REPORT SAMSO-TR-76-31, VOL II

(12)

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Spectroscopic Constants for Selected Homonuclear Diatomic Molecules

Volume II. K Through Z

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16 February 1976

Interim Report

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DARPA Order No. 2843

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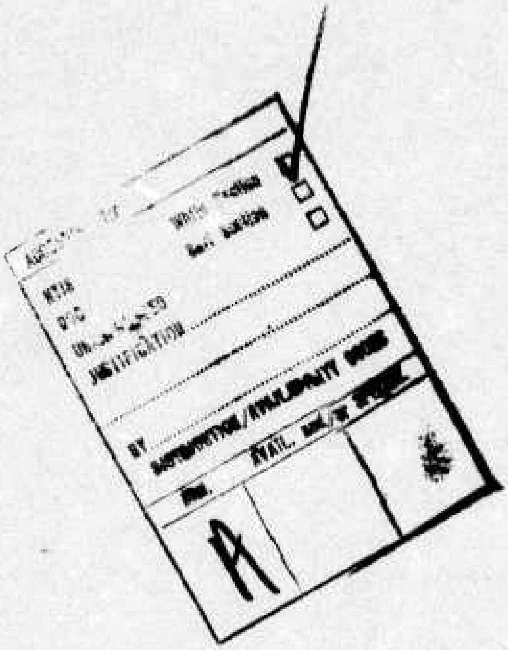
SPACE AND MISSILE SYSTEMS ORGANIZATION
AIR FORCE SYSTEMS COMMAND
Los Angeles Air Force Station
P.O. Box 92960, Worldway Postal Center
Los Angeles, Calif. 90009

This report was submitted by The Aerospace Corporation, El Segundo, CA 90245, under Contract F04701-75-C-0076 with the Space and Missile Systems Organization, Deputy for Advanced Space Programs, P.O. Box 92960, Worldway Postal Center, Los Angeles, CA 90009. It was reviewed and approved for The Aerospace Corporation by W. R. Warren, Jr., Director, Aerophysics Laboratory. Lt. Ronald C. Lawson, USAF, was the project officer. This research was supported by the Defense Advanced Research Projects Agency of the Department of Defense.

This report has been reviewed by the Information Office (OI) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication. Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.



FOR THE COMMANDER

Ronald C. Lawson

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Office of Research Applications
Deputy for Technology

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

19 REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

18

1. REPORT NUMBER
SAMSO-TR-76-31-Vol-[redacted]2

2. GOVT ACCESSION NO.

3. RECIPIENT'S CATALOG NUMBER

6

4. TITLE (and Subtitle)
SPECTROSCOPIC CONSTANTS FOR SELECTED HOMONUCLEAR DIATOMIC MOLECULES, Volume II. K Through Z,

9

5. TYPE OF REPORT & PERIOD COVERED
Interim Rept.,

14

6. PERFORMING ORG. REPORT NUMBER
TR-0076(6751)-1-Vol-[redacted]2

7. AUTHOR(s)

10

Steven N. Suchard [redacted] James E. Melzer

15

8. CONTRACT OR GRANT NUMBER(s)
F04701-75-C-0076,
DARPA Order-2843

9. PERFORMING ORGANIZATION NAME AND ADDRESS
The Aerospace Corporation
El Segundo, Calif. 90245

10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS

12 229p.

11. CONTROLLING OFFICE NAME AND ADDRESS
Defense Advanced Research Projects Agency
1400 Wilson Blvd.
Arlington, Va. 22209

11

12. REPORT DATE
16 Feb[redacted]76

13. NUMBER OF PAGES
272

14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)
Space and Missile Systems Organization
Air Force Systems Command
Los Angeles, Calif. 90009

15. SECURITY CLASS. (of this report)
Unclassified

15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Branching Ratio
Electron Transition
Electronic Quenching Rate
Franck-Condon Factor

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Spectroscopic information relevant to homonuclear diatomic molecules has been collected and is presented. This information includes not only the molecular band systems, but also Frank-Condon factors, oscillator strengths, potential energy curves, and reactive branching ratios, where available.

The information is arranged alphabetically by molecule in two volumes. This, the second volume, covers K through Z.

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1B

DD FORM 1473 (FACSIMILE)

409 367

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

19. KEY WORDS (Continued)

Molecular Band System
Potential Energy Diagram
Radiative Lifetime
Reaction Rate
Spectroscopic Constant
Spectroscopy

20. ABSTRACT (Continued)

PREFACE

During the preparation of this compilation, many people contributed; the compilers wish to thank all of them. In particular they appreciate the efforts of V. Gilbertson, the manuscript typist; and K. C. Bregand, J. A. Kiley, and W. H. McPherson, for their editorial assistance. They would like to thank Dr. J. R. Schwartz for his cooperation and encouragement. In addition, they extend their gratitude to Dr. L. Wilson of the Air Force Weapons Laboratory, who gave the initial impetus to this project.

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I. INTRODUCTION

A complete discussion of the purpose, organization, and notation used in this compilation and comments on the availability of spectroscopic information are presented in Volume I of this report. The only intent here is to outline the text of Volume I, to which the reader is referred.

Generally, the information on the alphabetically arranged molecules is broken into five separate sections: viz., methods of production and experimental technique, band systems, spectroscopic constants, perturbations and general information, and bibliography. These are described briefly.

METHODS OF PRODUCTION AND EXPERIMENTAL TECHNIQUE

Sources for the production of the molecule and techniques for study are presented.

BAND SYSTEMS

A general description is given of the molecular transition of each system or group. The system is analyzed in detail.

SPECTROSCOPIC CONSTANTS

The molecular constants that totally define the electronic states of the molecule are given. The bulk of the dissociation energy information is taken from Gaydon (Ref. 7 in Vol I); other sources are so noted.

PERTURBATIONS AND GENERAL INFORMATION

All other information deemed useful to the complete understanding of the molecule is included here.

BIBLIOGRAPHY

The referencing system (after Suchard, Ref. 4 in Vol I) is made up of two numbers: first, the year of publication; second, the running count of references cited for each molecule.

Also presented in Volume I is a section "Notation and Notational Conversion Formulas." Formulas are given for such molecular properties as total energy of a given state of the molecule T, electronic energy T_e, vibrational energy G, and rotational energy F. Nomenclature for other molecular constants reported is also given.

MOLECULE	VIBRATIONAL CONSTANTS	ROTATIONAL CONSTANTS	VIBRATIONAL LEVEL DISTRIBUTIONS	DISSOCIATION ENERGY	LIFETIMES	FRANCK-CONOON FACTORS	BRANCHING RATIOS	QUENCHING	LASER ACTION OBSERVED	
									VIBRATIONAL	ELECTRONIC
Ac_2										
Ag_2	X			X						
Al_2	X	X		X						
Am_2										
Ar_2	P	P		X						X
As_2	X	X		X		P		P		
At_2										
Au_2	X	X		X		P				
B_2	X	X		X						
Ba_2										
Be_2				P						
Bi_2	X	P		X						
Bk_2										
Br_2	X	X	P	X	P	X		P		
C_2	X	X	P	X	X					
Ca_2	P	P		X						
Cd_2										
Ce_2				X						
Cf_2										
Cl_2	X	P		X		P		P		
Cm_2										
Co_2				X						
Cr_2				X						
Cs_2	X			X	P					

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-1

MOLECULE	VIBRATIONAL CONSTANTS	ROTATIONAL CONSTANTS	VIBRATIONAL LEVEL DISTRIBUTIONS	DISSOCIATION ENERGY	LIFETIMES	FRANCK-CONDON FACTORS	BRANCHING RATIOS	QUENCHING	LASER ACTION OBSERVED	
									VIBRATIONAL	ELECTRONIC
Cu_2	X	P		X		P				
Dy_2				X						
Er_2				X						
Es_2										
Eu_2				X						
F_2	P	P		X						
Fe_2				X						
Fm_2										
Fr_2										
Ga_2				X						
Gd_2				X						
Ge_2				X						
H_2	X	X	P	X	X	X		X		X
He_2	X	X		X						X
Hf_2										
Hg_2				X						
Ho_2										
I_2	X	X	P	X	P	X		X		X
In_2	X			P						
Ir_2										
K_2	X	P		X	P					
Kr_2	X	P		X						X
La_2	P			X						
Li_2	X	X		X	P					

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-2

MOLECULE	VIBRATIONAL CONSTANTS	ROTATIONAL CONSTANTS	VIBRATIONAL LEVEL DISTRIBUTIONS	DISSOCIATION ENERGY	LIFETIMES	FRANCK-CONDON FACTORS	BRANCHING RATIOS	QUENCHING	LASER ACTION OBSERVED	
									VIBRATIONAL	ELECTRONIC
Lu_2										
Md_2										
Mg_2	X	X		X		X				
Mn_2				X						
Mo_2										
N_2	X	X	P	X	X	X		X		X
Na_2	X	X		X	P	P				
Nb_2										
Nd_2				X						
Ne_2	P	P		X	P					
Ni_2				X						
No_2										
Np_2										
O_2	X	X	P	X	X	X		X		
Os_2										
P_2	X	P		X				P		
Pa_2										
Pb_2	X			X						
Pd_2				X						
Pm_2										
Po_2	X			X						
Pr_2				X						
Pt_2										
Pu_2										

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-3

MOLECULE	VIBRATIONAL CONSTANTS	ROTATIONAL CONSTANTS	VIBRATIONAL LEVEL DISTRIBUTIONS	DISSOCIATION ENERGY	LIFETIMES	FRANCK-CONOON FACTORS	BRANCHING RATIOS	QUENCHING	LASER ACTION OBSERVED	
									VIBRATIONAL	ELECTRONIC
Ra_2										
Rb_2	X			X	P			P		
Re_2										
Rh_2										
Rn_2										
Ru_2										
S_2	X	X		X	P			P		
Sb_2	X	P		X				P		
Sc_2				X						
Se_2	X	X		X				P		
Si_2	X	X		X				P		
Sm_2				X						
Sn_2				X						
Sr_2										
Ta_2										
Tb_2				X						
Tc_2										
Te_2	X	X		X		X				
Th_2				X						
Ti_2				X						
Tl_2				X						
Tm_2				X						
U_2				X						
V_2				X						

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-4

MOLECULE	VIBRATIONAL CONSTANTS	ROTATIONAL CONSTANTS	VIBRATIONAL LEVEL DISTRIBUTIONS	DISSOCIATION ENERGY	LIFETIMES	FRANCK-CONDON FACTORS	BRANCHING RATIOS	QUENCHING	LASER ACTION OBSERVED	
									VIBRATIONAL	ELECTRONIC
W_2										
Xe_2	P			X	P			P		X
Y_2				X						
Yb_2				X						
Zn_2				P						
Zr_2										

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-5

K_2

Methods of Production and Experimental Technique

Absorption.

Emission from a heat pipe, laser fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A\,^1\Sigma_u^+ \rightleftarrows X\,^1\Sigma_g^+$	Heat Pipe	8850-7700	R			(71.47, 30.10)
	II	$B\,^1\Pi_u \rightleftarrows X\,^1\Sigma_g^+$	Absorption, laser fluorescence	6950-6250	R	6583.2(0,2) 6544.0(0,1) 6473.6(1,0)		(68.39, 32.15, 31.12)
	III	$C\,^1\Pi_u \rightleftarrows X\,^1\Sigma_g^+$	Absorption	4510-4220	R	4343.5(1,0)		(61.32, 48.29)
	IV	$D(^1\Pi_u) \leftarrow X\,^1\Sigma_g^+$	Absorption	4160-3940	R	4082.7(1,2)		(48.29)
	V	$E(^1\Pi_u) \leftarrow X\,^1\Sigma_g^+$	Absorption	3925-3700	R	3797.6(2,3) 3793.7(1,2)		(50.31)
	VI	$F \leftarrow X\,^1\Sigma_g^+$	Absorption	3700-3600	R			(37.20, 37.19)
	VII	$G \leftarrow X\,^1\Sigma_g^+$	Absorption	3600-3480	R			(37.19)

I. $A^1\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$ System

Most characteristic bands, λ (30.10):

(v', v'')	(0, 3)	(0, 2)	(1, 2)	(0, 1)	(0, 0)	(1, 0)	(2, 0)
λ	8773.15	8702.00	8651.79	8634.43	8566.30	8515.70	8468.23

II. $B^1\Pi_u \rightleftarrows X^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (32.15, 31.12):

v', v''	(0, 2)	(0, 1)	(1, 1)	(1, 0)	(2, 0)
λ	6583.19	6544.00	6512.19	6473.58	6443.00
(Intensity)	9	8	5	10	8

III. $C^1\Pi_u \rightleftarrows X^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (61.32, 48.29):

v', v''	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	4355.1	4343.5	4332.3	4320.9	4310.0
(Intensity)	8	10	7	7	7

