71126	0.06875	0.30529	0.82793	0.08964	0.37584	0.93446	2820
2830	0.04966	0.23582	0.70653	0.06792	0.30237	0.82319	0.08864	0.37254	0.92979	2830
2840	0.04901	0.23334	0.70182	0.06710	0.29947	0.81846	0.08764	0.36927	0.92514	2840
2850	0.04837	0.23088	0.69714	0.06628	0.29661	0.81374	0.08665	0.36602	0.92050	2850
2860	0.04773	0.22845	0.69247	0.06548	0.29376	0.80904	0.08568	0.36281	0.91587	2860
2870	0.04710	0.22604	0.68783	0.06469	0.29095	0.80436	0.08471	0.35962	0.91125	2870
2880	0.04648	0.22365	0.68320	0.06390	0.28816	0.79969	0.08376	0.35646	0.90664	2880
2890	0.04587	0.22129	0.67860	0.06313	0.28540	0.79503	0.08282	0.35332	0.90204	2890
2900	0.04527	0.21896	0.67401	0.06237	0.28266	0.79039	0.08189	0.35021	0.89746	2900
2910	0.04467	0.21664	0.66945	0.06161	0.27994	0.78577	0.08097	0.34713	0.89288	2910
2920	0.04409	0.21436	0.66491	0.06087	0.27726	0.78117	0.08006	0.34408	0.88832	2920
2930	0.04351	0.21209	0.66038	0.06013	0.27459	0.77658	0.07916	0.34105	0.88377	2930
2940	0.04294	0.20985	0.65588	0.05940	0.27196	0.77200	0.07827	0.33805	0.87924	2940
2950	0.04237	0.20763	0.65140	0.05868	0.26934	0.76744	0.07739	0.33507	0.87471	2950
2960	0.04182	0.20543	0.64694	0.05797	0.26675	0.76290	0.07653	0.33212	0.87020	2960
2970	0.04127	0.20326	0.64250	0.05727	0.26419	0.75838	0.07567	0.32919	0.86569	2970
2980	0.04073	0.20111	0.63808	0.05658	0.26165	0.75387	0.07482	0.32629	0.86121	2980
2990	0.04019	0.19897	0.63368	0.05590	0.25913	0.74937	0.07398	0.32341	0.85673	2990
3000	0.03966	0.19687	0.62930	0.05522	0.25663	0.74490	0.07315	0.32055	0.85226	3000
3010	0.03914	0.19478	0.62494	0.05455	0.25416	0.74044	0.07233	0.31773	0.84781	3010
3020	0.03863	0.19271	0.62061	0.05389	0.25171	0.73599	0.07152	0.31492	0.84337	3020
3030	0.03812	0.19067	0.61629	0.05324	0.24929	0.73156	0.07072	0.31214	0.83895	3030
3040	0.03762	0.18865	0.61200	0.05260	0.24688	0.72715	0.06993	0.30938	0.83453	3040
3050	0.03713	0.18664	0.60772	0.05196	0.24450	0.72276	0.06914	0.30665	0.83013	3050
3060	0.03664	0.18466	0.60347	0.05134	0.24214	0.71838	0.06837	0.30394	0.82574	3060
3070	0.03616	0.18270	0.59924	0.05072	0.23981	0.71402	0.06760	0.30125	0.82137	3070
3080	0.03569	0.18076	0.59502	0.05011	0.23749	0.70968	0.06685	0.29859	0.81700	3080
3090	0.03522	0.17883	0.59083	0.04950	0.23520	0.70535	0.06610	0.29595	0.81266	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹	
T=1100.			T=1200.			T=1300.					
3100	0.03476	0.17693	0.58666	0.04890	0.23293	0.70104	0.06536	0.29333	0.80832	3100	
3110	0.03430	0.17505	0.58251	0.04831	0.23068	0.69675	0.06463	0.29073	0.80400	3110	
3120	0.03385	0.17319	0.57839	0.04773	0.22845	0.69247	0.06390	0.28816	0.79969	3120	
3130	0.03341	0.17134	0.57428	0.04715	0.22624	0.68821	0.06319	0.28561	0.79539	3130	
3140	0.03297	0.16952	0.57019	0.04659	0.22405	0.68397	0.06248	0.28308	0.79111	3140	
3150	0.03254	0.16771	0.56613	0.04602	0.22188	0.67975	0.06178	0.28057	0.78684	3150	
3160	0.03211	0.16592	0.56208	0.04547	0.21973	0.67554	0.06109	0.27808	0.78258	3160	
3170	0.03169	0.16415	0.55806	0.04492	0.21761	0.67135	0.06041	0.27561	0.77834	3170	
3180	0.03128	0.16240	0.55406	0.04438	0.21550	0.66717	0.05974	0.27317	0.77411	3180	
3190	0.03087	0.16067	0.55007	0.04385	0.21341	0.66302	0.05907	0.27075	0.76990	3190	
3200	0.03046	0.15895	0.54611	0.04332	0.21134	0.65888	0.05841	0.26834	0.76569	3200	
3210	0.03006	0.15725	0.54217	0.04280	0.20929	0.65476	0.05776	0.26596	0.76151	3210	
3220	0.02967	0.15557	0.53825	0.04228	0.20726	0.65065	0.05711	0.26360	0.75733	3220	
3230	0.02928	0.15391	0.53436	0.04177	0.20525	0.64657	0.05647	0.26126	0.75317	3230	
3240	0.02890	0.15227	0.53048	0.04127	0.20326	0.64250	0.05584	0.25893	0.74903	3240	
3250	0.02852	0.15064	0.52662	0.04077	0.20128	0.63845	0.05522	0.25663	0.74490	3250	
3260	0.02815	0.14903	0.52278	0.04028	0.19933	0.63441	0.05460	0.25435	0.74078	3260	
3270	0.02778	0.14743	0.51897	0.03979	0.19739	0.63039	0.05399	0.25209	0.73667	3270	
3280	0.02742	0.14585	0.51517	0.03932	0.19547	0.62639	0.05339	0.24984	0.73258	3280	
3290	0.02706	0.14429	0.51140	0.03884	0.19357	0.62241	0.05280	0.24762	0.72851	3290	
3300	0.02670	0.14274	0.50765	0.03838	0.19169	0.61845	0.05221	0.24542	0.72445	3300	
3310	0.02635	0.14121	0.50391	0.03791	0.18982	0.61450	0.05163	0.24323	0.72040	3310	
3320	0.02601	0.13970	0.50020	0.03746	0.18798	0.61057	0.05105	0.24106	0.71637	3320	
3330	0.02567	0.13820	0.49651	0.03701	0.18615	0.60666	0.05048	0.23891	0.71235	3330	
3340	0.02533	0.13672	0.49284	0.03656	0.18433	0.60276	0.04992	0.23678	0.70834	3340	
3350	0.02500	0.13525	0.48919	0.03612	0.18254	0.59888	0.04936	0.23467	0.70435	3350	
3360	0.02467	0.13379	0.48556	0.03569	0.18076	0.59502	0.04881	0.23258	0.70038	3360	
3370	0.02435	0.13236	0.48195	0.03526	0.17899	0.59118	0.04827	0.23050	0.69642	3370	
3380	0.02403	0.13093	0.47836	0.03483	0.17725	0.58736	0.04773	0.22845	0.69247	3380	
3390	0.02372	0.12953	0.47479	0.03442	0.17552	0.58355	0.04720	0.22641	0.68854	3390	
3400	0.02341	0.12813	0.47124	0.03400	0.17381	0.57976	0.04667	0.22438	0.68462	3400	
3410	0.02310	0.12675	0.46772	0.03359	0.17211	0.57599	0.04615	0.22238	0.68072	3410	
3420	0.02280	0.12539	0.46421	0.03319	0.17043	0.57223	0.04564	0.22039	0.67683	3420	
3430	0.02250	0.12404	0.46072	0.03279	0.16876	0.56850	0.04513	0.21842	0.67296	3430	
3440	0.02221	0.12270	0.45726	0.03240	0.16711	0.56478	0.04463	0.21647	0.66910	3440	
3450	0.02192	0.12138	0.45381	0.03201	0.16548	0.56108	0.04413	0.21453	0.66525	3450	
3460	0.02163	0.12007	0.45038	0.03162	0.16386	0.55739	0.04364	0.21261	0.66142	3460	
3470	0.02135	0.11878	0.44698	0.03124	0.16226	0.55372	0.04316	0.21071	0.65761	3470	
3480	0.02107	0.11750	0.44359	0.03087	0.16067	0.55007	0.04268	0.20882	0.65381	3480	
3490	0.02080	0.11623	0.44022	0.03050	0.15910	0.54644	0.04220	0.20695	0.65002	3490	
3500	0.02052	0.11497	0.43688	0.03013	0.15754	0.54283	0.04173	0.20510	0.64625	3500	
3510	0.02026	0.11373	0.43355	0.02977	0.15599	0.53923	0.04127	0.20326	0.64250	3510	
3520	0.01999	0.11250	0.43024	0.02941	0.15446	0.53565	0.04081	0.20143	0.63876	3520	
3530	0.01973	0.11129	0.42696	0.02906	0.15295	0.53209	0.04035	0.19963	0.63503	3530	
3540	0.01947	0.11008	0.42369	0.02871	0.15145	0.52855	0.03991	0.19784	0.63132	3540	
3550	0.01922	0.10889	0.42044	0.02836	0.14996	0.52502	0.03946	0.19606	0.62762	3550	
3560	0.01897	0.10772	0.41721	0.02802	0.14849	0.52151	0.03902	0.19430	0.62394	3560	
3570	0.01872	0.10655	0.41400	0.02769	0.14703	0.51802	0.03859	0.19256	0.62027	3570	
3580	0.01848	0.10540	0.41082	0.02736	0.14559	0.51454	0.03816	0.19083	0.61662	3580	
3590	0.01823	0.10425	0.40765	0.02703	0.14416	0.51109	0.03774	0.18911	0.61299	3590	

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
	T=1100.			T=1200.			T=1300.			
3600	0.01800	0.10312	0.40450	0.02670	0.14274	0.50765	0.03732	0.18741	0.60936	3600
3610	0.01776	0.10201	0.40137	0.02638	0.14134	0.50422	0.03690	0.18573	0.60576	3610
3620	0.01753	0.10090	0.39826	0.02607	0.13995	0.50082	0.03649	0.18405	0.60216	3620
3630	0.01730	0.09981	0.39517	0.02575	0.13857	0.49743	0.03609	0.18240	0.59859	3630
3640	0.01708	0.09872	0.39209	0.02544	0.13721	0.49406	0.03569	0.18076	0.59502	3640
3650	0.01685	0.09765	0.38904	0.02514	0.13586	0.49071	0.03529	0.17913	0.59148	3650
3660	0.01663	0.09659	0.38601	0.02484	0.13452	0.48737	0.03490	0.17752	0.58794	3660
3670	0.01642	0.09554	0.38299	0.02454	0.13319	0.48405	0.03451	0.17592	0.58443	3670
3680	0.01620	0.09450	0.37999	0.02425	0.13188	0.48075	0.03413	0.17433	0.58092	3680
3690	0.01599	0.09348	0.37702	0.02396	0.13058	0.47747	0.03375	0.17276	0.57744	3690
3700	0.01578	0.09246	0.37406	0.02367	0.12929	0.47420	0.03337	0.17120	0.57396	3700
3710	0.01558	0.09146	0.37112	0.02338	0.12802	0.47095	0.03300	0.16966	0.57051	3710
3720	0.01537	0.09046	0.36820	0.02310	0.12675	0.46772	0.03264	0.16813	0.56706	3720
3730	0.01517	0.08948	0.36530	0.02283	0.12550	0.46450	0.03228	0.16661	0.56364	3730
3740	0.01497	0.08850	0.36241	0.02255	0.12426	0.46130	0.03192	0.16510	0.56022	3740
3750	0.01478	0.08754	0.35955	0.02228	0.12304	0.45812	0.03156	0.16361	0.55683	3750
3760	0.01459	0.08658	0.35670	0.02202	0.12182	0.45495	0.03121	0.16213	0.55344	3760
3770	0.01440	0.08564	0.35388	0.02175	0.12062	0.45181	0.03087	0.16067	0.55007	3770
3780	0.01421	0.08471	0.35107	0.02149	0.11942	0.44868	0.03053	0.15922	0.54672	3780
3790	0.01402	0.08378	0.34827	0.02123	0.11824	0.44556	0.03019	0.15778	0.54338	3790
3800	0.01384	0.08287	0.34550	0.02098	0.11707	0.44246	0.02985	0.15635	0.54006	3800
3810	0.01366	0.08196	0.34275	0.02073	0.11591	0.43938	0.02952	0.15493	0.53675	3810
3820	0.01348	0.08107	0.34001	0.02048	0.11477	0.43632	0.02919	0.15353	0.53346	3820
3830	0.01331	0.08018	0.33729	0.02023	0.11363	0.43327	0.02887	0.15214	0.53018	3830
3840	0.01313	0.07931	0.33459	0.01999	0.11250	0.43024	0.02855	0.15076	0.52692	3840
3850	0.01296	0.07844	0.33191	0.01975	0.11139	0.42723	0.02823	0.14940	0.52367	3850
3860	0.01279	0.07758	0.32924	0.01952	0.11028	0.42423	0.02792	0.14804	0.52043	3860
3870	0.01263	0.07674	0.32660	0.01928	0.10919	0.42125	0.02761	0.14670	0.51721	3870
3880	0.01246	0.07590	0.32397	0.01905	0.10811	0.41829	0.02730	0.14537	0.51401	3880
3890	0.01230	0.07507	0.32135	0.01882	0.10703	0.41534	0.02700	0.14405	0.51082	3890
3900	0.01214	0.07424	0.31876	0.01860	0.10597	0.41241	0.02670	0.14274	0.50765	3900
3910	0.01198	0.07343	0.31618	0.01838	0.10492	0.40949	0.02641	0.14145	0.50449	3910
3920	0.01182	0.07263	0.31362	0.01816	0.10388	0.40660	0.02611	0.14016	0.50134	3920
3930	0.01167	0.07183	0.31108	0.01794	0.10284	0.40371	0.02583	0.13889	0.49821	3930
3940	0.01152	0.07104	0.30855	0.01772	0.10182	0.40085	0.02554	0.13763	0.49510	3940
3950	0.01137	0.07026	0.30605	0.01751	0.10081	0.39800	0.02526	0.13638	0.49200	3950
3960	0.01122	0.06949	0.30356	0.01730	0.09981	0.39517	0.02498	0.13513	0.48891	3960
3970	0.01107	0.06873	0.30108	0.01709	0.09881	0.39235	0.02470	0.13391	0.48584	3970
3980	0.01093	0.06798	0.29862	0.01689	0.09783	0.38955	0.02443	0.13269	0.48278	3980
3990	0.01079	0.06723	0.29618	0.01669	0.09686	0.38676	0.02416	0.13148	0.47974	3990
4000	0.01065	0.06649	0.29376	0.01649	0.09589	0.38399	0.02389	0.13028	0.47671	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=1400.			T=1500.			T=1600.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
100	4.62254	6.50935	1.98542	4.75295	6.64634	1.98565	4.87533	6.77449	1.98583	100
110	4.44317	6.32013	1.98505	4.57292	6.45710	1.98533	4.69473	6.58524	1.98555	110
120	4.28028	6.14743	1.98465	4.40937	6.28437	1.98498	4.53060	6.41248	1.98524	120
130	4.13121	5.98859	1.98422	4.25965	6.12550	1.98460	4.38031	6.25359	1.98491	130
140	3.99392	5.84156	1.98375	4.12171	5.97844	1.98419	4.24180	6.10651	1.98455	140
150	3.86678	5.70471	1.98324	3.99392	5.84156	1.98375	4.11344	5.96960	1.98416	150
160	3.74847	5.57673	1.98270	3.87497	5.71355	1.98327	3.99392	5.84156	1.98375	160
170	3.63792	5.45655	1.98212	3.76377	5.59333	1.98277	3.88216	5.72131	1.98330	170
180	3.53424	5.34327	1.98151	3.65945	5.48001	1.98224	3.77728	5.60796	1.98284	180
190	3.43669	5.23616	1.98087	3.56126	5.37285	1.98168	3.67853	5.50077	1.98234	190
200	3.34463	5.13457	1.98019	3.46857	5.27122	1.98109	3.58527	5.39910	1.98182	200
210	3.25753	5.03797	1.97947	3.38083	5.17458	1.98046	3.49698	5.30242	1.98128	210
220	3.17492	4.94590	1.97873	3.29759	5.08246	1.97981	3.41318	5.21026	1.98070	220
230	3.09641	4.85796	1.97794	3.21845	4.99447	1.97913	3.33348	5.12223	1.98010	230
240	3.02163	4.77380	1.97713	3.14304	4.91025	1.97842	3.25753	5.03797	1.97947	240
250	2.95030	4.69311	1.97627	3.07108	4.82950	1.97767	3.18502	4.95718	1.97882	250
260	2.88212	4.61561	1.97539	3.00229	4.75195	1.97690	3.11567	4.87958	1.97814	260
270	2.81688	4.54108	1.97447	2.93642	4.67736	1.97610	3.04926	4.80494	1.97744	270
280	2.75434	4.46929	1.97351	2.87326	4.60551	1.97527	2.98555	4.73304	1.97670	280
290	2.69432	4.40005	1.97253	2.81262	4.53621	1.97441	2.92437	4.66368	1.97595	290
300	2.63665	4.33320	1.97150	2.75434	4.46929	1.97351	2.86555	4.59671	1.97516	300
310	2.58117	4.26857	1.97045	2.69825	4.40459	1.97259	2.80891	4.53196	1.97435	310
320	2.52774	4.20603	1.96936	2.64421	4.34198	1.97164	2.75434	4.46929	1.97351	320
330	2.47623	4.14544	1.96823	2.59209	4.28132	1.97066	2.70169	4.40857	1.97265	330
340	2.42654	4.08670	1.96707	2.54179	4.22251	1.96965	2.65085	4.34970	1.97176	340
350	2.37854	4.02970	1.96588	2.49319	4.16543	1.96861	2.60172	4.29255	1.97085	350
360	2.33215	3.97434	1.96466	2.44621	4.10999	1.96754	2.55420	4.23705	1.96991	360
370	2.28728	3.92052	1.96340	2.40073	4.05609	1.96644	2.50820	4.18308	1.96894	370
380	2.24384	3.86818	1.96211	2.35670	4.00366	1.96531	2.46364	4.13059	1.96795	380
390	2.20177	3.81723	1.96078	2.31403	3.95263	1.96416	2.42045	4.07948	1.96693	390
400	2.16098	3.76761	1.95942	2.27265	3.90292	1.96297	2.37854	4.02970	1.96588	400
410	2.12141	3.71924	1.95803	2.23249	3.85446	1.96175	2.33787	3.98117	1.96481	410
420	2.08302	3.67207	1.95660	2.19351	3.80720	1.96051	2.29836	3.93384	1.96372	420
430	2.04573	3.62605	1.95514	2.15563	3.76108	1.95924	2.25997	3.88764	1.96259	430
440	2.00950	3.58112	1.95365	2.11882	3.71606	1.95793	2.22264	3.84254	1.96145	440
450	1.97427	3.53723	1.95213	2.08302	3.67207	1.95660	2.18632	3.79847	1.96027	450
460	1.94002	3.49434	1.95057	2.04818	3.62908	1.95524	2.15097	3.75540	1.95908	460
470	1.90668	3.45241	1.94898	2.01427	3.58705	1.95385	2.11655	3.71328	1.95785	470
480	1.87423	3.41139	1.94736	1.98124	3.54593	1.95243	2.08302	3.67207	1.95660	480
490	1.84262	3.37126	1.94570	1.94906	3.50568	1.95099	2.05033	3.63174	1.95533	490
500	1.81182	3.33197	1.94402	1.91769	3.46628	1.94951	2.01846	3.59225	1.95403	500
510	1.78180	3.29349	1.94230	1.88711	3.42769	1.94801	1.98737	3.55357	1.95270	510
520	1.75253	3.25579	1.94054	1.85727	3.38988	1.94648	1.95703	3.51567	1.95135	520
530	1.72398	3.21884	1.93876	1.82815	3.35282	1.94492	1.92741	3.47851	1.94998	530
540	1.69611	3.18262	1.93694	1.79972	3.31648	1.94333	1.89849	3.44207	1.94858	540
550	1.66891	3.14709	1.93510	1.77197	3.28084	1.94172	1.87023	3.40633	1.94715	550
560	1.64235	3.11224	1.93322	1.74485	3.24586	1.94007	1.84262	3.37126	1.94570	560
570	1.61641	3.07804	1.93131	1.71835	3.21154	1.93840	1.81563	3.33683	1.94423	570
580	1.59106	3.04447	1.92936	1.69245	3.17784	1.93670	1.78924	3.30303	1.94273	580
590	1.56628	3.01151	1.92739	1.66712	3.14475	1.93497	1.76342	3.26984	1.94120	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	ν cm ⁻¹
	T=1400.			T=1500.			T=1600.			
600	1.54206	2.97913	1.92538	1.64235	3.11224	1.93322	1.73817	3.23722	1.93966	600
610	1.51838	2.94732	1.92335	1.61812	3.08030	1.93143	1.71345	3.20517	1.93808	610
620	1.49521	2.91606	1.92128	1.59441	3.04891	1.92962	1.68925	3.17367	1.93648	620
630	1.47254	2.88534	1.91918	1.57119	3.01805	1.92779	1.66556	3.14270	1.93486	630
640	1.45035	2.85513	1.91705	1.54847	2.98771	1.92592	1.64235	3.11224	1.93322	640
650	1.42863	2.82543	1.91489	1.52621	2.95786	1.92403	1.61962	3.08228	1.93155	650
660	1.40737	2.79621	1.91270	1.50441	2.92850	1.92211	1.59734	3.05281	1.92985	660
670	1.38654	2.76746	1.91048	1.48305	2.89961	1.92016	1.57551	3.02380	1.92813	670
680	1.36614	2.73917	1.90823	1.46212	2.87118	1.91819	1.55411	2.99525	1.92639	680
690	1.34615	2.71133	1.90595	1.44161	2.84319	1.91619	1.53312	2.96714	1.92462	690
700	1.32657	2.68392	1.90364	1.42149	2.81563	1.91417	1.51254	2.93946	1.92283	700
710	1.30737	2.65694	1.90130	1.40177	2.78850	1.91211	1.49235	2.91219	1.92102	710
720	1.28855	2.63036	1.89893	1.38243	2.76177	1.91003	1.47254	2.88534	1.91918	720
730	1.27009	2.60419	1.89653	1.36345	2.73544	1.90793	1.45310	2.85888	1.91732	730
740	1.25199	2.57840	1.89410	1.34484	2.70949	1.90580	1.43402	2.83281	1.91544	740
750	1.23424	2.55299	1.89164	1.32657	2.68392	1.90364	1.41529	2.80711	1.91353	750
760	1.21682	2.52795	1.88915	1.30864	2.65872	1.90146	1.39690	2.78178	1.91160	760
770	1.19973	2.50327	1.88664	1.29104	2.63388	1.89925	1.37884	2.75680	1.90964	770
780	1.18296	2.47895	1.88409	1.27375	2.60939	1.89701	1.36111	2.73217	1.90766	780
790	1.16650	2.45496	1.88152	1.25679	2.58524	1.89475	1.34368	2.70788	1.90566	790
800	1.15034	2.43131	1.87892	1.24012	2.56142	1.89246	1.32657	2.68392	1.90364	800
810	1.13447	2.40799	1.87629	1.22375	2.53792	1.89015	1.30975	2.66029	1.90159	810
820	1.11889	2.38498	1.87363	1.20767	2.51475	1.88782	1.29322	2.63697	1.89952	820
830	1.10359	2.36229	1.87094	1.19187	2.49188	1.88545	1.27697	2.61396	1.89743	830
840	1.08856	2.33989	1.86822	1.17634	2.46931	1.88307	1.26100	2.59125	1.89532	840
850	1.07380	2.31780	1.86548	1.16108	2.44704	1.88065	1.24530	2.56883	1.89318	850
860	1.05929	2.29600	1.86271	1.14608	2.42506	1.87822	1.22985	2.54670	1.89102	860
870	1.04503	2.27448	1.85991	1.13134	2.40336	1.87576	1.21467	2.52485	1.88884	870
880	1.03102	2.25324	1.85709	1.11684	2.38194	1.87327	1.19973	2.50327	1.88664	880
890	1.01725	2.23227	1.85424	1.10258	2.36078	1.87076	1.18504	2.48197	1.88441	890
900	1.00372	2.21157	1.85136	1.08856	2.33989	1.86822	1.17059	2.46093	1.88216	900
910	0.99041	2.19113	1.84845	1.07477	2.31927	1.86567	1.15637	2.44014	1.87990	910
920	0.97733	2.17094	1.84552	1.06121	2.29889	1.86308	1.14237	2.41961	1.87760	920
930	0.96446	2.15101	1.84256	1.04786	2.27876	1.86048	1.12860	2.39932	1.87529	930
940	0.95181	2.13132	1.83958	1.03474	2.25888	1.85784	1.11504	2.37928	1.87296	940
950	0.93936	2.11187	1.83657	1.02182	2.23923	1.85519	1.10170	2.35947	1.87060	950
960	0.92712	2.09265	1.83353	1.00910	2.21982	1.85251	1.08856	2.33989	1.86822	960
970	0.91508	2.07367	1.83047	0.99659	2.20064	1.84981	1.07563	2.32055	1.86583	970
980	0.90323	2.05491	1.82738	0.98428	2.18168	1.84709	1.06289	2.30142	1.86341	980
990	0.89157	2.03637	1.82427	0.97215	2.16294	1.84434	1.05035	2.28252	1.86097	990
1000	0.88010	2.01805	1.82113	0.96022	2.14442	1.84157	1.03800	2.26383	1.85850	1000
1010	0.86881	1.99995	1.81797	0.94847	2.12611	1.83878	1.02583	2.24535	1.85602	1010
1020	0.85770	1.98205	1.81478	0.93690	2.10800	1.83596	1.01385	2.22707	1.85352	1020
1030	0.84677	1.96436	1.81157	0.92550	2.09011	1.83312	1.00204	2.20900	1.85100	1030
1040	0.83600	1.94687	1.80833	0.91428	2.07241	1.83026	0.99041	2.19113	1.84845	1040
1050	0.82540	1.92958	1.80507	0.90323	2.05491	1.82738	0.97895	2.17345	1.84589	1050
1060	0.81497	1.91249	1.80178	0.89235	2.03760	1.82448	0.96766	2.15597	1.84330	1060
1070	0.80469	1.89559	1.79847	0.88162	2.02048	1.82155	0.95653	2.13867	1.84070	1070
1080	0.79458	1.87887	1.79514	0.87106	2.00355	1.81860	0.94556	2.12156	1.83808	1080
1090	0.78461	1.86234	1.79178	0.86065	1.98680	1.81563	0.93475	2.10463	1.83543	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	ν cm^{-1}
T=1400.			T=1500.			T=1600.				
1100	0.77480	1.84600	1.78840	0.85039	1.97024	1.81264	0.92409	2.08788	1.83277	1100
1110	0.76514	1.82983	1.78500	0.84029	1.95384	1.80963	0.91359	2.07131	1.83008	1110
1120	0.75562	1.81383	1.78157	0.83033	1.93763	1.80659	0.90323	2.05491	1.82738	1120
1130	0.74624	1.79801	1.77813	0.82051	1.92158	1.80354	0.89302	2.03868	1.82466	1130
1140	0.73700	1.78236	1.77465	0.81084	1.90571	1.80046	0.88295	2.02261	1.82192	1140
1150	0.72790	1.76688	1.77116	0.80130	1.89000	1.79736	0.87303	2.00671	1.81916	1150
1160	0.71893	1.75156	1.76765	0.79190	1.87445	1.79425	0.86324	1.99097	1.81638	1160
1170	0.71009	1.73640	1.76411	0.78264	1.85906	1.79111	0.85358	1.97539	1.81358	1170
1180	0.70138	1.72140	1.76055	0.77350	1.84383	1.78795	0.84406	1.95997	1.81076	1180
1190	0.69280	1.70656	1.75697	0.76450	1.82875	1.78477	0.83467	1.94470	1.80792	1190
1200	0.68435	1.69187	1.75336	0.75562	1.81383	1.78157	0.82540	1.92958	1.80507	1200
1210	0.67601	1.67733	1.74974	0.74686	1.79906	1.77836	0.81626	1.91462	1.80219	1210
1220	0.66779	1.66295	1.74610	0.73822	1.78444	1.77512	0.80725	1.89980	1.79930	1220
1230	0.65970	1.64871	1.74243	0.72971	1.76996	1.77186	0.79835	1.88512	1.79639	1230
1240	0.65171	1.63461	1.73874	0.72131	1.75563	1.76859	0.78958	1.87059	1.79346	1240
1250	0.64384	1.62066	1.73504	0.71302	1.74143	1.76529	0.78092	1.85619	1.79052	1250
1260	0.63608	1.60685	1.73131	0.70485	1.72738	1.76197	0.77237	1.84194	1.78756	1260
1270	0.62843	1.59318	1.72756	0.69679	1.71346	1.75864	0.76394	1.82782	1.78457	1270
1280	0.62089	1.57965	1.72380	0.68884	1.69968	1.75529	0.75562	1.81383	1.78157	1280
1290	0.61345	1.56625	1.72001	0.68100	1.68604	1.75192	0.74740	1.79998	1.77856	1290
1300	0.60612	1.55298	1.71621	0.67326	1.67252	1.74853	0.73930	1.78626	1.77552	1300
1310	0.59888	1.53984	1.71238	0.66562	1.65914	1.74512	0.73129	1.77266	1.77247	1310
1320	0.59175	1.52684	1.70854	0.65809	1.64588	1.74169	0.72340	1.75920	1.76941	1320
1330	0.58471	1.51396	1.70467	0.65066	1.63275	1.73825	0.71560	1.74585	1.76632	1330
1340	0.57778	1.50120	1.70079	0.64332	1.61974	1.73479	0.70790	1.73263	1.76322	1340
1350	0.57093	1.48857	1.69689	0.63608	1.60685	1.73131	0.70031	1.71954	1.76010	1350
1360	0.56418	1.47606	1.69297	0.62894	1.59409	1.72781	0.69280	1.70656	1.75697	1360
1370	0.55752	1.46367	1.68904	0.62189	1.58144	1.72430	0.68540	1.69370	1.75382	1370
1380	0.55095	1.45140	1.68509	0.61493	1.56892	1.72077	0.67808	1.68095	1.75065	1380
1390	0.54447	1.43925	1.68111	0.60806	1.55650	1.71722	0.67086	1.66833	1.74747	1390
1400	0.53808	1.42721	1.67713	0.60128	1.54421	1.71366	0.66373	1.65581	1.74427	1400
1410	0.53177	1.41529	1.67312	0.59459	1.53202	1.71008	0.65669	1.64341	1.74105	1410
1420	0.52554	1.40348	1.66910	0.58799	1.51995	1.70648	0.64973	1.63111	1.73782	1420
1430	0.51940	1.39178	1.66506	0.58146	1.50799	1.70286	0.64287	1.61893	1.73457	1430
1440	0.51334	1.38019	1.66100	0.57503	1.49613	1.69923	0.63608	1.60685	1.73131	1440
1450	0.50736	1.36871	1.65693	0.56867	1.48439	1.69559	0.62938	1.59488	1.72803	1450
1460	0.50146	1.35734	1.65284	0.56240	1.47275	1.69193	0.62277	1.58302	1.72474	1460
1470	0.49564	1.34607	1.64874	0.55620	1.46121	1.68825	0.61623	1.57126	1.72143	1470
1480	0.48989	1.33491	1.64462	0.55008	1.44978	1.68456	0.60977	1.55960	1.71811	1480
1490	0.48422	1.32385	1.64048	0.54404	1.43844	1.68085	0.60339	1.54804	1.71477	1490
1500	0.47862	1.31289	1.63633	0.53808	1.42721	1.67713	0.59709	1.53658	1.71142	1500
1510	0.47309	1.30203	1.63216	0.53219	1.41608	1.67339	0.59087	1.52522	1.70805	1510
1520	0.46764	1.29127	1.62798	0.52637	1.40505	1.66963	0.58471	1.51396	1.70467	1520
1530	0.46226	1.28061	1.62379	0.52062	1.39411	1.66587	0.57864	1.50279	1.70128	1530
1540	0.45694	1.27004	1.61957	0.51495	1.38327	1.66208	0.57263	1.49172	1.69787	1540
1550	0.45170	1.25957	1.61535	0.50935	1.37253	1.65829	0.56670	1.48074	1.69445	1550
1560	0.44652	1.24920	1.61111	0.50381	1.36188	1.65448	0.56084	1.46985	1.69101	1560
1570	0.44141	1.23892	1.60686	0.49835	1.35132	1.65065	0.55505	1.45906	1.68756	1570
1580	0.43636	1.22873	1.60259	0.49295	1.34085	1.64681	0.54932	1.44835	1.68409	1580
1590	0.43138	1.21863	1.59831	0.48761	1.33047	1.64296	0.54367	1.43774	1.68062	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=1400.			T=1500.			T=1600.				
1600	0.42646	1.20862	1.59402	0.48234	1.32018	1.63910	0.53808	1.42721	1.67713	1600
1610	0.42160	1.19870	1.58971	0.47714	1.30998	1.63522	0.53255	1.41678	1.67362	1610
1620	0.41680	1.18887	1.58540	0.47200	1.29987	1.63133	0.52709	1.40642	1.67010	1620
1630	0.41207	1.17913	1.58106	0.46692	1.28984	1.62742	0.52170	1.39616	1.66657	1630
1640	0.40739	1.16947	1.57672	0.46190	1.27990	1.62350	0.51636	1.38597	1.66303	1640
1650	0.40277	1.15990	1.57236	0.45694	1.27004	1.61957	0.51109	1.37588	1.65948	1650
1660	0.39821	1.15042	1.56800	0.45204	1.26027	1.61563	0.50588	1.36586	1.65591	1660
1670	0.39371	1.14101	1.56362	0.44720	1.25058	1.61168	0.50073	1.35592	1.65233	1670
1680	0.38926	1.13169	1.55922	0.44242	1.24097	1.60771	0.49564	1.34607	1.64874	1680
1690	0.38487	1.12245	1.55482	0.43770	1.23144	1.60373	0.49060	1.33630	1.64513	1690
1700	0.38053	1.11329	1.55041	0.43303	1.22199	1.59974	0.48563	1.32660	1.64151	1700
1710	0.37625	1.10421	1.54598	0.42842	1.21262	1.59574	0.48071	1.31698	1.63789	1710
1720	0.37202	1.09521	1.54155	0.42386	1.20332	1.59173	0.47585	1.30744	1.63425	1720
1730	0.36784	1.08628	1.53710	0.41935	1.19411	1.58770	0.47104	1.29798	1.63060	1730
1740	0.36371	1.07744	1.53264	0.41490	1.18497	1.58366	0.46629	1.28859	1.62693	1740
1750	0.35964	1.06867	1.52818	0.41050	1.17590	1.57962	0.46159	1.27928	1.62326	1750
1760	0.35561	1.05997	1.52370	0.40615	1.16691	1.57556	0.45694	1.27004	1.61957	1760
1770	0.35163	1.05135	1.51921	0.40186	1.15800	1.57149	0.45235	1.26088	1.61588	1770
1780	0.34770	1.04281	1.51472	0.39761	1.14916	1.56741	0.44781	1.25178	1.61217	1780
1790	0.34382	1.03433	1.51021	0.39341	1.14039	1.56332	0.44332	1.24276	1.60846	1790
1800	0.33999	1.02593	1.50570	0.38926	1.13169	1.55922	0.43887	1.23381	1.60473	1800
1810	0.33620	1.01760	1.50117	0.38516	1.12306	1.55512	0.43448	1.22493	1.60099	1810
1820	0.33246	1.00934	1.49664	0.38111	1.11451	1.55100	0.43014	1.21612	1.59724	1820
1830	0.32876	1.00115	1.49210	0.37710	1.10602	1.54687	0.42584	1.20738	1.59348	1830
1840	0.32511	0.99304	1.48755	0.37314	1.09760	1.54273	0.42160	1.19870	1.58971	1840
1850	0.32150	0.98499	1.48299	0.36923	1.08925	1.53858	0.41740	1.19010	1.58594	1850
1860	0.31794	0.97700	1.47843	0.36536	1.08097	1.53443	0.41324	1.18156	1.58215	1860
1870	0.31441	0.96909	1.47385	0.36153	1.07275	1.53026	0.40914	1.17309	1.57835	1870
1880	0.31093	0.96124	1.46927	0.35775	1.06460	1.52609	0.40507	1.16468	1.57454	1880
1890	0.30750	0.95346	1.46468	0.35401	1.05651	1.52191	0.40106	1.15634	1.57073	1890
1900	0.30410	0.94574	1.46009	0.35032	1.04849	1.51772	0.39708	1.14806	1.56690	1900
1910	0.30074	0.93809	1.45549	0.34666	1.04054	1.51352	0.39315	1.13984	1.56307	1910
1920	0.29742	0.93050	1.45088	0.34305	1.03265	1.50931	0.38926	1.13169	1.55922	1920
1930	0.29415	0.92297	1.44626	0.33948	1.02482	1.50509	0.38542	1.12360	1.55537	1930
1940	0.29091	0.91551	1.44164	0.33595	1.01705	1.50087	0.38161	1.11557	1.55151	1940
1950	0.28771	0.90811	1.43701	0.33246	1.00934	1.49664	0.37785	1.10760	1.54764	1950
1960	0.28454	0.90077	1.43238	0.32901	1.00170	1.49240	0.37413	1.09970	1.54377	1960
1970	0.28142	0.89350	1.42774	0.32559	0.99411	1.48816	0.37045	1.09185	1.53988	1970
1980	0.27833	0.88628	1.42309	0.32222	0.98659	1.48390	0.36680	1.08406	1.53599	1980
1990	0.27528	0.87912	1.41844	0.31888	0.97913	1.47965	0.36320	1.07634	1.53209	1990
2000	0.27226	0.87202	1.41378	0.31558	0.97172	1.47538	0.35964	1.06867	1.52818	2000
2010	0.26928	0.86498	1.40912	0.31232	0.96437	1.47111	0.35611	1.06105	1.52426	2010
2020	0.26633	0.85800	1.40446	0.30909	0.95708	1.46683	0.35262	1.05350	1.52034	2020
2030	0.26342	0.85108	1.39979	0.30590	0.94985	1.46254	0.34917	1.04600	1.51640	2030
2040	0.26054	0.84421	1.39511	0.30275	0.94267	1.45825	0.34576	1.03856	1.51247	2040
2050	0.25770	0.83740	1.39043	0.29963	0.93555	1.45395	0.34238	1.03117	1.50852	2050
2060	0.25489	0.83064	1.38575	0.29655	0.92849	1.44965	0.33904	1.02384	1.50457	2060
2070	0.25211	0.82395	1.38106	0.29350	0.92148	1.44534	0.33573	1.01657	1.50061	2070
2080	0.24936	0.81730	1.37637	0.29048	0.91452	1.44102	0.33246	1.00934	1.49664	2080
2090	0.24665	0.81071	1.37167	0.28749	0.90762	1.43670	0.32922	1.00217	1.49267	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
T=1400.			T=1500.			T=1600.				
2100	0.24396	0.80417	1.36698	0.28454	0.90077	1.43238	0.32602	0.99506	1.48869	2100
2110	0.24131	0.79769	1.36227	0.28163	0.89398	1.42805	0.32285	0.98800	1.48470	2110
2120	0.23869	0.79126	1.35757	0.27874	0.88724	1.42371	0.31971	0.98099	1.48071	2120
2130	0.23610	0.78488	1.35286	0.27589	0.88055	1.41937	0.31661	0.97403	1.47671	2130
2140	0.23354	0.77856	1.34815	0.27306	0.87391	1.41503	0.31354	0.96712	1.47271	2140
2150	0.23101	0.77228	1.34344	0.27027	0.86732	1.41068	0.31050	0.96026	1.46870	2150
2160	0.22850	0.76606	1.33872	0.26751	0.86079	1.40632	0.30750	0.95346	1.46468	2160
2170	0.22603	0.75989	1.33401	0.26478	0.85430	1.40197	0.30452	0.94670	1.46066	2170
2180	0.22358	0.75377	1.32929	0.26207	0.84787	1.39761	0.30158	0.93999	1.45664	2180
2190	0.22116	0.74769	1.32457	0.25940	0.84148	1.39324	0.29866	0.93334	1.45261	2190
2200	0.21877	0.74167	1.31985	0.25676	0.83514	1.38887	0.29578	0.92673	1.44857	2200
2210	0.21641	0.73569	1.31512	0.25414	0.82885	1.38450	0.29293	0.92017	1.44453	2210
2220	0.21407	0.72977	1.31040	0.25156	0.82261	1.38012	0.29010	0.91366	1.44048	2220
2230	0.21176	0.72389	1.30567	0.24900	0.81642	1.37574	0.28731	0.90719	1.43643	2230
2240	0.20948	0.71806	1.30095	0.24647	0.81027	1.37136	0.28454	0.90077	1.43238	2240
2250	0.20722	0.71227	1.29622	0.24396	0.80417	1.36698	0.28181	0.89440	1.42832	2250
2260	0.20499	0.70654	1.29149	0.24149	0.79812	1.36259	0.27910	0.88808	1.42425	2260
2270	0.20278	0.70084	1.28676	0.23904	0.79212	1.35820	0.27642	0.88180	1.42019	2270
2280	0.20060	0.69520	1.28203	0.23662	0.78616	1.35380	0.27376	0.87556	1.41611	2280
2290	0.19845	0.68960	1.27730	0.23422	0.78024	1.34941	0.27114	0.86938	1.41204	2290
2300	0.19631	0.68404	1.27257	0.23185	0.77437	1.34501	0.26854	0.86323	1.40796	2300
2310	0.19420	0.67853	1.26785	0.22950	0.76854	1.34061	0.26597	0.85713	1.40387	2310
2320	0.19212	0.67307	1.26312	0.22718	0.76276	1.33621	0.26342	0.85108	1.39979	2320
2330	0.19006	0.66764	1.25839	0.22488	0.75703	1.33181	0.26090	0.84507	1.39570	2330
2340	0.18802	0.66226	1.25366	0.22261	0.75133	1.32740	0.25841	0.83910	1.39160	2340
2350	0.18601	0.65693	1.24894	0.22036	0.74568	1.32299	0.25594	0.83317	1.38750	2350
2360	0.18401	0.65163	1.24421	0.21814	0.74007	1.31859	0.25349	0.82729	1.38340	2360
2370	0.18204	0.64638	1.23949	0.21594	0.73451	1.31418	0.25108	0.82145	1.37930	2370
2380	0.18009	0.64117	1.23477	0.21376	0.72898	1.30977	0.24868	0.81565	1.37520	2380
2390	0.17817	0.63601	1.23005	0.21161	0.72350	1.30536	0.24631	0.80989	1.37109	2390
2400	0.17626	0.63088	1.22533	0.20948	0.71806	1.30094	0.24396	0.80417	1.36698	2400
2410	0.17438	0.62580	1.22061	0.20737	0.71266	1.29653	0.24164	0.79850	1.36286	2410
2420	0.17252	0.62075	1.21590	0.20529	0.70730	1.29212	0.23934	0.79286	1.35875	2420
2430	0.17067	0.61575	1.21118	0.20322	0.70198	1.28771	0.23707	0.78727	1.35463	2430
2440	0.16885	0.61078	1.20647	0.20118	0.69670	1.28329	0.23482	0.78172	1.35051	2440
2450	0.16705	0.60586	1.20177	0.19916	0.69146	1.27888	0.23258	0.77620	1.34638	2450
2460	0.16527	0.60097	1.19706	0.19716	0.68626	1.27447	0.23038	0.77072	1.34226	2460
2470	0.16351	0.59613	1.19236	0.19519	0.68110	1.27005	0.22819	0.76529	1.33814	2470
2480	0.16177	0.59132	1.18766	0.19323	0.67598	1.26564	0.22603	0.75989	1.33401	2480
2490	0.16005	0.58655	1.18296	0.19129	0.67089	1.26123	0.22389	0.75453	1.32988	2490
2500	0.15834	0.58182	1.17827	0.18938	0.66585	1.25682	0.22177	0.74921	1.32575	2500
2510	0.15666	0.57712	1.17358	0.18748	0.66084	1.25240	0.21967	0.74392	1.32162	2510
2520	0.15499	0.57246	1.16889	0.18560	0.65587	1.24799	0.21759	0.73868	1.31748	2520
2530	0.15334	0.56784	1.16421	0.18375	0.65093	1.24358	0.21553	0.73347	1.31335	2530
2540	0.15171	0.56326	1.15953	0.18191	0.64604	1.23918	0.21349	0.72829	1.30922	2540
2550	0.15010	0.55871	1.15485	0.18009	0.64117	1.23477	0.21148	0.72316	1.30508	2550
2560	0.14851	0.55420	1.15018	0.17830	0.63635	1.23036	0.20948	0.71806	1.30094	2560
2570	0.14693	0.54973	1.14552	0.17652	0.63156	1.22596	0.20750	0.71299	1.29681	2570
2580	0.14538	0.54529	1.14085	0.17475	0.62681	1.22156	0.20555	0.70797	1.29267	2580
2590	0.14383	0.54088	1.13619	0.17301	0.62209	1.21715	0.20361	0.70297	1.28853	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
	T=1400.			T=1500.			T=1600.			
2600	0.14231	0.53651	1.13154	0.17129	0.61741	1.21276	0.20169	0.69802	1.28440	2600
2610	0.14080	0.53218	1.12689	0.16958	0.61276	1.20836	0.19979	0.69309	1.28026	2610
2620	0.13931	0.52788	1.12225	0.16789	0.60815	1.20396	0.19791	0.68821	1.27612	2620
2630	0.13784	0.52361	1.11761	0.16622	0.60357	1.19957	0.19605	0.68335	1.27198	2630
2640	0.13638	0.51938	1.11297	0.16456	0.59903	1.19518	0.19420	0.67853	1.26785	2640
2650	0.13493	0.51518	1.10834	0.16293	0.59452	1.19079	0.19238	0.67375	1.26371	2650
2660	0.13351	0.51102	1.10372	0.16131	0.59004	1.18641	0.19057	0.66899	1.25957	2660
2670	0.13210	0.50688	1.09910	0.15970	0.58560	1.18202	0.18878	0.66428	1.25544	2670
2680	0.13070	0.50278	1.09449	0.15812	0.58119	1.17764	0.18701	0.65959	1.25130	2680
2690	0.12932	0.49871	1.08988	0.15655	0.57681	1.17327	0.18526	0.65494	1.24717	2690
2700	0.12795	0.49468	1.08528	0.15499	0.57246	1.16889	0.18352	0.65032	1.24303	2700
2710	0.12660	0.49068	1.08069	0.15345	0.56815	1.16452	0.18180	0.64573	1.23890	2710
2720	0.12527	0.48670	1.07610	0.15193	0.56387	1.16015	0.18009	0.64117	1.23477	2720
2730	0.12394	0.48276	1.07151	0.15042	0.55962	1.15579	0.17841	0.63665	1.23064	2730
2740	0.12264	0.47885	1.06694	0.14893	0.55540	1.15143	0.17674	0.63216	1.22651	2740
2750	0.12134	0.47498	1.06237	0.14746	0.55122	1.14707	0.17508	0.62770	1.22238	2750
2760	0.12007	0.47113	1.05781	0.14600	0.54706	1.14272	0.17345	0.62327	1.21825	2760
2770	0.11880	0.46731	1.05325	0.14455	0.54294	1.13837	0.17182	0.61887	1.21413	2770
2780	0.11755	0.46352	1.04870	0.14312	0.53884	1.13402	0.17022	0.61450	1.21001	2780
2790	0.11631	0.45977	1.04416	0.14170	0.53478	1.12968	0.16863	0.61017	1.20589	2790
2800	0.11509	0.45604	1.03962	0.14030	0.53074	1.12534	0.16705	0.60586	1.20177	2800
2810	0.11388	0.45234	1.03509	0.13892	0.52674	1.12101	0.16549	0.60158	1.19765	2810
2820	0.11268	0.44867	1.03057	0.13754	0.52276	1.11668	0.16395	0.59733	1.19353	2820
2830	0.11149	0.44503	1.02605	0.13618	0.51882	1.11236	0.16242	0.59312	1.18942	2830
2840	0.11032	0.44142	1.02155	0.13484	0.51490	1.10804	0.16090	0.58893	1.18531	2840
2850	0.10916	0.43784	1.01705	0.13351	0.51102	1.10372	0.15940	0.58477	1.18120	2850
2860	0.10801	0.43428	1.01256	0.13219	0.50716	1.09941	0.15792	0.58064	1.17710	2860
2870	0.10688	0.43076	1.00807	0.13088	0.50333	1.09510	0.15645	0.57654	1.17299	2870
2880	0.10576	0.42726	1.00360	0.12959	0.49953	1.09080	0.15499	0.57246	1.16889	2880
2890	0.10465	0.42379	0.99913	0.12832	0.49575	1.08651	0.15355	0.56842	1.16479	2890
2900	0.10355	0.42034	0.99467	0.12705	0.49201	1.08222	0.15212	0.56440	1.16070	2900
2910	0.10246	0.41693	0.99021	0.12580	0.48829	1.07793	0.15071	0.56041	1.15661	2910
2920	0.10139	0.41354	0.98577	0.12456	0.48460	1.07365	0.14930	0.55645	1.15252	2920
2930	0.10032	0.41017	0.98134	0.12333	0.48093	1.06938	0.14792	0.55252	1.14843	2930
2940	0.09927	0.40684	0.97691	0.12212	0.47730	1.06511	0.14654	0.54861	1.14435	2940
2950	0.09823	0.40353	0.97249	0.12092	0.47369	1.06085	0.14518	0.54474	1.14027	2950
2960	0.09720	0.40024	0.96808	0.11973	0.47011	1.05659	0.14383	0.54088	1.13619	2960
2970	0.09618	0.39699	0.96368	0.11855	0.46655	1.05234	0.14250	0.53706	1.13212	2970
2980	0.09518	0.39376	0.95929	0.11738	0.46302	1.04809	0.14118	0.53326	1.12805	2980
2990	0.09418	0.39055	0.95490	0.11623	0.45952	1.04385	0.13987	0.52949	1.12399	2990
3000	0.09319	0.38737	0.95053	0.11509	0.45604	1.03962	0.13857	0.52574	1.11993	3000
3010	0.09222	0.38421	0.94616	0.11396	0.45258	1.03539	0.13729	0.52202	1.11587	3010
3020	0.09125	0.38108	0.94181	0.11284	0.44916	1.03117	0.13601	0.51833	1.11182	3020
3030	0.09030	0.37797	0.93746	0.11173	0.44576	1.02696	0.13475	0.51466	1.10777	3030
3040	0.08935	0.37489	0.93312	0.11063	0.44238	1.02275	0.13351	0.51102	1.10372	3040
3050	0.08842	0.37184	0.92879	0.10955	0.43903	1.01855	0.13227	0.50740	1.09968	3050
3060	0.08750	0.36880	0.92448	0.10847	0.43570	1.01435	0.13105	0.50380	1.09564	3060
3070	0.08658	0.36579	0.92017	0.10741	0.43240	1.01016	0.12983	0.50024	1.09161	3070
3080	0.08568	0.36281	0.91587	0.10635	0.42912	1.00598	0.12863	0.49669	1.08758	3080
3090	0.08478	0.35985	0.91158	0.10531	0.42586	1.00181	0.12744	0.49317	1.08356	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=1400.			T=1500.			T=1600.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S°	C _p °	$-(F^0-E_0^0)/T$	S°	C _p °	$-(F^0-E_0^0)/T$	S°	C _p °	
3100	0.08390	0.35691	0.90730	0.10428	0.42263	0.99764	0.12627	0.48968	1.07954	3100
3110	0.08302	0.35399	0.90303	0.10326	0.41943	0.99348	0.12510	0.48621	1.07552	3110
3120	0.08215	0.35110	0.89877	0.10225	0.41625	0.98933	0.12394	0.48276	1.07151	3120
3130	0.08130	0.34823	0.89452	0.10124	0.41309	0.98518	0.12280	0.47934	1.06751	3130
3140	0.08045	0.34538	0.89028	0.10025	0.40995	0.98104	0.12167	0.47594	1.06351	3140
3150	0.07961	0.34256	0.88605	0.09927	0.40684	0.97691	0.12054	0.47257	1.05952	3150
3160	0.07878	0.33976	0.88183	0.09830	0.40375	0.97278	0.11943	0.46921	1.05553	3160
3170	0.07796	0.33698	0.87762	0.09734	0.40068	0.96867	0.11833	0.46589	1.05154	3170
3180	0.07714	0.33422	0.87342	0.09639	0.39764	0.96456	0.11724	0.46258	1.04756	3180
3190	0.07634	0.33149	0.86923	0.09544	0.39461	0.96046	0.11616	0.45930	1.04359	3190
3200	0.07555	0.32877	0.86505	0.09451	0.39161	0.95636	0.11509	0.45604	1.03962	3200
3210	0.07476	0.32608	0.86088	0.09359	0.38864	0.95228	0.11403	0.45280	1.03566	3210
3220	0.07398	0.32341	0.85673	0.09267	0.38568	0.94820	0.11298	0.44958	1.03170	3220
3230	0.07321	0.32076	0.85258	0.09177	0.38275	0.94413	0.11194	0.44639	1.02775	3230
3240	0.07245	0.31813	0.84845	0.09087	0.37984	0.94007	0.11090	0.44322	1.02380	3240
3250	0.07169	0.31552	0.84432	0.08998	0.37694	0.93601	0.10988	0.44007	1.01986	3250
3260	0.07095	0.31293	0.84021	0.08910	0.37408	0.93197	0.10887	0.43694	1.01592	3260
3270	0.07021	0.31037	0.83611	0.08823	0.37123	0.92793	0.10787	0.43384	1.01199	3270
3280	0.06948	0.30782	0.83202	0.08737	0.36840	0.92390	0.10688	0.43076	1.00807	3280
3290	0.06875	0.30529	0.82793	0.08652	0.36559	0.91988	0.10590	0.42769	1.00415	3290
3300	0.06804	0.30279	0.82387	0.08568	0.36281	0.91587	0.10492	0.42465	1.00024	3300
3310	0.06733	0.30030	0.81981	0.08484	0.36004	0.91186	0.10396	0.42163	0.99634	3310
3320	0.06663	0.29783	0.81576	0.08401	0.35730	0.90787	0.10300	0.41863	0.99244	3320
3330	0.06594	0.29539	0.81172	0.08320	0.35457	0.90388	0.10206	0.41565	0.98855	3330
3340	0.06525	0.29296	0.80770	0.08238	0.35187	0.89990	0.10112	0.41269	0.98466	3340
3350	0.06458	0.29055	0.80369	0.08158	0.34918	0.89593	0.10019	0.40976	0.98078	3350
3360	0.06390	0.28816	0.79969	0.08079	0.34652	0.89197	0.09927	0.40684	0.97691	3360
3370	0.06324	0.28579	0.79570	0.08000	0.34388	0.88802	0.09836	0.40394	0.97304	3370
3380	0.06258	0.28344	0.79172	0.07922	0.34125	0.88408	0.09746	0.40106	0.96918	3380
3390	0.06193	0.28110	0.78775	0.07845	0.33864	0.88014	0.09656	0.39821	0.96533	3390
3400	0.06129	0.27879	0.78380	0.07769	0.33606	0.87622	0.09568	0.39537	0.96148	3400
3410	0.06065	0.27649	0.77985	0.07693	0.33349	0.87230	0.09480	0.39255	0.95764	3410
3420	0.06002	0.27422	0.77592	0.07618	0.33094	0.86839	0.09393	0.38975	0.95381	3420
3430	0.05940	0.27196	0.77200	0.07544	0.32841	0.86450	0.09307	0.38697	0.94998	3430
3440	0.05878	0.26971	0.76809	0.07471	0.32590	0.86061	0.09222	0.38421	0.94616	3440
3450	0.05817	0.26749	0.76420	0.07398	0.32341	0.85673	0.09137	0.38147	0.94235	3450
3460	0.05757	0.26528	0.76031	0.07326	0.32093	0.85286	0.09054	0.37875	0.93855	3460
3470	0.05697	0.26309	0.75644	0.07255	0.31848	0.84900	0.08971	0.37605	0.93475	3470
3480	0.05638	0.26092	0.75258	0.07184	0.31604	0.84515	0.08889	0.37336	0.93096	3480
3490	0.05580	0.25877	0.74873	0.07114	0.31362	0.84131	0.08807	0.37070	0.92717	3490
3500	0.05522	0.25663	0.74490	0.07045	0.31122	0.83747	0.08727	0.36805	0.92340	3500
3510	0.05465	0.25451	0.74107	0.06977	0.30884	0.83365	0.08647	0.36542	0.91963	3510
3520	0.05408	0.25241	0.73726	0.06909	0.30647	0.82984	0.08568	0.36281	0.91587	3520
3530	0.05352	0.25032	0.73346	0.06842	0.30412	0.82603	0.08489	0.36021	0.91211	3530
3540	0.05297	0.24825	0.72967	0.06775	0.30179	0.82224	0.08412	0.35764	0.90837	3540
3550	0.05242	0.24620	0.72590	0.06710	0.29947	0.81846	0.08335	0.35508	0.90463	3550
3560	0.05187	0.24416	0.72213	0.06645	0.29718	0.81468	0.08259	0.35254	0.90090	3560
3570	0.05134	0.24214	0.71838	0.06580	0.29490	0.81092	0.08183	0.35002	0.89717	3570
3580	0.05081	0.24014	0.71464	0.06516	0.29263	0.80717	0.08108	0.34752	0.89346	3580
3590	0.05028	0.23815	0.71092	0.06453	0.29039	0.80342	0.08034	0.34503	0.88975	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
T=1400.			T=1500.			T=1600.				
3600	0.04976	0.23618	0.70720	0.06390	0.28816	0.79969	0.07961	0.34256	0.88605	3600
3610	0.04924	0.23422	0.70350	0.06328	0.28595	0.79596	0.07888	0.34011	0.88235	3610
3620	0.04873	0.23228	0.69981	0.06267	0.28375	0.79225	0.07816	0.33767	0.87867	3620
3630	0.04823	0.23036	0.69614	0.06206	0.28157	0.78854	0.07745	0.33525	0.87499	3630
3640	0.04773	0.22845	0.69247	0.06146	0.27940	0.78485	0.07674	0.33285	0.87132	3640
3650	0.04724	0.22655	0.68882	0.06087	0.27726	0.78117	0.07604	0.33047	0.86766	3650
3660	0.04675	0.22467	0.68518	0.06028	0.27512	0.77749	0.07535	0.32810	0.86401	3660
3670	0.04626	0.22281	0.68155	0.05969	0.27301	0.77383	0.07466	0.32574	0.86036	3670
3680	0.04579	0.22096	0.67794	0.05911	0.27091	0.77018	0.07398	0.32341	0.85673	3680
3690	0.04531	0.21912	0.67434	0.05854	0.26882	0.76653	0.07330	0.32109	0.85310	3690
3700	0.04484	0.21730	0.67075	0.05797	0.26675	0.76290	0.07264	0.31878	0.84948	3700
3710	0.04438	0.21550	0.66717	0.05741	0.26470	0.75928	0.07197	0.31650	0.84587	3710
3720	0.04392	0.21371	0.66361	0.05686	0.26266	0.75567	0.07132	0.31422	0.84226	3720
3730	0.04347	0.21193	0.66006	0.05631	0.26064	0.75207	0.07067	0.31197	0.83867	3730
3740	0.04302	0.21017	0.65652	0.05576	0.25863	0.74848	0.07002	0.30973	0.83508	3740
3750	0.04257	0.20842	0.65300	0.05522	0.25663	0.74490	0.06939	0.30750	0.83150	3750
3760	0.04213	0.20668	0.64948	0.05469	0.25465	0.74133	0.06875	0.30529	0.82793	3760
3770	0.04170	0.20496	0.64598	0.05416	0.25269	0.73777	0.06813	0.30310	0.82437	3770
3780	0.04127	0.20326	0.64250	0.05363	0.25074	0.73422	0.06751	0.30092	0.82082	3780
3790	0.04084	0.20156	0.63902	0.05311	0.24880	0.73068	0.06689	0.29876	0.81728	3790
3800	0.04042	0.19989	0.63556	0.05260	0.24688	0.72715	0.06628	0.29661	0.81374	3800
3810	0.04000	0.19822	0.63211	0.05209	0.24498	0.72364	0.06568	0.29447	0.81021	3810
3820	0.03959	0.19657	0.62868	0.05159	0.24309	0.72013	0.06508	0.29235	0.80670	3820
3830	0.03918	0.19493	0.62525	0.05109	0.24121	0.71664	0.06449	0.29025	0.80319	3830
3840	0.03878	0.19330	0.62184	0.05059	0.23934	0.71315	0.06390	0.28816	0.79969	3840
3850	0.03838	0.19169	0.61845	0.05011	0.23749	0.70968	0.06332	0.28608	0.79619	3850
3860	0.03798	0.19009	0.61506	0.04962	0.23566	0.70621	0.06275	0.28402	0.79271	3860
3870	0.03759	0.18850	0.61169	0.04914	0.23383	0.70276	0.06218	0.28198	0.78924	3870
3880	0.03720	0.18693	0.60833	0.04867	0.23202	0.69932	0.06161	0.27994	0.78577	3880
3890	0.03682	0.18537	0.60499	0.04820	0.23023	0.69589	0.06105	0.27793	0.78232	3890
3900	0.03644	0.18382	0.60165	0.04773	0.22845	0.69247	0.06050	0.27592	0.77887	3900
3910	0.03606	0.18228	0.59833	0.04727	0.22668	0.68906	0.05995	0.27393	0.77543	3910
3920	0.03569	0.18076	0.59502	0.04681	0.22492	0.68567	0.05940	0.27196	0.77200	3920
3930	0.03532	0.17925	0.59173	0.04636	0.22318	0.68228	0.05886	0.26999	0.76858	3930
3940	0.03495	0.17775	0.58845	0.04591	0.22145	0.67890	0.05833	0.26804	0.76517	3940
3950	0.03459	0.17626	0.58518	0.04547	0.21973	0.67554	0.05780	0.26611	0.76177	3950
3960	0.03424	0.17478	0.58192	0.04503	0.21803	0.67218	0.05727	0.26419	0.75838	3960
3970	0.03388	0.17332	0.57868	0.04460	0.21634	0.66884	0.05675	0.26228	0.75499	3970
3980	0.03354	0.17187	0.57545	0.04417	0.21466	0.66551	0.05624	0.26038	0.75162	3980
3990	0.03319	0.17043	0.57223	0.04374	0.21299	0.66219	0.05573	0.25850	0.74825	3990
4000	0.03285	0.16900	0.56903	0.04332	0.21134	0.65888	0.05522	0.25663	0.74490	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ - E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ - E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ - E_0^\circ)/T$	S ^o	C _p ^o	ν cm ⁻¹
	T=1700.			T=1800.			T=1900.			
100	4.99062	6.89489	1.98598	5.09960	7.00841	1.98611	5.20292	7.11579	1.98622	100
110	4.80951	6.70561	1.98573	4.91803	6.81912	1.98589	5.02094	6.92650	1.98602	110
120	4.64488	6.53284	1.98546	4.75295	6.64634	1.98565	4.85545	6.75370	1.98580	120
130	4.49408	6.37393	1.98517	4.60170	6.48741	1.98538	4.70380	6.59476	1.98557	130
140	4.35506	6.22683	1.98485	4.46223	6.34029	1.98510	4.56393	6.44762	1.98531	140
150	4.22620	6.08990	1.98450	4.33292	6.20334	1.98479	4.43421	6.31066	1.98503	150
160	4.10618	5.96184	1.98414	4.21245	6.07526	1.98446	4.31334	6.18256	1.98474	160
170	3.99392	5.84156	1.98375	4.09975	5.95496	1.98412	4.20024	6.06224	1.98443	170
180	3.88854	5.72818	1.98333	3.99392	5.84156	1.98375	4.09401	5.94883	1.98410	180
190	3.78929	5.62096	1.98289	3.89423	5.73431	1.98335	3.99392	5.84156	1.98375	190
200	3.69554	5.51926	1.98243	3.80003	5.63259	1.98294	3.89933	5.73982	1.98338	200
210	3.60675	5.42255	1.98195	3.71080	5.53585	1.98251	3.80971	5.64306	1.98299	210
220	3.52246	5.33036	1.98144	3.62608	5.44364	1.98206	3.72458	5.55082	1.98258	220
230	3.44227	5.24230	1.98091	3.54545	5.35554	1.98158	3.64356	5.46270	1.98215	230
240	3.36583	5.15800	1.98035	3.46857	5.27122	1.98109	3.56629	5.37835	1.98171	240
250	3.29283	5.07717	1.97977	3.39513	5.19036	1.98057	3.49246	5.29746	1.98125	250
260	3.22299	4.99954	1.97917	3.32486	5.11269	1.98003	3.42180	5.21976	1.98076	260
270	3.15609	4.92485	1.97855	3.25753	5.03797	1.97947	3.35408	5.14502	1.98026	270
280	3.09191	4.85291	1.97790	3.19291	4.96599	1.97890	3.28907	5.07301	1.97974	280
290	3.03025	4.78351	1.97722	3.13082	4.89656	1.97830	3.22659	5.00355	1.97920	290
300	2.97094	4.71650	1.97653	3.07108	4.82950	1.97767	3.16647	4.93646	1.97865	300
310	2.91383	4.65170	1.97581	3.01354	4.76467	1.97703	3.10855	4.87159	1.97807	310
320	2.85877	4.58898	1.97507	2.95806	4.70191	1.97637	3.05268	4.80880	1.97747	320
330	2.80565	4.52821	1.97430	2.90451	4.64110	1.97569	2.99875	4.74796	1.97686	330
340	2.75434	4.46929	1.97351	2.85278	4.58213	1.97498	2.94663	4.68895	1.97623	340
350	2.70474	4.41209	1.97270	2.80275	4.52489	1.97426	2.89623	4.63167	1.97558	350
360	2.65674	4.35653	1.97187	2.75434	4.46929	1.97351	2.84743	4.57603	1.97491	360
370	2.61027	4.30252	1.97101	2.70745	4.41523	1.97275	2.80016	4.52193	1.97422	370
380	2.56525	4.24996	1.97013	2.66200	4.36263	1.97196	2.75434	4.46929	1.97351	380
390	2.52158	4.19880	1.96923	2.61792	4.31141	1.97115	2.70988	4.41803	1.97279	390
400	2.47921	4.14896	1.96830	2.57513	4.26152	1.97033	2.66672	4.36810	1.97205	400
410	2.43807	4.10036	1.96735	2.53358	4.21288	1.96948	2.62479	4.31941	1.97128	410
420	2.39811	4.05297	1.96638	2.49319	4.16543	1.96861	2.58403	4.27192	1.97050	420
430	2.35925	4.00671	1.96538	2.45393	4.11912	1.96772	2.54440	4.22556	1.96970	430
440	2.32146	3.96154	1.96436	2.41573	4.07389	1.96681	2.50582	4.18029	1.96889	440
450	2.28469	3.91740	1.96332	2.37854	4.02970	1.96588	2.46827	4.13605	1.96805	450
460	2.24888	3.87426	1.96226	2.34233	3.98650	1.96493	2.43169	4.09280	1.96720	460
470	2.21401	3.83208	1.96117	2.30704	3.94425	1.96396	2.39603	4.05051	1.96633	470
480	2.18002	3.79080	1.96006	2.27265	3.90292	1.96297	2.36127	4.00912	1.96543	480
490	2.14688	3.75039	1.95893	2.23910	3.86245	1.96196	2.32736	3.96860	1.96453	490
500	2.11456	3.71083	1.95778	2.20638	3.82283	1.96093	2.29427	3.92892	1.96360	500
510	2.08302	3.67207	1.95660	2.17443	3.78400	1.95988	2.26196	3.89005	1.96265	510
520	2.05223	3.63409	1.95540	2.14325	3.74596	1.95881	2.23041	3.85194	1.96169	520
530	2.02217	3.59686	1.95418	2.11278	3.70866	1.95771	2.19959	3.81459	1.96071	530
540	1.99280	3.56034	1.95294	2.08302	3.67207	1.95660	2.16946	3.77795	1.95971	540
550	1.96410	3.52452	1.95167	2.05392	3.63618	1.95547	2.14001	3.74200	1.95869	550
560	1.93605	3.48936	1.95038	2.02547	3.60096	1.95432	2.11120	3.70671	1.95766	560
570	1.90862	3.45485	1.94907	1.99765	3.56638	1.95315	2.08302	3.67207	1.95660	570
580	1.88179	3.42097	1.94774	1.97042	3.53242	1.95196	2.05544	3.63805	1.95553	580
590	1.85554	3.38768	1.94639	1.94378	3.49906	1.95074	2.02844	3.60463	1.95444	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	T=1700.			T=1800.			T=1900.			ν cm^{-1}
	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	
600	1.82984	3.35498	1.94501	1.91769	3.46628	1.94951	2.00200	3.57179	1.95333	600
610	1.80469	3.32284	1.94361	1.89215	3.43407	1.94826	1.97610	3.53952	1.95221	610
620	1.78006	3.29125	1.94219	1.86713	3.40240	1.94699	1.95073	3.50778	1.95107	620
630	1.75594	3.26018	1.94075	1.84262	3.37126	1.94570	1.92587	3.47657	1.94990	630
640	1.73230	3.22963	1.93929	1.81860	3.34063	1.94439	1.90150	3.44587	1.94873	640
650	1.70914	3.19958	1.93780	1.79505	3.31049	1.94306	1.87760	3.41567	1.94753	650
660	1.68644	3.17000	1.93630	1.77197	3.28084	1.94172	1.85417	3.38595	1.94632	660
670	1.66418	3.14090	1.93477	1.74932	3.25165	1.94035	1.83118	3.35669	1.94508	670
680	1.64235	3.11224	1.93322	1.72712	3.22291	1.93896	1.80863	3.32788	1.94384	680
690	1.62094	3.08403	1.93165	1.70533	3.19461	1.93755	1.78649	3.29951	1.94257	690
700	1.59994	3.05625	1.93005	1.68394	3.16675	1.93613	1.76477	3.27157	1.94129	700
710	1.57933	3.02888	1.92844	1.66296	3.13929	1.93468	1.74344	3.24404	1.93998	710
720	1.55910	3.00192	1.92680	1.64235	3.11224	1.93322	1.72249	3.21692	1.93867	720
730	1.53925	2.97536	1.92515	1.62212	3.08559	1.93173	1.70192	3.19019	1.93733	730
740	1.51976	2.94918	1.92347	1.60225	3.05932	1.93023	1.68172	3.16384	1.93598	740
750	1.50061	2.92337	1.92177	1.58274	3.03342	1.92871	1.66186	3.13786	1.93460	750
760	1.48181	2.89793	1.92005	1.56357	3.00788	1.92717	1.64235	3.11224	1.93322	760
770	1.46334	2.87284	1.91831	1.54473	2.98270	1.92561	1.62318	3.08698	1.93181	770
780	1.44520	2.84810	1.91655	1.52621	2.95786	1.92403	1.60433	3.06206	1.93039	780
790	1.42737	2.82369	1.91477	1.50802	2.93336	1.92243	1.58580	3.03748	1.92895	790
800	1.40985	2.79962	1.91296	1.49013	2.90919	1.92082	1.56757	3.01323	1.92749	800
810	1.39262	2.77587	1.91114	1.47254	2.88534	1.91918	1.54965	2.98929	1.92602	810
820	1.37569	2.75243	1.90929	1.45524	2.86180	1.91753	1.53203	2.96567	1.92453	820
830	1.35904	2.72930	1.90743	1.43823	2.83857	1.91586	1.51468	2.94235	1.92302	830
840	1.34267	2.70646	1.90555	1.42149	2.81563	1.91417	1.49762	2.91933	1.92150	840
850	1.32657	2.68392	1.90364	1.40503	2.79299	1.91246	1.48083	2.89660	1.91996	850
860	1.31073	2.66167	1.90171	1.38883	2.77063	1.91073	1.46431	2.87415	1.91840	860
870	1.29515	2.63970	1.89977	1.37290	2.74855	1.90899	1.44804	2.85198	1.91683	870
880	1.27982	2.61800	1.89780	1.35721	2.72675	1.90722	1.43203	2.83008	1.91524	880
890	1.26473	2.59656	1.89582	1.34177	2.70520	1.90544	1.41627	2.80845	1.91363	890
900	1.24989	2.57539	1.89381	1.32657	2.68392	1.90364	1.40074	2.78708	1.91201	900
910	1.23528	2.55448	1.89179	1.31160	2.66290	1.90182	1.38546	2.76596	1.91036	910
920	1.22089	2.53381	1.88974	1.29687	2.64212	1.89999	1.37040	2.74509	1.90871	920
930	1.20673	2.51339	1.88768	1.28236	2.62159	1.89813	1.35557	2.72447	1.90704	930
940	1.19279	2.49321	1.88559	1.26806	2.60130	1.89626	1.34096	2.70408	1.90535	940
950	1.17906	2.47327	1.88349	1.25399	2.58125	1.89437	1.32657	2.68392	1.90364	950
960	1.16554	2.45356	1.88137	1.24012	2.56142	1.89246	1.31238	2.66400	1.90192	960
970	1.15223	2.43408	1.87922	1.22646	2.54182	1.89054	1.29841	2.64430	1.90018	970
980	1.13911	2.41481	1.87706	1.21300	2.52244	1.88860	1.28463	2.62482	1.89843	980
990	1.12619	2.39577	1.87488	1.19973	2.50327	1.88664	1.27105	2.60555	1.89666	990
1000	1.11346	2.37693	1.87268	1.18666	2.48432	1.88466	1.25767	2.58650	1.89487	1000
1010	1.10092	2.35831	1.87046	1.17378	2.46558	1.88267	1.24448	2.56766	1.89307	1010
1020	1.08856	2.33989	1.86822	1.16108	2.44704	1.88065	1.23147	2.54901	1.89125	1020
1030	1.07638	2.32168	1.86597	1.14856	2.42870	1.87862	1.21864	2.53057	1.88942	1030
1040	1.06438	2.30366	1.86369	1.13622	2.41056	1.87658	1.20599	2.51232	1.88757	1040
1050	1.05255	2.28584	1.86140	1.12406	2.39261	1.87452	1.19352	2.49427	1.88570	1050
1060	1.04089	2.26820	1.85909	1.11206	2.37486	1.87244	1.18122	2.47641	1.88382	1060
1070	1.02939	2.25076	1.85675	1.10023	2.35728	1.87034	1.16908	2.45873	1.88193	1070
1080	1.01806	2.23350	1.85441	1.08856	2.33989	1.86822	1.15711	2.44123	1.88002	1080
1090	1.00688	2.21642	1.85204	1.07705	2.32269	1.86609	1.14530	2.42391	1.87809	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic
 Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm ⁻¹
	T=1700.			T=1800.			T=1900.			
1100	0.99586	2.19951	1.84965	1.06570	2.30565	1.86395	1.13365	2.40677	1.87615	1100
1110	0.98500	2.18279	1.84725	1.05451	2.28879	1.86178	1.12215	2.38980	1.87419	1110
1120	0.97428	2.16623	1.84483	1.04346	2.27211	1.85960	1.11081	2.37300	1.87222	1120
1130	0.96371	2.14984	1.84239	1.03257	2.25559	1.85740	1.09961	2.35636	1.87023	1130
1140	0.95329	2.13362	1.83993	1.02182	2.23923	1.85519	1.08856	2.33989	1.86822	1140
1150	0.94300	2.11756	1.83746	1.01121	2.22304	1.85296	1.07766	2.32359	1.86621	1150
1160	0.93286	2.10166	1.83496	1.00074	2.20701	1.85072	1.06689	2.30744	1.86417	1160
1170	0.92285	2.08592	1.83245	0.99041	2.19113	1.84845	1.05627	2.29145	1.86212	1170
1180	0.91297	2.07034	1.82993	0.98021	2.17541	1.84617	1.04578	2.27561	1.86006	1180
1190	0.90323	2.05491	1.82738	0.97015	2.15984	1.84388	1.03542	2.25992	1.85798	1190
1200	0.89362	2.03963	1.82482	0.96022	2.14442	1.84157	1.02520	2.24438	1.85589	1200
1210	0.88413	2.02449	1.82224	0.95041	2.12914	1.83924	1.01510	2.22899	1.85378	1210
1220	0.87477	2.00951	1.81964	0.94074	2.11401	1.83690	1.00513	2.21374	1.85166	1220
1230	0.86553	1.99466	1.81703	0.93118	2.09903	1.83455	0.99529	2.19863	1.84953	1230
1240	0.85641	1.97996	1.81440	0.92175	2.08418	1.83217	0.98556	2.18366	1.84738	1240
1250	0.84741	1.96540	1.81176	0.91243	2.06948	1.82978	0.97596	2.16883	1.84521	1250
1260	0.83852	1.95097	1.80909	0.90323	2.05491	1.82738	0.96648	2.15414	1.84303	1260
1270	0.82975	1.93668	1.80641	0.89415	2.04047	1.82496	0.95711	2.13958	1.84084	1270
1280	0.82109	1.92252	1.80372	0.88518	2.02617	1.82253	0.94786	2.12515	1.83863	1280
1290	0.81254	1.90850	1.80101	0.87632	2.01199	1.82008	0.93871	2.11085	1.83641	1290
1300	0.80409	1.89460	1.79828	0.86757	1.99795	1.81761	0.92968	2.09668	1.83417	1300
1310	0.79576	1.88083	1.79553	0.85893	1.98403	1.81513	0.92076	2.08263	1.83192	1310
1320	0.78753	1.86719	1.79277	0.85039	1.97024	1.81264	0.91194	2.06871	1.82966	1320
1330	0.77940	1.85367	1.79000	0.84196	1.95656	1.81013	0.90323	2.05491	1.82738	1330
1340	0.77137	1.84027	1.78721	0.83363	1.94301	1.80761	0.89462	2.04123	1.82509	1340
1350	0.76345	1.82699	1.78440	0.82540	1.92958	1.80507	0.88612	2.02767	1.82278	1350
1360	0.75562	1.81383	1.78157	0.81727	1.91627	1.80251	0.87771	2.01422	1.82047	1360
1370	0.74788	1.80079	1.77874	0.80924	1.90308	1.79995	0.86940	2.00089	1.81813	1370
1380	0.74024	1.78786	1.77588	0.80130	1.89000	1.79736	0.86119	1.98768	1.81579	1380
1390	0.73270	1.77505	1.77301	0.79346	1.87703	1.79477	0.85308	1.97458	1.81343	1390
1400	0.72525	1.76235	1.77013	0.78571	1.86417	1.79216	0.84506	1.96159	1.81106	1400
1410	0.71788	1.74976	1.76723	0.77805	1.85142	1.78953	0.83713	1.94871	1.80867	1410
1420	0.71061	1.73729	1.76432	0.77049	1.83879	1.78689	0.82929	1.93593	1.80627	1420
1430	0.70342	1.72491	1.76139	0.76301	1.82626	1.78424	0.82154	1.92326	1.80386	1430
1440	0.69632	1.71265	1.75844	0.75562	1.81383	1.78157	0.81388	1.91070	1.80143	1440
1450	0.68931	1.70049	1.75549	0.74831	1.80151	1.77889	0.80631	1.89824	1.79900	1450
1460	0.68237	1.68844	1.75251	0.74109	1.78930	1.77620	0.79882	1.88589	1.79655	1460
1470	0.67552	1.67648	1.74953	0.73395	1.77718	1.77349	0.79141	1.87363	1.79408	1470
1480	0.66876	1.66463	1.74653	0.72689	1.76517	1.77077	0.78409	1.86148	1.79161	1480
1490	0.66207	1.65288	1.74351	0.71992	1.75325	1.76804	0.77685	1.84942	1.78912	1490
1500	0.65546	1.64123	1.74048	0.71302	1.74143	1.76529	0.76970	1.83746	1.78662	1500
1510	0.64892	1.62967	1.73744	0.70621	1.72971	1.76253	0.76262	1.82560	1.78410	1510
1520	0.64246	1.61822	1.73438	0.69947	1.71809	1.75975	0.75562	1.81383	1.78157	1520
1530	0.63608	1.60685	1.73131	0.69280	1.70656	1.75697	0.74869	1.80216	1.77904	1530
1540	0.62977	1.59558	1.72823	0.68622	1.69512	1.75417	0.74184	1.79058	1.77648	1540
1550	0.62354	1.58441	1.72513	0.67970	1.68378	1.75135	0.73507	1.77909	1.77392	1550
1560	0.61738	1.57332	1.72202	0.67326	1.67252	1.74853	0.72837	1.76769	1.77135	1560
1570	0.61128	1.56233	1.71889	0.66689	1.66136	1.74569	0.72175	1.75638	1.76876	1570
1580	0.60526	1.55143	1.71576	0.66059	1.65028	1.74284	0.71519	1.74515	1.76616	1580
1590	0.59931	1.54061	1.71261	0.65436	1.63930	1.73998	0.70871	1.73402	1.76355	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	T=1700.			T=1800.			T=1900.			ν cm^{-1}
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
1600	0.59342	1.52988	1.70944	0.64820	1.62840	1.73710	0.70230	1.72297	1.76092	1600
1610	0.58760	1.51924	1.70627	0.64211	1.61758	1.73421	0.69595	1.71201	1.75829	1610
1620	0.58185	1.50869	1.70308	0.63608	1.60685	1.73131	0.68967	1.70113	1.75564	1620
1630	0.57616	1.49822	1.69988	0.63012	1.59621	1.72840	0.68346	1.69033	1.75298	1630
1640	0.57053	1.48783	1.69666	0.62423	1.58565	1.72547	0.67732	1.67962	1.75031	1640
1650	0.56497	1.47753	1.69344	0.61840	1.57517	1.72254	0.67124	1.66899	1.74763	1650
1660	0.55947	1.46730	1.69020	0.61263	1.56477	1.71959	0.66522	1.65844	1.74494	1660
1670	0.55403	1.45716	1.68695	0.60693	1.55445	1.71663	0.65927	1.64796	1.74224	1670
1680	0.54865	1.44710	1.68369	0.60128	1.54421	1.71366	0.65338	1.63757	1.73952	1680
1690	0.54334	1.43712	1.68041	0.59570	1.53405	1.71067	0.64756	1.62725	1.73680	1690
1700	0.53808	1.42721	1.67713	0.59018	1.52396	1.70768	0.64179	1.61702	1.73406	1700
1710	0.53288	1.41739	1.67383	0.58471	1.51396	1.70467	0.63608	1.60685	1.73131	1710
1720	0.52773	1.40764	1.67052	0.57931	1.50402	1.70166	0.63044	1.59677	1.72855	1720
1730	0.52264	1.39796	1.66720	0.57396	1.49417	1.69863	0.62485	1.58675	1.72578	1730
1740	0.51761	1.38836	1.66387	0.56867	1.48439	1.69559	0.61931	1.57681	1.72300	1740
1750	0.51263	1.37884	1.66052	0.56344	1.47468	1.69254	0.61384	1.56695	1.72021	1750
1760	0.50771	1.36939	1.65717	0.55826	1.46504	1.68948	0.60842	1.55716	1.71741	1760
1770	0.50284	1.36001	1.65380	0.55313	1.45548	1.68641	0.60306	1.54743	1.71460	1770
1780	0.49803	1.35070	1.65043	0.54806	1.44599	1.68332	0.59775	1.53778	1.71177	1780
1790	0.49326	1.34146	1.64704	0.54304	1.43657	1.68023	0.59250	1.52820	1.70894	1790
1800	0.48855	1.33229	1.64364	0.53808	1.42721	1.67713	0.58730	1.51869	1.70610	1800
1810	0.48389	1.32320	1.64024	0.53316	1.41793	1.67401	0.58215	1.50924	1.70325	1810
1820	0.47927	1.31417	1.63682	0.52830	1.40872	1.67089	0.57705	1.49987	1.70038	1820
1830	0.47471	1.30521	1.63339	0.52349	1.39957	1.66775	0.57201	1.49056	1.69751	1830
1840	0.47020	1.29632	1.62995	0.51873	1.39049	1.66461	0.56701	1.48131	1.69463	1840
1850	0.46573	1.28749	1.62650	0.51401	1.38148	1.66145	0.56207	1.47214	1.69173	1850
1860	0.46131	1.27873	1.62304	0.50935	1.37253	1.65829	0.55717	1.46302	1.68883	1860
1870	0.45694	1.27004	1.61957	0.50473	1.36364	1.65511	0.55233	1.45398	1.68592	1870
1880	0.45262	1.26141	1.61610	0.50016	1.35483	1.65193	0.54753	1.44499	1.68300	1880
1890	0.44834	1.25285	1.61261	0.49564	1.34607	1.64874	0.54278	1.43607	1.68007	1890
1900	0.44410	1.24435	1.60911	0.49116	1.33738	1.64553	0.53808	1.42721	1.67713	1900
1910	0.43991	1.23591	1.60561	0.48673	1.32875	1.64232	0.53342	1.41842	1.67418	1910
1920	0.43577	1.22754	1.60209	0.48234	1.32018	1.63910	0.52881	1.40968	1.67122	1920
1930	0.43167	1.21922	1.59856	0.47800	1.31167	1.63587	0.52424	1.40101	1.66825	1930
1940	0.42761	1.21097	1.59503	0.47370	1.30323	1.63263	0.51972	1.39240	1.66527	1940
1950	0.42359	1.20278	1.59149	0.46945	1.29484	1.62938	0.51525	1.38384	1.66228	1950
1960	0.41962	1.19465	1.58794	0.46524	1.28652	1.62612	0.51082	1.37535	1.65929	1960
1970	0.41568	1.18657	1.58438	0.46107	1.27825	1.62285	0.50643	1.36691	1.65628	1970
1980	0.41179	1.17856	1.58081	0.45694	1.27004	1.61957	0.50208	1.35853	1.65327	1980
1990	0.40794	1.17061	1.57723	0.45286	1.26189	1.61629	0.49777	1.35021	1.65025	1990
2000	0.40412	1.16271	1.57365	0.44881	1.25380	1.61300	0.49351	1.34195	1.64722	2000
2010	0.40035	1.15487	1.57005	0.44481	1.24576	1.60970	0.48929	1.33374	1.64418	2010
2020	0.39662	1.14709	1.56645	0.44084	1.23778	1.60639	0.48511	1.32559	1.64113	2020
2030	0.39292	1.13936	1.56284	0.43692	1.22986	1.60307	0.48097	1.31749	1.63808	2030
2040	0.38926	1.13169	1.55922	0.43303	1.22199	1.59974	0.47687	1.30945	1.63501	2040
2050	0.38564	1.12407	1.55560	0.42918	1.21417	1.59641	0.47281	1.30146	1.63194	2050
2060	0.38206	1.11651	1.55197	0.42537	1.20641	1.59306	0.46878	1.29352	1.62886	2060
2070	0.37851	1.10901	1.54833	0.42160	1.19870	1.58971	0.46480	1.28564	1.62577	2070
2080	0.37500	1.10155	1.54468	0.41786	1.19105	1.58636	0.46085	1.27782	1.62268	2080
2090	0.37152	1.09415	1.54102	0.41416	1.18345	1.58299	0.45694	1.27004	1.61957	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
T=1700.			T=1800.			T=1900.				
2100	0.36808	1.08681	1.53736	0.41050	1.17590	1.57962	0.45307	1.26232	1.61646	2100
2110	0.36468	1.07951	1.53369	0.40687	1.16841	1.57624	0.44924	1.25465	1.61334	2110
2120	0.36131	1.07227	1.53002	0.40328	1.16096	1.57285	0.44544	1.24703	1.61022	2120
2130	0.35797	1.06508	1.52633	0.39973	1.15357	1.56945	0.44167	1.23946	1.60708	2130
2140	0.35467	1.05794	1.52264	0.39620	1.14623	1.56605	0.43795	1.23194	1.60394	2140
2150	0.35140	1.05085	1.51895	0.39272	1.13893	1.56264	0.43425	1.22447	1.60079	2150
2160	0.34816	1.04381	1.51525	0.38926	1.13169	1.55922	0.43059	1.21704	1.59764	2160
2170	0.34496	1.03682	1.51154	0.38584	1.12450	1.55580	0.42697	1.20967	1.59447	2170
2180	0.34179	1.02988	1.50782	0.38245	1.11735	1.55237	0.42338	1.20235	1.59130	2180
2190	0.33864	1.02298	1.50410	0.37910	1.11025	1.54893	0.41982	1.19507	1.58812	2190
2200	0.33554	1.01614	1.50037	0.37578	1.10320	1.54549	0.41630	1.18785	1.58494	2200
2210	0.33246	1.00934	1.49664	0.37249	1.09620	1.54204	0.41281	1.18066	1.58175	2210
2220	0.32941	1.00259	1.49290	0.36923	1.08925	1.53858	0.40935	1.17353	1.57855	2220
2230	0.32639	0.99589	1.48916	0.36600	1.08234	1.53512	0.40592	1.16644	1.57535	2230
2240	0.32341	0.98924	1.48541	0.36280	1.07548	1.53165	0.40253	1.15940	1.57213	2240
2250	0.32045	0.98263	1.48165	0.35964	1.06867	1.52818	0.39917	1.15241	1.56892	2250
2260	0.31752	0.97607	1.47789	0.35650	1.06190	1.52470	0.39583	1.14546	1.56569	2260
2270	0.31462	0.96955	1.47412	0.35339	1.05517	1.52121	0.39253	1.13855	1.56246	2270
2280	0.31175	0.96308	1.47035	0.35032	1.04849	1.51772	0.38926	1.13169	1.55922	2280
2290	0.30891	0.95665	1.46657	0.34727	1.04186	1.51422	0.38602	1.12487	1.55598	2290
2300	0.30609	0.95027	1.46279	0.34425	1.03527	1.51071	0.38281	1.11810	1.55273	2300
2310	0.30330	0.94393	1.45901	0.34126	1.02872	1.50720	0.37963	1.11137	1.54948	2310
2320	0.30054	0.93764	1.45522	0.33830	1.02222	1.50369	0.37647	1.10468	1.54622	2320
2330	0.29781	0.93139	1.45142	0.33536	1.01576	1.50017	0.37335	1.09804	1.54295	2330
2340	0.29511	0.92518	1.44762	0.33246	1.00934	1.49664	0.37025	1.09144	1.53968	2340
2350	0.29243	0.91902	1.44382	0.32958	1.00297	1.49311	0.36718	1.08488	1.53640	2350
2360	0.28977	0.91289	1.44001	0.32673	0.99664	1.48957	0.36414	1.07836	1.53311	2360
2370	0.28715	0.90681	1.43619	0.32390	0.99034	1.48603	0.36113	1.07189	1.52982	2370
2380	0.28454	0.90077	1.43238	0.32110	0.98410	1.48249	0.35815	1.06545	1.52653	2380
2390	0.28197	0.89478	1.42856	0.31833	0.97789	1.47893	0.35519	1.05906	1.52323	2390
2400	0.27942	0.88882	1.42473	0.31558	0.97172	1.47538	0.35226	1.05271	1.51992	2400
2410	0.27689	0.88290	1.42090	0.31286	0.96559	1.47182	0.34935	1.04639	1.51661	2410
2420	0.27439	0.87703	1.41707	0.31017	0.95950	1.46825	0.34647	1.04012	1.51329	2420
2430	0.27191	0.87119	1.41324	0.30750	0.95346	1.46468	0.34362	1.03389	1.50997	2430
2440	0.26945	0.86540	1.40940	0.30485	0.94745	1.46111	0.34079	1.02769	1.50665	2440
2450	0.26702	0.85964	1.40556	0.30223	0.94148	1.45753	0.33799	1.02154	1.50332	2450
2460	0.26462	0.85392	1.40171	0.29963	0.93555	1.45395	0.33521	1.01542	1.49998	2460
2470	0.26223	0.84824	1.39786	0.29706	0.92966	1.45037	0.33246	1.00934	1.49664	2470
2480	0.25987	0.84260	1.39401	0.29451	0.92381	1.44678	0.32973	1.00330	1.49330	2480
2490	0.25753	0.83700	1.39016	0.29198	0.91799	1.44318	0.32703	0.99730	1.48995	2490
2500	0.25522	0.83144	1.38630	0.28948	0.91222	1.43958	0.32435	0.99134	1.48659	2500
2510	0.25292	0.82591	1.38244	0.28700	0.90648	1.43598	0.32169	0.98541	1.48323	2510
2520	0.25065	0.82042	1.37858	0.28454	0.90077	1.43238	0.31906	0.97952	1.47987	2520
2530	0.24840	0.81497	1.37471	0.28211	0.89511	1.42877	0.31645	0.97366	1.47650	2530
2540	0.24617	0.80955	1.37084	0.27970	0.88948	1.42516	0.31386	0.96784	1.47313	2540
2550	0.24396	0.80417	1.36698	0.27731	0.88389	1.42154	0.31130	0.96206	1.46976	2550
2560	0.24178	0.79883	1.36310	0.27494	0.87833	1.41792	0.30876	0.95632	1.46638	2560
2570	0.23961	0.79353	1.35923	0.27259	0.87281	1.41430	0.30624	0.95061	1.46299	2570
2580	0.23747	0.78825	1.35535	0.27027	0.86732	1.41068	0.30374	0.94493	1.45961	2580
2590	0.23534	0.78302	1.35148	0.26797	0.86187	1.40705	0.30127	0.93929	1.45621	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
	T=1700.			T=1800.			T=1900.			
2600	0.23324	0.77782	1.34760	0.26568	0.85646	1.40342	0.29882	0.93369	1.45282	2600
2610	0.23115	0.77265	1.34372	0.26342	0.85108	1.39979	0.29638	0.92812	1.44942	2610
2620	0.22909	0.76752	1.33983	0.26118	0.84573	1.39615	0.29397	0.92258	1.44602	2620
2630	0.22704	0.76242	1.33595	0.25896	0.84042	1.39251	0.29159	0.91708	1.44261	2630
2640	0.22502	0.75736	1.33206	0.25676	0.83514	1.38887	0.28922	0.91161	1.43921	2640
2650	0.22301	0.75233	1.32818	0.25458	0.82990	1.38523	0.28687	0.90617	1.43579	2650
2660	0.22102	0.74734	1.32429	0.25242	0.82469	1.38158	0.28454	0.90077	1.43238	2660
2670	0.21905	0.74238	1.32040	0.25027	0.81951	1.37793	0.28224	0.89540	1.42896	2670
2680	0.21710	0.73745	1.31651	0.24815	0.81437	1.37428	0.27995	0.89007	1.42554	2680
2690	0.21517	0.73255	1.31262	0.24605	0.80925	1.37063	0.27768	0.88477	1.42211	2690
2700	0.21326	0.72769	1.30873	0.24396	0.80417	1.36698	0.27544	0.87950	1.41869	2700
2710	0.21136	0.72286	1.30484	0.24190	0.79913	1.36332	0.27321	0.87426	1.41526	2710
2720	0.20948	0.71806	1.30095	0.23985	0.79411	1.35966	0.27100	0.86905	1.41182	2720
2730	0.20762	0.71329	1.29705	0.23782	0.78913	1.35600	0.26881	0.86388	1.40839	2730
2740	0.20578	0.70856	1.29316	0.23581	0.78418	1.35234	0.26664	0.85873	1.40495	2740
2750	0.20395	0.70385	1.28926	0.23382	0.77926	1.34868	0.26449	0.85362	1.40151	2750
2760	0.20214	0.69918	1.28537	0.23185	0.77437	1.34501	0.26236	0.84854	1.39806	2760
2770	0.20035	0.69454	1.28148	0.22989	0.76951	1.34134	0.26024	0.84349	1.39462	2770
2780	0.19857	0.68993	1.27758	0.22795	0.76469	1.33768	0.25815	0.83847	1.39117	2780
2790	0.19681	0.68535	1.27369	0.22603	0.75989	1.33401	0.25607	0.83348	1.38772	2790
2800	0.19507	0.68080	1.26979	0.22412	0.75512	1.33034	0.25401	0.82852	1.38427	2800
2810	0.19334	0.67628	1.26590	0.22224	0.75039	1.32667	0.25196	0.82359	1.38081	2810
2820	0.19163	0.67179	1.26201	0.22036	0.74568	1.32299	0.24994	0.81870	1.37736	2820
2830	0.18994	0.66733	1.25811	0.21851	0.74100	1.31932	0.24793	0.81383	1.37390	2830
2840	0.18826	0.66289	1.25422	0.21667	0.73636	1.31565	0.24594	0.80899	1.37044	2840
2850	0.18660	0.65849	1.25033	0.21485	0.73174	1.31197	0.24396	0.80417	1.36698	2850
2860	0.18495	0.65412	1.24644	0.21304	0.72715	1.30830	0.24201	0.79939	1.36351	2860
2870	0.18331	0.64978	1.24255	0.21125	0.72259	1.30462	0.24007	0.79464	1.36005	2870
2880	0.18170	0.64546	1.23866	0.20948	0.71806	1.30094	0.23814	0.78991	1.35658	2880
2890	0.18009	0.64117	1.23477	0.20772	0.71355	1.29727	0.23624	0.78522	1.35311	2890
2900	0.17851	0.63692	1.23088	0.20598	0.70908	1.29359	0.23434	0.78055	1.34964	2900
2910	0.17693	0.63269	1.22699	0.20425	0.70463	1.28991	0.23247	0.77591	1.34617	2910
2920	0.17537	0.62848	1.22311	0.20254	0.70021	1.28624	0.23061	0.77130	1.34270	2920
2930	0.17383	0.62431	1.21923	0.20084	0.69582	1.28256	0.22876	0.76671	1.33922	2930
2940	0.17230	0.62016	1.21534	0.19916	0.69146	1.27888	0.22694	0.76216	1.33575	2940
2950	0.17078	0.61604	1.21146	0.19750	0.68712	1.27520	0.22512	0.75763	1.33227	2950
2960	0.16928	0.61195	1.20758	0.19584	0.68281	1.27152	0.22333	0.75312	1.32879	2960
2970	0.16779	0.60788	1.20370	0.19420	0.67853	1.26785	0.22154	0.74865	1.32531	2970
2980	0.16632	0.60384	1.19983	0.19258	0.67428	1.26417	0.21978	0.74420	1.32183	2980
2990	0.16485	0.59983	1.19595	0.19097	0.67005	1.26049	0.21802	0.73978	1.31835	2990
3000	0.16341	0.59584	1.19208	0.18938	0.66585	1.25682	0.21629	0.73538	1.31487	3000
3010	0.16197	0.59188	1.18821	0.18780	0.66167	1.25314	0.21456	0.73101	1.31139	3010
3020	0.16055	0.58795	1.18434	0.18623	0.65752	1.24946	0.21286	0.72667	1.30791	3020
3030	0.15914	0.58404	1.18048	0.18467	0.65339	1.24579	0.21116	0.72235	1.30443	3030
3040	0.15775	0.58015	1.17661	0.18313	0.64930	1.24211	0.20948	0.71806	1.30094	3040
3050	0.15636	0.57630	1.17275	0.18161	0.64522	1.23844	0.20781	0.71379	1.29746	3050
3060	0.15499	0.57246	1.16889	0.18009	0.64117	1.23477	0.20616	0.70955	1.29398	3060
3070	0.15363	0.56866	1.16503	0.17859	0.63715	1.23110	0.20452	0.70533	1.29049	3070
3080	0.15229	0.56487	1.16118	0.17711	0.63315	1.22743	0.20290	0.70114	1.28701	3080
3090	0.15095	0.56112	1.15733	0.17563	0.62918	1.22376	0.20129	0.69698	1.28353	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	T=1700.			T=1800.			T=1900.			ν cm^{-1}
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
3100	0.14963	0.55738	1.15348	0.17417	0.62523	1.22009	0.19969	0.69283	1.28004	3100
3110	0.14832	0.55367	1.14963	0.17272	0.62131	1.21642	0.19811	0.68872	1.27656	3110
3120	0.14703	0.54999	1.14579	0.17129	0.61741	1.21276	0.19654	0.68463	1.27307	3120
3130	0.14574	0.54633	1.14195	0.16986	0.61354	1.20909	0.19498	0.68056	1.26959	3130
3140	0.14447	0.54269	1.13811	0.16845	0.60968	1.20543	0.19343	0.67651	1.26610	3140
3150	0.14320	0.53908	1.13428	0.16705	0.60586	1.20177	0.19190	0.67249	1.26262	3150
3160	0.14195	0.53549	1.13045	0.16566	0.60205	1.19811	0.19038	0.66850	1.25914	3160
3170	0.14071	0.53193	1.12662	0.16429	0.59827	1.19445	0.18888	0.66452	1.25565	3170
3180	0.13948	0.52838	1.12279	0.16293	0.59452	1.19079	0.18738	0.66057	1.25217	3180
3190	0.13827	0.52486	1.11897	0.16158	0.59079	1.18714	0.18590	0.65665	1.24869	3190
3200	0.13706	0.52137	1.11515	0.16024	0.58708	1.18348	0.18443	0.65275	1.24521	3200
3210	0.13587	0.51789	1.11134	0.15891	0.58339	1.17983	0.18297	0.64887	1.24173	3210
3220	0.13468	0.51444	1.10753	0.15759	0.57972	1.17618	0.18153	0.64501	1.23825	3220
3230	0.13351	0.51102	1.10372	0.15629	0.57608	1.17254	0.18009	0.64117	1.23477	3230
3240	0.13234	0.50761	1.09992	0.15499	0.57246	1.16889	0.17867	0.63736	1.23129	3240
3250	0.13119	0.50423	1.09612	0.15371	0.56887	1.16525	0.17726	0.63357	1.22781	3250
3260	0.13005	0.50086	1.09232	0.15244	0.56529	1.16161	0.17586	0.62981	1.22434	3260
3270	0.12892	0.49752	1.08853	0.15118	0.56174	1.15797	0.17448	0.62606	1.22086	3270
3280	0.12779	0.49421	1.08474	0.14993	0.55821	1.15433	0.17310	0.62234	1.21739	3280
3290	0.12668	0.49091	1.08096	0.14869	0.55470	1.15070	0.17174	0.61864	1.21391	3290
3300	0.12558	0.48764	1.07718	0.14746	0.55122	1.14707	0.17039	0.61496	1.21044	3300
3310	0.12449	0.48438	1.07340	0.14624	0.54775	1.14344	0.16904	0.61130	1.20697	3310
3320	0.12340	0.48115	1.06963	0.14503	0.54431	1.13982	0.16771	0.60767	1.20350	3320
3330	0.12233	0.47794	1.06586	0.14383	0.54088	1.13619	0.16639	0.60405	1.20003	3330
3340	0.12127	0.47475	1.06210	0.14265	0.53748	1.13257	0.16508	0.60046	1.19657	3340
3350	0.12021	0.47158	1.05834	0.14147	0.53410	1.12896	0.16379	0.59689	1.19310	3350
3360	0.11917	0.46843	1.05459	0.14030	0.53074	1.12534	0.16250	0.59334	1.18964	3360
3370	0.11814	0.46530	1.05084	0.13915	0.52740	1.12173	0.16122	0.58981	1.18618	3370
3380	0.11711	0.46219	1.04709	0.13800	0.52409	1.11812	0.15996	0.58630	1.18271	3380
3390	0.11609	0.45911	1.04335	0.13686	0.52079	1.11452	0.15870	0.58281	1.17926	3390
3400	0.11509	0.45604	1.03962	0.13573	0.51751	1.11092	0.15745	0.57934	1.17580	3400
3410	0.11409	0.45299	1.03589	0.13462	0.51425	1.10732	0.15622	0.57589	1.17234	3410
3420	0.11310	0.44996	1.03216	0.13351	0.51102	1.10372	0.15499	0.57246	1.16889	3420
3430	0.11212	0.44695	1.02844	0.13241	0.50780	1.10013	0.15378	0.56906	1.16544	3430
3440	0.11115	0.44396	1.02473	0.13132	0.50460	1.09654	0.15257	0.56567	1.16199	3440
3450	0.11018	0.44100	1.02102	0.13024	0.50142	1.09295	0.15137	0.56230	1.15854	3450
3460	0.10923	0.43805	1.01731	0.12917	0.49826	1.08937	0.15019	0.55895	1.15510	3460
3470	0.10828	0.43512	1.01361	0.12810	0.49513	1.08579	0.14901	0.55562	1.15166	3470
3480	0.10734	0.43220	1.00992	0.12705	0.49201	1.08222	0.14784	0.55231	1.14822	3480
3490	0.10642	0.42931	1.00623	0.12601	0.48891	1.07865	0.14669	0.54902	1.14478	3490
3500	0.10549	0.42644	1.00254	0.12497	0.48583	1.07508	0.14554	0.54575	1.14134	3500
3510	0.10458	0.42358	0.99886	0.12394	0.48276	1.07151	0.14440	0.54250	1.13791	3510
3520	0.10368	0.42075	0.99519	0.12293	0.47972	1.06795	0.14327	0.53927	1.13448	3520
3530	0.10278	0.41793	0.99152	0.12192	0.47670	1.06440	0.14215	0.53606	1.13105	3530
3540	0.10189	0.41513	0.98786	0.12092	0.47369	1.06085	0.14104	0.53286	1.12762	3540
3550	0.10101	0.41235	0.98420	0.11992	0.47070	1.05730	0.13994	0.52969	1.12420	3550
3560	0.10014	0.40958	0.98055	0.11894	0.46773	1.05375	0.13884	0.52653	1.12078	3560
3570	0.09927	0.40684	0.97691	0.11796	0.46478	1.05021	0.13776	0.52339	1.11736	3570
3580	0.09841	0.40411	0.97327	0.11700	0.46185	1.04668	0.13668	0.52027	1.11395	3580
3590	0.09756	0.40140	0.96964	0.11604	0.45893	1.04315	0.13562	0.51717	1.11054	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	ν cm ⁻¹
	T=1700.			T=1800.			T=1900.			
3600	0.09672	0.39871	0.96601	0.11509	0.45604	1.03962	0.13456	0.51408	1.10713	3600
3610	0.09589	0.39603	0.96239	0.11414	0.45316	1.03610	0.13351	0.51102	1.10372	3610
3620	0.09506	0.39338	0.95877	0.11321	0.45030	1.03258	0.13247	0.50797	1.10032	3620
3630	0.09424	0.39074	0.95516	0.11228	0.44745	1.02906	0.13143	0.50494	1.09692	3630
3640	0.09342	0.38811	0.95156	0.11136	0.44463	1.02555	0.13041	0.50192	1.09352	3640
3650	0.09262	0.38551	0.94796	0.11045	0.44182	1.02205	0.12939	0.49893	1.09013	3650
3660	0.09182	0.38292	0.94437	0.10955	0.43903	1.01855	0.12838	0.49595	1.08673	3660
3670	0.09103	0.38035	0.94078	0.10865	0.43625	1.01505	0.12738	0.49299	1.08335	3670
3680	0.09024	0.37779	0.93720	0.10776	0.43350	1.01156	0.12639	0.49005	1.07996	3680
3690	0.08947	0.37525	0.93363	0.10688	0.43076	1.00807	0.12541	0.48712	1.07658	3690
3700	0.08869	0.37273	0.93007	0.10601	0.42803	1.00459	0.12443	0.48421	1.07320	3700
3710	0.08793	0.37023	0.92651	0.10514	0.42532	1.00111	0.12346	0.48132	1.06983	3710
3720	0.08717	0.36774	0.92295	0.10428	0.42263	0.99764	0.12250	0.47844	1.06646	3720
3730	0.08642	0.36526	0.91941	0.10343	0.41996	0.99417	0.12155	0.47559	1.06309	3730
3740	0.08568	0.36281	0.91587	0.10258	0.41730	0.99071	0.12060	0.47274	1.05973	3740
3750	0.08494	0.36037	0.91233	0.10174	0.41466	0.98725	0.11966	0.46992	1.05637	3750
3760	0.08421	0.35794	0.90881	0.10091	0.41204	0.98380	0.11873	0.46711	1.05301	3760
3770	0.08348	0.35553	0.90529	0.10009	0.40943	0.98035	0.11781	0.46432	1.04966	3770
3780	0.08276	0.35314	0.90177	0.09927	0.40684	0.97691	0.11690	0.46154	1.04631	3780
3790	0.08205	0.35076	0.89827	0.09846	0.40426	0.97347	0.11599	0.45878	1.04296	3790
3800	0.08135	0.34840	0.89477	0.09766	0.40170	0.97004	0.11509	0.45604	1.03962	3800
3810	0.08065	0.34605	0.89127	0.09686	0.39916	0.96661	0.11419	0.45331	1.03628	3810
3820	0.07995	0.34372	0.88779	0.09607	0.39663	0.96319	0.11331	0.45060	1.03295	3820
3830	0.07927	0.34140	0.88431	0.09529	0.39411	0.95977	0.11243	0.44790	1.02962	3830
3840	0.07858	0.33910	0.88084	0.09451	0.39161	0.95636	0.11155	0.44522	1.02629	3840
3850	0.07791	0.33682	0.87737	0.09374	0.38913	0.95296	0.11069	0.44256	1.02297	3850
3860	0.07724	0.33454	0.87391	0.09298	0.38666	0.94956	0.10983	0.43991	1.01965	3860
3870	0.07658	0.33229	0.87046	0.09222	0.38421	0.94616	0.10898	0.43727	1.01634	3870
3880	0.07592	0.33005	0.86702	0.09147	0.38177	0.94277	0.10813	0.43465	1.01303	3880
3890	0.07527	0.32782	0.86358	0.09072	0.37935	0.93939	0.10730	0.43205	1.00972	3890
3900	0.07462	0.32561	0.86015	0.08998	0.37694	0.93601	0.10646	0.42946	1.00642	3900
3910	0.07398	0.32341	0.85673	0.08925	0.37455	0.93264	0.10564	0.42689	1.00312	3910
3920	0.07334	0.32122	0.85331	0.08852	0.37217	0.92927	0.10482	0.42433	0.99983	3920
3930	0.07271	0.31905	0.84991	0.08780	0.36981	0.92591	0.10401	0.42179	0.99654	3930
3940	0.07209	0.31690	0.84650	0.08709	0.36746	0.92256	0.10320	0.41926	0.99326	3940
3950	0.07147	0.31476	0.84311	0.08638	0.36513	0.91921	0.10240	0.41675	0.98998	3950
3960	0.07086	0.31263	0.83973	0.08568	0.36281	0.91587	0.10161	0.41425	0.98671	3960
3970	0.07025	0.31052	0.83635	0.08498	0.36050	0.91253	0.10083	0.41176	0.98344	3970
3980	0.06965	0.30842	0.83298	0.08429	0.35821	0.90920	0.10005	0.40929	0.98017	3980
3990	0.06905	0.30633	0.82961	0.08360	0.35593	0.90587	0.09927	0.40684	0.97691	3990
4000	0.06846	0.30426	0.82626	0.08292	0.35367	0.90255	0.09850	0.40440	0.97365	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	ν cm ⁻¹	
T=2000.			T=2100.			T=2200.					
100	5.30113	7.21768	1.98631	5.39472	7.31459	1.98639	5.48410	7.40700	1.98646	100	
110	5.11879	7.02837	1.98613	5.21205	7.12528	1.98623	5.30113	7.21768	1.98631	110	
120	4.95293	6.85556	1.98594	5.04586	6.95246	1.98605	5.13464	7.04485	1.98615	120	
130	4.80091	6.69661	1.98572	4.89351	6.79350	1.98586	4.98199	6.88588	1.98597	130	
140	4.66068	6.54946	1.98549	4.75295	6.64634	1.98565	4.84113	6.73871	1.98578	140	
150	4.53060	6.41248	1.98524	4.62254	6.50935	1.98542	4.71042	6.60171	1.98558	150	
160	4.40937	6.28437	1.98498	4.50098	6.38122	1.98518	4.58856	6.47357	1.98536	160	
170	4.29590	6.16404	1.98470	4.38719	6.26088	1.98492	4.47447	6.35322	1.98512	170	
180	4.18932	6.05060	1.98440	4.28028	6.14743	1.98465	4.36726	6.23976	1.98488	180	
190	4.08887	5.94332	1.98408	4.17950	6.04013	1.98437	4.26619	6.13245	1.98461	190	
200	3.99392	5.84156	1.98375	4.08423	5.93836	1.98406	4.17062	6.03066	1.98434	200	
210	3.90394	5.74478	1.98339	3.99392	5.84156	1.98375	4.08002	5.93385	1.98405	210	
220	3.81846	5.65252	1.98303	3.90812	5.74928	1.98341	3.99392	5.84156	1.98375	220	
230	3.73708	5.56438	1.98264	3.82642	5.66113	1.98306	3.91193	5.75339	1.98343	230	
240	3.65945	5.48001	1.98224	3.74847	5.57673	1.98270	3.83368	5.66898	1.98310	240	
250	3.58527	5.39910	1.98182	3.67397	5.49580	1.98232	3.75889	5.58803	1.98275	250	
260	3.51426	5.32138	1.98139	3.60264	5.41806	1.98192	3.68727	5.51027	1.98239	260	
270	3.44619	5.24661	1.98093	3.53424	5.34327	1.98151	3.61858	5.43547	1.98201	270	
280	3.38083	5.17458	1.98046	3.46857	5.27122	1.98109	3.55262	5.36339	1.98163	280	
290	3.31800	5.10509	1.97998	3.40542	5.20171	1.98065	3.48918	5.29386	1.98122	290	
300	3.25753	5.03797	1.97947	3.34463	5.13457	1.98019	3.42810	5.22670	1.98081	300	
310	3.19926	4.97307	1.97895	3.28604	5.06964	1.97972	3.36922	5.16176	1.98038	310	
320	3.14304	4.91025	1.97842	3.22951	5.00680	1.97923	3.31241	5.09889	1.97993	320	
330	3.08877	4.84938	1.97786	3.17492	4.94590	1.97873	3.25753	5.03797	1.97947	330	
340	3.03630	4.79034	1.97729	3.12215	4.88684	1.97821	3.20447	4.97888	1.97900	340	
350	2.98555	4.73304	1.97670	3.07108	4.82950	1.97767	3.15312	4.92153	1.97852	350	
360	2.93642	4.67736	1.97610	3.02163	4.77380	1.97713	3.10338	4.86580	1.97802	360	
370	2.88881	4.62322	1.97548	2.97371	4.71963	1.97656	3.05518	4.81161	1.97750	370	
380	2.84264	4.57055	1.97484	2.92723	4.66693	1.97598	3.00842	4.75888	1.97697	380	
390	2.79784	4.51926	1.97419	2.88212	4.61561	1.97539	2.96302	4.70753	1.97643	390	
400	2.75434	4.46929	1.97351	2.83831	4.56561	1.97478	2.91893	4.65750	1.97588	400	
410	2.71207	4.42056	1.97283	2.79574	4.51685	1.97415	2.87607	4.60872	1.97531	410	
420	2.67098	4.37303	1.97212	2.75434	4.46929	1.97351	2.83439	4.56112	1.97472	420	
430	2.63100	4.32664	1.97140	2.71406	4.42286	1.97286	2.79383	4.51466	1.97413	430	
440	2.59209	4.28132	1.97066	2.67484	4.37751	1.97219	2.75434	4.46929	1.97351	440	
450	2.55420	4.23705	1.96991	2.63665	4.33320	1.97150	2.71586	4.42494	1.97289	450	
460	2.51729	4.19376	1.96913	2.59943	4.28987	1.97080	2.67836	4.38159	1.97225	460	
470	2.48130	4.15142	1.96835	2.56314	4.24750	1.97009	2.64180	4.33918	1.97160	470	
480	2.44621	4.10999	1.96754	2.52774	4.20603	1.96936	2.60612	4.29768	1.97093	480	
490	2.41196	4.06942	1.96672	2.49319	4.16543	1.96861	2.57130	4.25705	1.97025	490	
500	2.37854	4.02970	1.96588	2.45947	4.12566	1.96785	2.53731	4.21725	1.96956	500	
510	2.34591	3.99078	1.96503	2.42654	4.08670	1.96707	2.50410	4.17825	1.96885	510	
520	2.31403	3.95263	1.96416	2.39436	4.04851	1.96628	2.47164	4.14003	1.96813	520	
530	2.28287	3.91522	1.96327	2.36291	4.01107	1.96548	2.43992	4.10255	1.96739	530	
540	2.25242	3.87854	1.96237	2.33215	3.97434	1.96466	2.40889	4.06578	1.96664	540	
550	2.22264	3.84254	1.96145	2.30208	3.93829	1.96382	2.37854	4.02970	1.96588	550	
560	2.19351	3.80720	1.96051	2.27265	3.90292	1.96297	2.34884	3.99428	1.96511	560	
570	2.16500	3.77251	1.95956	2.24384	3.86818	1.96211	2.31977	3.95951	1.96432	570	
580	2.13710	3.73844	1.95859	2.21565	3.83406	1.96123	2.29130	3.92535	1.96351	580	
590	2.10977	3.70497	1.95760	2.18803	3.80055	1.96033	2.26342	3.89180	1.96270	590	