IV. $D(^1\Pi_u) \leftarrow X^1\Sigma_g^+$ System

Possibly two independent systems, λ (Intensity) (27.20, 37.19):

v', v''	0	1	2	3	4	5
0			4092.3(8)	4107.3(7)	4122.7(6)	
1		4067.0(8)	4082.7(10)	4097.4(7)	4112.8(8)	
2				4087.5(6)	4103.0(6)	
3	4033.5(6)			4078.2(6)		4108.6(6)
4	4024.9(6)					

V. $E(^1\Pi_u) \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (50.31):

v', v''	0	1	2	3
0				
1			3793.7(10)	3806.2(7)
2		3771.5(8)	3784.4(7)	3797.6(10)
3		3762.8(7)	3776.0(7)	3789.2(7)
4				
5	3733.8(7)	3746.6(7)		
6		3738.1(7)		

VI. $F \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, analysis uncertain, λ (37.20, 37.19):

v', v''	0	1	2	3
0		3639.5	3651.7	
1		3631.6	3643.4	
2	3611.2	3623.5	3635.3	3647.3
3	3603.2			

VII. $G \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (37.19):

(v', v'')	(0, 2)	(1, 2)	(2, 2)	(3, 2)	(4, 2)	(3, 1)	(4, 1)
λ	3583.7	3575.6	3567.6	3559.9	3553.4	3548.6	3541.1
(Intensity)	4	4	4	3	4	3	3

Molecule K_2

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	$B_e \times 10^2$	$\alpha_e \times 10^4$	$D_e \times 10^8$	r_e	Remarks	Bibliography
G	28091	64.9	0.05						(37.19)
F	27571	62.2	0.24						(37.19)
$E(^1\Pi_u)$	26493.0	60.6	0.15						(50.31)
$D(^1\Pi_u)$	24627.7	61.6	0.90					(a)	(48.29)
$C^1\Pi_u$	22969.7	61.48	0.14	4.404	1.10		4.43		(61.32, 50.31)
$B^1\Pi_u$	15376.4	92.021	0.2829	5.6743	1.65	8.63	4.23	(b)	(68.39, 32.15, 31.13)
$A^1\Sigma_u^+$	11682.6	69.09	0.153						(30.10)
$X^1\Sigma_g^+$	0	92.64		5.622	2.19	8.28	3.92	(c)	(61.32, 48.29)

(a) $y_e\omega_e = 0.001$, $z_e\omega_e = -0.0003$; (b) $y_e\omega_e = -0.002055$, $\gamma_e = -7.2 \times 10^{-6}$, $\delta_e = 1.5 \times 10^{-7}$, $\beta = -7.4 \times 10^{-10}$;

(c) $\beta = -8.3 \times 10^{-11}$

Dissociation energy = 0.51 ± 0.05 eV, 11.8 kcal/mole, 4114 cm^{-1}.

Perturbations and General Information

Radiative lifetime of $B^1\Pi_u$ state (70.44, 70.41):

$$\tau(B^1\Pi_u) = 9.65 \pm 0.3 \text{ nsec.}$$

Absolute absorption cross sections (68.37, 66.35).

Potential energy curves, RKR potentials (69.40):

	State	v	$U(cm^{-1})$	r_{min}(Å)	r_{max}(Å)
T_e = 0.0	$X^1\Sigma_g^+$	0	46.2	3.7906	4.0643
		1	138.2	3.6996	4.1752
		2	229.4	3.6394	4.2554
		3	319.9	3.5918	4.3230
		4	409.7	3.5516	4.3835
		5	498.8	3.5164	4.4391
		6	587.2	3.4848	4.4912
		7	674.9	3.4560	4.5407
		8	761.9	3.4294	4.5880
		9	848.1	3.4047	4.6337
		10	933.7	3.3815	4.6780
		11	1018.5	3.3597	4.7212
		12	1102.7	3.3389	4.7633
		13	1186.1	3.3192	4.8047
		14	1268.9	3.3003	4.8453
		15	1350.9	3.2822	4.8852
T_e = 15376.4 cm^{-1}	$B^1\Pi_u$	0	37.4	4.0886	4.3929
		1	111.6	3.9885	4.5179
		2	185.1	3.9225	4.6089
		3	257.9	3.8706	4.6861
		4	330.0	3.8269	4.7553
		5	401.3	3.7886	4.8192
		6	472.0	3.7544	4.8794
		7	542.0	3.7233	4.9367
		8	611.2	3.6945	4.9917
		9	679.8	3.6678	5.0451
		10	747.6	3.6427	5.0970
		11	814.7	3.6190	5.1478
		12	881.0	3.5965	5.1978
		13	946.5	3.5749	5.2471
		14	1011.2	3.5542	5.2959
		15	1075.1	3.5341	5.3445

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Kr_2

Methods of Production and Experimental Technique

Absorption.

Emission: positive columns, condensed discharge, microwave discharge, electron beam discharge, α-particle irradiation.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$^{1,3}\Sigma_u \rightarrow {}^1\Sigma_g^+$	α irradiation	1250-1850		Max. ~1480Å, 1280Å	Continuum	(73.9, 65.4, 55.3, 55.2)
	II	$B(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$	Absorption	1252-1257	V	1254.8(3, 4)		(73.10)
	III	$C(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$	Absorption	1239-1245		1241.3(3, 4) 1242.3(4, 4)		(73.10)
	IV	$D(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$	Absorption	1167-1169		1168.1(2, 0) 1167.6(4, 1)		(73.10)
	V	$E \leftarrow X^1\Sigma_g^+$	Absorption	1161-1170				(73.10)
	VI		Emission	2000-8000			Continuum	(67.7, 42.1)
	VII			1064-1080			4 fragmented systems	(73.10)

Systems II - V correlate to separated atom limits in which one atom is excited to various levels of configuration $4p^55s$.

System VII systems are energetically close to various atom levels of configuration $4p^55p$.

Molecule Kr_2

II. $B(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0					1252.3(2)
1				1252.8(2)	1253.1(6)
2				1253.7(6)	1253.9(8)
3		1254.0(1)		1254.6(8)	1254.8(10)
4		1255.0(0)		1255.6(1)	1255.8(3)

III. $C(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0				1239.2(9)	1239.5(9)
1		1239.2(9)	1239.5(7)	1239.8(8)	1240.0(10)
2	1239.6(6)	1239.9(7)	1240.2(8)	1240.4(8)	1240.7(9)
3	1240.2(4)	1240.6(4)	1240.9(5)	1241.1(6)	1241.3(10)
4	1241.0(1)	1241.4(3)	1241.6(5)	1241.9(8)	1242.1(10)

IV. $D(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0	1169.2(5)	1169.5(4)	1169.7(3)	1170.0(2)	1170.1(1)
1	1168.6(8)	1168.9(5)	1169.2(5)	1169.4(2)	1169.6(2)
2	1168.1(8)	1168.4(2)	1168.7(3)	1168.9(5)	1169.1(3)
3	1167.7(6)	1168.0(7)	1168.2(2)	1168.4(2)	1168.7(3)
4	1167.3(7)	1167.6(8)	1167.8(5)		1168.2(2)

V. $E \leftarrow X^1\Sigma_g^+$ System

Band heads in absorption, λ (Intensity) (73.10):

λ	1161.4	1162.3	1163.1	1163.7	1164.1	1164.4
(Intensity)	10	9	8	7	6	6

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$D(0_u^+)$	85531.5 [a]	39.66 [b]							(73.10)
$C(0_u^+)$	80763.9 [a]	35.75 [b]							(73.10)
$B(1_u)$	79932.8	22.3 [b]							(73.10)
$X^1\Sigma_g^+$ (0_g^+)	0	23.99	1.3	0.024	1.0			$y_e\omega_e = 0.021$	(73.11, 73.10)

[a] T_o; [b] $\Delta G_{1/2}$

Dissociation energy = 0.02 eV, 0.39 kcal/mole, 138.4 cm^{-1} (73.10).

Kr_2

Perturbations and General Information

Laser action has been observed on the $^{1,3}\Sigma_u^+ \rightarrow X\,^1\Sigma_g^+$ transition at 1457 ± 8Å (73.13).

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La_2

Methods of Production and Experimental Technique

Thermal emission from a King furnace (T >2000° C).

Band Systems

Bands in the region 6100-6040Å have been attributed to La_2. The bands are degraded principally to the violet, but the series convergence is degraded red (69.2).

Characteristic bands:

λ	6075.3	6074.9	6074.7	6074.6	6069.4	6068.8	6049.6	6049.1

A vibrational analysis yields $\omega_o' = 82.6$ cm^{-1} and $\omega_o'' = 76.9$ cm^{-1}, but these values are in doubt.

Spectroscopic Constants

Dissociation energy = 2.50 ± 0.22 eV, 57.6 kcal/mole, 20200 cm^{-1} (64.1).

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Li_2

Methods of Production and Experimental Technique

Absorption, magnetic rotation.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Absorption	7700-6550	R	6883.9(2,0)		(72.64, 29.16, 28.1)
	II	$B^1\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	5590-4500	R	4800.6(3,1) 4778.8(2,0)		(33.13, 31.9)
	III	$C^1\Pi_u \leftarrow X^1\Sigma_g$	Absorption	3500-3100	R	3358.6(0,2) 3315.6(0,1)		(60.36, 38.31)
	IV	$D^1\Gamma_u \leftarrow X^1\Sigma_g^+$	Absorption	3100-2500	R			(60.36)

Several bands of the isotopic species $^7Li^6Li$ have been observed for Systems II and III.

Molecule Li_2

Li_2

I. $A\,^1\Sigma_u^+ \leftarrow X\,^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (36.16, 28.1):

(v', v'')	(0, 2)	(0, 1)	(1, 1)	(1, 0)	(2, 0)	(3, 0)
λ	7690.3	7309.2	7177.4	7003.7	6883.9	6768.7
(Intensity)	8	8	8	8	10	8

II. $B\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$ System

Most intense band heads of $^7Li_2$, λ (Intensity) (31.9):

(v', v'')	(2, 1)	(1, 0)	(3, 1)	(2, 0)	(4, 1)	(3, 0)
λ	4859.7	4838.2	4800.6	4778.8	4744.9	4722.0
(Intensity)	1.5	4	10	10	4	1.5

Most intense band heads of $^7Li^6Li$, λ (Intensity) (31.9):

(v', v'')	(0, 0)	(1, 0)	(4, 1)
λ	4901.8	4836.5	4739.7
(Intensity)	5	4	2

III. $C\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (60.36, 48.31):

(v', v'')	(0, 4)	(1, 4)	(0, 3)	(2, 4)	(0, 2)	(0, 1)	(0, 0)	(1, 0)
λ	3431.2	3404.4	3392.1	3378.5	3358.6	3315.6	3277.6	3253.1
(Intensity)	4	4	6	4	10	9	6	10

IV. $D\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$ System

Several systems are superimposed in the region 3100-2500Å. Simple Q branches here have been attributed to a $D\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$ system. The D state appears perturbed (60.36).

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$D^1\Pi_u$	≤34140	~205		0.465			3.18		(60.36)
$C^1\Pi_u$	30549	237.9	3.33	0.5068	9.39	9.9	3.08	$y_e\omega_e = 0.060$	(60.36)
$B^1\Pi_u$	20439.40	270.94	3.13	0.5577	8.88	9.45	2.93	$y_e\omega_e = -0.0637$	(33.13, 3.9)
$A^1\Sigma_u^+$	14069.9	255.50	1.59	0.4975	5.22		3.11	$y_e\omega_e = 0.0039$ (a)	(36.16, 28.1)
$X^1\Sigma_g^+$	0	351.43	2.55	0.672	6.8	9.87	2.67	(b)	(69.51, 36.16, 28.1)

(a) Spectroscopic constants for $^6Li_2$ (72.64); (b) spectroscopic constants for $^6Li_2$, $^7Li^6Li$ (69.31)

Dissociation energy = 1.026 ± 0.006 eV, 23.66 kcal/mole, 8275 cm^{-1} (69.51).

Perturbations and General Information

Gyromagnetic ratio (g_j) = 0.10797 nuclear magnetons (64.39).

Transition probabilities (70.53):

Transition	ν	f
$A\,^1\Sigma_u^+ - X\,^1\Sigma_u^+$	14068	0.8688
$C\,^1\Pi_u - X\,^1\Sigma_u^+$	30558	0.0158

Average polarizability (990° K) = 34×10^{-24} cm^3 (74.68).

Potential energy curves – RKR potentials (69.50):

	State	v	U(cm^{-1})	r_{min}(Å)	r_{max}(Å)
T_e = 0.0	$X\,^1\Sigma_g^+$	0	175.1	2.5163	2.8480
		1	521.3	2.4131	2.9911
		2	862.3	2.3470	3.0980
		3	1198.0	2.2961	3.1906
		4	1528.4	2.2542	3.2752
		5	1853.5	2.2183	3.3548
		6	2173.2	2.1868	3.4309
		7	2487.5	2.1588	3.5046
		8	2796.4	2.1336	3.5766
		9	3099.7	2.1107	3.6475
		10	3397.6	2.0897	3.7175
		11	3689.9	2.0704	3.7872
		12	3976.6	2.0526	3.8566
		13	4257.7	2.0361	3.9260
		14	4533.2	2.0208	3.9956
		15	4802.9	2.0066	4.0656
		16	5067.0	1.9935	4.1361
T_e = 14069.9 cm^{-1}	$A\,^1\Sigma_u^+$	0	127.3	2.9237	3.3125
		1	379.7	2.8043	3.4812
		2	628.8	2.7281	3.6066
		3	874.9	2.6693	3.7142
		4	1117.9	2.6205	3.8116
		5	1357.7	2.5782	3.9021

	State	v	$U(cm^{-1})$	r_{min}(Å)	r_{max}(Å)
$T_e = 20439.40\ cm^{-1}$	$B\,^1\Pi_u$	0	134.2	2.7598	3.1389
		1	398.2	2.6448	3.3074
		2	656.1	2.5714	3.4354
		3	907.6	2.5148	3.5480
		4	1152.2	2.4675	3.6526
		5	1389.7	2.4263	3.7528
		6	1619.6	2.3893	3.8506
		7	1841.5	2.3552	3.9476
		8	2055.0	2.3232	4.0449
		9	2259.8	2.2927	4.1434
		10	2455.5	2.2631	4.2441
		11	2641.7	2.2339	4.3479
		12	2814.6	2.2016	4.4635
		13	2976.8	2.1704	4.5812
		14	3127.9	2.1384	4.7059

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Mg_2

Methods of Production and Experimental Technique

Absorption ($T \sim 800°$ C).

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A\,^1\Sigma_u^+ \leftarrow X\,^1\Sigma_g^+$	Absorption	3853-3140	V	3790.9(0, 2) 3764.7(0, 3)		(70.7)
	II	$(^1\Pi_u) \leftarrow X\,^1\Sigma_g^+$	Absorption	2852-2660	-			(70.7)

Mg_2

I. $A\,^1\Sigma_u^+ \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (70.7):

v', v''	3	4	5	6	7
2	3790.9	3796.5	3801.6	3806.3	3810.7
3	3764.6	3770.2	3775.3	3779.9	3784.2
4	3739.2	3744.5	3749.5	3754.2	3758.3
5	3714.2	3719.5	3724.5	3729.0	

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$A\,^1\Sigma_u^+$	26068.76	190.615	1.14562	0.147999	1.31642	0.334286	3.082		(70.7)
$X\,^1\Sigma_g^+$	0	51.12	1.6448	0.0929	3.7758	1.2166	3.890		(70.7)

Dissociation energy = 0.05 eV, 1.15 kcal/mole, 404.1 cm^{-1} (73.10).

Mg_2

Perturbations and General Information

Potential energy curves - RKR potentials (72.8):

	State	v	$E(v) cm^{-1}$	r_{min}(Å)	r_{max}(Å)
T_e = 0.0	$X^1\Sigma_g^+$	0	25.156	3.6872	4.1626
		1	73.037	3.5698	4.4165
		2	117.757	3.5010	4.6260
		3	159.384	3.4509	4.8226
		4	197.971	3.4112	5.0166
		5	233.558	3.3786	5.2140
		6	266.168	3.3513	5.4195
		7	295.811	3.3285	5.6380
		8	322.482	4.4097	5.8750
		9	346.162	3.2948	6.1378
		10	366.806	3.2835	6.4364
		11	384.393	3.2762	6.7852
		12	398.831	3.2717	7.2110
T_e = 26068.76 cm^{-1}	$A^1\Sigma_u^+$	0	95.021	2.9676	3.2111
		1	283.350	2.8915	3.3154
		2	469.404	2.8426	3.3927
		3	653.193	2.8048	3.4591
		4	834.728	2.7736	3.5193
		5	1014.020	2.7467	3.5754
		6	1191.078	2.7231	3.6286
		7	1365.915	2.7018	3.6796
		8	1538.541	2.6826	3.7290
		9	1708.965	2.6649	3.7771
		10	1877.199	2.6486	3.8242
		11	2043.254	2.6335	3.8704
		12	2207.139	2.6193	3.9159
		13	2368.867	2.6060	3.9609
		14	2528.446	2.5935	4.0055
		15	2685.889	2.5818	4.0497

Franck-Condon factors – RKR potentials (72.8):

$A^1\Sigma_u^+ - X^1\Sigma_g^+$

v', v''	0	1	2	3	4	5	6	7	8
0	0.0000	0.0000	0.0001	0.0003	0.0006	0.0010	0.0014	0.0019	0.0022
1	0.0001	0.0004	0.0012	0.0027	0.0047	0.0070	0.0092	0.0110	0.0121
2	0.0004	0.0020	0.0053	0.0102	0.0159	0.0211	0.0249	0.0266	0.0264
3	0.0016	0.0065	0.0148	0.0245	0.0326	0.0370	0.0371	0.0337	0.0283
4	0.0044	0.0157	0.0301	0.0412	0.0448	0.0406	0.0316	0.0216	0.0130
5	0.0103	0.0302	0.0471	0.0508	0.0416	0.0264	0.0126	0.0039	0.0004
6	0.0204	0.0480	0.0578	0.0452	0.0235	0.0067	0.0002	0.0014	0.0055
7	0.0350	0.0636	0.0550	0.0259	0.0045	0.0004	0.0067	0.0138	0.0169
8	0.0530	0.0707	0.0381	0.0061	0.0011	0.0121	0.0210	0.0212	0.0156
9	0.0722	0.0653	0.0160	0.0004	0.0147	0.0261	0.0228	0.0124	0.0039
10	0.0895	0.0485	0.0015	0.0120	0.0297	0.0248	0.0099	0.0009	0.0008

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Mn_2

Spectroscopic Constants

Dissociation energy = 0.22 ± 0.17 eV, 5 kcal/mole, 1750 cm^{-1} (68.2).

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N_2

Methods of Production and Experimental Technique

Absorption (in the vacuum ultraviolet).

Emission from discharge into air, pure N_2, or N_2 in rare gases, hollow cathode discharge, high voltage arc, afterglow, aurora, laser emission, electron beam emission.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Vegard-Kaplan	I	$A^3\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$	Luminescence	5060-2100	R	2760.8(0, 6)		(71.105, 68.80, 68.75, 65.57, 62.40, 61.38, 59.31, 34.6, 34.5, 32.3)
Wilkinson	II	$B^3\Pi_g \leftarrow X^1\Sigma_g^+$	Absorption	1690-1630	R	1635(0, 0) 1638(1, 0)		(62.42)
Saum-Benesch	III	$W^3\Delta_u \leftarrow X^1\Sigma_g^+$	Absorption	4400-2400				(71.101)
Ogawa-Tanaka-Wilkinson	IV	$B'^3\Sigma_u^- \leftarrow X^1\Sigma_g^+$	Absorption	2240-1120	R			(65.51, 64.46

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Ogawa-Tanaka-Wilkinson-Mulliken	V	$a'^1\Sigma_u^- \rightleftarrows X^1\Sigma_g^+$	Absorption: N_2 + Ar	2000-1080	R			(66.62, 65.54, 64.46, 60.35, 59.32, 59.30)
Lyman-Birge-Hopfield	VI	$a^1\Pi_g \rightleftarrows X^1\Sigma_g^+$	Absorption and discharge	2600-1090	R	2125.0(5, 14) 2041.2(5, 13)		(66.63, 65.59, 65.55, 54.46, 56.25)
Tanaka	VII	$w^1\Delta_u \leftarrow X^1\Sigma_g^+$	Absorption	1400-1140	R			(64.46)
Tanaka	VIII	$C^3\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	1130-1070	R		5 heads	(65.53, 64.46)
	IX	$E^3\Sigma_g^+ \leftarrow X^1\Sigma_g^+$	Energy loss spectra	~ 1050		1043.9(0, 0)		(73.166)

Molecule N_2

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Dressler-Lutz	X	$a''^1\Sigma_g^+ \leftarrow X^1\Sigma_g^+$	Absorption	~ 1010		1011.5(0, 0)		(73.166, 67.67)
	XI	$b^1\Pi_u \rightleftarrows X^1\Sigma_g^+$	Absorption and discharge	995-855	R	979.5(2, 0)		(73.166, 69.83, 69.82, 69.81, 64.47)
	XII	$F^3\Pi_u \leftarrow X^1\Sigma_g^+$	Energy loss spectra	980-930		972.2(0, 0)		(73.166)
	XIII	$G^3\Pi_u \leftarrow X^1\Sigma_g^+$	Energy loss spectra	970-940		967.7(0, 0)		(73.166)
	XIV	$D^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Energy loss spectra	~ 960		965.4(0, 0)		(73.166)
	XV	$b'^1\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$	Absorption and discharge	965-830	R			(69.83, 69.82, 69.81, 64.47)
	XVI	$c^1\Pi_u \rightleftarrows X^1\Sigma_g^+$	Absorption and discharge	960-865	R			(69.83, 69.82, 69.81, 64.47)
	XVII	$c'^1\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$	Absorption and discharge	960-840	R			(69.83, 69.82, 69.81, 64.47)

Molecule N_2

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	XVIII	$o^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption and discharge	950-880	R			(69.83, 69.82, 69.81, 64.47)
	XIX	$e^1\Pi_u \leftarrow X^1\Sigma_g^+$	Energy loss spectra	~ 860		865. 1(0, 0)		(69.90)
	XX	$e'^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Energy loss spectra	~ 860		863. 8(0, 0)		(69.90)
First Positive	XXI	$B^3\Pi_g \rightarrow A^3\Sigma_u^+$	Positive column	Infrared - 4700	V	10510. 1(0, 0) 8912. 4(1, 0)		(61.38, 59.33)
Herman-Kaplan	XXII	$E^3\Sigma_g^+ \rightarrow A^3\Sigma_u^+$	Lumines-cence	2740-2130	V	2471. 4(0, 4) 2391. [illegible](0, 3)	Bands not resolved	(45.16, 35.9)
Wu-Benesch	XXIII	$W^3\Delta_u \rightleftharpoons B^3\Pi_g$	Discharge	69000-7000			Bands not resolved	(71.101, 68.73)
"Y" Bands	XXIV	$B'^3\Sigma_u^- \rightarrow B^3\Pi_g$	Lumines-cence from discharge	8920-6060	R		Complex structure	(64.45, 60.36, 60.34, 58.29)

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Second Positive	XXV	$C^3\Pi_u \rightarrow B^3\Pi_g$	Positive column	5450-2680	V	3371. 3(0, 0) 3576. 9(0, 1)		(65.56, 64.49, 60.37, 59.33)
Goldstein-Kaplan	XXVI	$C'^3\Pi_u \rightarrow B^3\Pi_g$	Lumines-cence	5060-2860	R	4728. 0(0, 11)		(64.45, 63.44, 61.38)
Fourth Positive	XXVII	$D^3\Sigma_u^+ \rightarrow B^3\Pi_g$	Lumines-cence from discharge	2910-2250	V	2448. 0(0, 2)	5 heads	(40.11)
	XXVIII	$E^3\Sigma_g^+ \rightarrow B^3\Pi_g$	Electron impact	3180-2740	V	2740(0, 0)		(69.88)
MacFarlane Infrared	XXIX	$a^1\Pi_g \rightarrow a'^1\Sigma_u^-$	Laser emission	82000-33000				(65.58)
Fifth Positive	XXX	$x^1\Sigma_g^- \rightarrow a'^1\Sigma_u^-$	Discharge	2850-2030	V	2411. 7(1, 4)		(56.26)

Molecule N_2

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
First Kaplan	XXXI	$y^1\Pi_g \rightarrow a'^1\Sigma_u^-$	Discharge	2470-2070	V	2225.9(0, 1)		(57.28)
MacFarlane Infrared	XXXII	$w^1\Delta_u \rightarrow a^1\Pi_g$	Laser emission	36500				(66.64)
Gaydon-Herman	XXXIII	$b^1\Pi_u \rightarrow a^1\Pi_g$	Discharge	3420-2740	R			(69.82, 69.81, 57.27)
Gaydon-Herman	XXXIV	$b'^1\Sigma_u^+ \rightarrow a^1\Pi_g$	Discharge	2500	R			(69.82, 69.81, 57.27)
Gaydon-Herman	XXXV	$c^1\Pi_u \rightarrow a^1\Pi_g$	Discharge	3010-2220	R, V			(69.82, 69.81, 57.27)
Gaydon-Herman	XXXVI	$c'^1\Sigma_u^+ \rightarrow a^1\Pi_g$	Discharge	3660-2280	R, V			(69.82, 69.81, 57.27)