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	ν cm ⁻¹
	T=2000.			T=2100.			T=2200.			
600	2.08302	3.67207	1.95660	2.16098	3.76761	1.95942	2.23609	3.85882	1.96187	600
610	2.05680	3.63974	1.95558	2.13447	3.73522	1.95850	2.20932	3.82639	1.96102	610
620	2.03111	3.60795	1.95455	2.10849	3.70339	1.95756	2.18307	3.79451	1.96017	620
630	2.00593	3.57668	1.95350	2.08302	3.67207	1.95660	2.15733	3.76316	1.95930	630
640	1.98124	3.54593	1.95243	2.05804	3.64127	1.95563	2.13209	3.73231	1.95841	640
650	1.95703	3.51567	1.95135	2.03353	3.61095	1.95465	2.10732	3.70195	1.95751	650
660	1.93328	3.48588	1.95025	2.00950	3.58112	1.95365	2.08302	3.67207	1.95660	660
670	1.90997	3.45656	1.94914	1.98591	3.55175	1.95264	2.05916	3.64266	1.95568	670
680	1.88711	3.42769	1.94801	1.96275	3.52283	1.95161	2.03574	3.61369	1.95474	680
690	1.86466	3.39926	1.94686	1.94002	3.49434	1.95057	2.01275	3.58516	1.95379	690
700	1.84262	3.37126	1.94570	1.91769	3.46628	1.94951	1.99016	3.55705	1.95282	700
710	1.82098	3.34367	1.94452	1.89577	3.43864	1.94844	1.96797	3.52936	1.95185	710
720	1.79972	3.31648	1.94333	1.87423	3.41139	1.94736	1.94618	3.50207	1.95086	720
730	1.77884	3.28968	1.94212	1.85306	3.38454	1.94626	1.92475	3.47517	1.94985	730
740	1.75833	3.26327	1.94090	1.83227	3.35807	1.94514	1.90369	3.44864	1.94883	740
750	1.73817	3.23722	1.93966	1.81182	3.33197	1.94402	1.88299	3.42249	1.94780	750
760	1.71835	3.21154	1.93840	1.79173	3.30623	1.94287	1.86264	3.39670	1.94676	760
770	1.69887	3.18621	1.93713	1.77197	3.28084	1.94172	1.84262	3.37126	1.94570	770
780	1.67971	3.16122	1.93584	1.75253	3.25579	1.94054	1.82293	3.34616	1.94463	780
790	1.66088	3.13657	1.93454	1.73342	3.23108	1.93936	1.80356	3.32139	1.94355	790
800	1.64235	3.11224	1.93322	1.71461	3.20669	1.93816	1.78450	3.29695	1.94245	800
810	1.62413	3.08824	1.93188	1.69611	3.18262	1.93694	1.76575	3.27283	1.94134	810
820	1.60620	3.06454	1.93053	1.67791	3.15886	1.93572	1.74729	3.24902	1.94022	820
830	1.58856	3.04115	1.92917	1.65999	3.13540	1.93447	1.72912	3.22550	1.93909	830
840	1.57119	3.01805	1.92779	1.64235	3.11224	1.93322	1.71123	3.20229	1.93794	840
850	1.55411	2.99525	1.92639	1.62499	3.08937	1.93195	1.69361	3.17936	1.93678	850
860	1.53728	2.97272	1.92498	1.60789	3.06678	1.93066	1.67627	3.15672	1.93560	860
870	1.52072	2.95048	1.92355	1.59106	3.04447	1.92936	1.65918	3.13434	1.93442	870
880	1.50441	2.92850	1.92211	1.57448	3.02243	1.92805	1.64235	3.11224	1.93322	880
890	1.48835	2.90679	1.92065	1.55815	3.00065	1.92672	1.62577	3.09041	1.93200	890
900	1.47254	2.88534	1.91918	1.54206	2.97913	1.92538	1.60944	3.06883	1.93078	900
910	1.45696	2.86414	1.91769	1.52621	2.95786	1.92403	1.59334	3.04750	1.92954	910
920	1.44161	2.84319	1.91619	1.51060	2.93684	1.92266	1.57748	3.02642	1.92829	920
930	1.42649	2.82248	1.91468	1.49521	2.91606	1.92128	1.56184	3.00558	1.92703	930
940	1.41158	2.80201	1.91314	1.48004	2.89552	1.91988	1.54643	2.98497	1.92575	940
950	1.39690	2.78178	1.91160	1.46509	2.87521	1.91848	1.53123	2.96460	1.92446	950
960	1.38243	2.76177	1.91003	1.45035	2.85513	1.91705	1.51625	2.94446	1.92316	960
970	1.36816	2.74198	1.90846	1.43582	2.83527	1.91562	1.50148	2.92453	1.92185	970
980	1.35410	2.72242	1.90687	1.42149	2.81563	1.91417	1.48691	2.90483	1.92052	980
990	1.34024	2.70306	1.90526	1.40737	2.79621	1.91270	1.47254	2.88534	1.91918	990
1000	1.32657	2.68392	1.90364	1.39344	2.77699	1.91123	1.45836	2.86606	1.91783	1000
1010	1.31309	2.66499	1.90200	1.37969	2.75798	1.90974	1.44438	2.84698	1.91647	1010
1020	1.29980	2.64626	1.90035	1.36614	2.73917	1.90823	1.43059	2.82811	1.91509	1020
1030	1.28669	2.62773	1.89869	1.35277	2.72056	1.90671	1.41698	2.80943	1.91370	1030
1040	1.27375	2.60939	1.89701	1.33958	2.70215	1.90518	1.40355	2.79095	1.91230	1040
1050	1.26100	2.59125	1.89532	1.32657	2.68392	1.90364	1.39030	2.77265	1.91089	1050
1060	1.24842	2.57329	1.89361	1.31373	2.66589	1.90208	1.37722	2.75455	1.90946	1060
1070	1.23600	2.55552	1.89189	1.30105	2.64804	1.90051	1.36431	2.73662	1.90803	1070
1080	1.22375	2.53792	1.89015	1.28855	2.63036	1.89893	1.35156	2.71888	1.90658	1080
1090	1.21166	2.52051	1.88840	1.27620	2.61287	1.89733	1.33899	2.70132	1.90511	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=2000.			T=2100.			T=2200.				
1100	1.19973	2.50327	1.88664	1.26402	2.59555	1.89572	1.32657	2.68392	1.90364	1100
1110	1.18796	2.48621	1.88486	1.25199	2.57840	1.89410	1.31431	2.66670	1.90215	1110
1120	1.17634	2.46931	1.88307	1.24012	2.56142	1.89246	1.30220	2.64965	1.90066	1120
1130	1.16487	2.45258	1.88126	1.22840	2.54460	1.89082	1.29024	2.63276	1.89915	1130
1140	1.15355	2.43601	1.87944	1.21682	2.52795	1.88915	1.27844	2.61604	1.89762	1140
1150	1.14237	2.41961	1.87760	1.20539	2.51146	1.88748	1.26678	2.59947	1.89609	1150
1160	1.13134	2.40336	1.87576	1.19411	2.49513	1.88579	1.25526	2.58306	1.89454	1160
1170	1.12044	2.38727	1.87389	1.18296	2.47895	1.88409	1.24388	2.56680	1.89299	1170
1180	1.10968	2.37133	1.87202	1.17195	2.46292	1.88238	1.23264	2.55070	1.89142	1180
1190	1.09905	2.35554	1.87013	1.16108	2.44704	1.88065	1.22154	2.53475	1.88984	1190
1200	1.08856	2.33989	1.86822	1.15034	2.43131	1.87892	1.21057	2.51894	1.88824	1200
1210	1.07820	2.32440	1.86631	1.13973	2.41572	1.87717	1.19973	2.50327	1.88664	1210
1220	1.06796	2.30905	1.86438	1.12925	2.40028	1.87540	1.18902	2.48775	1.88502	1220
1230	1.05785	2.29383	1.86243	1.11889	2.38498	1.87363	1.17844	2.47237	1.88339	1230
1240	1.04786	2.27876	1.86048	1.10866	2.36982	1.87184	1.16798	2.45713	1.88175	1240
1250	1.03800	2.26383	1.85850	1.09855	2.35479	1.87004	1.15765	2.44202	1.88010	1250
1260	1.02825	2.24902	1.85652	1.08856	2.33989	1.86822	1.14743	2.42705	1.87844	1260
1270	1.01862	2.23436	1.85452	1.07869	2.32513	1.86640	1.13734	2.41220	1.87677	1270
1280	1.00910	2.21982	1.85251	1.06893	2.31050	1.86456	1.12736	2.39749	1.87508	1280
1290	0.99970	2.20541	1.85049	1.05929	2.29600	1.86271	1.11749	2.38290	1.87338	1290
1300	0.99041	2.19113	1.84845	1.04976	2.28162	1.86085	1.10774	2.36844	1.87167	1300
1310	0.98123	2.17697	1.84640	1.04034	2.26737	1.85898	1.09809	2.35411	1.86996	1310
1320	0.97215	2.16294	1.84434	1.03102	2.25324	1.85709	1.08856	2.33989	1.86822	1320
1330	0.96319	2.14903	1.84227	1.02182	2.23923	1.85519	1.07913	2.32580	1.86648	1330
1340	0.95432	2.13524	1.84018	1.01272	2.22534	1.85328	1.06981	2.31183	1.86473	1340
1350	0.94556	2.12156	1.83808	1.00372	2.21157	1.85136	1.06060	2.29797	1.86296	1350
1360	0.93690	2.10800	1.83596	0.99482	2.19791	1.84942	1.05148	2.28423	1.86119	1360
1370	0.92834	2.09456	1.83384	0.98602	2.18437	1.84748	1.04247	2.27060	1.85940	1370
1380	0.91987	2.08123	1.83170	0.97733	2.17094	1.84552	1.03355	2.25708	1.85760	1380
1390	0.91150	2.06801	1.82955	0.96872	2.15762	1.84355	1.02473	2.24368	1.85580	1390
1400	0.90323	2.05491	1.82738	0.96022	2.14442	1.84157	1.01601	2.23038	1.85398	1400
1410	0.89505	2.04191	1.82520	0.95181	2.13132	1.83958	1.00739	2.21719	1.85215	1410
1420	0.88696	2.02902	1.82302	0.94349	2.11832	1.83757	0.99885	2.20411	1.85031	1420
1430	0.87897	2.01623	1.82081	0.93526	2.10543	1.83556	0.99041	2.19113	1.84845	1430
1440	0.87106	2.00355	1.81860	0.92712	2.09265	1.83353	0.98206	2.17825	1.84659	1440
1450	0.86324	1.99097	1.81638	0.91907	2.07997	1.83149	0.97380	2.16548	1.84472	1450
1460	0.85550	1.97850	1.81414	0.91111	2.06739	1.82944	0.96562	2.15281	1.84283	1460
1470	0.84785	1.96612	1.81189	0.90323	2.05491	1.82738	0.95753	2.14024	1.84094	1470
1480	0.84029	1.95384	1.80963	0.89544	2.04252	1.82531	0.94953	2.12776	1.83903	1480
1490	0.83280	1.94167	1.80735	0.88773	2.03024	1.82322	0.94161	2.11538	1.83712	1490
1500	0.82540	1.92958	1.80507	0.88010	2.01805	1.82113	0.93377	2.10310	1.83519	1500
1510	0.81808	1.91760	1.80277	0.87256	2.00596	1.81902	0.92602	2.09091	1.83325	1510
1520	0.81084	1.90571	1.80046	0.86509	1.99396	1.81691	0.91834	2.07882	1.83131	1520
1530	0.80367	1.89391	1.79814	0.85770	1.98205	1.81478	0.91075	2.06682	1.82935	1530
1540	0.79659	1.88220	1.79581	0.85039	1.97024	1.81264	0.90323	2.05491	1.82738	1540
1550	0.78958	1.87059	1.79346	0.84316	1.95851	1.81049	0.89579	2.04309	1.82540	1550
1560	0.78264	1.85906	1.79111	0.83600	1.94687	1.80833	0.88843	2.03135	1.82341	1560
1570	0.77578	1.84762	1.78874	0.82892	1.93533	1.80616	0.88114	2.01971	1.82142	1570
1580	0.76898	1.83627	1.78636	0.82191	1.92387	1.80398	0.87392	2.00815	1.81941	1580
1590	0.76226	1.82501	1.78398	0.81497	1.91249	1.80178	0.86678	1.99668	1.81739	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	T=2000.			T=2100.			T=2200.			ν cm^{-1}
	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	
1600	0.75562	1.81383	1.78157	0.80810	1.90120	1.79958	0.85971	1.98529	1.81536	1600
1610	0.74904	1.80274	1.77916	0.80130	1.89000	1.79736	0.85271	1.97399	1.81332	1610
1620	0.74253	1.79173	1.77674	0.79458	1.87887	1.79514	0.84578	1.96276	1.81127	1620
1630	0.73608	1.78080	1.77431	0.78792	1.86783	1.79290	0.83892	1.95162	1.80921	1630
1640	0.72971	1.76996	1.77186	0.78133	1.85687	1.79066	0.83213	1.94056	1.80715	1640
1650	0.72340	1.75920	1.76941	0.77480	1.84600	1.78840	0.82540	1.92958	1.80507	1650
1660	0.71715	1.74851	1.76694	0.76834	1.83520	1.78614	0.81874	1.91868	1.80298	1660
1670	0.71097	1.73791	1.76446	0.76195	1.82448	1.78386	0.81215	1.90786	1.80088	1670
1680	0.70485	1.72738	1.76197	0.75562	1.81383	1.78157	0.80562	1.89712	1.79877	1680
1690	0.69880	1.71693	1.75948	0.74935	1.80327	1.77928	0.79916	1.88645	1.79666	1690
1700	0.69280	1.70656	1.75697	0.74314	1.79278	1.77697	0.79275	1.87585	1.79453	1700
1710	0.68687	1.69626	1.75445	0.73700	1.78236	1.77465	0.78641	1.86534	1.79240	1710
1720	0.68100	1.68604	1.75192	0.73092	1.77202	1.77233	0.78013	1.85489	1.79025	1720
1730	0.67518	1.67589	1.74938	0.72489	1.76175	1.76999	0.77392	1.84452	1.78810	1730
1740	0.66943	1.66581	1.74683	0.71893	1.75156	1.76765	0.76776	1.83422	1.78593	1740
1750	0.66373	1.65581	1.74427	0.71302	1.74143	1.76529	0.76166	1.82399	1.78376	1750
1760	0.65809	1.64588	1.74169	0.70718	1.73138	1.76292	0.75562	1.81383	1.78157	1760
1770	0.65251	1.63602	1.73911	0.70138	1.72140	1.76055	0.74963	1.80374	1.77938	1770
1780	0.64698	1.62623	1.73652	0.69565	1.71149	1.75816	0.74370	1.79373	1.77718	1780
1790	0.64150	1.61651	1.73392	0.68997	1.70164	1.75577	0.73783	1.78378	1.77497	1790
1800	0.63608	1.60685	1.73131	0.68435	1.69187	1.75336	0.73202	1.77389	1.77275	1800
1810	0.63072	1.59727	1.72869	0.67878	1.68216	1.75095	0.72626	1.76408	1.77052	1810
1820	0.62540	1.58775	1.72606	0.67326	1.67252	1.74853	0.72055	1.75433	1.76829	1820
1830	0.62014	1.57830	1.72342	0.66779	1.66295	1.74610	0.71490	1.74465	1.76604	1830
1840	0.61493	1.56892	1.72077	0.66238	1.65344	1.74365	0.70930	1.73503	1.76379	1840
1850	0.60977	1.55960	1.71811	0.65702	1.64399	1.74120	0.70375	1.72547	1.76152	1850
1860	0.60466	1.55034	1.71544	0.65171	1.63461	1.73874	0.69825	1.71598	1.75925	1860
1870	0.59960	1.54115	1.71276	0.64645	1.62530	1.73628	0.69280	1.70656	1.75697	1870
1880	0.59459	1.53202	1.71008	0.64124	1.61604	1.73380	0.68741	1.69719	1.75468	1880
1890	0.58963	1.52296	1.70738	0.63608	1.60685	1.73131	0.68206	1.68789	1.75238	1890
1900	0.58471	1.51396	1.70467	0.63097	1.59772	1.72882	0.67676	1.67865	1.75007	1900
1910	0.57985	1.50501	1.70196	0.62591	1.58866	1.72631	0.67151	1.66947	1.74776	1910
1920	0.57503	1.49613	1.69923	0.62089	1.57965	1.72380	0.66631	1.66035	1.74543	1920
1930	0.57025	1.48731	1.69650	0.61592	1.57070	1.72128	0.66116	1.65129	1.74310	1930
1940	0.56552	1.47855	1.69376	0.61099	1.56181	1.71874	0.65605	1.64228	1.74076	1940
1950	0.56084	1.46985	1.69101	0.60612	1.55298	1.71621	0.65099	1.63334	1.73841	1950
1960	0.55620	1.46121	1.68825	0.60128	1.54421	1.71366	0.64598	1.62445	1.73605	1960
1970	0.55160	1.45262	1.68548	0.59649	1.53549	1.71110	0.64101	1.61563	1.73368	1970
1980	0.54705	1.44410	1.68270	0.59175	1.52684	1.70854	0.63608	1.60685	1.73131	1980
1990	0.54254	1.43563	1.67992	0.58705	1.51824	1.70596	0.63120	1.59814	1.72893	1990
2000	0.53808	1.42721	1.67713	0.58239	1.50969	1.70338	0.62636	1.58948	1.72654	2000
2010	0.53365	1.41886	1.67432	0.57778	1.50120	1.70079	0.62157	1.58087	1.72414	2010
2020	0.52927	1.41055	1.67151	0.57320	1.49277	1.69819	0.61682	1.57232	1.72173	2020
2030	0.52493	1.40231	1.66869	0.56867	1.48439	1.69559	0.61211	1.56382	1.71932	2030
2040	0.52062	1.39411	1.66587	0.56418	1.47606	1.69298	0.60744	1.55538	1.71690	2040
2050	0.51636	1.38597	1.66303	0.55973	1.46779	1.69035	0.60282	1.54699	1.71447	2050
2060	0.51214	1.37789	1.66019	0.55532	1.45957	1.68772	0.59823	1.53866	1.71203	2060
2070	0.50796	1.36986	1.65734	0.55095	1.45140	1.68509	0.59369	1.53037	1.70959	2070
2080	0.50381	1.36188	1.65448	0.54662	1.44329	1.68244	0.58918	1.52214	1.70713	2080
2090	0.49971	1.35395	1.65161	0.54233	1.43523	1.67979	0.58471	1.51396	1.70467	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=2000.			T=2100.			T=2200.				
2100	0.49564	1.34607	1.64874	0.53808	1.42721	1.67713	0.58029	1.50582	1.70221	2100
2110	0.49161	1.33824	1.64585	0.53386	1.41925	1.67446	0.57590	1.49774	1.69973	2110
2120	0.48761	1.33047	1.64296	0.52968	1.41134	1.67178	0.57155	1.48971	1.69725	2120
2130	0.48366	1.32275	1.64006	0.52554	1.40348	1.66910	0.56724	1.48173	1.69476	2130
2140	0.47973	1.31507	1.63716	0.52144	1.39567	1.66641	0.56296	1.47380	1.69226	2140
2150	0.47585	1.30744	1.63425	0.51737	1.38791	1.66371	0.55873	1.46592	1.68976	2150
2160	0.47200	1.29987	1.63133	0.51334	1.38019	1.66100	0.55452	1.45808	1.68724	2160
2170	0.46818	1.29234	1.62840	0.50935	1.37253	1.65829	0.55036	1.45029	1.68473	2170
2180	0.46440	1.28486	1.62547	0.50539	1.36491	1.65557	0.54623	1.44255	1.68220	2180
2190	0.46066	1.27743	1.62252	0.50146	1.35734	1.65284	0.54214	1.43486	1.67967	2190
2200	0.45694	1.27004	1.61957	0.49757	1.34982	1.65011	0.53808	1.42721	1.67713	2200
2210	0.45326	1.26270	1.61662	0.49371	1.34234	1.64736	0.53405	1.41961	1.67458	2210
2220	0.44962	1.25541	1.61366	0.48989	1.33491	1.64462	0.53006	1.41206	1.67202	2220
2230	0.44600	1.24817	1.61069	0.48610	1.32752	1.64186	0.52611	1.40455	1.66946	2230
2240	0.44242	1.24097	1.60771	0.48234	1.32018	1.63910	0.52218	1.39709	1.66690	2240
2250	0.43887	1.23381	1.60473	0.47862	1.31289	1.63633	0.51829	1.38967	1.66432	2250
2260	0.43536	1.22670	1.60174	0.47493	1.30564	1.63355	0.51444	1.38229	1.66174	2260
2270	0.43187	1.21964	1.59874	0.47127	1.29843	1.63077	0.51061	1.37496	1.65915	2270
2280	0.42842	1.21262	1.59574	0.46764	1.29127	1.62798	0.50682	1.36767	1.65656	2280
2290	0.42499	1.20564	1.59273	0.46404	1.28415	1.62519	0.50306	1.36043	1.65396	2290
2300	0.42160	1.19870	1.58971	0.46048	1.27707	1.62238	0.49933	1.35323	1.65135	2300
2310	0.41823	1.19181	1.58669	0.45694	1.27004	1.61957	0.49564	1.34607	1.64874	2310
2320	0.41490	1.18497	1.58366	0.45344	1.26305	1.61676	0.49197	1.33895	1.64612	2320
2330	0.41160	1.17816	1.58063	0.44996	1.25610	1.61394	0.48834	1.33188	1.64349	2330
2340	0.40832	1.17140	1.57759	0.44652	1.24920	1.61111	0.48473	1.32485	1.64086	2340
2350	0.40507	1.16468	1.57454	0.44310	1.24233	1.60828	0.48116	1.31786	1.63822	2350
2360	0.40186	1.15800	1.57149	0.43972	1.23551	1.60544	0.47761	1.31090	1.63557	2360
2370	0.39867	1.15136	1.56843	0.43636	1.22873	1.60259	0.47409	1.30399	1.63292	2370
2380	0.39550	1.14476	1.56537	0.43303	1.22199	1.59974	0.47061	1.29712	1.63026	2380
2390	0.39237	1.13821	1.56230	0.42973	1.21528	1.59688	0.46715	1.29029	1.62760	2390
2400	0.38926	1.13169	1.55922	0.42646	1.20862	1.59402	0.46372	1.28350	1.62493	2400
2410	0.38618	1.12521	1.55614	0.42321	1.20200	1.59115	0.46032	1.27675	1.62226	2410
2420	0.38313	1.11878	1.55306	0.41999	1.19542	1.58828	0.45694	1.27004	1.61957	2420
2430	0.38010	1.11238	1.54997	0.41680	1.18887	1.58540	0.45360	1.26337	1.61689	2430
2440	0.37710	1.10602	1.54687	0.41364	1.18237	1.58251	0.45028	1.25673	1.61420	2440
2450	0.37413	1.09970	1.54377	0.41050	1.17590	1.57962	0.44699	1.25014	1.61150	2450
2460	0.37118	1.09342	1.54066	0.40739	1.16947	1.57672	0.44372	1.24358	1.60879	2460
2470	0.36826	1.08717	1.53755	0.40430	1.16308	1.57382	0.44048	1.23706	1.60608	2470
2480	0.36536	1.08097	1.53443	0.40125	1.15673	1.57091	0.43727	1.23057	1.60337	2480
2490	0.36248	1.07480	1.53130	0.39821	1.15042	1.56800	0.43409	1.22413	1.60065	2490
2500	0.35964	1.06867	1.52818	0.39520	1.14414	1.56508	0.43093	1.21772	1.59792	2500
2510	0.35681	1.06257	1.52504	0.39222	1.13789	1.56215	0.42779	1.21134	1.59519	2510
2520	0.35401	1.05651	1.52191	0.38926	1.13169	1.55922	0.42468	1.20501	1.59246	2520
2530	0.35124	1.05049	1.51876	0.38633	1.12552	1.55629	0.42160	1.19870	1.58971	2530
2540	0.34848	1.04451	1.51562	0.38342	1.11939	1.55335	0.41854	1.19244	1.58697	2540
2550	0.34576	1.03856	1.51247	0.38053	1.11329	1.55041	0.41550	1.18621	1.58422	2550
2560	0.34305	1.03265	1.50931	0.37767	1.10723	1.54746	0.41249	1.18001	1.58146	2560
2570	0.34037	1.02677	1.50615	0.37483	1.10120	1.54451	0.40951	1.17385	1.57870	2570
2580	0.33771	1.02092	1.50298	0.37202	1.09521	1.54155	0.40655	1.16773	1.57593	2580
2590	0.33507	1.01512	1.49981	0.36923	1.08925	1.53858	0.40361	1.16164	1.57316	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=2000.			T=2100.			T=2200.				
2600	0.33246	1.00934	1.49664	0.36646	1.08333	1.53562	0.40069	1.15558	1.57038	2600
2610	0.32967	1.00360	1.49346	0.36371	1.07744	1.53264	0.39780	1.14956	1.56760	2610
2620	0.32729	0.99790	1.49028	0.36099	1.07158	1.52967	0.39493	1.14357	1.56481	2620
2630	0.32475	0.99223	1.48709	0.35829	1.06576	1.52669	0.39209	1.13761	1.56202	2630
2640	0.32222	0.98659	1.48390	0.35561	1.05997	1.52370	0.38926	1.13169	1.55922	2640
2650	0.31971	0.98099	1.48071	0.35295	1.05422	1.52071	0.38646	1.12580	1.55642	2650
2660	0.31723	0.97541	1.47751	0.35032	1.04849	1.51772	0.38368	1.11994	1.55362	2660
2670	0.31476	0.96988	1.47431	0.34770	1.04281	1.51472	0.38092	1.11412	1.55081	2670
2680	0.31232	0.96437	1.47111	0.34511	1.03715	1.51171	0.37819	1.10833	1.54800	2680
2690	0.30990	0.95890	1.46790	0.34254	1.03152	1.50871	0.37548	1.10257	1.54518	2690
2700	0.30750	0.95346	1.46468	0.33999	1.02593	1.50570	0.37278	1.09684	1.54235	2700
2710	0.30511	0.94805	1.46147	0.33746	1.02037	1.50268	0.37011	1.09114	1.53953	2710
2720	0.30275	0.94267	1.45825	0.33495	1.01484	1.49966	0.36746	1.08548	1.53670	2720
2730	0.30041	0.93733	1.45503	0.33246	1.00934	1.49664	0.36483	1.07984	1.53386	2730
2740	0.29808	0.93201	1.45180	0.32999	1.00388	1.49361	0.36222	1.07424	1.53102	2740
2750	0.29578	0.92673	1.44857	0.32754	0.99844	1.49058	0.35964	1.06867	1.52818	2750
2760	0.29350	0.92148	1.44534	0.32511	0.99304	1.48755	0.35707	1.06312	1.52533	2760
2770	0.29123	0.91626	1.44210	0.32270	0.98766	1.48451	0.35452	1.05761	1.52248	2770
2780	0.28898	0.91106	1.43886	0.32031	0.98232	1.48147	0.35199	1.05213	1.51962	2780
2790	0.28675	0.90590	1.43562	0.31794	0.97700	1.47843	0.34948	1.04668	1.51676	2790
2800	0.28454	0.90077	1.43238	0.31558	0.97172	1.47538	0.34699	1.04126	1.51390	2800
2810	0.28235	0.89567	1.42913	0.31325	0.96646	1.47233	0.34452	1.03587	1.51103	2810
2820	0.28018	0.89060	1.42588	0.31093	0.96124	1.46927	0.34207	1.03050	1.50816	2820
2830	0.27802	0.88556	1.42263	0.30864	0.95604	1.46621	0.33964	1.02517	1.50529	2830
2840	0.27589	0.88055	1.41937	0.30636	0.95088	1.46315	0.33723	1.01987	1.50241	2840
2850	0.27376	0.87556	1.41611	0.30410	0.94574	1.46009	0.33483	1.01459	1.49953	2850
2860	0.27166	0.87061	1.41285	0.30186	0.94063	1.45702	0.33246	1.00934	1.49664	2860
2870	0.26958	0.86568	1.40959	0.29963	0.93555	1.45395	0.33010	1.00412	1.49375	2870
2880	0.26751	0.86079	1.40632	0.29742	0.93050	1.45088	0.32776	0.99893	1.49086	2880
2890	0.26546	0.85592	1.40306	0.29523	0.92548	1.44780	0.32544	0.99377	1.48796	2890
2900	0.26342	0.85108	1.39979	0.29306	0.92048	1.44472	0.32314	0.98864	1.48506	2900
2910	0.26140	0.84626	1.39651	0.29091	0.91551	1.44164	0.32085	0.98353	1.48216	2910
2920	0.25940	0.84148	1.39324	0.28877	0.91057	1.43856	0.31858	0.97845	1.47926	2920
2930	0.25742	0.83672	1.38996	0.28665	0.90566	1.43547	0.31633	0.97340	1.47635	2930
2940	0.25545	0.83199	1.38668	0.28454	0.90077	1.43238	0.31410	0.96837	1.47344	2940
2950	0.25349	0.82729	1.38340	0.28246	0.89591	1.42929	0.31188	0.96337	1.47052	2950
2960	0.25156	0.82261	1.38012	0.28038	0.89108	1.42619	0.30968	0.95840	1.46761	2960
2970	0.24964	0.81796	1.37684	0.27833	0.88628	1.42309	0.30750	0.95346	1.46468	2970
2980	0.24773	0.81334	1.37355	0.27629	0.88150	1.41999	0.30533	0.94854	1.46176	2980
2990	0.24584	0.80874	1.37026	0.27427	0.87675	1.41689	0.30318	0.94365	1.45883	2990
3000	0.24396	0.80417	1.36698	0.27226	0.87202	1.41378	0.30104	0.93878	1.45591	3000
3010	0.24211	0.79963	1.36368	0.27027	0.86732	1.41068	0.29893	0.93394	1.45297	3010
3020	0.24026	0.79511	1.36039	0.26829	0.86265	1.40757	0.29683	0.92913	1.45004	3020
3030	0.23843	0.79062	1.35710	0.26633	0.85800	1.40446	0.29474	0.92434	1.44710	3030
3040	0.23662	0.78616	1.35380	0.26439	0.85338	1.40134	0.29267	0.91957	1.44416	3040
3050	0.23482	0.78172	1.35051	0.26246	0.84878	1.39823	0.29061	0.91484	1.44122	3050
3060	0.23303	0.77730	1.34721	0.26054	0.84421	1.39511	0.28858	0.91012	1.43828	3060
3070	0.23126	0.77291	1.34391	0.25864	0.83966	1.39199	0.28655	0.90544	1.43533	3070
3080	0.22950	0.76854	1.34061	0.25676	0.83514	1.38887	0.28454	0.90077	1.43238	3080
3090	0.22776	0.76420	1.33731	0.25489	0.83064	1.38575	0.28255	0.89614	1.42943	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	T=2000.			T=2100.			T=2200.			ν cm^{-1}
	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	
3100	0.22603	0.75989	1.33401	0.25303	0.82617	1.38262	0.28057	0.89152	1.42647	3100
3110	0.22431	0.75560	1.33070	0.25119	0.82172	1.37950	0.27861	0.88693	1.42351	3110
3120	0.22261	0.75133	1.32740	0.24936	0.81730	1.37637	0.27666	0.88237	1.42056	3120
3130	0.22092	0.74709	1.32410	0.24755	0.81290	1.37324	0.27473	0.87783	1.41759	3130
3140	0.21925	0.74287	1.32079	0.24575	0.80853	1.37011	0.27281	0.87331	1.41463	3140
3150	0.21759	0.73868	1.31748	0.24396	0.80417	1.36698	0.27090	0.86882	1.41167	3150
3160	0.21594	0.73451	1.31418	0.24219	0.79985	1.36384	0.26901	0.86435	1.40870	3160
3170	0.21431	0.73036	1.31087	0.24044	0.79554	1.36071	0.26713	0.85990	1.40573	3170
3180	0.21269	0.72623	1.30756	0.23869	0.79126	1.35757	0.26527	0.85548	1.40276	3180
3190	0.21108	0.72213	1.30425	0.23696	0.78700	1.35443	0.26342	0.85108	1.39979	3190
3200	0.20948	0.71806	1.30094	0.23524	0.78277	1.35129	0.26159	0.84670	1.39681	3200
3210	0.20790	0.71400	1.29764	0.23354	0.77856	1.34815	0.25976	0.84235	1.39384	3210
3220	0.20633	0.70997	1.29433	0.23185	0.77437	1.34501	0.25796	0.83802	1.39086	3220
3230	0.20477	0.70596	1.29102	0.23017	0.77020	1.34187	0.25616	0.83371	1.38788	3230
3240	0.20322	0.70198	1.28771	0.22850	0.76606	1.33872	0.25438	0.82942	1.38490	3240
3250	0.20169	0.69802	1.28440	0.22685	0.76194	1.33558	0.25261	0.82516	1.38191	3250
3260	0.20017	0.69407	1.28109	0.22521	0.75784	1.33243	0.25086	0.82092	1.37893	3260
3270	0.19866	0.69016	1.27778	0.22358	0.75377	1.32929	0.24911	0.81670	1.37594	3270
3280	0.19716	0.68626	1.27447	0.22197	0.74971	1.32614	0.24739	0.81250	1.37295	3280
3290	0.19568	0.68239	1.27116	0.22036	0.74568	1.32299	0.24567	0.80833	1.36997	3290
3300	0.19420	0.67853	1.26785	0.21877	0.74167	1.31985	0.24396	0.80417	1.36698	3300
3310	0.19274	0.67470	1.26454	0.21720	0.73768	1.31670	0.24227	0.80004	1.36398	3310
3320	0.19129	0.67089	1.26123	0.21563	0.73371	1.31355	0.24059	0.79593	1.36099	3320
3330	0.18985	0.66710	1.25792	0.21407	0.72977	1.31040	0.23893	0.79184	1.35800	3330
3340	0.18843	0.66334	1.25461	0.21253	0.72584	1.30725	0.23727	0.78778	1.35500	3340
3350	0.18701	0.65959	1.25130	0.21100	0.72194	1.30410	0.23563	0.78373	1.35201	3350
3360	0.18560	0.65587	1.24799	0.20948	0.71806	1.30095	0.23400	0.77971	1.34901	3360
3370	0.18421	0.65216	1.24469	0.20797	0.71420	1.29779	0.23238	0.77570	1.34601	3370
3380	0.18283	0.64848	1.24138	0.20648	0.71036	1.29464	0.23078	0.77172	1.34301	3380
3390	0.18146	0.64482	1.23807	0.20499	0.70654	1.29149	0.22918	0.76775	1.34001	3390
3400	0.18009	0.64117	1.23477	0.20352	0.70274	1.28834	0.22760	0.76381	1.33701	3400
3410	0.17874	0.63755	1.23146	0.20205	0.69896	1.28518	0.22603	0.75989	1.33401	3410
3420	0.17740	0.63395	1.22816	0.20060	0.69520	1.28203	0.22447	0.75599	1.33101	3420
3430	0.17607	0.63037	1.22486	0.19916	0.69146	1.27888	0.22292	0.75211	1.32800	3430
3440	0.17475	0.62681	1.22156	0.19773	0.68774	1.27573	0.22138	0.74824	1.32500	3440
3450	0.17345	0.62327	1.21825	0.19631	0.68404	1.27257	0.21986	0.74440	1.32199	3450
3460	0.17215	0.61975	1.21495	0.19491	0.68036	1.26942	0.21834	0.74058	1.31899	3460
3470	0.17086	0.61625	1.21166	0.19351	0.67671	1.26627	0.21684	0.73678	1.31598	3470
3480	0.16958	0.61276	1.20836	0.19212	0.67307	1.26312	0.21535	0.73299	1.31298	3480
3490	0.16831	0.60930	1.20506	0.19074	0.66945	1.25997	0.21386	0.72923	1.30997	3490
3500	0.16705	0.60586	1.20177	0.18938	0.66585	1.25682	0.21239	0.72549	1.30696	3500
3510	0.16580	0.60243	1.19847	0.18802	0.66226	1.25366	0.21093	0.72176	1.30395	3510
3520	0.16456	0.59903	1.19518	0.18667	0.65870	1.25051	0.20948	0.71806	1.30095	3520
3530	0.16333	0.59564	1.19189	0.18534	0.65516	1.24736	0.20804	0.71437	1.29794	3530
3540	0.16211	0.59228	1.18860	0.18401	0.65163	1.24421	0.20661	0.71070	1.29493	3540
3550	0.16090	0.58893	1.18531	0.18270	0.64813	1.24106	0.20519	0.70706	1.29192	3550
3560	0.15970	0.58560	1.18202	0.18139	0.64464	1.23792	0.20378	0.70343	1.28891	3560
3570	0.15851	0.58229	1.17874	0.18009	0.64117	1.23477	0.20239	0.69981	1.28590	3570
3580	0.15733	0.57899	1.17545	0.17881	0.63773	1.23162	0.20100	0.69622	1.28289	3580
3590	0.15616	0.57572	1.17217	0.17753	0.63429	1.22848	0.19962	0.69265	1.27988	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm ⁻¹
T=2000.			T=2100.			T=2200.				
3600	0.15499	0.57246	1.16889	0.17626	0.63088	1.22533	0.19825	0.68909	1.27687	3600
3610	0.15384	0.56923	1.16561	0.17500	0.62749	1.22218	0.19689	0.68555	1.27386	3610
3620	0.15269	0.56601	1.16234	0.17376	0.62411	1.21904	0.19554	0.68203	1.27086	3620
3630	0.15155	0.56280	1.15906	0.17252	0.62075	1.21590	0.19420	0.67853	1.26785	3630
3640	0.15042	0.55962	1.15579	0.17129	0.61741	1.21276	0.19288	0.67505	1.26484	3640
3650	0.14930	0.55645	1.15252	0.17007	0.61409	1.20961	0.19156	0.67158	1.26183	3650
3660	0.14819	0.55331	1.14925	0.16885	0.61078	1.20647	0.19025	0.66813	1.25882	3660
3670	0.14709	0.55017	1.14598	0.16765	0.60750	1.20334	0.18894	0.66470	1.25581	3670
3680	0.14600	0.54706	1.14272	0.16646	0.60423	1.20020	0.18765	0.66129	1.25281	3680
3690	0.14491	0.54396	1.13945	0.16527	0.60097	1.19706	0.18637	0.65789	1.24980	3690
3700	0.14383	0.54088	1.13619	0.16409	0.59774	1.19393	0.18510	0.65452	1.24679	3700
3710	0.14276	0.53782	1.13294	0.16293	0.59452	1.19079	0.18383	0.65116	1.24378	3710
3720	0.14170	0.53478	1.12968	0.16177	0.59132	1.18766	0.18258	0.64781	1.24078	3720
3730	0.14065	0.53175	1.12643	0.16062	0.58813	1.18453	0.18133	0.64448	1.23777	3730
3740	0.13961	0.52874	1.12318	0.15948	0.58497	1.18140	0.18009	0.64117	1.23477	3740
3750	0.13857	0.52574	1.11993	0.15834	0.58182	1.17827	0.17887	0.63788	1.23176	3750
3760	0.13754	0.52276	1.11668	0.15722	0.57868	1.17514	0.17765	0.63461	1.22876	3760
3770	0.13652	0.51980	1.11344	0.15610	0.57556	1.17202	0.17643	0.63135	1.22576	3770
3780	0.13551	0.51686	1.11020	0.15499	0.57246	1.16889	0.17523	0.62810	1.22276	3780
3790	0.13450	0.51393	1.10696	0.15389	0.56938	1.16577	0.17404	0.62488	1.21976	3790
3800	0.13351	0.51102	1.10372	0.15280	0.56631	1.16265	0.17285	0.62167	1.21675	3800
3810	0.13252	0.50812	1.10049	0.15171	0.56326	1.15953	0.17168	0.61847	1.21376	3810
3820	0.13153	0.50524	1.09726	0.15064	0.56023	1.15641	0.17051	0.61529	1.21076	3820
3830	0.13056	0.50237	1.09403	0.14957	0.55721	1.15330	0.16935	0.61213	1.20776	3830
3840	0.12959	0.49953	1.09080	0.14851	0.55420	1.15018	0.16820	0.60899	1.20476	3840
3850	0.12863	0.49669	1.08758	0.14746	0.55122	1.14707	0.16705	0.60586	1.20177	3850
3860	0.12768	0.49388	1.08436	0.14641	0.54824	1.14396	0.16592	0.60274	1.19877	3860
3870	0.12674	0.49107	1.08115	0.14538	0.54529	1.14085	0.16479	0.59965	1.19578	3870
3880	0.12580	0.48829	1.07793	0.14435	0.54235	1.13775	0.16367	0.59656	1.19279	3880
3890	0.12487	0.48552	1.07472	0.14332	0.53942	1.13464	0.16256	0.59350	1.18979	3890
3900	0.12394	0.48276	1.07151	0.14231	0.53651	1.13154	0.16145	0.59045	1.18680	3900
3910	0.12303	0.48002	1.06831	0.14130	0.53362	1.12844	0.16036	0.58741	1.18382	3910
3920	0.12212	0.47730	1.06511	0.14030	0.53074	1.12534	0.15927	0.58439	1.18083	3920
3930	0.12122	0.47459	1.06191	0.13931	0.52788	1.12225	0.15819	0.58139	1.17784	3930
3940	0.12032	0.47189	1.05872	0.13833	0.52503	1.11915	0.15712	0.57840	1.17486	3940
3950	0.11943	0.46921	1.05553	0.13735	0.52220	1.11606	0.15605	0.57542	1.17187	3950
3960	0.11855	0.46655	1.05234	0.13638	0.51938	1.11297	0.15499	0.57246	1.16889	3960
3970	0.11767	0.46390	1.04915	0.13541	0.51658	1.10989	0.15394	0.56952	1.16591	3970
3980	0.11680	0.46126	1.04597	0.13446	0.51379	1.10680	0.15290	0.56659	1.16293	3980
3990	0.11594	0.45864	1.04279	0.13351	0.51102	1.10372	0.15186	0.56368	1.15995	3990
4000	0.11509	0.45604	1.03962	0.13256	0.50826	1.10064	0.15083	0.56078	1.15698	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=2300.			T=2400.			T=2500.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
100	5.56964	7.49530	1.98652	5.65165	7.57985	1.98657	5.73041	7.66095	1.98662	100
110	5.38639	7.30597	1.98639	5.46815	7.39052	1.98645	5.54667	7.47161	1.98651	110
120	5.21962	7.13314	1.98624	5.30113	7.21768	1.98631	5.37942	7.29876	1.98638	120
130	5.06670	6.97416	1.98607	5.14795	7.05869	1.98616	5.22601	7.13977	1.98624	130
140	4.92556	6.82699	1.98590	5.00656	6.91151	1.98600	5.08439	6.99258	1.98610	140
150	4.79458	6.68998	1.98571	4.87533	6.77449	1.98583	4.95293	6.85556	1.98594	150
160	4.67245	6.56183	1.98551	4.75295	6.64634	1.98565	4.83032	6.72740	1.98577	160
170	4.55809	6.44147	1.98530	4.63833	6.52596	1.98545	4.71547	6.60702	1.98559	170
180	4.45061	6.32800	1.98507	4.53060	6.41248	1.98524	4.60751	6.49353	1.98539	180
190	4.34926	6.22068	1.98483	4.42901	6.30515	1.98502	4.50569	6.38619	1.98519	190
200	4.25342	6.11887	1.98458	4.33292	6.20334	1.98479	4.40937	6.28437	1.98498	200
210	4.16255	6.02205	1.98431	4.24180	6.10651	1.98455	4.31802	6.18753	1.98475	210
220	4.07618	5.92975	1.98404	4.15519	6.01419	1.98429	4.23118	6.09520	1.98452	220
230	3.99392	5.84156	1.98375	4.07268	5.92599	1.98402	4.14844	6.00699	1.98427	230
240	3.91541	5.75714	1.98344	3.99392	5.84156	1.98375	4.06946	5.92255	1.98401	240
250	3.84035	5.67618	1.98312	3.91861	5.76059	1.98345	3.99392	5.84156	1.98375	250
260	3.76846	5.59840	1.98279	3.84648	5.68280	1.98315	3.92156	5.76376	1.98347	260
270	3.69951	5.52358	1.98245	3.77728	5.60796	1.98284	3.85214	5.68891	1.98318	270
280	3.63328	5.45149	1.98210	3.71080	5.53585	1.98251	3.78544	5.61679	1.98288	280
290	3.56957	5.38194	1.98173	3.64686	5.46629	1.98217	3.72127	5.54722	1.98256	290
300	3.50823	5.31476	1.98135	3.58527	5.39910	1.98182	3.65945	5.48001	1.98224	300
310	3.44909	5.24980	1.98095	3.52589	5.33412	1.98146	3.59985	5.41502	1.98191	310
320	3.39201	5.18691	1.98055	3.46857	5.27122	1.98109	3.54230	5.35210	1.98156	320
330	3.33687	5.12598	1.98013	3.41318	5.21026	1.98070	3.48669	5.29113	1.98121	330
340	3.28354	5.06687	1.97970	3.35962	5.15114	1.98030	3.43290	5.23199	1.98084	340
350	3.23193	5.00949	1.97925	3.30776	5.09374	1.97990	3.38083	5.17458	1.98046	350
360	3.18194	4.95374	1.97879	3.25753	5.03797	1.97947	3.33037	5.11879	1.98008	360
370	3.13347	4.89953	1.97832	3.20882	4.98374	1.97904	3.28145	5.06454	1.97968	370
380	3.08645	4.84678	1.97784	3.16156	4.93097	1.97860	3.23396	5.01175	1.97927	380
390	3.04080	4.79541	1.97734	3.11567	4.87958	1.97814	3.18785	4.96035	1.97885	390
400	2.99645	4.74535	1.97683	3.07108	4.82950	1.97767	3.14304	4.91025	1.97842	400
410	2.95333	4.69655	1.97631	3.02773	4.78068	1.97720	3.09947	4.86140	1.97798	410
420	2.91139	4.64893	1.97578	2.98555	4.73304	1.97670	3.05708	4.81375	1.97752	420
430	2.87057	4.60244	1.97523	2.94450	4.68653	1.97620	3.01580	4.76722	1.97706	430
440	2.83082	4.55704	1.97467	2.90451	4.64110	1.97569	2.97560	4.72177	1.97658	440
450	2.79209	4.51267	1.97410	2.86555	4.59671	1.97516	2.93642	4.67736	1.97610	450
460	2.75434	4.46929	1.97351	2.82756	4.55330	1.97462	2.89821	4.63393	1.97560	460
470	2.71752	4.42685	1.97292	2.79050	4.51084	1.97407	2.86094	4.59145	1.97510	470
480	2.68159	4.38532	1.97231	2.75434	4.46929	1.97351	2.82456	4.54987	1.97458	480
490	2.64652	4.34466	1.97168	2.71903	4.42860	1.97294	2.78904	4.50916	1.97405	490
500	2.61226	4.30483	1.97105	2.68455	4.38875	1.97236	2.75434	4.46929	1.97351	500
510	2.57880	4.26581	1.97040	2.65085	4.34970	1.97176	2.72043	4.43021	1.97296	510
520	2.54610	4.22755	1.96974	2.61792	4.31141	1.97115	2.68728	4.39191	1.97240	520
530	2.51412	4.19004	1.96907	2.58571	4.27387	1.97054	2.65486	4.35434	1.97183	530
540	2.48285	4.15324	1.96838	2.55420	4.23705	1.96991	2.62314	4.31749	1.97125	540
550	2.45225	4.11713	1.96768	2.52337	4.20091	1.96926	2.59209	4.28132	1.97066	550
560	2.42230	4.08168	1.96697	2.49319	4.16543	1.96861	2.56170	4.24582	1.97006	560
570	2.39298	4.04687	1.96625	2.46364	4.13059	1.96795	2.53194	4.21096	1.96944	570
580	2.36426	4.01268	1.96551	2.43470	4.09637	1.96727	2.50278	4.17671	1.96882	580
590	2.33613	3.97909	1.96476	2.40634	4.06275	1.96658	2.47421	4.14306	1.96819	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
	T=2300.			T=2400.			T=2500.			
600	2.30856	3.94607	1.96400	2.37854	4.02970	1.96588	2.44621	4.10999	1.96754	600
610	2.28154	3.91361	1.96323	2.35129	3.99721	1.96517	2.41875	4.07747	1.96689	610
620	2.25504	3.88170	1.96245	2.32457	3.96526	1.96445	2.39182	4.04549	1.96622	620
630	2.22906	3.85030	1.96165	2.29836	3.93384	1.96372	2.36540	4.01404	1.96554	630
640	2.20357	3.81942	1.96084	2.27265	3.90292	1.96297	2.33947	3.98309	1.96486	640
650	2.17856	3.78902	1.96002	2.24741	3.87249	1.96221	2.31403	3.95263	1.96416	650
660	2.15401	3.75910	1.95918	2.22264	3.84254	1.96145	2.28905	3.92265	1.96345	660
670	2.12991	3.72965	1.95833	2.19832	3.81305	1.96067	2.26452	3.89313	1.96273	670
680	2.10625	3.70064	1.95747	2.17443	3.78400	1.95988	2.24043	3.86405	1.96200	680
690	2.08302	3.67207	1.95660	2.15097	3.75540	1.95908	2.21676	3.83542	1.96126	690
700	2.06019	3.64393	1.95572	2.12793	3.72722	1.95826	2.19351	3.80720	1.96051	700
710	2.03776	3.61619	1.95482	2.10528	3.69944	1.95744	2.17065	3.77940	1.95975	710
720	2.01572	3.58886	1.95391	2.08302	3.67207	1.95660	2.14819	3.75199	1.95898	720
730	1.99406	3.56191	1.95299	2.06113	3.64509	1.95576	2.12610	3.72498	1.95820	730
740	1.97276	3.53535	1.95206	2.03962	3.61849	1.95490	2.10438	3.69834	1.95740	740
750	1.95183	3.50915	1.95112	2.01846	3.59225	1.95403	2.08302	3.67207	1.95660	750
760	1.93123	3.48331	1.95016	1.99765	3.56638	1.95315	2.06200	3.64616	1.95579	760
770	1.91098	3.45783	1.94919	1.97717	3.54085	1.95226	2.04132	3.62060	1.95497	770
780	1.89105	3.43268	1.94821	1.95703	3.51567	1.95135	2.02098	3.59538	1.95413	780
790	1.87145	3.40787	1.94722	1.93720	3.49081	1.95044	2.00095	3.57049	1.95329	790
800	1.85215	3.38338	1.94621	1.91769	3.46628	1.94951	1.98124	3.54593	1.95243	800
810	1.83316	3.35921	1.94519	1.89849	3.44207	1.94858	1.96183	3.52168	1.95157	810
820	1.81447	3.33535	1.94416	1.87958	3.41817	1.94763	1.94272	3.49774	1.95070	820
830	1.79607	3.31179	1.94312	1.86096	3.39457	1.94667	1.92390	3.47410	1.94981	830
840	1.77794	3.28853	1.94207	1.84262	3.37126	1.94570	1.90537	3.45075	1.94892	840
850	1.76010	3.26555	1.94100	1.82456	3.34824	1.94472	1.88711	3.42769	1.94801	850
860	1.74252	3.24285	1.93993	1.80677	3.32550	1.94373	1.86911	3.40491	1.94710	860
870	1.72520	3.22043	1.93884	1.78924	3.30303	1.94273	1.85139	3.38241	1.94617	870
880	1.70814	3.19828	1.93774	1.77197	3.28084	1.94172	1.83392	3.36017	1.94523	880
890	1.69134	3.17639	1.93662	1.75494	3.25890	1.94069	1.81670	3.33820	1.94429	890
900	1.67477	3.15476	1.93550	1.73817	3.23722	1.93966	1.79972	3.31648	1.94333	900
910	1.65844	3.13338	1.93436	1.72163	3.21580	1.93861	1.78299	3.29501	1.94236	910
920	1.64235	3.11224	1.93322	1.70533	3.19461	1.93755	1.76649	3.27379	1.94139	920
930	1.62649	3.09135	1.93206	1.68925	3.17367	1.93648	1.75022	3.25281	1.94040	930
940	1.61085	3.07069	1.93089	1.67340	3.15297	1.93541	1.73418	3.23206	1.93941	940
950	1.59543	3.05027	1.92970	1.65777	3.13249	1.93432	1.71835	3.21154	1.93840	950
960	1.58022	3.03007	1.92851	1.64235	3.11224	1.93322	1.70274	3.19125	1.93738	960
970	1.56522	3.01009	1.92730	1.62715	3.09222	1.93211	1.68734	3.17118	1.93636	970
980	1.55043	2.99033	1.92608	1.61214	3.07241	1.93098	1.67214	3.15132	1.93532	980
990	1.53583	2.97078	1.92486	1.59734	3.05281	1.92985	1.65715	3.13168	1.93427	990
1000	1.52144	2.95144	1.92361	1.58274	3.03342	1.92871	1.54235	3.11224	1.93322	1000
1010	1.50723	2.93230	1.92236	1.56833	3.01423	1.92755	1.62775	3.09301	1.93215	1010
1020	1.49322	2.91337	1.92110	1.55411	2.99525	1.92639	1.61334	3.07398	1.93107	1020
1030	1.47938	2.89463	1.91982	1.54007	2.97646	1.92522	1.59911	3.05515	1.92999	1030
1040	1.46573	2.87609	1.91854	1.52621	2.95786	1.92403	1.58506	3.03651	1.92889	1040
1050	1.45226	2.85774	1.91724	1.51254	2.93946	1.92283	1.57119	3.01805	1.92779	1050
1060	1.43896	2.83957	1.91593	1.49903	2.92124	1.92163	1.55750	2.99978	1.92667	1060
1070	1.42583	2.82159	1.91461	1.48570	2.90320	1.92041	1.54398	2.98170	1.92555	1070
1080	1.41287	2.80378	1.91328	1.47254	2.88534	1.91918	1.53063	2.96379	1.92441	1080
1090	1.40007	2.78616	1.91193	1.45954	2.86766	1.91794	1.51744	2.94606	1.92327	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=2300.			T=2400.			T=2500.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	
1100	1.38744	2.76870	1.91058	1.44670	2.85015	1.91670	1.50441	2.92850	1.92211	1100
1110	1.37496	2.75142	1.90921	1.43402	2.83281	1.91544	1.49155	2.91111	1.92095	1110
1120	1.36264	2.73430	1.90784	1.42149	2.81563	1.91417	1.47883	2.89389	1.91977	1120
1130	1.35046	2.71735	1.90645	1.40912	2.79862	1.91289	1.46628	2.87683	1.91859	1130
1140	1.33844	2.70056	1.90505	1.39690	2.78178	1.91160	1.45387	2.85993	1.91740	1140
1150	1.32657	2.68392	1.90364	1.38483	2.76509	1.91030	1.44161	2.84319	1.91619	1150
1160	1.31484	2.66745	1.90222	1.37290	2.74855	1.90899	1.42949	2.82660	1.91498	1160
1170	1.30325	2.65113	1.90079	1.36111	2.73217	1.90766	1.41752	2.81017	1.91376	1170
1180	1.29179	2.63496	1.89934	1.34946	2.71594	1.90633	1.40569	2.79389	1.91253	1180
1190	1.28048	2.61893	1.89789	1.33794	2.69986	1.90499	1.39399	2.77776	1.91129	1190
1200	1.26930	2.60306	1.89642	1.32657	2.68392	1.90364	1.38243	2.76177	1.91003	1200
1210	1.25825	2.58733	1.89495	1.31532	2.66813	1.90228	1.37100	2.74592	1.90877	1210
1220	1.24733	2.57174	1.89346	1.30421	2.65248	1.90091	1.35970	2.73022	1.90751	1220
1230	1.23654	2.55628	1.89196	1.29322	2.63697	1.89952	1.34853	2.71465	1.90623	1230
1240	1.22587	2.54097	1.89046	1.28236	2.62159	1.89813	1.33749	2.69922	1.90494	1240
1250	1.21532	2.52579	1.88894	1.27162	2.60635	1.89673	1.32657	2.68392	1.90364	1250
1260	1.20490	2.51075	1.88741	1.26100	2.59125	1.89532	1.31577	2.66876	1.90233	1260
1270	1.19460	2.49583	1.88587	1.25050	2.57627	1.89390	1.30509	2.65373	1.90102	1270
1280	1.18441	2.48105	1.88431	1.24012	2.56142	1.89246	1.29453	2.63882	1.89969	1280
1290	1.17434	2.46639	1.88275	1.22985	2.54670	1.89102	1.28409	2.62404	1.89836	1290
1300	1.16438	2.45186	1.88118	1.21970	2.53210	1.88957	1.27375	2.60939	1.89701	1300
1310	1.15453	2.43745	1.87960	1.20966	2.51763	1.88811	1.26354	2.59486	1.89566	1310
1320	1.14479	2.42316	1.87800	1.19973	2.50327	1.88664	1.25343	2.58045	1.89430	1320
1330	1.13516	2.40899	1.87640	1.18991	2.48904	1.88516	1.24343	2.56616	1.89292	1330
1340	1.12563	2.39494	1.87479	1.18020	2.47493	1.88367	1.23354	2.55198	1.89154	1340
1350	1.11621	2.38101	1.87316	1.17059	2.46093	1.88216	1.22375	2.53792	1.89015	1350
1360	1.10689	2.36719	1.87153	1.16108	2.44704	1.88065	1.21407	2.52398	1.88875	1360
1370	1.09768	2.35349	1.86988	1.15168	2.43327	1.87913	1.20449	2.51015	1.88735	1370
1380	1.08856	2.33989	1.86822	1.14237	2.41961	1.87760	1.19501	2.49643	1.88593	1380
1390	1.07954	2.32641	1.86656	1.13316	2.40606	1.87606	1.18562	2.48282	1.88450	1390
1400	1.07062	2.31304	1.86488	1.12406	2.39261	1.87452	1.17634	2.46931	1.88307	1400
1410	1.06179	2.29977	1.86320	1.11504	2.37928	1.87296	1.16715	2.45591	1.88162	1410
1420	1.05306	2.28661	1.86150	1.10612	2.36605	1.87139	1.15806	2.44262	1.88017	1420
1430	1.04442	2.27355	1.85979	1.09730	2.35292	1.86981	1.14906	2.42943	1.87871	1430
1440	1.03587	2.26060	1.85807	1.08856	2.33989	1.86822	1.14015	2.41635	1.87724	1440
1450	1.02741	2.24774	1.85635	1.07992	2.32697	1.86663	1.13134	2.40336	1.87576	1450
1460	1.01904	2.23499	1.85461	1.07136	2.31415	1.86502	1.12261	2.39047	1.87427	1460
1470	1.01075	2.22234	1.85286	1.06289	2.30142	1.86341	1.11397	2.37768	1.87277	1470
1480	1.00255	2.20978	1.85111	1.05451	2.28879	1.86178	1.10541	2.36499	1.87126	1480
1490	0.99444	2.19732	1.84934	1.04621	2.27626	1.86015	1.09694	2.35240	1.86975	1490
1500	0.98640	2.18496	1.84756	1.03800	2.26383	1.85850	1.08856	2.33989	1.86822	1500
1510	0.97846	2.17269	1.84578	1.02987	2.25148	1.85685	1.08026	2.32749	1.86669	1510
1520	0.97059	2.16051	1.84398	1.02182	2.23923	1.85519	1.07204	2.31517	1.86515	1520
1530	0.96280	2.14842	1.84217	1.01385	2.22707	1.85352	1.06390	2.30294	1.86360	1530
1540	0.95509	2.13643	1.84036	1.00596	2.21500	1.85184	1.05584	2.29081	1.86204	1540
1550	0.94746	2.12452	1.83853	0.99815	2.20302	1.85015	1.04786	2.27876	1.86048	1550
1560	0.93990	2.11271	1.83670	0.99041	2.19113	1.84845	1.03996	2.26680	1.85890	1560
1570	0.93242	2.10098	1.83485	0.98275	2.17932	1.84675	1.03213	2.25493	1.85732	1570
1580	0.92501	2.08933	1.83300	0.97517	2.16760	1.84503	1.02438	2.24314	1.85572	1580
1590	0.91768	2.07777	1.83114	0.96766	2.15597	1.84330	1.01671	2.23144	1.85412	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
T=2300.			T=2400.			T=2500.				
1600	0.91042	2.06630	1.82926	0.96022	2.14442	1.84157	1.00910	2.21982	1.85251	1600
1610	0.90323	2.05491	1.82738	0.95285	2.13295	1.83983	1.00157	2.20828	1.85090	1610
1620	0.89611	2.04360	1.82549	0.94556	2.12156	1.83808	0.99411	2.19683	1.84927	1620
1630	0.88906	2.03237	1.82359	0.93833	2.11026	1.83632	0.98672	2.18545	1.84763	1630
1640	0.88208	2.02122	1.82168	0.93118	2.09903	1.83455	0.97940	2.17416	1.84599	1640
1650	0.87517	2.01015	1.81976	0.92409	2.08788	1.83277	0.97215	2.16294	1.84434	1650
1660	0.86833	1.99916	1.81783	0.91707	2.07681	1.83098	0.96497	2.15180	1.84268	1660
1670	0.86155	1.98825	1.81589	0.91012	2.06582	1.82919	0.95785	2.14074	1.84101	1670
1680	0.85483	1.97742	1.81394	0.90323	2.05491	1.82738	0.95080	2.12975	1.83934	1680
1690	0.84818	1.96666	1.81199	0.89641	2.04407	1.82557	0.94382	2.11884	1.83765	1690
1700	0.84160	1.95597	1.81002	0.88965	2.03330	1.82375	0.93690	2.10800	1.83596	1700
1710	0.83507	1.94536	1.80805	0.88295	2.02261	1.82192	0.93004	2.09724	1.83426	1710
1720	0.82861	1.93483	1.80606	0.87632	2.01199	1.82008	0.92325	2.08655	1.83255	1720
1730	0.82221	1.92436	1.80407	0.86975	2.00145	1.81823	0.91651	2.07593	1.83084	1730
1740	0.81587	1.91397	1.80207	0.86324	1.99097	1.81638	0.90984	2.06538	1.82911	1740
1750	0.80959	1.90365	1.80006	0.85679	1.98057	1.81451	0.90323	2.05491	1.82738	1750
1760	0.80337	1.89340	1.79804	0.85039	1.97024	1.81264	0.89668	2.04450	1.82564	1760
1770	0.79720	1.88322	1.79601	0.84406	1.95997	1.81076	0.89019	2.03416	1.82389	1770
1780	0.79109	1.87310	1.79398	0.83778	1.94977	1.80887	0.88375	2.02389	1.82214	1780
1790	0.78504	1.86306	1.79193	0.83157	1.93965	1.80697	0.87738	2.01369	1.82037	1790
1800	0.77905	1.85308	1.78988	0.82540	1.92958	1.80507	0.87106	2.00355	1.81860	1800
1810	0.77311	1.84317	1.78781	0.81930	1.91959	1.80315	0.86479	1.99348	1.81682	1810
1820	0.76722	1.83333	1.78574	0.81324	1.90966	1.80123	0.85859	1.98348	1.81503	1820
1830	0.76139	1.82355	1.78366	0.80725	1.89980	1.79930	0.85243	1.97353	1.81324	1830
1840	0.75562	1.81383	1.78157	0.80130	1.89000	1.79736	0.84633	1.96366	1.81144	1840
1850	0.74989	1.80418	1.77948	0.79541	1.88026	1.79542	0.84029	1.95384	1.80963	1850
1860	0.74422	1.79459	1.77737	0.78958	1.87059	1.79346	0.83429	1.94409	1.80781	1860
1870	0.73860	1.78507	1.77526	0.78379	1.86097	1.79150	0.82835	1.93441	1.80598	1870
1880	0.73303	1.77561	1.77314	0.77805	1.85142	1.78953	0.82246	1.92478	1.80415	1880
1890	0.72750	1.76621	1.77101	0.77237	1.84194	1.78756	0.81663	1.91521	1.80231	1890
1900	0.72203	1.75687	1.76887	0.76674	1.83251	1.78557	0.81084	1.90571	1.80046	1900
1910	0.71661	1.74759	1.76672	0.76115	1.82314	1.78358	0.80510	1.89626	1.79861	1910
1920	0.71124	1.73837	1.76457	0.75562	1.81383	1.78157	0.79941	1.88687	1.79674	1920
1930	0.70591	1.72921	1.76241	0.75013	1.80458	1.77957	0.79377	1.87754	1.79487	1930
1940	0.70063	1.72010	1.76024	0.74469	1.79539	1.77755	0.78818	1.86827	1.79299	1940
1950	0.69540	1.71106	1.75806	0.73930	1.78626	1.77552	0.78264	1.85906	1.79111	1950
1960	0.69022	1.70207	1.75587	0.73395	1.77718	1.77349	0.77714	1.84990	1.78922	1960
1970	0.68508	1.69314	1.75368	0.72865	1.76816	1.77145	0.77169	1.84080	1.78732	1970
1980	0.67998	1.68427	1.75148	0.72340	1.75920	1.76941	0.76629	1.83176	1.78541	1980
1990	0.67493	1.67545	1.74927	0.71819	1.75029	1.76735	0.76093	1.82277	1.78350	1990
2000	0.66993	1.66669	1.74705	0.71302	1.74143	1.76529	0.75562	1.81383	1.78157	2000
2010	0.66496	1.65798	1.74482	0.70790	1.73263	1.76322	0.75035	1.80495	1.77965	2010
2020	0.66005	1.64932	1.74259	0.70283	1.72389	1.76114	0.74512	1.79612	1.77771	2020
2030	0.65517	1.64072	1.74035	0.69779	1.71520	1.75906	0.73994	1.78735	1.77577	2030
2040	0.65034	1.63218	1.73810	0.69280	1.70656	1.75697	0.73480	1.77863	1.77382	2040
2050	0.64554	1.62368	1.73585	0.68786	1.69797	1.75487	0.72971	1.76996	1.77186	2050
2060	0.64079	1.61524	1.73358	0.68295	1.68944	1.75276	0.72465	1.76134	1.76990	2060
2070	0.63608	1.60685	1.73131	0.67808	1.68095	1.75065	0.71964	1.75278	1.76793	2070
2080	0.63141	1.59852	1.72903	0.67326	1.67252	1.74853	0.71467	1.74426	1.76595	2080
2090	0.62678	1.59023	1.72675	0.66847	1.66414	1.74640	0.70974	1.73580	1.76397	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=2300.			T=2400.			T=2500.				
2100	0.62219	1.58199	1.72445	0.66373	1.65581	1.74427	0.70485	1.72738	1.76197	2100
2110	0.61764	1.57380	1.72215	0.65903	1.64753	1.74212	0.70000	1.71901	1.75998	2110
2120	0.61313	1.56567	1.71985	0.65436	1.63930	1.73998	0.69519	1.71070	1.75797	2120
2130	0.60866	1.55758	1.71753	0.64973	1.63111	1.73782	0.69042	1.70243	1.75596	2130
2140	0.60422	1.54954	1.71521	0.64515	1.62298	1.73566	0.68569	1.69421	1.75394	2140
2150	0.59982	1.54155	1.71288	0.64060	1.61489	1.73349	0.68100	1.68604	1.75192	2150
2160	0.59546	1.53361	1.71054	0.63608	1.60685	1.73131	0.67634	1.67791	1.74989	2160
2170	0.59113	1.52571	1.70820	0.63161	1.59886	1.72913	0.67172	1.66983	1.74785	2170
2180	0.58685	1.51786	1.70585	0.62717	1.59092	1.72694	0.66714	1.66180	1.74580	2180
2190	0.58259	1.51006	1.70349	0.62277	1.58302	1.72474	0.66260	1.65382	1.74375	2190
2200	0.57838	1.50231	1.70113	0.61840	1.57517	1.72254	0.65809	1.64588	1.74169	2200
2210	0.57419	1.49460	1.69876	0.61407	1.56736	1.72033	0.65362	1.63798	1.73963	2210
2220	0.57005	1.48693	1.69638	0.60977	1.55960	1.71811	0.64918	1.63014	1.73756	2220
2230	0.56593	1.47931	1.69400	0.60551	1.55188	1.71589	0.64478	1.62233	1.73548	2230
2240	0.56185	1.47174	1.69161	0.60128	1.54421	1.71366	0.64041	1.61457	1.73340	2240
2250	0.55781	1.46421	1.68921	0.59709	1.53658	1.71142	0.63608	1.60685	1.73131	2250
2260	0.55380	1.45672	1.68681	0.59293	1.52899	1.70918	0.63179	1.59918	1.72922	2260
2270	0.54982	1.44928	1.68440	0.58881	1.52145	1.70693	0.62752	1.59155	1.72711	2270
2280	0.54587	1.44188	1.68198	0.58471	1.51396	1.70467	0.62329	1.58396	1.72500	2280
2290	0.54196	1.43453	1.67956	0.58066	1.50650	1.70241	0.61909	1.57642	1.72289	2290
2300	0.53808	1.42721	1.67713	0.57663	1.49909	1.70014	0.61493	1.56892	1.72077	2300
2310	0.53423	1.41994	1.67469	0.57263	1.49172	1.69787	0.61080	1.56146	1.71864	2310
2320	0.53041	1.41271	1.67225	0.56867	1.48439	1.69559	0.60670	1.55404	1.71651	2320
2330	0.52662	1.40553	1.66980	0.56474	1.47710	1.69330	0.60263	1.54666	1.71437	2330
2340	0.52286	1.39838	1.66734	0.56084	1.46985	1.69101	0.59860	1.53932	1.71223	2340
2350	0.51914	1.39128	1.66488	0.55697	1.46265	1.68871	0.59459	1.53202	1.71008	2350
2360	0.51544	1.38421	1.66241	0.55313	1.45548	1.68641	0.59062	1.52477	1.70792	2360
2370	0.51177	1.37719	1.65994	0.54932	1.44835	1.68409	0.58667	1.51755	1.70576	2370
2380	0.50814	1.37020	1.65746	0.54554	1.44127	1.68178	0.58276	1.51037	1.70359	2380
2390	0.50453	1.36326	1.65498	0.54180	1.43422	1.67945	0.57888	1.50323	1.70141	2390
2400	0.50095	1.35635	1.65248	0.53808	1.42721	1.67713	0.57503	1.49613	1.69923	2400
2410	0.49740	1.34949	1.64999	0.53439	1.42025	1.67479	0.57120	1.48907	1.69705	2410
2420	0.49388	1.34266	1.64748	0.53073	1.41332	1.67245	0.56741	1.48205	1.69486	2420
2430	0.49039	1.33587	1.64497	0.52709	1.40642	1.67010	0.56364	1.47507	1.69266	2430
2440	0.48692	1.32912	1.64246	0.52349	1.39957	1.66775	0.55991	1.46812	1.69046	2440
2450	0.48348	1.32241	1.63994	0.51991	1.39275	1.66539	0.55620	1.46121	1.68825	2450
2460	0.48007	1.31574	1.63741	0.51636	1.38597	1.66303	0.55252	1.45434	1.68604	2460
2470	0.47669	1.30910	1.63488	0.51284	1.37923	1.66066	0.54887	1.44750	1.68382	2470
2480	0.47333	1.30250	1.63234	0.50935	1.37253	1.65829	0.54524	1.44070	1.68159	2480
2490	0.47000	1.29593	1.62980	0.50588	1.36586	1.65591	0.54165	1.43394	1.67936	2490
2500	0.46670	1.28941	1.62725	0.50244	1.35923	1.65352	0.53808	1.42721	1.67713	2500
2510	0.46342	1.28292	1.62470	0.49903	1.35263	1.65113	0.53453	1.42052	1.67488	2510
2520	0.46017	1.27646	1.62214	0.49564	1.34607	1.64874	0.53102	1.41387	1.67264	2520
2530	0.45694	1.27004	1.61957	0.49228	1.33955	1.64633	0.52753	1.40725	1.67039	2530
2540	0.45374	1.26366	1.61700	0.48894	1.33306	1.64393	0.52406	1.40066	1.66813	2540
2550	0.45057	1.25731	1.61443	0.48563	1.32660	1.64151	0.52062	1.39411	1.66587	2550
2560	0.44741	1.25100	1.61185	0.48234	1.32018	1.63910	0.51721	1.38760	1.66360	2560
2570	0.44429	1.24472	1.60926	0.47908	1.31380	1.63667	0.51382	1.38112	1.66133	2570
2580	0.44118	1.23847	1.60667	0.47585	1.30744	1.63425	0.51046	1.37467	1.65905	2580
2590	0.43811	1.23226	1.60408	0.47264	1.30113	1.63181	0.50713	1.36826	1.65677	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=2300.			T=2400.			T=2500.				
2600	0.43505	1.22609	1.60148	0.46945	1.29484	1.62938	0.50381	1.36188	1.65448	2600
2610	0.43202	1.21994	1.59887	0.46629	1.28859	1.62693	0.50052	1.35553	1.65218	2610
2620	0.42901	1.21383	1.59626	0.46315	1.28238	1.62449	0.49726	1.34922	1.64989	2620
2630	0.42603	1.20776	1.59365	0.46003	1.27619	1.62203	0.49402	1.34293	1.64758	2630
2640	0.42307	1.20171	1.59103	0.45694	1.27004	1.61957	0.49081	1.33669	1.64528	2640
2650	0.42013	1.19570	1.58840	0.45387	1.26392	1.61711	0.48761	1.33047	1.64296	2650
2660	0.41722	1.18973	1.58577	0.45083	1.25784	1.61464	0.48444	1.32429	1.64065	2660
2670	0.41432	1.18378	1.58314	0.44781	1.25178	1.61217	0.48130	1.31813	1.63832	2670
2680	0.41145	1.17787	1.58050	0.44481	1.24576	1.60970	0.47818	1.31201	1.63600	2680
2690	0.40860	1.17199	1.57785	0.44183	1.23977	1.60721	0.47508	1.30593	1.63366	2690
2700	0.40578	1.16614	1.57521	0.43887	1.23381	1.60473	0.47200	1.29987	1.63133	2700
2710	0.40297	1.16032	1.57255	0.43594	1.22788	1.60224	0.46894	1.29384	1.62899	2710
2720	0.40019	1.15453	1.56990	0.43303	1.22199	1.59974	0.46591	1.28785	1.62664	2720
2730	0.39742	1.14877	1.56723	0.43014	1.21612	1.59724	0.46290	1.28188	1.62429	2730
2740	0.39468	1.14305	1.56457	0.42727	1.21028	1.59474	0.45991	1.27595	1.62193	2740
2750	0.39196	1.13735	1.56190	0.42442	1.20448	1.59223	0.45694	1.27004	1.61957	2750
2760	0.38926	1.13169	1.55922	0.42160	1.19870	1.58971	0.45400	1.26417	1.61721	2760
2770	0.38658	1.12606	1.55655	0.41879	1.19296	1.58720	0.45107	1.25832	1.61484	2770
2780	0.38392	1.12045	1.55386	0.41601	1.18724	1.58467	0.44817	1.25251	1.61247	2780
2790	0.38128	1.11488	1.55118	0.41324	1.18156	1.58215	0.44529	1.24672	1.61009	2790
2800	0.37866	1.10933	1.54848	0.41050	1.17590	1.57962	0.44242	1.24097	1.60771	2800
2810	0.37606	1.10382	1.54579	0.40778	1.17028	1.57708	0.43958	1.23524	1.60532	2810
2820	0.37348	1.09833	1.54309	0.40507	1.16468	1.57454	0.43676	1.22954	1.60293	2820
2830	0.37092	1.09287	1.54039	0.40239	1.15911	1.57200	0.43396	1.22387	1.60054	2830
2840	0.36838	1.08744	1.53768	0.39973	1.15357	1.56945	0.43118	1.21823	1.59814	2840
2850	0.36586	1.08204	1.53497	0.39708	1.14806	1.56690	0.42842	1.21262	1.59574	2850
2860	0.36336	1.07667	1.53226	0.39446	1.14257	1.56435	0.42567	1.20703	1.59333	2860
2870	0.36087	1.07133	1.52954	0.39185	1.13712	1.56179	0.42295	1.20147	1.59092	2870
2880	0.35841	1.06601	1.52682	0.38926	1.13169	1.55922	0.42025	1.19594	1.58851	2880
2890	0.35596	1.06072	1.52409	0.38669	1.12629	1.55666	0.41756	1.19044	1.58609	2890
2900	0.35353	1.05546	1.52136	0.38414	1.12092	1.55409	0.41490	1.18497	1.58366	2900
2910	0.35112	1.05023	1.51863	0.38161	1.11557	1.55151	0.41225	1.17952	1.58124	2910
2920	0.34872	1.04503	1.51589	0.37910	1.11025	1.54893	0.40963	1.17410	1.57881	2920
2930	0.34635	1.03985	1.51315	0.37660	1.10496	1.54635	0.40702	1.16871	1.57637	2930
2940	0.34399	1.03470	1.51041	0.37413	1.09970	1.54377	0.40443	1.16334	1.57393	2940
2950	0.34165	1.02957	1.50766	0.37167	1.09446	1.54118	0.40186	1.15800	1.57149	2950
2960	0.33932	1.02448	1.50491	0.36923	1.08925	1.53858	0.39930	1.15269	1.56905	2960
2970	0.33702	1.01941	1.50216	0.36680	1.08406	1.53599	0.39676	1.14740	1.56660	2970
2980	0.33473	1.01436	1.49940	0.36440	1.07891	1.53339	0.39425	1.14214	1.56414	2980
2990	0.33246	1.00934	1.49664	0.36201	1.07377	1.53078	0.39175	1.13690	1.56169	2990
3000	0.33020	1.00435	1.49388	0.35964	1.06867	1.52818	0.38926	1.13169	1.55922	3000
3010	0.32796	0.99938	1.49111	0.35728	1.06359	1.52557	0.38680	1.12650	1.55676	3010
3020	0.32574	0.99444	1.48834	0.35494	1.05853	1.52295	0.38435	1.12135	1.55429	3020
3030	0.32353	0.98953	1.48557	0.35262	1.05350	1.52034	0.38191	1.11621	1.55182	3030
3040	0.32134	0.98464	1.48279	0.35032	1.04849	1.51772	0.37950	1.11110	1.54935	3040
3050	0.31917	0.97977	1.48002	0.34803	1.04351	1.51509	0.37710	1.10602	1.54687	3050
3060	0.31701	0.97493	1.47723	0.34576	1.03856	1.51247	0.37472	1.10096	1.54439	3060
3070	0.31487	0.97012	1.47445	0.34350	1.03363	1.50984	0.37235	1.09592	1.54190	3070
3080	0.31274	0.96533	1.47166	0.34126	1.02872	1.50720	0.37001	1.09091	1.53941	3080
3090	0.31063	0.96056	1.46887	0.33904	1.02384	1.50457	0.36767	1.08593	1.53692	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=2300.			T=2400.			T=2500.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
3100	0.30854	0.95582	1.46608	0.33683	1.01898	1.50193	0.36536	1.08097	1.53443	3100
3110	0.30646	0.95110	1.46329	0.33463	1.01415	1.49929	0.36306	1.07603	1.53193	3110
3120	0.30439	0.94641	1.46049	0.33246	1.00934	1.49664	0.36077	1.07111	1.52943	3120
3130	0.30234	0.94174	1.45769	0.33030	1.00456	1.49399	0.35850	1.06622	1.52692	3130
3140	0.30031	0.93709	1.45489	0.32815	0.99980	1.49134	0.35625	1.06136	1.52442	3140
3150	0.29829	0.93247	1.45208	0.32602	0.99506	1.48869	0.35401	1.05651	1.52191	3150
3160	0.29628	0.92787	1.44927	0.32390	0.99034	1.48603	0.35179	1.05169	1.51939	3160
3170	0.29429	0.92330	1.44646	0.32180	0.98565	1.48337	0.34958	1.04690	1.51688	3170
3180	0.29231	0.91875	1.44365	0.31971	0.98099	1.48071	0.34739	1.04212	1.51436	3180
3190	0.29035	0.91422	1.44084	0.31764	0.97634	1.47805	0.34521	1.03737	1.51183	3190
3200	0.28840	0.90972	1.43802	0.31558	0.97172	1.47538	0.34305	1.03265	1.50931	3200
3210	0.28646	0.90523	1.43520	0.31354	0.96712	1.47271	0.34090	1.02794	1.50678	3210
3220	0.28454	0.90077	1.43238	0.31151	0.96254	1.47004	0.33877	1.02326	1.50425	3220
3230	0.28264	0.89634	1.42955	0.30950	0.95799	1.46736	0.33665	1.01860	1.50172	3230
3240	0.28074	0.89192	1.42673	0.30750	0.95346	1.46468	0.33455	1.01396	1.49918	3240
3250	0.27886	0.88753	1.42390	0.30551	0.94895	1.46201	0.33246	1.00934	1.49664	3250
3260	0.27700	0.88316	1.42107	0.30354	0.94446	1.45932	0.33038	1.00475	1.49410	3260
3270	0.27515	0.87881	1.41824	0.30158	0.93999	1.45664	0.32832	1.00018	1.49155	3270
3280	0.27331	0.87448	1.41541	0.29963	0.93555	1.45395	0.32627	0.99563	1.48901	3280
3290	0.27148	0.87018	1.41257	0.29770	0.93113	1.45126	0.32424	0.99110	1.48646	3290
3300	0.26967	0.86590	1.40973	0.29578	0.92673	1.44857	0.32222	0.98659	1.48390	3300
3310	0.26787	0.86164	1.40689	0.29387	0.92235	1.44588	0.32021	0.98210	1.48135	3310
3320	0.26608	0.85740	1.40405	0.29198	0.91799	1.44318	0.31822	0.97764	1.47879	3320
3330	0.26430	0.85318	1.40121	0.29010	0.91366	1.44048	0.31624	0.97320	1.47623	3330
3340	0.26254	0.84898	1.39836	0.28824	0.90934	1.43778	0.31427	0.96877	1.47367	3340
3350	0.26079	0.84480	1.39552	0.28638	0.90505	1.43508	0.31232	0.96437	1.47111	3350
3360	0.25906	0.84065	1.39267	0.28454	0.90077	1.43238	0.31038	0.95999	1.46854	3360
3370	0.25733	0.83652	1.38982	0.28272	0.89652	1.42967	0.30845	0.95563	1.46597	3370
3380	0.25562	0.83240	1.38697	0.28090	0.89229	1.42696	0.30654	0.95129	1.46340	3380
3390	0.25392	0.82831	1.38412	0.27910	0.88808	1.42425	0.30464	0.94697	1.46083	3390
3400	0.25223	0.82424	1.38126	0.27731	0.88389	1.42154	0.30275	0.94267	1.45825	3400
3410	0.25055	0.82018	1.37841	0.27553	0.87971	1.41883	0.30087	0.93839	1.45567	3410
3420	0.24889	0.81615	1.37555	0.27376	0.87556	1.41611	0.29901	0.93413	1.45309	3420
3430	0.24724	0.81214	1.37269	0.27201	0.87143	1.41340	0.29716	0.92990	1.45051	3430
3440	0.24559	0.80815	1.36984	0.27027	0.86732	1.41068	0.29532	0.92568	1.44792	3440
3450	0.24396	0.80417	1.36698	0.26854	0.86323	1.40796	0.29350	0.92148	1.44534	3450
3460	0.24235	0.80022	1.36411	0.26682	0.85916	1.40524	0.29168	0.91730	1.44275	3460
3470	0.24074	0.79629	1.36125	0.26512	0.85511	1.40251	0.28988	0.91314	1.44016	3470
3480	0.23914	0.79238	1.35839	0.26342	0.85108	1.39979	0.28809	0.90900	1.43757	3480
3490	0.23756	0.78848	1.35552	0.26174	0.84706	1.39706	0.28631	0.90488	1.43497	3490
3500	0.23599	0.78461	1.35266	0.26007	0.84307	1.39433	0.28454	0.90077	1.43238	3500
3510	0.23443	0.78075	1.34979	0.25841	0.83910	1.39160	0.28279	0.89669	1.42978	3510
3520	0.23287	0.77692	1.34692	0.25676	0.83514	1.38887	0.28105	0.89263	1.42718	3520
3530	0.23133	0.77310	1.34405	0.25512	0.83121	1.38614	0.27931	0.88858	1.42458	3530
3540	0.22981	0.76930	1.34118	0.25349	0.82729	1.38340	0.27759	0.88456	1.42198	3540
3550	0.22829	0.76552	1.33831	0.25188	0.82339	1.38067	0.27589	0.88055	1.41937	3550
3560	0.22678	0.76176	1.33544	0.25027	0.81951	1.37793	0.27419	0.87656	1.41677	3560
3570	0.22528	0.75802	1.33257	0.24868	0.81565	1.37520	0.27250	0.87259	1.41416	3570
3580	0.22379	0.75430	1.32970	0.24710	0.81181	1.37246	0.27083	0.86864	1.41155	3580
3590	0.22232	0.75059	1.32683	0.24553	0.80798	1.36972	0.26916	0.86470	1.40894	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=2300.			T=2400.			T=2500.			ν cm ⁻¹
	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	
3600	0.22085	0.74690	1.32395	0.24396	0.80417	1.36698	0.26751	0.86079	1.40632	3600
3610	0.21939	0.74324	1.32108	0.24241	0.80039	1.36423	0.26587	0.85689	1.40371	3610
3620	0.21795	0.73959	1.31820	0.24087	0.79662	1.36149	0.26423	0.85301	1.40109	3620
3630	0.21651	0.73595	1.31533	0.23934	0.79286	1.35875	0.26261	0.84915	1.39848	3630
3640	0.21509	0.73234	1.31245	0.23782	0.78913	1.35600	0.26100	0.84530	1.39586	3640
3650	0.21367	0.72874	1.30958	0.23631	0.78541	1.35325	0.25940	0.84148	1.39324	3650
3660	0.21226	0.72516	1.30670	0.23482	0.78172	1.35051	0.25781	0.83767	1.39062	3660
3670	0.21087	0.72160	1.30382	0.23333	0.77803	1.34776	0.25623	0.83388	1.38800	3670
3680	0.20948	0.71806	1.30095	0.23185	0.77437	1.34501	0.25466	0.83011	1.38537	3680
3690	0.20810	0.71453	1.29807	0.23038	0.77072	1.34226	0.25311	0.82635	1.38275	3690
3700	0.20674	0.71102	1.29519	0.22892	0.76710	1.33951	0.25156	0.82261	1.38012	3700
3710	0.20538	0.70753	1.29231	0.22747	0.76348	1.33676	0.25002	0.81889	1.37749	3710
3720	0.20403	0.70403	1.28943	0.22603	0.75989	1.33401	0.24849	0.81519	1.37487	3720
3730	0.20269	0.70060	1.28656	0.22460	0.75631	1.33126	0.24697	0.81150	1.37224	3730
3740	0.20136	0.69716	1.28368	0.22318	0.75275	1.32850	0.24546	0.80783	1.36961	3740
3750	0.20004	0.69373	1.28080	0.22177	0.74921	1.32575	0.24396	0.80417	1.36698	3750
3760	0.19873	0.69033	1.27792	0.22036	0.74568	1.32299	0.24248	0.80054	1.36434	3760
3770	0.19742	0.68694	1.27504	0.21897	0.74217	1.32024	0.24100	0.79692	1.36171	3770
3780	0.19613	0.68356	1.27216	0.21759	0.73868	1.31748	0.23953	0.79331	1.35907	3780
3790	0.19484	0.68020	1.26929	0.21621	0.73520	1.31473	0.23807	0.78973	1.35644	3790
3800	0.19357	0.67686	1.26641	0.21485	0.73174	1.31197	0.23662	0.78616	1.35380	3800
3810	0.19230	0.67354	1.26353	0.21349	0.72829	1.30922	0.23517	0.78260	1.35117	3810
3820	0.19104	0.67023	1.26065	0.21215	0.72487	1.30646	0.23374	0.77906	1.34853	3820
3830	0.18979	0.66694	1.25777	0.21081	0.72145	1.30370	0.23232	0.77554	1.34589	3830
3840	0.18855	0.66366	1.25490	0.20948	0.71806	1.30094	0.23091	0.77203	1.34325	3840
3850	0.18732	0.66040	1.25202	0.20816	0.71468	1.29819	0.22950	0.76854	1.34061	3850
3860	0.18609	0.65716	1.24914	0.20685	0.71131	1.29543	0.22810	0.76507	1.33797	3860
3870	0.18488	0.65393	1.24627	0.20555	0.70797	1.29267	0.22672	0.76161	1.33533	3870
3880	0.18367	0.65072	1.24339	0.20425	0.70463	1.28991	0.22534	0.75817	1.33269	3880
3890	0.18247	0.64752	1.24052	0.20297	0.70132	1.28715	0.22397	0.75474	1.33004	3890
3900	0.18128	0.64434	1.23764	0.20169	0.69802	1.28440	0.22261	0.75133	1.32740	3900
3910	0.18009	0.64117	1.23477	0.20042	0.69473	1.28164	0.22126	0.74794	1.32476	3910
3920	0.17892	0.63802	1.23190	0.19916	0.69146	1.27888	0.21992	0.74455	1.32211	3920
3930	0.17775	0.63489	1.22902	0.19791	0.68821	1.27612	0.21858	0.74119	1.31947	3930
3940	0.17659	0.63177	1.22615	0.19667	0.68497	1.27336	0.21726	0.73784	1.31682	3940
3950	0.17544	0.62867	1.22328	0.19543	0.68174	1.27060	0.21594	0.73451	1.31418	3950
3960	0.17430	0.62558	1.22041	0.19420	0.67853	1.26785	0.21463	0.73119	1.31153	3960
3970	0.17316	0.62250	1.21754	0.19299	0.67534	1.26509	0.21333	0.72788	1.30889	3970
3980	0.17203	0.61944	1.21467	0.19177	0.67216	1.26233	0.21204	0.72459	1.30624	3980
3990	0.17091	0.61640	1.21180	0.19057	0.66899	1.25957	0.21076	0.72132	1.30359	3990
4000	0.16980	0.61337	1.20893	0.18938	0.66585	1.25682	0.20948	0.71806	1.30094	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$T=2600.$			$T=2700.$			$T=2800.$			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
100	5.80617	7.73886	1.98666	5.87915	7.81384	1.98670	5.94954	7.88609	1.98673	100
110	5.62222	7.54952	1.98656	5.69500	7.62449	1.98660	5.76520	7.69674	1.98664	110
120	5.45475	7.37667	1.98644	5.52733	7.45164	1.98649	5.59735	7.52389	1.98654	120
130	5.30113	7.21768	1.98631	5.37351	7.29264	1.98638	5.44335	7.36488	1.98643	130
140	5.15929	7.07048	1.98618	5.23147	7.14544	1.98625	5.30113	7.21768	1.98631	140
150	5.02762	6.93345	1.98603	5.09960	7.00841	1.98611	5.16907	7.08064	1.98619	150
160	4.90479	6.80528	1.98587	4.97657	6.88023	1.98597	5.04586	6.95246	1.98605	160
170	4.78973	6.68489	1.98570	4.86132	6.75984	1.98581	4.93042	6.83206	1.98591	170
180	4.68156	6.57140	1.98553	4.75295	6.64634	1.98565	4.82187	6.71855	1.98575	180
190	4.57952	6.46405	1.98534	4.65071	6.53898	1.98547	4.71945	6.61119	1.98559	190
200	4.48299	6.36222	1.98514	4.55399	6.43715	1.98529	4.62254	6.50935	1.98542	200
210	4.39143	6.26537	1.98493	4.46223	6.34029	1.98510	4.53060	6.41248	1.98524	210
220	4.30438	6.17304	1.98472	4.37498	6.24795	1.98490	4.44317	6.32013	1.98505	220
230	4.22143	6.08482	1.98449	4.29184	6.15972	1.98468	4.35985	6.23190	1.98486	230
240	4.14224	6.00037	1.98425	4.21245	6.07526	1.98446	4.28028	6.14743	1.98465	240
250	4.06649	5.91937	1.98400	4.13651	5.99425	1.98423	4.20415	6.06642	1.98444	250
260	3.99392	5.84156	1.98375	4.06375	5.91643	1.98399	4.13121	5.98859	1.98422	260
270	3.92429	5.76670	1.98348	3.99392	5.84156	1.98375	4.06120	5.91371	1.98399	270
280	3.85738	5.69457	1.98320	3.92682	5.76942	1.98349	3.99392	5.84156	1.98375	280
290	3.79300	5.62498	1.98291	3.86224	5.69982	1.98322	3.92917	5.77195	1.98350	290
300	3.73098	5.55776	1.98261	3.80003	5.63259	1.98294	3.86678	5.70471	1.98324	300
310	3.67116	5.49276	1.98230	3.74003	5.56758	1.98266	3.80659	5.63969	1.98297	310
320	3.61341	5.42983	1.98199	3.68208	5.50463	1.98236	3.74847	5.57673	1.98270	320
330	3.55760	5.36884	1.98166	3.62608	5.44364	1.98206	3.69228	5.51573	1.98242	330
340	3.50360	5.30969	1.98132	3.57189	5.38447	1.98174	3.63792	5.45655	1.98212	340
350	3.45132	5.25226	1.98097	3.51942	5.32703	1.98142	3.58527	5.39910	1.98182	350
360	3.40066	5.19646	1.98061	3.46857	5.27122	1.98109	3.53424	5.34327	1.98151	360
370	3.35153	5.14220	1.98024	3.41924	5.21694	1.98074	3.48474	5.28899	1.98119	370
380	3.30384	5.08939	1.97986	3.37137	5.16412	1.98039	3.43669	5.23616	1.98087	380
390	3.25753	5.03797	1.97947	3.32486	5.11269	1.98003	3.39001	5.18471	1.98053	390
400	3.21252	4.98786	1.97908	3.27966	5.06256	1.97966	3.34463	5.13457	1.98019	400
410	3.16874	4.93900	1.97867	3.23570	5.01368	1.97928	3.30049	5.08568	1.97984	410
420	3.12614	4.89132	1.97825	3.19291	4.96599	1.97890	3.25753	5.03797	1.97947	420
430	3.08467	4.84478	1.97782	3.15125	4.91943	1.97850	3.21569	4.99140	1.97910	430
440	3.04426	4.79931	1.97738	3.11065	4.87395	1.97809	3.17492	4.94590	1.97873	440
450	3.00488	4.75488	1.97693	3.07108	4.82950	1.97767	3.13518	4.90144	1.97834	450
460	2.96647	4.71143	1.97647	3.03249	4.78604	1.97725	3.09641	4.85796	1.97794	460
470	2.92900	4.66893	1.97601	2.99483	4.74352	1.97681	3.05857	4.81543	1.97754	470
480	2.89242	4.62734	1.97553	2.95806	4.70191	1.97637	3.02163	4.77380	1.97713	480
490	2.85669	4.58661	1.97504	2.92215	4.66116	1.97592	2.98555	4.73304	1.97670	490
500	2.82180	4.54671	1.97454	2.88707	4.62125	1.97546	2.95030	4.69311	1.97627	500
510	2.78769	4.50761	1.97403	2.85278	4.58213	1.97498	2.91583	4.65397	1.97584	510
520	2.75434	4.46929	1.97351	2.81924	4.54379	1.97450	2.88212	4.61561	1.97539	520
530	2.72172	4.43170	1.97299	2.78644	4.50618	1.97401	2.84915	4.57799	1.97493	530
540	2.68980	4.39483	1.97245	2.75434	4.46929	1.97351	2.81688	4.54108	1.97447	540
550	2.65856	4.35864	1.97190	2.72291	4.43308	1.97301	2.78528	4.50485	1.97400	550
560	2.62797	4.32311	1.97134	2.69214	4.39753	1.97249	2.75434	4.46929	1.97351	560
570	2.59801	4.28823	1.97078	2.66200	4.36263	1.97196	2.72402	4.43436	1.97302	570
580	2.56866	4.25396	1.97020	2.63246	4.32834	1.97143	2.69432	4.40005	1.97253	580
590	2.53989	4.22028	1.96961	2.60351	4.29464	1.97088	2.66520	4.36634	1.97202	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
	T=2600.			T=2700.			T=2800.			
600	2.51169	4.18718	1.96901	2.57513	4.26152	1.97033	2.63665	4.33320	1.97150	600
610	2.48404	4.15464	1.96841	2.54730	4.22896	1.96976	2.60864	4.30061	1.97098	610
620	2.45691	4.12264	1.96779	2.51999	4.19693	1.96919	2.58117	4.26857	1.97045	620
630	2.43030	4.09116	1.96716	2.49319	4.16543	1.96861	2.55420	4.23705	1.96991	630
640	2.40418	4.06018	1.96653	2.46690	4.13443	1.96802	2.52774	4.20603	1.96936	640
650	2.37854	4.02970	1.96588	2.44108	4.10392	1.96742	2.50175	4.17550	1.96880	650
660	2.35337	3.99969	1.96523	2.41573	4.07389	1.96681	2.47623	4.14544	1.96823	660
670	2.32865	3.97014	1.96456	2.39083	4.04432	1.96619	2.45117	4.11585	1.96766	670
680	2.30437	3.94104	1.96389	2.36637	4.01519	1.96557	2.42654	4.08670	1.96707	680
690	2.28051	3.91238	1.96320	2.34233	3.98650	1.96493	2.40233	4.05799	1.96648	690
700	2.25706	3.88413	1.96251	2.31870	3.95823	1.96429	2.37854	4.02970	1.96588	700
710	2.23402	3.85630	1.96180	2.29548	3.93038	1.96363	2.35515	4.00182	1.96527	710
720	2.21136	3.82887	1.96109	2.27265	3.90292	1.96297	2.33215	3.97434	1.96466	720
730	2.18908	3.80182	1.96036	2.25019	3.87585	1.96230	2.30953	3.94724	1.96403	730
740	2.16717	3.77516	1.95963	2.22811	3.84915	1.96162	2.28728	3.92052	1.96340	740
750	2.14562	3.74886	1.95889	2.20638	3.82283	1.96093	2.26539	3.89417	1.96276	750
760	2.12442	3.72292	1.95814	2.18500	3.79686	1.96023	2.24384	3.86818	1.96211	760
770	2.10355	3.69732	1.95737	2.16396	3.77124	1.95952	2.22264	3.84254	1.96145	770
780	2.08302	3.67207	1.95660	2.14325	3.74596	1.95881	2.20177	3.81723	1.96078	780
790	2.06280	3.64715	1.95582	2.12286	3.72101	1.95808	2.18121	3.79226	1.96010	790
800	2.04290	3.62256	1.95503	2.10278	3.69638	1.95735	2.16098	3.76761	1.95942	800
810	2.02331	3.59827	1.95423	2.08302	3.67207	1.95660	2.14105	3.74327	1.95873	810
820	2.00401	3.57430	1.95342	2.06355	3.64807	1.95585	2.12141	3.71924	1.95803	820
830	1.98501	3.55063	1.95260	2.04437	3.62437	1.95509	2.10207	3.69551	1.95732	830
840	1.96628	3.52725	1.95177	2.02547	3.60096	1.95432	2.08302	3.67207	1.95660	840
850	1.94784	3.50415	1.95093	2.00685	3.57783	1.95354	2.06424	3.64892	1.95588	850
860	1.92966	3.48134	1.95008	1.98850	3.55499	1.95275	2.04573	3.62605	1.95514	860
870	1.91175	3.45880	1.94923	1.97042	3.53242	1.95196	2.02748	3.60345	1.95440	870
880	1.89410	3.43653	1.94836	1.95259	3.51011	1.95115	2.00950	3.58112	1.95365	880
890	1.87669	3.41452	1.94748	1.93502	3.48807	1.95034	1.99176	3.55905	1.95289	890
900	1.85954	3.39276	1.94660	1.91769	3.46628	1.94951	1.97427	3.53723	1.95213	900
910	1.84262	3.37126	1.94570	1.90061	3.44475	1.94868	1.95703	3.51567	1.95135	910
920	1.82594	3.35000	1.94480	1.88375	3.42345	1.94784	1.94002	3.49434	1.95057	920
930	1.80949	3.32898	1.94388	1.86713	3.40240	1.94699	1.92324	3.47326	1.94978	930
940	1.79326	3.30819	1.94296	1.85074	3.38158	1.94613	1.90668	3.45241	1.94898	940
950	1.77725	3.28764	1.94203	1.83456	3.36099	1.94527	1.89035	3.43179	1.94817	950
960	1.76146	3.26731	1.94109	1.81860	3.34063	1.94439	1.87423	3.41139	1.94736	960
970	1.74588	3.24720	1.94013	1.80285	3.32048	1.94351	1.85832	3.39122	1.94653	970
980	1.73050	3.22730	1.93917	1.78731	3.30055	1.94262	1.84262	3.37126	1.94570	980
990	1.71533	3.20762	1.93820	1.77197	3.28084	1.94172	1.82712	3.35151	1.94486	990
1000	1.70036	3.18815	1.93723	1.75682	3.26133	1.94081	1.81182	3.33197	1.94402	1000
1010	1.68557	3.16887	1.93624	1.74187	3.24202	1.93989	1.79672	3.31263	1.94316	1010
1020	1.67098	3.14980	1.93524	1.72712	3.22291	1.93896	1.78180	3.29349	1.94230	1020
1030	1.65658	3.13093	1.93423	1.71254	3.20400	1.93802	1.76708	3.27454	1.94142	1030
1040	1.64235	3.11224	1.93322	1.69815	3.18528	1.93708	1.75253	3.25579	1.94054	1040
1050	1.62831	3.09375	1.93219	1.68394	3.16675	1.93613	1.73817	3.23722	1.93966	1050
1060	1.61444	3.07544	1.93116	1.66991	3.14840	1.93517	1.72398	3.21884	1.93876	1060
1070	1.60074	3.05731	1.93011	1.65605	3.13023	1.93420	1.70996	3.20064	1.93786	1070
1080	1.58721	3.03936	1.92906	1.64235	3.11224	1.93322	1.69611	3.18262	1.93694	1080
1090	1.57385	3.02159	1.92800	1.62882	3.09443	1.93223	1.68243	3.16477	1.93602	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
T=2600.			T=2700.			T=2800.				
1100	1.56065	3.00398	1.92693	1.61546	3.07679	1.93123	1.66891	3.14709	1.93510	1100
1110	1.54760	2.98655	1.92585	1.60225	3.05932	1.93023	1.65555	3.12959	1.93416	1110
1120	1.53472	2.96928	1.92476	1.58921	3.04201	1.92922	1.64235	3.11224	1.93322	1120
1130	1.52199	2.95218	1.92366	1.57631	3.02487	1.92820	1.62931	3.09506	1.93227	1130
1140	1.50940	2.93523	1.92256	1.56357	3.00788	1.92717	1.61641	3.07804	1.93131	1140
1150	1.49697	2.91845	1.92144	1.55097	2.99105	1.92613	1.60366	3.06118	1.93034	1150
1160	1.48468	2.90182	1.92032	1.53852	2.97438	1.92508	1.59106	3.04447	1.92936	1160
1170	1.47254	2.88534	1.91918	1.52621	2.95786	1.92403	1.57860	3.02791	1.92838	1170
1180	1.46053	2.86901	1.91804	1.51405	2.94149	1.92297	1.56628	3.01151	1.92739	1180
1190	1.44866	2.85283	1.91689	1.50202	2.92527	1.92190	1.55411	2.99525	1.92639	1190
1200	1.43693	2.83679	1.91573	1.49013	2.90919	1.92082	1.54206	2.97913	1.92538	1200
1210	1.42533	2.82090	1.91456	1.47837	2.89325	1.91973	1.53015	2.96316	1.92437	1210
1220	1.41386	2.80515	1.91338	1.46674	2.87746	1.91863	1.51838	2.94732	1.92335	1220
1230	1.40252	2.78953	1.91219	1.45524	2.86180	1.91753	1.50673	2.93162	1.92232	1230
1240	1.39131	2.77405	1.91100	1.44387	2.84628	1.91642	1.49521	2.91606	1.92128	1240
1250	1.38022	2.75871	1.90979	1.43262	2.83089	1.91530	1.48381	2.90064	1.92023	1250
1260	1.36925	2.74350	1.90858	1.42149	2.81563	1.91417	1.47254	2.88534	1.91918	1260
1270	1.35841	2.72841	1.90736	1.41049	2.80051	1.91303	1.46138	2.87017	1.91812	1270
1280	1.34768	2.71346	1.90613	1.39960	2.78551	1.91188	1.45035	2.85513	1.91705	1280
1290	1.33706	2.69863	1.90489	1.38883	2.77063	1.91073	1.43943	2.84022	1.91598	1290
1300	1.32657	2.68392	1.90364	1.37818	2.75588	1.90957	1.42863	2.82543	1.91489	1300
1310	1.31618	2.66934	1.90238	1.36764	2.74125	1.90840	1.41794	2.81076	1.91380	1310
1320	1.30591	2.65488	1.90112	1.35721	2.72675	1.90722	1.40737	2.79621	1.91270	1320
1330	1.29574	2.64054	1.89984	1.34689	2.71236	1.90604	1.39690	2.78178	1.91160	1330
1340	1.28568	2.62631	1.89856	1.33667	2.69808	1.90484	1.38654	2.76746	1.91048	1340
1350	1.27573	2.61220	1.89727	1.32657	2.68392	1.90364	1.37629	2.75326	1.90936	1350
1360	1.26588	2.59820	1.89597	1.31656	2.66988	1.90243	1.36614	2.73917	1.90823	1360
1370	1.25614	2.58432	1.89466	1.30666	2.65595	1.90121	1.35610	2.72520	1.90710	1370
1380	1.24649	2.57054	1.89335	1.29687	2.64212	1.89999	1.34615	2.71133	1.90595	1380
1390	1.23695	2.55688	1.89202	1.28717	2.62841	1.89875	1.33631	2.69757	1.90480	1390
1400	1.22750	2.54332	1.89069	1.27757	2.61480	1.89751	1.32657	2.68392	1.90364	1400
1410	1.21815	2.52987	1.88935	1.26806	2.60130	1.89626	1.31692	2.67038	1.90247	1410
1420	1.20890	2.51652	1.88800	1.25866	2.58791	1.89500	1.30737	2.65694	1.90130	1420
1430	1.19973	2.50327	1.88664	1.24934	2.57461	1.89374	1.29791	2.64360	1.90012	1430
1440	1.19066	2.49013	1.88527	1.24012	2.56142	1.89246	1.28855	2.63036	1.89893	1440
1450	1.18169	2.47709	1.88390	1.23099	2.54833	1.89118	1.27927	2.61723	1.89773	1450
1460	1.17280	2.46415	1.88251	1.22195	2.53533	1.88989	1.27009	2.60419	1.89653	1460
1470	1.16400	2.45130	1.88112	1.21300	2.52244	1.88860	1.26100	2.59125	1.89532	1470
1480	1.15528	2.43855	1.87972	1.20413	2.50964	1.88729	1.25199	2.57840	1.89410	1480
1490	1.14665	2.42590	1.87831	1.19536	2.49693	1.88598	1.24307	2.56565	1.89287	1490
1500	1.13811	2.41334	1.87689	1.18666	2.48432	1.88466	1.23424	2.55299	1.89164	1500
1510	1.12965	2.40087	1.87547	1.17805	2.47180	1.88333	1.22549	2.54043	1.89040	1510
1520	1.12127	2.38850	1.87404	1.16953	2.45938	1.88200	1.21682	2.52795	1.88915	1520
1530	1.11298	2.37621	1.87260	1.16108	2.44704	1.88065	1.20824	2.51557	1.88790	1530
1540	1.10476	2.36402	1.87115	1.15272	2.43479	1.87930	1.19973	2.50327	1.88664	1540
1550	1.09662	2.35191	1.86969	1.14443	2.42263	1.87794	1.19131	2.49107	1.88537	1550
1560	1.08856	2.33989	1.86822	1.13622	2.41056	1.87658	1.18296	2.47895	1.88409	1560
1570	1.08058	2.32796	1.86675	1.12809	2.39857	1.87521	1.17469	2.46691	1.88281	1570
1580	1.07267	2.31611	1.86527	1.12004	2.38667	1.87382	1.16650	2.45496	1.88152	1580
1590	1.06484	2.30435	1.86378	1.11206	2.37486	1.87244	1.15838	2.44309	1.88022	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
	T=2600.			T=2700.			T=2800.			
1600	1.05708	2.29267	1.86228	1.10415	2.36312	1.87104	1.15034	2.43131	1.87892	1600
1610	1.04939	2.28107	1.86078	1.09632	2.35147	1.86964	1.14237	2.41961	1.87760	1610
1620	1.04178	2.26955	1.85926	1.08856	2.33989	1.86822	1.13447	2.40799	1.87629	1620
1630	1.03423	2.25812	1.85774	1.08087	2.32840	1.86681	1.12665	2.39644	1.87496	1630
1640	1.02676	2.24676	1.85621	1.07325	2.31699	1.86538	1.11889	2.38498	1.87363	1640
1650	1.01936	2.23548	1.85468	1.06570	2.30565	1.86395	1.11121	2.37359	1.87229	1650
1660	1.01202	2.22428	1.85313	1.05822	2.29440	1.86251	1.10359	2.36229	1.87094	1660
1670	1.00475	2.21315	1.85158	1.05081	2.28321	1.86106	1.09604	2.35105	1.86959	1670
1680	0.99755	2.20210	1.85002	1.04346	2.27211	1.85960	1.08856	2.33989	1.86822	1680
1690	0.99041	2.19113	1.84845	1.03618	2.26107	1.85814	1.08115	2.32881	1.86686	1690
1700	0.98334	2.18023	1.84688	1.02897	2.25012	1.85667	1.07380	2.31780	1.86548	1700
1710	0.97633	2.16940	1.84529	1.02182	2.23923	1.85519	1.06651	2.30686	1.86410	1710
1720	0.96938	2.15865	1.84370	1.01473	2.22842	1.85371	1.05929	2.29600	1.86271	1720
1730	0.96250	2.14796	1.84211	1.00770	2.21768	1.85221	1.05213	2.28520	1.86132	1730
1740	0.95568	2.13735	1.84050	1.00074	2.20701	1.85072	1.04503	2.27448	1.85991	1740
1750	0.94892	2.12681	1.83889	0.99384	2.19640	1.84921	1.03800	2.26383	1.85850	1750
1760	0.94222	2.11633	1.83726	0.98700	2.18587	1.84770	1.03102	2.25324	1.85709	1760
1770	0.93557	2.10593	1.83564	0.98021	2.17541	1.84617	1.02411	2.24272	1.85567	1770
1780	0.92899	2.09559	1.83400	0.97349	2.16501	1.84465	1.01725	2.23227	1.85424	1780
1790	0.92247	2.08532	1.83236	0.96683	2.15468	1.84311	1.01046	2.22189	1.85280	1790
1800	0.91600	2.07512	1.83071	0.96022	2.14442	1.84157	1.00372	2.21157	1.85136	1800
1810	0.90959	2.06498	1.82905	0.95367	2.13422	1.84002	0.99704	2.20132	1.84991	1810
1820	0.90323	2.05491	1.82738	0.94717	2.12408	1.83847	0.99041	2.19113	1.84845	1820
1830	0.89693	2.04490	1.82571	0.94074	2.11401	1.83690	0.98384	2.18100	1.84699	1830
1840	0.89069	2.03495	1.82403	0.93435	2.10401	1.83533	0.97733	2.17094	1.84552	1840
1850	0.88449	2.02507	1.82234	0.92802	2.09407	1.83376	0.97087	2.16094	1.84405	1850
1860	0.87835	2.01525	1.82064	0.92175	2.08418	1.83217	0.96446	2.15101	1.84256	1860
1870	0.87227	2.00549	1.81894	0.91552	2.07436	1.83058	0.95811	2.14113	1.84107	1870
1880	0.86623	1.99580	1.81723	0.90935	2.06461	1.82899	0.95181	2.13132	1.83958	1880
1890	0.86025	1.98616	1.81552	0.90323	2.05491	1.82738	0.94556	2.12156	1.83808	1890
1900	0.85432	1.97659	1.81379	0.89716	2.04527	1.82577	0.93936	2.11187	1.83657	1900
1910	0.84844	1.96707	1.81206	0.89115	2.03569	1.82415	0.93322	2.10223	1.83505	1910
1920	0.84261	1.95761	1.81032	0.88518	2.02617	1.82253	0.92712	2.09265	1.83353	1920
1930	0.83682	1.94821	1.80858	0.87926	2.01670	1.82090	0.92108	2.08313	1.83200	1930
1940	0.83109	1.93887	1.80683	0.87339	2.00730	1.81926	0.91508	2.07367	1.83047	1940
1950	0.82540	1.92958	1.80507	0.86757	1.99795	1.81761	0.90913	2.06426	1.82893	1950
1960	0.81976	1.92036	1.80330	0.86180	1.98865	1.81596	0.90323	2.05491	1.82738	1960
1970	0.81417	1.91118	1.80153	0.85607	1.97942	1.81430	0.89738	2.04561	1.82583	1970
1980	0.80863	1.90207	1.79975	0.85039	1.97024	1.81264	0.89157	2.03637	1.82427	1980
1990	0.80313	1.89300	1.79796	0.84476	1.96111	1.81097	0.88582	2.02718	1.82270	1990
2000	0.79767	1.88400	1.79617	0.83917	1.95203	1.80929	0.88010	2.01805	1.82113	2000
2010	0.79226	1.87504	1.79437	0.83363	1.94301	1.80761	0.87444	2.00897	1.81955	2010
2020	0.78690	1.86614	1.79256	0.82813	1.93405	1.80592	0.86881	1.99995	1.81797	2020
2030	0.78158	1.85729	1.79075	0.82268	1.92513	1.80422	0.86324	1.99097	1.81638	2030
2040	0.77630	1.84850	1.78893	0.81727	1.91627	1.80251	0.85770	1.98205	1.81478	2040
2050	0.77107	1.83976	1.78710	0.81191	1.90746	1.80080	0.85221	1.97318	1.81318	2050
2060	0.76587	1.83106	1.78526	0.80658	1.89870	1.79909	0.84677	1.96426	1.81157	2060
2070	0.76072	1.82242	1.78342	0.80130	1.89000	1.79736	0.84136	1.95559	1.80995	2070
2080	0.75562	1.81383	1.78157	0.79607	1.88134	1.79564	0.83600	1.94687	1.80833	2080
2090	0.75055	1.80529	1.77972	0.79087	1.87273	1.79390	0.83068	1.93820	1.80670	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}	
T=2600.			T=2700.			T=2800.					
2100	0.74552	1.79680	1.77786	0.78571	1.86417	1.79216	0.82540	1.92958	1.80507	2100	
2110	0.74054	1.78836	1.77599	0.78060	1.85566	1.79041	0.82017	1.92101	1.80343	2110	
2120	0.73559	1.77997	1.77412	0.77552	1.84720	1.78865	0.81497	1.91249	1.80178	2120	
2130	0.73068	1.77162	1.77224	0.77049	1.83879	1.78689	0.80981	1.90402	1.80013	2130	
2140	0.72582	1.76333	1.77035	0.76549	1.83042	1.78513	0.80469	1.89559	1.79847	2140	
2150	0.72099	1.75508	1.76846	0.76053	1.82210	1.78335	0.79962	1.88721	1.79681	2150	
2160	0.71620	1.74688	1.76656	0.75562	1.81383	1.78157	0.79458	1.87887	1.79514	2160	
2170	0.71144	1.73872	1.76465	0.75074	1.80561	1.77979	0.78958	1.87059	1.79346	2170	
2180	0.70673	1.73061	1.76274	0.74589	1.79743	1.77800	0.78461	1.86234	1.79178	2180	
2190	0.70205	1.72255	1.76082	0.74109	1.78930	1.77620	0.77969	1.85415	1.79010	2190	
2200	0.69741	1.71453	1.75890	0.73632	1.78121	1.77440	0.77480	1.84600	1.78840	2200	
2210	0.69280	1.70656	1.75697	0.73159	1.77316	1.77259	0.76995	1.83789	1.78671	2210	
2220	0.68823	1.69863	1.75503	0.72689	1.76517	1.77077	0.76514	1.82983	1.78500	2220	
2230	0.68370	1.69075	1.75309	0.72224	1.75721	1.76895	0.76036	1.82181	1.78329	2230	
2240	0.67920	1.68291	1.75114	0.71761	1.74930	1.76712	0.75562	1.81383	1.78157	2240	
2250	0.67474	1.67511	1.74918	0.71302	1.74143	1.76529	0.75091	1.80590	1.77985	2250	
2260	0.67031	1.66736	1.74722	0.70847	1.73361	1.76345	0.74624	1.79801	1.77813	2260	
2270	0.66592	1.65965	1.74525	0.70395	1.72583	1.76161	0.74160	1.79016	1.77639	2270	
2280	0.66155	1.65198	1.74328	0.69947	1.71809	1.75975	0.73700	1.78236	1.77465	2280	
2290	0.65723	1.64436	1.74130	0.69502	1.71039	1.75790	0.73243	1.77460	1.77291	2290	
2300	0.65293	1.63677	1.73931	0.69060	1.70273	1.75604	0.72790	1.76688	1.77116	2300	
2310	0.64867	1.62923	1.73732	0.68622	1.69512	1.75417	0.72340	1.75920	1.76941	2310	
2320	0.64444	1.62173	1.73532	0.68186	1.68755	1.75229	0.71893	1.75156	1.76765	2320	
2330	0.64025	1.61427	1.73332	0.67755	1.68001	1.75041	0.71449	1.74396	1.76588	2330	
2340	0.63608	1.60685	1.73131	0.67326	1.67252	1.74853	0.71009	1.73640	1.76411	2340	
2350	0.63195	1.59947	1.72930	0.66900	1.66507	1.74664	0.70572	1.72888	1.76233	2350	
2360	0.62785	1.59214	1.72728	0.66478	1.65766	1.74474	0.70138	1.72140	1.76055	2360	
2370	0.62378	1.58484	1.72525	0.66059	1.65028	1.74284	0.69708	1.71396	1.75876	2370	
2380	0.61974	1.57758	1.72322	0.65643	1.64295	1.74093	0.69280	1.70656	1.75697	2380	
2390	0.61573	1.57036	1.72118	0.65230	1.63565	1.73902	0.68856	1.69919	1.75517	2390	
2400	0.61175	1.56317	1.71913	0.64820	1.62840	1.73710	0.68435	1.69187	1.75336	2400	
2410	0.60780	1.55603	1.71709	0.64413	1.62118	1.73518	0.68016	1.68458	1.75156	2410	
2420	0.60388	1.54892	1.71503	0.64009	1.61400	1.73325	0.67601	1.67733	1.74974	2420	
2430	0.59999	1.54186	1.71297	0.63608	1.60685	1.73131	0.67189	1.67012	1.74792	2430	
2440	0.59613	1.53483	1.71090	0.63210	1.59975	1.72937	0.66779	1.66295	1.74610	2440	
2450	0.59230	1.52783	1.70883	0.62815	1.59268	1.72742	0.66373	1.65581	1.74427	2450	
2460	0.58849	1.52088	1.70676	0.62423	1.58565	1.72547	0.65970	1.64871	1.74243	2460	
2470	0.58471	1.51396	1.70467	0.62033	1.57865	1.72352	0.65569	1.64164	1.74059	2470	
2480	0.58097	1.50707	1.70259	0.61647	1.57169	1.72156	0.65171	1.63461	1.73874	2480	
2490	0.57725	1.50023	1.70049	0.61263	1.56477	1.71959	0.64776	1.62762	1.73689	2490	
2500	0.57355	1.49341	1.69839	0.60882	1.55788	1.71762	0.64384	1.62066	1.73504	2500	
2510	0.56989	1.48664	1.69629	0.60504	1.55103	1.71564	0.63995	1.61374	1.73318	2510	
2520	0.56625	1.47990	1.69418	0.60128	1.54421	1.71366	0.63608	1.60685	1.73131	2520	
2530	0.56264	1.47319	1.69207	0.59755	1.53742	1.71167	0.63224	1.60000	1.72944	2530	
2540	0.55905	1.46652	1.68995	0.59385	1.53068	1.70968	0.62843	1.59318	1.72756	2540	
2550	0.55549	1.45989	1.68782	0.59018	1.52396	1.70768	0.62465	1.58640	1.72568	2550	
2560	0.55196	1.45328	1.68569	0.58653	1.51728	1.70568	0.62089	1.57965	1.72380	2560	
2570	0.54845	1.44672	1.68356	0.58291	1.51064	1.70367	0.61716	1.57293	1.72191	2570	
2580	0.54497	1.44018	1.68142	0.57931	1.50402	1.70166	0.61345	1.56625	1.72001	2580	
2590	0.54151	1.43368	1.67928	0.57574	1.49745	1.69964	0.60977	1.55960	1.71811	2590	