Molecule N_2

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Gaydon-Herman	XXXVII	$d'^1?_u \rightarrow a^1\Pi_g$	Discharge	2550-2350				(69.82, 69.81, 57.27)
Gaydon-Herman	XXXVIII	$b^1\Pi_u \rightarrow a^1\Pi_g$	Discharge	2860-2720	R			(69.82, 69.81, 57.27)
Second Kaplan	XXXIX	$y^1\Pi_g \rightarrow w^1\Delta_u$	Discharge	2860-2260	V	2536.6(0, 2)		(57.28)
	XL	$z^1\Delta_g \rightarrow w^1\Delta_u$	Discharge	2480-2360	V			(57.27)
	XLI	$E^3\Sigma_g^+ \rightarrow C^3\Pi_u$	Electron impact	12850	V	12843.6(0, 0)	One band observed	(69.88)
Gaydon Green	XLII	?	Discharge	6340-5040	V	5815(0, 1)	Bands not resolved	(54.23, 53.22, 44.15)
Herman Infrared	XLIII	?	Discharge	8550-7000	V	8057(0, 0)		(53.22, 51.18)

Molecule N_2

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Worley-Jenkins	XLIV	$X^2\Sigma_g^+ \leftarrow X^1\Sigma_g^+$ (N_2^+)	Absorption	< 960			Rydberg series	(69.82, 69.81, 67.66, 62.39, 53.21, 53.20, 43.14, 42.13)
Carroll-Yoshino	XLV	$X^2\Sigma_g^+ \leftarrow X^1\Sigma_g^+$ (N_2^+)	Absorption				Rydberg series	(69.82, 69.81, 67.66)
Worley	XLVI	$A^2\Pi_u \leftarrow X^1\Sigma_g^+$ (N_2^+)	Absorption	< 960			Rydberg series	(62.39, 53.21, 53.20)
Hopfield	XLVII	$B^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ (N_2^+)	Absorption	< 960			Rydberg series	(62.39, 43.14, 42.13, 38.10, 34.9, 30.1)
	XLVIII	$C^2\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ (N_2^+)	Absorption	570-470			Rydberg series	(66.60, 52.19)
	XLIX	Continuum	Absorption	1000-610				(73.151)

I. $A^3\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$ (Vegard-Kaplan) System

Band heads, λ (61.38, 50.17):

v', v''	2	3	4	5	6	7	8	9
0	2215.1	2332.8	2461.6	2603.6	2760.8	2935.7		3351.5
1	2146.6	2257.2	2377.5	2509.8	2655.5	2817.1	2997.0	3197.5
2		2187.8	2300.7	2424.2	2560.1	2710.1		
3		2123.5	2229.9	2346.0	2472.5	2612.8	2766.9	
4			2164.5	2274.0		2523.4	2666.6	
5				2207.2	2319.7	2441.8	2576.0	2722.5

II. $B^3\Pi_g \leftarrow X^1\Sigma_g^+$ (Wilkinson) System

Band heads: (v', v'')	(0,0)	(1,0)
λ	1685	1638

III. $W^3\Delta_u \leftarrow X^1\Sigma_g^+$ (Saum-Benesch) System

Band heads, λ (70.101, 70.94):

v', v''	0	1	2	3	4	5	6	7	8
0	1683.6	1752.4	1826.0	1905.1	1990.2	2082.0	2181.4	2289.1	2406.4
1	1642.7	1708.1	1778.0	1852.9	1933.3	2019.9	2113.2	2214.2	2323.8
2	1604.4	1666.7	1733.2	1804.3	1880.4	1962.2	2050.2	2145.1	2247.7
3	1568.3	1627.8	1691.2	1758.8	1831.1	1908.5	1991.7	2081.1	2177.6
4	1534.4	1591.3	1651.8	1716.3	1785.0	1858.6	1937.3	2021.9	2112.8
5	1502.9	1557.0	1614.9	1676.4	1742.0	1811.9	1886.7	1966.8	2052.7
6	1472.8	1524.6	1580.1	1639.0	1701.6	1768.3	1839.4	1915.4	1996.9
7	1444.2	1494.1	1547.4	1603.8	1663.7	1727.4	1795.2	1867.5	1944.9
8	1416.9	1465.3	1516.5	1570.6	1628.0	1689.0	1753.7	1822.7	1896.3
9	1391.5	1438.1	1487.3	1539.4	1594.5	1652.9	1714.9	1780.8	1851.0
10	1367.3	1412.3	1459.8	1509.9	1562.8	1618.9	1678.3	1741.4	1808.5

IV. $B'\,^3\Sigma_u^- \leftarrow X\,^1\Sigma_g^+$ (Ogawa-Tanaka-Wilkinson) System

Band heads, λ (66.61, 60.35, 59.30):

v', v''	0	1	2	3	4	5	6	7	8
0	1518.1			1695.6	1762.6	1834.2		1993.0	2081.2
1	1484.4		1593.9	1653.8	1717.5			1935.4	2018.6
2	1452.8						1808.6	1881.9	
3	1422.9								
4	1394.7								
5	1368.1								
6	1342.8								
7	1318.9								
8	1296.2								
9	1274.7								
10	1254.2								

V. $a'\,^1\Sigma_u^- \rightleftarrows X\,^1\Sigma_g^+$ (Ogawa-Tanaka-Wilkinson-Mulliken) System

Band heads in absorption, λ (Intensity) (66.61):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)	(6, 0)
λ	1477.1	1446.5	1414.7	1387.6	1360.5	1335.0	1310.7
(Intensity)	(2)	(4)	(8)	(16)	(22)	(30)	(30)

(v', v'')	(7, 0)	(8, 0)	(9, 0)	(10, 0)	(11, 0)	(12, 0)	(13, 0)
λ	1287.7	1265.8	1245.0	1225.3	1206.4	1188.5	1171.3
(Intensity)	(52)	(60)	(48)	(42)	(33)	(34)	(28)

(v', v'')	(14, 0)	(15, 0)	(16, 0)	(17, 0)	(18, 0)	(19, 0)
λ	1155.0	1139.3	1124.6	1110.0	1096.3	1083.2
(Intensity)	(24)	(20)	(16)	(10)	(6)	(4)

Band heads in emission, λ (Intensity) (60.33, 59.33):

(v', v'')	(0, 8)	(0, 7)	(0, 6)	(0, 5)	(0, 4)	(0, 3)
λ	2004.2	1922.2	1845.6	1774.0	1707.0	1643.8
(Intensity)	(1)	(2)	(3)	(4)	(4)	(3)

VI. $a^1\Pi_g \rightleftarrows X^1\Sigma_g^+$ (Lyman-Birge-Hopfield) System

Band heads in emission, λ (66.61):

v', v''	9	10	11	12	13	14	15	16	17
0									
1	1972.6								
2		1988.9	2073.0						
3			2006.0	2089.7	2181.1	2278.3			
4			1944.3	2023.5	2108.1	2198.7	2296.1		
5				1961.8	2041.2	2125.9	2216.6	2314.0	2418.4
6					1979.5	2059.0	2144.0	2234.8	2332.2
7									2253.4

VII. $w^1\Delta_u \leftarrow X^1\Sigma_g^+$ (Tanaka) System

Band heads, λ (Intensity) (64.46):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)
λ	1393.9	1364.7	1337.1	1311.0	1286.3	1262.9
(Intensity)		(1)	(2)	(3)	(3)	(4)

(v', v'')	(6, 0)	(7, 0)	(8, 0)	(9, 0)	(10, 0)	(11, 0)
λ	1240.6	1219.4	1199.3	1180.3	1162.1	1144.7
(Intensity)	(5)	(7)	(6)	(6)	(5)	(4)

VIII. $C^3\Pi_u \leftarrow X^1\Sigma_g^+$ (Tanaka) System

Band heads, λ (Intensity) (66.61):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	1124.2	1099.6	1076.3
(Intensity)	(45)	(60)	(30)

IX. $E^3\Sigma_g^+ \leftarrow X^1\Sigma_g^+$ System

Represents a part of a Rydberg series corresponding to a N_2^+ $X^2\Sigma_g^+$ core.

Band heads, λ (74.188, 73.166):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	1043.9	1020.7	998.9

X. $a''\,{}^1\Sigma_g^+ \leftarrow X\,{}^1\Sigma_g^+$ (Dressler-Lutz) System

Represents part of a Rydberg series corresponding to a N_2^+ $X^2\Sigma_g^+$ core.

Band heads, λ (67.67):

(v', v'')	(0, 0)	(1, 0)
λ	1011.5	990.9

XI. $b\,{}^1\Pi_u \rightleftarrows X\,{}^1\Sigma_g^+$ System

Band heads, λ (73.166, 69.83, 69.82, 69.81):

(v', v'')	λ	(v', v'')	λ
(0, 0)	991.9	(8, 0)	935.1
(1, 0)	985.6	(9, 0)	929.0
(2, 0)	978.9	(10, 0)	922.7
(3, 0)	972.1	(11, 0)	916.4
(4, 0)	965.7	(12, 0)	910.5
(5, 0)	955.1	(13, 0)	904.7
(6, 0)	949.2	(14, 0)	899.2
(7, 0)	942.4	(15, 0)	895.9

XII. $F\,{}^3\Pi_u \leftarrow X\,{}^1\Sigma_g^+$ System

Represents a part of a Rydberg series corresponding to a N_2^+ $A^2\Pi_u$ core.

Band heads, λ (73.166):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	972.2	955.0	938.4

XIII. $G^3\Pi_u \leftarrow X^1\Sigma_g^+$ System

Represents part of a Rydberg series corresponding to a N_2^+ $X^2\Sigma_g^+$ core.

Band heads, λ (73.166):

(v', v'')	(0, 0)	(1, 0)
λ	967.7	949.2

XIV. $D^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ System

Represents part of a Rydberg series corresponding to a N_2^+ $X^2\Sigma_g^+$ core.

Band head, λ (73.166):

(v', v'')	(0, 0)
λ	965.4

XV. $b'^1\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$ System

Band heads, λ (69.83, 69.82, 69.81, 64.47):

(v', v'')	λ	(v', v'')	λ
(0, 0)	964.6	(8, 0)	-
(1, 0)	957.7	(9, 0)	907.5
(2, 0)	951.0	(10, 0)	901.4
(3, 0)	944.6	(11, 0)	896.2
(4, 0)	937.9	(12, 0)	891.0
(5, 0)	931.9	(13, 0)	885.7
(6, 0)	926.1	(14, 0)	880.7
(7, 0)	917.8	(15, 0)	875.9

XVI. $c^1\Pi_u \rightleftarrows X^1\Sigma_g^+$ System

c_3 represents the first member of a Rydberg series corresponding to a N_2^+ $X^2\Sigma_g^+$ core.

Band heads, λ (69.83, 69.82, 69.81, 64.47):

(v', v'')	λ
(0, 0)	960.3
(1, 0)	920.0

XVII. $c'^1\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$ System

c_4' represents the first member of a Rydberg series corresponding to a N_2^+ $X^2\Sigma_g^+$ core.

Band heads, λ (69.83, 69.82, 69.81, 64.47):

(v', v'')	λ	(v', v'')	λ
(0, 0)	958.6	(4, 0)	886.8
(1, 0)	940.1	(5, 0)	870.8
(2, 0)	921.2	(6, 0)	856.0
(3, 0)	903.7	(7, 0)	841.9

XVIII. $o^1\Pi_u \rightleftarrows X^1\Sigma_g^+$ System

Represents the first member of the Worley Rydberg series corresponding to a N_2^+ $A^2\Pi_u$ core.

Band heads, λ (69.83, 69.82, 69.81, 64.47):

(v', v'')	λ
(0, 0)	946.1
(1, 0)	928.9
(2, 0)	912.6
(3, 0)	897.2
(4, 0)	882.5

XIX. $e^1\Pi_u \leftarrow X^1\Sigma_g^+$ System

e_4 represents a member of the Worley-Jenkins Rydberg series corresponding to a N_2^+ $X^2\Sigma_g^+$ core.

Band heads, λ (69.90):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	865.1	849.9	834.2

XX. $e'^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ System

e_4' represents a member of the Worley-Jenkins Rydberg series corresponding to a N_2^+ $X^2\Sigma_g^+$ core.

Band head, λ (69.90):

(v', v'')	(0, 0)
λ	863.8

XXI. $B^3\Pi_g \rightarrow A^3\Sigma_u^+$ (First Positive) System

Band heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4	5	6
0	10510.0(10)						
1	8912.4(10)						
2	7753.2(6)	8722.3(8)	9942.0(2)				
3	6875.0(2)	7626.2(7)	8541.8(6)	9682.1(3)			
4	6186.8(3)	6788.6(6)	7503.9(7)	8369.2(2)	9436.4(3)		
5	5632.7(1)	6127.4(3)	6704.8(8)	7386.6(5)	8204.8(3)	9203.9(2)	
6		5592.9(1)	6069.7(7)	6623.6(9)	7273.3(3)	8047.4(2)	
7			5553.7(1)	6013.6(7)	6544.8(10)	7164.8(2)	7896.4(2)
8				5515.6(2)	5959.0(8)	6468.5(10)	7059.0(2)
9					5478.5(2)	5906.0(8)	6394.7(9)
10						5442.3(3)	5854.4(8)
11						5053.6	5407.1(3)
12							5030.8

XXII. $E^3\Sigma_g^+ \rightarrow A^3\Sigma_u^+$ (Herman-Kaplan) System

Band heads, λ (74.188, 45.16, 35.9):

v', v''	0	1	2	3	4	5	6	7
0		2242.3	2315.3	2391.6	2471.4	2554.9	2642.1	2733.2
1		2137.6	2203.8	2272.9		2419.8	2497.8	

XXIII. $W^3\Delta_u \rightleftarrows B^3\Pi_g$ (Wu-Benesch) System

Band heads, λ (n.p. 218, 71.101, 70.92, 68.73):

v', v''	0	1	2	3	4	5	6
0	629373.3	-65875.5	-31578.9	-20889.5	-15675.8	-12589.4	-10549.8
1	61962.2	586939.5	-58422.4	-30011.2	-20307.6	-15412.6	-12462.8
2	32833.3	73057.5	-357305.2	-52623.6	-28633.1	-19777.0	-15169.8
3	22450.3	36005.1	88595.4	-203381.4	-47987.9	-27413.9	-19292.1
4	17124.2	24002.4	39775.2	111892.7	-143172.7	-44201.2	-26329.2
5	13885.3	18099.6	25797.6	44328.0	150660.7	-111088.6	-41053.2
6	11708.4	14568.8	19174.3	27817.1	49931.5	227885.3	-91169.0
7	10145.4	12225.3	15311.3	20363.6	30133.7	56992.5	456755.3
8	8969.2	10557.0	12781.6	16120.4	21686.6	32816.8	66157.9
9	8052.4	9309.4	10997.3	13382.0	17005.2	23166.3	35959.1
10	7318.0	8341.7	9671.8	11469.3	140[illegible]1.7	17976.5	24831.6

XXIV. $B'^3\Sigma_u^- \rightarrow B^3\Pi_g$ ("Y" Bands) System

Band heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4
4	8058(2)				
5	7243(2)	8262(5)			
6	6587(1)	7420(6)	8473(8)		
7	6062(1)	6744(6)	7602(10)	8691(10)	
8		6203(3)	6905(10)	7791(10)	8917(2)

XXV. $C^3\Pi_u \rightarrow B^3\Pi_g$ (Second Positive) System

Band heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4	5
0	3371.3(10)	3576.9(10)	3804.9(10)	4059.4(8)	4343.6(4)	4667.3(0)
1	3159.3(9)	3338.9(2)	3536.7(8)	3755.4(10)	3998.4(9)	4269.7(5)
2	2976.8(6)	3136.0(8)	3309 (2)	3500.5(4)	3710.5(8)	3943.0(8)
3	2819.8(1)	2962.0(6)	3116.7(6)	3285.3(3)	3469 (0)	3671.9(6)
4	2687	2814.3(1)	2953.2(6)	3104.0(3)	3268.1(4)	3446 (0)

XXVI. $C'^3\Pi_u \rightarrow B^3\Pi_g$ (Goldstein-Kaplan) System

Band heads, λ (50.17):

v', v''	2	3	4	5	6	7	8	9	10
0	2863.5	3005.4	3159.2	3326.1	3504.0	3707.1	3925.4	4166.0	4432.2
1			3025.8	3178.4					

XXVII. $D^3\Sigma_u^+ \rightarrow B^3\Pi_g$ (Fourth Positive) System

Band heads, λ (Intensity) (50.17):

(v', v'')	(0, 6)	(0, 5)	(0, 4)	(0, 3)	(0, 2)	(0, 1)	(0, 0)
λ	2903.9	2777.9	2660.5	2550.7	2448.0	2351.4	2260.8
(Intensity)	(1)	(2)	(5)	(8)	(10)	(6)	(2)

XXVIII. $E^3\Sigma_g^+ \rightarrow B^3\Pi_g$ System

Band heads, λ (69.88):

(v', v")	(0,0)	(0,1)	(0,2)	(0,3)
λ	2740	2880	3020	3180

XXIX. $a^1\Pi_g \rightarrow a'^1\Sigma_u^-$ (MacFarlane Infrared) System

Band heads, λ (65.58):

(v', v")	(0, 0)	(1, 0)	(2, 1)
λ	82439.2	34739.4	33214.5

XXX. $x^1\Sigma_g^- \rightarrow a'^1\Sigma_u^-$ (Fifth Positive) System

Band heads, λ (Intensity) (50.17):

v', v"	0	1	2	3	4	5	6
0	2198.9(4)	2274.3(6)	2353.6(4)		2525.6(2)	2619.3(4)	
1	2112.1(5)	2181.5(4)		2331.3(2)	2411.8(7)	2496.7(3)	2586.6(7)
2	2033.6(5)	2097.9(2)	2165.2(5)	2235.9(3)		2387.9	2469.9(4)

XXXI. $y^1\Pi_g \rightarrow a'^1\Sigma_u^-$ (First Kaplan) System

Band heads, λ (Intensity) (50.17):

v', v"	0	1	2	3	4
0	2153.6(4)	2225.9(5)	2301.9(4)	2381.7(3)	2466.0(2)
1	2077.3			2288.6(1)	2366.4(2)

XXXII. $w^1\Delta_u \rightarrow a^1\Pi_g$ (MacFarlane Infrared) System

Band head, λ (66.64):

(v', v")	(0, 0)
λ	36399.5

XXXIII. $b\,^1\Pi_u \rightarrow a\,^1\Pi_g$ (Gaydon-Herman) System

Band heads, λ (69.82, 69.81, 57.27):

v', v''	0	1	2	3	4
0					
1	3075.1	3241.3			
...					
5	2795.4	2932.0	3079.9	3240.8	3416.5
6	2746.2	2877.9	3020.3	3175.0	

XXXIV. $b'\,^1\Sigma_g^+ \rightarrow a\,^1\Pi_g$ (Gaydon-Herman) System

Band head, λ (69.82, 69.81, 57.27): (v', v'') (0, 7)
λ 2498.6

XXXV. $c\,^1\Pi_u \rightarrow a\,^1\Pi_g$ (Gaydon-Herman) System

c_3 and c_4 are the two first members of a $c\,^1\Pi_u$ Rydberg series that converges at $N_2^+\ X^2\Sigma_g^+$.

Band heads, λ (69.82, 69.81, 57.27):

$c_3\,^1\Pi_u \rightarrow a\,^1\Pi_g$

v', v''	0	1	2	3	4
0	2839.4	2980.1			
1					
2	2516.0	2626.2	2744.3	2871.1	3008.1

$c_4\,^1\Pi_u \rightarrow a\,^1\Pi_g$

v', v''	0	1	2	3	4	5	6
0		2224.4	2308.6	2397.8	2492.4	2592.8	2699.9

XXXVI. $c'\,{}^1\Sigma_u^+ \rightarrow a\,{}^1\Pi_g$ (Gaydon-Herman) System

c_4' is the first member of a $c'\,{}^1\Sigma_u^+$ Rydberg series that converges at $N_2^+\ X^2\Sigma_g^+$.

Band heads, λ (69.82, 69.81, 57.27):

v', v''	0	1	2	3	4	5
0	2827.1	2967.0	3118.6	3283.3	3463.3	3661.1
1	2671.7	2796.0				
2	2524.9		2753.8			
3	2397.1	2496.8	2603.3			
4	2281.5	2371.6	2467.7	2569.6	2678.5	2795.6

XXXVII. $d'({}^1\Sigma_u^-$ or ${}^1\Delta_u?) \rightarrow a\,{}^1\Pi_g$ (Gaydon-Herman) System

Band heads, λ (69.82, 69.81, 57.27):

v', v''	0	1	2
0	2358.8	2455.1	2558

XXXVIII. $o\,{}^1\Pi_u \rightarrow a\,{}^1\Pi_g$ (Gaydon-Herman) System

o is the first member of the Worley Rydberg series that converges at $N_2^+\ A^2\Pi_u$.

Band heads, λ (69.82, 69.81, 57.27):

(v', v'')	(0, 0)	(0, 1)
λ	2723.6	2853.3

XXXIX $y\,{}^1\Pi_g \rightarrow w\,{}^1\Delta_u$ (Second Kaplan) System

Band heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4	5	6
0	2354.5(4)		2536.6(5)	2636.2(5)	2741.9(3)	2854.9	
1	2263.4(4)		2431.0	2522.3(3)	2619.3(5)	2722.0(3)	2831.7

XL. $z\,^1\Delta_g \rightarrow w\,^1\Delta_u$ System

Band heads, λ (57.27):

(v', v'')	(n, 2)	(n+3, 4)	for n = 2?
λ	2477.3	2368.8	

XLI. $E\,^3\Sigma_g^+ \rightarrow C\,^3\Pi_u$ System

Band head, λ (69.88):

(v', v'')	(0, 0)
λ	12843.6

XLII. Gaydon Green System

Band heads, λ (54.23, 53.22, 44.15):

v', v''	0	1	2	3	4	5
0	5574.4(9)	5815.1(10)	6068.6(8)	6336.3(5)		
1	5308.6(8)	5527.1(2)	5755.1(3)	5994.5(6)	6246.3(5)	
2	5073.4(4)	5272.0(5)	5479.6(6)		5924 (1)	6160.5(3)
3		5047.0(2)		5435.0(3)	5640 (1)	

XLIII. Herman Infrared System

Band heads, λ (53.22, 51.18):

v', v''	0	1	2
0	8057.6(10)	8549 (2)	
1	7521.0(0)		8397 (1)
2	7061.7(6)	7435.0(5)	7828.5(8)
3		7001.2(4)	

XLIV. $X\,^2\Sigma_g^+(N_2^+) \leftarrow X\,^1\Sigma_g^+$ (Worley-Jenkins) System

Represents a $^1\Pi_u$ Rydberg series, the first state of which is $c\,^1\Pi_u$ (69.82, 69.81, 67.66, 62.39)

$$\nu = 125665.8 - R\left[m + 0.3450 - (0.1000/m) - (0.100/m^2)\right]^{-2}$$

where m = 2, 3, ⋯ 26

XLV. $X^2\Sigma_g^+(N_2^+) \leftarrow X^1\Sigma_g^+$ (Carroll-Yoshino) System

Represents a $^1\Sigma_u^+$ Rydberg series, the first member of which is $c'\,^1\Sigma_u^+$ (69.82, 69.81, 67.66)

m	2	3	4	5	6	7
λ	958.559	(863.6)	833.746	820.592	(813.2)	808.672
n*	2.2675		4.3776	5.3713		7.394

XLVI. $A^2\Pi_u(N_2^+) \leftarrow X^1\Sigma_g^+$ (Worley) System

Represents a $^1\Pi_u$ Rydberg series, the first of which is $o\,^1\Pi_u$ (62.39, 53.21, 53.20)

$\nu = 136607 - R\left[m - 0.0441 - (0.018/m^2)\right]^{-2}$ where m = 2, 3, ⋯ 6

XLVII. $B^2\Sigma_u^+(N_2^+) \leftarrow X^1\Sigma_g^+$ (Hopfield) System

Represents a Rydberg series (62.39, 43.14, 42.13, 38.10, 24.8, 30.1)

$\nu = 151240 - R(m - 0.092)^{-2}$ where m = 3, 4, ⋯ 7

XLVIII. $C^2\Sigma_u^+(N_2^+) \leftarrow X^1\Sigma_g^+$ System

Represents a Rydberg series

Band heads, λ (66.60, 52.19):

n* = 3.040

(v', v'')	λ	(v', v'')	λ
(0, 0)	560.48	(7, 0)	520.46
(1, 0)	554.10	(8, 0)	515.61
(2, 0)	548.00	(9, 0)	510.93
(3, 0)	542.11	(10, 0)	506.35
(4, 0)	536.41	(11, 0)	502.02
(5, 0)	530.86	(12, 0)	497.77
(6, 0)	525.54	(13, 0)	493.71

$n^* = 4.059$	(v', v'')	λ
	(3, 0)	527.33
	(4, 0)	521.89
	(5, 0)	516.71
	(6, 0)	
	(7, 0)	506.71
	(8, 0)	502.02

$n^* = 5.05$	(v', v'')	λ
	(8, 0)	496.15

XLIX. Continuum

There are two weak continua between 825 and 1000 Å with maximums of approximately 5 cm^{-1} at 970 Å and 15 cm^{-1} at 910 Å. At approximately 850 Å a dissociation continuum increases gradually to a maximum of ~ 120 cm^{-1} at 805 Å. This is followed by a secondary peak with a maximum value of 75 cm^{-1} occurring at 775 Å. The continuum then decreases to 0 at ~ 750 Å. The most prominent dissociation continuum starts at approximately 730 Å and decreases to 90 cm^{-1} at 660 Å. Below 660 Å there is another continuum with a broad maximum at 610 Å, this continuum overlapping the previous one. (73.151)