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$T=2600.$			$T=2700.$			$T=2800.$			ν cm ⁻¹
	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	
2600	0.53808	1.42721	1.67713	0.57219	1.49090	1.69762	0.60612	1.55298	1.71621	2600
2610	0.53467	1.42078	1.67497	0.56867	1.48439	1.69559	0.60249	1.54640	1.71430	2610
2620	0.53129	1.41438	1.67281	0.56518	1.47791	1.69356	0.59888	1.53984	1.71238	2620
2630	0.52793	1.40801	1.67065	0.56170	1.47146	1.69152	0.59530	1.53332	1.71046	2630
2640	0.52459	1.40167	1.66848	0.55826	1.46504	1.68948	0.59175	1.52684	1.70854	2640
2650	0.52128	1.39537	1.66630	0.55483	1.45866	1.68743	0.58822	1.52038	1.70661	2650
2660	0.51800	1.38910	1.66412	0.55144	1.45231	1.68538	0.58471	1.51396	1.70467	2660
2670	0.51473	1.38286	1.66194	0.54806	1.44599	1.68332	0.58123	1.50756	1.70274	2670
2680	0.51149	1.37665	1.65975	0.54471	1.43970	1.68126	0.57778	1.50120	1.70079	2680
2690	0.50828	1.37047	1.65756	0.54138	1.43344	1.67920	0.57434	1.49487	1.69884	2690
2700	0.50508	1.36433	1.65536	0.53808	1.42721	1.67713	0.57093	1.48857	1.69689	2700
2710	0.50191	1.35821	1.65316	0.53480	1.42102	1.67505	0.56754	1.48230	1.69494	2710
2720	0.49876	1.35213	1.65095	0.53154	1.41485	1.67297	0.56418	1.47606	1.69297	2720
2730	0.49564	1.34607	1.64874	0.52830	1.40872	1.67089	0.56084	1.46985	1.69101	2730
2740	0.49253	1.34005	1.64652	0.52509	1.40261	1.66880	0.55752	1.46367	1.68904	2740
2750	0.48945	1.33405	1.64430	0.52189	1.39654	1.66670	0.55423	1.45752	1.68706	2750
2760	0.48639	1.32809	1.64207	0.51873	1.39049	1.66461	0.55095	1.45140	1.68509	2760
2770	0.48335	1.32215	1.63984	0.51558	1.38447	1.66251	0.54770	1.44531	1.68310	2770
2780	0.48033	1.31625	1.63761	0.51245	1.37849	1.66040	0.54447	1.43925	1.68111	2780
2790	0.47734	1.31037	1.63537	0.50935	1.37253	1.65829	0.54126	1.43322	1.67912	2790
2800	0.47436	1.30452	1.63312	0.50626	1.36660	1.65617	0.53808	1.42721	1.67713	2800
2810	0.47141	1.29871	1.63088	0.50320	1.36070	1.65405	0.53491	1.42124	1.67512	2810
2820	0.46847	1.29292	1.62863	0.50016	1.35483	1.65193	0.53177	1.41529	1.67312	2820
2830	0.46556	1.28716	1.62637	0.49714	1.34898	1.64980	0.52865	1.40937	1.67111	2830
2840	0.46267	1.28142	1.62411	0.49414	1.34317	1.64767	0.52554	1.40348	1.66910	2840
2850	0.45980	1.27572	1.62184	0.49116	1.33738	1.64553	0.52246	1.39762	1.66708	2850
2860	0.45694	1.27004	1.61957	0.48820	1.33162	1.64339	0.51940	1.39178	1.66506	2860
2870	0.45411	1.26439	1.61730	0.48526	1.32589	1.64125	0.51636	1.38597	1.66303	2870
2880	0.45130	1.25877	1.61502	0.48234	1.32018	1.63910	0.51334	1.38019	1.66100	2880
2890	0.44850	1.25318	1.61274	0.47944	1.31450	1.63694	0.51034	1.37444	1.65897	2890
2900	0.44573	1.24761	1.61046	0.47657	1.30885	1.63479	0.50736	1.36871	1.65693	2900
2910	0.44297	1.24207	1.60817	0.47370	1.30323	1.63263	0.50440	1.36301	1.65489	2910
2920	0.44024	1.23656	1.60588	0.47086	1.29763	1.63046	0.50146	1.35734	1.65284	2920
2930	0.43752	1.23107	1.60358	0.46804	1.29206	1.62829	0.49854	1.35169	1.65079	2930
2940	0.43482	1.22561	1.60128	0.46524	1.28652	1.62612	0.49564	1.34607	1.64874	2940
2950	0.43214	1.22018	1.59897	0.46245	1.28100	1.62394	0.49275	1.34048	1.64668	2950
2960	0.42948	1.21477	1.59666	0.45969	1.27551	1.62176	0.48989	1.33491	1.64462	2960
2970	0.42683	1.20939	1.59435	0.45694	1.27004	1.61957	0.48705	1.32936	1.64255	2970
2980	0.42421	1.20403	1.59203	0.45421	1.26460	1.61739	0.48422	1.32385	1.64048	2980
2990	0.42160	1.19870	1.58971	0.45150	1.25919	1.61519	0.48141	1.31835	1.63841	2990
3000	0.41901	1.19340	1.58739	0.44881	1.25380	1.61300	0.47862	1.31289	1.63633	3000
3010	0.41644	1.18812	1.58506	0.44614	1.24843	1.61080	0.47585	1.30744	1.63425	3010
3020	0.41388	1.18287	1.58273	0.44348	1.24309	1.60859	0.47309	1.30203	1.63216	3020
3030	0.41134	1.17764	1.58040	0.44084	1.23778	1.60639	0.47036	1.29664	1.63007	3030
3040	0.40882	1.17244	1.57806	0.43822	1.23249	1.60417	0.46764	1.29127	1.62798	3040
3050	0.40632	1.16726	1.57572	0.43562	1.22723	1.60196	0.46494	1.28592	1.62588	3050
3060	0.40383	1.16210	1.57337	0.43303	1.22199	1.59974	0.46226	1.28061	1.62379	3060
3070	0.40136	1.15698	1.57102	0.43046	1.21677	1.59752	0.45959	1.27531	1.62168	3070
3080	0.39891	1.15187	1.56867	0.42791	1.21158	1.59529	0.45694	1.27004	1.61957	3080
3090	0.39647	1.14679	1.56631	0.42537	1.20641	1.59306	0.45431	1.26480	1.61746	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	$-(F^\circ-E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
	T=2600.			T=2700.			T=2800.			
3100	0.39405	1.14173	1.56395	0.42285	1.20127	1.59083	0.45170	1.25957	1.61535	3100
3110	0.39165	1.13670	1.56159	0.42035	1.19615	1.58860	0.44910	1.25437	1.61323	3110
3120	0.38926	1.13169	1.55922	0.41786	1.19105	1.58636	0.44652	1.24920	1.61111	3120
3130	0.38689	1.12670	1.55686	0.41539	1.18598	1.58411	0.44395	1.24405	1.60899	3130
3140	0.38453	1.12174	1.55448	0.41294	1.18093	1.58187	0.44141	1.23892	1.60686	3140
3150	0.38219	1.11680	1.55211	0.41050	1.17590	1.57962	0.43887	1.23381	1.60473	3150
3160	0.37987	1.11189	1.54973	0.40808	1.17090	1.57736	0.43636	1.22873	1.60259	3160
3170	0.37756	1.10699	1.54735	0.40567	1.16592	1.57511	0.43386	1.22367	1.60045	3170
3180	0.37527	1.10212	1.54496	0.40328	1.16096	1.57285	0.43138	1.21863	1.59831	3180
3190	0.37299	1.09728	1.54257	0.40091	1.15603	1.57059	0.42891	1.21362	1.59617	3190
3200	0.37073	1.09245	1.54018	0.39855	1.15112	1.56832	0.42646	1.20862	1.59402	3200
3210	0.36848	1.08765	1.53779	0.39620	1.14623	1.56605	0.42402	1.20365	1.59187	3210
3220	0.36625	1.08287	1.53539	0.39387	1.14136	1.56378	0.42160	1.19870	1.58971	3220
3230	0.36403	1.07811	1.53299	0.39156	1.13651	1.56150	0.41919	1.19378	1.58756	3230
3240	0.36182	1.07338	1.53058	0.38926	1.13169	1.55922	0.41680	1.18887	1.58540	3240
3250	0.35964	1.06867	1.52818	0.38698	1.12689	1.55694	0.41443	1.18399	1.58323	3250
3260	0.35746	1.06398	1.52577	0.38471	1.12211	1.55466	0.41207	1.17913	1.58106	3260
3270	0.35530	1.05931	1.52335	0.38245	1.11735	1.55237	0.40972	1.17429	1.57889	3270
3280	0.35316	1.05466	1.52094	0.38021	1.11261	1.55008	0.40739	1.16947	1.57672	3280
3290	0.35102	1.05003	1.51852	0.37799	1.10790	1.54779	0.40507	1.16468	1.57454	3290
3300	0.34891	1.04543	1.51610	0.37578	1.10320	1.54549	0.40277	1.15990	1.57236	3300
3310	0.34680	1.04084	1.51368	0.37358	1.09853	1.54319	0.40048	1.15515	1.57018	3310
3320	0.34471	1.03628	1.51125	0.37140	1.09388	1.54089	0.39821	1.15042	1.56800	3320
3330	0.34264	1.03174	1.50882	0.36923	1.08925	1.53858	0.39595	1.14570	1.56581	3330
3340	0.34057	1.02722	1.50639	0.36707	1.08464	1.53628	0.39371	1.14101	1.56362	3340
3350	0.33852	1.02272	1.50396	0.36493	1.08005	1.53397	0.39148	1.13634	1.56142	3350
3360	0.33649	1.01824	1.50152	0.36280	1.07548	1.53165	0.38926	1.13169	1.55922	3360
3370	0.33447	1.01378	1.49908	0.36069	1.07093	1.52934	0.38706	1.12706	1.55702	3370
3380	0.33246	1.00934	1.49664	0.35859	1.06640	1.52702	0.38487	1.12245	1.55482	3380
3390	0.33046	1.00493	1.49420	0.35650	1.06190	1.52470	0.38269	1.11786	1.55262	3390
3400	0.32848	1.00053	1.49175	0.35443	1.05741	1.52237	0.38053	1.11329	1.55041	3400
3410	0.32651	0.99615	1.48930	0.35236	1.05294	1.52004	0.37838	1.10874	1.54820	3410
3420	0.32455	0.99179	1.48685	0.35032	1.04849	1.51772	0.37625	1.10421	1.54598	3420
3430	0.32261	0.98746	1.48440	0.34828	1.04407	1.51538	0.37413	1.09970	1.54377	3430
3440	0.32067	0.98314	1.48194	0.34626	1.03966	1.51305	0.37202	1.09521	1.54155	3440
3450	0.31875	0.97884	1.47948	0.34425	1.03527	1.51071	0.36992	1.09074	1.53932	3450
3460	0.31685	0.97456	1.47702	0.34225	1.03090	1.50837	0.36784	1.08628	1.53710	3460
3470	0.31495	0.97030	1.47456	0.34027	1.02655	1.50603	0.36577	1.08185	1.53487	3470
3480	0.31307	0.96606	1.47209	0.33830	1.02222	1.50369	0.36371	1.07744	1.53264	3480
3490	0.31120	0.96184	1.46963	0.33634	1.01791	1.50134	0.36167	1.07304	1.53041	3490
3500	0.30934	0.95764	1.46716	0.33439	1.01362	1.49899	0.35964	1.06867	1.52818	3500
3510	0.30750	0.95346	1.46468	0.33246	1.00934	1.49664	0.35762	1.06431	1.52594	3510
3520	0.30566	0.94929	1.46221	0.33054	1.00509	1.49429	0.35561	1.05997	1.52370	3520
3530	0.30384	0.94515	1.45974	0.32862	1.00085	1.49193	0.35361	1.05565	1.52146	3530
3540	0.30203	0.94102	1.45726	0.32673	0.99664	1.48957	0.35163	1.05135	1.51921	3540
3550	0.30023	0.93692	1.45478	0.32484	0.99244	1.48721	0.34966	1.04707	1.51697	3550
3560	0.29844	0.93283	1.45230	0.32297	0.98826	1.48485	0.34770	1.04281	1.51472	3560
3570	0.29666	0.92876	1.44981	0.32110	0.98410	1.48249	0.34576	1.03856	1.51247	3570
3580	0.29490	0.92471	1.44733	0.31925	0.97995	1.48012	0.34382	1.03433	1.51021	3580
3590	0.29315	0.92067	1.44484	0.31741	0.97583	1.47775	0.34190	1.03012	1.50795	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
T=2600.			T=2700.			T=2800.				
3600	0.29140	0.91666	1.44235	0.31558	0.97172	1.47538	0.33999	1.02593	1.50570	3600
3610	0.28967	0.91266	1.43986	0.31377	0.96763	1.47301	0.33809	1.02176	1.50344	3610
3620	0.28795	0.90868	1.43737	0.31196	0.96356	1.47063	0.33620	1.01760	1.50117	3620
3630	0.28624	0.90472	1.43487	0.31017	0.95950	1.46825	0.33432	1.01346	1.49891	3630
3640	0.28454	0.90077	1.43238	0.30838	0.95547	1.46588	0.33246	1.00934	1.49664	3640
3650	0.28286	0.89685	1.42988	0.30661	0.95145	1.46349	0.33060	1.00524	1.49437	3650
3660	0.28118	0.89294	1.42738	0.30485	0.94745	1.46111	0.32876	1.00115	1.49210	3660
3670	0.27951	0.88905	1.42488	0.30310	0.94347	1.45873	0.32693	0.99709	1.48983	3670
3680	0.27786	0.88517	1.42238	0.30136	0.93950	1.45634	0.32511	0.99304	1.48755	3680
3690	0.27621	0.88132	1.41987	0.29963	0.93555	1.45395	0.32330	0.98900	1.48527	3690
3700	0.27458	0.87748	1.41737	0.29791	0.93162	1.45156	0.32150	0.98499	1.48299	3700
3710	0.27295	0.87366	1.41486	0.29621	0.92771	1.44917	0.31971	0.98099	1.48071	3710
3720	0.27134	0.86985	1.41235	0.29451	0.92381	1.44678	0.31794	0.97700	1.47843	3720
3730	0.26974	0.86606	1.40984	0.29282	0.91993	1.44438	0.31617	0.97304	1.47614	3730
3740	0.26814	0.86229	1.40733	0.29115	0.91606	1.44198	0.31441	0.96909	1.47385	3740
3750	0.26656	0.85854	1.40482	0.28948	0.91222	1.43958	0.31267	0.96516	1.47156	3750
3760	0.26499	0.85480	1.40230	0.28782	0.90838	1.43718	0.31093	0.96124	1.46927	3760
3770	0.26342	0.85108	1.39979	0.28618	0.90457	1.43478	0.30921	0.95734	1.46698	3770
3780	0.26187	0.84737	1.39727	0.28454	0.90077	1.43238	0.30750	0.95346	1.46468	3780
3790	0.26032	0.84368	1.39475	0.28292	0.89699	1.42997	0.30579	0.94959	1.46239	3790
3800	0.25879	0.84001	1.39223	0.28130	0.89323	1.42757	0.30410	0.94574	1.46009	3800
3810	0.25726	0.83636	1.38971	0.27970	0.88948	1.42516	0.30241	0.94191	1.45779	3810
3820	0.25575	0.83272	1.38719	0.27810	0.88575	1.42275	0.30074	0.93809	1.45549	3820
3830	0.25424	0.82909	1.38467	0.27652	0.88203	1.42034	0.29908	0.93429	1.45318	3830
3840	0.25275	0.82549	1.38214	0.27494	0.87833	1.41792	0.29742	0.93050	1.45088	3840
3850	0.25126	0.82189	1.37962	0.27337	0.87464	1.41551	0.29578	0.92673	1.44857	3850
3860	0.24978	0.81832	1.37709	0.27182	0.87098	1.41309	0.29415	0.92297	1.44626	3860
3870	0.24831	0.81476	1.37456	0.27027	0.86732	1.41068	0.29252	0.91924	1.44395	3870
3880	0.24686	0.81122	1.37203	0.26873	0.86369	1.40826	0.29091	0.91551	1.44164	3880
3890	0.24541	0.80769	1.36951	0.26720	0.86006	1.40584	0.28930	0.91180	1.43933	3890
3900	0.24396	0.80417	1.36698	0.26568	0.85646	1.40342	0.28771	0.90811	1.43701	3900
3910	0.24253	0.80068	1.36444	0.26417	0.85287	1.40100	0.28612	0.90443	1.43470	3910
3920	0.24111	0.79720	1.36191	0.26267	0.84929	1.39857	0.28454	0.90077	1.43238	3920
3930	0.23970	0.79373	1.35938	0.26118	0.84573	1.39615	0.28298	0.89713	1.43006	3930
3940	0.23829	0.79028	1.35685	0.25970	0.84219	1.39372	0.28142	0.89350	1.42774	3940
3950	0.23689	0.78684	1.35431	0.25822	0.83866	1.39130	0.27987	0.88988	1.42542	3950
3960	0.23551	0.78342	1.35178	0.25676	0.83514	1.38887	0.27833	0.88628	1.42309	3960
3970	0.23413	0.78001	1.34924	0.25530	0.83164	1.38644	0.27680	0.88269	1.42077	3970
3980	0.23276	0.77662	1.34670	0.25385	0.82816	1.38401	0.27528	0.87912	1.41844	3980
3990	0.23139	0.77325	1.34416	0.25242	0.82469	1.38158	0.27376	0.87556	1.41611	3990
4000	0.23004	0.76989	1.34163	0.25099	0.82123	1.37915	0.27226	0.87202	1.41378	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=2900.			T=3000.			T=3100.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
100	6.01753	7.95581	1.98676	6.08327	8.02317	1.98679	6.14690	8.08831	1.98681	100
110	5.83302	7.76646	1.98668	5.89860	7.83381	1.98671	5.96208	7.89895	1.98674	110
120	5.66499	7.59360	1.98658	5.73041	7.66095	1.98662	5.79374	7.72609	1.98666	120
130	5.51082	7.43459	1.98648	5.57607	7.50194	1.98653	5.63925	7.56707	1.98657	130
140	5.36842	7.28738	1.98637	5.43352	7.35472	1.98642	5.49655	7.41986	1.98647	140
150	5.23619	7.15034	1.98625	5.30113	7.21768	1.98631	5.36401	7.28281	1.98637	150
160	5.11281	7.02215	1.98613	5.17759	7.08949	1.98620	5.24032	7.15461	1.98626	160
170	4.99720	6.90175	1.98599	5.06182	6.96908	1.98607	5.12440	7.03420	1.98614	170
180	4.88848	6.78824	1.98585	4.95293	6.85556	1.98594	5.01536	6.92068	1.98601	180
190	4.78589	6.68087	1.98570	4.85019	6.74819	1.98579	4.91247	6.81331	1.98588	190
200	4.68881	6.57902	1.98554	4.75295	6.64634	1.98565	4.81508	6.71145	1.98574	200
210	4.59670	6.48215	1.98537	4.66068	6.54946	1.98549	4.72266	6.61457	1.98560	210
220	4.50910	6.38980	1.98520	4.57292	6.45710	1.98533	4.63476	6.52220	1.98544	220
230	4.42561	6.30155	1.98501	4.48927	6.36885	1.98516	4.55095	6.43395	1.98528	230
240	4.34587	6.21708	1.98482	4.40937	6.28437	1.98498	4.47091	6.34946	1.98512	240
250	4.26958	6.13606	1.98462	4.33292	6.20334	1.98479	4.39431	6.26842	1.98494	250
260	4.19647	6.05822	1.98442	4.25965	6.12550	1.98460	4.32090	6.19058	1.98476	260
270	4.12629	5.98333	1.98420	4.18932	6.05060	1.98440	4.25042	6.11567	1.98457	270
280	4.05884	5.91118	1.98398	4.12171	5.97844	1.98419	4.18266	6.04350	1.98438	280
290	3.99392	5.84156	1.98375	4.05664	5.90882	1.98397	4.11744	5.97387	1.98417	290
300	3.93136	5.77431	1.98351	3.99392	5.84156	1.98375	4.05458	5.90661	1.98396	300
310	3.87101	5.70928	1.98326	3.93341	5.77652	1.98351	3.99392	5.84156	1.98375	310
320	3.81272	5.64632	1.98300	3.87497	5.71355	1.98327	3.93533	5.77858	1.98352	320
330	3.75637	5.58530	1.98274	3.81846	5.65252	1.98303	3.87868	5.71755	1.98329	330
340	3.70184	5.52611	1.98246	3.76377	5.59333	1.98277	3.82385	5.65835	1.98305	340
350	3.64902	5.46865	1.98218	3.71080	5.53585	1.98251	3.77073	5.60087	1.98281	350
360	3.59783	5.41281	1.98190	3.65945	5.48001	1.98224	3.71924	5.54501	1.98255	360
370	3.54816	5.35852	1.98160	3.60963	5.42570	1.98196	3.66927	5.49070	1.98229	370
380	3.49994	5.30567	1.98129	3.56126	5.37285	1.98168	3.62075	5.43783	1.98203	380
390	3.45310	5.25421	1.98098	3.51426	5.32138	1.98139	3.57361	5.38635	1.98175	390
400	3.40756	5.20406	1.98066	3.46857	5.27122	1.98109	3.52777	5.33618	1.98147	400
410	3.36325	5.15516	1.98033	3.42411	5.22230	1.98078	3.48317	5.28726	1.98118	410
420	3.32013	5.10744	1.97999	3.38083	5.17458	1.98046	3.43975	5.23952	1.98089	420
430	3.27813	5.06086	1.97965	3.33867	5.12798	1.98014	3.39745	5.19291	1.98059	430
440	3.23719	5.01535	1.97930	3.29759	5.08246	1.97981	3.35622	5.14738	1.98028	440
450	3.19728	4.97087	1.97894	3.25753	5.03797	1.97947	3.31602	5.10289	1.97996	450
460	3.15835	4.92738	1.97857	3.21845	4.99447	1.97913	3.27679	5.05937	1.97964	460
470	3.12036	4.88483	1.97819	3.18030	4.95191	1.97878	3.23850	5.01680	1.97931	470
480	3.08326	4.84319	1.97780	3.14304	4.91025	1.97842	3.20110	4.97513	1.97897	480
490	3.04701	4.80241	1.97741	3.10665	4.86946	1.97805	3.16457	4.93433	1.97863	490
500	3.01160	4.76247	1.97701	3.07108	4.82950	1.97767	3.12886	4.89436	1.97828	500
510	2.97697	4.72332	1.97660	3.03630	4.79034	1.97729	3.09394	4.85519	1.97792	510
520	2.94310	4.68494	1.97618	3.00229	4.75195	1.97690	3.05978	4.81679	1.97755	520
530	2.90997	4.64731	1.97576	2.96900	4.71430	1.97650	3.02635	4.77912	1.97718	530
540	2.87753	4.61038	1.97533	2.93642	4.67736	1.97610	2.99363	4.74217	1.97680	540
550	2.84578	4.57414	1.97489	2.90451	4.64110	1.97569	2.96158	4.70590	1.97641	550
560	2.81468	4.53856	1.97444	2.87326	4.60551	1.97527	2.93019	4.67029	1.97602	560
570	2.78420	4.50361	1.97398	2.84264	4.57055	1.97484	2.89943	4.63532	1.97562	570
580	2.75434	4.46929	1.97351	2.81262	4.53621	1.97441	2.86927	4.60096	1.97521	580
590	2.72506	4.43556	1.97304	2.78320	4.50246	1.97396	2.83971	4.56720	1.97480	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹	
T=2900.			T=3000.			T=3100.					
600	2.69635	4.40240	1.97256	2.75434	4.46929	1.97351	2.81071	4.53401	1.97438	600	
610	2.66819	4.36980	1.97207	2.72603	4.43667	1.97306	2.78226	4.50138	1.97395	610	
620	2.64055	4.33773	1.97157	2.69825	4.40459	1.97259	2.75434	4.46929	1.97351	620	
630	2.61343	4.30619	1.97107	2.67098	4.37303	1.97212	2.72693	4.43771	1.97307	630	
640	2.58681	4.27516	1.97056	2.64421	4.34198	1.97164	2.70002	4.40665	1.97262	640	
650	2.56067	4.24461	1.97004	2.61792	4.31141	1.97115	2.67359	4.37606	1.97217	650	
660	2.53499	4.21453	1.96951	2.59209	4.28132	1.97066	2.64763	4.34596	1.97170	660	
670	2.50977	4.18492	1.96897	2.56672	4.25169	1.97016	2.62213	4.31631	1.97123	670	
680	2.48498	4.15575	1.96843	2.54179	4.22251	1.96965	2.59706	4.28711	1.97076	680	
690	2.46062	4.12702	1.96788	2.51729	4.19376	1.96913	2.57241	4.25834	1.97027	690	
700	2.43668	4.09871	1.96732	2.49319	4.16543	1.96861	2.54818	4.23000	1.96978	700	
710	2.41313	4.07081	1.96675	2.46950	4.13751	1.96808	2.52436	4.20206	1.96928	710	
720	2.38998	4.04331	1.96617	2.44621	4.10999	1.96754	2.50092	4.17452	1.96878	720	
730	2.36720	4.01619	1.96559	2.42329	4.08285	1.96700	2.47787	4.14737	1.96827	730	
740	2.34480	3.98945	1.96500	2.40073	4.05609	1.96644	2.45518	4.12059	1.96775	740	
750	2.32275	3.96308	1.96440	2.37854	4.02970	1.96588	2.43285	4.09418	1.96723	750	
760	2.30105	3.93706	1.96379	2.35670	4.00366	1.96531	2.41087	4.06813	1.96669	760	
770	2.27969	3.91140	1.96318	2.33520	3.97798	1.96474	2.38924	4.04242	1.96615	770	
780	2.25867	3.88607	1.96255	2.31403	3.95263	1.96416	2.36793	4.01706	1.96561	780	
790	2.23796	3.86107	1.96192	2.29318	3.92761	1.96357	2.34695	3.99202	1.96506	790	
800	2.21757	3.83640	1.96129	2.27265	3.90292	1.96297	2.32628	3.96731	1.96450	800	
810	2.19749	3.81204	1.96064	2.25242	3.87854	1.96237	2.30592	3.94291	1.96393	810	
820	2.17770	3.78798	1.95999	2.23249	3.85446	1.96175	2.28586	3.91881	1.96336	820	
830	2.15821	3.76423	1.95933	2.21286	3.83069	1.96114	2.26609	3.89502	1.96278	830	
840	2.13900	3.74077	1.95866	2.19351	3.80720	1.96051	2.24661	3.87151	1.96219	840	
850	2.12007	3.71759	1.95798	2.17443	3.78400	1.95988	2.22740	3.84830	1.96160	850	
860	2.10141	3.69470	1.95729	2.15563	3.76108	1.95924	2.20846	3.82536	1.96100	860	
870	2.08302	3.67207	1.95660	2.13710	3.73844	1.95859	2.18979	3.80269	1.96039	870	
880	2.06488	3.64971	1.95590	2.11882	3.71606	1.95793	2.17138	3.78029	1.95977	880	
890	2.04699	3.62762	1.95519	2.10079	3.69394	1.95727	2.15323	3.75815	1.95915	890	
900	2.02936	3.60578	1.95448	2.08302	3.67207	1.95660	2.13532	3.73626	1.95853	900	
910	2.01196	3.58418	1.95376	2.06548	3.65046	1.95593	2.11765	3.71462	1.95789	910	
920	1.99480	3.56283	1.95303	2.04818	3.62908	1.95524	2.10022	3.69323	1.95725	920	
930	1.97787	3.54172	1.95229	2.03111	3.60795	1.95455	2.08302	3.67207	1.95660	930	
940	1.96117	3.52085	1.95154	2.01427	3.58705	1.95385	2.06604	3.65115	1.95595	940	
950	1.94469	3.50020	1.95079	1.99765	3.56638	1.95315	2.04929	3.63045	1.95529	950	
960	1.92842	3.47978	1.95003	1.98124	3.54593	1.95243	2.03275	3.60998	1.95462	960	
970	1.91236	3.45957	1.94926	1.96505	3.52570	1.95172	2.01643	3.58973	1.95394	970	
980	1.89652	3.43959	1.94848	1.94906	3.50568	1.95099	2.00031	3.56969	1.95326	980	
990	1.88087	3.41981	1.94770	1.93328	3.48588	1.95025	1.98440	3.54987	1.95257	990	
1000	1.86543	3.40024	1.94690	1.91769	3.46628	1.94951	1.96868	3.53025	1.95188	1000	
1010	1.85017	3.38087	1.94611	1.90230	3.44689	1.94877	1.95317	3.51083	1.95118	1010	
1020	1.83511	3.36170	1.94530	1.88711	3.42769	1.94801	1.93784	3.49161	1.95047	1020	
1030	1.82024	3.34272	1.94448	1.87209	3.40869	1.94725	1.92270	3.47258	1.94975	1030	
1040	1.80555	3.32394	1.94366	1.85727	3.38988	1.94648	1.90774	3.45375	1.94903	1040	
1050	1.79104	3.30534	1.94283	1.84262	3.37126	1.94570	1.89297	3.43510	1.94830	1050	
1060	1.77670	3.28693	1.94200	1.82815	3.35282	1.94492	1.87837	3.41664	1.94757	1060	
1070	1.76254	3.26870	1.94115	1.81385	3.33456	1.94413	1.86394	3.39835	1.94683	1070	
1080	1.74855	3.25065	1.94030	1.79972	3.31648	1.94333	1.84969	3.38025	1.94608	1080	
1090	1.73473	3.23277	1.93944	1.78576	3.29857	1.94253	1.83560	3.36231	1.94532	1090	