Molecule N_2

SPECTROSCOPIC CONSTANTS

State	T_o	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$e'\,^1\Sigma_u^+$	115767.5							Rydberg	(69.90)
$e\,^1\Pi_u$	115593.6							Rydberg	(69.90)
$z\,^1\Delta_g$	115365.9	(1700)		(1.76)	15.3		(1.16)	Rydberg	(57.27)
$y\,^1\Pi_g$	114166.3	1707.9[a]		1.78[b]			1.16[c]	Rydberg	(57.28)
$x\,^1\Sigma_g^-$	113212.1	1910.0		1.750	22.5	5.88	1.168	Rydberg	(56.26)
$d'\,^1?_u$	111333								(45.16)
$o\,^1\Pi_u$	105682	2020.0	32.28	1.694[b]			1.19[c]	Rydberg	(69.82, 69.81)
$c'\,^1\Sigma_u^+$	104322.4	2046[a]		1.929[b]			1.12[c]	Rydberg	(69.82, 69.81)
$c'\Pi_u$	104[illegible]39.2	2410[a]		1.50[b]			1.27[c]	Rydberg	(69.82, 69.81)
$b'\,^1\Sigma_u^+$	103672	746[a]		1.154	4.8		1.444		(69.82, 69.81)
$D\,^3\Sigma_u^+$	103573			1.961[b]		20	1.108[c]	Rydberg	(40.11)

SPECTROSCOPIC CONSTANTS

State	T_o	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$G^3\Pi_u$	103338							Rydberg	(73.166)
$F^3\Pi_u$	102854							Rydberg	(73.166)
$b^1\Pi_u$	100816	635[(a)]		1.448[(b)]	4.8	29	1.230[(c)]		(69.86, 69.81)
$a''^1\Sigma_g^+$	99032							Rydberg	(67.67)
$C'^3\Pi_u$	97580			1.0496[(b)]		10.9	1.508[(c)]		(63.44)
$E^3\Sigma_g^+$	95774.50	2185[(a)]		1.927[(b)]		6.0	1.117[(c)]	Rydberg	(74.188, 54.50)
$C^3\Pi_u$	88977.9	2047.18	28.4450	1.82473	18.683	5.80	1.1487		(65.50)
$^5\Sigma^-$	77925	650				0.0011	1.55		(62.41)
$w^1\Delta_u$	71698.8	1559.24	11.8874	1.498	16.6	5.53	1.2678		(65.50)
$a^1\Pi_g$	68951.2	1694.20	13.9491	1.61688	17.933	5.89	1.2203		(65.50)
$a'^1\Sigma_u^-$	67739.3	1530.25	12.0747	1.47988	16.574	5.54	1.2755		(65.50)

Molecule N_2

SPECTROSCOPIC CONSTANTS

State	T_o	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$B'^3\Sigma_u^-$	65852.4	1516.88	12.1810	1.47359	16.861	5.56	1.2782		(65.50)
$W^3\Delta_u$	60555.8	1501.4	11.6				1.28		(71.101, 65.50)
$B^3\Pi_g$	59306.8	1733.39	14.1221	1.6374	17.91	5.84	1.2126		(65.50)
$A^3\Sigma_u^+$	49754.8	1460.52	13.8313	1.45455	18.009	5.77	1.2866		(65.50)
$X^1\Sigma_g^+$	0	2358.03	14.1351	1.9980	17.72	5.74	1.0977		(65.50)

(a) ΔG_0, (b) B_o, (c) r_o

Dissociation energy = 9.76 ± 0.01 eV, 225.07 kcal/mole, 78710 cm^{-1} (63.43, 56.24).

Perturbations and General Information

The $D^3\Sigma_u^+$ state is predissociated by the shallow $C'^3\Pi_u$ state (74.188).

The $b^1\Pi_u$ state is perturbed by the $c^1\Pi_u$ state (73.166)

The $b'^1\Sigma_u^+$ state is perturbed by the $c'^1\Sigma_u^+$ state (73.166)

The $o^1\Pi_u$ level is predissociated possibly by the $C'^3\Pi_u$ state (73.166).

The $B^3\Pi_g$ (v' ~ 12) and a $^1\Pi_g$ (v' ~ 6) levels are predissociated by the $^5\Sigma^+$ level (68.80).

The higher levels of the $C^3\Pi_u$ and $C'^3\Pi_u$ states are predissociated by the $^3\Pi_u$ continuum (69.82).

Perturbations and predissociation have been observed in the y state (57.28).

Lifetimes:

$A^3\Sigma_u^+$	v' = 0	τ = 1.36 $\pm$ 0.27 sec for Σ = 0 substate levels	(69.L2, 69.L3)
		τ = 2.70 $\pm$ 0.54 sec for Σ = 1, -1 substate levels	
$B^3\Pi_g$	v' = 0	τ = 10 $\pm$ 2 μsec	(n.p. 217)
	v' - 2	τ = 7.0 $\pm$ 0.4 μsec	(66.L1)
	v' = 3	τ = 6.8 $\pm$ 0.3 μsec	
	v' = 4	τ = 6.7 $\pm$ 0.7 μsec	
	v' = 5	τ = 6.7 $\pm$ 1.0 μsec	
	v' = 6	τ = 7.0 $\pm$ 0.7 μsec	
	v' = 7	τ = 5.4 $\pm$ 0.8 μsec	
	v' = 8	τ = 5.4 $\pm$ 0.8 μsec	
	v' = 9	τ = 5.4 $\pm$ 0.5 μsec	
$W^3\Delta_u$	v' = 0	τ = 1.668 msec	(73.167)
	v' = 1	τ = 2.000 msec	
$a'\Pi_g$	v' = 0	τ = 0.17 msec	(65.52)
$C^3\Pi_u$	v' = 0	τ = 40.4 $\pm$ 0.5 nsec	(73.177)
	v' = 1	τ = 40.6 $\pm$ 0.5 nsec	
$D^3\Sigma_u^+$	v' = 0	τ = 14.1 nsec	(73.182)

Oscillator Strengths:

$A^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	$f_{0,0} = 2 \times 10^{-3}$	(66.L1)
$a'\Pi_g \leftarrow X^1\Sigma_g^+$	$f_{0,0} = 1.3 \times 10^{-6}$	(67.68)
	$f_{1,0} = 3.0 \times 10^{-6}$	
	$f_{2,0} = 4.1 \times 10^{-6}$	
$C^3\Pi_u \leftarrow X^1\Sigma_g^+$	$f_{0,0} = 2.2 \times 10^{-6}$	
	$f_{1,0} = 1.1 \times 10^{-6}$	
	$f_{2,0} = 5.6 \times 10^{-7}$	

$$w^1\Delta_u \leftarrow X^1\Sigma_g^+ \qquad \left.\begin{aligned} f_{3,0} &= (3.5 + 0.18p) \times 10^{-8} \\ f_{4,0} &= (6.1 + 0.21p) \times 10^{-8} \\ f_{5.0} &= (4.0 + 0.26p) \times 10^{-8} \end{aligned}\right\} \text{ for pressure p in psi}$$

Franck-Condon factors for the $C^3\Pi_u$ - $B^3\Pi_g$ (Second Positive) system (65.52):

v'', v'	0	1	2	3	4
0	4.55-1	3.88-1	1.34-1	2.16-2	1.16-3
1	3.31-1	2.29-2	3.35-1	2.52-1	5.66-2
2	1.45-1	2.12-1	2.30-2	2.04-1	3.26-1
3	4.94-2	2.02-1	6.91-2	8.81-2	1.13-1
4	1.45-2	1.09-1	1.69-1	6.56-3	1.16-1
5	3.87-3	4.43-2	1.41-1	1.02-1	2.45-3
6	9.68-4	1.52-2	7.72-2	1.37-1	4.70-2
7	2.31-4	4.68-3	3.32-2	9.93-2	1.09-1
8	5.36-5	1.33-3	1.23-2	5.26-2	1.04-1
9	1.21-5	3.57-4	4.12-3	2.31-2	6.67-2
10	2.61-6	9.15-5	1.27-3	8.95-3	3.40-2

Franck-Condon factors followed by a factor of ten

Franck-Condon factors for the $B^3\Pi_g - A^3\Sigma_g^+$ (First Positive) system (65.52):

v'', v'	0	1	2	3	4	5	6	7	8
0	4.06-1	4.01-1	1.58-1	3.17-2	3.47-3	2.01-4	5.72-6	8.81-8	8.28-11
1	3.27-1	3.71-3	2.85-1	2.77-1	9.18-2	1.41-2	1.07-3	3.70-5	5.14-7
2	1.64-1	1.59-1	6.59-2	1.05-1	3.06-1	1.63-1	3.41-2	3.26-3	1.35-4
3	6.67-2	1.93-1	2.25-2	1.50-1	1.11-2	2.59-1	2.26-2	6.36-2	7.50-3
4	2.44-2	1.29-1	1.22-1	4.67-3	1.53-1	6.94-3	1.76-1	2.68-1	1.01-1
5	8.38-3	6.57-2	1.39-1	4.09-2	4.94-2	1.00-1	5.05-2	9.30-2	2.83-1
6	2.80-3	2.92-2	9.94-2	1.03-1	2.04-3	9.29-2	4.02-2	9.90-2	3.20-2
7	9.26-4	1.20-2	5.66-2	1.08-1	5.13-2	8.81-3	1.04-1	5.00-3	1.26-1
8	3.07-4	4.73-3	2.83-2	7.88-2	8.85-2	1.22-2	3.92-2	8.29-2	2.75-3
9	1.03-4	1.83-3	1.31-2	4.78-2	8.58-2	5.37-2	4.73-5	6.71-2	4.68-2

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the $A^3\Sigma_u^+ - X^1\Sigma_g^+$ (Vegard-Kaplan) system (65.52):

v'', v'	0	1	2	3	4	5	6	7	8
0	1.06-3	5.55-3	1.57-2	3.15-2	5.07-2	6.93-2	8.38-2	9.21-2	9.38-2
1	8.41-3	3.27-2	6.65-2	9.31-2	9.91-2	8.35-2	5.57-2	2.78-2	8.41-3
2	3.34-2	8.88-2	1.15-1	8.91-2	4.00-2	5.73-3	1.92-3	1.90-2	3.87-2
3	8.29-2	1.33-1	8.12-2	1.35-2	3.65-3	3.44-2	5.52-2	4.64-2	2.21-2
4	1.44-1	1.09-1	9.45-3	1.74-2	6.05-2	5.16-2	1.45-2	1.60-4	1.52-2
5	1.89-1	3.67-2	1.77-2	7.36-2	3.88-2	4.23-4	1.88-2	4.41-2	3.63-2
6	1.92-1	8.43-5	8.13-2	4.21-2	1.05-2	4.10-2	4.70-2	1.23-2	1.06-3
7	1.55-1	4.26-2	7.92-2	1.22-4	5.28-2	4.21-2	8.71-4	1.90-2	4.11-2
8	1.02-1	1.17-1	1.76-2	4.83-2	5.01-2	5.30-5	3.71-2	4.04-2	5.56-3
9	5.47-2	1.53-1	6.52-3	8.10-2	8.41-4	4.56-2	3.70-2	8.28-6	2.58-2
10	2.46-2	1.32-1	7.06-2	3.10-2	3.70-2	4.73-2	5.09-4	4.04-2	3.06-2

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the $a^1\Pi_g - X^1\Sigma_g^+$ (Lyman-Birge-Hopfield) system (65.52):

v'', v'	0	1	2	3	4	5	6
0	4.43-2	1.18-1	1.73-1	1.85-1	1.60-1	1.20-1	8.08-2
1	1.51-1	1.90-1	9.44-2	1.15-2	6.67-3	4.75-2	8.52-2
2	2.50-1	8.02-2	3.30-3	7.51-2	9.62-2	4.70-2	4.94-3
3	2.53-1	5.84-4	1.08-1	6.81-2	4.43-4	3.47-2	7.32-2
4	1.73-1	9.22-2	8.41-2	4.39-3	7.81-2	5.51-2	2.37-3
5	8.61-2	1.91-1	3.19-4	9.76-2	3.47-2	9.80-3	6.39-2
6	3.22-2	1.76-1	7.30-2	6.18-2	2.05-2	7.84-2	1.24-2
7	9.17-3	9.93-2	1.73-1	1.17-3	9.90-2	5.16-3	4.47-2
8	1.99-3	3.87-2	1.60-1	9.17-2	2.93-2	5.50-2	5.01-2
9	3.37-4	1.10-2	8.76-2	1.71-1	1.64-2	8.17-2	5.19-3
10	4.75-5	2.33-3	3.23-2	1.38-1	1.25-1	3.08-3	8.54-2

Franck-Condon factors followed by a factor of ten

Franck-Condon factors for the $C^3\Pi_u - X^1\Sigma_g^+$ (Tanaka) system (65.52):

v'', v'	0	1	2	3	4
0	5.5[illegible]-1	3.03-1	1.01-1	2.76-2	7.16-3
1	3.36-1	8.73-2	2.71-1	1.82-1	7.88-2
2	9.03-2	3.64-1	1.82-3	1.30-1	1.82-1
3	1.33-2	1.95-1	2.44-1	7.11-2	2.42-2
4	1.12-3	4.47-2	2.67-1	9.92-2	1.48-1
5	6.28-5	5.84-3	9.52-2	2.80-1	9.47-3
6	6.12-6	5.13-4	1.80-2	1.58-1	2.19-1
7	6.77-7	4.90-5	2.27-3	4.32-2	2.13-1
8	4.83-9	5.17-6	2.79-4	8.06-3	8.76-2
9	1.44-10	1.48-7	4.21-5	1.39-3	2.40-2
10	1.68-8	9.72-8	4.41-6	2.59-4	5.66-3