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=2900.			T=3000.			T=3100.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
1100	1.72106	3.21506	1.93857	1.77197	3.28084	1.94172	1.82167	3.34455	1.94456	1100
1110	1.70756	3.19752	1.93770	1.75833	3.26327	1.94090	1.80791	3.32696	1.94380	1110
1120	1.69422	3.18015	1.93682	1.74485	3.24586	1.94007	1.79430	3.30953	1.94302	1120
1130	1.68103	3.16293	1.93593	1.73152	3.22862	1.93924	1.78085	3.29226	1.94224	1130
1140	1.66799	3.14588	1.93503	1.71835	3.21154	1.93840	1.76755	3.27515	1.94145	1140
1150	1.65510	3.12899	1.93413	1.70533	3.19461	1.93755	1.75440	3.25820	1.94066	1150
1160	1.64235	3.11224	1.93322	1.69245	3.17784	1.93670	1.74139	3.24140	1.93986	1160
1170	1.62975	3.09565	1.93230	1.67971	3.16122	1.93584	1.72854	3.22475	1.93905	1170
1180	1.61729	3.07921	1.93137	1.66712	3.14475	1.93497	1.71582	3.20825	1.93824	1180
1190	1.60497	3.06292	1.93044	1.65467	3.12843	1.93410	1.70324	3.19190	1.93742	1190
1200	1.59279	3.04677	1.92950	1.64235	3.11224	1.93322	1.69080	3.17569	1.93659	1200
1210	1.58074	3.03076	1.92855	1.63017	3.09620	1.93233	1.67849	3.15962	1.93576	1210
1220	1.56882	3.01489	1.92759	1.61812	3.08030	1.93143	1.66631	3.14369	1.93492	1220
1230	1.55703	2.99916	1.92663	1.60620	3.06454	1.93053	1.65427	3.12790	1.93407	1230
1240	1.54537	2.98356	1.92566	1.59441	3.04891	1.92962	1.64235	3.11224	1.93322	1240
1250	1.53384	2.96810	1.92469	1.58274	3.03342	1.92871	1.63056	3.09672	1.93236	1250
1260	1.52242	2.95277	1.92370	1.57119	3.01805	1.92779	1.61889	3.08133	1.93149	1260
1270	1.51113	2.93756	1.92271	1.55977	3.00282	1.92686	1.60735	3.06606	1.93062	1270
1280	1.49996	2.92249	1.92171	1.54847	2.98771	1.92592	1.59592	3.05092	1.92974	1280
1290	1.48890	2.90754	1.92070	1.53728	2.97272	1.92498	1.58461	3.03591	1.92886	1290
1300	1.47796	2.89271	1.91969	1.52621	2.95786	1.92403	1.57342	3.02102	1.92797	1300
1310	1.46714	2.87800	1.91867	1.51526	2.94312	1.92307	1.56234	3.00625	1.92707	1310
1320	1.45642	2.86341	1.91764	1.50441	2.92850	1.92211	1.55137	2.99159	1.92616	1320
1330	1.44582	2.84895	1.91661	1.49368	2.91400	1.92114	1.54052	2.97706	1.92525	1330
1340	1.43532	2.83459	1.91557	1.48305	2.89961	1.92016	1.52977	2.96264	1.92434	1340
1350	1.42493	2.82035	1.91452	1.47254	2.88534	1.91918	1.51913	2.94834	1.92341	1350
1360	1.41465	2.80623	1.91346	1.46212	2.87118	1.91819	1.50860	2.93415	1.92248	1360
1370	1.40447	2.79221	1.91240	1.45181	2.85713	1.91720	1.49817	2.92007	1.92155	1370
1380	1.39439	2.77831	1.91133	1.44161	2.84319	1.91619	1.48784	2.90609	1.92061	1380
1390	1.38441	2.76451	1.91025	1.43150	2.82936	1.91518	1.47761	2.89223	1.91966	1390
1400	1.37453	2.75082	1.90917	1.42149	2.81563	1.91417	1.46749	2.87847	1.91870	1400
1410	1.36475	2.73724	1.90808	1.41158	2.80201	1.91314	1.45746	2.86482	1.91774	1410
1420	1.35506	2.72376	1.90698	1.40177	2.78850	1.91211	1.44752	2.85127	1.91678	1420
1430	1.34547	2.71038	1.90587	1.39205	2.77508	1.91108	1.43768	2.83782	1.91580	1430
1440	1.33597	2.69710	1.90476	1.38243	2.76177	1.91003	1.42794	2.82448	1.91482	1440
1450	1.32657	2.68392	1.90364	1.37290	2.74855	1.90899	1.41829	2.81123	1.91384	1450
1460	1.31725	2.67084	1.90251	1.36345	2.73544	1.90793	1.40873	2.79808	1.91285	1460
1470	1.30802	2.65786	1.90138	1.35410	2.72242	1.90687	1.39925	2.78502	1.91185	1470
1480	1.29889	2.64498	1.90024	1.34484	2.70949	1.90580	1.38987	2.77207	1.91084	1480
1490	1.28983	2.63218	1.89909	1.33566	2.69666	1.90472	1.38058	2.75920	1.90983	1490
1500	1.28087	2.61948	1.89794	1.32657	2.68392	1.90364	1.37137	2.74643	1.90882	1500
1510	1.27198	2.60688	1.89678	1.31756	2.67128	1.90255	1.36224	2.73375	1.90779	1510
1520	1.26319	2.59436	1.89561	1.30864	2.65872	1.90146	1.35320	2.72116	1.90676	1520
1530	1.25447	2.58193	1.89444	1.29980	2.64626	1.90035	1.34424	2.70866	1.90573	1530
1540	1.24583	2.56960	1.89326	1.29104	2.63388	1.89925	1.33536	2.69625	1.90469	1540
1550	1.23728	2.55735	1.89207	1.28236	2.62159	1.89813	1.32657	2.68392	1.90364	1550
1560	1.22880	2.54518	1.89087	1.27375	2.60939	1.89701	1.31785	2.67169	1.90259	1560
1570	1.22040	2.53310	1.88967	1.26523	2.59727	1.89588	1.30921	2.65953	1.90153	1570
1580	1.21208	2.52111	1.88846	1.25679	2.58524	1.89475	1.30065	2.64746	1.90046	1580
1590	1.20383	2.50920	1.88725	1.24842	2.57329	1.89361	1.29216	2.63548	1.89939	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$T=2900.$			$T=3000.$			$T=3100.$			ν cm^{-1}
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
1600	1.19566	2.49737	1.88603	1.24012	2.56142	1.89246	1.28375	2.62357	1.89831	1600
1610	1.18756	2.48562	1.88480	1.23190	2.54963	1.89131	1.27541	2.61175	1.89723	1610
1620	1.17953	2.47396	1.88356	1.22375	2.53792	1.89015	1.26715	2.60000	1.89614	1620
1630	1.17158	2.46237	1.88232	1.21567	2.52630	1.88899	1.25896	2.58834	1.89504	1630
1640	1.16369	2.45086	1.88107	1.20767	2.51475	1.88782	1.25084	2.57675	1.89394	1640
1650	1.15588	2.43943	1.87982	1.19973	2.50327	1.88664	1.24279	2.56524	1.89283	1650
1660	1.14813	2.42807	1.87855	1.19187	2.49188	1.88545	1.23481	2.55381	1.89172	1660
1670	1.14046	2.41680	1.87729	1.18407	2.48056	1.88426	1.22690	2.54245	1.89060	1670
1680	1.13285	2.40559	1.87601	1.17634	2.46931	1.88307	1.21905	2.53116	1.88948	1680
1690	1.12531	2.39446	1.87473	1.16868	2.45814	1.88186	1.21128	2.51995	1.88835	1690
1700	1.11783	2.38340	1.87344	1.16108	2.44704	1.88065	1.20356	2.50882	1.88721	1700
1710	1.11042	2.37242	1.87215	1.15355	2.43601	1.87944	1.19592	2.49775	1.88607	1710
1720	1.10307	2.36151	1.87085	1.14608	2.42506	1.87822	1.18834	2.48676	1.88492	1720
1730	1.09578	2.35067	1.86954	1.13868	2.41417	1.87699	1.18082	2.47583	1.88376	1730
1740	1.08856	2.33989	1.86822	1.13134	2.40336	1.87576	1.17337	2.46498	1.88260	1740
1750	1.08140	2.32919	1.86690	1.12406	2.39261	1.87452	1.16597	2.45419	1.88143	1750
1760	1.07430	2.31856	1.86558	1.11684	2.38194	1.87327	1.15864	2.44348	1.88026	1760
1770	1.06726	2.30799	1.86424	1.10968	2.37133	1.87202	1.15137	2.43283	1.87908	1770
1780	1.06028	2.29749	1.86290	1.10258	2.36078	1.87076	1.14416	2.42224	1.87790	1780
1790	1.05336	2.28706	1.86156	1.09554	2.35031	1.86949	1.13701	2.41173	1.87671	1790
1800	1.04650	2.27669	1.86020	1.08856	2.33989	1.86822	1.12992	2.40127	1.87552	1800
1810	1.03969	2.26639	1.85885	1.08164	2.32955	1.86695	1.12289	2.39089	1.87431	1810
1820	1.03294	2.25615	1.85748	1.07477	2.31927	1.86567	1.11591	2.38056	1.87311	1820
1830	1.02625	2.24598	1.85611	1.06796	2.30905	1.86438	1.10899	2.37030	1.87190	1830
1840	1.01961	2.23587	1.85473	1.06121	2.29889	1.86308	1.10213	2.36011	1.87068	1840
1850	1.01303	2.22582	1.85335	1.05451	2.28879	1.86178	1.09532	2.34997	1.86945	1850
1860	1.00650	2.21583	1.85196	1.04786	2.27876	1.86048	1.08856	2.33989	1.86822	1860
1870	1.00002	2.20591	1.85056	1.04127	2.26879	1.85916	1.08186	2.32988	1.86699	1870
1880	0.99360	2.19604	1.84916	1.03474	2.25888	1.85784	1.07521	2.31993	1.86575	1880
1890	0.98723	2.18623	1.84775	1.02825	2.24902	1.85652	1.06862	2.31003	1.86450	1890
1900	0.98091	2.17649	1.84633	1.02182	2.23923	1.85519	1.06208	2.30020	1.86325	1900
1910	0.97465	2.16680	1.84491	1.01543	2.22950	1.85385	1.05559	2.29042	1.86199	1910
1920	0.96843	2.15717	1.84348	1.00910	2.21982	1.85251	1.04915	2.28070	1.86073	1920
1930	0.96226	2.14759	1.84205	1.00282	2.21020	1.85117	1.04276	2.27104	1.85946	1930
1940	0.95615	2.13808	1.84061	0.99659	2.20064	1.84981	1.03642	2.26143	1.85819	1940
1950	0.95008	2.12862	1.83916	0.99041	2.19113	1.84845	1.03013	2.25188	1.85691	1950
1960	0.94406	2.11922	1.83771	0.98428	2.18168	1.84709	1.02389	2.24238	1.85562	1960
1970	0.93809	2.10987	1.83625	0.97819	2.17228	1.84572	1.01769	2.23294	1.85433	1970
1980	0.93216	2.10057	1.83479	0.97215	2.16294	1.84434	1.01155	2.22356	1.85303	1980
1990	0.92628	2.09133	1.83332	0.96616	2.15365	1.84296	1.00545	2.21423	1.85173	1990
2000	0.92045	2.08215	1.83184	0.96022	2.14442	1.84157	0.99940	2.20495	1.85042	2000
2010	0.91467	2.07301	1.83036	0.95432	2.13524	1.84018	0.99340	2.19572	1.84911	2010
2020	0.90893	2.06393	1.82887	0.94847	2.12611	1.83878	0.98744	2.18655	1.84779	2020
2030	0.90323	2.05491	1.82738	0.94266	2.11703	1.83737	0.98152	2.17743	1.84647	2030
2040	0.89758	2.04593	1.82588	0.93690	2.10800	1.83596	0.97565	2.16836	1.84514	2040
2050	0.89197	2.03701	1.82438	0.93118	2.09903	1.83455	0.96983	2.15934	1.84381	2050
2060	0.88641	2.02813	1.82286	0.92550	2.09011	1.83312	0.96405	2.15037	1.84247	2060
2070	0.88089	2.01931	1.82135	0.91987	2.08123	1.83170	0.95831	2.14145	1.84112	2070
2080	0.87541	2.01053	1.81982	0.91428	2.07241	1.83026	0.95262	2.13258	1.83977	2080
2090	0.86997	2.00181	1.81829	0.90874	2.06363	1.82883	0.94697	2.12376	1.83842	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic
 Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=2900.			T=3000.			T=3100.				
2100	0.86458	1.99313	1.81676	0.90323	2.05491	1.82738	0.94136	2.11499	1.83705	2100
2110	0.85923	1.98451	1.81522	0.89777	2.04623	1.82593	0.93579	2.10626	1.83569	2110
2120	0.85391	1.97593	1.81367	0.89235	2.03760	1.82448	0.93026	2.09759	1.83432	2120
2130	0.84864	1.96740	1.81212	0.88696	2.02902	1.82302	0.92478	2.08896	1.83294	2130
2140	0.84341	1.95891	1.81056	0.88162	2.02048	1.82155	0.91933	2.08038	1.83156	2140
2150	0.83821	1.95048	1.80900	0.87632	2.01199	1.82008	0.91392	2.07184	1.83017	2150
2160	0.83306	1.94208	1.80743	0.87106	2.00355	1.81860	0.90856	2.06335	1.82878	2160
2170	0.82795	1.93374	1.80586	0.86583	1.99515	1.81712	0.90323	2.05491	1.82738	2170
2180	0.82287	1.92544	1.80428	0.86065	1.98680	1.81563	0.89794	2.04651	1.82598	2180
2190	0.81783	1.91719	1.80269	0.85550	1.97850	1.81414	0.89269	2.03815	1.82457	2190
2200	0.81283	1.90898	1.80110	0.85039	1.97024	1.81264	0.88748	2.02985	1.82316	2200
2210	0.80787	1.90081	1.79950	0.84532	1.96202	1.81114	0.88231	2.02158	1.82174	2210
2220	0.80294	1.89269	1.79790	0.84029	1.95384	1.80963	0.87717	2.01336	1.82032	2220
2230	0.79805	1.88462	1.79629	0.83529	1.94572	1.80811	0.87207	2.00518	1.81889	2230
2240	0.79319	1.87658	1.79468	0.83033	1.93763	1.80659	0.86701	1.99705	1.81745	2240
2250	0.78837	1.86859	1.79306	0.82540	1.92958	1.80507	0.86198	1.98895	1.81602	2250
2260	0.78359	1.86064	1.79143	0.82051	1.92158	1.80354	0.85699	1.98090	1.81457	2260
2270	0.77884	1.85274	1.78981	0.81566	1.91362	1.80200	0.85204	1.97290	1.81312	2270
2280	0.77413	1.84487	1.78817	0.81084	1.90571	1.80046	0.84712	1.96493	1.81167	2280
2290	0.76945	1.83705	1.78653	0.80605	1.89783	1.79892	0.84223	1.95700	1.81021	2290
2300	0.76481	1.82927	1.78488	0.80130	1.89000	1.79736	0.83738	1.94912	1.80875	2300
2310	0.76019	1.82153	1.78323	0.79659	1.88220	1.79581	0.83256	1.94128	1.80728	2310
2320	0.75562	1.81383	1.78157	0.79190	1.87445	1.79425	0.82778	1.93347	1.80581	2320
2330	0.75107	1.80617	1.77991	0.78726	1.86673	1.79268	0.82303	1.92571	1.80433	2330
2340	0.74656	1.79855	1.77825	0.78264	1.85906	1.79111	0.81832	1.91798	1.80284	2340
2350	0.74208	1.79097	1.77657	0.77805	1.85142	1.78953	0.81363	1.91030	1.80136	2350
2360	0.73763	1.78343	1.77490	0.77350	1.84383	1.78795	0.80898	1.90265	1.79986	2360
2370	0.73322	1.77593	1.77321	0.76898	1.83627	1.78636	0.80436	1.89505	1.79837	2370
2380	0.72883	1.76847	1.77152	0.76450	1.82875	1.78477	0.79978	1.88748	1.79686	2380
2390	0.72448	1.76105	1.76983	0.76004	1.82127	1.78318	0.79522	1.87995	1.79536	2390
2400	0.72016	1.75366	1.76813	0.75562	1.81383	1.78157	0.79070	1.87245	1.79384	2400
2410	0.71587	1.74631	1.76643	0.75122	1.80643	1.77997	0.78621	1.86500	1.79233	2410
2420	0.71161	1.73900	1.76472	0.74686	1.79906	1.77836	0.78175	1.85758	1.79080	2420
2430	0.70738	1.73173	1.76301	0.74253	1.79173	1.77674	0.77732	1.85020	1.78928	2430
2440	0.70318	1.72449	1.76129	0.73822	1.78444	1.77512	0.77292	1.84285	1.78775	2440
2450	0.69901	1.71729	1.75956	0.73395	1.77718	1.77349	0.76855	1.83554	1.78621	2450
2460	0.69486	1.71013	1.75783	0.72971	1.76996	1.77186	0.76421	1.82827	1.78467	2460
2470	0.69075	1.70300	1.75610	0.72549	1.76277	1.77023	0.75990	1.82103	1.78312	2470
2480	0.68667	1.69591	1.75436	0.72131	1.75563	1.76859	0.75562	1.81383	1.78157	2480
2490	0.68261	1.68885	1.75262	0.71715	1.74851	1.76694	0.75136	1.80667	1.78002	2490
2500	0.67858	1.68183	1.75087	0.71302	1.74143	1.76529	0.74714	1.79953	1.77846	2500
2510	0.67459	1.67484	1.74911	0.70892	1.73439	1.76363	0.74294	1.79244	1.77690	2510
2520	0.67061	1.66789	1.74736	0.70485	1.72738	1.76197	0.73878	1.78538	1.77533	2520
2530	0.66667	1.66098	1.74559	0.70081	1.72041	1.76031	0.73464	1.77835	1.77376	2530
2540	0.66275	1.65409	1.74382	0.69679	1.71346	1.75864	0.73053	1.77135	1.77218	2540
2550	0.65886	1.64724	1.74205	0.69280	1.70656	1.75697	0.72644	1.76439	1.77060	2550
2560	0.65500	1.64043	1.74027	0.68884	1.69968	1.75529	0.72239	1.75747	1.76901	2560
2570	0.65117	1.63365	1.73849	0.68491	1.69284	1.75361	0.71836	1.75057	1.76742	2570
2580	0.64736	1.62690	1.73670	0.68100	1.68604	1.75192	0.71435	1.74371	1.76582	2580
2590	0.64357	1.62019	1.73491	0.67712	1.67926	1.75023	0.71038	1.73688	1.76422	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	T=2900.			T=3000.			T=3100.			ν cm^{-1}
	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	
2600	0.63981	1.61350	1.73311	0.67326	1.67252	1.74853	0.70643	1.73009	1.76262	2600
2610	0.63608	1.60685	1.73131	0.66943	1.66581	1.74683	0.70250	1.72333	1.76101	2610
2620	0.63238	1.60024	1.72950	0.66562	1.65914	1.74512	0.69860	1.71659	1.75940	2620
2630	0.62869	1.59365	1.72769	0.66184	1.65249	1.74341	0.69473	1.70990	1.75778	2630
2640	0.62504	1.58710	1.72588	0.65809	1.64588	1.74169	0.69088	1.70323	1.75616	2640
2650	0.62141	1.58058	1.72406	0.65436	1.63930	1.73998	0.68706	1.69659	1.75453	2650
2660	0.61780	1.57409	1.72223	0.65066	1.63275	1.73825	0.68326	1.68999	1.75290	2660
2670	0.61422	1.56763	1.72040	0.64698	1.62623	1.73652	0.67949	1.68341	1.75126	2670
2680	0.61066	1.56120	1.71857	0.64332	1.61974	1.73479	0.67574	1.67687	1.74962	2680
2690	0.60712	1.55480	1.71673	0.63969	1.61328	1.73305	0.67202	1.67035	1.74798	2690
2700	0.60361	1.54844	1.71489	0.63608	1.60685	1.73131	0.66832	1.66387	1.74633	2700
2710	0.60012	1.54210	1.71304	0.63250	1.60046	1.72956	0.66465	1.65742	1.74468	2710
2720	0.59666	1.53579	1.71119	0.62894	1.59409	1.72781	0.66099	1.65100	1.74302	2720
2730	0.59322	1.52952	1.70933	0.62540	1.58775	1.72606	0.65737	1.64460	1.74136	2730
2740	0.58980	1.52327	1.70747	0.62189	1.58144	1.72430	0.65376	1.63824	1.73970	2740
2750	0.58640	1.51705	1.70561	0.61840	1.57517	1.72254	0.65018	1.63190	1.73803	2750
2760	0.58303	1.51087	1.70374	0.61493	1.56892	1.72077	0.64662	1.62560	1.73636	2760
2770	0.57968	1.50471	1.70187	0.61149	1.56270	1.71900	0.64309	1.61932	1.73468	2770
2780	0.57635	1.49858	1.69999	0.60806	1.55650	1.71722	0.63957	1.61307	1.73300	2780
2790	0.57305	1.49248	1.69811	0.60466	1.55034	1.71544	0.63608	1.60685	1.73131	2790
2800	0.56976	1.48640	1.69622	0.60128	1.54421	1.71366	0.63261	1.60066	1.72962	2800
2810	0.56650	1.48036	1.69433	0.59793	1.53810	1.71187	0.62917	1.59450	1.72793	2810
2820	0.56326	1.47435	1.69243	0.59459	1.53202	1.71008	0.62574	1.58836	1.72623	2820
2830	0.56004	1.46836	1.69053	0.59128	1.52597	1.70828	0.62234	1.58226	1.72453	2830
2840	0.55684	1.46240	1.68863	0.58799	1.51995	1.70648	0.61896	1.57618	1.72282	2840
2850	0.55366	1.45647	1.68672	0.58471	1.51396	1.70467	0.61560	1.57012	1.72111	2850
2860	0.55050	1.45056	1.68481	0.58146	1.50799	1.70286	0.61226	1.56410	1.71940	2860
2870	0.54737	1.44468	1.68290	0.57824	1.50205	1.70105	0.60894	1.55810	1.71768	2870
2880	0.54425	1.43883	1.68098	0.57503	1.49613	1.69923	0.60565	1.55213	1.71596	2880
2890	0.54115	1.43301	1.67905	0.57184	1.49025	1.69741	0.60237	1.54618	1.71423	2890
2900	0.53808	1.42721	1.67713	0.56867	1.48439	1.69559	0.59912	1.54026	1.71250	2900
2910	0.53502	1.42144	1.67519	0.56552	1.47855	1.69376	0.59588	1.53437	1.71077	2910
2920	0.53198	1.41570	1.67326	0.56240	1.47275	1.69193	0.59267	1.52851	1.70903	2920
2930	0.52897	1.40998	1.67132	0.55929	1.46696	1.69009	0.58947	1.52267	1.70729	2930
2940	0.52597	1.40429	1.66937	0.55620	1.46121	1.68825	0.58630	1.51685	1.70555	2940
2950	0.52299	1.39863	1.66743	0.55313	1.45548	1.68641	0.58314	1.51106	1.70380	2950
2960	0.52003	1.39299	1.66548	0.55008	1.44978	1.68456	0.58000	1.50530	1.70205	2960
2970	0.51709	1.38737	1.66352	0.54705	1.44410	1.68270	0.57689	1.49956	1.70029	2970
2980	0.51417	1.38179	1.66156	0.54404	1.43844	1.68085	0.57379	1.49385	1.69853	2980
2990	0.51127	1.37622	1.65960	0.54105	1.43282	1.67899	0.57071	1.48816	1.69677	2990
3000	0.50839	1.37068	1.65763	0.53808	1.42721	1.67713	0.56765	1.48250	1.69500	3000
3010	0.50552	1.36517	1.65566	0.53512	1.42164	1.67526	0.56461	1.47686	1.69323	3010
3020	0.50268	1.35968	1.65369	0.53219	1.41608	1.67339	0.56159	1.47125	1.69145	3020
3030	0.49985	1.35422	1.65171	0.52927	1.41055	1.67151	0.55859	1.46566	1.68968	3030
3040	0.49704	1.34878	1.64973	0.52637	1.40505	1.66963	0.55560	1.46010	1.68789	3040
3050	0.49424	1.34337	1.64774	0.52349	1.39957	1.66775	0.55264	1.45456	1.68611	3050
3060	0.49147	1.33798	1.64575	0.52062	1.39411	1.66587	0.54969	1.44904	1.68432	3060
3070	0.48871	1.33261	1.64376	0.51778	1.38868	1.66398	0.54676	1.44355	1.68253	3070
3080	0.48597	1.32727	1.64176	0.51495	1.38327	1.66208	0.54385	1.43808	1.68073	3080
3090	0.48325	1.32195	1.63976	0.51214	1.37789	1.66019	0.54095	1.43264	1.67893	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
	T=2900.			T=3000.			T=3100.			
3100	0.48054	1.31665	1.63776	0.50935	1.37253	1.65829	0.53808	1.42721	1.67713	3100
3110	0.47785	1.31138	1.63575	0.50657	1.36719	1.65638	0.53522	1.42182	1.67532	3110
3120	0.47518	1.30613	1.63374	0.50381	1.36188	1.65448	0.53238	1.41644	1.67351	3120
3130	0.47253	1.30091	1.63173	0.50107	1.35658	1.65257	0.52955	1.41109	1.67169	3130
3140	0.46989	1.29571	1.62971	0.49835	1.35132	1.65065	0.52674	1.40576	1.66988	3140
3150	0.46727	1.29053	1.62769	0.49564	1.34607	1.64874	0.52395	1.40045	1.66806	3150
3160	0.46466	1.28537	1.62567	0.49295	1.34085	1.64681	0.52118	1.39517	1.66623	3160
3170	0.46207	1.28024	1.62364	0.49027	1.33565	1.64489	0.51842	1.38991	1.66440	3170
3180	0.45950	1.27513	1.62161	0.48761	1.33047	1.64296	0.51568	1.38467	1.66257	3180
3190	0.45694	1.27004	1.61957	0.48497	1.32531	1.64103	0.51295	1.37945	1.66074	3190
3200	0.45440	1.26498	1.61754	0.48234	1.32018	1.63910	0.51025	1.37425	1.65890	3200
3210	0.45188	1.25993	1.61550	0.47973	1.31507	1.63716	0.50755	1.36908	1.65706	3210
3220	0.44937	1.25491	1.61345	0.47714	1.30998	1.63522	0.50488	1.36393	1.65522	3220
3230	0.44687	1.24991	1.61140	0.47456	1.30491	1.63327	0.50222	1.35880	1.65337	3230
3240	0.44439	1.24493	1.60935	0.47200	1.29987	1.63133	0.49957	1.35369	1.65152	3240
3250	0.44193	1.23998	1.60730	0.46945	1.29484	1.62938	0.49695	1.34861	1.64966	3250
3260	0.43948	1.23504	1.60524	0.46692	1.28984	1.62742	0.49433	1.34354	1.64781	3260
3270	0.43705	1.23013	1.60318	0.46440	1.28486	1.62547	0.49174	1.33850	1.64595	3270
3280	0.43463	1.22524	1.60112	0.46190	1.27990	1.62350	0.48915	1.33347	1.64408	3280
3290	0.43223	1.22037	1.59905	0.45941	1.27496	1.62154	0.48659	1.32847	1.64222	3290
3300	0.42984	1.21552	1.59698	0.45694	1.27004	1.61957	0.48404	1.32349	1.64035	3300
3310	0.42747	1.21069	1.59491	0.45449	1.26514	1.61760	0.48150	1.31853	1.63847	3310
3320	0.42511	1.20588	1.59283	0.45204	1.26027	1.61563	0.47898	1.31359	1.63660	3320
3330	0.42276	1.20109	1.59075	0.44962	1.25541	1.61366	0.47647	1.30867	1.63472	3330
3340	0.42043	1.19632	1.58867	0.44720	1.25058	1.61168	0.47398	1.30377	1.63283	3340
3350	0.41812	1.19158	1.58659	0.44481	1.24576	1.60970	0.47150	1.29889	1.63095	3350
3360	0.41582	1.18685	1.58450	0.44242	1.24097	1.60771	0.46904	1.29404	1.62906	3360
3370	0.41353	1.18215	1.58241	0.44005	1.23619	1.60572	0.46659	1.28920	1.62717	3370
3380	0.41126	1.17746	1.58032	0.43770	1.23144	1.60373	0.46416	1.28438	1.62528	3380
3390	0.40900	1.17280	1.57822	0.43536	1.22670	1.60174	0.46174	1.27958	1.62338	3390
3400	0.40675	1.16815	1.57612	0.43303	1.22199	1.59974	0.45933	1.27480	1.62148	3400
3410	0.40452	1.16352	1.57402	0.43072	1.21729	1.59774	0.45694	1.27004	1.61957	3410
3420	0.40230	1.15892	1.57191	0.42842	1.21262	1.59574	0.45457	1.26530	1.61767	3420
3430	0.40009	1.15433	1.56980	0.42613	1.20796	1.59373	0.45220	1.26058	1.61576	3430
3440	0.39790	1.14976	1.56769	0.42386	1.20332	1.59173	0.44985	1.25588	1.61385	3440
3450	0.39572	1.14522	1.56558	0.42160	1.19870	1.58971	0.44752	1.25120	1.61193	3450
3460	0.39355	1.14069	1.56346	0.41935	1.19411	1.58770	0.44519	1.24654	1.61002	3460
3470	0.39140	1.13618	1.56135	0.41712	1.18953	1.58568	0.44288	1.24189	1.60809	3470
3480	0.38926	1.13169	1.55922	0.41490	1.18497	1.58366	0.44059	1.23727	1.60617	3480
3490	0.38713	1.12722	1.55710	0.41269	1.18043	1.58164	0.43830	1.23266	1.60425	3490
3500	0.38502	1.12277	1.55497	0.41050	1.17590	1.57962	0.43603	1.22807	1.60232	3500
3510	0.38292	1.11833	1.55284	0.40832	1.17140	1.57759	0.43378	1.22351	1.60039	3510
3520	0.38083	1.11392	1.55071	0.40615	1.16691	1.57556	0.43154	1.21895	1.59845	3520
3530	0.37875	1.10952	1.54858	0.40400	1.16245	1.57353	0.42930	1.21442	1.59651	3530
3540	0.37669	1.10514	1.54644	0.40186	1.15800	1.57149	0.42709	1.20991	1.59457	3540
3550	0.37464	1.10078	1.54430	0.39973	1.15357	1.56945	0.42488	1.20541	1.59263	3550
3560	0.37260	1.09644	1.54216	0.39761	1.14916	1.56741	0.42269	1.20094	1.59069	3560
3570	0.37057	1.09212	1.54001	0.39550	1.14476	1.56537	0.42051	1.19648	1.58874	3570
3580	0.36856	1.08782	1.53787	0.39341	1.14039	1.56332	0.41834	1.19204	1.58679	3580
3590	0.36655	1.08353	1.53572	0.39133	1.13603	1.56128	0.41619	1.18761	1.58484	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
	T=2900.			T=3000.			T=3100.			
3600	0.36456	1.07926	1.53357	0.38926	1.13169	1.55922	0.41404	1.18321	1.58288	3600
3610	0.36258	1.07501	1.53141	0.38721	1.12737	1.55717	0.41191	1.17882	1.58092	3610
3620	0.36062	1.07078	1.52926	0.38516	1.12306	1.55512	0.40980	1.17445	1.57896	3620
3630	0.35866	1.06656	1.52710	0.38313	1.11878	1.55306	0.40769	1.17010	1.57700	3630
3640	0.35671	1.06236	1.52494	0.38111	1.11451	1.55100	0.40560	1.16576	1.57504	3640
3650	0.35478	1.05818	1.52277	0.37910	1.11025	1.54893	0.40351	1.16144	1.57307	3650
3660	0.35286	1.05402	1.52061	0.37710	1.10602	1.54687	0.40144	1.15714	1.57110	3660
3670	0.35095	1.04987	1.51844	0.37512	1.10180	1.54480	0.39938	1.15286	1.56912	3670
3680	0.34905	1.04574	1.51627	0.37314	1.09760	1.54273	0.39734	1.14859	1.56715	3680
3690	0.34716	1.04163	1.51410	0.37118	1.09342	1.54066	0.39530	1.14434	1.56517	3690
3700	0.34529	1.03754	1.51192	0.36923	1.08925	1.53858	0.39328	1.14011	1.56319	3700
3710	0.34342	1.03346	1.50974	0.36729	1.08510	1.53651	0.39126	1.13589	1.56121	3710
3720	0.34157	1.02940	1.50757	0.36536	1.08097	1.53443	0.38926	1.13169	1.55922	3720
3730	0.33972	1.02535	1.50538	0.36344	1.07685	1.53235	0.38727	1.12751	1.55724	3730
3740	0.33789	1.02133	1.50320	0.36153	1.07275	1.53026	0.38529	1.12334	1.55525	3740
3750	0.33607	1.01732	1.50102	0.35964	1.06867	1.52818	0.38332	1.11919	1.55326	3750
3760	0.33426	1.01332	1.49883	0.35775	1.06460	1.52609	0.38137	1.11506	1.55126	3760
3770	0.33246	1.00934	1.49664	0.35588	1.06055	1.52400	0.37942	1.11094	1.54927	3770
3780	0.33067	1.00538	1.49445	0.35401	1.05651	1.52191	0.37749	1.10684	1.54727	3780
3790	0.32889	1.00144	1.49226	0.35216	1.05250	1.51981	0.37556	1.10275	1.54527	3790
3800	0.32712	0.99751	1.49006	0.35032	1.04849	1.51772	0.37365	1.09868	1.54327	3800
3810	0.32536	0.99359	1.48786	0.34848	1.04451	1.51562	0.37175	1.09463	1.54126	3810
3820	0.32361	0.98970	1.48567	0.34666	1.04054	1.51352	0.36986	1.09059	1.53925	3820
3830	0.32187	0.98582	1.48346	0.34485	1.03658	1.51141	0.36797	1.08657	1.53724	3830
3840	0.32014	0.98195	1.48126	0.34305	1.03265	1.50931	0.36610	1.08256	1.53523	3840
3850	0.31842	0.97810	1.47906	0.34126	1.02872	1.50720	0.36424	1.07857	1.53322	3850
3860	0.31672	0.97427	1.47685	0.33948	1.02482	1.50509	0.36239	1.07460	1.53120	3860
3870	0.31502	0.97045	1.47464	0.33771	1.02092	1.50298	0.36055	1.07064	1.52919	3870
3880	0.31333	0.96665	1.47243	0.33595	1.01705	1.50087	0.35872	1.06670	1.52717	3880
3890	0.31165	0.96286	1.47022	0.33420	1.01319	1.49876	0.35690	1.06277	1.52514	3890
3900	0.30998	0.95909	1.46801	0.33246	1.00934	1.49664	0.35509	1.05886	1.52312	3900
3910	0.30832	0.95533	1.46579	0.33073	1.00551	1.49452	0.35329	1.05496	1.52110	3910
3920	0.30667	0.95159	1.46358	0.32901	1.00170	1.49240	0.35150	1.05107	1.51907	3920
3930	0.30503	0.94786	1.46136	0.32729	0.99790	1.49028	0.34972	1.04721	1.51704	3930
3940	0.30340	0.94415	1.45914	0.32559	0.99411	1.48816	0.34795	1.04335	1.51501	3940
3950	0.30178	0.94046	1.45692	0.32390	0.99034	1.48603	0.34619	1.03952	1.51297	3950
3960	0.30017	0.93677	1.45469	0.32222	0.98659	1.48390	0.34444	1.03569	1.51094	3960
3970	0.29856	0.93311	1.45247	0.32055	0.98285	1.48178	0.34270	1.03189	1.50890	3970
3980	0.29697	0.92946	1.45024	0.31888	0.97913	1.47965	0.34097	1.02809	1.50686	3980
3990	0.29538	0.92582	1.44801	0.31723	0.97541	1.47751	0.33925	1.02431	1.50482	3990
4000	0.29381	0.92220	1.44578	0.31558	0.97172	1.47538	0.33754	1.02055	1.50278	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=3200.			T=3300.			T=3400.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	
100	6.20856	8.15139	1.98683	6.26837	8.21253	1.98685	6.32642	8.27184	1.98687	100
110	6.02360	7.96203	1.98676	6.08327	8.02317	1.98679	6.14120	8.08248	1.98681	110
120	5.85512	7.78916	1.98669	5.91466	7.85030	1.98672	5.97246	7.90961	1.98674	120
130	5.70049	7.63015	1.98660	5.75989	7.69128	1.98664	5.81757	7.75059	1.98667	130
140	5.55764	7.48293	1.98651	5.61692	7.54405	1.98655	5.67447	7.60336	1.98659	140
150	5.42496	7.34587	1.98642	5.48410	7.40700	1.98646	5.54153	7.46630	1.98650	150
160	5.30113	7.21768	1.98631	5.36014	7.27880	1.98636	5.41744	7.33810	1.98641	160
170	5.18507	7.09726	1.98620	5.24394	7.15838	1.98626	5.30113	7.21768	1.98631	170
180	5.07589	6.98373	1.98609	5.13464	7.04485	1.98615	5.19170	7.10414	1.98621	180
190	4.97286	6.87636	1.98596	5.03147	6.93747	1.98603	5.08841	6.99676	1.98610	190
200	4.87533	6.77449	1.98583	4.93381	6.83560	1.98591	4.99062	6.89489	1.98598	200
210	4.78278	6.67761	1.98569	4.84113	6.73871	1.98578	4.89781	6.79799	1.98586	210
220	4.69473	6.58524	1.98555	4.75295	6.64634	1.98565	4.80951	6.70561	1.98573	220
230	4.61079	6.49698	1.98540	4.66888	6.55807	1.98551	4.72532	6.61735	1.98560	230
240	4.53060	6.41248	1.98524	4.58856	6.47357	1.98536	4.64488	6.53284	1.98546	240
250	4.45387	6.33145	1.98508	4.51170	6.39253	1.98520	4.56789	6.45180	1.98532	250
260	4.38031	6.25359	1.98491	4.43801	6.31467	1.98504	4.49408	6.37393	1.98517	260
270	4.30969	6.17868	1.98473	4.36726	6.23976	1.98488	4.42321	6.29902	1.98501	270
280	4.24180	6.10651	1.98455	4.29924	6.16758	1.98470	4.35506	6.22683	1.98485	280
290	4.17644	6.03687	1.98436	4.23375	6.09794	1.98452	4.28945	6.15718	1.98468	290
300	4.11344	5.96960	1.98416	4.17062	6.03066	1.98434	4.22620	6.08990	1.98450	300
310	4.05265	5.90454	1.98396	4.10970	5.96560	1.98415	4.16516	6.02483	1.98432	310
320	3.99392	5.84156	1.98375	4.05084	5.90261	1.98395	4.10618	5.96184	1.98414	320
330	3.93713	5.78052	1.98353	3.99392	5.84156	1.98375	4.04914	5.90078	1.98394	330
340	3.88216	5.72131	1.98330	3.93882	5.78234	1.98353	3.99392	5.84156	1.98375	340
350	3.82891	5.66382	1.98307	3.88544	5.72485	1.98332	3.94042	5.78406	1.98354	350
360	3.77728	5.60796	1.98284	3.83368	5.66898	1.98310	3.88854	5.72818	1.98333	360
370	3.72718	5.55364	1.98259	3.78345	5.61465	1.98287	3.83819	5.67385	1.98312	370
380	3.67853	5.50077	1.98234	3.73467	5.56177	1.98263	3.78929	5.62096	1.98289	380
390	3.63125	5.44928	1.98209	3.68727	5.51027	1.98239	3.74176	5.56946	1.98267	390
400	3.58527	5.39910	1.98182	3.64116	5.46009	1.98214	3.69554	5.51926	1.98243	400
410	3.54053	5.35017	1.98155	3.59630	5.41115	1.98189	3.65055	5.47032	1.98219	410
420	3.49698	5.30242	1.98128	3.55262	5.36339	1.98163	3.60675	5.42255	1.98195	420
430	3.45454	5.25580	1.98099	3.51006	5.31677	1.98136	3.56407	5.37592	1.98170	430
440	3.41318	5.21026	1.98070	3.46857	5.27122	1.98109	3.52246	5.33036	1.98144	440
450	3.37284	5.16575	1.98040	3.42810	5.22670	1.98081	3.48188	5.28584	1.98118	450
460	3.33348	5.12223	1.98010	3.38861	5.18317	1.98052	3.44227	5.24230	1.98091	460
470	3.29506	5.07965	1.97979	3.35006	5.14058	1.98023	3.40360	5.19970	1.98063	470
480	3.25753	5.03797	1.97947	3.31241	5.09889	1.97993	3.36583	5.15800	1.98035	480
490	3.22086	4.99716	1.97915	3.27561	5.05807	1.97963	3.32891	5.11717	1.98007	490
500	3.18502	4.95718	1.97882	3.23965	5.01808	1.97932	3.29283	5.07717	1.97977	500
510	3.14996	4.91800	1.97849	3.20447	4.97888	1.97900	3.25753	5.03797	1.97947	510
520	3.11567	4.87958	1.97814	3.17005	4.94046	1.97868	3.22299	4.99954	1.97917	520
530	3.08211	4.84190	1.97779	3.13636	4.90277	1.97835	3.18919	4.96184	1.97886	530
540	3.04926	4.80494	1.97744	3.10338	4.86580	1.97802	3.15609	4.92485	1.97855	540
550	3.01708	4.76866	1.97707	3.07108	4.82950	1.97767	3.12367	4.88855	1.97822	550
560	2.98555	4.73304	1.97670	3.03943	4.79387	1.97733	3.09191	4.85291	1.97790	560
570	2.95466	4.69805	1.97633	3.00842	4.75888	1.97697	3.06077	4.81790	1.97756	570
580	2.92437	4.66368	1.97595	2.97801	4.72450	1.97661	3.03025	4.78351	1.97722	580
590	2.89468	4.62991	1.97556	2.94819	4.69071	1.97625	3.00031	4.74972	1.97688	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=3200.			T=3300.			T=3400.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
600	2.86555	4.59671	1.97516	2.91893	4.65750	1.97588	2.97094	4.71650	1.97653	600
610	2.83697	4.56406	1.97476	2.89023	4.62484	1.97550	2.94212	4.68383	1.97617	610
620	2.80891	4.53196	1.97435	2.86205	4.59272	1.97511	2.91383	4.65170	1.97581	620
630	2.78138	4.50037	1.97394	2.83439	4.56112	1.97472	2.88605	4.62009	1.97544	630
640	2.75434	4.46929	1.97351	2.80723	4.53003	1.97433	2.85877	4.58898	1.97507	640
650	2.72778	4.43869	1.97309	2.78055	4.49942	1.97392	2.83198	4.55836	1.97469	650
660	2.70169	4.40857	1.97265	2.75434	4.46929	1.97351	2.80565	4.52821	1.97430	660
670	2.67605	4.37891	1.97221	2.72858	4.43961	1.97310	2.77977	4.49853	1.97391	670
680	2.65085	4.34970	1.97176	2.70326	4.41038	1.97268	2.75434	4.46929	1.97351	680
690	2.62608	4.32091	1.97131	2.67836	4.38159	1.97225	2.72933	4.44048	1.97311	690
700	2.60172	4.29255	1.97085	2.65389	4.35321	1.97182	2.70474	4.41209	1.97270	700
710	2.57777	4.26460	1.97038	2.62981	4.32525	1.97138	2.68054	4.38411	1.97229	710
720	2.55420	4.23705	1.96991	2.60612	4.29768	1.97093	2.65674	4.35653	1.97187	720
730	2.53102	4.20988	1.96943	2.58282	4.27050	1.97048	2.63332	4.32934	1.97144	730
740	2.50820	4.18308	1.96894	2.55988	4.24369	1.97002	2.61027	4.30252	1.97101	740
750	2.48575	4.15666	1.96845	2.53731	4.21725	1.96956	2.58758	4.27606	1.97057	750
760	2.46364	4.13059	1.96795	2.51508	4.19116	1.96909	2.56525	4.24996	1.97013	760
770	2.44188	4.10487	1.96744	2.49319	4.16543	1.96861	2.54325	4.22421	1.96968	770
780	2.42045	4.07948	1.96693	2.47164	4.14003	1.96813	2.52158	4.19880	1.96923	780
790	2.39934	4.05443	1.96641	2.45041	4.11496	1.96764	2.50024	4.17372	1.96877	790
800	2.37854	4.02970	1.96588	2.42950	4.09021	1.96715	2.47921	4.14896	1.96830	800
810	2.35806	4.00528	1.96535	2.40889	4.06578	1.96664	2.45849	4.12451	1.96783	810
820	2.33787	3.98117	1.96481	2.38859	4.04165	1.96614	2.43807	4.10036	1.96735	820
830	2.31797	3.95736	1.96427	2.36857	4.01782	1.96562	2.41795	4.07652	1.96687	830
840	2.29836	3.93384	1.96372	2.34884	3.99428	1.96511	2.39811	4.05297	1.96638	840
850	2.27903	3.91060	1.96316	2.32939	3.97103	1.96458	2.37854	4.02970	1.96588	850
860	2.25997	3.88764	1.96259	2.31021	3.94806	1.96405	2.35925	4.00671	1.96538	860
870	2.24118	3.86496	1.96202	2.29130	3.92535	1.96351	2.34023	3.98399	1.96488	870
880	2.22264	3.84254	1.96145	2.27265	3.90292	1.96297	2.32146	3.96154	1.96436	880
890	2.20436	3.82038	1.96086	2.25425	3.88074	1.96242	2.30295	3.93934	1.96385	890
900	2.18632	3.79847	1.96027	2.23609	3.85882	1.96187	2.28469	3.91740	1.96332	900
910	2.16853	3.77681	1.95968	2.21818	3.83714	1.96131	2.26667	3.89571	1.96279	910
920	2.15097	3.75540	1.95908	2.20051	3.81571	1.96074	2.24888	3.87426	1.96226	920
930	2.13365	3.73422	1.95847	2.18307	3.79451	1.96017	2.23133	3.85305	1.96172	930
940	2.11655	3.71328	1.95785	2.16586	3.77355	1.95959	2.21401	3.83208	1.96117	940
950	2.09968	3.69256	1.95723	2.14886	3.75282	1.95900	2.19690	3.81132	1.96062	950
960	2.08302	3.67207	1.95660	2.13209	3.73231	1.95841	2.18002	3.79080	1.96006	960
970	2.06657	3.65180	1.95597	2.11552	3.71202	1.95781	2.16334	3.77049	1.95950	970
980	2.05033	3.63174	1.95533	2.09917	3.69194	1.95721	2.14688	3.75039	1.95893	980
990	2.03429	3.61189	1.95468	2.08302	3.67207	1.95660	2.13062	3.73051	1.95836	990
1000	2.01846	3.59225	1.95403	2.06706	3.65241	1.95599	2.11456	3.71083	1.95778	1000
1010	2.00282	3.57281	1.95337	2.05131	3.63295	1.95537	2.09869	3.69135	1.95719	1010
1020	1.98737	3.55357	1.95270	2.03574	3.61369	1.95474	2.08302	3.67207	1.95660	1020
1030	1.97211	3.53452	1.95203	2.02037	3.59462	1.95411	2.06753	3.65299	1.95601	1030
1040	1.95703	3.51567	1.95135	2.00517	3.57574	1.95347	2.05223	3.63409	1.95540	1040
1050	1.94213	3.49700	1.95067	1.99016	3.55705	1.95282	2.03711	3.61538	1.95480	1050
1060	1.92741	3.47851	1.94998	1.97533	3.53855	1.95217	2.02217	3.59686	1.95418	1060
1070	1.91286	3.46020	1.94928	1.96067	3.52022	1.95152	2.00740	3.57851	1.95356	1070
1080	1.89849	3.44207	1.94858	1.94618	3.50207	1.95086	1.99280	3.56034	1.95294	1080
1090	1.88428	3.42412	1.94787	1.93185	3.48409	1.95019	1.97837	3.54234	1.95231	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=3200.			T=3300.			T=3400.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S°	C _p °	$-(F^0-E_0^0)/T$	S°	C _p °	$-(F^0-E_0^0)/T$	S°	C _p °	
1100	1.87023	3.40633	1.94715	1.91769	3.46628	1.94951	1.96410	3.52452	1.95167	1100
1110	1.85635	3.38871	1.94643	1.90369	3.44864	1.94883	1.94999	3.50686	1.95103	1110
1120	1.84262	3.37126	1.94570	1.88985	3.43117	1.94815	1.93605	3.48936	1.95038	1120
1130	1.82905	3.35397	1.94497	1.87617	3.41386	1.94746	1.92226	3.47203	1.94973	1130
1140	1.81563	3.33683	1.94423	1.86264	3.39670	1.94676	1.90862	3.45485	1.94907	1140
1150	1.80236	3.31986	1.94348	1.84926	3.37970	1.94606	1.89513	3.43783	1.94841	1150
1160	1.78924	3.30303	1.94273	1.83602	3.36285	1.94535	1.88179	3.42097	1.94774	1160
1170	1.77626	3.28636	1.94197	1.82293	3.34616	1.94463	1.86859	3.40425	1.94707	1170
1180	1.76342	3.26984	1.94120	1.80998	3.32961	1.94391	1.85554	3.38768	1.94639	1180
1190	1.75073	3.25346	1.94043	1.79717	3.31321	1.94319	1.84262	3.37126	1.94570	1190
1200	1.73817	3.23722	1.93966	1.78450	3.29695	1.94245	1.82984	3.35498	1.94501	1200
1210	1.72574	3.22113	1.93887	1.77197	3.28084	1.94172	1.81720	3.33884	1.94432	1210
1220	1.71345	3.20517	1.93808	1.75956	3.26486	1.94097	1.80469	3.32284	1.94361	1220
1230	1.70129	3.18936	1.93729	1.74729	3.24902	1.94022	1.79231	3.30698	1.94291	1230
1240	1.68925	3.17367	1.93648	1.73514	3.23331	1.93947	1.78006	3.29125	1.94219	1240
1250	1.67734	3.15812	1.93568	1.72312	3.21773	1.93871	1.76794	3.27565	1.94148	1250
1260	1.66556	3.14270	1.93486	1.71123	3.20229	1.93794	1.75594	3.26018	1.94075	1260
1270	1.65390	3.12741	1.93404	1.69945	3.18697	1.93717	1.74406	3.24485	1.94002	1270
1280	1.64235	3.11224	1.93322	1.68780	3.17178	1.93639	1.73230	3.22963	1.93929	1280
1290	1.63093	3.09720	1.93238	1.67627	3.15672	1.93560	1.72066	3.21454	1.93855	1290
1300	1.61962	3.08228	1.93155	1.66485	3.14177	1.93481	1.70914	3.19958	1.93780	1300
1310	1.60842	3.06749	1.93070	1.65354	3.12695	1.93402	1.69773	3.18473	1.93705	1310
1320	1.59734	3.05281	1.92985	1.64235	3.11224	1.93322	1.68644	3.17000	1.93630	1320
1330	1.58637	3.03825	1.92900	1.63127	3.09766	1.93241	1.67525	3.15539	1.93553	1330
1340	1.57551	3.02380	1.92813	1.62030	3.08318	1.93160	1.66418	3.14090	1.93477	1340
1350	1.56475	3.00947	1.92726	1.60944	3.06883	1.93078	1.65321	3.12651	1.93399	1350
1360	1.55411	2.99525	1.92639	1.59868	3.05458	1.92996	1.64235	3.11224	1.93322	1360
1370	1.54356	2.98114	1.92551	1.58803	3.04044	1.92913	1.63160	3.09808	1.93243	1370
1380	1.53312	2.96714	1.92462	1.57748	3.02642	1.92829	1.62094	3.08403	1.93165	1380
1390	1.52278	2.95324	1.92373	1.56703	3.01250	1.92745	1.61039	3.07009	1.93085	1390
1400	1.51254	2.93946	1.92283	1.55668	2.99868	1.92660	1.59994	3.05625	1.93005	1400
1410	1.50239	2.92577	1.92193	1.54643	2.98497	1.92575	1.58959	3.04252	1.92925	1410
1420	1.49235	2.91219	1.92102	1.53627	2.97137	1.92489	1.57933	3.02888	1.92844	1420
1430	1.48239	2.89872	1.92010	1.52621	2.95786	1.92403	1.56917	3.01535	1.92762	1430
1440	1.47254	2.88534	1.91918	1.51625	2.94446	1.92316	1.55910	3.00192	1.92680	1440
1450	1.46277	2.87206	1.91825	1.50638	2.93115	1.92229	1.54913	2.98859	1.92598	1450
1460	1.45310	2.85888	1.91732	1.49660	2.91794	1.92141	1.53925	2.97536	1.92515	1460
1470	1.44351	2.84580	1.91638	1.48691	2.90483	1.92052	1.52946	2.96222	1.92431	1470
1480	1.43402	2.83281	1.91544	1.47730	2.89181	1.91963	1.51976	2.94918	1.92347	1480
1490	1.42461	2.81991	1.91448	1.46779	2.87889	1.91873	1.51014	2.93623	1.92262	1490
1500	1.41529	2.80711	1.91353	1.45836	2.86606	1.91783	1.50061	2.92337	1.92177	1500
1510	1.40605	2.79440	1.91257	1.44902	2.85332	1.91692	1.49117	2.91060	1.92091	1510
1520	1.39690	2.78178	1.91160	1.43976	2.84067	1.91601	1.48181	2.89793	1.92005	1520
1530	1.38783	2.76924	1.91062	1.43059	2.82811	1.91509	1.47254	2.88534	1.91918	1530
1540	1.37884	2.75680	1.90964	1.42149	2.81563	1.91417	1.46334	2.87284	1.91831	1540
1550	1.36993	2.74444	1.90866	1.41248	2.80325	1.91324	1.45423	2.86043	1.91743	1550
1560	1.36111	2.73217	1.90766	1.40355	2.79095	1.91230	1.44520	2.84810	1.91655	1560
1570	1.35236	2.71999	1.90667	1.39469	2.77873	1.91136	1.43624	2.83585	1.91566	1570
1580	1.34368	2.70788	1.90566	1.38592	2.76660	1.91041	1.42737	2.82369	1.91477	1580
1590	1.33509	2.69586	1.90465	1.37722	2.75455	1.90946	1.41857	2.81162	1.91387	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=3200.			T=3300.			T=3400.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
1600	1.32657	2.68392	1.90364	1.36859	2.74258	1.90851	1.40985	2.79962	1.91296	1600
1610	1.31812	2.67207	1.90262	1.36004	2.73069	1.90754	1.40120	2.78770	1.91205	1610
1620	1.30975	2.66029	1.90159	1.35157	2.71888	1.90658	1.39262	2.77587	1.91114	1620
1630	1.30145	2.64859	1.90056	1.34316	2.70715	1.90560	1.38412	2.76411	1.91022	1630
1640	1.29322	2.63697	1.89952	1.33483	2.69550	1.90462	1.37569	2.75243	1.90929	1640
1650	1.28506	2.62542	1.89848	1.32657	2.68392	1.90364	1.36733	2.74082	1.90837	1650
1660	1.27697	2.61396	1.89743	1.31838	2.67243	1.90265	1.35904	2.72930	1.90743	1660
1670	1.26895	2.60256	1.89638	1.31025	2.66100	1.90166	1.35082	2.71784	1.90649	1670
1680	1.26100	2.59125	1.89532	1.30220	2.64965	1.90066	1.34267	2.70646	1.90555	1680
1690	1.25311	2.58000	1.89425	1.29421	2.63837	1.89965	1.33458	2.69516	1.90460	1690
1700	1.24530	2.56883	1.89318	1.28629	2.62717	1.89864	1.32657	2.68392	1.90364	1700
1710	1.23754	2.55773	1.89210	1.27844	2.61604	1.89762	1.31862	2.67276	1.90268	1710
1720	1.22985	2.54670	1.89102	1.27065	2.60497	1.89660	1.31073	2.66167	1.90171	1720
1730	1.22223	2.53574	1.88993	1.26292	2.59398	1.89558	1.30291	2.65065	1.90074	1730
1740	1.21467	2.52485	1.88884	1.25526	2.58306	1.89454	1.29515	2.63970	1.89977	1740
1750	1.20717	2.51403	1.88774	1.24766	2.57221	1.89351	1.28745	2.62881	1.89879	1750
1760	1.19973	2.50327	1.88664	1.24012	2.56142	1.89246	1.27982	2.61800	1.89780	1760
1770	1.19236	2.49259	1.88553	1.23264	2.55070	1.89142	1.27224	2.60725	1.89681	1770
1780	1.18504	2.48197	1.88441	1.22523	2.54005	1.89036	1.26473	2.59656	1.89582	1780
1790	1.17779	2.47141	1.88329	1.21787	2.52946	1.88931	1.25728	2.58594	1.89482	1790
1800	1.17059	2.46093	1.88216	1.21057	2.51894	1.88824	1.24989	2.57539	1.89381	1800
1810	1.16345	2.45050	1.88103	1.20333	2.50848	1.88717	1.24255	2.56490	1.89280	1810
1820	1.15637	2.44014	1.87990	1.19615	2.49808	1.88610	1.23528	2.55448	1.89179	1820
1830	1.14934	2.42984	1.87875	1.18902	2.48775	1.88502	1.22806	2.54411	1.89077	1830
1840	1.14237	2.41961	1.87760	1.18196	2.47748	1.88394	1.22089	2.53381	1.88974	1840
1850	1.13546	2.40943	1.87645	1.17494	2.46728	1.88285	1.21378	2.52357	1.88871	1850
1860	1.12860	2.39932	1.87529	1.16798	2.45713	1.88175	1.20673	2.51339	1.88768	1860
1870	1.12179	2.38927	1.87413	1.16108	2.44704	1.88065	1.19973	2.50327	1.88664	1870
1880	1.11504	2.37928	1.87296	1.15423	2.43701	1.87955	1.19279	2.49321	1.88559	1880
1890	1.10834	2.36934	1.87178	1.14743	2.42705	1.87844	1.18590	2.48321	1.88454	1890
1900	1.10170	2.35947	1.87060	1.14069	2.41714	1.87732	1.17906	2.47327	1.88349	1900
1910	1.09510	2.34965	1.86942	1.13400	2.40728	1.87620	1.17228	2.46339	1.88243	1910
1920	1.08856	2.33989	1.86822	1.12736	2.39749	1.87508	1.16554	2.45356	1.88137	1920
1930	1.08207	2.33019	1.86703	1.12077	2.38775	1.87395	1.15886	2.44379	1.88030	1930
1940	1.07563	2.32055	1.86583	1.11423	2.37807	1.87281	1.15223	2.43408	1.87922	1940
1950	1.06923	2.31096	1.86462	1.10774	2.36844	1.87167	1.14564	2.42442	1.87815	1950
1960	1.06289	2.30142	1.86341	1.10130	2.35887	1.87053	1.13911	2.41481	1.87706	1960
1970	1.05660	2.29194	1.86219	1.09490	2.34936	1.86938	1.13263	2.40526	1.87597	1970
1980	1.05035	2.28252	1.86097	1.08856	2.33989	1.86822	1.12619	2.39577	1.87488	1980
1990	1.04415	2.27314	1.85974	1.08226	2.33049	1.86706	1.11980	2.38632	1.87378	1990
2000	1.03800	2.26383	1.85850	1.07602	2.32113	1.86590	1.11346	2.37693	1.87268	2000
2010	1.03189	2.25456	1.85727	1.06981	2.31183	1.86473	1.10717	2.36760	1.87157	2010
2020	1.02583	2.24535	1.85602	1.06366	2.30258	1.86355	1.10092	2.35831	1.87046	2020
2030	1.01982	2.23618	1.85477	1.05755	2.29338	1.86237	1.09472	2.34908	1.86935	2030
2040	1.01385	2.22707	1.85352	1.05148	2.28423	1.86119	1.08856	2.33989	1.86822	2040
2050	1.00792	2.21801	1.85226	1.04546	2.27513	1.86000	1.08245	2.33076	1.86710	2050
2060	1.00204	2.20900	1.85100	1.03948	2.26608	1.85880	1.07638	2.32168	1.86597	2060
2070	0.99620	2.20004	1.84973	1.03355	2.25708	1.85760	1.07036	2.31265	1.86483	2070
2080	0.99041	2.19113	1.84845	1.02766	2.24813	1.85640	1.06438	2.30366	1.86369	2080
2090	0.98466	2.18227	1.84717	1.02182	2.23923	1.85519	1.05844	2.29473	1.86255	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=3200.			T=3300.			T=3400.				
2100	0.97895	2.17345	1.84589	1.01601	2.23038	1.85398	1.05255	2.28584	1.86140	2100
2110	0.97328	2.16469	1.84460	1.01025	2.22157	1.85276	1.04670	2.27700	1.86024	2110
2120	0.96766	2.15597	1.84330	1.00453	2.21282	1.85153	1.04089	2.26820	1.85909	2120
2130	0.96207	2.14730	1.84201	0.99885	2.20411	1.85031	1.03512	2.25946	1.85792	2130
2140	0.95653	2.13867	1.84070	0.99321	2.19544	1.84907	1.02939	2.25076	1.85675	2140
2150	0.95102	2.13009	1.83939	0.98762	2.18683	1.84783	1.02370	2.24211	1.85558	2150
2160	0.94556	2.12156	1.83808	0.98206	2.17825	1.84659	1.01806	2.23350	1.85441	2160
2170	0.94013	2.11307	1.83676	0.97654	2.16973	1.84534	1.01245	2.22494	1.85322	2170
2180	0.93475	2.10463	1.83543	0.97106	2.16125	1.84409	1.00688	2.21642	1.85204	2180
2190	0.92940	2.09624	1.83410	0.96562	2.15281	1.84283	1.00135	2.20794	1.85085	2190
2200	0.92409	2.08788	1.83277	0.96022	2.14442	1.84157	0.99586	2.19951	1.84965	2200
2210	0.91882	2.07957	1.83143	0.95486	2.13607	1.84030	0.99041	2.19113	1.84845	2210
2220	0.91359	2.07131	1.83008	0.94953	2.12776	1.83903	0.98500	2.18279	1.84725	2220
2230	0.90839	2.06309	1.82873	0.94424	2.11950	1.83776	0.97962	2.17449	1.84604	2230
2240	0.90323	2.05491	1.82738	0.93899	2.11128	1.83648	0.97428	2.16623	1.84483	2240
2250	0.89811	2.04677	1.82602	0.93377	2.10310	1.83519	0.96898	2.15801	1.84361	2250
2260	0.89302	2.03868	1.82466	0.92859	2.09497	1.83390	0.96371	2.14984	1.84239	2260
2270	0.88797	2.03062	1.82329	0.92345	2.08687	1.83261	0.95848	2.14171	1.84116	2270
2280	0.88295	2.02261	1.82192	0.91834	2.07882	1.83131	0.95329	2.13362	1.83993	2280
2290	0.87797	2.01464	1.82054	0.91327	2.07081	1.83000	0.94813	2.12557	1.83870	2290
2300	0.87303	2.00671	1.81916	0.90823	2.06284	1.82869	0.94300	2.11756	1.83746	2300
2310	0.86811	1.99882	1.81777	0.90323	2.05491	1.82738	0.93791	2.10959	1.83621	2310
2320	0.86324	1.99097	1.81638	0.89826	2.04702	1.82606	0.93286	2.10166	1.83496	2320
2330	0.85839	1.98316	1.81498	0.89333	2.03916	1.82474	0.92784	2.09377	1.83371	2330
2340	0.85358	1.97539	1.81358	0.88843	2.03135	1.82341	0.92285	2.08592	1.83245	2340
2350	0.84880	1.96766	1.81217	0.88356	2.02358	1.82208	0.91790	2.07811	1.83119	2350
2360	0.84406	1.95997	1.81076	0.87873	2.01585	1.82075	0.91297	2.07034	1.82993	2360
2370	0.83935	1.95232	1.80934	0.87392	2.00815	1.81941	0.90809	2.06260	1.82866	2370
2380	0.83467	1.94470	1.80792	0.86915	2.00049	1.81806	0.90323	2.05491	1.82738	2380
2390	0.83002	1.93712	1.80650	0.86442	1.99287	1.81671	0.89841	2.04725	1.82610	2390
2400	0.82540	1.92958	1.80507	0.85971	1.98529	1.81536	0.89362	2.03963	1.82482	2400
2410	0.82082	1.92208	1.80363	0.85504	1.97774	1.81400	0.88886	2.03204	1.82353	2410
2420	0.81626	1.91462	1.80219	0.85039	1.97024	1.81264	0.88413	2.02449	1.82224	2420
2430	0.81174	1.90719	1.80075	0.84578	1.96276	1.81127	0.87943	2.01698	1.82094	2430
2440	0.80725	1.89980	1.79930	0.84120	1.95533	1.80990	0.87477	2.00951	1.81964	2440
2450	0.80278	1.89244	1.79785	0.83665	1.94793	1.80853	0.87013	2.00207	1.81834	2450
2460	0.79835	1.88512	1.79639	0.83213	1.94056	1.80715	0.86553	1.99466	1.81703	2460
2470	0.79395	1.87783	1.79493	0.82764	1.93324	1.80576	0.86095	1.98729	1.81572	2470
2480	0.78958	1.87059	1.79346	0.82318	1.92594	1.80437	0.85641	1.97996	1.81440	2480
2490	0.78523	1.86337	1.79199	0.81874	1.91868	1.80298	0.85189	1.97266	1.81308	2490
2500	0.78092	1.85619	1.79052	0.81434	1.91146	1.80158	0.84741	1.96540	1.81176	2500
2510	0.77663	1.84905	1.78904	0.80997	1.90427	1.80018	0.84295	1.95817	1.81043	2510
2520	0.77237	1.84194	1.78756	0.80562	1.89712	1.79877	0.83852	1.95097	1.80909	2520
2530	0.76814	1.83486	1.78607	0.80130	1.89000	1.79736	0.83412	1.94381	1.80776	2530
2540	0.76394	1.82782	1.78457	0.79701	1.88291	1.79595	0.82975	1.93668	1.80641	2540
2550	0.75976	1.82081	1.78308	0.79275	1.87585	1.79453	0.82540	1.92958	1.80507	2550
2560	0.75562	1.81383	1.78157	0.78852	1.86883	1.79311	0.82109	1.92252	1.80372	2560
2570	0.75150	1.80689	1.78007	0.78431	1.86185	1.79168	0.81680	1.91549	1.80236	2570
2580	0.74740	1.79998	1.77856	0.78013	1.85489	1.79025	0.81254	1.90850	1.80101	2580
2590	0.74334	1.79310	1.77704	0.77598	1.84797	1.78881	0.80830	1.90153	1.79964	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=3200.			T=3300.			T=3400.				
2600	0.73930	1.78626	1.77552	0.77186	1.84108	1.78737	0.80409	1.89460	1.79828	2600
2610	0.73528	1.77944	1.77400	0.76776	1.83422	1.78593	0.79991	1.88770	1.79691	2610
2620	0.73129	1.77266	1.77247	0.76368	1.82739	1.78448	0.79576	1.88083	1.79553	2620
2630	0.72733	1.76591	1.77094	0.75964	1.82060	1.78303	0.79163	1.87399	1.79416	2630
2640	0.72340	1.75920	1.76941	0.75562	1.81383	1.78157	0.78753	1.86719	1.79277	2640
2650	0.71949	1.75251	1.76787	0.75162	1.80710	1.78011	0.78345	1.86041	1.79139	2650
2660	0.71560	1.74585	1.76632	0.74765	1.80040	1.77865	0.77940	1.85367	1.79000	2660
2670	0.71174	1.73923	1.76477	0.74370	1.79373	1.77718	0.77537	1.84695	1.78860	2670
2680	0.70790	1.73263	1.76322	0.73978	1.78708	1.77571	0.77137	1.84027	1.78721	2680
2690	0.70409	1.72607	1.76166	0.73589	1.78047	1.77423	0.76740	1.83361	1.78580	2690
2700	0.70031	1.71954	1.76010	0.73202	1.77389	1.77275	0.76345	1.82699	1.78440	2700
2710	0.69654	1.71303	1.75854	0.72817	1.76734	1.77127	0.75952	1.82040	1.78299	2710
2720	0.69280	1.70656	1.75697	0.72435	1.76082	1.76978	0.75562	1.81383	1.78157	2720
2730	0.68909	1.70011	1.75539	0.72055	1.75433	1.76829	0.75174	1.80730	1.78016	2730
2740	0.68540	1.69370	1.75382	0.71678	1.74787	1.76679	0.74788	1.80079	1.77874	2740
2750	0.68173	1.68731	1.75223	0.71302	1.74143	1.76529	0.74405	1.79431	1.77731	2750
2760	0.67808	1.68095	1.75065	0.70930	1.73503	1.76379	0.74024	1.78786	1.77588	2760
2770	0.67446	1.67463	1.74906	0.70559	1.72865	1.76228	0.73646	1.78144	1.77445	2770
2780	0.67086	1.66833	1.74747	0.70191	1.72230	1.76076	0.73270	1.77505	1.77301	2780
2790	0.66729	1.66205	1.74587	0.69825	1.71598	1.75925	0.72896	1.76869	1.77157	2790
2800	0.66373	1.65581	1.74427	0.69461	1.70969	1.75773	0.72525	1.76235	1.77013	2800
2810	0.66020	1.64959	1.74266	0.69100	1.70343	1.75620	0.72155	1.75604	1.76868	2810
2820	0.65669	1.64341	1.74105	0.68741	1.69719	1.75468	0.71788	1.74976	1.76723	2820
2830	0.65320	1.63725	1.73944	0.68384	1.69098	1.75315	0.71424	1.74351	1.76578	2830
2840	0.64973	1.63111	1.73782	0.68029	1.68480	1.75161	0.71061	1.73729	1.76432	2840
2850	0.64629	1.62501	1.73620	0.67676	1.67865	1.75007	0.70700	1.73109	1.76285	2850
2860	0.64287	1.61893	1.73457	0.67326	1.67252	1.74853	0.70342	1.72491	1.76139	2860
2870	0.63946	1.61288	1.73294	0.66978	1.66642	1.74698	0.69986	1.71877	1.75992	2870
2880	0.63608	1.60685	1.73131	0.66631	1.66035	1.74543	0.69632	1.71265	1.75844	2880
2890	0.63272	1.60086	1.72967	0.66287	1.65430	1.74388	0.69280	1.70656	1.75697	2890
2900	0.62938	1.59488	1.72803	0.65945	1.64828	1.74232	0.68931	1.70049	1.75549	2900
2910	0.62606	1.58894	1.72639	0.65605	1.64228	1.74076	0.68583	1.69445	1.75400	2910
2920	0.62277	1.58302	1.72474	0.65267	1.63632	1.73919	0.68237	1.68844	1.75251	2920
2930	0.61949	1.57712	1.72309	0.64932	1.63037	1.73762	0.67894	1.68245	1.75102	2930
2940	0.61623	1.57126	1.72143	0.64598	1.62445	1.73605	0.67552	1.67648	1.74953	2940
2950	0.61299	1.56541	1.71977	0.64266	1.61856	1.73447	0.67213	1.67055	1.74803	2950
2960	0.60977	1.55960	1.71811	0.63936	1.61270	1.73289	0.66876	1.66463	1.74653	2960
2970	0.60657	1.55381	1.71644	0.63608	1.60685	1.73131	0.66540	1.65874	1.74502	2970
2980	0.60339	1.54804	1.71477	0.63282	1.60104	1.72972	0.66207	1.65288	1.74351	2980
2990	0.60023	1.54230	1.71310	0.62958	1.59524	1.72813	0.65875	1.64704	1.74200	2990
3000	0.59709	1.53658	1.71142	0.62636	1.58948	1.72654	0.65546	1.64123	1.74048	3000
3010	0.59397	1.53089	1.70974	0.62316	1.58373	1.72494	0.65218	1.63544	1.73896	3010
3020	0.59087	1.52522	1.70805	0.61998	1.57802	1.72334	0.64892	1.62967	1.73744	3020
3030	0.58778	1.51958	1.70637	0.61682	1.57232	1.72173	0.64568	1.62393	1.73591	3030
3040	0.58471	1.51396	1.70467	0.61368	1.56665	1.72013	0.64246	1.61822	1.73438	3040
3050	0.58167	1.50836	1.70298	0.61055	1.56100	1.71851	0.63926	1.61252	1.73285	3050
3060	0.57864	1.50279	1.70128	0.60744	1.55538	1.71690	0.63608	1.60685	1.73131	3060
3070	0.57563	1.49724	1.69958	0.60435	1.54978	1.71528	0.63292	1.60121	1.72977	3070
3080	0.57263	1.49172	1.69787	0.60128	1.54421	1.71366	0.62977	1.59558	1.72823	3080
3090	0.56966	1.48622	1.69616	0.59823	1.53866	1.71203	0.62665	1.58999	1.72668	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	T=3200.			T=3300.			T=3400.			ν cm^{-1}
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
3100	0.56670	1.48074	1.69445	0.59520	1.53313	1.71040	0.62354	1.58441	1.72513	3100
3110	0.56376	1.47528	1.69273	0.59218	1.52762	1.70877	0.62045	1.57886	1.72358	3110
3120	0.56084	1.46985	1.69101	0.58918	1.52214	1.70713	0.61738	1.57332	1.72202	3120
3130	0.55793	1.46444	1.68929	0.58620	1.51668	1.70549	0.61432	1.56782	1.72046	3130
3140	0.55505	1.45906	1.68756	0.58324	1.51124	1.70385	0.61128	1.56233	1.71889	3140
3150	0.55218	1.45369	1.68583	0.58029	1.50582	1.70221	0.60826	1.55687	1.71733	3150
3160	0.54932	1.44835	1.68409	0.57736	1.50043	1.70056	0.60526	1.55143	1.71576	3160
3170	0.54649	1.44304	1.68236	0.57445	1.49506	1.69890	0.60227	1.54601	1.71418	3170
3180	0.54367	1.43774	1.68062	0.57155	1.48971	1.69725	0.59931	1.54061	1.71261	3180
3190	0.54086	1.43247	1.67887	0.56867	1.48439	1.69559	0.59635	1.53524	1.71103	3190
3200	0.53808	1.42721	1.67713	0.56581	1.47908	1.69393	0.59342	1.52988	1.70944	3200
3210	0.53531	1.42198	1.67538	0.56296	1.47380	1.69226	0.59050	1.52455	1.70786	3210
3220	0.53255	1.41678	1.67362	0.56013	1.46854	1.69059	0.58760	1.51924	1.70627	3220
3230	0.52981	1.41159	1.67186	0.55732	1.46330	1.68892	0.58471	1.51396	1.70467	3230
3240	0.52709	1.40642	1.67010	0.55452	1.45808	1.68724	0.58185	1.50869	1.70308	3240
3250	0.52439	1.40128	1.66834	0.55174	1.45288	1.68557	0.57899	1.50344	1.70148	3250
3260	0.52170	1.39616	1.66657	0.54898	1.44771	1.68388	0.57616	1.49822	1.69988	3260
3270	0.51902	1.39106	1.66480	0.54623	1.44255	1.68220	0.57334	1.49301	1.69827	3270
3280	0.51636	1.38597	1.66303	0.54350	1.43742	1.68051	0.57053	1.48783	1.69666	3280
3290	0.51372	1.38091	1.66126	0.54078	1.43231	1.67882	0.56774	1.48267	1.69505	3290
3300	0.51109	1.37588	1.65948	0.53808	1.42721	1.67713	0.56497	1.47753	1.69344	3300
3310	0.50848	1.37086	1.65769	0.53539	1.42214	1.67543	0.56221	1.47241	1.69182	3310
3320	0.50588	1.36586	1.65591	0.53272	1.41709	1.67373	0.55947	1.46730	1.69020	3320
3330	0.50330	1.36088	1.65412	0.53006	1.41206	1.67202	0.55674	1.46222	1.68857	3330
3340	0.50073	1.35592	1.65233	0.52742	1.40705	1.67032	0.55403	1.45716	1.68695	3340
3350	0.49818	1.35099	1.65053	0.52480	1.40206	1.66861	0.55134	1.45212	1.68532	3350
3360	0.49564	1.34607	1.64874	0.52218	1.39709	1.66690	0.54865	1.44710	1.68369	3360
3370	0.49311	1.34117	1.64693	0.51959	1.39214	1.66518	0.54599	1.44210	1.68205	3370
3380	0.49060	1.33630	1.64513	0.51701	1.38720	1.66346	0.54334	1.43712	1.68041	3380
3390	0.48811	1.33144	1.64332	0.51444	1.38229	1.66174	0.54070	1.43216	1.67877	3390
3400	0.48563	1.32660	1.64151	0.51189	1.37740	1.66002	0.53808	1.42721	1.67713	3400
3410	0.48316	1.32178	1.63970	0.50935	1.37253	1.65829	0.53547	1.42229	1.67548	3410
3420	0.48071	1.31698	1.63789	0.50682	1.36767	1.65656	0.53288	1.41739	1.67383	3420
3430	0.47827	1.31220	1.63607	0.50431	1.36284	1.65482	0.53030	1.41250	1.67217	3430
3440	0.47585	1.30744	1.63425	0.50182	1.35803	1.65309	0.52773	1.40764	1.67052	3440
3450	0.47344	1.30270	1.63242	0.49933	1.35323	1.65135	0.52518	1.40279	1.66886	3450
3460	0.47104	1.29798	1.63060	0.49687	1.34845	1.64961	0.52264	1.39796	1.66720	3460
3470	0.46866	1.29328	1.62877	0.49441	1.34369	1.64786	0.52012	1.39315	1.66553	3470
3480	0.46629	1.28859	1.62693	0.49197	1.33895	1.64612	0.51761	1.38836	1.66387	3480
3490	0.46393	1.28393	1.62510	0.48954	1.33423	1.64436	0.51512	1.38359	1.66220	3490
3500	0.46159	1.27928	1.62326	0.48713	1.32953	1.64261	0.51263	1.37884	1.66052	3500
3510	0.45926	1.27465	1.62142	0.48473	1.32485	1.64086	0.51017	1.37410	1.65885	3510
3520	0.45694	1.27004	1.61957	0.48234	1.32018	1.63910	0.50771	1.36939	1.65717	3520
3530	0.45464	1.26545	1.61773	0.47997	1.31553	1.63734	0.50527	1.36469	1.65549	3530
3540	0.45235	1.26088	1.61588	0.47761	1.31090	1.63557	0.50284	1.36001	1.65380	3540
3550	0.45007	1.25632	1.61403	0.47526	1.30629	1.63381	0.50043	1.35534	1.65212	3550
3560	0.44781	1.25178	1.61217	0.47293	1.30170	1.63204	0.49803	1.35070	1.65043	3560
3570	0.44555	1.24726	1.61032	0.47061	1.29712	1.63026	0.49564	1.34607	1.64874	3570
3580	0.44332	1.24276	1.60846	0.46830	1.29257	1.62849	0.49326	1.34146	1.64704	3580
3590	0.44109	1.23828	1.60659	0.46600	1.28803	1.62671	0.49090	1.33687	1.64534	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm ⁻¹
T=3200.			T=3300.			T=3400.				
3600	0.43887	1.23381	1.60473	0.46372	1.28350	1.62493	0.48855	1.33229	1.64364	3600
3610	0.43667	1.22936	1.60286	0.46145	1.27900	1.62315	0.48621	1.32774	1.64194	3610
3620	0.43448	1.22493	1.60099	0.45919	1.27451	1.62136	0.48389	1.32320	1.64024	3620
3630	0.43230	1.22052	1.59912	0.45694	1.27004	1.61957	0.48157	1.31868	1.63853	3630
3640	0.43014	1.21612	1.59724	0.45471	1.26559	1.61778	0.47927	1.31417	1.63682	3640
3650	0.42799	1.21174	1.59536	0.45249	1.26115	1.61599	0.47699	1.30968	1.63510	3650
3660	0.42584	1.20738	1.59348	0.45028	1.25673	1.61420	0.47471	1.30521	1.63339	3660
3670	0.42372	1.20303	1.59160	0.44808	1.25233	1.61240	0.47245	1.30076	1.63167	3670
3680	0.42160	1.19870	1.58971	0.44589	1.24795	1.61060	0.47020	1.29632	1.62995	3680
3690	0.41949	1.19439	1.58783	0.44372	1.24358	1.60879	0.46796	1.29190	1.62823	3690
3700	0.41740	1.19010	1.58594	0.44156	1.23923	1.60699	0.46573	1.28749	1.62650	3700
3710	0.41532	1.18582	1.58404	0.43941	1.23489	1.60518	0.46352	1.28311	1.62477	3710
3720	0.41324	1.18156	1.58215	0.43727	1.23057	1.60337	0.46131	1.27873	1.62304	3720
3730	0.41118	1.17731	1.58025	0.43514	1.22627	1.60156	0.45912	1.27438	1.62131	3730
3740	0.40914	1.17309	1.57835	0.43303	1.22199	1.59974	0.45694	1.27004	1.61957	3740
3750	0.40710	1.16887	1.57645	0.43093	1.21772	1.59792	0.45477	1.26572	1.61784	3750
3760	0.40507	1.16468	1.57454	0.42883	1.21346	1.59610	0.45262	1.26141	1.61610	3760
3770	0.40306	1.16050	1.57264	0.42675	1.20923	1.59428	0.45047	1.25712	1.61435	3770
3780	0.40106	1.15634	1.57073	0.42468	1.20501	1.59246	0.44834	1.25285	1.61261	3780
3790	0.39906	1.15219	1.56882	0.42262	1.20080	1.59063	0.44622	1.24859	1.61086	3790
3800	0.39708	1.14806	1.56690	0.42058	1.19661	1.58880	0.44410	1.24435	1.60911	3800
3810	0.39511	1.14394	1.56499	0.41854	1.19244	1.58697	0.44200	1.24012	1.60736	3810
3820	0.39315	1.13984	1.56307	0.41651	1.18828	1.58513	0.43991	1.23591	1.60561	3820
3830	0.39120	1.13576	1.56115	0.41450	1.18414	1.58330	0.43784	1.23172	1.60385	3830
3840	0.38926	1.13169	1.55922	0.41249	1.18001	1.58146	0.43577	1.22754	1.60209	3840
3850	0.38733	1.12764	1.55730	0.41050	1.17590	1.57962	0.43371	1.22337	1.60033	3850
3860	0.38542	1.12360	1.55537	0.40852	1.17181	1.57777	0.43167	1.21922	1.59856	3860
3870	0.38351	1.11958	1.55344	0.40655	1.16773	1.57593	0.42963	1.21509	1.59680	3870
3880	0.38161	1.11557	1.55151	0.40458	1.16366	1.57408	0.42761	1.21097	1.59503	3880
3890	0.37973	1.11158	1.54958	0.40263	1.15961	1.57223	0.42559	1.20687	1.59326	3890
3900	0.37785	1.10760	1.54764	0.40069	1.15558	1.57038	0.42359	1.20278	1.59149	3900
3910	0.37598	1.10364	1.54571	0.39876	1.15156	1.56853	0.42160	1.19870	1.58971	3910
3920	0.37413	1.09970	1.54377	0.39684	1.14756	1.56667	0.41962	1.19465	1.58794	3920
3930	0.37228	1.09577	1.54182	0.39493	1.14357	1.56481	0.41764	1.19060	1.58616	3930
3940	0.37045	1.09185	1.53988	0.39303	1.13959	1.56295	0.41568	1.18657	1.58438	3940
3950	0.36862	1.08795	1.53793	0.39114	1.13563	1.56109	0.41373	1.18256	1.58259	3950
3960	0.36680	1.08406	1.53599	0.38926	1.13169	1.55922	0.41179	1.17856	1.58081	3960
3970	0.36500	1.08019	1.53404	0.38739	1.12776	1.55736	0.40986	1.17458	1.57902	3970
3980	0.36320	1.07634	1.53209	0.38553	1.12384	1.55549	0.40794	1.17061	1.57723	3980
3990	0.36141	1.07249	1.53013	0.38368	1.11994	1.55362	0.40603	1.16665	1.57544	3990
4000	0.35964	1.06867	1.52818	0.38184	1.11606	1.55175	0.40412	1.16271	1.57365	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic
 Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
	T=3500.			T=3600.			T=3700.			
100	6.38283	8.32944	1.98689	6.43769	8.38541	1.98691	6.49107	8.43985	1.98692	100
110	6.19749	8.14007	1.98683	6.25223	8.19604	1.98685	6.30551	8.25048	1.98687	110
120	6.02864	7.96720	1.98677	6.08327	8.02317	1.98679	6.13644	8.07760	1.98681	120
130	5.87363	7.80817	1.98670	5.92815	7.86414	1.98672	5.98121	7.91858	1.98675	130
140	5.73041	7.66095	1.98662	5.78482	7.71691	1.98665	5.83778	7.77134	1.98668	140
150	5.59735	7.52389	1.98654	5.65165	7.57985	1.98657	5.70450	7.63428	1.98661	150
160	5.47315	7.39568	1.98645	5.52733	7.45164	1.98649	5.58008	7.50607	1.98653	160
170	5.35671	7.27525	1.98636	5.41079	7.33121	1.98641	5.46343	7.38564	1.98645	170
180	5.24716	7.16172	1.98626	5.30113	7.21768	1.98631	5.35367	7.27210	1.98636	180
190	5.14376	7.05433	1.98616	5.19761	7.11028	1.98622	5.25004	7.16471	1.98627	190
200	5.04586	6.95246	1.98605	5.09960	7.00841	1.98611	5.15193	7.06283	1.98617	200
210	4.95293	6.85556	1.98594	5.00656	6.91151	1.98600	5.05879	6.96592	1.98607	210
220	4.86451	6.76318	1.98582	4.91803	6.81912	1.98589	4.97015	6.87353	1.98596	220
230	4.78020	6.67491	1.98569	4.83361	6.73085	1.98577	4.88563	6.78526	1.98585	230
240	4.69965	6.59040	1.98556	4.75295	6.64634	1.98565	4.80486	6.70074	1.98573	240
250	4.62254	6.50935	1.98542	4.67573	6.56528	1.98552	4.72754	6.61968	1.98561	250
260	4.54862	6.43148	1.98528	4.60170	6.48741	1.98538	4.65340	6.54181	1.98548	260
270	4.47763	6.35656	1.98513	4.53060	6.41248	1.98524	4.58220	6.46688	1.98535	270
280	4.40937	6.28437	1.98498	4.46223	6.34029	1.98510	4.51373	6.39468	1.98521	280
290	4.34364	6.21471	1.98482	4.39640	6.27063	1.98495	4.44779	6.32502	1.98507	290
300	4.28028	6.14743	1.98465	4.33292	6.20334	1.98479	4.38421	6.25772	1.98492	300
310	4.21912	6.08236	1.98448	4.27165	6.13826	1.98463	4.32284	6.19264	1.98477	310
320	4.16002	6.01935	1.98431	4.21245	6.07526	1.98446	4.26353	6.12963	1.98461	320
330	4.10287	5.95830	1.98413	4.15519	6.01419	1.98429	4.20617	6.06856	1.98444	330
340	4.04754	5.89907	1.98394	4.09975	5.95496	1.98412	4.15063	6.00932	1.98428	340
350	3.99392	5.84156	1.98375	4.04602	5.89745	1.98393	4.09680	5.95181	1.98411	350
360	3.94192	5.78568	1.98355	3.99392	5.84156	1.98375	4.04459	5.89591	1.98393	360
370	3.89146	5.73133	1.98334	3.94335	5.78721	1.98355	3.99392	5.84156	1.98375	370
380	3.84245	5.67844	1.98313	3.89423	5.73431	1.98335	3.94470	5.78866	1.98356	380
390	3.79481	5.62693	1.98292	3.84648	5.68280	1.98315	3.89685	5.73714	1.98337	390
400	3.74847	5.57673	1.98270	3.80003	5.63259	1.98294	3.85030	5.68693	1.98317	400
410	3.70337	5.52778	1.98247	3.75483	5.58363	1.98273	3.80499	5.63796	1.98297	410
420	3.65945	5.48001	1.98224	3.71080	5.53585	1.98251	3.76087	5.59018	1.98276	420
430	3.61666	5.43337	1.98200	3.66790	5.48921	1.98229	3.71787	5.54352	1.98255	430
440	3.57494	5.38781	1.98176	3.62608	5.44364	1.98206	3.67594	5.49795	1.98233	440
450	3.53424	5.34327	1.98151	3.58527	5.39910	1.98182	3.63503	5.45340	1.98211	450
460	3.49452	5.29972	1.98126	3.54545	5.35554	1.98158	3.59510	5.40984	1.98188	460
470	3.45574	5.25712	1.98100	3.50656	5.31293	1.98134	3.55612	5.36722	1.98165	470
480	3.41786	5.21541	1.98073	3.46857	5.27122	1.98109	3.51802	5.32550	1.98141	480
490	3.38083	5.17458	1.98046	3.43144	5.23037	1.98083	3.48079	5.28465	1.98117	490
500	3.34463	5.13457	1.98019	3.39513	5.19036	1.98057	3.44439	5.24463	1.98092	500
510	3.30922	5.09536	1.97991	3.35962	5.15114	1.98030	3.40877	5.20540	1.98067	510
520	3.27458	5.05691	1.97962	3.32486	5.11269	1.98003	3.37392	5.16694	1.98041	520
530	3.24066	5.01921	1.97933	3.29084	5.07497	1.97976	3.33980	5.12922	1.98015	530
540	3.20745	4.98221	1.97903	3.25753	5.03797	1.97947	3.30639	5.09221	1.97988	540
550	3.17492	4.94590	1.97873	3.22489	5.00165	1.97919	3.27365	5.05589	1.97961	550
560	3.14304	4.91025	1.97842	3.19291	4.96599	1.97890	3.24157	5.02022	1.97934	560
570	3.11180	4.87524	1.97810	3.16156	4.93097	1.97860	3.21012	4.98519	1.97905	570
580	3.08116	4.84084	1.97778	3.13082	4.89656	1.97830	3.17928	4.95077	1.97877	580
590	3.05111	4.80703	1.97746	3.10067	4.86275	1.97799	3.14903	4.91695	1.97848	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
	T=3500.			T=3600.			T=3700.			
600	3.02163	4.77380	1.97713	3.07108	4.82950	1.97767	3.11934	4.88370	1.97818	600
610	2.99270	4.74112	1.97679	3.04205	4.79682	1.97736	3.09021	4.85100	1.97788	610
620	2.96430	4.70898	1.97645	3.01354	4.76467	1.97703	3.06161	4.81884	1.97757	620
630	2.93642	4.67736	1.97610	2.98555	4.73304	1.97670	3.03352	4.78720	1.97726	630
640	2.90903	4.64624	1.97575	2.95806	4.70191	1.97637	3.00593	4.75607	1.97694	640
650	2.88212	4.61561	1.97539	2.93105	4.67127	1.97603	2.97882	4.72542	1.97662	650
660	2.85569	4.58546	1.97502	2.90451	4.64110	1.97569	2.95218	4.69524	1.97630	660
670	2.82970	4.55576	1.97466	2.87842	4.61140	1.97534	2.92600	4.66553	1.97597	670
680	2.80416	4.52651	1.97428	2.85278	4.58213	1.97498	2.90025	4.63625	1.97563	680
690	2.77904	4.49769	1.97390	2.82756	4.55330	1.97462	2.87493	4.60742	1.97529	690
700	2.75434	4.46929	1.97351	2.80275	4.52489	1.97426	2.85003	4.57900	1.97495	700
710	2.73004	4.44130	1.97312	2.77835	4.49689	1.97389	2.82553	4.55098	1.97459	710
720	2.70613	4.41370	1.97273	2.75434	4.46929	1.97351	2.80142	4.52337	1.97424	720
730	2.68260	4.38650	1.97232	2.73071	4.44207	1.97313	2.77769	4.49614	1.97388	730
740	2.65944	4.35966	1.97192	2.70745	4.41523	1.97275	2.75434	4.46929	1.97351	740
750	2.63665	4.33320	1.97150	2.68455	4.38875	1.97236	2.73134	4.44280	1.97314	750
760	2.61420	4.30709	1.97108	2.66200	4.36263	1.97196	2.70870	4.41667	1.97277	760
770	2.59209	4.28132	1.97066	2.63979	4.33685	1.97156	2.68639	4.39088	1.97239	770
780	2.57032	4.25590	1.97023	2.61792	4.31141	1.97115	2.66442	4.36543	1.97200	780
790	2.54887	4.23080	1.96980	2.59637	4.28631	1.97074	2.64277	4.34031	1.97162	790
800	2.52774	4.20603	1.96936	2.57513	4.26152	1.97033	2.62144	4.31552	1.97122	800
810	2.50691	4.18157	1.96891	2.55420	4.23705	1.96991	2.60042	4.29103	1.97082	810
820	2.48639	4.15741	1.96846	2.53358	4.21288	1.96948	2.57970	4.26685	1.97042	820
830	2.46615	4.13355	1.96800	2.51324	4.18901	1.96905	2.55927	4.24297	1.97001	830
840	2.44621	4.10999	1.96754	2.49319	4.16543	1.96861	2.53912	4.21938	1.96959	840
850	2.42654	4.08670	1.96707	2.47343	4.14213	1.96817	2.51926	4.19607	1.96918	850
860	2.40714	4.06370	1.96660	2.45393	4.11912	1.96772	2.49967	4.17304	1.96875	860
870	2.38801	4.04097	1.96612	2.43470	4.09637	1.96727	2.48034	4.15029	1.96832	870
880	2.36914	4.01850	1.96564	2.41573	4.07389	1.96681	2.46127	4.12779	1.96789	880
890	2.35052	3.99629	1.96515	2.39701	4.05167	1.96635	2.44246	4.10556	1.96745	890
900	2.33215	3.97434	1.96466	2.37854	4.02970	1.96588	2.42390	4.08358	1.96701	900
910	2.31403	3.95263	1.96416	2.36032	4.00798	1.96541	2.40558	4.06185	1.96656	910
920	2.29614	3.93117	1.96365	2.34233	3.98650	1.96493	2.38750	4.04036	1.96611	920
930	2.27848	3.90994	1.96314	2.32457	3.96526	1.96445	2.36965	4.01910	1.96565	930
940	2.26105	3.88895	1.96263	2.30704	3.94425	1.96396	2.35202	3.99808	1.96519	940
950	2.24384	3.86818	1.96211	2.28974	3.92347	1.96347	2.33462	3.97729	1.96472	950
960	2.22685	3.84764	1.96158	2.27265	3.90292	1.96297	2.31744	3.95672	1.96425	960
970	2.21008	3.82731	1.96105	2.25577	3.88258	1.96247	2.30047	3.93636	1.96378	970
980	2.19351	3.80720	1.96051	2.23910	3.86245	1.96196	2.28371	3.91623	1.96329	980
990	2.17714	3.78730	1.95997	2.22264	3.84254	1.96145	2.26715	3.89630	1.96281	990
1000	2.16098	3.76761	1.95942	2.20638	3.82283	1.96093	2.25079	3.87657	1.96232	1000
1010	2.14501	3.74811	1.95887	2.19031	3.80332	1.96041	2.23463	3.85705	1.96182	1010
1020	2.12923	3.72881	1.95831	2.17443	3.78400	1.95988	2.21867	3.83772	1.96132	1020
1030	2.11364	3.70971	1.95775	2.15875	3.76489	1.95934	2.20289	3.81859	1.96082	1030
1040	2.09824	3.69080	1.95718	2.14325	3.74596	1.95881	2.18729	3.79965	1.96031	1040
1050	2.08302	3.67207	1.95660	2.12793	3.72722	1.95826	2.17188	3.78089	1.95979	1050
1060	2.06797	3.65353	1.95602	2.11278	3.70866	1.95771	2.15664	3.76232	1.95927	1060
1070	2.05310	3.63517	1.95544	2.09781	3.69028	1.95716	2.14158	3.74392	1.95875	1070
1080	2.03840	3.61698	1.95485	2.08302	3.67207	1.95660	2.12669	3.72570	1.95822	1080
1090	2.02386	3.59896	1.95425	2.06839	3.65404	1.95604	2.11197	3.70766	1.95768	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=3500.			T=3600.			T=3700.				
1100	2.00950	3.58112	1.95365	2.05392	3.63618	1.95547	2.09741	3.68978	1.95715	1100
1110	1.99529	3.56344	1.95305	2.03962	3.61849	1.95490	2.08302	3.67207	1.95660	1110
1120	1.98124	3.54593	1.95243	2.02547	3.60096	1.95432	2.06878	3.65453	1.95605	1120
1130	1.96735	3.52858	1.95182	2.01148	3.58359	1.95374	2.05470	3.63714	1.95550	1130
1140	1.95361	3.51138	1.95120	1.99765	3.56638	1.95315	2.04077	3.61992	1.95494	1140
1150	1.94002	3.49434	1.95057	1.98396	3.54932	1.95255	2.02699	3.60284	1.95438	1150
1160	1.92657	3.47746	1.94994	1.97042	3.53242	1.95196	2.01336	3.58592	1.95381	1160
1170	1.91328	3.46072	1.94930	1.95703	3.51567	1.95135	1.99988	3.56916	1.95324	1170
1180	1.90012	3.44414	1.94866	1.94378	3.49906	1.95074	1.98654	3.55254	1.95267	1180
1190	1.88711	3.42769	1.94801	1.93067	3.48260	1.95013	1.97334	3.53606	1.95209	1190
1200	1.87423	3.41139	1.94736	1.91769	3.46628	1.94951	1.96027	3.51973	1.95150	1200
1210	1.86149	3.39524	1.94670	1.90486	3.45011	1.94889	1.94734	3.50353	1.95091	1210
1220	1.84888	3.37922	1.94604	1.89215	3.43407	1.94826	1.93455	3.48748	1.95031	1220
1230	1.83640	3.36333	1.94537	1.87958	3.41817	1.94763	1.92189	3.47156	1.94971	1230
1240	1.82405	3.34758	1.94469	1.86713	3.40240	1.94699	1.90935	3.45578	1.94911	1240
1250	1.81182	3.33197	1.94402	1.85481	3.38676	1.94635	1.89694	3.44012	1.94850	1250
1260	1.79972	3.31648	1.94333	1.84262	3.37126	1.94570	1.88466	3.42460	1.94789	1260
1270	1.78775	3.30112	1.94264	1.83055	3.35588	1.94505	1.87250	3.40920	1.94727	1270
1280	1.77589	3.28589	1.94195	1.81860	3.34063	1.94439	1.86046	3.39393	1.94665	1280
1290	1.76415	3.27078	1.94125	1.80677	3.32550	1.94373	1.84854	3.37879	1.94602	1290
1300	1.75253	3.25579	1.94054	1.79505	3.31049	1.94306	1.83673	3.36376	1.94539	1300
1310	1.74103	3.24092	1.93983	1.78345	3.29560	1.94239	1.82504	3.34886	1.94475	1310
1320	1.72963	3.22617	1.93912	1.77197	3.28084	1.94172	1.81347	3.33407	1.94411	1320
1330	1.71835	3.21154	1.93840	1.76059	3.26618	1.94103	1.80200	3.31940	1.94346	1330
1340	1.70718	3.19702	1.93767	1.74932	3.25165	1.94035	1.79065	3.30484	1.94281	1340
1350	1.69611	3.18262	1.93694	1.73817	3.23722	1.93966	1.77940	3.29040	1.94215	1350
1360	1.68515	3.16833	1.93621	1.72712	3.22291	1.93896	1.76826	3.27607	1.94149	1360
1370	1.67430	3.15414	1.93547	1.71617	3.20871	1.93826	1.75723	3.26185	1.94083	1370
1380	1.66355	3.14007	1.93472	1.70533	3.19461	1.93755	1.74630	3.24774	1.94016	1380
1390	1.65290	3.12610	1.93397	1.69458	3.18063	1.93684	1.73547	3.23373	1.93949	1390
1400	1.64235	3.11224	1.93322	1.68394	3.16675	1.93613	1.72474	3.21983	1.93881	1400
1410	1.63190	3.09849	1.93246	1.67340	3.15297	1.93541	1.71411	3.20603	1.93813	1410
1420	1.62155	3.08483	1.93169	1.66296	3.13929	1.93468	1.70358	3.19234	1.93744	1420
1430	1.61129	3.07128	1.93092	1.65261	3.12572	1.93395	1.69314	3.17875	1.93675	1430
1440	1.60113	3.05783	1.93014	1.64235	3.11224	1.93322	1.68280	3.16525	1.93605	1440
1450	1.59106	3.04447	1.92936	1.63219	3.09887	1.93248	1.67255	3.15186	1.93535	1450
1460	1.58108	3.03121	1.92858	1.62212	3.08559	1.93173	1.66239	3.13856	1.93464	1460
1470	1.57119	3.01805	1.92779	1.61214	3.07241	1.93098	1.65233	3.12535	1.93393	1470
1480	1.56140	3.00499	1.92699	1.60225	3.05932	1.93023	1.64235	3.11224	1.93322	1480
1490	1.55169	2.99201	1.92619	1.59245	3.04632	1.92947	1.63246	3.09923	1.93250	1490
1500	1.54206	2.97913	1.92538	1.58274	3.03342	1.92871	1.62266	3.08630	1.93177	1500
1510	1.53253	2.96634	1.92457	1.57311	3.02060	1.92794	1.61295	3.07347	1.93104	1510
1520	1.52307	2.95364	1.92376	1.56357	3.00788	1.92717	1.60332	3.06073	1.93031	1520
1530	1.51370	2.94103	1.92294	1.55411	2.99525	1.92639	1.59377	3.04807	1.92957	1530
1540	1.50441	2.92850	1.92211	1.54473	2.98270	1.92561	1.58431	3.03550	1.92883	1540
1550	1.49521	2.91606	1.92128	1.53543	2.97024	1.92482	1.57493	3.02302	1.92809	1550
1560	1.48608	2.90371	1.92044	1.52621	2.95786	1.92403	1.56562	3.01062	1.92734	1560
1570	1.47703	2.89144	1.91960	1.51708	2.94557	1.92323	1.55640	2.99831	1.92658	1570
1580	1.46806	2.87926	1.91876	1.50802	2.93336	1.92243	1.54725	2.98608	1.92582	1580
1590	1.45917	2.86715	1.91791	1.49903	2.92124	1.92163	1.53819	2.97393	1.92506	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
	T=3500.			T=3600.			T=3700.			
1600	1.45035	2.85513	1.91705	1.49013	2.90919	1.92082	1.52919	2.96187	1.92429	1600
1610	1.44161	2.84319	1.91619	1.48129	2.89723	1.92000	1.52028	2.94988	1.92351	1610
1620	1.43294	2.83133	1.91533	1.47254	2.88534	1.91918	1.51143	2.93797	1.92274	1620
1630	1.42434	2.81954	1.91446	1.46385	2.87353	1.91836	1.50267	2.92614	1.92195	1630
1640	1.41582	2.80784	1.91358	1.45524	2.86180	1.91753	1.49397	2.91439	1.92117	1640
1650	1.40737	2.79621	1.91270	1.44670	2.85015	1.91670	1.48534	2.90271	1.92038	1650
1660	1.39899	2.78465	1.91182	1.43823	2.83857	1.91586	1.47679	2.89111	1.91958	1660
1670	1.39067	2.77317	1.91093	1.42983	2.82706	1.91501	1.46830	2.87959	1.91878	1670
1680	1.38243	2.76177	1.91003	1.42149	2.81563	1.91417	1.45989	2.86813	1.91798	1680
1690	1.37425	2.75043	1.90914	1.41323	2.80428	1.91331	1.45154	2.85675	1.91717	1690
1700	1.36614	2.73917	1.90823	1.40503	2.79299	1.91246	1.44326	2.84544	1.91636	1700
1710	1.35810	2.72798	1.90732	1.39690	2.78178	1.91160	1.43504	2.83421	1.91554	1710
1720	1.35012	2.71687	1.90641	1.38883	2.77063	1.91073	1.42689	2.82304	1.91472	1720
1730	1.34221	2.70582	1.90549	1.38083	2.75956	1.90986	1.41881	2.81194	1.91389	1730
1740	1.33435	2.69484	1.90457	1.37290	2.74855	1.90899	1.41079	2.80091	1.91306	1740
1750	1.32657	2.68392	1.90364	1.36502	2.73762	1.90811	1.40283	2.78995	1.91223	1750
1760	1.31884	2.67308	1.90271	1.35721	2.72675	1.90722	1.39493	2.77906	1.91139	1760
1770	1.31118	2.66230	1.90177	1.34946	2.71594	1.90633	1.38710	2.76823	1.91054	1770
1780	1.30357	2.65159	1.90083	1.34177	2.70520	1.90544	1.37933	2.75747	1.90970	1780
1790	1.29603	2.64094	1.89988	1.33414	2.69453	1.90454	1.37161	2.74677	1.90884	1790
1800	1.28855	2.63036	1.89893	1.32657	2.68392	1.90364	1.36396	2.73614	1.90799	1800
1810	1.28112	2.61985	1.89797	1.31906	2.67338	1.90273	1.35637	2.72557	1.90713	1810
1820	1.27375	2.60939	1.89701	1.31160	2.66290	1.90182	1.34883	2.71507	1.90626	1820
1830	1.26644	2.59900	1.89605	1.30421	2.65248	1.90091	1.34135	2.70463	1.90539	1830
1840	1.25919	2.58867	1.89508	1.29687	2.64212	1.89999	1.33393	2.69424	1.90452	1840
1850	1.25199	2.57840	1.89410	1.28958	2.63183	1.89906	1.32657	2.68392	1.90364	1850
1860	1.24485	2.56819	1.89312	1.28236	2.62159	1.89813	1.31926	2.67366	1.90276	1860
1870	1.23776	2.55804	1.89214	1.27518	2.61142	1.89720	1.31200	2.66346	1.90187	1870
1880	1.23073	2.54795	1.89115	1.26806	2.60130	1.89626	1.30480	2.65332	1.90098	1880
1890	1.22375	2.53792	1.89015	1.26100	2.59125	1.89532	1.29766	2.64324	1.90009	1890
1900	1.21682	2.52795	1.88915	1.25399	2.58125	1.89437	1.29056	2.63322	1.89919	1900
1910	1.20995	2.51804	1.88815	1.24703	2.57130	1.89342	1.28352	2.62325	1.89828	1910
1920	1.20313	2.50818	1.88714	1.24012	2.56142	1.89246	1.27654	2.61334	1.89738	1920
1930	1.19635	2.49838	1.88613	1.23326	2.55159	1.89150	1.26960	2.60349	1.89646	1930
1940	1.18963	2.48864	1.88511	1.22646	2.54182	1.89054	1.26271	2.59369	1.89555	1940
1950	1.18296	2.47895	1.88409	1.21970	2.53210	1.88957	1.25588	2.58394	1.89463	1950
1960	1.17634	2.46931	1.88307	1.21300	2.52244	1.88860	1.24909	2.57425	1.89370	1960
1970	1.16977	2.45973	1.88204	1.20634	2.51283	1.88762	1.24235	2.56462	1.89277	1970
1980	1.16324	2.45020	1.88100	1.19973	2.50327	1.88664	1.23567	2.55504	1.89184	1980
1990	1.15677	2.44073	1.87996	1.19317	2.49377	1.88565	1.22903	2.54551	1.89091	1990
2000	1.15034	2.43131	1.87892	1.18666	2.48432	1.88466	1.22244	2.53603	1.88996	2000
2010	1.14396	2.42194	1.87787	1.18020	2.47493	1.88367	1.21589	2.52661	1.88902	2010
2020	1.13762	2.41262	1.87681	1.17378	2.46558	1.88267	1.20939	2.51724	1.88807	2020
2030	1.13134	2.40336	1.87576	1.16741	2.45628	1.88166	1.20294	2.50792	1.88712	2030
2040	1.12509	2.39414	1.87469	1.16108	2.44704	1.88065	1.19654	2.49864	1.88616	2040
2050	1.11889	2.38498	1.87363	1.15480	2.43785	1.87964	1.19018	2.48942	1.88520	2050
2060	1.11274	2.37587	1.87255	1.14856	2.42870	1.87862	1.18386	2.48025	1.88423	2060
2070	1.10663	2.36680	1.87148	1.14237	2.41961	1.87760	1.17759	2.47113	1.88326	2070
2080	1.10056	2.35778	1.87040	1.13622	2.41056	1.87658	1.17136	2.46206	1.88229	2080
2090	1.09454	2.34881	1.86931	1.13012	2.40156	1.87555	1.16518	2.45303	1.88131	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=3500.			T=3600.			T=3700.				
2100	1.08856	2.33989	1.86822	1.12406	2.39261	1.87452	1.15904	2.44405	1.88033	2100
2110	1.08262	2.33102	1.86713	1.11804	2.38371	1.87348	1.15294	2.43512	1.87934	2110
2120	1.07673	2.32220	1.86603	1.11206	2.37486	1.87244	1.14689	2.42624	1.87835	2120
2130	1.07087	2.31342	1.86493	1.10612	2.36605	1.87139	1.14087	2.41740	1.87736	2130
2140	1.06506	2.30469	1.86382	1.10023	2.35728	1.87034	1.13490	2.40861	1.87636	2140
2150	1.05929	2.29600	1.86271	1.09437	2.34857	1.86928	1.12897	2.39987	1.87535	2150
2160	1.05356	2.28736	1.86160	1.08856	2.33989	1.86822	1.12308	2.39117	1.87435	2160
2170	1.04786	2.27876	1.86048	1.08279	2.33127	1.86716	1.11723	2.38251	1.87334	2170
2180	1.04221	2.27021	1.85935	1.07705	2.32269	1.86609	1.11141	2.37390	1.87232	2180
2190	1.03660	2.26170	1.85822	1.07136	2.31415	1.86502	1.10564	2.36533	1.87130	2190
2200	1.03102	2.25324	1.85709	1.06570	2.30565	1.86395	1.09991	2.35681	1.87028	2200
2210	1.02549	2.24482	1.85595	1.06009	2.29720	1.86287	1.09422	2.34833	1.86925	2210
2220	1.01999	2.23644	1.85481	1.05451	2.28879	1.86178	1.08856	2.33989	1.86822	2220
2230	1.01453	2.22811	1.85366	1.04897	2.28043	1.86069	1.08294	2.33150	1.86719	2230
2240	1.00910	2.21982	1.85251	1.04346	2.27211	1.85960	1.07736	2.32315	1.86615	2240
2250	1.00372	2.21157	1.85136	1.03800	2.26383	1.85850	1.07182	2.31484	1.86511	2250
2260	0.99837	2.20336	1.85020	1.03257	2.25559	1.85740	1.06631	2.30657	1.86406	2260
2270	0.99305	2.19520	1.84904	1.02717	2.24739	1.85630	1.06084	2.29834	1.86301	2270
2280	0.98778	2.18707	1.84787	1.02182	2.23923	1.85519	1.05541	2.29016	1.86196	2280
2290	0.98253	2.17899	1.84670	1.01649	2.23111	1.85408	1.05001	2.28201	1.86090	2290
2300	0.97733	2.17094	1.84552	1.01121	2.22304	1.85296	1.04465	2.27390	1.85984	2300
2310	0.97215	2.16294	1.84434	1.00596	2.21500	1.85184	1.03932	2.26584	1.85877	2310
2320	0.96702	2.15497	1.84316	1.00074	2.20701	1.85072	1.03403	2.25781	1.85770	2320
2330	0.96191	2.14705	1.84197	0.99556	2.19905	1.84959	1.02877	2.24982	1.85663	2330
2340	0.95684	2.13916	1.84078	0.99041	2.19113	1.84845	1.02355	2.24187	1.85555	2340
2350	0.95181	2.13132	1.83958	0.98530	2.18325	1.84732	1.01836	2.23396	1.85447	2350
2360	0.94680	2.12351	1.83838	0.98021	2.17541	1.84617	1.01320	2.22609	1.85338	2360
2370	0.94184	2.11574	1.83717	0.97517	2.16760	1.84503	1.00808	2.21826	1.85230	2370
2380	0.93690	2.10800	1.83596	0.97015	2.15984	1.84388	1.00299	2.21046	1.85120	2380
2390	0.93199	2.10031	1.83475	0.96517	2.15211	1.84273	0.99794	2.20270	1.85011	2390
2400	0.92712	2.09265	1.83353	0.96022	2.14442	1.84157	0.99291	2.19498	1.84900	2400
2410	0.92228	2.08503	1.83231	0.95530	2.13676	1.84041	0.98792	2.18729	1.84790	2410
2420	0.91747	2.07744	1.83108	0.95041	2.12914	1.83924	0.98296	2.17964	1.84679	2420
2430	0.91269	2.06990	1.82985	0.94556	2.12156	1.83808	0.97803	2.17203	1.84568	2430
2440	0.90795	2.06238	1.82862	0.94074	2.11401	1.83690	0.97313	2.16445	1.84456	2440
2450	0.90323	2.05491	1.82738	0.93594	2.10650	1.83573	0.96826	2.15691	1.84344	2450
2460	0.89855	2.04747	1.82614	0.93118	2.09903	1.83455	0.96343	2.14940	1.84232	2460
2470	0.89389	2.04006	1.82489	0.92645	2.09159	1.83336	0.95862	2.14193	1.84119	2470
2480	0.88927	2.03269	1.82364	0.92175	2.08418	1.83217	0.95384	2.13449	1.84006	2480
2490	0.88467	2.02535	1.82239	0.91707	2.07681	1.83098	0.94910	2.12709	1.83893	2490
2500	0.88010	2.01805	1.82113	0.91243	2.06948	1.82978	0.94438	2.11972	1.83779	2500
2510	0.87557	2.01078	1.81987	0.90782	2.06218	1.82858	0.93970	2.11239	1.83665	2510
2520	0.87106	2.00355	1.81860	0.90323	2.05491	1.82738	0.93504	2.10509	1.83550	2520
2530	0.86658	1.99635	1.81733	0.89868	2.04767	1.82617	0.93041	2.09782	1.83435	2530
2540	0.86213	1.98918	1.81606	0.89415	2.04047	1.82496	0.92581	2.09059	1.83320	2540
2550	0.85770	1.98205	1.81478	0.88965	2.03330	1.82375	0.92124	2.08339	1.83204	2550
2560	0.85331	1.97495	1.81350	0.88518	2.02617	1.82253	0.91670	2.07622	1.83088	2560
2570	0.84894	1.96788	1.81221	0.88074	2.01906	1.82130	0.91218	2.06908	1.82972	2570
2580	0.84460	1.96085	1.81092	0.87632	2.01199	1.82008	0.90769	2.06198	1.82855	2580
2590	0.84029	1.95384	1.80963	0.87193	2.00495	1.81885	0.90323	2.05491	1.82738	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=3500.			T=3600.			T=3700.				
2600	0.83600	1.94687	1.80833	0.86757	1.99795	1.81761	0.89880	2.04787	1.82621	2600
2610	0.83174	1.93993	1.80703	0.86324	1.99097	1.81638	0.89439	2.04086	1.82503	2610
2620	0.82751	1.93303	1.80572	0.85893	1.98403	1.81513	0.89001	2.03388	1.82385	2620
2630	0.82330	1.92615	1.80441	0.85465	1.97712	1.81389	0.88566	2.02694	1.82266	2630
2640	0.81912	1.91930	1.80310	0.85039	1.97024	1.81264	0.88133	2.02002	1.82147	2640
2650	0.81497	1.91249	1.80178	0.84616	1.96338	1.81139	0.87703	2.01314	1.82028	2650
2660	0.81084	1.90571	1.80046	0.84196	1.95656	1.81013	0.87276	2.00628	1.81908	2660
2670	0.80674	1.89895	1.79914	0.83778	1.94977	1.80887	0.86851	1.99946	1.81788	2670
2680	0.80266	1.89223	1.79781	0.83363	1.94301	1.80761	0.86429	1.99267	1.81668	2680
2690	0.79860	1.88554	1.79648	0.82950	1.93628	1.80634	0.86009	1.98590	1.81547	2690
2700	0.79458	1.87887	1.79514	0.82540	1.92958	1.80507	0.85592	1.97917	1.81426	2700
2710	0.79057	1.87224	1.79380	0.82133	1.92291	1.80379	0.85177	1.97246	1.81305	2710
2720	0.78659	1.86563	1.79246	0.81727	1.91627	1.80251	0.84765	1.96579	1.81183	2720
2730	0.78264	1.85906	1.79111	0.81324	1.90966	1.80123	0.84355	1.95914	1.81061	2730
2740	0.77871	1.85251	1.78976	0.80924	1.90308	1.79995	0.83947	1.95252	1.80938	2740
2750	0.77480	1.84600	1.78840	0.80526	1.89652	1.79866	0.83542	1.94593	1.80815	2750
2760	0.77092	1.83951	1.78705	0.80130	1.89000	1.79736	0.83140	1.93937	1.80692	2760
2770	0.76706	1.83305	1.78568	0.79737	1.88350	1.79607	0.82740	1.93284	1.80569	2770
2780	0.76322	1.82661	1.78432	0.79346	1.87703	1.79477	0.82342	1.92634	1.80445	2780
2790	0.75941	1.82021	1.78295	0.78958	1.87059	1.79346	0.81946	1.91986	1.80321	2790
2800	0.75562	1.81383	1.78157	0.78571	1.86417	1.79216	0.81553	1.91341	1.80196	2800
2810	0.75185	1.80748	1.78020	0.78187	1.85778	1.79085	0.81162	1.90699	1.80071	2810
2820	0.74810	1.80116	1.77882	0.77805	1.85142	1.78953	0.80773	1.90059	1.79946	2820
2830	0.74438	1.79487	1.77743	0.77426	1.84509	1.78822	0.80387	1.89423	1.79820	2830
2840	0.74068	1.78860	1.77605	0.77049	1.83879	1.78689	0.80003	1.88788	1.79694	2840
2850	0.73700	1.78236	1.77465	0.76674	1.83251	1.78557	0.79621	1.88157	1.79568	2850
2860	0.73334	1.77615	1.77326	0.76301	1.82626	1.78424	0.79241	1.87528	1.79442	2860
2870	0.72971	1.76996	1.77186	0.75930	1.82003	1.78291	0.78863	1.86902	1.79315	2870
2880	0.72609	1.76380	1.77046	0.75562	1.81383	1.78157	0.78488	1.86279	1.79187	2880
2890	0.72250	1.75766	1.76905	0.75195	1.80766	1.78024	0.78115	1.85658	1.79060	2890
2900	0.71893	1.75156	1.76765	0.74831	1.80151	1.77889	0.77744	1.85040	1.78932	2900
2910	0.71538	1.74547	1.76623	0.74469	1.79539	1.77755	0.77375	1.84424	1.78804	2910
2920	0.71185	1.73942	1.76482	0.74109	1.78930	1.77620	0.77008	1.83811	1.78675	2920
2930	0.70834	1.73339	1.76340	0.73751	1.78322	1.77485	0.76643	1.83200	1.78546	2930
2940	0.70485	1.72738	1.76197	0.73395	1.77718	1.77349	0.76281	1.82592	1.78417	2940
2950	0.70138	1.72140	1.76055	0.73041	1.77116	1.77213	0.75920	1.81986	1.78287	2950
2960	0.69794	1.71544	1.75912	0.72689	1.76517	1.77077	0.75562	1.81383	1.78157	2960
2970	0.69451	1.70951	1.75769	0.72340	1.75920	1.76941	0.75205	1.80783	1.78027	2970
2980	0.69110	1.70361	1.75625	0.71992	1.75325	1.76804	0.74851	1.80184	1.77897	2980
2990	0.68771	1.69773	1.75481	0.71646	1.74733	1.76667	0.74498	1.79589	1.77766	2990
3000	0.68435	1.69187	1.75336	0.71302	1.74143	1.76529	0.74148	1.78995	1.77635	3000
3010	0.68100	1.68604	1.75192	0.70961	1.73556	1.76391	0.73799	1.78404	1.77503	3010
3020	0.67767	1.68023	1.75047	0.70621	1.72971	1.76253	0.73453	1.77816	1.77371	3020
3030	0.67436	1.67444	1.74901	0.70283	1.72389	1.76114	0.73108	1.77230	1.77239	3030
3040	0.67107	1.66868	1.74756	0.69947	1.71809	1.75975	0.72765	1.76646	1.77107	3040
3050	0.66779	1.66295	1.74610	0.69613	1.71231	1.75836	0.72425	1.76065	1.76974	3050
3060	0.66454	1.65723	1.74463	0.69280	1.70656	1.75697	0.72086	1.75485	1.76841	3060
3070	0.66131	1.65154	1.74317	0.68950	1.70083	1.75557	0.71749	1.74909	1.76707	3070
3080	0.65809	1.64588	1.74169	0.68622	1.69512	1.75417	0.71414	1.74334	1.76574	3080
3090	0.65489	1.64024	1.74022	0.68295	1.68944	1.75276	0.71080	1.73762	1.76440	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
T=3500.			T=3600.			T=3700.				
3100	0.65171	1.63461	1.73874	0.67970	1.68378	1.75135	0.70749	1.73192	1.76305	3100
3110	0.64855	1.62902	1.73726	0.67647	1.67814	1.74994	0.70420	1.72625	1.76171	3110
3120	0.64541	1.62344	1.73578	0.67326	1.67252	1.74853	0.70092	1.72059	1.76036	3120
3130	0.64228	1.61789	1.73429	0.67007	1.66693	1.74711	0.69766	1.71496	1.75900	3130
3140	0.63917	1.61236	1.73280	0.66689	1.66136	1.74569	0.69442	1.70935	1.75765	3140
3150	0.63608	1.60685	1.73131	0.66373	1.65581	1.74427	0.69119	1.70377	1.75629	3150
3160	0.63301	1.60137	1.72981	0.66059	1.65028	1.74284	0.68799	1.69820	1.75493	3160
3170	0.62995	1.59591	1.72832	0.65747	1.64478	1.74141	0.68480	1.69266	1.75356	3170
3180	0.62692	1.59046	1.72681	0.65436	1.63930	1.73998	0.68163	1.68714	1.75219	3180
3190	0.62389	1.58504	1.72531	0.65127	1.63384	1.73854	0.67848	1.68164	1.75082	3190
3200	0.62089	1.57965	1.72380	0.64820	1.62840	1.73710	0.67534	1.67616	1.74945	3200
3210	0.61790	1.57427	1.72229	0.64515	1.62298	1.73566	0.67222	1.67071	1.74807	3210
3220	0.61493	1.56892	1.72077	0.64211	1.61758	1.73421	0.66912	1.66527	1.74669	3220
3230	0.61198	1.56358	1.71925	0.63909	1.61221	1.73276	0.66603	1.65986	1.74531	3230
3240	0.60904	1.55827	1.71773	0.63608	1.60685	1.73131	0.66297	1.65446	1.74392	3240
3250	0.60612	1.55298	1.71621	0.63309	1.60152	1.72986	0.65991	1.64909	1.74253	3250
3260	0.60321	1.54771	1.71468	0.63012	1.59621	1.72840	0.65688	1.64374	1.74114	3260
3270	0.60032	1.54246	1.71315	0.62717	1.59092	1.72694	0.65386	1.63841	1.73974	3270
3280	0.59745	1.53723	1.71161	0.62423	1.58565	1.72547	0.65086	1.63310	1.73834	3280
3290	0.59459	1.53202	1.71008	0.62131	1.58040	1.72401	0.64787	1.62781	1.73694	3290
3300	0.59175	1.52684	1.70854	0.61840	1.57517	1.72254	0.64490	1.62254	1.73554	3300
3310	0.58892	1.52167	1.70699	0.61551	1.56996	1.72106	0.64194	1.61729	1.73413	3310
3320	0.58611	1.51652	1.70545	0.61263	1.56477	1.71959	0.63901	1.61206	1.73272	3320
3330	0.58332	1.51139	1.70390	0.60977	1.55960	1.71811	0.63608	1.60685	1.73131	3330
3340	0.58054	1.50629	1.70235	0.60693	1.55445	1.71663	0.63318	1.60166	1.72990	3340
3350	0.57778	1.50120	1.70079	0.60410	1.54932	1.71514	0.63028	1.59649	1.72848	3350
3360	0.57503	1.49613	1.69923	0.60128	1.54421	1.71366	0.62741	1.59135	1.72706	3360
3370	0.57229	1.49109	1.69767	0.59848	1.53912	1.71217	0.62455	1.58621	1.72563	3370
3380	0.56957	1.48606	1.69611	0.59570	1.53405	1.71067	0.62170	1.58110	1.72421	3380
3390	0.56687	1.48105	1.69454	0.59293	1.52899	1.70918	0.61887	1.57601	1.72278	3390
3400	0.56418	1.47606	1.69297	0.59018	1.52396	1.70768	0.61605	1.57094	1.72134	3400
3410	0.56151	1.47109	1.69140	0.58744	1.51895	1.70618	0.61325	1.56589	1.71991	3410
3420	0.55885	1.46614	1.68983	0.58471	1.51396	1.70467	0.61047	1.56085	1.71847	3420
3430	0.55620	1.46121	1.68825	0.58201	1.50898	1.70317	0.60769	1.55584	1.71703	3430
3440	0.55357	1.45630	1.68667	0.57931	1.50402	1.70166	0.60494	1.55084	1.71559	3440
3450	0.55095	1.45140	1.68509	0.57663	1.49909	1.70014	0.60219	1.54586	1.71414	3450
3460	0.54835	1.44653	1.68350	0.57396	1.49417	1.69863	0.59947	1.54090	1.71269	3460
3470	0.54576	1.44167	1.68191	0.57131	1.48927	1.69711	0.59675	1.53596	1.71124	3470
3480	0.54319	1.43683	1.68032	0.56867	1.48439	1.69559	0.59405	1.53104	1.70979	3480
3490	0.54062	1.43202	1.67872	0.56605	1.47952	1.69407	0.59137	1.52614	1.70833	3490
3500	0.53808	1.42721	1.67713	0.56344	1.47468	1.69254	0.58870	1.52125	1.70687	3500
3510	0.53554	1.42243	1.67553	0.56084	1.46985	1.69101	0.58604	1.51638	1.70541	3510
3520	0.53302	1.41767	1.67392	0.55826	1.46504	1.68948	0.58339	1.51153	1.70394	3520
3530	0.53052	1.41292	1.67232	0.55569	1.46025	1.68794	0.58076	1.50670	1.70247	3530
3540	0.52802	1.40819	1.67071	0.55313	1.45548	1.68641	0.57815	1.50189	1.70100	3540
3550	0.52554	1.40348	1.66910	0.55059	1.45073	1.68487	0.57555	1.49709	1.69953	3550
3560	0.52308	1.39879	1.66748	0.54806	1.44599	1.68332	0.57296	1.49231	1.69805	3560
3570	0.52062	1.39411	1.66587	0.54554	1.44127	1.68178	0.57038	1.48755	1.69658	3570
3580	0.51818	1.38946	1.66425	0.54304	1.43657	1.68023	0.56782	1.48281	1.69510	3580
3590	0.51576	1.38482	1.66263	0.54055	1.43188	1.67868	0.56527	1.47808	1.69361	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=3500.			T=3600.			T=3700.				
3600	0.51334	1.38019	1.66100	0.53808	1.42721	1.67713	0.56273	1.47337	1.69213	3600
3610	0.51094	1.37559	1.65937	0.53561	1.42256	1.67557	0.56021	1.46868	1.69064	3610
3620	0.50855	1.37100	1.65774	0.53316	1.41793	1.67401	0.55770	1.46401	1.68915	3620
3630	0.50618	1.36643	1.65611	0.53073	1.41332	1.67245	0.55520	1.45935	1.68765	3630
3640	0.50381	1.36188	1.65448	0.52830	1.40872	1.67089	0.55272	1.45471	1.68616	3640
3650	0.50146	1.35734	1.65284	0.52589	1.40413	1.66932	0.55025	1.45008	1.68466	3650
3660	0.49912	1.35282	1.65120	0.52349	1.39957	1.66775	0.54779	1.44548	1.68316	3660
3670	0.49680	1.34832	1.64956	0.52110	1.39502	1.66618	0.54534	1.44089	1.68165	3670
3680	0.49448	1.34383	1.64791	0.51873	1.39049	1.66461	0.54291	1.43631	1.68015	3680
3690	0.49218	1.33936	1.64627	0.51636	1.38597	1.66303	0.54049	1.43176	1.67864	3690
3700	0.48989	1.33491	1.64462	0.51401	1.38148	1.66145	0.53808	1.42721	1.67713	3700
3710	0.48761	1.33047	1.64296	0.51167	1.37699	1.65987	0.53568	1.42269	1.67561	3710
3720	0.48535	1.32605	1.64131	0.50935	1.37253	1.65829	0.53330	1.41818	1.67410	3720
3730	0.48309	1.32165	1.63965	0.50703	1.36808	1.65670	0.53092	1.41369	1.67258	3730
3740	0.48085	1.31726	1.63799	0.50473	1.36364	1.65511	0.52856	1.40921	1.67106	3740
3750	0.47862	1.31289	1.63633	0.50244	1.35923	1.65352	0.52621	1.40475	1.66953	3750
3760	0.47640	1.30853	1.63466	0.50016	1.35483	1.65193	0.52388	1.40031	1.66801	3760
3770	0.47419	1.30419	1.63300	0.49789	1.35044	1.65033	0.52155	1.39588	1.66648	3770
3780	0.47200	1.29987	1.63133	0.49564	1.34607	1.64874	0.51924	1.39147	1.66495	3780
3790	0.46981	1.29556	1.62966	0.49339	1.34172	1.64713	0.51694	1.38707	1.66341	3790
3800	0.46764	1.29127	1.62798	0.49116	1.33738	1.64553	0.51465	1.38269	1.66188	3800
3810	0.46548	1.28699	1.62630	0.48894	1.33306	1.64393	0.51237	1.37832	1.66034	3810
3820	0.46333	1.28273	1.62463	0.48673	1.32875	1.64232	0.51010	1.37397	1.65880	3820
3830	0.46119	1.27849	1.62294	0.48453	1.32446	1.64071	0.50784	1.36964	1.65726	3830
3840	0.45906	1.27426	1.62126	0.48234	1.32018	1.63910	0.50560	1.36532	1.65571	3840
3850	0.45694	1.27004	1.61957	0.48017	1.31592	1.63748	0.50337	1.36102	1.65417	3850
3860	0.45484	1.26584	1.61789	0.47800	1.31167	1.63587	0.50114	1.35673	1.65262	3860
3870	0.45274	1.26166	1.61620	0.47585	1.30744	1.63425	0.49893	1.35245	1.65107	3870
3880	0.45066	1.25749	1.61450	0.47370	1.30323	1.63263	0.49673	1.34819	1.64951	3880
3890	0.44858	1.25334	1.61281	0.47157	1.29903	1.63100	0.49454	1.34395	1.64796	3890
3900	0.44652	1.24920	1.61111	0.46945	1.29484	1.62938	0.49237	1.33972	1.64640	3900
3910	0.44447	1.24507	1.60941	0.46734	1.29067	1.62775	0.49020	1.33551	1.64484	3910
3920	0.44242	1.24097	1.60771	0.46524	1.28652	1.62612	0.48804	1.33131	1.64328	3920
3930	0.44039	1.23687	1.60601	0.46315	1.28238	1.62449	0.48590	1.32712	1.64171	3930
3940	0.43837	1.23279	1.60430	0.46107	1.27825	1.62285	0.48376	1.32295	1.64014	3940
3950	0.43636	1.22873	1.60259	0.45900	1.27414	1.62121	0.48164	1.31880	1.63857	3950
3960	0.43436	1.22468	1.60088	0.45694	1.27004	1.61957	0.47952	1.31466	1.63700	3960
3970	0.43237	1.22064	1.59917	0.45489	1.26596	1.61793	0.47742	1.31053	1.63543	3970
3980	0.43039	1.21662	1.59746	0.45286	1.26189	1.61629	0.47533	1.30642	1.63385	3980
3990	0.42842	1.21262	1.59574	0.45083	1.25784	1.61464	0.47324	1.30232	1.63227	3990
4000	0.42646	1.20862	1.59402	0.44881	1.25380	1.61300	0.47117	1.29824	1.63069	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=3800.			T=3900.			T=4000.				
100	6.54305	8.49284	1.98693	6.59371	8.54445	1.98695	6.64311	8.59476	1.98696	100
110	6.35739	8.30347	1.98688	6.40796	8.35508	1.98690	6.45726	8.40538	1.98691	110
120	6.18822	8.13059	1.98683	6.23869	8.18220	1.98685	6.28791	8.23250	1.98686	120
130	6.03289	7.97156	1.98677	6.08327	8.02317	1.98679	6.13240	8.07347	1.98681	130
140	5.88936	7.82433	1.98670	5.93964	7.87593	1.98673	5.98868	7.92623	1.98675	140
150	5.75599	7.68726	1.98664	5.80617	7.73886	1.98666	5.85512	7.78916	1.98669	150
160	5.63146	7.55905	1.98656	5.68155	7.61065	1.98659	5.73041	7.66095	1.98662	160
170	5.51471	7.43862	1.98648	5.56471	7.49022	1.98652	5.61348	7.54051	1.98655	170
180	5.40485	7.32507	1.98640	5.45475	7.37667	1.98644	5.50343	7.42696	1.98648	180
190	5.30113	7.21768	1.98631	5.35093	7.26927	1.98636	5.39952	7.31956	1.98640	190
200	5.20292	7.11579	1.98622	5.25263	7.16739	1.98627	5.30113	7.21768	1.98631	200
210	5.10967	7.01889	1.98612	5.15929	7.07048	1.98618	5.20770	7.12077	1.98622	210
220	5.02094	6.92650	1.98602	5.07047	6.97809	1.98608	5.11879	7.02837	1.98613	220
230	4.93632	6.83822	1.98591	4.98575	6.88980	1.98598	5.03398	6.94008	1.98604	230
240	4.85545	6.75370	1.98580	4.90479	6.80528	1.98587	4.95293	6.85556	1.98594	240
250	4.77803	6.67264	1.98569	4.82728	6.72422	1.98576	4.87533	6.77449	1.98583	250
260	4.70380	6.59476	1.98557	4.75295	6.64634	1.98565	4.80091	6.69661	1.98572	260
270	4.63250	6.51983	1.98544	4.68156	6.57140	1.98553	4.72943	6.62167	1.98561	270
280	4.56393	6.44762	1.98531	4.61289	6.49919	1.98540	4.66068	6.54946	1.98549	280
290	4.49789	6.37796	1.98517	4.54676	6.42952	1.98528	4.59446	6.47979	1.98537	290
300	4.43421	6.31066	1.98503	4.48299	6.36222	1.98514	4.53060	6.41248	1.98524	300
310	4.37274	6.24557	1.98489	4.42143	6.29713	1.98501	4.46895	6.34739	1.98511	310
320	4.31334	6.18256	1.98474	4.36193	6.23411	1.98486	4.40937	6.28437	1.98498	320
330	4.25588	6.12149	1.98459	4.30438	6.17304	1.98472	4.35173	6.22329	1.98484	330
340	4.20024	6.06224	1.98443	4.24865	6.11379	1.98457	4.29590	6.16404	1.98470	340
350	4.14631	6.00472	1.98426	4.19463	6.05627	1.98441	4.24180	6.10651	1.98455	350
360	4.09401	5.94883	1.98410	4.14224	6.00037	1.98425	4.18932	6.05060	1.98440	360
370	4.04324	5.89447	1.98392	4.09137	5.94600	1.98409	4.13837	5.99624	1.98424	370
380	3.99392	5.84156	1.98375	4.04196	5.89309	1.98392	4.08887	5.94332	1.98408	380
390	3.94597	5.79003	1.98356	3.99392	5.84156	1.98375	4.04074	5.89179	1.98391	390
400	3.89933	5.73982	1.98338	3.94719	5.79134	1.98357	3.99392	5.84156	1.98375	400
410	3.85393	5.69084	1.98318	3.90169	5.74236	1.98339	3.94834	5.79258	1.98357	410
420	3.80971	5.64306	1.98299	3.85738	5.69457	1.98320	3.90394	5.74478	1.98339	420
430	3.76661	5.59640	1.98279	3.81419	5.64790	1.98301	3.86066	5.69811	1.98321	430
440	3.72458	5.55082	1.98258	3.77207	5.60232	1.98281	3.81846	5.65252	1.98303	440
450	3.68358	5.50627	1.98237	3.73098	5.55776	1.98261	3.77728	5.60796	1.98284	450
460	3.64356	5.46270	1.98215	3.69087	5.51419	1.98241	3.73708	5.56438	1.98264	460
470	3.60447	5.42007	1.98193	3.65169	5.47156	1.98220	3.69782	5.52174	1.98244	470
480	3.56629	5.37835	1.98171	3.61341	5.42983	1.98199	3.65945	5.48001	1.98224	480
490	3.52896	5.33749	1.98148	3.57600	5.38896	1.98177	3.62195	5.43914	1.98203	490
500	3.49246	5.29746	1.98125	3.53940	5.34893	1.98154	3.58527	5.39910	1.98182	500
510	3.45675	5.25823	1.98101	3.50360	5.30969	1.98132	3.54939	5.35986	1.98161	510
520	3.42180	5.21976	1.98076	3.46857	5.27122	1.98109	3.51426	5.32138	1.98139	520
530	3.38759	5.18203	1.98051	3.43426	5.23348	1.98085	3.47987	5.28364	1.98116	530
540	3.35408	5.14502	1.98026	3.40066	5.19646	1.98061	3.44619	5.24661	1.98093	540
550	3.32125	5.10868	1.98000	3.36774	5.16012	1.98037	3.41318	5.21026	1.98070	550
560	3.28907	5.07301	1.97974	3.33548	5.12444	1.98012	3.38083	5.17458	1.98046	560
570	3.25753	5.03797	1.97947	3.30384	5.08939	1.97986	3.34911	5.13952	1.98022	570
580	3.22659	5.00355	1.97920	3.27282	5.05496	1.97961	3.31800	5.10509	1.97998	580
590	3.19625	4.96972	1.97893	3.24238	5.02112	1.97934	3.28748	5.07124	1.97973	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
T=3800.			T=3900.			T=4000.				
600	3.16647	4.93646	1.97865	3.21252	4.98786	1.97908	3.25753	5.03797	1.97947	600
610	3.13724	4.90375	1.97836	3.18320	4.95515	1.97880	3.22813	5.00525	1.97922	610
620	3.10855	4.87159	1.97807	3.15441	4.92298	1.97853	3.19926	4.97307	1.97895	620
630	3.08036	4.83994	1.97777	3.12614	4.89132	1.97825	3.17090	4.94141	1.97869	630
640	3.05268	4.80880	1.97747	3.09837	4.86017	1.97796	3.14304	4.91025	1.97842	640
650	3.02548	4.77814	1.97717	3.07108	4.82950	1.97767	3.11567	4.87958	1.97814	650
660	2.99875	4.74796	1.97686	3.04426	4.79931	1.97738	3.08877	4.84938	1.97786	660
670	2.97247	4.71823	1.97655	3.01789	4.76958	1.97708	3.06231	4.81964	1.97758	670
680	2.94663	4.68895	1.97623	2.99197	4.74029	1.97678	3.03630	4.79034	1.97729	680
690	2.92122	4.66010	1.97591	2.96647	4.71143	1.97647	3.01072	4.76148	1.97700	690
700	2.89623	4.63167	1.97558	2.94138	4.68300	1.97616	2.98555	4.73304	1.97670	700
710	2.87163	4.60365	1.97525	2.91670	4.65497	1.97585	2.96079	4.70500	1.97640	710
720	2.84743	4.57603	1.97491	2.89242	4.62734	1.97553	2.93642	4.67736	1.97610	720
730	2.82361	4.54879	1.97457	2.86851	4.60009	1.97520	2.91243	4.65010	1.97579	730
740	2.80016	4.52193	1.97422	2.84497	4.57322	1.97487	2.88881	4.62322	1.97548	740
750	2.77708	4.49543	1.97387	2.82180	4.54671	1.97454	2.86555	4.59671	1.97516	750
760	2.75434	4.46929	1.97351	2.79897	4.52056	1.97420	2.84264	4.57055	1.97484	760
770	2.73194	4.44349	1.97315	2.77649	4.49475	1.97386	2.82007	4.54474	1.97452	770
780	2.70988	4.41803	1.97279	2.75434	4.46929	1.97351	2.79784	4.51926	1.97419	780
790	2.68814	4.39290	1.97242	2.73251	4.44415	1.97316	2.77593	4.49411	1.97385	790
800	2.66672	4.36810	1.97205	2.71100	4.41933	1.97281	2.75434	4.46929	1.97351	800
810	2.64560	4.34360	1.97167	2.68980	4.39483	1.97245	2.73305	4.44477	1.97317	810
820	2.62479	4.31941	1.97128	2.66890	4.37063	1.97208	2.71207	4.42056	1.97283	820
830	2.60427	4.29552	1.97090	2.64829	4.34672	1.97172	2.69138	4.39665	1.97248	830
840	2.58403	4.27192	1.97050	2.62797	4.32311	1.97134	2.67098	4.37303	1.97212	840
850	2.56408	4.24860	1.97011	2.60793	4.29979	1.97097	2.65035	4.34970	1.97176	850
860	2.54440	4.22556	1.96970	2.58816	4.27674	1.97058	2.63100	4.32664	1.97140	860
870	2.52498	4.20279	1.96930	2.56866	4.25396	1.97020	2.61142	4.30385	1.97103	870
880	2.50582	4.18029	1.96889	2.54942	4.23144	1.96981	2.59209	4.28132	1.97066	880
890	2.48692	4.15804	1.96847	2.53043	4.20919	1.96941	2.57302	4.25906	1.97029	890
900	2.46827	4.13605	1.96805	2.51169	4.18718	1.96901	2.55420	4.23705	1.96991	900
910	2.44986	4.11430	1.96763	2.49319	4.16543	1.96861	2.53563	4.21528	1.96952	910
920	2.43169	4.09280	1.96720	2.47494	4.14391	1.96820	2.51729	4.19376	1.96913	920
930	2.41375	4.07154	1.96676	2.45691	4.12264	1.96779	2.49918	4.17247	1.96874	930
940	2.39603	4.05051	1.96633	2.43911	4.10159	1.96737	2.48130	4.15142	1.96835	940
950	2.37854	4.02970	1.96588	2.42154	4.08078	1.96695	2.46364	4.13059	1.96795	950
960	2.36127	4.00912	1.96543	2.40418	4.06018	1.96653	2.44621	4.10999	1.96754	960
970	2.34421	3.98875	1.96498	2.38704	4.03981	1.96610	2.42898	4.08960	1.96713	970
980	2.32736	3.96860	1.96453	2.37010	4.01964	1.96566	2.41196	4.06942	1.96672	980
990	2.31071	3.94866	1.96406	2.35337	3.99969	1.96523	2.39515	4.04946	1.96630	990
1000	2.29427	3.92892	1.96360	2.33684	3.97994	1.96478	2.37854	4.02970	1.96588	1000
1010	2.27802	3.90938	1.96313	2.32051	3.96039	1.96434	2.36213	4.01014	1.96546	1010
1020	2.26196	3.89005	1.96265	2.30437	3.94104	1.96389	2.34591	3.99078	1.96503	1020
1030	2.24610	3.87090	1.96217	2.28841	3.92188	1.96343	2.32988	3.97161	1.96459	1030
1040	2.23041	3.85194	1.96169	2.27265	3.90292	1.96297	2.31403	3.95263	1.96416	1040
1050	2.21491	3.83317	1.96120	2.25706	3.88413	1.96251	2.29836	3.93384	1.96372	1050
1060	2.19959	3.81459	1.96071	2.24165	3.86553	1.96204	2.28287	3.91522	1.96327	1060
1070	2.18444	3.79618	1.96021	2.22642	3.84711	1.96157	2.26756	3.89679	1.96282	1070
1080	2.16946	3.77795	1.95971	2.21136	3.82887	1.96109	2.25242	3.87854	1.96237	1080
1090	2.15465	3.75989	1.95920	2.19647	3.81080	1.96061	2.23745	3.86045	1.96191	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
T=3800.			T=3900.			T=4000.				
1100	2.14001	3.74200	1.95869	2.18174	3.79289	1.96012	2.22264	3.84254	1.96145	1100
1110	2.12552	3.72427	1.95818	2.16717	3.77516	1.95963	2.20799	3.82479	1.96098	1110
1120	2.11120	3.70671	1.95766	2.15276	3.75758	1.95914	2.19351	3.80720	1.96051	1120
1130	2.09703	3.68931	1.95713	2.13851	3.74017	1.95864	2.17918	3.78978	1.96004	1130
1140	2.08302	3.67207	1.95660	2.12442	3.72292	1.95814	2.16500	3.77251	1.95956	1140
1150	2.06915	3.65499	1.95607	2.11047	3.70582	1.95763	2.15097	3.75540	1.95908	1150
1160	2.05544	3.63805	1.95553	2.09667	3.68887	1.95712	2.13710	3.73844	1.95859	1160
1170	2.04186	3.62127	1.95499	2.08302	3.67207	1.95660	2.12336	3.72163	1.95810	1170
1180	2.02844	3.60463	1.95444	2.06951	3.65542	1.95608	2.10977	3.70497	1.95760	1180
1190	2.01515	3.58814	1.95389	2.05614	3.63892	1.95556	2.09633	3.68845	1.95711	1190
1200	2.00200	3.57179	1.95333	2.04290	3.62256	1.95503	2.08302	3.67207	1.95660	1200
1210	1.98898	3.55559	1.95277	2.02981	3.60633	1.95450	2.06984	3.65584	1.95610	1210
1220	1.97610	3.53952	1.95221	2.01684	3.59025	1.95396	2.05680	3.63974	1.95558	1220
1230	1.96335	3.52358	1.95164	2.00401	3.57430	1.95342	2.04389	3.62378	1.95507	1230
1240	1.95073	3.50778	1.95107	1.99131	3.55848	1.95287	2.03111	3.60795	1.95455	1240
1250	1.93824	3.49211	1.95049	1.97873	3.54280	1.95232	2.01846	3.59225	1.95403	1250
1260	1.92587	3.47657	1.94990	1.96628	3.52725	1.95177	2.00593	3.57668	1.95350	1260
1270	1.91362	3.46116	1.94932	1.95396	3.51182	1.95121	1.99352	3.56124	1.95297	1270
1280	1.90150	3.44587	1.94873	1.94175	3.49652	1.95065	1.98124	3.54593	1.95243	1280
1290	1.88949	3.43071	1.94813	1.92966	3.48134	1.95008	1.96907	3.53074	1.95190	1290
1300	1.87760	3.41567	1.94753	1.91769	3.46628	1.94951	1.95703	3.51567	1.95135	1300
1310	1.86583	3.40075	1.94693	1.90584	3.45135	1.94894	1.94510	3.50071	1.95081	1310
1320	1.85417	3.38595	1.94632	1.89410	3.43653	1.94836	1.93328	3.48588	1.95025	1320
1330	1.84262	3.37126	1.94570	1.88247	3.42183	1.94778	1.92157	3.47116	1.94970	1330
1340	1.83118	3.35669	1.94508	1.87095	3.40724	1.94719	1.90997	3.45656	1.94914	1340
1350	1.81985	3.34223	1.94446	1.85954	3.39276	1.94660	1.89849	3.44207	1.94858	1350
1360	1.80863	3.32788	1.94384	1.84823	3.37840	1.94600	1.88711	3.42769	1.94801	1360
1370	1.79751	3.31364	1.94320	1.83703	3.36415	1.94540	1.87583	3.41342	1.94744	1370
1380	1.78649	3.29951	1.94257	1.82594	3.35000	1.94480	1.86466	3.39926	1.94686	1380
1390	1.77558	3.28549	1.94193	1.81495	3.33596	1.94419	1.85359	3.38521	1.94629	1390
1400	1.76477	3.27157	1.94129	1.80405	3.32202	1.94358	1.84262	3.37126	1.94570	1400
1410	1.75405	3.25775	1.94064	1.79326	3.30819	1.94296	1.83175	3.35741	1.94512	1410
1420	1.74344	3.24404	1.93998	1.78256	3.29446	1.94234	1.82098	3.34367	1.94452	1420
1430	1.73292	3.23043	1.93933	1.77197	3.28084	1.94172	1.81030	3.33002	1.94393	1430
1440	1.72249	3.21692	1.93867	1.76146	3.26731	1.94109	1.79972	3.31648	1.94333	1440
1450	1.71216	3.20350	1.93800	1.75105	3.25388	1.94045	1.78924	3.30303	1.94273	1450
1460	1.70192	3.19019	1.93733	1.74073	3.24054	1.93982	1.77884	3.28968	1.94212	1460
1470	1.69177	3.17696	1.93665	1.73050	3.22730	1.93917	1.76854	3.27643	1.94151	1470
1480	1.68172	3.16384	1.93598	1.72037	3.21416	1.93853	1.75833	3.26327	1.94090	1480
1490	1.67175	3.15080	1.93529	1.71032	3.20111	1.93788	1.74820	3.25020	1.94028	1490
1500	1.66186	3.13786	1.93460	1.70036	3.18815	1.93723	1.73817	3.23722	1.93966	1500
1510	1.65207	3.12501	1.93391	1.69048	3.17528	1.93657	1.72822	3.22434	1.93903	1510
1520	1.64235	3.11224	1.93322	1.68069	3.16250	1.93591	1.71835	3.21154	1.93840	1520
1530	1.63272	3.09957	1.93252	1.67098	3.14980	1.93524	1.70857	3.19883	1.93777	1530
1540	1.62318	3.08698	1.93181	1.66136	3.13720	1.93457	1.69887	3.18621	1.93713	1540
1550	1.61371	3.07448	1.93110	1.65182	3.12468	1.93390	1.68925	3.17367	1.93648	1550
1560	1.60433	3.06206	1.93039	1.64235	3.11224	1.93322	1.67971	3.16122	1.93584	1560
1570	1.59502	3.04973	1.92967	1.63297	3.09989	1.93253	1.67026	3.14885	1.93519	1570
1580	1.58580	3.03748	1.92895	1.62367	3.08763	1.93185	1.66088	3.13657	1.93454	1580
1590	1.57665	3.02531	1.92822	1.61444	3.07544	1.93116	1.65158	3.12437	1.93388	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
T=3800.			T=3900.			T=4000.				
1600	1.56757	3.01323	1.92749	1.60529	3.06333	1.93046	1.64235	3.11224	1.93322	1600
1610	1.55858	3.00122	1.92676	1.59621	3.05131	1.92976	1.63320	3.10020	1.93255	1610
1620	1.54965	2.98929	1.92602	1.58721	3.03936	1.92906	1.62413	3.08824	1.93188	1620
1630	1.54080	2.97744	1.92528	1.57828	3.02749	1.92835	1.61513	3.07635	1.93121	1630
1640	1.53203	2.96567	1.92453	1.56943	3.01570	1.92764	1.60620	3.06454	1.93053	1640
1650	1.52332	2.95397	1.92378	1.56065	3.00398	1.92693	1.59734	3.05281	1.92985	1650
1660	1.51468	2.94235	1.92302	1.55193	2.99234	1.92621	1.58856	3.04115	1.92917	1660
1670	1.50612	2.93080	1.92226	1.54329	2.98078	1.92549	1.57984	3.02956	1.92848	1670
1680	1.49762	2.91933	1.92150	1.53472	2.96928	1.92476	1.57119	3.01805	1.92779	1680
1690	1.48919	2.90793	1.92073	1.52621	2.95786	1.92403	1.56262	3.00661	1.92709	1690
1700	1.48083	2.89660	1.91996	1.51778	2.94651	1.92329	1.55411	2.99525	1.92639	1700
1710	1.47254	2.88534	1.91918	1.50940	2.93523	1.92256	1.54566	2.98395	1.92569	1710
1720	1.46431	2.87415	1.91840	1.50110	2.92403	1.92181	1.53728	2.97272	1.92498	1720
1730	1.45614	2.86303	1.91762	1.49286	2.91289	1.92107	1.52897	2.96157	1.92427	1730
1740	1.44804	2.85198	1.91683	1.48468	2.90182	1.92032	1.52072	2.95048	1.92355	1740
1750	1.44001	2.84100	1.91603	1.47657	2.89082	1.91956	1.51254	2.93946	1.92283	1750
1760	1.43203	2.83008	1.91524	1.46852	2.87988	1.91880	1.50441	2.92850	1.92211	1760
1770	1.42412	2.81923	1.91443	1.46053	2.86901	1.91804	1.49635	2.91761	1.92138	1770
1780	1.41627	2.80845	1.91363	1.45260	2.85821	1.91727	1.48835	2.90679	1.92065	1780
1790	1.40848	2.79773	1.91282	1.44474	2.84747	1.91650	1.48042	2.89603	1.91992	1790
1800	1.40074	2.78708	1.91201	1.43693	2.83679	1.91573	1.47254	2.88534	1.91918	1800
1810	1.39307	2.77649	1.91119	1.42918	2.82618	1.91495	1.46472	2.87471	1.91844	1810
1820	1.38546	2.76596	1.91036	1.42149	2.81563	1.91417	1.45696	2.86414	1.91769	1820
1830	1.37790	2.75550	1.90954	1.41386	2.80515	1.91338	1.44925	2.85363	1.91695	1830
1840	1.37040	2.74509	1.90871	1.40629	2.79472	1.91259	1.44161	2.84319	1.91619	1840
1850	1.36296	2.73475	1.90787	1.39877	2.78436	1.91180	1.43402	2.83281	1.91544	1850
1860	1.35557	2.72447	1.90704	1.39131	2.77405	1.91100	1.42649	2.82248	1.91468	1860
1870	1.34824	2.71424	1.90619	1.38390	2.76381	1.91020	1.41901	2.81222	1.91391	1870
1880	1.34096	2.70408	1.90535	1.37655	2.75362	1.90939	1.41158	2.80201	1.91314	1880
1890	1.33374	2.69397	1.90450	1.36925	2.74350	1.90858	1.40422	2.79187	1.91237	1890
1900	1.32657	2.68392	1.90364	1.36201	2.73343	1.90777	1.39690	2.78178	1.91160	1900
1910	1.31945	2.67393	1.90278	1.35482	2.72341	1.90695	1.38964	2.77174	1.91082	1910
1920	1.31238	2.66400	1.90192	1.34768	2.71346	1.90613	1.38243	2.76177	1.91003	1920
1930	1.30537	2.65412	1.90105	1.34059	2.70356	1.90530	1.37527	2.75185	1.90925	1930
1940	1.29841	2.64430	1.90018	1.33355	2.69371	1.90447	1.36816	2.74198	1.90846	1940
1950	1.29149	2.63453	1.89931	1.32657	2.68392	1.90364	1.36111	2.73217	1.90766	1950
1960	1.28463	2.62482	1.89843	1.31963	2.67419	1.90280	1.35410	2.72242	1.90687	1960
1970	1.27782	2.61516	1.89754	1.31274	2.66451	1.90196	1.34714	2.71271	1.90607	1970
1980	1.27105	2.60555	1.89666	1.30591	2.65488	1.90112	1.34024	2.70306	1.90526	1980
1990	1.26434	2.59600	1.89577	1.29912	2.64530	1.90027	1.33338	2.69347	1.90445	1990
2000	1.25767	2.58650	1.89487	1.29238	2.63578	1.89942	1.32657	2.68392	1.90364	2000
2010	1.25105	2.57705	1.89397	1.28568	2.62631	1.89856	1.31980	2.67443	1.90282	2010
2020	1.24448	2.56766	1.89307	1.27904	2.61689	1.89770	1.31309	2.66499	1.90200	2020
2030	1.23795	2.55831	1.89216	1.27244	2.60752	1.89684	1.30642	2.65560	1.90118	2030
2040	1.23147	2.54901	1.89125	1.26588	2.59820	1.89597	1.29980	2.64626	1.90035	2040
2050	1.22503	2.53977	1.89034	1.25938	2.58893	1.89510	1.29322	2.63697	1.89952	2050
2060	1.21864	2.53057	1.88942	1.25291	2.57971	1.89423	1.28669	2.62773	1.89869	2060
2070	1.21229	2.52142	1.88849	1.24649	2.57054	1.89335	1.28020	2.61854	1.89785	2070
2080	1.20599	2.51232	1.88757	1.24012	2.56142	1.89246	1.27375	2.60939	1.89701	2080
2090	1.19973	2.50327	1.88664	1.23379	2.55235	1.89158	1.26736	2.60029	1.89617	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ^o	C _p ^o	$-(F^0-E_0^0)/T$	S ^o	C _p ^o	$-(F^0-E_0^0)/T$	S ^o	C _p ^o	ν cm ⁻¹
T=3800.			T=3900.			T=4000.				
2100	1.19352	2.49427	1.88570	1.22750	2.54332	1.89069	1.26100	2.59125	1.89532	2100
2110	1.18735	2.48531	1.88476	1.22126	2.53434	1.88979	1.25469	2.58224	1.89447	2110
2120	1.18122	2.47641	1.88382	1.21506	2.52541	1.88890	1.24842	2.57329	1.89361	2120
2130	1.17513	2.46754	1.88288	1.20890	2.51652	1.88800	1.24219	2.56438	1.89275	2130
2140	1.16908	2.45873	1.88193	1.20278	2.50768	1.88709	1.23600	2.55552	1.89189	2140
2150	1.16307	2.44995	1.88097	1.19670	2.49888	1.88618	1.22985	2.54670	1.89102	2150
2160	1.15711	2.44123	1.88002	1.19066	2.49013	1.88527	1.22375	2.53792	1.89015	2160
2170	1.15118	2.43255	1.87905	1.18467	2.48143	1.88435	1.21769	2.52920	1.88928	2170
2180	1.14530	2.42391	1.87809	1.17871	2.47276	1.88344	1.21166	2.52051	1.88840	2180
2190	1.13945	2.41532	1.87712	1.17280	2.46415	1.88251	1.20568	2.51187	1.88752	2190
2200	1.13365	2.40677	1.87615	1.16692	2.45557	1.88158	1.19973	2.50327	1.88664	2200
2210	1.12788	2.39826	1.87517	1.16108	2.44704	1.88065	1.19383	2.49472	1.88575	2210
2220	1.12215	2.38980	1.87419	1.15528	2.43855	1.87972	1.18796	2.48621	1.88486	2220
2230	1.11646	2.38138	1.87320	1.14952	2.43011	1.87878	1.18213	2.47774	1.88396	2230
2240	1.11081	2.37300	1.87222	1.14380	2.42170	1.87784	1.17634	2.46931	1.88307	2240
2250	1.10519	2.36466	1.87122	1.13811	2.41334	1.87689	1.17059	2.46093	1.88216	2250
2260	1.09961	2.35636	1.87023	1.13246	2.40502	1.87595	1.16487	2.45258	1.88126	2260
2270	1.09407	2.34811	1.86923	1.12685	2.39674	1.87499	1.15919	2.44428	1.88035	2270
2280	1.08856	2.33989	1.86822	1.12127	2.38850	1.87404	1.15355	2.43601	1.87944	2280
2290	1.08309	2.33172	1.86722	1.11573	2.38030	1.87308	1.14794	2.42779	1.87852	2290
2300	1.07766	2.32359	1.86621	1.11023	2.37214	1.87211	1.14237	2.41961	1.87760	2300
2310	1.07226	2.31549	1.86519	1.10476	2.36402	1.87115	1.13684	2.41146	1.87668	2310
2320	1.06689	2.30744	1.86417	1.09932	2.35594	1.87018	1.13134	2.40336	1.87576	2320
2330	1.06156	2.29942	1.86315	1.09393	2.34790	1.86920	1.12587	2.39529	1.87483	2330
2340	1.05627	2.29145	1.86212	1.08856	2.33989	1.86822	1.12044	2.38727	1.87389	2340
2350	1.05100	2.28351	1.86110	1.08323	2.33193	1.86724	1.11504	2.37928	1.87296	2350
2360	1.04578	2.27561	1.86006	1.07793	2.32400	1.86626	1.10968	2.37133	1.87202	2360
2370	1.04058	2.26774	1.85902	1.07267	2.31611	1.86527	1.10435	2.36341	1.87107	2370
2380	1.03542	2.25992	1.85798	1.06744	2.30826	1.86428	1.09905	2.35554	1.87013	2380
2390	1.03029	2.25213	1.85694	1.06224	2.30045	1.86328	1.09379	2.34770	1.86918	2390
2400	1.02520	2.24438	1.85589	1.05708	2.29267	1.86228	1.08856	2.33989	1.86822	2400
2410	1.02013	2.23666	1.85484	1.05195	2.28493	1.86128	1.08336	2.33213	1.86727	2410
2420	1.01510	2.22899	1.85378	1.04685	2.27722	1.86027	1.07820	2.32440	1.86631	2420
2430	1.01010	2.22134	1.85273	1.04178	2.26955	1.85926	1.07306	2.31670	1.86534	2430
2440	1.00513	2.21374	1.85166	1.03674	2.26192	1.85825	1.06796	2.30905	1.86438	2440
2450	1.00019	2.20617	1.85060	1.03174	2.25432	1.85723	1.06289	2.30142	1.86341	2450
2460	0.99529	2.19863	1.84953	1.02676	2.24676	1.85621	1.05785	2.29383	1.86243	2460
2470	0.99041	2.19113	1.84845	1.02182	2.23923	1.85519	1.05284	2.28628	1.86146	2470
2480	0.98556	2.18366	1.84738	1.01690	2.23174	1.85416	1.04786	2.27876	1.86048	2480
2490	0.98075	2.17623	1.84630	1.01202	2.22428	1.85313	1.04292	2.27128	1.85949	2490
2500	0.97596	2.16883	1.84521	1.00717	2.21685	1.85210	1.03800	2.26383	1.85850	2500
2510	0.97120	2.16147	1.84412	1.00234	2.20946	1.85106	1.03311	2.25641	1.85751	2510
2520	0.96648	2.15414	1.84303	0.99755	2.20210	1.85002	1.02825	2.24902	1.85652	2520
2530	0.96178	2.14684	1.84194	0.99278	2.19478	1.84898	1.02342	2.24167	1.85552	2530
2540	0.95711	2.13958	1.84084	0.98805	2.18749	1.84793	1.01862	2.23436	1.85452	2540
2550	0.95247	2.13235	1.83974	0.98334	2.18023	1.84688	1.01385	2.22707	1.85352	2550
2560	0.94786	2.12515	1.83863	0.97866	2.17300	1.84582	1.00910	2.21982	1.85251	2560
2570	0.94327	2.11798	1.83752	0.97401	2.16581	1.84477	1.00439	2.21260	1.85150	2570
2580	0.93871	2.11085	1.83641	0.96938	2.15865	1.84370	0.99970	2.20541	1.85049	2580
2590	0.93418	2.10375	1.83529	0.96479	2.15152	1.84264	0.99504	2.19825	1.84947	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=3800.			T=3900.			T=4000.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S°	C° _P	$-(F^0-E_0^0)/T$	S°	C° _P	$-(F^0-E_0^0)/T$	S°	C° _P	
2600	0.92968	2.09668	1.83417	0.96022	2.14442	1.84157	0.99041	2.19113	1.84845	2600
2610	0.92521	2.08964	1.83305	0.95568	2.13735	1.84050	0.98581	2.18403	1.84743	2610
2620	0.92076	2.08263	1.83192	0.95116	2.13031	1.83942	0.98123	2.17697	1.84640	2620
2630	0.91634	2.07565	1.83079	0.94668	2.12331	1.83835	0.97668	2.16994	1.84537	2630
2640	0.91194	2.06871	1.82966	0.94222	2.11633	1.83726	0.97215	2.16294	1.84434	2640
2650	0.90757	2.06179	1.82852	0.93778	2.10939	1.83618	0.96766	2.15597	1.84330	2650
2660	0.90323	2.05491	1.82738	0.93337	2.10248	1.83509	0.96319	2.14903	1.84227	2660
2670	0.89892	2.04805	1.82624	0.92899	2.09559	1.83400	0.95874	2.14212	1.84122	2670
2680	0.89462	2.04123	1.82509	0.92464	2.08874	1.83290	0.95432	2.13524	1.84018	2680
2690	0.89036	2.03443	1.82394	0.92030	2.08191	1.83181	0.94993	2.12838	1.83913	2690
2700	0.88612	2.02767	1.82278	0.91600	2.07512	1.83071	0.94556	2.12156	1.83808	2700
2710	0.88190	2.02093	1.82163	0.91172	2.06835	1.82960	0.94122	2.11477	1.83702	2710
2720	0.87771	2.01422	1.82047	0.90746	2.06162	1.82849	0.93690	2.10800	1.83596	2720
2730	0.87355	2.00754	1.81930	0.90323	2.05491	1.82738	0.93261	2.10127	1.83490	2730
2740	0.86940	2.00089	1.81813	0.89903	2.04823	1.82627	0.92834	2.09456	1.83384	2740
2750	0.86529	1.99427	1.81696	0.89484	2.04158	1.82515	0.92409	2.08788	1.83277	2750
2760	0.86119	1.98768	1.81579	0.89069	2.03495	1.82403	0.91987	2.08123	1.83170	2760
2770	0.85712	1.98112	1.81461	0.88655	2.02836	1.82290	0.91568	2.07461	1.83062	2770
2780	0.85308	1.97458	1.81343	0.88244	2.02179	1.82178	0.91150	2.06801	1.82955	2780
2790	0.84905	1.96807	1.81224	0.87835	2.01525	1.82064	0.90736	2.06145	1.82846	2790
2800	0.84506	1.96159	1.81106	0.87429	2.00874	1.81951	0.90323	2.05491	1.82738	2800
2810	0.84108	1.95513	1.80987	0.87025	2.00226	1.81837	0.89913	2.04839	1.82629	2810
2820	0.83713	1.94871	1.80867	0.86623	1.99580	1.81723	0.89505	2.04191	1.82520	2820
2830	0.83320	1.94230	1.80747	0.86224	1.98937	1.81609	0.89100	2.03545	1.82411	2830
2840	0.82929	1.93593	1.80627	0.85827	1.98296	1.81494	0.88696	2.02902	1.82302	2840
2850	0.82540	1.92958	1.80507	0.85432	1.97659	1.81379	0.88295	2.02261	1.82192	2850
2860	0.82154	1.92326	1.80386	0.85039	1.97024	1.81264	0.87897	2.01623	1.82081	2860
2870	0.81770	1.91697	1.80265	0.84649	1.96391	1.81148	0.87500	2.00988	1.81971	2870
2880	0.81388	1.91070	1.80143	0.84261	1.95761	1.81032	0.87106	2.00355	1.81860	2880
2890	0.81008	1.90446	1.80022	0.83875	1.95134	1.80916	0.86714	1.99725	1.81749	2890
2900	0.80631	1.89824	1.79900	0.83491	1.94509	1.80800	0.86324	1.99097	1.81638	2900
2910	0.80255	1.89205	1.79777	0.83109	1.93887	1.80683	0.85936	1.98472	1.81526	2910
2920	0.79882	1.88589	1.79655	0.82729	1.93267	1.80565	0.85550	1.97850	1.81414	2920
2930	0.79510	1.87975	1.79532	0.82352	1.92650	1.80448	0.85167	1.97230	1.81301	2930
2940	0.79141	1.87363	1.79408	0.81976	1.92036	1.80330	0.84785	1.96612	1.81189	2940
2950	0.78774	1.86754	1.79285	0.81603	1.91423	1.80212	0.84406	1.95997	1.81076	2950
2960	0.78409	1.86148	1.79161	0.81232	1.90814	1.80094	0.84029	1.95384	1.80963	2960
2970	0.78046	1.85544	1.79036	0.80863	1.90207	1.79975	0.83654	1.94774	1.80849	2970
2980	0.77685	1.84942	1.78912	0.80496	1.89602	1.79856	0.83280	1.94167	1.80735	2980
2990	0.77326	1.84343	1.78787	0.80130	1.89000	1.79736	0.82909	1.93561	1.80621	2990
3000	0.76970	1.83746	1.78662	0.79767	1.88400	1.79617	0.82540	1.92958	1.80507	3000
3010	0.76615	1.83152	1.78536	0.79406	1.87802	1.79497	0.82173	1.92358	1.80392	3010
3020	0.76262	1.82560	1.78410	0.79047	1.87207	1.79377	0.81808	1.91760	1.80277	3020
3030	0.75911	1.81970	1.78284	0.78690	1.86614	1.79256	0.81445	1.91164	1.80162	3030
3040	0.75562	1.81383	1.78157	0.78335	1.86024	1.79135	0.81084	1.90571	1.80046	3040
3050	0.75214	1.80798	1.78031	0.77981	1.85436	1.79014	0.80725	1.89980	1.79930	3050
3060	0.74869	1.80216	1.77904	0.77630	1.84850	1.78893	0.80367	1.89391	1.79814	3060
3070	0.74526	1.79636	1.77776	0.77281	1.84266	1.78771	0.80012	1.88804	1.79698	3070
3080	0.74184	1.79058	1.77648	0.76933	1.83685	1.78649	0.79659	1.88220	1.79581	3080
3090	0.73845	1.78482	1.77520	0.76587	1.83106	1.78526	0.79307	1.87638	1.79464	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
	T=3800.			T=3900.			T=4000.			
3100	0.73507	1.77909	1.77392	0.76244	1.82530	1.78404	0.78958	1.87059	1.79346	3100
3110	0.73171	1.77338	1.77264	0.75902	1.81955	1.78281	0.78610	1.86481	1.79229	3110
3120	0.72837	1.76769	1.77135	0.75562	1.81383	1.78157	0.78264	1.85906	1.79111	3120
3130	0.72505	1.76202	1.77005	0.75223	1.80813	1.78034	0.77920	1.85333	1.78993	3130
3140	0.72175	1.75638	1.76876	0.74887	1.80246	1.77910	0.77578	1.84762	1.78874	3140
3150	0.71846	1.75075	1.76746	0.74552	1.79680	1.77786	0.77237	1.84194	1.78756	3150
3160	0.71519	1.74515	1.76616	0.74219	1.79117	1.77662	0.76898	1.83627	1.78636	3160
3170	0.71194	1.73958	1.76485	0.73888	1.78556	1.77537	0.76562	1.83063	1.78517	3170
3180	0.70871	1.73402	1.76355	0.73559	1.77997	1.77412	0.76226	1.82501	1.78398	3180
3190	0.70549	1.72848	1.76224	0.73231	1.77440	1.77287	0.75893	1.81941	1.78278	3190
3200	0.70230	1.72297	1.76092	0.72906	1.76885	1.77161	0.75562	1.81383	1.78157	3200
3210	0.69911	1.71748	1.75961	0.72582	1.76333	1.77035	0.75232	1.80828	1.78037	3210
3220	0.69595	1.71201	1.75829	0.72259	1.75782	1.76909	0.74904	1.80274	1.77916	3220
3230	0.69280	1.70656	1.75697	0.71939	1.75234	1.76783	0.74577	1.79722	1.77795	3230
3240	0.68967	1.70113	1.75564	0.71620	1.74688	1.76656	0.74253	1.79173	1.77674	3240
3250	0.68656	1.69572	1.75431	0.71302	1.74143	1.76529	0.73930	1.78626	1.77552	3250
3260	0.68346	1.69033	1.75298	0.70987	1.73601	1.76402	0.73608	1.78080	1.77431	3260
3270	0.68038	1.68497	1.75165	0.70673	1.73061	1.76274	0.73289	1.77537	1.77309	3270
3280	0.67732	1.67962	1.75031	0.70361	1.72523	1.76146	0.72971	1.76996	1.77186	3280
3290	0.67427	1.67429	1.74898	0.70050	1.71987	1.76018	0.72654	1.76457	1.77064	3290
3300	0.67124	1.66899	1.74763	0.69741	1.71453	1.75890	0.72340	1.75920	1.76941	3300
3310	0.66822	1.66370	1.74629	0.69433	1.70921	1.75761	0.72027	1.75384	1.76817	3310
3320	0.66522	1.65844	1.74494	0.69128	1.70391	1.75632	0.71715	1.74851	1.76694	3320
3330	0.66224	1.65319	1.74359	0.68823	1.69863	1.75503	0.71405	1.74320	1.76570	3330
3340	0.65927	1.64796	1.74224	0.68521	1.69337	1.75374	0.71097	1.73791	1.76446	3340
3350	0.65632	1.64276	1.74088	0.68220	1.68813	1.75244	0.70790	1.73263	1.76322	3350
3360	0.65338	1.63757	1.73952	0.67920	1.68291	1.75114	0.70485	1.72738	1.76197	3360
3370	0.65046	1.63240	1.73816	0.67622	1.67770	1.74983	0.70182	1.72215	1.76073	3370
3380	0.64756	1.62725	1.73680	0.67326	1.67252	1.74853	0.69880	1.71693	1.75948	3380
3390	0.64467	1.62213	1.73543	0.67031	1.66736	1.74722	0.69579	1.71173	1.75822	3390
3400	0.64179	1.61702	1.73406	0.66738	1.66221	1.74591	0.69280	1.70656	1.75697	3400
3410	0.63893	1.61193	1.73269	0.66446	1.65709	1.74459	0.68983	1.70140	1.75571	3410
3420	0.63608	1.60685	1.73131	0.66155	1.65198	1.74328	0.68687	1.69626	1.75445	3420
3430	0.63325	1.60180	1.72993	0.65867	1.64689	1.74196	0.68393	1.69114	1.75318	3430
3440	0.63044	1.59677	1.72855	0.65579	1.64182	1.74064	0.68100	1.68604	1.75192	3440
3450	0.62763	1.59175	1.72717	0.65293	1.63677	1.73931	0.67808	1.68095	1.75065	3450
3460	0.62485	1.58675	1.72578	0.65009	1.63174	1.73799	0.67518	1.67589	1.74938	3460
3470	0.62207	1.58178	1.72439	0.64726	1.62673	1.73666	0.67230	1.67084	1.74810	3470
3480	0.61931	1.57681	1.72300	0.64444	1.62173	1.73532	0.66943	1.66581	1.74683	3480
3490	0.61657	1.57187	1.72161	0.64164	1.61675	1.73399	0.66657	1.66080	1.74555	3490
3500	0.61384	1.56695	1.72021	0.63886	1.61180	1.73265	0.66373	1.65581	1.74427	3500
3510	0.61112	1.56204	1.71881	0.63608	1.60685	1.73131	0.66090	1.65084	1.74298	3510
3520	0.60842	1.55716	1.71741	0.63332	1.60193	1.72997	0.65809	1.64588	1.74169	3520
3530	0.60573	1.55229	1.71600	0.63058	1.59702	1.72862	0.65529	1.64094	1.74041	3530
3540	0.60306	1.54743	1.71460	0.62785	1.59214	1.72728	0.65251	1.63602	1.73911	3540
3550	0.60040	1.54260	1.71319	0.62513	1.58727	1.72592	0.64973	1.63111	1.73782	3550
3560	0.59775	1.53778	1.71177	0.62243	1.58241	1.72457	0.64698	1.62623	1.73652	3560
3570	0.59512	1.53298	1.71036	0.61974	1.57758	1.72322	0.64423	1.62136	1.73522	3570
3580	0.59250	1.52820	1.70894	0.61706	1.57276	1.72186	0.64150	1.61651	1.73392	3580
3590	0.58989	1.52343	1.70752	0.61440	1.56796	1.72050	0.63879	1.61167	1.73262	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ - E_0^\circ)/T$	S°	C _p ^o	$-(F^\circ - E_0^\circ)/T$	S°	C _p ^o	$-(F^\circ - E_0^\circ)/T$	S°	C _p ^o	ν cm ⁻¹
	T=3800.			T=3900.			T=4000.			
3600	0.58730	1.51869	1.70610	0.61175	1.56317	1.71913	0.63608	1.60685	1.73131	3600
3610	0.58471	1.51396	1.70467	0.60911	1.55841	1.71777	0.63339	1.60205	1.73000	3610
3620	0.58215	1.50924	1.70325	0.60649	1.55366	1.71640	0.63072	1.59727	1.72869	3620
3630	0.57959	1.50455	1.70182	0.60388	1.54892	1.71503	0.62805	1.59250	1.72738	3630
3640	0.57705	1.49987	1.70038	0.60128	1.54421	1.71366	0.62540	1.58775	1.72606	3640
3650	0.57452	1.49520	1.69895	0.59870	1.53951	1.71228	0.62277	1.58302	1.72474	3650
3660	0.57201	1.49056	1.69751	0.59613	1.53483	1.71090	0.62014	1.57830	1.72342	3660
3670	0.56950	1.48593	1.69607	0.59357	1.53016	1.70952	0.61753	1.57360	1.72210	3670
3680	0.56701	1.48131	1.69463	0.59102	1.52551	1.70814	0.61493	1.56892	1.72077	3680
3690	0.56453	1.47672	1.69318	0.58849	1.52088	1.70676	0.61234	1.56425	1.71944	3690
3700	0.56207	1.47214	1.69173	0.58597	1.51626	1.70537	0.60977	1.55960	1.71811	3700
3710	0.55961	1.46757	1.69028	0.58346	1.51166	1.70398	0.60721	1.55496	1.71678	3710
3720	0.55717	1.46302	1.68883	0.58097	1.50707	1.70259	0.60466	1.55034	1.71544	3720
3730	0.55474	1.45849	1.68738	0.57848	1.50250	1.70119	0.60213	1.54574	1.71410	3730
3740	0.55233	1.45398	1.68592	0.57601	1.49795	1.69979	0.59960	1.54115	1.71276	3740
3750	0.54992	1.44948	1.68446	0.57355	1.49341	1.69839	0.59709	1.53658	1.71142	3750
3760	0.54753	1.44499	1.68300	0.57111	1.48889	1.69699	0.59459	1.53202	1.71008	3760
3770	0.54515	1.44052	1.68153	0.56867	1.48439	1.69559	0.59210	1.52748	1.70873	3770
3780	0.54278	1.43607	1.68007	0.56625	1.47990	1.69418	0.58963	1.52296	1.70738	3780
3790	0.54042	1.43164	1.67860	0.56384	1.47542	1.69277	0.58717	1.51845	1.70603	3790
3800	0.53808	1.42721	1.67713	0.56144	1.47096	1.69136	0.58471	1.51396	1.70467	3800
3810	0.53574	1.42281	1.67565	0.55905	1.46652	1.68995	0.58228	1.50948	1.70332	3810
3820	0.53342	1.41842	1.67418	0.55667	1.46209	1.68853	0.57985	1.50501	1.70196	3820
3830	0.53111	1.41404	1.67270	0.55431	1.45768	1.68712	0.57743	1.50057	1.70060	3830
3840	0.52881	1.40968	1.67122	0.55196	1.45328	1.68569	0.57503	1.49613	1.69923	3840
3850	0.52652	1.40534	1.66973	0.54962	1.44890	1.68427	0.57263	1.49172	1.69787	3850
3860	0.52424	1.40101	1.66825	0.54729	1.44453	1.68285	0.57025	1.48731	1.69650	3860
3870	0.52198	1.39669	1.66676	0.54497	1.44018	1.68142	0.56788	1.48293	1.69513	3870
3880	0.51972	1.39240	1.66527	0.54266	1.43584	1.67999	0.56552	1.47855	1.69376	3880
3890	0.51748	1.38811	1.66378	0.54036	1.43152	1.67856	0.56318	1.47420	1.69239	3890
3900	0.51525	1.38384	1.66228	0.53808	1.42721	1.67713	0.56084	1.46985	1.69101	3900
3910	0.51303	1.37959	1.66079	0.53580	1.42292	1.67569	0.55851	1.46552	1.68963	3910
3920	0.51082	1.37535	1.65929	0.53354	1.41864	1.67425	0.55620	1.46121	1.68825	3920
3930	0.50861	1.37112	1.65779	0.53129	1.41438	1.67281	0.55390	1.45691	1.68687	3930
3940	0.50643	1.36691	1.65628	0.52904	1.41013	1.67137	0.55160	1.45262	1.68548	3940
3950	0.50425	1.36271	1.65478	0.52681	1.40589	1.66992	0.54932	1.44835	1.68409	3950
3960	0.50208	1.35853	1.65327	0.52459	1.40167	1.66848	0.54705	1.44410	1.68270	3960
3970	0.49992	1.35436	1.65176	0.52238	1.39747	1.66703	0.54479	1.43986	1.68131	3970
3980	0.49777	1.35021	1.65025	0.52019	1.39328	1.66558	0.54254	1.43563	1.67992	3980
3990	0.49564	1.34607	1.64874	0.51800	1.38910	1.66412	0.54030	1.43141	1.67852	3990
4000	0.49351	1.34195	1.64722	0.51582	1.38493	1.66267	0.53808	1.42721	1.67713	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=4100.			T=4200.			T=4300.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	$-(F^0-E_0^0)/T$	S°	C _p ^o	
100	6.69131	8.64382	1.98696	6.73837	8.69170	1.98698	6.78435	8.73846	1.98699	100
110	6.50538	8.45444	1.98692	6.55236	8.50232	1.98694	6.59825	8.54908	1.98695	110
120	6.33594	8.28156	1.98688	6.38283	8.32944	1.98689	6.42865	8.37619	1.98690	120
130	6.18034	8.12253	1.98682	6.22716	8.17041	1.98684	6.27289	8.21716	1.98686	130
140	6.03653	7.97529	1.98677	6.08327	8.02317	1.98679	6.12893	8.06992	1.98681	140
150	5.90289	7.83822	1.98671	5.94954	7.88609	1.98673	5.99512	7.93284	1.98675	150
160	5.77810	7.71000	1.98665	5.82467	7.75787	1.98667	5.87017	7.80462	1.98669	160
170	5.66108	7.58956	1.98658	5.70757	7.63744	1.98661	5.75299	7.68418	1.98663	170
180	5.55095	7.47602	1.98651	5.59735	7.52389	1.98654	5.64270	7.57063	1.98657	180
190	5.44696	7.36861	1.98643	5.49328	7.41648	1.98647	5.53855	7.46322	1.98650	190
200	5.34847	7.26672	1.98635	5.39472	7.31459	1.98639	5.43991	7.36133	1.98643	200
210	5.25496	7.16981	1.98627	5.30113	7.21768	1.98631	5.34624	7.26442	1.98635	210
220	5.16596	7.07741	1.98618	5.21205	7.12528	1.98623	5.25709	7.17201	1.98627	220
230	5.08107	6.98912	1.98609	5.12707	7.03699	1.98614	5.17204	7.08372	1.98619	230
240	4.99994	6.90460	1.98600	5.04586	6.95246	1.98605	5.09074	6.99919	1.98610	240
250	4.92225	6.82353	1.98590	4.96809	6.87139	1.98596	5.01290	6.91812	1.98601	250
260	4.84775	6.74564	1.98579	4.89351	6.79350	1.98586	4.93824	6.84023	1.98592	260
270	4.77619	6.67070	1.98568	4.82187	6.71855	1.98575	4.86652	6.76528	1.98582	270
280	4.70735	6.59849	1.98557	4.75295	6.64634	1.98565	4.79753	6.69306	1.98572	280
290	4.64104	6.52881	1.98546	4.68656	6.57666	1.98554	4.73107	6.62338	1.98561	290
300	4.57710	6.46151	1.98534	4.62254	6.50935	1.98542	4.66697	6.55607	1.98550	300
310	4.51537	6.39641	1.98521	4.56073	6.44425	1.98530	4.60508	6.49096	1.98539	310
320	4.45570	6.33338	1.98508	4.50098	6.38122	1.98518	4.54525	6.42793	1.98527	320
330	4.39797	6.27230	1.98495	4.44317	6.32013	1.98505	4.48737	6.36685	1.98515	330
340	4.34207	6.21305	1.98481	4.38719	6.26088	1.98492	4.43131	6.30758	1.98503	340
350	4.28788	6.15551	1.98467	4.33292	6.20334	1.98479	4.37696	6.25004	1.98490	350
360	4.23532	6.09960	1.98453	4.28028	6.14743	1.98465	4.32424	6.19413	1.98477	360
370	4.18428	6.04523	1.98438	4.22916	6.09305	1.98451	4.27305	6.13975	1.98463	370
380	4.13470	5.99232	1.98423	4.17950	6.04013	1.98437	4.22331	6.08683	1.98449	380
390	4.08649	5.94078	1.98407	4.13121	5.98859	1.98422	4.17495	6.03528	1.98435	390
400	4.03958	5.89055	1.98391	4.08423	5.93836	1.98406	4.12789	5.98504	1.98421	400
410	3.99392	5.84156	1.98375	4.03848	5.88937	1.98391	4.08207	5.93605	1.98406	410
420	3.94944	5.79376	1.98358	3.99392	5.84156	1.98375	4.03743	5.88824	1.98390	420
430	3.90608	5.74709	1.98340	3.95048	5.79488	1.98358	3.99392	5.84156	1.98375	430
440	3.86379	5.70149	1.98323	3.90812	5.74928	1.98341	3.95148	5.79596	1.98358	440
450	3.82253	5.65692	1.98305	3.86678	5.70471	1.98324	3.91006	5.75138	1.98342	450
460	3.78225	5.61334	1.98286	3.82642	5.66113	1.98306	3.86963	5.70779	1.98325	460
470	3.74290	5.57070	1.98267	3.78699	5.61848	1.98288	3.83013	5.66514	1.98308	470
480	3.70446	5.52896	1.98248	3.74847	5.57673	1.98270	3.79153	5.62339	1.98290	480
490	3.66687	5.48808	1.98228	3.71080	5.53585	1.98251	3.75379	5.58251	1.98272	490
500	3.63011	5.44804	1.98208	3.67397	5.49580	1.98232	3.71688	5.54245	1.98254	500
510	3.59414	5.40879	1.98187	3.63792	5.45655	1.98212	3.68076	5.50319	1.98235	510
520	3.55894	5.37031	1.98166	3.60264	5.41806	1.98192	3.64540	5.46470	1.98216	520
530	3.52447	5.33256	1.98145	3.56809	5.38031	1.98172	3.61078	5.42695	1.98197	530
540	3.49070	5.29553	1.98123	3.53424	5.34327	1.98151	3.57686	5.38990	1.98177	540
550	3.45761	5.25918	1.98101	3.50108	5.30692	1.98130	3.54362	5.35354	1.98157	550
560	3.42518	5.22348	1.98079	3.46857	5.27122	1.98109	3.51103	5.31784	1.98137	560
570	3.39338	5.18843	1.98056	3.43669	5.23616	1.98087	3.47908	5.28277	1.98116	570
580	3.36219	5.15398	1.98032	3.40542	5.20171	1.98065	3.44774	5.24822	1.98094	580
590	3.33159	5.12013	1.98009	3.37474	5.16785	1.98042	3.41699	5.21445	1.98073	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹	
T=4100.			T=4200.			T=4300.					
600	3.30155	5.08685	1.97984	3.34463	5.13457	1.98019	3.38680	5.18117	1.98051	600	
610	3.27207	5.05413	1.97960	3.31507	5.10184	1.97995	3.35717	5.14843	1.98029	610	
620	3.24312	5.02194	1.97935	3.28604	5.06964	1.97972	3.32807	5.11623	1.98006	620	
630	3.21468	4.99027	1.97910	3.25753	5.03797	1.97947	3.29948	5.08455	1.97983	630	
640	3.18675	4.95911	1.97884	3.22951	5.00680	1.97923	3.27139	5.05338	1.97959	640	
650	3.15929	4.92843	1.97858	3.20198	4.97611	1.97898	3.24379	5.02269	1.97936	650	
660	3.13231	4.89823	1.97831	3.17492	4.94590	1.97873	3.21665	4.99247	1.97911	660	
670	3.10577	4.86848	1.97804	3.14831	4.91615	1.97847	3.18997	4.96271	1.97887	670	
680	3.07968	4.83917	1.97777	3.12215	4.88684	1.97821	3.16373	4.93339	1.97862	680	
690	3.05402	4.81030	1.97749	3.09641	4.85796	1.97794	3.13792	4.90451	1.97837	690	
700	3.02877	4.78185	1.97721	3.07108	4.82950	1.97767	3.11252	4.87604	1.97811	700	
710	3.00393	4.75381	1.97692	3.04616	4.80145	1.97740	3.08753	4.84799	1.97785	710	
720	2.97948	4.72616	1.97663	3.02163	4.77380	1.97713	3.06292	4.82033	1.97759	720	
730	2.95541	4.69890	1.97634	2.99749	4.74653	1.97685	3.03871	4.79305	1.97732	730	
740	2.93171	4.67201	1.97604	2.97371	4.71963	1.97656	3.01486	4.76615	1.97705	740	
750	2.90837	4.64549	1.97574	2.95030	4.69311	1.97627	2.99137	4.73961	1.97677	750	
760	2.88538	4.61932	1.97543	2.92723	4.66693	1.97598	2.96823	4.71343	1.97650	760	
770	2.86273	4.59350	1.97512	2.90451	4.64110	1.97569	2.94544	4.68760	1.97621	770	
780	2.84042	4.56802	1.97481	2.88212	4.61561	1.97539	2.92298	4.66210	1.97593	780	
790	2.81843	4.54286	1.97449	2.86006	4.59045	1.97509	2.90084	4.63693	1.97564	790	
800	2.79676	4.51803	1.97417	2.83831	4.56561	1.97478	2.87903	4.61208	1.97535	800	
810	2.77540	4.49350	1.97384	2.81688	4.54108	1.97447	2.85752	4.58754	1.97505	810	
820	2.75434	4.46929	1.97351	2.79574	4.51685	1.97415	2.83631	4.56331	1.97475	820	
830	2.73357	4.44537	1.97318	2.77490	4.49292	1.97384	2.81539	4.53938	1.97445	830	
840	2.71309	4.42174	1.97284	2.75434	4.46929	1.97351	2.79476	4.51573	1.97414	840	
850	2.69289	4.39839	1.97250	2.73406	4.44593	1.97319	2.77441	4.49237	1.97383	850	
860	2.67296	4.37532	1.97216	2.71406	4.42286	1.97286	2.75434	4.46929	1.97351	860	
870	2.65329	4.35253	1.97181	2.69432	4.40005	1.97253	2.73453	4.44647	1.97320	870	
880	2.63389	4.32999	1.97145	2.67484	4.37751	1.97219	2.71498	4.42392	1.97287	880	
890	2.61474	4.30772	1.97109	2.65562	4.35523	1.97185	2.69569	4.40163	1.97255	890	
900	2.59584	4.28570	1.97073	2.63665	4.33320	1.97150	2.67664	4.37960	1.97222	900	
910	2.57719	4.26392	1.97037	2.61792	4.31141	1.97115	2.65784	4.35780	1.97189	910	
920	2.55877	4.24239	1.97000	2.59943	4.28987	1.97080	2.63928	4.33626	1.97155	920	
930	2.54059	4.22110	1.96963	2.58117	4.26857	1.97045	2.62095	4.31494	1.97121	930	
940	2.52263	4.20003	1.96925	2.56314	4.24750	1.97009	2.60285	4.29386	1.97087	940	
950	2.50490	4.17920	1.96887	2.54533	4.22665	1.96972	2.58497	4.27301	1.97052	950	
960	2.48738	4.15858	1.96848	2.52774	4.20603	1.96936	2.56731	4.25238	1.97017	960	
970	2.47008	4.13818	1.96809	2.51036	4.18562	1.96899	2.54986	4.23196	1.96982	970	
980	2.45298	4.11800	1.96770	2.49319	4.16543	1.96861	2.53262	4.21176	1.96946	980	
990	2.43610	4.09803	1.96730	2.47623	4.14544	1.96823	2.51559	4.19177	1.96910	990	
1000	2.41941	4.07825	1.96690	2.45947	4.12566	1.96785	2.49876	4.17198	1.96873	1000	
1010	2.40292	4.05869	1.96650	2.44291	4.10609	1.96746	2.48213	4.15239	1.96836	1010	
1020	2.38662	4.03931	1.96609	2.42654	4.08670	1.96707	2.46569	4.13300	1.96799	1020	
1030	2.37051	4.02013	1.96568	2.41035	4.06751	1.96668	2.44943	4.11380	1.96762	1030	
1040	2.35459	4.00114	1.96526	2.39436	4.04851	1.96628	2.43337	4.09479	1.96724	1040	
1050	2.33885	3.98234	1.96484	2.37854	4.02970	1.96588	2.41748	4.07597	1.96685	1050	
1060	2.32328	3.96372	1.96441	2.36291	4.01107	1.96548	2.40178	4.05733	1.96647	1060	
1070	2.30789	3.94527	1.96399	2.34744	3.99261	1.96507	2.38624	4.03887	1.96608	1070	
1080	2.29268	3.92701	1.96355	2.33215	3.97434	1.96466	2.37088	4.02058	1.96568	1080	
1090	2.27763	3.90891	1.96312	2.31703	3.95623	1.96424	2.35569	4.00246	1.96529	1090	