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the $W^3\Delta_u - X^1\Sigma_g^+$ system (70.94):

v', v''	0	1	2	3	4	5	6	7
0	.1713-2	.1310-1	.4721-1	.1065-6	.1691-0	.2005-0	.1846-0	.1354-0
1	.8568-2	.4711-1	.1107-0	.1384-0	.8733-1	.1401-1	.9521-2	.7826-1
2	.2295-1	.8741-1	.1204-0	.5727-1	.1253-3	.4533-1	.9516-1	.5355-1
3	.4383-1	.1099-0	.7206-1	.1040-2	.4385-1	.7576-1	.1548-1	.1425-1
4	.6680-1	.1025-0	.1818-1	.2143-1	.6970-1	.1385-1	.1912-1	.6786-1
5	.8696-1	.7284-1	.7807-4	.5735-1	.3075-1	.7809-2	.5891-1	.1536-1
6	.1003-0	.3743-1	.1649-1	.5698-1	.5108-3	.4486-1	.2615-1	.8806-2
7	.1050-0	.1106-1	.4202-1	.2820-1	.1368-1	.4519-1	.2614-4	.4465-1
8	.1021-0	.3046-3	.5511-1	.4007-2	.3909-1	.1477-1	.2141-1	.3225-1
9	.9325-1	.3737-2	.4992-1	.1816-2	.4350-1	.1630-4	.4062-1	.2814-2
10	.8129-1	.1581-1	.3329-1	.1623-1	.2659-1	.1279-1	.2831-1	.6968-2

Franck-Condon factors followed by a factor of ten

r-Centroids for the $B'^3\Sigma_u^- - X^1\Sigma_g^+$ system (66.65a).

v', v''	0	1	2	3	4	5	6	7	8
0	1.182	1.199	1.216	1.234	1.252	1.271	1.290	1.310	1.330
1	1.171	1.188	1.205	1.222	1.240	1.258	1.277	1.296	1.316
2	1.161	1.177	1.194	1.211	1.228	1.246	1.264	1.283	1.302
3	1.151	1.167	1.183	1.200	1.217	1.234	1.252	1.270	1.289

Lasing from the First Positive system has been observed (n.p. 217, 67.68a, 63.43a).

Lasing from the Second Positive system has been observed (n.p. 217, 74.206, 74.204, 74.199, 74.197, 74.195, 74.193, 74.191, 74.190, 74.189, 73.168, 73.165, 73.163, 68.74a, 67.68a, 66.64a, 64.47a).

Lasing from the Lyman-Birge-Hopfield system has been observed (73.168).

The two MacFarlane infrared systems have only been seen in lasing (n.p. 217 66.65, 66.63a, 65.58).

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Na_2

Methods of Production and Experimental Technique

Absorption.

Emission from a discharge in Na_2 vapor, heat pipe.

Fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$	Absorption, discharge, fluorescence	8000-6000	R			(70.44, 33.20, 29.13)
	II	$B^1\Pi_u \rightleftarrows X^1\Sigma_g^+$	Absorption, discharge, fluorescence	5040-4560	R			(69.41, 32.17, 28.10)
	III	$C^1\Pi_u \rightleftarrows X^1\Sigma_g^+$	Absorption, discharge	3600-3200	R	3338.8(5,0) 3326.3(6,0)		(50.34, 49.33)
	IV	$D^1\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	3325-3030	R			(50.34)
	V	$E \rightleftarrows ?$	Absorption, discharge	3120-2880	R	2945.5(7,0)		(47.31)
	VI	?	Absorption, discharge	3050-2500	R	2750, 2735		(47.31)

Molecule Na_2

I. $A\,^1\Sigma_u^+ \rightleftarrows X\,^1\Sigma_g^+$ System

Most intense band heads in absorption, λ (33.20, 29.13):

(v', v'')	(4, 2)	(4, 1)	(5, 1)	(6, 0)	(7, 0)	(8, 0)	(9, 0)
λ	6751.2	6679.7	6561.5	6513.2	6465.8	6418.4	6374.2

II. $B\,^1\Pi_u \rightleftarrows X\,^1\Sigma_g^+$ System

Most intense band heads in absorption, λ (32.17, 28.10):

(v', v'')	(0, 3)	(0, 2)	(0, 1)	(1, 1)	(0, 0)	(1, 0)	(2, 0)	(3, 0)
λ	5040.4	5001.4	4962.8	4932.6	4924.2	4894.5	4865.5	4837.2

III. $C\,^1\Pi_u \rightleftarrows X\,^1\Sigma_g^+$ System

Most intense band heads, λ (absorption intensity, emission intensity) (50.34, 49.3[illegible]):

(v', v'')	(5, 1)	(4, 0)	(5, 0)	(6, 0)	(7, 0)	(9, 0)	(10, 0)
λ	3356.5	3351.5	3338.8	3326.3	3314.0	3290.0	3278.4
Absorption intensity	8	7	10	10	10	9	8
Emission intensity	4	4	5	4	4	4	4

IV. $D\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (50.34):

(v', v'')	(1, 2)	(3, 3)	(2, 2)	(1, 1)	(0, 0)	(2, 1)	(1, 0)	(2, 0)
λ	3151.6	3145.2	3140.0	3135.7	3131.2	3125.1	3120.5	3109.5
(Intensity)	2	2	2	2	2	2	2	2

V. E ⇄ ? System

Most intense band heads, λ (absorption intensity, emission intensity) (47.31):

λ	2983.1	2959.6	2945.5	2936.2	2932.5	2928.6	2927.6
Absorption intensity	6	6	10	8	6	6	8
Emission intensity	0	0	0	4	2	2	4

VI. 3050-2500Å Bands

Possibly four fragmentary systems (4-7), preliminary vibrational analysis, λ (Intensity) (47.31):

(v', v'')	(0, 3)	(1, 3)	(0, 1)	(2, 1)	(0, 0)	(1, 0)	(2, 0)	(8, 0)	(0, 6)
λ	2986.4	2977.0	2958.6	2948.2	2944.0	2935.6	2970.6	2750.0	2735.0
Intensity	6	5	5	6	5	8	5	5	5
System	4	4	4	4	4	4	4	5	6

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^4$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$D^1\Pi_u$	33486.9	111.93	0.573	0.1152	11.0				(60.35)
$C^1\Pi_u$	29384.8	119.53	0.782	0.1185	9.6				(60.35, 32.17)
$B^1\Pi_u$	20319.596	124.065	0.6863	0.125829	8.6754	0.3614	3.41398	(a)	(69.41, 32.17)
$A^1\Sigma_u^+$	14680.4	117.6	0.38	0.1107	5.4		3.64		(29.13)
$b\Pi(0_u^+)$ (b)	<14680.4	~ 145		~ 0.14					(33.21)
$X^1\Sigma_g^+$	0	159.126	0.7262	0.154853	8.5637	0.6552	3.07745	(c)	(69.41, 33.20)

(a) $y_e\omega_e = -5.441 \times 10^{-3}$, $z_e\omega_e = -1.15 \times 10^{-4}$, $\gamma_e = -1.535 \times 10^{-5}$; (b) calculated by deperturbation analysis of $A^1\Sigma_u^+$; (c) $y_e\omega_e = -9.145 \times 10^{-3}$, $z_e\omega_e = -5.02 \times 10^{-5}$, $\gamma_e = -7.646 \times 10^{-6}$

Dissociation energy = 0.75 ± 0.03 eV, 17.3 kcal/mole, 6049 cm^{-1}.

Perturbations and General Information

Gyromagnetic ratio (g_j) = 0.03892 nuclear magnetons (64.36).

$A^1\Sigma_u^+$ state is perturbed by the $b\Pi\left(0_u^+\right)$ state (33.21).

Radiative lifetimes:

$$A^1\Sigma_u^+, \quad \tau_r = 10^{-7} - 10^{-6} \text{ sec (70.44)}$$

$$B^1\Pi_u, \quad \tau_r = 6.41 \text{ nsec (69.43)}$$

Average polarizability (736°K) = 30×10^{-24} cm^3 (74.55).

Transition moment for $B^1\Pi_u \rightarrow X^1\Sigma_g^+$ system (74.56):

$$D = 6.8 + 0.5r \qquad 2.6Å \leq r \leq 5.0Å$$

Potential energy curves – RKR potential (69.40):

	State	v	$E(v)cm^{-1}$	r_{min}(Å)	r_{max}(Å)
$T_e = 0.0$	$X^1\Sigma_g^+$	0	79.4	2.9481	3.2200
		1	237.2	2.8593	3.3320
		2	393.5	2.8014	3.4141
		3	548.3	2.7563	3.4841
		4	701.6	2.7187	3.5475
		5	853.4	2.6864	3.6065
		6	1003.6	2.6581	3.6624
		7	1152.3	2.6327	3.7163
		8	1299.3	2.6099	3.7686
		9	1444.9	2.5893	3.8196
		10	1588.8	2.5705	3.8699
		11	1731.0	2.5533	2.9195
		12	1871.7	2.5375	3.9687
		13	2010.7	2.5231	4.0176
		14	2148.0	2.5100	4.0665
		15	2283.6	2.4979	4.1153

	State	v	$E(v) cm^{-1}$	r_{min}(A)	r_{max}(A)
T_e = 14680.4 cm^{-1}	$A\,^1\Sigma_u^+$	0	58.7	3.4875	3.8037
		1	175.5	3.3839	3.9330
		2	291.6	3.3159	4.0268
		3	406.9	3.2626	4.1060
		4	521.5	3.2179	4.1769
		5	635.3	3.1789	4.2421
		6	748.3	3.1442	4.3032
		7	860.6	3.1128	4.3612
		8	972.1	3.0839	4.4168
		9	1082.9	3.0573	4.4703
		10	1192.9	3.0324	4.5222
		11	1302.1	3.0091	4.5728
		12	1410.6	2.9871	4.6221
		13	1518.3	2.9663	4.6704
		14	1625.3	2.9466	4.7178
		15	1731.5	2.9278	4.7645
T_e = 20319.596	$B\,^1\Pi_u$	0	61.7	3.2663	3.5747
		1	184.2	3.1678	3.7044
		2	305.4	3.1038	3.7998
		3	425.1	3.0539	3.8814
		4	543.4	3.0122	3.9553
		5	660.2	2.9759	4.0242
		6	775.4	2.9435	4.0895
		7	889.0	2.9141	4.1523
		8	1000.9	2.8870	4.2132
		9	1111.1	2.8618	4.2727
		10	1219.5	2.8381	4.3313
		11	1326.0	2.8157	4.3892
		12	1430.6	2.7943	4.4467
		13	1533.2	2.7737	5.5039
		14	1633.9	2.7539	4.5612
		15	1732.4	2.7347	4.6186

Na_2

Franck-Condon factors – RKR potential (69.41):

$B^1\Pi_u - X^1\Sigma_g^+$

v', v''	0	1	2	3	4	5	6	7	8
0	6.55-1	1.61-1	2.13-1	2.00-1	1.51-1	9.77-2	5.61-2	2.94-2	1.44-2
1	1.93-1	1.92-1	5.53-2	2.47-4	4.52-2	1.03-1	1.23-1	1.07-1	7.68-2
2	2.69-1	4.05-2	3.19-2	1.15-1	7.40-2	8.32-3	9.19-3	5.28-2	8.78-2
3	2.35-1	1.67-2	1.30-1	2.68-2	1.69-2	8.17-2	6.84-2	1.56-2	1.46-3
4	1.43-1	1.36-1	4.39-2	3.84-2	9.15-2	1.41-2	1.53-2	6.60-2	5.99-2
5	6.44-2	1.96-1	9.62-3	1.08-1	2.86-3	5.45-2	6.53-2	5.72-3	1.66-2
6	2.22-2	1.49-1	1.16-1	2.24-2	6.54-2	5.29-2	3.20-3	6.06-2	4.46-2
7	5.95-3	7.41-2	1.77-1	2.28-2	8.28-2	6.65-3	7.60-2	1.46-2	1.68-2
8	1.26-3	2.63-2	1.33-1	1.31-1	2.55-3	8.92-3	9.94-3	4.16-2	5.20-2

Franck-Condon factor followed by a factor of ten

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Nd_2

Spectroscopic Constants

Dissociation energy = 0.82 ± 0.30 eV, 19 kcal/mole, 6614 cm^{-1} (72.1).

Nd_2

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Ne_2

Methods of Production and Experimental Technique

Absorption.