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=4100.			T=4200.			T=4300.			ν cm ⁻¹
	$-(F^\circ - E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ - E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ - E_0^\circ)/T$	S ^o	C _p ^o	
1100	2.26274	3.89098	1.96268	2.30208	3.93829	1.96382	2.34067	3.98452	1.96489	1100
1110	2.24802	3.87322	1.96223	2.28728	3.92052	1.96340	2.32580	3.96674	1.96448	1110
1120	2.23346	3.85563	1.96178	2.27265	3.90292	1.96297	2.31110	3.94912	1.96408	1120
1130	2.21905	3.83819	1.96133	2.25817	3.88547	1.96254	2.29655	3.93166	1.96366	1130
1140	2.20480	3.82091	1.96088	2.24384	3.86818	1.96211	2.28216	3.91436	1.96325	1140
1150	2.19070	3.80379	1.96042	2.22967	3.85105	1.96167	2.26792	3.89722	1.96283	1150
1160	2.17675	3.78682	1.95995	2.21565	3.83406	1.96123	2.25382	3.88023	1.96241	1160
1170	2.16294	3.77000	1.95949	2.20177	3.81723	1.96078	2.23987	3.86338	1.96198	1170
1180	2.14927	3.75332	1.95902	2.18803	3.80055	1.96033	2.22607	3.84669	1.96155	1180
1190	2.13575	3.73679	1.95854	2.17443	3.78400	1.95988	2.21241	3.83014	1.96112	1190
1200	2.12237	3.72040	1.95806	2.16098	3.76761	1.95942	2.19888	3.81373	1.96069	1200
1210	2.10912	3.70416	1.95758	2.14766	3.75135	1.95896	2.18549	3.79746	1.96025	1210
1220	2.09600	3.68805	1.95709	2.13447	3.73522	1.95850	2.17223	3.78132	1.95980	1220
1230	2.08302	3.67207	1.95660	2.12141	3.71924	1.95803	2.15911	3.76533	1.95936	1230
1240	2.07016	3.65623	1.95611	2.10849	3.70339	1.95756	2.14612	3.74946	1.95891	1240
1250	2.05743	3.64052	1.95561	2.09569	3.68766	1.95708	2.13325	3.73373	1.95845	1250
1260	2.04483	3.62494	1.95511	2.08302	3.67207	1.95660	2.12051	3.71813	1.95800	1260
1270	2.03235	3.60949	1.95460	2.07047	3.65661	1.95612	2.10789	3.70265	1.95753	1270
1280	2.01999	3.59416	1.95409	2.05804	3.64127	1.95563	2.09539	3.68730	1.95707	1280
1290	2.00775	3.57895	1.95358	2.04573	3.62605	1.95514	2.08302	3.67207	1.95660	1290
1300	1.99563	3.56387	1.95306	2.03353	3.61095	1.95465	2.07076	3.65697	1.95613	1300
1310	1.98363	3.54891	1.95254	2.02146	3.59598	1.95415	2.05861	3.64198	1.95566	1310
1320	1.97174	3.53406	1.95201	2.00950	3.58112	1.95365	2.04658	3.62711	1.95518	1320
1330	1.95996	3.51933	1.95149	1.99765	3.56638	1.95315	2.03466	3.61235	1.95470	1330
1340	1.94829	3.50471	1.95095	1.98591	3.55175	1.95264	2.02286	3.59771	1.95421	1340
1350	1.93672	3.49021	1.95042	1.97427	3.53723	1.95213	2.01116	3.58319	1.95372	1350
1360	1.92527	3.47582	1.94988	1.96275	3.52283	1.95161	1.99957	3.56877	1.95323	1360
1370	1.91392	3.46154	1.94933	1.95133	3.50853	1.95109	1.98808	3.55446	1.95273	1370
1380	1.90268	3.44736	1.94878	1.94002	3.49434	1.95057	1.97670	3.54026	1.95223	1380
1390	1.89153	3.43329	1.94823	1.92880	3.48026	1.95004	1.96542	3.52617	1.95173	1390
1400	1.88049	3.41933	1.94768	1.91769	3.46628	1.94951	1.95424	3.51218	1.95123	1400
1410	1.86955	3.40547	1.94712	1.90668	3.45241	1.94898	1.94316	3.49829	1.95072	1410
1420	1.85871	3.39171	1.94655	1.89577	3.43864	1.94844	1.93218	3.48451	1.95020	1420
1430	1.84796	3.37805	1.94599	1.88495	3.42497	1.94790	1.92130	3.47082	1.94969	1430
1440	1.83731	3.36449	1.94542	1.87423	3.41139	1.94736	1.91051	3.45724	1.94917	1440
1450	1.82675	3.35103	1.94484	1.86360	3.39792	1.94681	1.89982	3.44375	1.94864	1450
1460	1.81628	3.33767	1.94426	1.85306	3.38454	1.94626	1.88922	3.43036	1.94812	1460
1470	1.80591	3.32440	1.94368	1.84262	3.37126	1.94570	1.87870	3.41706	1.94759	1470
1480	1.79562	3.31122	1.94310	1.83227	3.35807	1.94514	1.86828	3.40386	1.94705	1480
1490	1.78542	3.29814	1.94251	1.82200	3.34497	1.94458	1.85795	3.39075	1.94652	1490
1500	1.77532	3.28515	1.94191	1.81182	3.33197	1.94402	1.84771	3.37773	1.94597	1500
1510	1.76529	3.27225	1.94132	1.80173	3.31905	1.94345	1.83755	3.36481	1.94543	1510
1520	1.75536	3.25943	1.94072	1.79173	3.30623	1.94287	1.82748	3.35197	1.94488	1520
1530	1.74550	3.24671	1.94011	1.78180	3.29349	1.94230	1.81749	3.33921	1.94433	1530
1540	1.73573	3.23407	1.93950	1.77197	3.28084	1.94172	1.80759	3.32655	1.94378	1540
1550	1.72604	3.22152	1.93889	1.76221	3.26827	1.94113	1.79777	3.31397	1.94322	1550
1560	1.71643	3.20905	1.93828	1.75253	3.25579	1.94054	1.78802	3.30148	1.94266	1560
1570	1.70691	3.19667	1.93766	1.74294	3.24339	1.93995	1.77836	3.28906	1.94209	1570
1580	1.69746	3.18437	1.93703	1.73342	3.23108	1.93936	1.76878	3.27674	1.94153	1580
1590	1.68808	3.17215	1.93641	1.72398	3.21884	1.93876	1.75927	3.26449	1.94095	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=4100.			T=4200.			T=4300.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S°	C _p ⁰	$-(F^0-E_0^0)/T$	S°	C _p ⁰	$-(F^0-E_0^0)/T$	S°	C _p ⁰	
1600	1.67879	3.16001	1.93578	1.71461	3.20669	1.93816	1.74985	3.25232	1.94038	1600
1610	1.66957	3.14795	1.93514	1.70533	3.19461	1.93755	1.74049	3.24023	1.93980	1610
1620	1.66042	3.13597	1.93450	1.69611	3.18262	1.93694	1.73121	3.22822	1.93922	1620
1630	1.65135	3.12407	1.93386	1.68697	3.17070	1.93633	1.72201	3.21629	1.93863	1630
1640	1.64235	3.11224	1.93322	1.67791	3.15886	1.93572	1.71288	3.20444	1.93805	1640
1650	1.63343	3.10049	1.93257	1.66891	3.14709	1.93510	1.70382	3.19266	1.93745	1650
1660	1.62457	3.08882	1.93192	1.65999	3.13540	1.93447	1.69483	3.18095	1.93686	1660
1670	1.61578	3.07722	1.93126	1.65114	3.12379	1.93385	1.68592	3.16932	1.93626	1670
1680	1.60707	3.06569	1.93060	1.64235	3.11224	1.93322	1.67707	3.15776	1.93566	1680
1690	1.59842	3.05423	1.92993	1.63364	3.10077	1.93258	1.66829	3.14628	1.93505	1690
1700	1.58984	3.04285	1.92927	1.62499	3.08937	1.93195	1.65958	3.13486	1.93444	1700
1710	1.58132	3.03154	1.92860	1.61641	3.07804	1.93131	1.65093	3.12352	1.93383	1710
1720	1.57288	3.02029	1.92792	1.60789	3.06678	1.93066	1.64235	3.11224	1.93322	1720
1730	1.56449	3.00912	1.92724	1.59945	3.05559	1.93001	1.63384	3.10104	1.93260	1730
1740	1.55618	2.99801	1.92656	1.59106	3.04447	1.92936	1.62539	3.08990	1.93198	1740
1750	1.54792	2.98697	1.92588	1.58274	3.03342	1.92871	1.61701	3.07883	1.93135	1750
1760	1.53973	2.97600	1.92519	1.57448	3.02243	1.92805	1.60868	3.06783	1.93072	1760
1770	1.53160	2.96510	1.92449	1.56628	3.01151	1.92739	1.60042	3.05689	1.93009	1770
1780	1.52353	2.95426	1.92380	1.55815	3.00065	1.92672	1.59223	3.04602	1.92945	1780
1790	1.51552	2.94348	1.92310	1.55008	2.98986	1.92606	1.58409	3.03521	1.92882	1790
1800	1.50758	2.93277	1.92239	1.54206	2.97913	1.92538	1.57601	3.02447	1.92817	1800
1810	1.49969	2.92212	1.92169	1.53411	2.96846	1.92471	1.56800	3.01379	1.92753	1810
1820	1.49186	2.91153	1.92098	1.52621	2.95786	1.92403	1.56004	3.00317	1.92688	1820
1830	1.48409	2.90101	1.92026	1.51838	2.94732	1.92335	1.55214	2.99261	1.92623	1830
1840	1.47637	2.89055	1.91954	1.51060	2.93684	1.92266	1.54429	2.98212	1.92557	1840
1850	1.46871	2.88015	1.91882	1.50287	2.92642	1.92197	1.53651	2.97168	1.92491	1850
1860	1.46111	2.86980	1.91810	1.49521	2.91606	1.92128	1.52878	2.96131	1.92425	1860
1870	1.45357	2.85952	1.91737	1.48760	2.90576	1.92058	1.52110	2.95099	1.92359	1870
1880	1.44608	2.84930	1.91663	1.48004	2.89552	1.91988	1.51348	2.94073	1.92292	1880
1890	1.43864	2.83913	1.91590	1.47254	2.88534	1.91918	1.50592	2.93053	1.92225	1890
1900	1.43126	2.82902	1.91516	1.46509	2.87521	1.91848	1.49841	2.92039	1.92157	1900
1910	1.42393	2.81897	1.91441	1.45769	2.86514	1.91777	1.49095	2.91031	1.92089	1910
1920	1.41665	2.80898	1.91367	1.45035	2.85513	1.91705	1.48355	2.90028	1.92021	1920
1930	1.40942	2.79904	1.91292	1.44306	2.84517	1.91634	1.47619	2.89031	1.91953	1930
1940	1.40225	2.78915	1.91216	1.43582	2.83527	1.91562	1.46889	2.88039	1.91884	1940
1950	1.39512	2.77932	1.91141	1.42863	2.82543	1.91489	1.46164	2.87052	1.91815	1950
1960	1.38805	2.76955	1.91065	1.42149	2.81563	1.91417	1.45444	2.86071	1.91745	1960
1970	1.38103	2.75983	1.90988	1.41441	2.80589	1.91344	1.44729	2.85096	1.91675	1970
1980	1.37405	2.75016	1.90911	1.40737	2.79621	1.91270	1.44019	2.84125	1.91605	1980
1990	1.36713	2.74054	1.90834	1.40038	2.78657	1.91197	1.43314	2.83160	1.91535	1990
2000	1.36025	2.73098	1.90757	1.39344	2.77699	1.91123	1.42614	2.82200	1.91464	2000
2010	1.35342	2.72147	1.90679	1.38654	2.76746	1.91048	1.41918	2.81246	1.91393	2010
2020	1.34664	2.71201	1.90601	1.37969	2.75798	1.90974	1.41227	2.80296	1.91322	2020
2030	1.33990	2.70260	1.90522	1.37290	2.74855	1.90899	1.40541	2.79351	1.91250	2030
2040	1.33321	2.69324	1.90443	1.36614	2.73917	1.90823	1.39860	2.78412	1.91178	2040
2050	1.32657	2.68392	1.90364	1.35943	2.72984	1.90747	1.39183	2.77477	1.91105	2050
2060	1.31997	2.67466	1.90284	1.35277	2.72056	1.90671	1.38510	2.76547	1.91033	2060
2070	1.31341	2.66545	1.90204	1.34615	2.71133	1.90595	1.37843	2.75622	1.90960	2070
2080	1.30691	2.65629	1.90124	1.33958	2.70215	1.90518	1.37179	2.74702	1.90886	2080
2090	1.30044	2.64717	1.90044	1.33305	2.69301	1.90441	1.36520	2.73787	1.90813	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	ν cm ⁻¹	
T=4100.			T=4200.			T=4300.					
2100	1.29402	2.63810	1.89963	1.32657	2.68392	1.90364	1.35866	2.72876	1.90739	2100	
2110	1.28764	2.62908	1.89881	1.32012	2.67488	1.90286	1.35215	2.71970	1.90664	2110	
2120	1.28130	2.62010	1.89800	1.31373	2.66589	1.90208	1.34569	2.71069	1.90590	2120	
2130	1.27501	2.61117	1.89718	1.30737	2.65694	1.90130	1.33928	2.70172	1.90515	2130	
2140	1.26876	2.60229	1.89635	1.30105	2.64804	1.90051	1.33290	2.69280	1.90440	2140	
2150	1.26255	2.59345	1.89553	1.29478	2.63918	1.89972	1.32657	2.68392	1.90364	2150	
2160	1.25638	2.58465	1.89470	1.28855	2.63036	1.89893	1.32027	2.67509	1.90288	2160	
2170	1.25025	2.57590	1.89386	1.28236	2.62159	1.89813	1.31402	2.66631	1.90212	2170	
2180	1.24416	2.56720	1.89302	1.27620	2.61287	1.89733	1.30781	2.65756	1.90135	2180	
2190	1.23811	2.55854	1.89218	1.27009	2.60419	1.89653	1.30164	2.64886	1.90059	2190	
2200	1.23210	2.54992	1.89134	1.26402	2.59555	1.89572	1.29551	2.64020	1.89981	2200	
2210	1.22613	2.54134	1.89049	1.25799	2.58695	1.89491	1.28941	2.63159	1.89904	2210	
2220	1.22020	2.53281	1.88964	1.25199	2.57840	1.89410	1.28336	2.62302	1.89826	2220	
2230	1.21430	2.52432	1.88879	1.24604	2.56989	1.89328	1.27735	2.61449	1.89748	2230	
2240	1.20845	2.51587	1.88793	1.24012	2.56142	1.89246	1.27137	2.60600	1.89670	2240	
2250	1.20263	2.50746	1.88707	1.23424	2.55299	1.89164	1.26543	2.59755	1.89591	2250	
2260	1.19685	2.49910	1.88621	1.22840	2.54460	1.89082	1.25953	2.58915	1.89512	2260	
2270	1.19110	2.49077	1.88534	1.22259	2.53626	1.88999	1.25366	2.58078	1.89433	2270	
2280	1.18540	2.48248	1.88447	1.21682	2.52795	1.88915	1.24783	2.57246	1.89353	2280	
2290	1.17973	2.47424	1.88359	1.21109	2.51969	1.88832	1.24204	2.56417	1.89273	2290	
2300	1.17409	2.46603	1.88271	1.20539	2.51146	1.88748	1.23629	2.55593	1.89193	2300	
2310	1.16849	2.45787	1.88183	1.19973	2.50327	1.88664	1.23057	2.54772	1.89112	2310	
2320	1.16293	2.44974	1.88095	1.19411	2.49513	1.88579	1.22488	2.53955	1.89031	2320	
2330	1.15740	2.44165	1.88006	1.18852	2.48702	1.88494	1.21923	2.53142	1.88950	2330	
2340	1.15190	2.43360	1.87917	1.18296	2.47895	1.88409	1.21362	2.52333	1.88869	2340	
2350	1.14644	2.42559	1.87828	1.17744	2.47091	1.88324	1.20804	2.51528	1.88787	2350	
2360	1.14102	2.41762	1.87738	1.17195	2.46292	1.88238	1.20249	2.50727	1.88705	2360	
2370	1.13563	2.40968	1.87648	1.16650	2.45496	1.88152	1.19698	2.49929	1.88623	2370	
2380	1.13027	2.40178	1.87557	1.16108	2.44704	1.88065	1.19150	2.49135	1.88540	2380	
2390	1.12494	2.39392	1.87467	1.15569	2.43916	1.87979	1.18606	2.48345	1.88457	2390	
2400	1.11965	2.38609	1.87376	1.15034	2.43131	1.87892	1.18065	2.47558	1.88373	2400	
2410	1.11439	2.37831	1.87284	1.14502	2.42350	1.87804	1.17527	2.46775	1.88290	2410	
2420	1.10916	2.37055	1.87193	1.13973	2.41572	1.87717	1.16992	2.45995	1.88206	2420	
2430	1.10396	2.36283	1.87100	1.13447	2.40799	1.87629	1.16461	2.45219	1.88122	2430	
2440	1.09880	2.35515	1.87008	1.12925	2.40028	1.87540	1.15932	2.44447	1.88037	2440	
2450	1.09366	2.34751	1.86915	1.12406	2.39261	1.87452	1.15407	2.43678	1.87952	2450	
2460	1.08856	2.33989	1.86822	1.11889	2.38498	1.87363	1.14885	2.42913	1.87867	2460	
2470	1.08349	2.33232	1.86729	1.11376	2.37738	1.87273	1.14366	2.42151	1.87782	2470	
2480	1.07845	2.32477	1.86635	1.10866	2.36982	1.87184	1.13851	2.41392	1.87696	2480	
2490	1.07344	2.31727	1.86541	1.10359	2.36229	1.87094	1.13338	2.40637	1.87610	2490	
2500	1.06846	2.30979	1.86447	1.09855	2.35479	1.87004	1.12828	2.39885	1.87524	2500	
2510	1.06351	2.30235	1.86352	1.09354	2.34732	1.86913	1.12321	2.39137	1.87437	2510	
2520	1.05859	2.29494	1.86258	1.08856	2.33989	1.86822	1.11818	2.38392	1.87350	2520	
2530	1.05370	2.28757	1.86162	1.08361	2.33250	1.86731	1.11317	2.37650	1.87263	2530	
2540	1.04883	2.28023	1.86067	1.07869	2.32513	1.86640	1.10819	2.36911	1.87175	2540	
2550	1.04400	2.27292	1.85971	1.07380	2.31780	1.86548	1.10324	2.36176	1.87088	2550	
2560	1.03919	2.26564	1.85875	1.06893	2.31050	1.86456	1.09832	2.35444	1.87000	2560	
2570	1.03442	2.25840	1.85778	1.06410	2.30323	1.86364	1.09343	2.34715	1.86911	2570	
2580	1.02967	2.25118	1.85681	1.05929	2.29600	1.86271	1.08856	2.33989	1.86822	2580	
2590	1.02495	2.24400	1.85584	1.05451	2.28879	1.86178	1.08372	2.33267	1.86733	2590	

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	ν cm ⁻¹
	T=4100.			T=4200.			T=4300.			
2600	1.02026	2.23685	1.85487	1.04976	2.28162	1.86085	1.07892	2.32547	1.86644	2600
2610	1.01559	2.22973	1.85389	1.04503	2.27448	1.85991	1.07414	2.31831	1.86555	2610
2620	1.01095	2.22265	1.85291	1.04034	2.26737	1.85898	1.06938	2.31118	1.86465	2620
2630	1.00634	2.21559	1.85192	1.03567	2.26029	1.85803	1.06466	2.30408	1.86375	2630
2640	1.00176	2.20856	1.85093	1.03102	2.25324	1.85709	1.05996	2.29701	1.86284	2640
2650	0.99720	2.20157	1.84994	1.02641	2.24622	1.85614	1.05528	2.28997	1.86193	2650
2660	0.99267	2.19460	1.84895	1.02182	2.23923	1.85519	1.05064	2.28295	1.86102	2660
2670	0.98816	2.18766	1.84795	1.01725	2.23227	1.85424	1.04602	2.27597	1.86011	2670
2680	0.98368	2.18076	1.84695	1.01272	2.22534	1.85328	1.04143	2.26902	1.85919	2680
2690	0.97923	2.17388	1.84595	1.00820	2.21844	1.85232	1.03686	2.26210	1.85827	2690
2700	0.97480	2.16703	1.84495	1.00372	2.21157	1.85136	1.03232	2.25520	1.85735	2700
2710	0.97040	2.16021	1.84394	0.99926	2.20473	1.85039	1.02780	2.24834	1.85643	2710
2720	0.96602	2.15342	1.84292	0.99482	2.19791	1.84942	1.02331	2.24150	1.85550	2720
2730	0.96166	2.14666	1.84191	0.99041	2.19113	1.84845	1.01884	2.23470	1.85457	2730
2740	0.95734	2.13993	1.84089	0.98602	2.18437	1.84748	1.01440	2.22792	1.85364	2740
2750	0.95303	2.13323	1.83987	0.98166	2.17764	1.84650	1.00998	2.22117	1.85270	2750
2760	0.94875	2.12655	1.83885	0.97733	2.17094	1.84552	1.00559	2.21444	1.85176	2760
2770	0.94450	2.11990	1.83782	0.97301	2.16427	1.84454	1.00122	2.20775	1.85082	2770
2780	0.94027	2.11328	1.83679	0.96872	2.15762	1.84355	0.99688	2.20108	1.84988	2780
2790	0.93606	2.10669	1.83576	0.96446	2.15101	1.84256	0.99256	2.19444	1.84893	2790
2800	0.93187	2.10012	1.83472	0.96022	2.14442	1.84157	0.98827	2.18783	1.84798	2800
2810	0.92771	2.09358	1.83368	0.95600	2.13785	1.84058	0.98399	2.18124	1.84702	2810
2820	0.92358	2.08707	1.83264	0.95181	2.13132	1.83958	0.97974	2.17468	1.84607	2820
2830	0.91946	2.08058	1.83159	0.94764	2.12481	1.83858	0.97552	2.16815	1.84511	2830
2840	0.91537	2.07413	1.83054	0.94349	2.11832	1.83757	0.97132	2.16164	1.84415	2840
2850	0.91130	2.06769	1.82949	0.93936	2.11187	1.83657	0.96714	2.15516	1.84318	2850
2860	0.90726	2.06129	1.82844	0.93526	2.10543	1.83556	0.96298	2.14870	1.84222	2860
2870	0.90323	2.05491	1.82738	0.93118	2.09903	1.83455	0.95884	2.14228	1.84125	2870
2880	0.89923	2.04855	1.82632	0.92712	2.09265	1.83353	0.95473	2.13587	1.84027	2880
2890	0.89525	2.04222	1.82526	0.92309	2.08630	1.83251	0.95064	2.12950	1.83930	2890
2900	0.89129	2.03592	1.82419	0.91907	2.07997	1.83149	0.94657	2.12315	1.83832	2900
2910	0.88736	2.02964	1.82312	0.91508	2.07367	1.83047	0.94253	2.11682	1.83734	2910
2920	0.88344	2.02339	1.82205	0.91111	2.06739	1.82944	0.93850	2.11052	1.83636	2920
2930	0.87955	2.01716	1.82098	0.90716	2.06113	1.82841	0.93450	2.10424	1.83537	2930
2940	0.87568	2.01096	1.81990	0.90323	2.05491	1.82738	0.93052	2.09799	1.83438	2940
2950	0.87183	2.00478	1.81882	0.89932	2.04870	1.82635	0.92656	2.09176	1.83339	2950
2960	0.86800	1.99863	1.81773	0.89544	2.04252	1.82531	0.92262	2.08556	1.83239	2960
2970	0.86419	1.99250	1.81665	0.89157	2.03637	1.82427	0.91870	2.07938	1.83140	2970
2980	0.86040	1.98640	1.81556	0.88773	2.03024	1.82322	0.91480	2.07323	1.83040	2980
2990	0.85663	1.98032	1.81447	0.88391	2.02413	1.82218	0.91092	2.06710	1.82939	2990
3000	0.85288	1.97426	1.81337	0.88010	2.01805	1.82113	0.90707	2.06099	1.82839	3000
3010	0.84915	1.96823	1.81227	0.87632	2.01199	1.82008	0.90323	2.05491	1.82738	3010
3020	0.84544	1.96222	1.81117	0.87256	2.00596	1.81902	0.89942	2.04885	1.82637	3020
3030	0.84176	1.95623	1.81007	0.86881	1.99995	1.81797	0.89562	2.04281	1.82536	3030
3040	0.83809	1.95027	1.80896	0.86509	1.99396	1.81691	0.89184	2.03680	1.82434	3040
3050	0.83444	1.94433	1.80785	0.86139	1.98799	1.81584	0.88809	2.03081	1.82332	3050
3060	0.83081	1.93842	1.80674	0.85770	1.98205	1.81478	0.88435	2.02484	1.82230	3060
3070	0.82720	1.93252	1.80563	0.85404	1.97613	1.81371	0.88063	2.01890	1.82128	3070
3080	0.82361	1.92665	1.80451	0.85039	1.97024	1.81264	0.87693	2.01298	1.82025	3080
3090	0.82004	1.92080	1.80339	0.84677	1.96436	1.81157	0.87326	2.00708	1.81922	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm ⁻¹
T=4100.			T=4200.			T=4300.				
3100	0.81648	1.91498	1.80226	0.84316	1.95851	1.81049	0.86960	2.00120	1.81819	3100
3110	0.81295	1.90918	1.80114	0.83957	1.95268	1.80941	0.86595	1.99535	1.81715	3110
3120	0.80944	1.90340	1.80001	0.83600	1.94687	1.80833	0.86233	1.98952	1.81612	3120
3130	0.80594	1.89764	1.79888	0.83245	1.94109	1.80724	0.85873	1.98371	1.81508	3130
3140	0.80246	1.89190	1.79774	0.82892	1.93533	1.80616	0.85514	1.97792	1.81403	3140
3150	0.79900	1.88619	1.79661	0.82540	1.92958	1.80507	0.85158	1.97215	1.81299	3150
3160	0.79556	1.88050	1.79547	0.82191	1.92387	1.80398	0.84803	1.96641	1.81194	3160
3170	0.79213	1.87482	1.79432	0.81843	1.91817	1.80288	0.84450	1.96068	1.81089	3170
3180	0.78873	1.86917	1.79318	0.81497	1.91249	1.80178	0.84099	1.95498	1.80984	3180
3190	0.78534	1.86355	1.79203	0.81153	1.90684	1.80068	0.83749	1.94930	1.80878	3190
3200	0.78197	1.85794	1.79088	0.80810	1.90120	1.79958	0.83402	1.94364	1.80772	3200
3210	0.77861	1.85235	1.78973	0.80469	1.89559	1.79847	0.83056	1.93800	1.80666	3210
3220	0.77528	1.84679	1.78857	0.80130	1.89000	1.79736	0.82712	1.93239	1.80560	3220
3230	0.77196	1.84124	1.78741	0.79793	1.88442	1.79625	0.82369	1.92679	1.80453	3230
3240	0.76865	1.83572	1.78625	0.79458	1.87887	1.79514	0.82029	1.92121	1.80347	3240
3250	0.76537	1.83022	1.78508	0.79124	1.87334	1.79402	0.81690	1.91566	1.80240	3250
3260	0.76210	1.82474	1.78392	0.78792	1.86783	1.79290	0.81352	1.91012	1.80132	3260
3270	0.75885	1.81927	1.78275	0.78461	1.86234	1.79178	0.81017	1.90461	1.80025	3270
3280	0.75562	1.81383	1.78157	0.78133	1.85687	1.79066	0.80683	1.89911	1.79917	3280
3290	0.75240	1.80841	1.78040	0.77805	1.85142	1.78953	0.80351	1.89363	1.79809	3290
3300	0.74920	1.80301	1.77922	0.77480	1.84600	1.78840	0.80020	1.88818	1.79700	3300
3310	0.74601	1.79763	1.77804	0.77156	1.84059	1.78727	0.79692	1.88274	1.79592	3310
3320	0.74284	1.79227	1.77686	0.76834	1.83520	1.78614	0.79364	1.87733	1.79483	3320
3330	0.73969	1.78692	1.77567	0.76514	1.82983	1.78500	0.79039	1.87193	1.79374	3330
3340	0.73655	1.78160	1.77449	0.76195	1.82448	1.78386	0.78715	1.86655	1.79264	3340
3350	0.73343	1.77630	1.77329	0.75877	1.81914	1.78272	0.78392	1.86120	1.79155	3350
3360	0.73033	1.77101	1.77210	0.75562	1.81383	1.78157	0.78072	1.85586	1.79045	3360
3370	0.72724	1.76575	1.77090	0.75247	1.80854	1.78043	0.77752	1.85054	1.78935	3370
3380	0.72416	1.76050	1.76971	0.74935	1.80327	1.77928	0.77435	1.84524	1.78825	3380
3390	0.72110	1.75528	1.76851	0.74624	1.79801	1.77813	0.77119	1.83996	1.78714	3390
3400	0.71806	1.75007	1.76730	0.74314	1.79278	1.77697	0.76804	1.83470	1.78603	3400
3410	0.71503	1.74488	1.76610	0.74006	1.78756	1.77581	0.76491	1.82945	1.78492	3410
3420	0.71202	1.73971	1.76489	0.73700	1.78236	1.77465	0.76180	1.82423	1.78381	3420
3430	0.70902	1.73456	1.76367	0.73395	1.77718	1.77349	0.75870	1.81902	1.78269	3430
3440	0.70604	1.72943	1.76246	0.73092	1.77202	1.77233	0.75562	1.81383	1.78157	3440
3450	0.70307	1.72431	1.76124	0.72790	1.76688	1.77116	0.75255	1.80866	1.78045	3450
3460	0.70012	1.71922	1.76003	0.72489	1.76175	1.76999	0.74949	1.80351	1.77933	3460
3470	0.69718	1.71414	1.75880	0.72190	1.75664	1.76882	0.74645	1.79838	1.77821	3470
3480	0.69426	1.70908	1.75758	0.71893	1.75156	1.76765	0.74343	1.79326	1.77708	3480
3490	0.69135	1.70404	1.75635	0.71597	1.74649	1.76647	0.74042	1.78816	1.77595	3490
3500	0.68846	1.69902	1.75512	0.71302	1.74143	1.76529	0.73743	1.78308	1.77482	3500
3510	0.68558	1.69401	1.75389	0.71009	1.73640	1.76411	0.73445	1.77802	1.77368	3510
3520	0.68271	1.68902	1.75266	0.70718	1.73138	1.76292	0.73148	1.77298	1.77255	3520
3530	0.67986	1.68405	1.75142	0.70427	1.72638	1.76174	0.72853	1.76795	1.77141	3530
3540	0.67702	1.67910	1.75018	0.70138	1.72140	1.76055	0.72559	1.76294	1.77026	3540
3550	0.67420	1.67416	1.74894	0.69851	1.71644	1.75936	0.72267	1.75795	1.76912	3550
3560	0.67139	1.66925	1.74770	0.69565	1.71149	1.75816	0.71976	1.75297	1.76797	3560
3570	0.66859	1.66434	1.74645	0.69280	1.70656	1.75697	0.71686	1.74802	1.76682	3570
3580	0.66581	1.65946	1.74520	0.68997	1.70164	1.75577	0.71398	1.74308	1.76567	3580
3590	0.66304	1.65460	1.74395	0.68715	1.69675	1.75457	0.71111	1.73815	1.76452	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=4100.			T=4200.			T=4300.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S°	C _p ⁰	$-(F^0-E_0^0)/T$	S°	C _p ⁰	$-(F^0-E_0^0)/T$	S°	C _p ⁰	
3600	0.66028	1.64975	1.74270	0.68435	1.69187	1.75336	0.70826	1.73325	1.76336	3600
3610	0.65754	1.64491	1.74144	0.68155	1.68701	1.75216	0.70542	1.72836	1.76221	3610
3620	0.65481	1.64010	1.74019	0.67878	1.68216	1.75095	0.70259	1.72348	1.76105	3620
3630	0.65210	1.63530	1.73892	0.67601	1.67733	1.74974	0.69978	1.71863	1.75988	3630
3640	0.64940	1.63052	1.73766	0.67326	1.67252	1.74853	0.69698	1.71379	1.75872	3640
3650	0.64671	1.62575	1.73640	0.67052	1.66773	1.74731	0.69419	1.70896	1.75755	3650
3660	0.64403	1.62100	1.73513	0.66779	1.66295	1.74610	0.69142	1.70416	1.75638	3660
3670	0.64137	1.61627	1.73386	0.66508	1.65819	1.74488	0.68866	1.69937	1.75521	3670
3680	0.63872	1.61155	1.73259	0.66238	1.65344	1.74365	0.68591	1.69459	1.75404	3680
3690	0.63608	1.60685	1.73131	0.65970	1.64871	1.74243	0.68318	1.68983	1.75286	3690
3700	0.63346	1.60217	1.73003	0.65702	1.64399	1.74120	0.68045	1.68509	1.75168	3700
3710	0.63085	1.59750	1.72875	0.65436	1.63930	1.73998	0.67775	1.68036	1.75050	3710
3720	0.62825	1.59285	1.72747	0.65171	1.63461	1.73874	0.67505	1.67565	1.74932	3720
3730	0.62566	1.58821	1.72619	0.64908	1.62995	1.73751	0.67237	1.67096	1.74813	3730
3740	0.62309	1.58359	1.72490	0.64645	1.62530	1.73628	0.66969	1.66628	1.74695	3740
3750	0.62052	1.57899	1.72361	0.64384	1.62066	1.73504	0.66704	1.66162	1.74576	3750
3760	0.61797	1.57440	1.72232	0.64124	1.61604	1.73380	0.66439	1.65697	1.74456	3760
3770	0.61544	1.56983	1.72103	0.63866	1.61144	1.73256	0.66176	1.65234	1.74337	3770
3780	0.61291	1.56527	1.71973	0.63608	1.60685	1.73131	0.65914	1.64772	1.74217	3780
3790	0.61040	1.56073	1.71844	0.63352	1.60228	1.73006	0.65653	1.64312	1.74098	3790
3800	0.60790	1.55620	1.71714	0.63097	1.59772	1.72882	0.65393	1.63853	1.73978	3800
3810	0.60541	1.55169	1.71583	0.62843	1.59318	1.72756	0.65134	1.63396	1.73857	3810
3820	0.60293	1.54720	1.71453	0.62591	1.58866	1.72631	0.64877	1.62941	1.73737	3820
3830	0.60046	1.54272	1.71322	0.62339	1.58414	1.72506	0.64621	1.62487	1.73616	3830
3840	0.59801	1.53825	1.71191	0.62089	1.57965	1.72380	0.64366	1.62034	1.73495	3840
3850	0.59557	1.53380	1.71060	0.61840	1.57517	1.72254	0.64112	1.61583	1.73374	3850
3860	0.59313	1.52936	1.70929	0.61592	1.57070	1.72128	0.63860	1.61133	1.73253	3860
3870	0.59071	1.52494	1.70797	0.61345	1.56625	1.72001	0.63608	1.60685	1.73131	3870
3880	0.58831	1.52054	1.70665	0.61099	1.56181	1.71874	0.63358	1.60239	1.73009	3880
3890	0.58591	1.51615	1.70533	0.60855	1.55739	1.71748	0.63109	1.59794	1.72887	3890
3900	0.58352	1.51177	1.70401	0.60612	1.55298	1.71621	0.62861	1.59350	1.72765	3900
3910	0.58115	1.50741	1.70269	0.60369	1.54859	1.71493	0.62614	1.58908	1.72643	3910
3920	0.57879	1.50306	1.70136	0.60128	1.54421	1.71366	0.62368	1.58467	1.72520	3920
3930	0.57643	1.49873	1.70003	0.59888	1.53984	1.71238	0.62124	1.58027	1.72397	3930
3940	0.57409	1.49441	1.69870	0.59649	1.53549	1.71110	0.61880	1.57589	1.72274	3940
3950	0.57176	1.49010	1.69737	0.59412	1.53116	1.70982	0.61638	1.57153	1.72151	3950
3960	0.56944	1.48581	1.69603	0.59175	1.52684	1.70854	0.61397	1.56718	1.72028	3960
3970	0.56713	1.48154	1.69470	0.58939	1.52253	1.70725	0.61157	1.56284	1.71904	3970
3980	0.56484	1.47728	1.69336	0.58705	1.51824	1.70596	0.60917	1.55852	1.71780	3980
3990	0.56255	1.47303	1.69202	0.58471	1.51396	1.70467	0.60679	1.55421	1.71656	3990
4000	0.56027	1.46880	1.69067	0.58239	1.50969	1.70338	0.60443	1.54991	1.71532	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=4400.			T=4500.			T=4600.			ν cm ⁻¹
	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	$-(F^\circ-E_0^\circ)/T$	S ^o	C _p ^o	
100	6.82928	8.78414	1.98699	6.87322	8.82879	1.98700	6.91621	8.87246	1.98701	100
110	6.64311	8.59476	1.98696	6.68698	8.63941	1.98697	6.72990	8.68308	1.98697	110
120	6.47343	8.42187	1.98692	6.51723	8.46652	1.98693	6.56008	8.51019	1.98694	120
130	6.31760	8.26283	1.98687	6.36133	8.30748	1.98688	6.40411	8.35115	1.98690	130
140	6.17356	8.11559	1.98682	6.21722	8.16024	1.98684	6.25993	8.20391	1.98685	140
150	6.03969	7.97852	1.98677	6.08327	8.02317	1.98679	6.12592	8.06683	1.98681	150
160	5.91466	7.85030	1.98672	5.95817	7.89494	1.98674	6.00075	7.93861	1.98676	160
170	5.79741	7.72985	1.98666	5.84085	7.77450	1.98668	5.88336	7.81816	1.98670	170
180	5.68704	7.61630	1.98660	5.73041	7.66095	1.98662	5.77286	7.70461	1.98665	180
190	5.58282	7.50889	1.98653	5.62612	7.55354	1.98656	5.66849	7.59720	1.98658	190
200	5.48410	7.40700	1.98646	5.52733	7.45164	1.98649	5.56964	7.49530	1.98652	200
210	5.39036	7.31008	1.98639	5.43352	7.35472	1.98642	5.47576	7.39838	1.98646	210
220	5.30113	7.21768	1.98631	5.34422	7.26232	1.98635	5.38639	7.30597	1.98639	220
230	5.21600	7.12938	1.98623	5.25902	7.17402	1.98627	5.30113	7.21768	1.98631	230
240	5.13464	7.04485	1.98615	5.17759	7.08949	1.98620	5.21962	7.13314	1.98624	240
250	5.05672	6.96377	1.98606	5.09960	7.00841	1.98611	5.14157	7.05206	1.98616	250
260	4.98199	6.88588	1.98597	5.02480	6.93051	1.98603	5.06670	6.97416	1.98607	260
270	4.91020	6.81093	1.98588	4.95293	6.85556	1.98594	4.99477	6.89921	1.98599	270
280	4.84113	6.73871	1.98578	4.88379	6.78334	1.98584	4.92556	6.82699	1.98590	280
290	4.77459	6.66903	1.98568	4.81719	6.71365	1.98575	4.85889	6.75730	1.98581	290
300	4.71042	6.60171	1.98558	4.75295	6.64634	1.98565	4.79458	6.68998	1.98571	300
310	4.64846	6.53661	1.98547	4.69091	6.58123	1.98554	4.73248	6.62487	1.98561	310
320	4.58856	6.47357	1.98536	4.63095	6.51819	1.98544	4.67245	6.56183	1.98551	320
330	4.53060	6.41248	1.98524	4.57292	6.45710	1.98533	4.61436	6.50073	1.98541	330
340	4.47447	6.35322	1.98512	4.51672	6.39783	1.98521	4.55809	6.44147	1.98530	340
350	4.42006	6.29568	1.98500	4.46223	6.34029	1.98510	4.50354	6.38392	1.98519	350
360	4.36726	6.23976	1.98488	4.40937	6.28437	1.98498	4.45061	6.32800	1.98507	360
370	4.31600	6.18538	1.98475	4.35804	6.22998	1.98485	4.39921	6.27361	1.98495	370
380	4.26619	6.13245	1.98461	4.30816	6.17705	1.98473	4.34926	6.22068	1.98483	380
390	4.21775	6.08090	1.98448	4.25965	6.12550	1.98460	4.30069	6.16912	1.98471	390
400	4.17062	6.03066	1.98434	4.21245	6.07526	1.98446	4.25342	6.11887	1.98458	400
410	4.12473	5.98166	1.98420	4.16649	6.02626	1.98433	4.20740	6.06987	1.98445	410
420	4.08002	5.93385	1.98405	4.12171	5.97844	1.98419	4.16255	6.02205	1.98431	420
430	4.03643	5.88717	1.98390	4.07806	5.93175	1.98404	4.11883	5.97536	1.98418	430
440	3.99392	5.84156	1.98375	4.03548	5.88614	1.98390	4.07618	5.92975	1.98404	440
450	3.95243	5.79698	1.98359	3.99392	5.84156	1.98375	4.03456	5.88516	1.98389	450
460	3.91193	5.75339	1.98343	3.95334	5.79796	1.98359	3.99392	5.84156	1.98375	460
470	3.87236	5.71073	1.98326	3.91371	5.75530	1.98343	3.95422	5.79890	1.98359	470
480	3.83368	5.66898	1.98310	3.87497	5.71355	1.98327	3.91541	5.75714	1.98344	480
490	3.79587	5.62809	1.98292	3.83709	5.67265	1.98311	3.87747	5.71624	1.98328	490
500	3.75889	5.58803	1.98275	3.80003	5.63259	1.98294	3.84035	5.67618	1.98312	500
510	3.72270	5.54877	1.98257	3.76377	5.59333	1.98277	3.80402	5.63691	1.98296	510
520	3.68727	5.51027	1.98239	3.72828	5.55483	1.98260	3.76846	5.59840	1.98279	520
530	3.65257	5.47251	1.98220	3.69351	5.51706	1.98242	3.73363	5.56064	1.98263	530
540	3.61858	5.43547	1.98201	3.65945	5.48001	1.98224	3.69951	5.52358	1.98245	540
550	3.58527	5.39910	1.98182	3.62608	5.44364	1.98206	3.66606	5.48720	1.98228	550
560	3.55262	5.36339	1.98163	3.59335	5.40793	1.98187	3.63328	5.45149	1.98210	560
570	3.52059	5.32832	1.98143	3.56126	5.37285	1.98168	3.60112	5.41641	1.98191	570
580	3.48918	5.29386	1.98122	3.52978	5.33839	1.98148	3.56957	5.38194	1.98173	580
590	3.45836	5.25999	1.98102	3.49889	5.30452	1.98129	3.53862	5.34807	1.98154	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=4400.			T=4500.			T=4600.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
600	3.42810	5.22670	1.98081	3.46857	5.27122	1.98109	3.50823	5.31476	1.98135	600
610	3.39840	5.19396	1.98059	3.43879	5.23847	1.98088	3.47839	5.28201	1.98115	610
620	3.36922	5.16176	1.98038	3.40955	5.20627	1.98068	3.44909	5.24980	1.98095	620
630	3.34057	5.13007	1.98016	3.38083	5.17458	1.98046	3.42030	5.21811	1.98075	630
640	3.31241	5.09889	1.97993	3.35261	5.14339	1.98025	3.39201	5.18691	1.98055	640
650	3.28473	5.06819	1.97971	3.32486	5.11269	1.98003	3.36420	5.15621	1.98034	650
660	3.25753	5.03797	1.97947	3.29759	5.08246	1.97981	3.33687	5.12598	1.98013	660
670	3.23078	5.00821	1.97924	3.27077	5.05269	1.97959	3.30998	5.09620	1.97991	670
680	3.20447	4.97888	1.97900	3.24439	5.02336	1.97936	3.28354	5.06687	1.97970	680
690	3.17858	4.95000	1.97876	3.21845	4.99447	1.97913	3.25753	5.03797	1.97947	690
700	3.15312	4.92153	1.97852	3.19291	4.96599	1.97890	3.23193	5.00949	1.97925	700
710	3.12805	4.89346	1.97827	3.16778	4.93792	1.97866	3.20674	4.98142	1.97902	710
720	3.10338	4.86580	1.97802	3.14304	4.91025	1.97842	3.18194	4.95374	1.97879	720
730	3.07910	4.83851	1.97776	3.11869	4.88296	1.97817	3.15752	4.92645	1.97856	730
740	3.05518	4.81161	1.97750	3.09471	4.85605	1.97793	3.13347	4.89953	1.97832	740
750	3.03162	4.78506	1.97724	3.07108	4.82950	1.97767	3.10978	4.87298	1.97808	750
760	3.00842	4.75888	1.97697	3.04781	4.80331	1.97742	3.08645	4.84678	1.97784	760
770	2.98555	4.73304	1.97670	3.02488	4.77746	1.97716	3.06346	4.82092	1.97759	770
780	2.96302	4.70753	1.97643	3.00229	4.75195	1.97690	3.04080	4.79541	1.97734	780
790	2.94082	4.68236	1.97616	2.98002	4.72677	1.97664	3.01846	4.77022	1.97709	790
800	2.91893	4.65750	1.97588	2.95806	4.70191	1.97637	2.99645	4.74535	1.97683	800
810	2.89735	4.63296	1.97559	2.93642	4.67736	1.97610	2.97474	4.72080	1.97657	810
820	2.87607	4.60872	1.97531	2.91507	4.65311	1.97583	2.95333	4.69655	1.97631	820
830	2.85509	4.58478	1.97502	2.89402	4.62917	1.97555	2.93222	4.67259	1.97605	830
840	2.83439	4.56112	1.97472	2.87326	4.60551	1.97527	2.91139	4.64893	1.97578	840
850	2.81398	4.53776	1.97443	2.85278	4.58213	1.97498	2.89085	4.62555	1.97551	850
860	2.79383	4.51466	1.97413	2.83257	4.55904	1.97470	2.87057	4.60244	1.97523	860
870	2.77395	4.49184	1.97382	2.81262	4.53621	1.97441	2.85057	4.57961	1.97495	870
880	2.75434	4.46929	1.97351	2.79294	4.51364	1.97411	2.83082	4.55704	1.97467	880
890	2.73498	4.44699	1.97320	2.77352	4.49134	1.97381	2.81133	4.53473	1.97439	890
900	2.71586	4.42494	1.97289	2.75434	4.46929	1.97351	2.79209	4.51267	1.97410	900
910	2.69700	4.40315	1.97257	2.73540	4.44748	1.97321	2.77310	4.49086	1.97381	910
920	2.67836	4.38159	1.97225	2.71671	4.42592	1.97290	2.75434	4.46929	1.97351	920
930	2.65997	4.36027	1.97193	2.69825	4.40459	1.97259	2.73581	4.44795	1.97322	930
940	2.64180	4.33918	1.97160	2.68001	4.38350	1.97228	2.71752	4.42685	1.97292	940
950	2.62385	4.31832	1.97127	2.66200	4.36263	1.97196	2.69944	4.40598	1.97261	950
960	2.60612	4.29768	1.97093	2.64421	4.34198	1.97164	2.68159	4.38532	1.97231	960
970	2.58861	4.27726	1.97059	2.62663	4.32155	1.97132	2.66395	4.36488	1.97200	970
980	2.57130	4.25705	1.97025	2.60926	4.30133	1.97099	2.64652	4.34466	1.97168	980
990	2.55420	4.23705	1.96991	2.59209	4.28132	1.97066	2.62929	4.32464	1.97137	990
1000	2.53731	4.21725	1.96956	2.57513	4.26152	1.97033	2.61226	4.30483	1.97105	1000
1010	2.52060	4.19765	1.96920	2.55837	4.24192	1.96999	2.59544	4.28522	1.97073	1010
1020	2.50410	4.17825	1.96885	2.54179	4.22251	1.96965	2.57880	4.26581	1.97040	1020
1030	2.48778	4.15905	1.96849	2.52541	4.20329	1.96931	2.56236	4.24659	1.97007	1030
1040	2.47164	4.14003	1.96813	2.50921	4.18427	1.96896	2.54610	4.22755	1.96974	1040
1050	2.45569	4.12120	1.96776	2.49319	4.16543	1.96861	2.53002	4.20870	1.96940	1050
1060	2.43992	4.10255	1.96739	2.47736	4.14677	1.96826	2.51412	4.19004	1.96907	1060
1070	2.42432	4.08407	1.96702	2.46170	4.12829	1.96790	2.49840	4.17155	1.96872	1070
1080	2.40889	4.06578	1.96664	2.44621	4.10999	1.96754	2.48285	4.15324	1.96838	1080
1090	2.39363	4.04765	1.96626	2.43088	4.09185	1.96718	2.46746	4.13510	1.96803	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	ν cm ⁻¹
T=4400.			T=4500.			T=4600.				
1100	2.37854	4.02970	1.96588	2.41573	4.07389	1.96681	2.45225	4.11713	1.96768	1100
1110	2.36361	4.01191	1.96550	2.40073	4.05609	1.96644	2.43719	4.09932	1.96733	1110
1120	2.34884	3.99428	1.96511	2.38590	4.03846	1.96607	2.42230	4.08168	1.96697	1120
1130	2.33423	3.97682	1.96471	2.37122	4.02098	1.96569	2.40756	4.06420	1.96661	1130
1140	2.31977	3.95951	1.96432	2.35670	4.00366	1.96531	2.39298	4.04687	1.96625	1140
1150	2.30546	3.94236	1.96392	2.34233	3.98650	1.96493	2.37854	4.02970	1.96588	1150
1160	2.29130	3.92535	1.96351	2.32811	3.96949	1.96455	2.36426	4.01268	1.96551	1160
1170	2.27729	3.90850	1.96311	2.31403	3.95263	1.96416	2.35012	3.99581	1.96514	1170
1180	2.26342	3.89180	1.96270	2.30009	3.93592	1.96376	2.33613	3.97909	1.96476	1180
1190	2.24969	3.87523	1.96228	2.28630	3.91934	1.96337	2.32227	3.96251	1.96439	1190
1200	2.23609	3.85882	1.96187	2.27265	3.90292	1.96297	2.30856	3.94607	1.96400	1200
1210	2.22264	3.84254	1.96145	2.25913	3.88663	1.96257	2.29498	3.92977	1.96362	1210
1220	2.20932	3.82639	1.96102	2.24575	3.87048	1.96216	2.28154	3.91361	1.96323	1220
1230	2.19613	3.81039	1.96060	2.23249	3.85446	1.96175	2.26822	3.89759	1.96284	1230
1240	2.18307	3.79451	1.96017	2.21937	3.83858	1.96134	2.25504	3.88170	1.96245	1240
1250	2.17014	3.77877	1.95973	2.20638	3.82283	1.96093	2.24199	3.86594	1.96205	1250
1260	2.15733	3.76316	1.95930	2.19351	3.80720	1.96051	2.22906	3.85030	1.96165	1260
1270	2.14465	3.74767	1.95885	2.18076	3.79171	1.96009	2.21625	3.83480	1.96124	1270
1280	2.13209	3.73231	1.95841	2.16814	3.77633	1.95966	2.20357	3.81942	1.96084	1280
1290	2.11964	3.71707	1.95796	2.15563	3.76108	1.95924	2.19100	3.80416	1.96043	1290
1300	2.10732	3.70195	1.95751	2.14325	3.74596	1.95881	2.17856	3.78902	1.96002	1300
1310	2.09511	3.68695	1.95706	2.13098	3.73095	1.95837	2.16623	3.77401	1.95960	1310
1320	2.08302	3.67207	1.95660	2.11882	3.71606	1.95793	2.15401	3.75910	1.95918	1320
1330	2.07103	3.65731	1.95614	2.10677	3.70128	1.95749	2.14191	3.74432	1.95876	1330
1340	2.05916	3.64266	1.95568	2.09484	3.68662	1.95705	2.12991	3.72965	1.95833	1340
1350	2.04740	3.62812	1.95521	2.08302	3.67207	1.95660	2.11803	3.71509	1.95791	1350
1360	2.03574	3.61369	1.95474	2.07130	3.65763	1.95615	2.10625	3.70064	1.95747	1360
1370	2.02419	3.59937	1.95427	2.05969	3.64330	1.95570	2.09458	3.68630	1.95704	1370
1380	2.01275	3.58516	1.95379	2.04818	3.62908	1.95524	2.08302	3.67207	1.95660	1380
1390	2.00140	3.57105	1.95331	2.03677	3.61497	1.95478	2.07155	3.65795	1.95616	1390
1400	1.99016	3.55705	1.95282	2.02547	3.60096	1.95432	2.06019	3.64393	1.95572	1400
1410	1.97902	3.54316	1.95234	2.01427	3.58705	1.95385	2.04893	3.63001	1.95527	1410
1420	1.96797	3.52936	1.95185	2.00316	3.57324	1.95338	2.03776	3.61619	1.95482	1420
1430	1.95703	3.51567	1.95135	1.99215	3.55954	1.95291	2.02669	3.60247	1.95437	1430
1440	1.94618	3.50207	1.95086	1.98124	3.54593	1.95243	2.01572	3.58886	1.95391	1440
1450	1.93542	3.48857	1.95036	1.97042	3.53242	1.95196	2.00485	3.57534	1.95346	1450
1460	1.92475	3.47517	1.94985	1.95969	3.51900	1.95147	1.99406	3.56191	1.95299	1460
1470	1.91418	3.46186	1.94934	1.94906	3.50568	1.95099	1.98337	3.54858	1.95253	1470
1480	1.90369	3.44864	1.94883	1.93852	3.49246	1.95050	1.97276	3.53535	1.95206	1480
1490	1.89330	3.43552	1.94832	1.92806	3.47933	1.95001	1.96225	3.52220	1.95159	1490
1500	1.88299	3.42249	1.94780	1.91769	3.46628	1.94951	1.95183	3.50915	1.95112	1500
1510	1.87277	3.40955	1.94728	1.90741	3.45333	1.94902	1.94149	3.49619	1.95064	1510
1520	1.86264	3.39670	1.94676	1.89722	3.44047	1.94851	1.93123	3.48331	1.95016	1520
1530	1.85259	3.38394	1.94623	1.88711	3.42769	1.94801	1.92106	3.47053	1.94968	1530
1540	1.84262	3.37126	1.94570	1.87708	3.41500	1.94750	1.91098	3.45783	1.94919	1540
1550	1.83273	3.35867	1.94517	1.86713	3.40240	1.94699	1.90097	3.44521	1.94870	1550
1560	1.82293	3.34616	1.94463	1.85727	3.38988	1.94648	1.89105	3.43268	1.94821	1560
1570	1.81321	3.33374	1.94409	1.84748	3.37745	1.94596	1.88121	3.42024	1.94771	1570
1580	1.80356	3.32139	1.94355	1.83778	3.36509	1.94544	1.87145	3.40787	1.94722	1580
1590	1.79399	3.30913	1.94300	1.82815	3.35282	1.94492	1.86176	3.39559	1.94671	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _P ⁰	ν cm ⁻¹
	T=4400.			T=4500.			T=4600.			
1600	1.78450	3.29695	1.94245	1.81860	3.34063	1.94439	1.85215	3.38338	1.94621	1600
1610	1.77509	3.28485	1.94190	1.80912	3.32851	1.94386	1.84262	3.37126	1.94570	1610
1620	1.76575	3.27283	1.94134	1.79972	3.31648	1.94333	1.83316	3.35921	1.94519	1620
1630	1.75648	3.26088	1.94078	1.79040	3.30452	1.94280	1.82378	3.34724	1.94468	1630
1640	1.74729	3.24902	1.94022	1.78115	3.29264	1.94226	1.81447	3.33535	1.94416	1640
1650	1.73817	3.23722	1.93966	1.77197	3.28084	1.94172	1.80523	3.32353	1.94364	1650
1660	1.72912	3.22550	1.93909	1.76286	3.26911	1.94117	1.79607	3.31179	1.94312	1660
1670	1.72014	3.21386	1.93851	1.75382	3.25745	1.94062	1.78697	3.30012	1.94260	1670
1680	1.71123	3.20229	1.93794	1.74485	3.24586	1.94007	1.77794	3.28853	1.94207	1680
1690	1.70239	3.19079	1.93736	1.73595	3.23435	1.93952	1.76899	3.27700	1.94154	1690
1700	1.69361	3.17936	1.93678	1.72712	3.22291	1.93896	1.76010	3.26555	1.94100	1700
1710	1.68491	3.16800	1.93619	1.71835	3.21154	1.93840	1.75128	3.25417	1.94047	1710
1720	1.67627	3.15672	1.93560	1.70965	3.20024	1.93784	1.74252	3.24285	1.93993	1720
1730	1.66769	3.14550	1.93501	1.70102	3.18901	1.93727	1.73383	3.23161	1.93938	1730
1740	1.65918	3.13434	1.93442	1.69245	3.17784	1.93670	1.72520	3.22043	1.93884	1740
1750	1.65074	3.12326	1.93382	1.68394	3.16675	1.93613	1.71664	3.20932	1.93829	1750
1760	1.64235	3.11224	1.93322	1.67550	3.15572	1.93555	1.70814	3.19828	1.93774	1760
1770	1.63403	3.10129	1.93261	1.66712	3.14475	1.93497	1.69971	3.18730	1.93718	1770
1780	1.62577	3.09041	1.93200	1.65881	3.13385	1.93439	1.69134	3.17639	1.93662	1780
1790	1.61758	3.07958	1.93139	1.65055	3.12302	1.93380	1.68302	3.16554	1.93606	1790
1800	1.60944	3.06883	1.93078	1.64235	3.11224	1.93322	1.67477	3.15476	1.93550	1800
1810	1.60136	3.05813	1.93016	1.63422	3.10154	1.93263	1.66658	3.14404	1.93493	1810
1820	1.59334	3.04750	1.92954	1.62614	3.09089	1.93203	1.65844	3.13338	1.93436	1820
1830	1.58538	3.03693	1.92892	1.61812	3.08030	1.93143	1.65037	3.12278	1.93379	1830
1840	1.57748	3.02642	1.92829	1.61016	3.06978	1.93083	1.64235	3.11224	1.93322	1840
1850	1.56963	3.01597	1.92766	1.60225	3.05932	1.93023	1.63439	3.10177	1.93264	1850
1860	1.56184	3.00558	1.92703	1.59441	3.04891	1.92962	1.62649	3.09135	1.93206	1860
1870	1.55411	2.99525	1.92639	1.58661	3.03857	1.92901	1.61864	3.08099	1.93147	1870
1880	1.54643	2.98497	1.92575	1.57888	3.02828	1.92840	1.61085	3.07069	1.93089	1880
1890	1.53880	2.97476	1.92511	1.57119	3.01805	1.92779	1.60311	3.06045	1.93030	1890
1900	1.53123	2.96460	1.92446	1.56357	3.00788	1.92717	1.59543	3.05027	1.92970	1900
1910	1.52371	2.95450	1.92381	1.55599	2.99777	1.92655	1.58780	3.04014	1.92911	1910
1920	1.51625	2.94446	1.92316	1.54847	2.98771	1.92592	1.58022	3.03007	1.92851	1920
1930	1.50884	2.93447	1.92251	1.54100	2.97770	1.92529	1.57269	3.02005	1.92791	1930
1940	1.50148	2.92453	1.92185	1.53358	2.96776	1.92466	1.56522	3.01009	1.92730	1940
1950	1.49417	2.91466	1.92119	1.52621	2.95786	1.92403	1.55780	3.00018	1.92670	1950
1960	1.48691	2.90483	1.92052	1.51890	2.94802	1.92339	1.55043	2.99033	1.92608	1960
1970	1.47970	2.89506	1.91985	1.51163	2.93824	1.92275	1.54310	2.98053	1.92547	1970
1980	1.47254	2.88534	1.91918	1.50441	2.92850	1.92211	1.53583	2.97078	1.92486	1980
1990	1.46543	2.87567	1.91851	1.49725	2.91882	1.92147	1.52861	2.96108	1.92424	1990
2000	1.45836	2.86606	1.91783	1.49013	2.90919	1.92082	1.52144	2.95144	1.92361	2000
2010	1.45135	2.85649	1.91715	1.48305	2.89961	1.92016	1.51431	2.94185	1.92299	2010
2020	1.44438	2.84698	1.91647	1.47603	2.89008	1.91951	1.50723	2.93230	1.92236	2020
2030	1.43746	2.83752	1.91578	1.46905	2.88061	1.91885	1.50020	2.92281	1.92173	2030
2040	1.43059	2.82811	1.91509	1.46212	2.87118	1.91819	1.49322	2.91337	1.92110	2040
2050	1.42376	2.81874	1.91440	1.45524	2.86180	1.91753	1.48628	2.90398	1.92046	2050
2060	1.41698	2.80943	1.91370	1.44840	2.85247	1.91686	1.47938	2.89463	1.91982	2060
2070	1.41024	2.80016	1.91300	1.44161	2.84319	1.91619	1.47254	2.88534	1.91918	2070
2080	1.40355	2.79095	1.91230	1.43486	2.83396	1.91552	1.46573	2.87609	1.91854	2080
2090	1.39690	2.78178	1.91160	1.42815	2.82477	1.91484	1.45898	2.86689	1.91789	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=4400.			T=4500.			T=4600.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
2100	1.39030	2.77265	1.91089	1.42149	2.81563	1.91417	1.45226	2.85774	1.91724	2100
2110	1.38373	2.76358	1.91018	1.41488	2.80654	1.91349	1.44559	2.84863	1.91659	2110
2120	1.37722	2.75455	1.90946	1.40830	2.79750	1.91280	1.43896	2.83957	1.91593	2120
2130	1.37074	2.74556	1.90875	1.40177	2.78850	1.91211	1.43238	2.83056	1.91527	2130
2140	1.36431	2.73662	1.90803	1.39528	2.77954	1.91142	1.42583	2.82159	1.91461	2140
2150	1.35792	2.72773	1.90730	1.38883	2.77063	1.91073	1.41933	2.81266	1.91394	2150
2160	1.35156	2.71888	1.90658	1.38243	2.76177	1.91003	1.41287	2.80378	1.91328	2160
2170	1.34526	2.71008	1.90585	1.37606	2.75295	1.90934	1.40645	2.79495	1.91261	2170
2180	1.33899	2.70132	1.90511	1.36974	2.74417	1.90863	1.40007	2.78616	1.91193	2180
2190	1.33276	2.69260	1.90438	1.36345	2.73544	1.90793	1.39374	2.77741	1.91126	2190
2200	1.32657	2.68392	1.90364	1.35721	2.72675	1.90722	1.38744	2.76870	1.91058	2200
2210	1.32042	2.67529	1.90290	1.35100	2.71810	1.90651	1.38118	2.76004	1.90990	2210
2220	1.31431	2.66670	1.90215	1.34484	2.70949	1.90580	1.37496	2.75142	1.90921	2220
2230	1.30823	2.65816	1.90141	1.33871	2.70093	1.90508	1.36878	2.74284	1.90853	2230
2240	1.30220	2.64965	1.90066	1.33262	2.69241	1.90436	1.36264	2.73430	1.90784	2240
2250	1.29620	2.64119	1.89990	1.32657	2.68392	1.90364	1.35653	2.72580	1.90714	2250
2260	1.29024	2.63276	1.89915	1.32055	2.67548	1.90292	1.35046	2.71735	1.90645	2260
2270	1.28432	2.62438	1.89839	1.31458	2.66708	1.90219	1.34444	2.70893	1.90575	2270
2280	1.27844	2.61604	1.89762	1.30864	2.65872	1.90146	1.33844	2.70056	1.90505	2280
2290	1.27259	2.60773	1.89686	1.30273	2.65040	1.90072	1.33249	2.69222	1.90435	2290
2300	1.26678	2.59947	1.89609	1.29687	2.64212	1.89999	1.32657	2.68392	1.90364	2300
2310	1.26100	2.59125	1.89532	1.29104	2.63388	1.89925	1.32068	2.67567	1.90293	2310
2320	1.25526	2.58306	1.89454	1.28524	2.62568	1.89850	1.31484	2.66745	1.90222	2320
2330	1.24955	2.57491	1.89377	1.27948	2.61752	1.89776	1.30902	2.65927	1.90150	2330
2340	1.24388	2.56680	1.89299	1.27375	2.60939	1.89701	1.30325	2.65113	1.90079	2340
2350	1.23825	2.55873	1.89220	1.26806	2.60130	1.89626	1.29750	2.64302	1.90007	2350
2360	1.23264	2.55070	1.89142	1.26241	2.59325	1.89551	1.29179	2.63496	1.89934	2360
2370	1.22708	2.54270	1.89063	1.25679	2.58524	1.89475	1.28612	2.62693	1.89862	2370
2380	1.22154	2.53475	1.88984	1.25120	2.57726	1.89399	1.28048	2.61893	1.89789	2380
2390	1.21604	2.52682	1.88904	1.24564	2.56932	1.89323	1.27487	2.61098	1.89716	2390
2400	1.21057	2.51894	1.88824	1.24012	2.56142	1.89246	1.26930	2.60306	1.89642	2400
2410	1.20514	2.51109	1.88744	1.23463	2.55355	1.89170	1.26376	2.59517	1.89569	2410
2420	1.19973	2.50327	1.88664	1.22917	2.54572	1.89093	1.25825	2.58733	1.89495	2420
2430	1.19436	2.49550	1.88583	1.22375	2.53792	1.89015	1.25277	2.57951	1.89421	2430
2440	1.18902	2.48775	1.88502	1.21836	2.53016	1.88938	1.24733	2.57174	1.89346	2440
2450	1.18372	2.48004	1.88421	1.21300	2.52244	1.88860	1.24192	2.56399	1.89271	2450
2460	1.17844	2.47237	1.88339	1.20767	2.51475	1.88782	1.23654	2.55628	1.89196	2460
2470	1.17320	2.46473	1.88257	1.20237	2.50709	1.88703	1.23119	2.54861	1.89121	2470
2480	1.16798	2.45713	1.88175	1.19710	2.49947	1.88624	1.22587	2.54097	1.89046	2480
2490	1.16280	2.44956	1.88093	1.19187	2.49188	1.88545	1.22058	2.53337	1.88970	2490
2500	1.15765	2.44202	1.88010	1.18666	2.48432	1.88466	1.21532	2.52579	1.88894	2500
2510	1.15253	2.43452	1.87927	1.18149	2.47680	1.88386	1.21010	2.51825	1.88817	2510
2520	1.14743	2.42705	1.87844	1.17634	2.46931	1.88307	1.20490	2.51075	1.88741	2520
2530	1.14237	2.41961	1.87760	1.17122	2.46186	1.88226	1.19973	2.50327	1.88664	2530
2540	1.13734	2.41220	1.87677	1.16614	2.45443	1.88146	1.19460	2.49583	1.88587	2540
2550	1.13233	2.40483	1.87592	1.16108	2.44704	1.88065	1.18949	2.48842	1.88509	2550
2560	1.12736	2.39749	1.87508	1.15605	2.43968	1.87984	1.18441	2.48105	1.88431	2560
2570	1.12241	2.39018	1.87423	1.15105	2.43235	1.87903	1.17936	2.47370	1.88354	2570
2580	1.11749	2.38290	1.87338	1.14608	2.42506	1.87822	1.17434	2.46639	1.88275	2580
2590	1.11260	2.37566	1.87253	1.14114	2.41779	1.87740	1.16934	2.45911	1.88197	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm^{-1}
T=4400.			T=4500.			T=4600.				
2600	1.10774	2.36844	1.87167	1.13622	2.41056	1.87658	1.16438	2.45186	1.88118	2600
2610	1.10290	2.36126	1.87082	1.13134	2.40336	1.87576	1.15944	2.44464	1.88039	2610
2620	1.09809	2.35411	1.86996	1.12648	2.39619	1.87493	1.15453	2.43745	1.87960	2620
2630	1.09331	2.34699	1.86909	1.12164	2.38905	1.87410	1.14964	2.43029	1.87880	2630
2640	1.08856	2.33989	1.86822	1.11684	2.38194	1.87327	1.14479	2.42316	1.87800	2640
2650	1.08383	2.33283	1.86735	1.11206	2.37486	1.87244	1.13996	2.41606	1.87720	2650
2660	1.07913	2.32580	1.86648	1.10731	2.36780	1.87160	1.13516	2.40899	1.87640	2660
2670	1.07446	2.31880	1.86561	1.10258	2.36078	1.87076	1.13038	2.40195	1.87559	2670
2680	1.06981	2.31183	1.86473	1.09788	2.35379	1.86992	1.12563	2.39494	1.87479	2680
2690	1.06519	2.30488	1.86385	1.09321	2.34683	1.86907	1.12091	2.38796	1.87397	2690
2700	1.06060	2.29797	1.86296	1.08856	2.33989	1.86822	1.11621	2.38101	1.87316	2700
2710	1.05603	2.29108	1.86208	1.08394	2.33299	1.86737	1.11154	2.37409	1.87234	2710
2720	1.05148	2.28423	1.86119	1.07934	2.32611	1.86652	1.10689	2.36719	1.87153	2720
2730	1.04696	2.27740	1.86030	1.07477	2.31927	1.86567	1.10227	2.36033	1.87070	2730
2740	1.04247	2.27060	1.85940	1.07023	2.31245	1.86481	1.09768	2.35349	1.86988	2740
2750	1.03800	2.26383	1.85850	1.06570	2.30565	1.86395	1.09311	2.34668	1.86905	2750
2760	1.03355	2.25708	1.85760	1.06121	2.29889	1.86308	1.08856	2.33989	1.86822	2760
2770	1.02913	2.25036	1.85670	1.05674	2.29215	1.86222	1.08404	2.33314	1.86739	2770
2780	1.02473	2.24368	1.85580	1.05229	2.28544	1.86135	1.07954	2.32641	1.86656	2780
2790	1.02036	2.23701	1.85489	1.04786	2.27876	1.86048	1.07507	2.31971	1.86572	2790
2800	1.01601	2.23038	1.85398	1.04346	2.27211	1.85960	1.07062	2.31304	1.86488	2800
2810	1.01169	2.22377	1.85306	1.03909	2.26548	1.85872	1.06619	2.30639	1.86404	2810
2820	1.00739	2.21719	1.85215	1.03474	2.25888	1.85784	1.06179	2.29977	1.86320	2820
2830	1.00311	2.21064	1.85123	1.03041	2.25230	1.85696	1.05741	2.29318	1.86235	2830
2840	0.99885	2.20411	1.85031	1.02610	2.24575	1.85608	1.05306	2.28661	1.86150	2840
2850	0.99462	2.19760	1.84938	1.02182	2.23923	1.85519	1.04873	2.28007	1.86065	2850
2860	0.99041	2.19113	1.84845	1.01756	2.23273	1.85430	1.04442	2.27355	1.85979	2860
2870	0.98622	2.18468	1.84752	1.01332	2.22626	1.85341	1.04013	2.26706	1.85893	2870
2880	0.98206	2.17825	1.84659	1.00910	2.21982	1.85251	1.03587	2.26060	1.85807	2880
2890	0.97792	2.17185	1.84565	1.00491	2.21340	1.85162	1.03163	2.25416	1.85721	2890
2900	0.97380	2.16548	1.84472	1.00074	2.20701	1.85072	1.02741	2.24774	1.85635	2900
2910	0.96970	2.15913	1.84378	0.99659	2.20064	1.84981	1.02321	2.24136	1.85548	2910
2920	0.96562	2.15281	1.84283	0.99247	2.19429	1.84891	1.01904	2.23499	1.85461	2920
2930	0.96157	2.14651	1.84189	0.98836	2.18797	1.84800	1.01488	2.22865	1.85374	2930
2940	0.95753	2.14024	1.84094	0.98428	2.18168	1.84709	1.01075	2.22234	1.85286	2940
2950	0.95352	2.13399	1.83999	0.98021	2.17541	1.84617	1.00664	2.21605	1.85199	2950
2960	0.94953	2.12776	1.83903	0.97617	2.16916	1.84526	1.00255	2.20978	1.85111	2960
2970	0.94556	2.12156	1.83808	0.97215	2.16294	1.84434	0.99848	2.20354	1.85022	2970
2980	0.94161	2.11538	1.83712	0.96815	2.15674	1.84342	0.99444	2.19732	1.84934	2980
2990	0.93768	2.10923	1.83615	0.96418	2.15057	1.84250	0.99041	2.19113	1.84845	2990
3000	0.93377	2.10310	1.83519	0.96022	2.14442	1.84157	0.98640	2.18496	1.84756	3000
3010	0.92989	2.09700	1.83422	0.95628	2.13829	1.84064	0.98242	2.17881	1.84667	3010
3020	0.92602	2.09091	1.83325	0.95237	2.13219	1.83971	0.97846	2.17269	1.84578	3020
3030	0.92217	2.08486	1.83228	0.94847	2.12611	1.83878	0.97451	2.16659	1.84488	3030
3040	0.91834	2.07882	1.83131	0.94459	2.12005	1.83784	0.97059	2.16051	1.84398	3040
3050	0.91454	2.07281	1.83033	0.94074	2.11401	1.83690	0.96668	2.15446	1.84308	3050
3060	0.91075	2.06682	1.82935	0.93690	2.10800	1.83596	0.96280	2.14842	1.84217	3060
3070	0.90698	2.06085	1.82837	0.93308	2.10202	1.83502	0.95893	2.14242	1.84127	3070
3080	0.90323	2.05491	1.82738	0.92928	2.09605	1.83407	0.95509	2.13643	1.84036	3080
3090	0.89950	2.04899	1.82639	0.92550	2.09011	1.83312	0.95126	2.13047	1.83945	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic
Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	$-(F^\circ - E_0^\circ)/T$	S°	C_p°	ν cm^{-1}
	T=4400.			T=4500.			T=4600.			
3100	0.89579	2.04309	1.82540	0.92175	2.08418	1.83217	0.94746	2.12452	1.83853	3100
3110	0.89210	2.03721	1.82441	0.91800	2.07829	1.83122	0.94367	2.11860	1.83762	3110
3120	0.88843	2.03135	1.82341	0.91428	2.07241	1.83026	0.93990	2.11271	1.83670	3120
3130	0.88477	2.02552	1.82242	0.91058	2.06655	1.82931	0.93615	2.10683	1.83578	3130
3140	0.88114	2.01971	1.82142	0.90690	2.06072	1.82834	0.93242	2.10098	1.83485	3140
3150	0.87752	2.01392	1.82041	0.90323	2.05491	1.82738	0.92871	2.09514	1.83393	3150
3160	0.87392	2.00815	1.81941	0.89958	2.04912	1.82642	0.92501	2.08933	1.83300	3160
3170	0.87034	2.00240	1.81840	0.89596	2.04335	1.82545	0.92134	2.08354	1.83207	3170
3180	0.86678	1.99668	1.81739	0.89235	2.03760	1.82448	0.91768	2.07777	1.83114	3180
3190	0.86324	1.99097	1.81638	0.88875	2.03187	1.82350	0.91404	2.07203	1.83020	3190
3200	0.85971	1.98529	1.81536	0.88518	2.02617	1.82253	0.91042	2.06630	1.82926	3200
3210	0.85620	1.97963	1.81434	0.88162	2.02048	1.82155	0.90682	2.06059	1.82832	3210
3220	0.85271	1.97399	1.81332	0.87808	2.01482	1.82057	0.90323	2.05491	1.82738	3220
3230	0.84924	1.96836	1.81230	0.87456	2.00917	1.81959	0.89966	2.04924	1.82644	3230
3240	0.84578	1.96276	1.81127	0.87106	2.00355	1.81860	0.89611	2.04360	1.82549	3240
3250	0.84234	1.95718	1.81024	0.86757	1.99795	1.81761	0.89258	2.03797	1.82454	3250
3260	0.83892	1.95162	1.80921	0.86410	1.99237	1.81662	0.88906	2.03237	1.82359	3260
3270	0.83552	1.94608	1.80818	0.86065	1.98680	1.81563	0.88557	2.02679	1.82263	3270
3280	0.83213	1.94056	1.80715	0.85721	1.98126	1.81464	0.88208	2.02122	1.82168	3280
3290	0.82876	1.93506	1.80611	0.85379	1.97574	1.81364	0.87862	2.01568	1.82072	3290
3300	0.82540	1.92958	1.80507	0.85039	1.97024	1.81264	0.87517	2.01015	1.81976	3300
3310	0.82206	1.92412	1.80402	0.84701	1.96475	1.81164	0.87174	2.00465	1.81879	3310
3320	0.81874	1.91868	1.80298	0.84364	1.95929	1.81063	0.86833	1.99916	1.81783	3320
3330	0.81544	1.91326	1.80193	0.84029	1.95384	1.80963	0.86493	1.99370	1.81686	3330
3340	0.81215	1.90786	1.80088	0.83695	1.94842	1.80862	0.86155	1.98825	1.81589	3340
3350	0.80888	1.90248	1.79983	0.83363	1.94301	1.80761	0.85818	1.98282	1.81492	3350
3360	0.80562	1.89712	1.79877	0.83033	1.93763	1.80659	0.85483	1.97742	1.81394	3360
3370	0.80238	1.89177	1.79772	0.82704	1.93226	1.80558	0.85150	1.97203	1.81297	3370
3380	0.79916	1.88645	1.79666	0.82377	1.92691	1.80456	0.84818	1.96666	1.81199	3380
3390	0.79595	1.88114	1.79560	0.82051	1.92158	1.80354	0.84488	1.96131	1.81100	3390
3400	0.79275	1.87585	1.79453	0.81727	1.91627	1.80251	0.84160	1.95597	1.81002	3400
3410	0.78958	1.87059	1.79346	0.81405	1.91098	1.80149	0.83833	1.95066	1.80903	3410
3420	0.78641	1.86534	1.79240	0.81084	1.90571	1.80046	0.83507	1.94536	1.80805	3420
3430	0.78327	1.86010	1.79132	0.80765	1.90045	1.79943	0.83183	1.94009	1.80706	3430
3440	0.78013	1.85489	1.79025	0.80447	1.89521	1.79840	0.82861	1.93483	1.80606	3440
3450	0.77702	1.84969	1.78917	0.80130	1.89000	1.79736	0.82540	1.92958	1.80507	3450
3460	0.77392	1.84452	1.78810	0.79816	1.88479	1.79633	0.82221	1.92436	1.80407	3460
3470	0.77083	1.83936	1.78701	0.79502	1.87961	1.79529	0.81903	1.91916	1.80307	3470
3480	0.76776	1.83422	1.78593	0.79190	1.87445	1.79425	0.81587	1.91397	1.80207	3480
3490	0.76470	1.82910	1.78485	0.78880	1.86930	1.79320	0.81272	1.90880	1.80106	3490
3500	0.76166	1.82399	1.78376	0.78571	1.86417	1.79216	0.80959	1.90365	1.80006	3500
3510	0.75863	1.81890	1.78267	0.78264	1.85906	1.79111	0.80647	1.89851	1.79905	3510
3520	0.75562	1.81383	1.78157	0.77958	1.85397	1.79006	0.80337	1.89340	1.79804	3520
3530	0.75262	1.80878	1.78048	0.77653	1.84889	1.78901	0.80028	1.88830	1.79703	3530
3540	0.74963	1.80374	1.77938	0.77350	1.84383	1.78795	0.79720	1.88322	1.79601	3540
3550	0.74666	1.79873	1.77828	0.77049	1.83879	1.78689	0.79414	1.87815	1.79499	3550
3560	0.74370	1.79373	1.77718	0.76748	1.83376	1.78583	0.79109	1.87310	1.79398	3560
3570	0.74076	1.78874	1.77608	0.76450	1.82875	1.78477	0.78806	1.86807	1.79295	3570
3580	0.73783	1.78378	1.77497	0.76152	1.82376	1.78371	0.78504	1.86306	1.79193	3580
3590	0.73492	1.77883	1.77386	0.75856	1.81879	1.78264	0.78204	1.85806	1.79090	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	ν cm ⁻¹
T=4400.			T=4500.			T=4600.				
3600	0.73202	1.77389	1.77275	0.75562	1.81383	1.78157	0.77905	1.85308	1.78988	3600
3610	0.72913	1.76898	1.77164	0.75268	1.80889	1.78050	0.77607	1.84812	1.78885	3610
3620	0.72626	1.76408	1.77052	0.74976	1.80397	1.77943	0.77311	1.84317	1.78781	3620
3630	0.72340	1.75920	1.76941	0.74686	1.79906	1.77836	0.77016	1.83824	1.78678	3630
3640	0.72055	1.75433	1.76829	0.74397	1.79417	1.77728	0.76722	1.83333	1.78574	3640
3650	0.71772	1.74948	1.76716	0.74109	1.78930	1.77620	0.76430	1.82843	1.78470	3650
3660	0.71490	1.74465	1.76604	0.73822	1.78444	1.77512	0.76139	1.82355	1.78366	3660
3670	0.71209	1.73983	1.76491	0.73537	1.77960	1.77404	0.75850	1.81868	1.78262	3670
3680	0.70930	1.73503	1.76379	0.73253	1.77477	1.77295	0.75562	1.81383	1.78157	3680
3690	0.70652	1.73024	1.76265	0.72971	1.76996	1.77186	0.75275	1.80900	1.78053	3690
3700	0.70375	1.72547	1.76152	0.72689	1.76517	1.77077	0.74989	1.80418	1.77948	3700
3710	0.70099	1.72072	1.76039	0.72409	1.76039	1.76968	0.74705	1.79938	1.77843	3710
3720	0.69825	1.71598	1.75925	0.72131	1.75563	1.76859	0.74422	1.79459	1.77737	3720
3730	0.69552	1.71126	1.75811	0.71853	1.75088	1.76749	0.74140	1.78982	1.77632	3730
3740	0.69280	1.70656	1.75697	0.71577	1.74615	1.76639	0.73860	1.78507	1.77526	3740
3750	0.69010	1.70187	1.75582	0.71302	1.74143	1.76529	0.73580	1.78033	1.77420	3750
3760	0.68741	1.69719	1.75468	0.71029	1.73673	1.76419	0.73303	1.77561	1.77314	3760
3770	0.68473	1.69253	1.75353	0.70756	1.73205	1.76308	0.73026	1.77090	1.77207	3770
3780	0.68206	1.68789	1.75238	0.70485	1.72738	1.76197	0.72750	1.76621	1.77101	3780
3790	0.67941	1.68326	1.75123	0.70215	1.72273	1.76087	0.72476	1.76153	1.76994	3790
3800	0.67676	1.67865	1.75007	0.69947	1.71809	1.75975	0.72203	1.75687	1.76887	3800
3810	0.67413	1.67405	1.74891	0.69679	1.71346	1.75864	0.71932	1.75222	1.76780	3810
3820	0.67151	1.66947	1.74776	0.69413	1.70886	1.75753	0.71661	1.74759	1.76672	3820
3830	0.66891	1.66490	1.74659	0.69148	1.70426	1.75641	0.71392	1.74297	1.76565	3830
3840	0.66631	1.66035	1.74543	0.68884	1.69968	1.75529	0.71124	1.73837	1.76457	3840
3850	0.66373	1.65581	1.74427	0.68622	1.69512	1.75417	0.70857	1.73378	1.76349	3850
3860	0.66116	1.65129	1.74310	0.68360	1.69057	1.75304	0.70591	1.72921	1.76241	3860
3870	0.65860	1.64678	1.74193	0.68100	1.68604	1.75192	0.70327	1.72465	1.76132	3870
3880	0.65605	1.64228	1.74076	0.67841	1.68152	1.75079	0.70063	1.72010	1.76024	3880
3890	0.65352	1.63781	1.73958	0.67583	1.67701	1.74966	0.69801	1.71557	1.75915	3890
3900	0.65099	1.63334	1.73841	0.67326	1.67252	1.74853	0.69540	1.71106	1.75806	3900
3910	0.64848	1.62889	1.73723	0.67070	1.66805	1.74739	0.69280	1.70656	1.75697	3910
3920	0.64598	1.62445	1.73605	0.66816	1.66358	1.74626	0.69022	1.70207	1.75587	3920
3930	0.64349	1.62003	1.73487	0.66562	1.65914	1.74512	0.68764	1.69760	1.75478	3930
3940	0.64101	1.61563	1.73368	0.66310	1.65470	1.74398	0.68508	1.69314	1.75368	3940
3950	0.63854	1.61123	1.73250	0.66059	1.65028	1.74284	0.68252	1.68870	1.75258	3950
3960	0.63608	1.60685	1.73131	0.65809	1.64588	1.74169	0.67998	1.68427	1.75148	3960
3970	0.63364	1.60249	1.73012	0.65560	1.64149	1.74055	0.67745	1.67985	1.75037	3970
3980	0.63120	1.59814	1.72893	0.65312	1.63711	1.73940	0.67493	1.67545	1.74927	3980
3990	0.62878	1.59380	1.72773	0.65066	1.63275	1.73825	0.67242	1.67106	1.74816	3990
4000	0.62636	1.58948	1.72654	0.64820	1.62840	1.73710	0.66993	1.66669	1.74705	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	T=4700.			T=4800.			T=4900.			ν cm ⁻¹
	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	
100	6.95829	8.91520	1.98702	6.99949	8.95703	1.98702	7.03986	8.99800	1.98703	100
110	6.77191	8.72581	1.98698	6.81306	8.76765	1.98699	6.85337	8.80862	1.98700	110
120	6.60203	8.55292	1.98695	6.64311	8.59476	1.98696	6.68336	8.63573	1.98696	120
130	6.44599	8.39388	1.98691	6.48701	8.43572	1.98692	6.52720	8.47669	1.98693	130
140	6.30175	8.24664	1.98687	6.34271	8.28847	1.98688	6.38283	8.32944	1.98689	140
150	6.16767	8.10956	1.98682	6.20856	8.15139	1.98683	6.24863	8.19236	1.98685	150
160	6.04244	7.98134	1.98677	6.08327	8.02317	1.98679	6.12328	8.06413	1.98680	160
170	5.92498	7.86089	1.98672	5.96575	7.90272	1.98674	6.00570	7.94368	1.98676	170
180	5.81441	7.74734	1.98667	5.85512	7.78916	1.98669	5.89501	7.83013	1.98671	180
190	5.70998	7.63992	1.98661	5.75063	7.68175	1.98663	5.79046	7.72271	1.98665	190
200	5.61107	7.53803	1.98655	5.65165	7.57985	1.98657	5.69142	7.62081	1.98660	200
210	5.51712	7.44110	1.98649	5.55764	7.48293	1.98651	5.59735	7.52389	1.98654	210
220	5.42769	7.34869	1.98642	5.46815	7.39052	1.98645	5.50780	7.43147	1.98648	220
230	5.34236	7.26039	1.98635	5.38276	7.30221	1.98638	5.42235	7.34317	1.98641	230
240	5.26079	7.17586	1.98628	5.30113	7.21768	1.98631	5.34066	7.25863	1.98635	240
250	5.18268	7.09478	1.98620	5.22295	7.13659	1.98624	5.26242	7.17755	1.98628	250
260	5.10774	7.01688	1.98612	5.14795	7.05869	1.98616	5.18737	7.09965	1.98621	260
270	5.03575	6.94192	1.98604	5.07589	6.98374	1.98609	5.11525	7.02469	1.98613	270
280	4.96648	6.86970	1.98595	5.00656	6.91151	1.98600	5.04586	6.95246	1.98605	280
290	4.89974	6.80001	1.98587	4.93977	6.84182	1.98592	4.97900	6.88277	1.98597	290
300	4.83537	6.73269	1.98577	4.87533	6.77449	1.98583	4.91451	6.81544	1.98589	300
310	4.77320	6.66757	1.98568	4.81311	6.70938	1.98574	4.85223	6.75032	1.98580	310
320	4.71311	6.60453	1.98558	4.75295	6.64634	1.98565	4.79201	6.68728	1.98571	320
330	4.65495	6.54343	1.98548	4.69473	6.58524	1.98555	4.73373	6.62618	1.98562	330
340	4.59862	6.48416	1.98538	4.63833	6.52596	1.98545	4.67728	6.56690	1.98552	340
350	4.54400	6.42661	1.98527	4.58366	6.46841	1.98535	4.62254	6.50935	1.98542	350
360	4.49101	6.37069	1.98516	4.53060	6.41248	1.98524	4.56943	6.45342	1.98532	360
370	4.43955	6.31630	1.98505	4.47908	6.35809	1.98513	4.51785	6.39902	1.98522	370
380	4.38953	6.26336	1.98493	4.42901	6.30515	1.98502	4.46772	6.34608	1.98511	380
390	4.34090	6.21180	1.98481	4.38031	6.25359	1.98491	4.41896	6.29452	1.98500	390
400	4.29357	6.16156	1.98469	4.33292	6.20334	1.98479	4.37151	6.24427	1.98489	400
410	4.24748	6.11255	1.98456	4.28677	6.15433	1.98467	4.32530	6.19526	1.98477	410
420	4.20257	6.06473	1.98443	4.24180	6.10651	1.98455	4.28028	6.14743	1.98465	420
430	4.15879	6.01803	1.98430	4.19796	6.05981	1.98442	4.23637	6.10073	1.98453	430
440	4.11608	5.97242	1.98417	4.15519	6.01419	1.98429	4.19354	6.05511	1.98441	440
450	4.07439	5.92783	1.98403	4.11344	5.96960	1.98416	4.15174	6.01051	1.98428	450
460	4.03369	5.88422	1.98389	4.07268	5.92599	1.98402	4.11092	5.96690	1.98415	460
470	3.99392	5.84156	1.98375	4.03285	5.88333	1.98389	4.07103	5.92423	1.98402	470
480	3.95505	5.79980	1.98360	3.99392	5.84156	1.98375	4.03205	5.88246	1.98388	480
490	3.91704	5.75890	1.98345	3.95585	5.80066	1.98360	3.99392	5.84156	1.98375	490
500	3.87986	5.71883	1.98329	3.91861	5.76059	1.98345	3.95662	5.80148	1.98360	500
510	3.84347	5.67956	1.98314	3.88216	5.72131	1.98330	3.92011	5.76220	1.98346	510
520	3.80785	5.64105	1.98298	3.84648	5.68280	1.98315	3.88437	5.72369	1.98331	520
530	3.77296	5.60328	1.98282	3.81153	5.64502	1.98300	3.84936	5.68591	1.98316	530
540	3.73877	5.56622	1.98265	3.77728	5.60796	1.98284	3.81506	5.64885	1.98301	540
550	3.70527	5.52984	1.98248	3.74371	5.57158	1.98268	3.78144	5.61246	1.98286	550
560	3.67242	5.49412	1.98231	3.71080	5.53585	1.98251	3.74847	5.57673	1.98270	560
570	3.64020	5.45903	1.98214	3.67853	5.50077	1.98234	3.71613	5.54164	1.98254	570
580	3.60859	5.42456	1.98196	3.64686	5.46629	1.98217	3.68441	5.50716	1.98237	580
590	3.57757	5.39068	1.98178	3.61578	5.43241	1.98200	3.65327	5.47328	1.98221	590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
	T=4700.			T=4800.			T=4900.			
600	3.54712	5.35738	1.98159	3.58527	5.39910	1.98182	3.62271	5.43996	1.98204	600
610	3.51722	5.32462	1.98141	3.55531	5.36634	1.98164	3.59269	5.40720	1.98187	610
620	3.48786	5.29241	1.98122	3.52589	5.33412	1.98146	3.56321	5.37498	1.98169	620
630	3.45901	5.26071	1.98102	3.49698	5.30242	1.98128	3.53424	5.34327	1.98151	630
640	3.43065	5.22951	1.98083	3.46857	5.27122	1.98109	3.50577	5.31207	1.98133	640
650	3.40279	5.19880	1.98063	3.44064	5.24050	1.98090	3.47779	5.28135	1.98115	650
660	3.37539	5.16856	1.98042	3.41318	5.21026	1.98070	3.45027	5.25111	1.98096	660
670	3.34844	5.13878	1.98022	3.38618	5.18048	1.98050	3.42321	5.22132	1.98077	670
680	3.32194	5.10945	1.98001	3.35962	5.15114	1.98030	3.39660	5.19197	1.98058	680
690	3.29587	5.08055	1.97980	3.33348	5.12223	1.98010	3.37041	5.16306	1.98039	690
700	3.27021	5.05206	1.97958	3.30776	5.09374	1.97990	3.34463	5.13457	1.98019	700
710	3.24495	5.02398	1.97937	3.28245	5.06566	1.97969	3.31926	5.10648	1.97999	710
720	3.22009	4.99630	1.97914	3.25753	5.03797	1.97947	3.29428	5.07879	1.97978	720
730	3.19561	4.96900	1.97892	3.23299	5.01067	1.97926	3.26969	5.05148	1.97958	730
740	3.17150	4.94208	1.97869	3.20882	4.98374	1.97904	3.24546	5.02455	1.97937	740
750	3.14775	4.91552	1.97846	3.18502	4.95718	1.97882	3.22160	4.99798	1.97916	750
760	3.12436	4.88932	1.97823	3.16156	4.93097	1.97860	3.19809	4.97177	1.97894	760
770	3.10130	4.86346	1.97799	3.13845	4.90511	1.97837	3.17492	4.94590	1.97873	770
780	3.07858	4.83794	1.97776	3.11567	4.87958	1.97814	3.15209	4.92037	1.97851	780
790	3.05619	4.81274	1.97751	3.09322	4.85438	1.97791	3.12958	4.89517	1.97828	790
800	3.03411	4.78787	1.97727	3.07108	4.82950	1.97767	3.10739	4.87029	1.97806	800
810	3.01234	4.76331	1.97702	3.04926	4.80494	1.97744	3.08550	4.84571	1.97783	810
820	2.99087	4.73905	1.97677	3.02773	4.78068	1.97720	3.06392	4.82145	1.97760	820
830	2.96970	4.71509	1.97651	3.00650	4.75671	1.97695	3.04263	4.79748	1.97736	830
840	2.94881	4.69142	1.97626	2.98555	4.73304	1.97670	3.02163	4.77380	1.97713	840
850	2.92821	4.66804	1.97600	2.96489	4.70964	1.97645	3.00091	4.75040	1.97689	850
860	2.90787	4.64493	1.97573	2.94450	4.68653	1.97620	2.98047	4.72728	1.97664	860
870	2.88781	4.62209	1.97547	2.92437	4.66368	1.97595	2.96029	4.70443	1.97640	870
880	2.86800	4.59951	1.97520	2.90451	4.64110	1.97569	2.94037	4.68184	1.97615	880
890	2.84845	4.57720	1.97492	2.88490	4.61878	1.97543	2.92071	4.65952	1.97590	890
900	2.82915	4.55513	1.97465	2.86555	4.59671	1.97516	2.90129	4.63744	1.97565	900
910	2.81010	4.53331	1.97437	2.84643	4.57489	1.97489	2.88212	4.61561	1.97539	910
920	2.79128	4.51174	1.97409	2.82756	4.55330	1.97462	2.86319	4.59402	1.97513	920
930	2.77269	4.49040	1.97380	2.80891	4.53196	1.97435	2.84450	4.57267	1.97487	930
940	2.75434	4.46929	1.97351	2.79050	4.51084	1.97407	2.82603	4.55155	1.97460	940
950	2.73620	4.44841	1.97322	2.77231	4.48995	1.97380	2.80778	4.53066	1.97433	950
960	2.71829	4.42774	1.97293	2.75434	4.46929	1.97351	2.78975	4.50999	1.97406	960
970	2.70059	4.40730	1.97263	2.73658	4.44884	1.97323	2.77194	4.48953	1.97379	970
980	2.68310	4.38707	1.97233	2.71903	4.42860	1.97294	2.75434	4.46929	1.97351	980
990	2.66581	4.36705	1.97203	2.70169	4.40857	1.97265	2.73694	4.44925	1.97324	990
1000	2.64873	4.34723	1.97172	2.68455	4.38875	1.97236	2.71974	4.42942	1.97295	1000
1010	2.63184	4.32761	1.97141	2.66760	4.36912	1.97206	2.70275	4.40979	1.97267	1010
1020	2.61515	4.30819	1.97110	2.65085	4.34970	1.97176	2.68594	4.39036	1.97238	1020
1030	2.59864	4.28896	1.97079	2.63429	4.33046	1.97146	2.66932	4.37112	1.97209	1030
1040	2.58233	4.26992	1.97047	2.61792	4.31141	1.97115	2.65289	4.35206	1.97180	1040
1050	2.56619	4.25107	1.97015	2.60172	4.29255	1.97085	2.63665	4.33320	1.97150	1050
1060	2.55023	4.23239	1.96982	2.58571	4.27387	1.97054	2.62058	4.31451	1.97120	1060
1070	2.53445	4.21390	1.96950	2.56987	4.25537	1.97022	2.60468	4.29600	1.97090	1070
1080	2.51884	4.19558	1.96917	2.55420	4.23705	1.96991	2.58896	4.27767	1.97060	1080
1090	2.50340	4.17743	1.96883	2.53871	4.21889	1.96959	2.57341	4.25951	1.97029	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic

Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_p°	ν cm^{-1}
T=4700.			T=4800.			T=4900.				
1100	2.48812	4.15945	1.96850	2.52337	4.20091	1.96926	2.55803	4.24152	1.96998	1100
1110	2.47301	4.14164	1.96816	2.50820	4.18308	1.96894	2.54280	4.22369	1.96967	1110
1120	2.45805	4.12399	1.96782	2.49319	4.16543	1.96861	2.52774	4.20603	1.96936	1120
1130	2.44326	4.10650	1.96747	2.47834	4.14793	1.96828	2.51283	4.18852	1.96904	1130
1140	2.42862	4.08917	1.96712	2.46364	4.13059	1.96795	2.49808	4.17118	1.96872	1140
1150	2.41412	4.07199	1.96677	2.44910	4.11340	1.96761	2.48348	4.15398	1.96839	1150
1160	2.39978	4.05496	1.96642	2.43470	4.09637	1.96727	2.46903	4.13694	1.96807	1160
1170	2.38559	4.03808	1.96606	2.42045	4.07948	1.96693	2.45472	4.12005	1.96774	1170
1180	2.37153	4.02135	1.96570	2.40634	4.06275	1.96658	2.44056	4.10330	1.96741	1180
1190	2.35762	4.00477	1.96534	2.39237	4.04615	1.96623	2.42654	4.08670	1.96707	1190
1200	2.34385	3.98832	1.96497	2.37854	4.02970	1.96588	2.41265	4.07024	1.96674	1200
1210	2.33021	3.97202	1.96460	2.36485	4.01339	1.96553	2.39891	4.05392	1.96640	1210
1220	2.31671	3.95585	1.96423	2.35129	3.99721	1.96517	2.38530	4.03774	1.96605	1220
1230	2.30334	3.93981	1.96386	2.33787	3.98117	1.96481	2.37182	4.02169	1.96571	1230
1240	2.29010	3.92391	1.96348	2.32457	3.96526	1.96445	2.35847	4.00578	1.96536	1240
1250	2.27699	3.90814	1.96310	2.31140	3.94948	1.96408	2.34525	3.98999	1.96501	1250
1260	2.26400	3.89250	1.96271	2.29836	3.93384	1.96372	2.33215	3.97434	1.96466	1260
1270	2.25114	3.87699	1.96233	2.28544	3.91831	1.96334	2.31918	3.95881	1.96430	1270
1280	2.23840	3.86160	1.96194	2.27265	3.90292	1.96297	2.30633	3.94340	1.96394	1280
1290	2.22578	3.84633	1.96155	2.25997	3.88764	1.96259	2.29360	3.92812	1.96358	1290
1300	2.21327	3.83119	1.96115	2.24741	3.87249	1.96221	2.28099	3.91296	1.96322	1300
1310	2.20089	3.81616	1.96075	2.23497	3.85745	1.96183	2.26849	3.89792	1.96285	1310
1320	2.18861	3.80125	1.96035	2.22264	3.84254	1.96145	2.25611	3.88299	1.96248	1320
1330	2.17645	3.78646	1.95994	2.21042	3.82773	1.96106	2.24384	3.86818	1.96211	1330
1340	2.16440	3.77178	1.95954	2.19832	3.81305	1.96067	2.23169	3.85348	1.96173	1340
1350	2.15246	3.75721	1.95913	2.18632	3.79847	1.96027	2.21964	3.83890	1.96135	1350
1360	2.14063	3.74275	1.95871	2.17443	3.78400	1.95988	2.20770	3.82443	1.96097	1360
1370	2.12890	3.72841	1.95830	2.16265	3.76965	1.95948	2.19586	3.81006	1.96059	1370
1380	2.11727	3.71417	1.95788	2.15097	3.75540	1.95908	2.18413	3.79580	1.96020	1380
1390	2.10575	3.70003	1.95746	2.13940	3.74125	1.95867	2.17250	3.78165	1.95981	1390
1400	2.09434	3.68600	1.95703	2.12793	3.72722	1.95826	2.16098	3.76761	1.95942	1400
1410	2.08302	3.67207	1.95660	2.11655	3.71328	1.95785	2.14955	3.75366	1.95903	1410
1420	2.07179	3.65825	1.95617	2.10528	3.69944	1.95744	2.13822	3.73982	1.95863	1420
1430	2.06067	3.64452	1.95574	2.09410	3.68571	1.95702	2.12699	3.72607	1.95823	1430
1440	2.04964	3.63089	1.95530	2.08302	3.67207	1.95660	2.11586	3.71243	1.95783	1440
1450	2.03871	3.61736	1.95486	2.07203	3.65853	1.95618	2.10482	3.69888	1.95742	1450
1460	2.02787	3.60393	1.95442	2.06113	3.64509	1.95576	2.09387	3.68543	1.95701	1460
1470	2.01712	3.59059	1.95397	2.05033	3.63174	1.95533	2.08302	3.67207	1.95660	1470
1480	2.00646	3.57734	1.95352	2.03962	3.61849	1.95490	2.07225	3.65881	1.95619	1480
1490	1.99589	3.56419	1.95307	2.02899	3.60532	1.95446	2.06158	3.64564	1.95577	1490
1500	1.98541	3.55113	1.95262	2.01846	3.59225	1.95403	2.05099	3.63256	1.95535	1500
1510	1.97501	3.53815	1.95216	2.00801	3.57927	1.95359	2.04049	3.61957	1.95493	1510
1520	1.96470	3.52527	1.95170	1.99765	3.56638	1.95315	2.03007	3.60666	1.95451	1520
1530	1.95448	3.51247	1.95124	1.98737	3.55357	1.95270	2.01974	3.59385	1.95408	1530
1540	1.94434	3.49976	1.95077	1.97717	3.54085	1.95226	2.00950	3.58112	1.95365	1540
1550	1.93428	3.48714	1.95030	1.96706	3.52822	1.95181	1.99933	3.56848	1.95322	1550
1560	1.92430	3.47460	1.94983	1.95703	3.51567	1.95135	1.98925	3.55592	1.95278	1560
1570	1.91440	3.46214	1.94936	1.94708	3.50320	1.95090	1.97925	3.54344	1.95235	1570
1580	1.90458	3.44977	1.94888	1.93720	3.49081	1.95044	1.96932	3.53104	1.95191	1580
1590	1.89484	3.43747	1.94840	1.92741	3.47851	1.94998	1.95948	3.51873	1.95146	1590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
	T=4700.			T=4800.			T=4900.			
1600	1.88518	3.42526	1.94791	1.91769	3.46628	1.94951	1.94971	3.50650	1.95102	1600
1610	1.87559	3.41312	1.94743	1.90805	3.45414	1.94905	1.94002	3.49434	1.95057	1610
1620	1.86608	3.40107	1.94694	1.89849	3.44207	1.94858	1.93040	3.48227	1.95012	1620
1630	1.85664	3.38909	1.94645	1.88900	3.43008	1.94811	1.92086	3.47027	1.94967	1630
1640	1.84728	3.37718	1.94595	1.87958	3.41817	1.94763	1.91139	3.45834	1.94921	1640
1650	1.83798	3.36535	1.94545	1.87023	3.40633	1.94715	1.90199	3.44650	1.94875	1650
1660	1.82876	3.35360	1.94495	1.86096	3.39457	1.94667	1.89267	3.43472	1.94829	1660
1670	1.81961	3.34192	1.94445	1.85175	3.38288	1.94619	1.88341	3.42302	1.94782	1670
1680	1.81053	3.33031	1.94394	1.84262	3.37126	1.94570	1.87423	3.41139	1.94736	1680
1690	1.80152	3.31878	1.94343	1.83356	3.35971	1.94521	1.86511	3.39984	1.94689	1690
1700	1.79257	3.30731	1.94292	1.82456	3.34824	1.94472	1.85607	3.38835	1.94642	1700
1710	1.78370	3.29592	1.94241	1.81563	3.33683	1.94423	1.84709	3.37694	1.94594	1710
1720	1.77489	3.28460	1.94189	1.80677	3.32550	1.94373	1.83817	3.36559	1.94546	1720
1730	1.76614	3.27334	1.94137	1.79797	3.31423	1.94323	1.82932	3.35432	1.94498	1730
1740	1.75746	3.26215	1.94084	1.78924	3.30303	1.94273	1.82054	3.34311	1.94450	1740
1750	1.74885	3.25103	1.94032	1.78057	3.29190	1.94222	1.81182	3.33197	1.94402	1750
1760	1.74029	3.23998	1.93979	1.77197	3.28084	1.94172	1.80317	3.32089	1.94353	1760
1770	1.73180	3.22899	1.93926	1.76342	3.26984	1.94120	1.79458	3.30988	1.94304	1770
1780	1.72338	3.21806	1.93872	1.75494	3.25890	1.94069	1.78605	3.29894	1.94254	1780
1790	1.71501	3.20720	1.93818	1.74652	3.24803	1.94017	1.77758	3.28805	1.94205	1790
1800	1.70670	3.19641	1.93764	1.73817	3.23722	1.93966	1.76917	3.27724	1.94155	1800
1810	1.69846	3.18567	1.93710	1.72987	3.22648	1.93913	1.76082	3.26648	1.94105	1810
1820	1.69027	3.17500	1.93655	1.72163	3.21580	1.93861	1.75253	3.25579	1.94054	1820
1830	1.68214	3.16439	1.93600	1.71345	3.20517	1.93808	1.74430	3.24516	1.94004	1830
1840	1.67407	3.15384	1.93545	1.70533	3.19461	1.93755	1.73613	3.23459	1.93953	1840
1850	1.66606	3.14336	1.93490	1.69726	3.18411	1.93702	1.72801	3.22407	1.93902	1850
1860	1.65810	3.13293	1.93434	1.68925	3.17367	1.93648	1.71995	3.21362	1.93850	1860
1870	1.65020	3.12256	1.93378	1.68130	3.16329	1.93595	1.71195	3.20323	1.93799	1870
1880	1.64235	3.11224	1.93322	1.67340	3.15297	1.93541	1.70401	3.19290	1.93747	1880
1890	1.63456	3.10199	1.93265	1.66556	3.14270	1.93486	1.69611	3.18262	1.93694	1890
1900	1.62682	3.09179	1.93208	1.65777	3.13249	1.93432	1.68827	3.17240	1.93642	1900
1910	1.61914	3.08165	1.93151	1.65003	3.12234	1.93377	1.68049	3.16224	1.93589	1910
1920	1.61151	3.07157	1.93094	1.64235	3.11224	1.93322	1.67276	3.15213	1.93536	1920
1930	1.60393	3.06154	1.93036	1.63472	3.10220	1.93266	1.66508	3.14208	1.93483	1930
1940	1.59640	3.05156	1.92978	1.62715	3.09222	1.93211	1.65745	3.13208	1.93429	1940
1950	1.58893	3.04164	1.92920	1.61962	3.08228	1.93155	1.64988	3.12213	1.93376	1950
1960	1.58151	3.03178	1.92861	1.61214	3.07241	1.93098	1.64235	3.11224	1.93322	1960
1970	1.57413	3.02196	1.92802	1.60472	3.06258	1.93042	1.63488	3.10241	1.93267	1970
1980	1.56681	3.01220	1.92743	1.59734	3.05281	1.92985	1.62745	3.09262	1.93213	1980
1990	1.55953	3.00249	1.92684	1.59002	3.04309	1.92928	1.62008	3.08289	1.93158	1990
2000	1.55230	2.99284	1.92624	1.58274	3.03342	1.92871	1.61275	3.07321	1.93103	2000
2010	1.54513	2.98323	1.92564	1.57551	3.02380	1.92813	1.60547	3.06358	1.93048	2010
2020	1.53799	2.97368	1.92504	1.56833	3.01423	1.92755	1.59824	3.05400	1.92992	2020
2030	1.53091	2.96417	1.92443	1.56119	3.00471	1.92697	1.59106	3.04447	1.92936	2030
2040	1.52387	2.95472	1.92383	1.55411	2.99525	1.92639	1.58392	3.03499	1.92880	2040
2050	1.51688	2.94531	1.92322	1.54706	2.98583	1.92580	1.57683	3.02556	1.92824	2050
2060	1.50994	2.93595	1.92260	1.54007	2.97646	1.92522	1.56979	3.01618	1.92767	2060
2070	1.50304	2.92664	1.92199	1.53312	2.96714	1.92462	1.56279	3.00685	1.92710	2070
2080	1.49618	2.91738	1.92137	1.52621	2.95786	1.92403	1.55584	2.99756	1.92653	2080
2090	1.48937	2.90817	1.92075	1.51935	2.94864	1.92343	1.54893	2.98832	1.92596	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	T=4700.			T=4800.			T=4900.			ν cm^{-1}
	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	
2100	1.48261	2.89900	1.92012	1.51254	2.93946	1.92283	1.54206	2.97913	1.92538	2100
2110	1.47588	2.88988	1.91950	1.50576	2.93032	1.92223	1.53524	2.96998	1.92481	2110
2120	1.46920	2.88081	1.91887	1.49903	2.92124	1.92163	1.52846	2.96089	1.92422	2120
2130	1.46256	2.87178	1.91823	1.49235	2.91219	1.92102	1.52173	2.95183	1.92364	2130
2140	1.45597	2.86280	1.91760	1.48570	2.90320	1.92041	1.51504	2.94282	1.92305	2140
2150	1.44942	2.85386	1.91696	1.47910	2.89425	1.91980	1.50838	2.93386	1.92247	2150
2160	1.44291	2.84496	1.91632	1.47254	2.88534	1.91918	1.50177	2.92494	1.92187	2160
2170	1.43643	2.83611	1.91568	1.46602	2.87648	1.91856	1.49521	2.91606	1.92128	2170
2180	1.43000	2.82731	1.91503	1.45954	2.86766	1.91794	1.48868	2.90723	1.92068	2180
2190	1.42362	2.81854	1.91438	1.45310	2.85888	1.91732	1.48219	2.89844	1.92008	2190
2200	1.41727	2.80982	1.91373	1.44670	2.85015	1.91670	1.47575	2.88970	1.91948	2200
2210	1.41096	2.80115	1.91308	1.44034	2.84146	1.91607	1.46934	2.88099	1.91888	2210
2220	1.40468	2.79251	1.91242	1.43402	2.83281	1.91544	1.46297	2.87233	1.91827	2220
2230	1.39845	2.78392	1.91176	1.42774	2.82420	1.91480	1.45664	2.86371	1.91766	2230
2240	1.39226	2.77537	1.91110	1.42149	2.81563	1.91417	1.45035	2.85513	1.91705	2240
2250	1.38610	2.76685	1.91043	1.41529	2.80711	1.91353	1.44410	2.84659	1.91644	2250
2260	1.37999	2.75838	1.90977	1.40912	2.79862	1.91289	1.43788	2.83810	1.91582	2260
2270	1.37390	2.74995	1.90910	1.40299	2.79018	1.91224	1.43171	2.82964	1.91520	2270
2280	1.36786	2.74156	1.90842	1.39690	2.78178	1.91160	1.42557	2.82122	1.91458	2280
2290	1.36185	2.73321	1.90775	1.39084	2.77341	1.91095	1.41946	2.81284	1.91396	2290
2300	1.35588	2.72490	1.90707	1.38483	2.76509	1.91030	1.41340	2.80451	1.91333	2300
2310	1.34995	2.71663	1.90639	1.37884	2.75680	1.90964	1.40737	2.79621	1.91270	2310
2320	1.34405	2.70840	1.90571	1.37290	2.74855	1.90899	1.40137	2.78795	1.91207	2320
2330	1.33819	2.70020	1.90502	1.36698	2.74034	1.90833	1.39541	2.77972	1.91144	2330
2340	1.33236	2.69204	1.90433	1.36111	2.73217	1.90766	1.38949	2.77154	1.91080	2340
2350	1.32657	2.68392	1.90364	1.35526	2.72404	1.90700	1.38360	2.76339	1.91016	2350
2360	1.32081	2.67584	1.90295	1.34946	2.71594	1.90633	1.37775	2.75528	1.90952	2360
2370	1.31508	2.66780	1.90225	1.34368	2.70788	1.90566	1.37193	2.74721	1.90888	2370
2380	1.30939	2.65979	1.90155	1.33794	2.69986	1.90499	1.36614	2.73917	1.90823	2380
2390	1.30374	2.65182	1.90085	1.33224	2.69187	1.90432	1.36039	2.73117	1.90758	2390
2400	1.29811	2.64388	1.90014	1.32657	2.68392	1.90364	1.35467	2.72321	1.90693	2400
2410	1.29252	2.63598	1.89944	1.32093	2.67601	1.90296	1.34898	2.71528	1.90628	2410
2420	1.28696	2.62812	1.89873	1.31532	2.66813	1.90228	1.34333	2.70739	1.90562	2420
2430	1.28144	2.62029	1.89801	1.30975	2.66029	1.90159	1.33771	2.69953	1.90496	2430
2440	1.27594	2.61250	1.89730	1.30421	2.65248	1.90091	1.33212	2.69171	1.90430	2440
2450	1.27048	2.60474	1.89658	1.29870	2.64471	1.90022	1.32657	2.68392	1.90364	2450
2460	1.26505	2.59702	1.89586	1.29322	2.63697	1.89952	1.32104	2.67617	1.90297	2460
2470	1.25965	2.58933	1.89514	1.28777	2.62926	1.89883	1.31555	2.66845	1.90231	2470
2480	1.25428	2.58167	1.89441	1.28236	2.62159	1.89813	1.31009	2.66077	1.90164	2480
2490	1.24895	2.57405	1.89368	1.27697	2.61396	1.89743	1.30466	2.65312	1.90096	2490
2500	1.24364	2.56646	1.89295	1.27162	2.60635	1.89673	1.29926	2.64550	1.90029	2500
2510	1.23836	2.55890	1.89222	1.26629	2.59878	1.89603	1.29389	2.63791	1.89961	2510
2520	1.23312	2.55138	1.89148	1.26100	2.59125	1.89532	1.28855	2.63036	1.89893	2520
2530	1.22790	2.54389	1.89075	1.25574	2.58374	1.89461	1.28324	2.62284	1.89825	2530
2540	1.22272	2.53644	1.89000	1.25050	2.57627	1.89390	1.27796	2.61536	1.89756	2540
2550	1.21756	2.52901	1.88926	1.24530	2.56883	1.89318	1.27271	2.60790	1.89687	2550
2560	1.21243	2.52162	1.88851	1.24012	2.56142	1.89246	1.26749	2.60048	1.89618	2560
2570	1.20733	2.51426	1.88777	1.23497	2.55404	1.89174	1.26229	2.59309	1.89549	2570
2580	1.20226	2.50693	1.88701	1.22985	2.54670	1.89102	1.25713	2.58573	1.89480	2580
2590	1.19722	2.49963	1.88626	1.22477	2.53938	1.89030	1.25199	2.57840	1.89410	2590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
	T=4700.			T=4800.			T=4900.			
2600	1.19220	2.49236	1.88550	1.21970	2.53210	1.88957	1.24689	2.57110	1.89340	2600
2610	1.18721	2.48512	1.88474	1.21467	2.52485	1.88884	1.24181	2.56384	1.89270	2610
2620	1.18226	2.47792	1.88398	1.20966	2.51763	1.88811	1.23676	2.55660	1.89199	2620
2630	1.17732	2.47074	1.88322	1.20469	2.51044	1.88737	1.23173	2.54939	1.89129	2630
2640	1.17242	2.46360	1.88245	1.19973	2.50327	1.88664	1.22674	2.54222	1.89058	2640
2650	1.16754	2.45648	1.88168	1.19481	2.49614	1.88590	1.22177	2.53507	1.88987	2650
2660	1.16269	2.44940	1.88091	1.18991	2.48904	1.88516	1.21682	2.52795	1.88915	2660
2670	1.15787	2.44234	1.88014	1.18504	2.48197	1.88441	1.21191	2.52087	1.88844	2670
2680	1.15307	2.43531	1.87936	1.18020	2.47493	1.88367	1.20702	2.51381	1.88772	2680
2690	1.14830	2.42831	1.87858	1.17538	2.46791	1.88292	1.20216	2.50678	1.88700	2690
2700	1.14355	2.42135	1.87780	1.17059	2.46093	1.88216	1.19732	2.49978	1.88628	2700
2710	1.13883	2.41440	1.87702	1.16582	2.45397	1.88141	1.19251	2.49281	1.88555	2710
2720	1.13414	2.40749	1.87623	1.16108	2.44704	1.88065	1.18772	2.48586	1.88482	2720
2730	1.12947	2.40061	1.87544	1.15637	2.44014	1.87990	1.18296	2.47895	1.88409	2730
2740	1.12483	2.39375	1.87465	1.15168	2.43327	1.87913	1.17823	2.47206	1.88336	2740
2750	1.12021	2.38693	1.87385	1.14701	2.42642	1.87837	1.17352	2.46520	1.88262	2750
2760	1.11561	2.38013	1.87306	1.14237	2.41961	1.87760	1.16883	2.45837	1.88189	2760
2770	1.11105	2.37335	1.87226	1.13776	2.41282	1.87684	1.16417	2.45156	1.88115	2770
2780	1.10650	2.36661	1.87146	1.13316	2.40606	1.87606	1.15954	2.44478	1.88041	2780
2790	1.10198	2.35989	1.87065	1.12860	2.39932	1.87529	1.15493	2.43803	1.87966	2790
2800	1.09748	2.35320	1.86984	1.12406	2.39261	1.87452	1.15034	2.43131	1.87892	2800
2810	1.09301	2.34653	1.86904	1.11954	2.38593	1.87374	1.14578	2.42461	1.87817	2810
2820	1.08856	2.33989	1.86822	1.11504	2.37928	1.87296	1.14124	2.41794	1.87742	2820
2830	1.08414	2.33328	1.86741	1.11057	2.37265	1.87217	1.13672	2.41130	1.87666	2830
2840	1.07973	2.32670	1.86659	1.10612	2.36605	1.87139	1.13223	2.40468	1.87591	2840
2850	1.07535	2.32014	1.86577	1.10170	2.35947	1.87060	1.12776	2.39809	1.87515	2850
2860	1.07100	2.31360	1.86495	1.09730	2.35292	1.86981	1.12332	2.39152	1.87439	2860
2870	1.06666	2.30710	1.86413	1.09292	2.34639	1.86902	1.11889	2.38498	1.87363	2870
2880	1.06235	2.30061	1.86330	1.08856	2.33989	1.86822	1.11449	2.37846	1.87286	2880
2890	1.05807	2.29416	1.86247	1.08423	2.33342	1.86743	1.11012	2.37197	1.87209	2890
2900	1.05380	2.28772	1.86164	1.07992	2.32697	1.86663	1.10576	2.36551	1.87132	2900
2910	1.04956	2.28132	1.86081	1.07563	2.32055	1.86583	1.10143	2.35907	1.87055	2910
2920	1.04533	2.27494	1.85997	1.07136	2.31415	1.86502	1.09712	2.35265	1.86978	2920
2930	1.04113	2.26858	1.85914	1.06711	2.30777	1.86422	1.09283	2.34626	1.86900	2930
2940	1.03695	2.26224	1.85829	1.06289	2.30142	1.86341	1.08856	2.33989	1.86822	2940
2950	1.03280	2.25594	1.85745	1.05869	2.29510	1.86260	1.08432	2.33355	1.86744	2950
2960	1.02866	2.24965	1.85661	1.05451	2.28879	1.86178	1.08009	2.32723	1.86666	2960
2970	1.02455	2.24339	1.85576	1.05035	2.28252	1.86097	1.07589	2.32094	1.86588	2970
2980	1.02045	2.23716	1.85491	1.04621	2.27626	1.86015	1.07171	2.31467	1.86509	2980
2990	1.01638	2.23094	1.85405	1.04209	2.27003	1.85933	1.06755	2.30842	1.86430	2990
3000	1.01233	2.22475	1.85320	1.03800	2.26383	1.85850	1.06341	2.30220	1.86351	3000
3010	1.00830	2.21859	1.85234	1.03392	2.25764	1.85768	1.05929	2.29600	1.86271	3010
3020	1.00429	2.21245	1.85148	1.02987	2.25148	1.85685	1.05519	2.28982	1.86191	3020
3030	1.00030	2.20633	1.85062	1.02583	2.24535	1.85602	1.05111	2.28367	1.86112	3030
3040	0.99633	2.20023	1.84975	1.02182	2.23923	1.85519	1.04705	2.27754	1.86032	3040
3050	0.99238	2.19416	1.84889	1.01782	2.23314	1.85436	1.04302	2.27143	1.85951	3050
3060	0.98845	2.18811	1.84802	1.01385	2.22707	1.85352	1.03900	2.26534	1.85871	3060
3070	0.98454	2.18208	1.84715	1.00989	2.22103	1.85268	1.03500	2.25928	1.85790	3070
3080	0.98065	2.17607	1.84627	1.00596	2.21500	1.85184	1.03102	2.25324	1.85709	3080
3090	0.97677	2.17009	1.84540	1.00204	2.20900	1.85100	1.02706	2.24722	1.85628	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic
 Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
	T=4700.			T=4800.			T=4900.			
3100	0.97292	2.16413	1.84452	0.99815	2.20302	1.85015	1.02313	2.24123	1.85546	3100
3110	0.96909	2.15819	1.84364	0.99427	2.19706	1.84930	1.01921	2.23525	1.85465	3110
3120	0.96527	2.15227	1.84275	0.99041	2.19113	1.84845	1.01531	2.22930	1.85383	3120
3130	0.96148	2.14638	1.84187	0.98657	2.18522	1.84760	1.01142	2.22337	1.85301	3130
3140	0.95770	2.14050	1.84098	0.98275	2.17932	1.84675	1.00756	2.21746	1.85218	3140
3150	0.95395	2.13465	1.84009	0.97895	2.17345	1.84589	1.00372	2.21157	1.85136	3150
3160	0.95021	2.12882	1.83920	0.97517	2.16760	1.84503	0.99989	2.20570	1.85053	3160
3170	0.94649	2.12301	1.83830	0.97140	2.16177	1.84417	0.99609	2.19986	1.84970	3170
3180	0.94278	2.11722	1.83740	0.96766	2.15597	1.84330	0.99230	2.19403	1.84887	3180
3190	0.93910	2.11145	1.83650	0.96393	2.15018	1.84244	0.98853	2.18823	1.84804	3190
3200	0.93543	2.10571	1.83560	0.96022	2.14442	1.84157	0.98478	2.18245	1.84720	3200
3210	0.93179	2.09998	1.83470	0.95653	2.13867	1.84070	0.98104	2.17668	1.84636	3210
3220	0.92816	2.09428	1.83379	0.95285	2.13295	1.83983	0.97733	2.17094	1.84552	3220
3230	0.92454	2.08859	1.83288	0.94920	2.12724	1.83895	0.97363	2.16522	1.84468	3230
3240	0.92095	2.08293	1.83197	0.94556	2.12156	1.83808	0.96995	2.15952	1.84383	3240
3250	0.91737	2.07728	1.83106	0.94194	2.11590	1.83720	0.96629	2.15384	1.84299	3250
3260	0.91381	2.07166	1.83014	0.93833	2.11026	1.83632	0.96264	2.14818	1.84214	3260
3270	0.91027	2.06606	1.82922	0.93475	2.10463	1.83543	0.95901	2.14254	1.84129	3270
3280	0.90674	2.06047	1.82830	0.93118	2.09903	1.83455	0.95540	2.13692	1.84043	3280
3290	0.90323	2.05491	1.82738	0.92763	2.09345	1.83366	0.95181	2.13132	1.83958	3290
3300	0.89974	2.04936	1.82646	0.92409	2.08788	1.83277	0.94823	2.12573	1.83872	3300
3310	0.89626	2.04384	1.82553	0.92057	2.08234	1.83188	0.94467	2.12017	1.83786	3310
3320	0.89281	2.03833	1.82460	0.91707	2.07681	1.83098	0.94113	2.11463	1.83700	3320
3330	0.88936	2.03285	1.82367	0.91359	2.07131	1.83008	0.93760	2.10911	1.83614	3330
3340	0.88594	2.02738	1.82274	0.91012	2.06582	1.82919	0.93409	2.10360	1.83527	3340
3350	0.88253	2.02193	1.82180	0.90667	2.06036	1.82828	0.93060	2.09812	1.83440	3350
3360	0.87914	2.01650	1.82086	0.90323	2.05491	1.82738	0.92712	2.09265	1.83353	3360
3370	0.87576	2.01109	1.81992	0.89981	2.04948	1.82648	0.92366	2.08720	1.83266	3370
3380	0.87240	2.00570	1.81898	0.89641	2.04407	1.82557	0.92022	2.08177	1.83178	3380
3390	0.86905	2.00033	1.81803	0.89302	2.03868	1.82466	0.91679	2.07636	1.83091	3390
3400	0.86572	1.99498	1.81709	0.88965	2.03330	1.82375	0.91338	2.07097	1.83003	3400
3410	0.86241	1.98964	1.81614	0.88629	2.02795	1.82283	0.90998	2.06560	1.82915	3410
3420	0.85911	1.98432	1.81519	0.88295	2.02261	1.82192	0.90660	2.06024	1.82827	3420
3430	0.85583	1.97903	1.81423	0.87963	2.01729	1.82100	0.90323	2.05491	1.82738	3430
3440	0.85256	1.97375	1.81328	0.87632	2.01199	1.82008	0.89988	2.04959	1.82649	3440
3450	0.84931	1.96848	1.81232	0.87303	2.00671	1.81916	0.89655	2.04429	1.82561	3450
3460	0.84607	1.96324	1.81136	0.86975	2.00145	1.81823	0.89323	2.03901	1.82471	3460
3470	0.84285	1.95801	1.81040	0.86648	1.99620	1.81730	0.88992	2.03374	1.82382	3470
3480	0.83965	1.95280	1.80943	0.86324	1.99097	1.81638	0.88664	2.02849	1.82293	3480
3490	0.83646	1.94761	1.80847	0.86000	1.98576	1.81544	0.88336	2.02326	1.82203	3490
3500	0.83328	1.94244	1.80750	0.85679	1.98057	1.81451	0.88010	2.01805	1.82113	3500
3510	0.83012	1.93729	1.80653	0.85358	1.97539	1.81358	0.87686	2.01286	1.82023	3510
3520	0.82697	1.93215	1.80555	0.85039	1.97024	1.81264	0.87363	2.00768	1.81933	3520
3530	0.82384	1.92703	1.80458	0.84722	1.96509	1.81170	0.87042	2.00252	1.81842	3530
3540	0.82072	1.92192	1.80360	0.84406	1.95997	1.81076	0.86722	1.99738	1.81751	3540
3550	0.81762	1.91684	1.80262	0.84091	1.95486	1.80982	0.86403	1.99225	1.81660	3550
3560	0.81453	1.91177	1.80164	0.83778	1.94977	1.80887	0.86086	1.98714	1.81569	3560
3570	0.81145	1.90671	1.80066	0.83467	1.94470	1.80792	0.85770	1.98205	1.81478	3570
3580	0.80839	1.90168	1.79967	0.83157	1.93965	1.80697	0.85456	1.97698	1.81386	3580
3590	0.80534	1.89666	1.79868	0.82848	1.93461	1.80602	0.85143	1.97192	1.81295	3590

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
	T=4700.			T=4800.			T=4900.			
3600	0.80231	1.89166	1.79769	0.82540	1.92958	1.80507	0.84832	1.96688	1.81203	3600
3610	0.79929	1.88667	1.79670	0.82234	1.92458	1.80411	0.84522	1.96185	1.81110	3610
3620	0.79629	1.88170	1.79571	0.81930	1.91959	1.80315	0.84213	1.95684	1.81018	3620
3630	0.79330	1.87675	1.79471	0.81626	1.91462	1.80219	0.83906	1.95185	1.80926	3630
3640	0.79032	1.87182	1.79371	0.81324	1.90966	1.80123	0.83600	1.94687	1.80833	3640
3650	0.78735	1.86690	1.79271	0.81024	1.90472	1.80027	0.83296	1.94191	1.80740	3650
3660	0.78440	1.86199	1.79171	0.80725	1.89980	1.79930	0.82992	1.93697	1.80647	3660
3670	0.78147	1.85711	1.79071	0.80427	1.89489	1.79833	0.82691	1.93204	1.80553	3670
3680	0.77854	1.85223	1.78970	0.80130	1.89000	1.79736	0.82390	1.92713	1.80460	3680
3690	0.77563	1.84738	1.78869	0.79835	1.88512	1.79639	0.82091	1.92223	1.80366	3690
3700	0.77273	1.84254	1.78768	0.79541	1.88026	1.79542	0.81793	1.91735	1.80272	3700
3710	0.76985	1.83772	1.78667	0.79249	1.87541	1.79444	0.81497	1.91249	1.80178	3710
3720	0.76698	1.83291	1.78565	0.78958	1.87059	1.79346	0.81202	1.90764	1.80084	3720
3730	0.76412	1.82812	1.78464	0.78668	1.86577	1.79248	0.80908	1.90281	1.79989	3730
3740	0.76127	1.82334	1.78362	0.78379	1.86097	1.79150	0.80615	1.89799	1.79895	3740
3750	0.75844	1.81858	1.78260	0.78092	1.85619	1.79052	0.80324	1.89319	1.79800	3750
3760	0.75562	1.81383	1.78157	0.77805	1.85142	1.78953	0.80034	1.88840	1.79705	3760
3770	0.75281	1.80910	1.78055	0.77521	1.84667	1.78854	0.79745	1.88363	1.79609	3770
3780	0.75001	1.80439	1.77952	0.77237	1.84194	1.78756	0.79458	1.87887	1.79514	3780
3790	0.74723	1.79969	1.77849	0.76955	1.83721	1.78656	0.79171	1.87413	1.79418	3790
3800	0.74446	1.79500	1.77746	0.76674	1.83251	1.78557	0.78886	1.86941	1.79322	3800
3810	0.74170	1.79033	1.77643	0.76394	1.82782	1.78457	0.78603	1.86469	1.79226	3810
3820	0.73895	1.78568	1.77540	0.76115	1.82314	1.78358	0.78320	1.86000	1.79130	3820
3830	0.73622	1.78104	1.77436	0.75838	1.81848	1.78258	0.78039	1.85531	1.79034	3830
3840	0.73350	1.77641	1.77332	0.75562	1.81383	1.78157	0.77759	1.85065	1.78937	3840
3850	0.73079	1.77180	1.77228	0.75287	1.80920	1.78057	0.77480	1.84600	1.78840	3850
3860	0.72809	1.76720	1.77124	0.75013	1.80458	1.77957	0.77202	1.84136	1.78743	3860
3870	0.72540	1.76262	1.77019	0.74740	1.79998	1.77856	0.76926	1.83673	1.78646	3870
3880	0.72273	1.75806	1.76914	0.74469	1.79539	1.77755	0.76651	1.83212	1.78549	3880
3890	0.72007	1.75350	1.76810	0.74199	1.79082	1.77654	0.76377	1.82753	1.78451	3890
3900	0.71742	1.74896	1.76704	0.73930	1.78626	1.77552	0.76104	1.82295	1.78354	3900
3910	0.71478	1.74444	1.76599	0.73662	1.78171	1.77451	0.75832	1.81838	1.78256	3910
3920	0.71215	1.73993	1.76494	0.73395	1.77718	1.77349	0.75562	1.81383	1.78157	3920
3930	0.70953	1.73544	1.76388	0.73129	1.77266	1.77247	0.75292	1.80929	1.78059	3930
3940	0.70693	1.73095	1.76282	0.72865	1.76816	1.77145	0.75024	1.80477	1.77961	3940
3950	0.70433	1.72649	1.76176	0.72602	1.76367	1.77043	0.74757	1.80026	1.77862	3950
3960	0.70175	1.72203	1.76070	0.72340	1.75920	1.76941	0.74491	1.79576	1.77763	3960
3970	0.69918	1.71760	1.75964	0.72079	1.75473	1.76838	0.74226	1.79128	1.77664	3970
3980	0.69662	1.71317	1.75857	0.71819	1.75029	1.76735	0.73963	1.78681	1.77565	3980
3990	0.69407	1.70876	1.75750	0.71560	1.74585	1.76632	0.73700	1.78236	1.77465	3990
4000	0.69154	1.70436	1.75643	0.71302	1.74143	1.76529	0.73439	1.77792	1.77366	4000

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=5000.				T=5000.				
100	7.07943	9.03814	1.98703	100	3.65945	5.48001	1.98224	600
110	6.89287	8.84876	1.98700	110	3.62938	5.44725	1.98208	610
120	6.72281	8.67587	1.98697	120	3.59985	5.41502	1.98191	620
130	6.56659	8.51683	1.98694	130	3.57082	5.38331	1.98174	630
140	6.42217	8.36958	1.98690	140	3.54230	5.35210	1.98156	640
150	6.28791	8.23250	1.98686	150	3.51426	5.32138	1.98139	650
160	6.16250	8.10427	1.98682	160	3.48669	5.29113	1.98121	660
170	6.04486	7.98382	1.98677	170	3.45958	5.26134	1.98103	670
180	5.93411	7.87026	1.98673	180	3.43290	5.23199	1.98084	680
190	5.82951	7.76285	1.98668	190	3.40666	5.20307	1.98065	690
200	5.73041	7.66095	1.98662	200	3.38083	5.17458	1.98046	700
210	5.63629	7.56402	1.98657	210	3.35541	5.14648	1.98027	710
220	5.54667	7.47161	1.98651	220	3.33037	5.11879	1.98008	720
230	5.46117	7.38330	1.98644	230	3.30572	5.09148	1.97988	730
240	5.37942	7.29876	1.98638	240	3.28145	5.06454	1.97968	740
250	5.30113	7.21768	1.98631	250	3.25753	5.03797	1.97947	750
260	5.22601	7.13977	1.98624	260	3.23396	5.01175	1.97927	760
270	5.15384	7.06481	1.98617	270	3.21074	4.98588	1.97906	770
280	5.08439	6.99258	1.98610	280	3.18785	4.96035	1.97885	780
290	5.01748	6.92289	1.98602	290	3.16529	4.93514	1.97863	790
300	4.95293	6.85556	1.98594	300	3.14304	4.91025	1.97842	800
310	4.89059	6.79044	1.98585	310	3.12111	4.88568	1.97820	810
320	4.83032	6.72740	1.98577	320	3.09947	4.86140	1.97798	820
330	4.77198	6.66629	1.98568	330	3.07813	4.83743	1.97775	830
340	4.71547	6.60702	1.98559	340	3.05708	4.81375	1.97752	840
350	4.66068	6.54946	1.98549	350	3.03630	4.79034	1.97729	850
360	4.60751	6.49353	1.98539	360	3.01580	4.76722	1.97706	860
370	4.55587	6.43913	1.98529	370	2.99557	4.74436	1.97682	870
380	4.50569	6.38619	1.98519	380	2.97560	4.72177	1.97658	880
390	4.45688	6.33462	1.98509	390	2.95588	4.69944	1.97634	890
400	4.40937	6.28437	1.98498	400	2.93642	4.67736	1.97610	900
410	4.36310	6.23535	1.98487	410	2.91719	4.65552	1.97585	910
420	4.31802	6.18753	1.98475	420	2.89821	4.63393	1.97560	920
430	4.27406	6.14082	1.98464	430	2.87946	4.61258	1.97535	930
440	4.23118	6.09520	1.98452	440	2.86094	4.59145	1.97510	940
450	4.18932	6.05060	1.98440	450	2.84264	4.57055	1.97484	950
460	4.14844	6.00699	1.98427	460	2.82456	4.54987	1.97458	960
470	4.10850	5.96432	1.98414	470	2.80669	4.52941	1.97432	970
480	4.06946	5.92255	1.98401	480	2.78904	4.50916	1.97405	980
490	4.03127	5.88164	1.98388	490	2.77159	4.48912	1.97378	990
500	3.99392	5.84156	1.98375	500	2.75434	4.46929	1.97351	1000
510	3.95736	5.80228	1.98361	510	2.73729	4.44965	1.97324	1010
520	3.92156	5.76376	1.98347	520	2.72043	4.43021	1.97296	1020
530	3.88650	5.72598	1.98332	530	2.70376	4.41096	1.97269	1030
540	3.85214	5.68891	1.98318	540	2.68728	4.39191	1.97240	1040
550	3.81846	5.65252	1.98303	550	2.67098	4.37303	1.97212	1050
560	3.78544	5.61679	1.98288	560	2.65486	4.35434	1.97183	1060
570	3.75305	5.58170	1.98272	570	2.63891	4.33583	1.97154	1070
580	3.72127	5.54722	1.98256	580	2.62314	4.31749	1.97125	1080
590	3.69007	5.51333	1.98240	590	2.60753	4.29932	1.97096	1090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹	ν cm ⁻¹	$-(F^0-E_0^0)/T$	S ⁰	C _p ⁰	ν cm ⁻¹
T=5000.					T=5000.				
1100	2.59209	4.28132	1.97066	1100	1600	1.98124	3.54593	1.95243	1600
1110	2.57682	4.26349	1.97036	1110	1610	1.97150	3.53376	1.95200	1610
1120	2.56170	4.24582	1.97006	1120	1620	1.96183	3.52168	1.95157	1620
1130	2.54674	4.22831	1.96975	1130	1630	1.95224	3.50967	1.95113	1630
1140	2.53194	4.21096	1.96944	1140	1640	1.94272	3.49774	1.95070	1640
1150	2.51729	4.19376	1.96913	1150	1650	1.93328	3.48588	1.95025	1650
1160	2.50278	4.17671	1.96882	1160	1660	1.92390	3.47410	1.94981	1660
1170	2.48843	4.15981	1.96850	1170	1670	1.91460	3.46239	1.94936	1670
1180	2.47421	4.14306	1.96819	1180	1680	1.90537	3.45075	1.94892	1680
1190	2.46014	4.12645	1.96787	1190	1690	1.89620	3.43919	1.94846	1690
1200	2.44621	4.10999	1.96754	1200	1700	1.88711	3.42769	1.94801	1700
1210	2.43241	4.09366	1.96721	1210	1710	1.87808	3.41627	1.94755	1710
1220	2.41875	4.07747	1.96689	1220	1720	1.86911	3.40491	1.94710	1720
1230	2.40522	4.06141	1.96655	1230	1730	1.86022	3.39363	1.94663	1730
1240	2.39182	4.04549	1.96622	1240	1740	1.85139	3.38241	1.94617	1740
1250	2.37854	4.02970	1.96588	1250	1750	1.84262	3.37126	1.94570	1750
1260	2.36540	4.01404	1.96554	1260	1760	1.83392	3.36017	1.94523	1760
1270	2.35237	3.99850	1.96520	1270	1770	1.82528	3.34915	1.94476	1770
1280	2.33947	3.98309	1.96486	1280	1780	1.81670	3.33820	1.94429	1780
1290	2.32669	3.96780	1.96451	1290	1790	1.80818	3.32731	1.94381	1790
1300	2.31403	3.95263	1.96416	1300	1800	1.79972	3.31648	1.94333	1800
1310	2.30148	3.93758	1.96380	1310	1810	1.79133	3.30571	1.94285	1810
1320	2.28905	3.92265	1.96345	1320	1820	1.78299	3.29501	1.94236	1820
1330	2.27673	3.90783	1.96309	1330	1830	1.77471	3.28437	1.94188	1830
1340	2.26452	3.89313	1.96273	1340	1840	1.76649	3.27379	1.94139	1840
1350	2.25242	3.87854	1.96237	1350	1850	1.75833	3.26327	1.94090	1850
1360	2.24043	3.86405	1.96200	1360	1860	1.75022	3.25281	1.94040	1860
1370	2.22854	3.84968	1.96163	1370	1870	1.74217	3.24240	1.93991	1870
1380	2.21676	3.83542	1.96126	1380	1880	1.73418	3.23206	1.93941	1880
1390	2.20508	3.82126	1.96089	1390	1890	1.72624	3.22177	1.93890	1890
1400	2.19351	3.80720	1.96051	1400	1900	1.71835	3.21154	1.93840	1900
1410	2.18203	3.79325	1.96013	1410	1910	1.71052	3.20137	1.93789	1910
1420	2.17065	3.77940	1.95975	1420	1920	1.70274	3.19125	1.93738	1920
1430	2.15937	3.76565	1.95937	1430	1930	1.69501	3.18118	1.93687	1930
1440	2.14819	3.75199	1.95898	1440	1940	1.68734	3.17118	1.93636	1940
1450	2.13710	3.73844	1.95859	1450	1950	1.67971	3.16122	1.93584	1950
1460	2.12610	3.72498	1.95820	1460	1960	1.67214	3.15132	1.93532	1960
1470	2.11519	3.71161	1.95780	1470	1970	1.66462	3.14147	1.93480	1970
1480	2.10438	3.69834	1.95740	1480	1980	1.65715	3.13168	1.93427	1980
1490	2.09365	3.68516	1.95700	1490	1990	1.64973	3.12194	1.93375	1990
1500	2.08302	3.67207	1.95660	1500	2000	1.64235	3.11224	1.93322	2000
1510	2.07247	3.65907	1.95620	1510	2010	1.63503	3.10260	1.93268	2010
1520	2.06200	3.64616	1.95579	1520	2020	1.62775	3.09301	1.93215	2020
1530	2.05162	3.63334	1.95538	1530	2030	1.62052	3.08347	1.93161	2030
1540	2.04132	3.62060	1.95497	1540	2040	1.61334	3.07398	1.93107	2040
1550	2.03111	3.60795	1.95455	1550	2050	1.60620	3.06454	1.93053	2050
1560	2.02098	3.59538	1.95413	1560	2060	1.59911	3.05515	1.92999	2060
1570	2.01093	3.58290	1.95371	1570	2070	1.59206	3.04580	1.92944	2070
1580	2.00095	3.57049	1.95329	1580	2080	1.58506	3.03651	1.92889	2080
1590	1.99106	3.55817	1.95286	1590	2090	1.57811	3.02726	1.92834	2090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	ν cm ⁻¹	ν cm ⁻¹	$-(F^0-E_0^0)/T$	S^0	C_p^0	ν cm ⁻¹
T=5000.				T=5000.				
2100	1.57119	3.01805	1.92779	2100	1.27375	2.60939	1.89701	2600
2110	1.56433	3.00890	1.92723	2110	1.26863	2.60211	1.89634	2610
2120	1.55750	2.99978	1.92667	2120	1.26354	2.59486	1.89566	2620
2130	1.55072	2.99072	1.92611	2130	1.25847	2.58764	1.89498	2630
2140	1.54398	2.98170	1.92555	2140	1.25343	2.58045	1.89430	2640
2150	1.53728	2.97272	1.92498	2150	1.24842	2.57329	1.89361	2650
2160	1.53063	2.96379	1.92441	2160	1.24343	2.56616	1.89292	2660
2170	1.52401	2.95490	1.92384	2170	1.23847	2.55906	1.89223	2670
2180	1.51744	2.94606	1.92327	2180	1.23354	2.55198	1.89154	2680
2190	1.51091	2.93726	1.92269	2190	1.22863	2.54494	1.89085	2690
2200	1.50441	2.92850	1.92211	2200	1.22375	2.53792	1.89015	2700
2210	1.49796	2.91979	1.92153	2210	1.21890	2.53094	1.88945	2710
2220	1.49155	2.91111	1.92095	2220	1.21407	2.52398	1.88875	2720
2230	1.48517	2.90248	1.92036	2230	1.20926	2.51705	1.88805	2730
2240	1.47883	2.89389	1.91977	2240	1.20449	2.51015	1.88735	2740
2250	1.47254	2.88534	1.91918	2250	1.19973	2.50327	1.88664	2750
2260	1.46628	2.87683	1.91859	2260	1.19501	2.49643	1.88593	2760
2270	1.46005	2.86836	1.91799	2270	1.19030	2.48961	1.88522	2770
2280	1.45387	2.85993	1.91740	2280	1.18562	2.48282	1.88450	2780
2290	1.44772	2.85154	1.91680	2290	1.18097	2.47605	1.88378	2790
2300	1.44161	2.84319	1.91619	2300	1.17634	2.46931	1.88307	2800
2310	1.43553	2.83488	1.91559	2310	1.17174	2.46260	1.88235	2810
2320	1.42949	2.82660	1.91498	2320	1.16715	2.45591	1.88162	2820
2330	1.42349	2.81837	1.91437	2330	1.16260	2.44925	1.88090	2830
2340	1.41752	2.81017	1.91376	2340	1.15806	2.44262	1.88017	2840
2350	1.41158	2.80201	1.91314	2350	1.15355	2.43601	1.87944	2850
2360	1.40569	2.79389	1.91253	2360	1.14906	2.42943	1.87871	2860
2370	1.39982	2.78580	1.91191	2370	1.14460	2.42288	1.87797	2870
2380	1.39399	2.77776	1.91129	2380	1.14015	2.41635	1.87724	2880
2390	1.38819	2.76974	1.91066	2390	1.13573	2.40984	1.87650	2890
2400	1.38243	2.76177	1.91003	2400	1.13134	2.40336	1.87576	2900
2410	1.37670	2.75383	1.90941	2410	1.12696	2.39690	1.87501	2910
2420	1.37100	2.74592	1.90877	2420	1.12261	2.39047	1.87427	2920
2430	1.36533	2.73805	1.90814	2430	1.11828	2.38407	1.87352	2930
2440	1.35970	2.73022	1.90751	2440	1.11397	2.37768	1.87277	2940
2450	1.35410	2.72242	1.90687	2450	1.10968	2.37133	1.87202	2950
2460	1.34853	2.71465	1.90623	2460	1.10541	2.36499	1.87126	2960
2470	1.34299	2.70692	1.90558	2470	1.10117	2.35868	1.87051	2970
2480	1.33749	2.69922	1.90494	2480	1.09694	2.35240	1.86975	2980
2490	1.33201	2.69156	1.90429	2490	1.09274	2.34613	1.86899	2990
2500	1.32657	2.68392	1.90364	2500	1.08856	2.33989	1.86822	3000
2510	1.32115	2.67633	1.90299	2510	1.08440	2.33368	1.86746	3010
2520	1.31577	2.66876	1.90233	2520	1.08026	2.32749	1.86669	3020
2530	1.31041	2.66123	1.90168	2530	1.07614	2.32132	1.86592	3030
2540	1.30509	2.65373	1.90102	2540	1.07204	2.31517	1.86515	3040
2550	1.29980	2.64626	1.90035	2550	1.06796	2.30905	1.86438	3050
2560	1.29453	2.63882	1.89969	2560	1.06390	2.30294	1.86360	3060
2570	1.28929	2.63142	1.89902	2570	1.05986	2.29687	1.86282	3070
2580	1.28409	2.62404	1.89836	2580	1.05584	2.29081	1.86204	3080
2590	1.27891	2.61670	1.89769	2590	1.05184	2.28477	1.86126	3090

Table II Harmonic Oscillator Contributions to the Thermodynamic Functions (in units of calories, moles, and °K)

ν cm^{-1}	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_P°	ν cm^{-1}	ν cm^{-1}	$-(F^{\circ}-E_0^{\circ})/T$	S°	C_P°	ν cm^{-1}
T=5000.				T=5000.					
3100	1.04786	2.27876	1.86048	3100	3600	0.87106	2.00355	1.81860	3600
3110	1.04390	2.27277	1.85969	3110	3610	0.86792	1.99851	1.81771	3610
3120	1.03996	2.26680	1.85890	3120	3620	0.86479	1.99348	1.81682	3620
3130	1.03604	2.26085	1.85811	3130	3630	0.86168	1.98847	1.81593	3630
3140	1.03213	2.25493	1.85732	3140	3640	0.85859	1.98348	1.81503	3640
3150	1.02825	2.24902	1.85652	3150	3650	0.85550	1.97850	1.81414	3650
3160	1.02438	2.24314	1.85572	3160	3660	0.85243	1.97353	1.81324	3660
3170	1.02054	2.23728	1.85492	3170	3670	0.84938	1.96859	1.81234	3670
3180	1.01671	2.23144	1.85412	3180	3680	0.84633	1.96366	1.81144	3680
3190	1.01290	2.22562	1.85332	3190	3690	0.84330	1.95874	1.81053	3690
3200	1.00910	2.21982	1.85251	3200	3700	0.84029	1.95384	1.80963	3700
3210	1.00533	2.21404	1.85171	3210	3710	0.83728	1.94896	1.80872	3710
3220	1.00157	2.20828	1.85090	3220	3720	0.83429	1.94409	1.80781	3720
3230	0.99783	2.20254	1.85008	3230	3730	0.83132	1.93924	1.80690	3730
3240	0.99411	2.19683	1.84927	3240	3740	0.82835	1.93441	1.80598	3740
3250	0.99041	2.19113	1.84845	3250	3750	0.82540	1.92958	1.80507	3750
3260	0.98672	2.18545	1.84763	3260	3760	0.82246	1.92478	1.80415	3760
3270	0.98306	2.17979	1.84681	3270	3770	0.81954	1.91999	1.80323	3770
3280	0.97940	2.17416	1.84599	3280	3780	0.81663	1.91521	1.80231	3780
3290	0.97577	2.16854	1.84517	3290	3790	0.81373	1.91045	1.80139	3790
3300	0.97215	2.16294	1.84434	3300	3800	0.81084	1.90571	1.80046	3800
3310	0.96855	2.15736	1.84351	3310	3810	0.80796	1.90098	1.79953	3810
3320	0.96497	2.15180	1.84268	3320	3820	0.80510	1.89626	1.79861	3820
3330	0.96140	2.14626	1.84185	3330	3830	0.80225	1.89156	1.79768	3830
3340	0.95785	2.14074	1.84101	3340	3840	0.79941	1.88687	1.79674	3840
3350	0.95432	2.13524	1.84018	3350	3850	0.79659	1.88220	1.79581	3850
3360	0.95080	2.12975	1.83934	3360	3860	0.79377	1.87754	1.79487	3860
3370	0.94730	2.12429	1.83850	3370	3870	0.79097	1.87290	1.79393	3870
3380	0.94382	2.11884	1.83765	3380	3880	0.78818	1.86827	1.79299	3880
3390	0.94035	2.11341	1.83681	3390	3890	0.78540	1.86366	1.79205	3890
3400	0.93690	2.10800	1.83596	3400	3900	0.78264	1.85906	1.79111	3900
3410	0.93346	2.10261	1.83511	3410	3910	0.77988	1.85447	1.79016	3910
3420	0.93004	2.09724	1.83426	3420	3920	0.77714	1.84990	1.78922	3920
3430	0.92664	2.09189	1.83341	3430	3930	0.77441	1.84535	1.78827	3930
3440	0.92325	2.08655	1.83255	3440	3940	0.77169	1.84080	1.78732	3940
3450	0.91987	2.08123	1.83170	3450	3950	0.76898	1.83627	1.78636	3950
3460	0.91651	2.07593	1.83084	3460	3960	0.76629	1.83176	1.78541	3960
3470	0.91317	2.07065	1.82998	3470	3970	0.76360	1.82726	1.78445	3970
3480	0.90984	2.06538	1.82911	3480	3980	0.76093	1.82277	1.78350	3980
3490	0.90653	2.06014	1.82825	3490	3990	0.75827	1.81829	1.78254	3990
3500	0.90323	2.05491	1.82738	3500	4000	0.75562	1.81383	1.78157	4000
3510	0.89995	2.04969	1.82651	3510					
3520	0.89668	2.04450	1.82564	3520					
3530	0.89343	2.03932	1.82477	3530					
3540	0.89019	2.03416	1.82389	3540					
3550	0.88696	2.02902	1.82302	3550					
3560	0.88375	2.02389	1.82214	3560					
3570	0.88056	2.01878	1.82126	3570					
3580	0.87738	2.01369	1.82037	3580					
3590	0.87421	2.00861	1.81949	3590					

THE NATIONAL BUREAU OF STANDARDS

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The functions of the National Bureau of Standards are set forth in the Act of Congress, March 3, 1901, as amended by Congress in Public Law 619, 1950. These include the development and maintenance of the national standards of measurement and the provision of means and methods for making measurements consistent with these standards; the determination of physical constants and properties of materials; the development of methods and instruments for testing materials, devices, and structures; advisory services to government agencies on scientific and technical problems; invention and development of devices to serve special needs of the Government; and the development of standard practices, codes, and specifications. The work includes basic and applied research, development, engineering, instrumentation, testing, evaluation, calibration services, and various consultation and information services. Research projects are also performed for other government agencies when the work relates to and supplements the basic program of the Bureau or when the Bureau's unique competence is required. The scope of activities is suggested by the listing of divisions and sections on the next page.

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U.S. DEPARTMENT OF COMMERCE

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THE NATIONAL BUREAU OF STANDARDS

The scope of activities of the National Bureau of Standards at its major laboratories in Washington, D.C., and Boulder Colorado, is suggested in the following listing of the divisions and sections engaged in technical work. In general, each section carries out specialized research, development, and engineering in the field indicated by its title. A brief description of the activities, and of the resultant publications, appears on the preceding page.

WASHINGTON, D.C.

Electricity. Resistance and Reactance. Electrochemistry. Electrical Instruments. Magnetic Measurements. Di-electrics. High Voltage.

Metrology. Photometry and Colorimetry. Refractometry. Photographic Research. Length. Engineering Metrology. Mass and Scale. Volumetry and Densimetry.

Heat. Temperature Physics. Heat Measurements. Cryogenic Physics. Equation of State. Statistical Physics.

Radiation Physics. X-ray. Radioactivity. Radiation Theory. High Energy Radiation. Radiological Equipment. Nucleonic Instrumentation. Neutron Physics.

Analytical and Inorganic Chemistry. Pure Substances. Spectrochemistry. Solution Chemistry. Standard Reference Materials. Applied Analytical Research.

Mechanics. Sound. Pressure and Vacuum. Fluid Mechanics. Engineering Mechanics. Rheology. Combustion Controls.

Polymers. Macromolecules: Synthesis and Structure. Polymer Chemistry. Polymer Physics. Polymer Characterization. Polymer Evaluation and Testing. Applied Polymer Standards and Research. Dental Research.

Metallurgy. Engineering Metallurgy. Microscopy and Diffraction. Metal Reactions. Metal Physics. Electrolysis and Metal Deposition.

Mineral Products. Engineering Ceramics. Glass. Refractories. Crystal Growth. Physical Properties. Constitution and Microstructure.

Building Research. Structural Engineering. Fire Research. Mechanical Systems. Organic Building Materials. Codes and Safety Standards. Heat Transfer. Inorganic Building Materials. Metallic Building Materials.

Applied Mathematics. Numerical Analysis. Computation. Statistical Engineering. Mathematical Physics. Operations Research.

Data Processing Systems. Components and Techniques. Computer Technology. Measurements Automation. Engineering Applications. Systems Analysis.

Atomic Physics. Spectroscopy. Infrared Spectroscopy. Solid State Physics. Electron Physics. Atomic Physics.

Instrumentation. Engineering Electronics. Electron Devices. Electronic Instrumentation. Mechanical Instruments. Basic Instrumentation.

Physical Chemistry. Thermochemistry. Surface Chemistry. Organic Chemistry. Molecular Spectroscopy. Molecular Kinetics. Mass Spectrometry.

Office of Weights and Measures.

BOULDER, COLO.

Cryogenic Engineering. Cryogenic Equipment. Cryogenic Processes. Properties of Materials. Cryogenic Technical Services.

Ionosphere Research and Propagation. Low Frequency and Very Low Frequency Research. Ionosphere Research. Prediction Services. Sun-Earth Relationships. Field Engineering. Radio Warning Services. Vertical Soundings Research.

Radio Propagation Engineering. Data Reduction Instrumentation. Radio Noise. Tropospheric Measurements. Tropospheric Analysis. Propagation-Terrain Effects. Radio-Meteorology. Lower Atmosphere Physics.

Radio Standards. High Frequency Electrical Standards. Radio Broadcast Service. Radio and Microwave Materials. Atomic Frequency and Time Interval Standards. Electronic Calibration Center. Millimeter-Wave Research. Microwave Circuit Standards.

Radio Systems. Applied Electromagnetic Theory. High Frequency and Very High Frequency Research. Modulation Research. Antenna Research. Navigation Systems.

Upper Atmosphere and Space Physics. Upper Atmosphere and Plasma Physics. Ionosphere and Exosphere Scatter. Airglow and Aurora. Ionospheric Radio Astronomy.

Radio Physics.

Circuit Standards.