Discharge.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$A(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$	Absorption	747-745	V			(72.5)
	II	$B(0_u^+) \leftarrow X^1\Sigma_g^+$	Absorption	737-736	V			(72.5)
	III	$C(1_u) \leftarrow X^1\Sigma_g^+$	Absorption	639-630				(72.5)
	IV	$D(0_u^+) \leftarrow X^1\Sigma_g^+$	Absorption	631-629				(72.5)
	V	$E(0_u^+) \leftarrow X^1\Sigma_g^+$	Absorption	628-626				(72.5)
	VI	$F(0_u^-)? \leftarrow X^1\Sigma_g^+$	Absorption	629-627				(72.5)
	VII	$G(0_u^+) \leftarrow X^1\Sigma_g^+$	Absorption	624-619				(72.5)
	VIII	$H(0_u^+) \leftarrow X^1\Sigma_g^+$	Absorption	624-619				(72.5)
	IX	$I(0_u^+)? \leftarrow X^1\Sigma_g^+$	Absorption	618-615				(72.5)
	X	$J(1_u) \leftarrow X^1\Sigma_g^+$	Absorption	609-603				(72.5)
	XI	$K(0_u^+) \leftarrow X^1\Sigma_g^+$	Absorption	604-602				(72.5)

Ne_2

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	XII	L$(0_u^+,0_u^-) \leftarrow$	Absorption	601-600				(72.5)

Molecule Ne_2

I. $A(0_u^+) \leftarrow X\,^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)	(v-3,0)
λ	745.11	745.34	745.85	746.83
(Intensity)	10	3	4	0

II. $B(0_u^+) \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v,1)	(v-1,0)	(v-1,1)
λ	736.18	736.25	736.49	736.57
(Intensity)	10	8	3	1

III. $C(1_u) \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)	(v-3,0)	(v-4,0)	(v-5,0)
λ	630.98	631.49	632.05	632.71	633.45	634.26
(Intensity)	10	9	8	6	4	2

VI. $D(0_u^+) \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)
λ	629.87	630.06	630.27
(Intensity)	4	6	10

V. $E(0_u^+) \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)	(v-3,0)
λ	626.92	627.03	627.23	627.46
(Intensity)	2	5	6	10

VI. $F(0_u^-)? \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)	(v-2,1)	(v-3,0)
λ	619.26	619.62	620.07	620.13	620.61
(Intensity)	10	7	6	2	5

VII. $G(0_u^+) \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)	(v-3,0)
λ	619.42	619.80	620.28	620.82
(Intensity)	10	7	4	2

VIII. $H(0_u^+) \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)	(v-3,0)
λ	619.42	619.80	620.28	620.82
(Intensity)	10	7	4	2

IX. $I(0_u^+)? \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)	(v-3,0)
λ	616.30	616.53	616.81	617.06
(Intensity)	10	5	8	3

X. $J(1_u) \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v-1,0)	(v-2,0)	(v-3,0)	(v-4,0)
λ	603.57	603.85	604.28	604.74
(Intensity)	10	8	7	7

XI. $K(0_u^+) \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v,0)	(v-1,0)	(v-2,0)	(v-3,0)	(v-4,0)
λ	602.88	602.90	602.97	603.08	603.23
(Intensity)	6	4	5	6	10

Molecule Ne_2

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$X^1\Sigma_g^+$	0	31.3	6.84	0.20	60		2.91		(72.5)

Dissociation energy = 3.74×10^{-3} eV, 10.6 cal/mole, 30.2 cm^{-1} (72.5).

Perturbations and General Information

Radiative lifetimes - calculated (74.15):

$$1_u(^3P_2) \rightarrow X^1\Sigma_g^+ \qquad \tau = 11.9\ \mu sec$$

$$0_u^+(^3P_1) \rightarrow X^1\Sigma_g^+ \qquad \tau = 2.8\ nsec$$

$$0_u^+(^1P_1) \rightarrow X^1\Sigma_g^+ \qquad \tau = 1.2\ nsec$$

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Ni_2

Spectroscopic Constants

Dissociation energy = 2.37 ± 0.22 eV, 54.5 kcal/mole, 19100 cm^{-1} (64.1).

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O_2

Methods of Production and Experimental Technique

Absorption: in high frequency discharges, pulsed discharges, ac discharges, flash photolysis.

Emission: all types of discharges, flames, explosions, luminescence.

In astrophysics.

Ground state studied by microwave spectroscopy.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
Infrared atmospheric	I	$a^1\Delta_g \rightleftarrows X^3\Sigma_g^-$	Absorption, emission	15800-9240	R	7882.39		(72.73, 62.39, 59.32, 58.29, 47.14, 33.6)
Atmospheric	II	$b^1\Sigma_g^+ \rightleftarrows X^3\Sigma_g^-$	Absorption, emission	9970-5380	R	13120.9085		(72.73, 69.57, 64.41, 61.36, 50.18, 49.17)
Noxon	III	$b^1\Sigma_g^+ \rightarrow a^1\Delta_g$	Discharge	19080		5240 (head)	Only a single band	(69.57)
Herzberg II	IV	$c^1\Sigma_u^- \rightleftarrows X^3\Sigma_g^-$	Absorption, lumines-cence	4790-4490 2715-2540	R	32664.1 (calculated)		(68.49, 53.22)
Herzberg III, High pressure	V	$C^3\Delta_u \leftarrow X^3\Sigma_g^-$	Absorption at high pressure	2630-2570 2924-2440	R	34319 (head)		(53.22, 39.11, 34.8, 32.5, 28.1)

Molecule O_2

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
Chamberlain	VI	$C^3\Delta_u \rightarrow a^1\Delta_g$	Luminescence	4380-3700	R			(58.27)
Herzberg I	VII	$A^3\Sigma_u^+ \rightleftharpoons X^3\Sigma_g^-$	Absorption, luminescence	4880-2430	R	35007.15 (calculated)		(60.33, 59.31, 57.26, 55.25)
Schumann-Runge	VIII	$B^3\Sigma_u^- \rightleftharpoons X^3\Sigma_g^-$	All sources	5350-1750 1750-1300	R Continuum	49358.15		(72.73, 68.54, 68.52, 66.45, 64.43, 64.42, 61.35, 59.30, 54.24, 54.23, 50.19)
	IX	$\alpha^1\Sigma_u^+ \leftarrow b^1\Sigma_g^+$		1585-1538	V	63141.5		(68.48)
		$\alpha^1\Sigma_u^+ \leftarrow X^3\Sigma_g^-$		1280-1196	V			(69.58, 68.48)
		$\beta^3\Sigma_u^+ \leftarrow X^3\Sigma_g^-$	Absorption	1294-1181	V			(69.58, 68.48, 52.21)
		$^1\Delta_u \leftarrow a^1\Delta_g$		1243.8 (only a single band)		80396.0		(68.48)

Molecule O_2

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
Rydberg Series	IX (cont)	$^1\Pi_u \leftarrow a^1\Delta_g$		1229.0 (only a single band)		81362.5		(68.48)
		$^3\Sigma_u^+ \leftarrow X^3\Sigma_g^-$		1144.6 (only a single band)	V	87369.1		(69.58)
	X	$X^2\Pi_g(O_2^+) \leftarrow X^3\Sigma_g^-$		1290-1180	V			(61.38, 52.21)
		$b^4\Sigma_g^-(O_2^+) \leftarrow X^3\Sigma_g^-$	Absorption	730-660	R			(68.51, 33.9)
		$B^2\Sigma_g^-(O_2^+) \leftarrow X^3\Sigma_g^-$		650-600	R			(68.51, 68.50, 42.12)
		$c^4\Sigma_u^-(O_2^+) \leftarrow X^3\Sigma_g^-$		595-510				(69.61)
	XI	Many bands that are unclassified or whose identification is doubtful						(68.51, 68.48, 67.47, 61.37, 54.24, 52.21, 48.16, 43.13)

Molecule O_2

I. $a^1\Delta_g \rightleftarrows X^3\Sigma_g^-$ System (Infrared Atmospheric)

Band origins, λ (58.29, 47.14, 33.6):

(v', v'')	(0, 1)	(0, 0)	(1, 0)	(2, 0)
λ	(15800)	1263.0	10674.1	(9240)

II. $b^1\Sigma_g^+ \rightleftarrows X^3\Sigma_g^-$ System (Atmospheric)

Band heads in emission, λ (69.57, 64.41, 61.36, 50.18, 49.17):

v', v''	0	1	2	3	4
0	7593.73	(8623)	(9970)		
1	6867.2	7683.85	8697.8		
2	6276.6	6953	7779.03		
3			7043	7879.17	
4				7141	7987

III. $b^1\Sigma_g^+ \rightarrow a^1\Delta_g$ System (Noxon)

Only a single band, Q branch (69.57):

λ(0, 0)	19080

IV. $c^1\Sigma_u^- \rightleftarrows X^3\Sigma_g^-$ System (Herzberg II)

Band origins (calculated), λ (68.49):

v', v''	0	1	2	3	4	5	6	7	8
0	3060.6	3213.7	3380.3	3562.0	3761.2	3980.3	4222.4	4491.2[a]	4791.5[a]
1	2990.3	3136.3	3294.7	3467.2	3655.6	3862.2	4089.7	4341.5	4621.4
2	2925.5	3065.1	3216.2	3380.4	3559.2	3754.8	3969.5	4206.2	4468.5
3	2865.8	2999.7	3144.3	3301.0	3471.3	3657.1	3860.5	4084.0	4330.8
4	2811.0	2939.6	3078.4	3228.4	3391.1	3568.2	3761.6	3973.5	4206.7
5	2760.6	2884.6	3018.1	3162.1	3318.1	3487.5	3671.9	3873.6	4094.9
6	2714.5[b]	2834.2	2963.0	3101.8	3251.7	3414.2	3590.8	3783.4	3994.2
7	2672.3[b]	2788.3	2912.9	3046.9	3191.4	3347.8	3517.4	3702.0	3903.6
8	2634.0[b]	2746.6	2867.4	2997.1	3136.9	3287.8	3451.3	3628.8	3822.4
9	2599.2[b]	2708.9	2826.2	2952.2	3087.7	3233.9	3391.9	3563.2	3749.6
10	2568.0[b]	2674.9	2789.3	2911.9	3043.7	3185.6	3338.8	3504.7	3684.9

[a] Observed in luminescence, [b] observed in absorption (53.22)

V. $C^3\Delta_u \leftarrow X^3\Sigma_g^-$ System (Herzberg III, High Pressure Bands)

Herzberg III

Two fragments with three heads have been observed (53.24). Vibrational numbering is uncertain.

(v', v'')	$F_2(6, 0)$	$F_3(6, 0)$	(5, 0)
λ	2589.14	2579.39	2620.71

High Pressure Bands (diffuse)

Maxima in absorption (no heads), λ (39.11). Vibrational numbering is uncertain.

(v',v'')	(0,0)	(1,0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)	(6, 0)	(7, 0)	(8, 0)	(9, 0)
λ	2924	2855	2795	2739.8	2689.8	2642.7	2598.8	2555.9	2525.4	2497.4
	2913	2842	2783.9	2729.9	2679.3	2632.7	2590.3	2553.5	2517	2488.7
	2904	2832	2769.1	2720.7	2671.6	2626	2582.4	2537	2510	2482

VI. $C^3\Delta_u \rightarrow a^1\Delta_g$ System (Chamberlain)

27 weak bands have been observed, but the identification is uncertain. Vibrational numbering of the lower state is uncertain.

Possible band heads, λ (53.24):

			$^3\Delta_1$			
v', v''	0	1	2	3	4	5
0						
1			4135			
2						
3			3887	4114		
4					4244	
5			3698		4127	4378
6				3813	4031	

$\underline{^3\Delta_2}$

v', v''	0	1	2	3	4	5
0						
1			4107			
2						
3			3866	4090		
4					4221	
5					4107	
6				3792	4009	4240

$\underline{^3\Delta_3}$

v', v''	0	1	2	3	4	5
0						
1			4086			
2						
3			3844	4071	4317	
4						
5				3861	4086	4326
6				3771	3985	4215

VII. $A^3\Sigma_u^+ \rightleftarrows X^3\Sigma_g^-$ System (Herzberg I)

Band heads in emission, λ (Intensity) (59.31):

v', v''	0	1	2	3	4	5	6	7	8
0							3840 (5)	4064 (5)	4309 (7)
1					(3366.5) (2)	3542 (8)	3734 (8)	3938 (7)	4170 (6)
2					3285 (7)	3453 (8)	3633 (8)	3829 (8)	4044 (2)
3			2931 (1)	3066 (5)	3211 (10)	3370 (10)	3542 (8)	(3726.1) (2)	(3842.2) (2)
4			2873 (2)	3002 (5)	3142 (7)	3292 (4)	3459 (2)	(3634.6) (2)	
5			2820 (3)	2945 (5)	3080	(3225.0) (2)		(3552.5) (4)	(3737.7) (4)
6			2775 (3)	2895 (6)	3026 (2)		(3315.7) (2)	(3479.3) (4)	3657 (2)
7		2622 (3)	2734 (5)	2850 (5)			(3257.1) (4)	(3414.7) (4)	
8		2588 (2)	2696 (4)						

VIII. $B^3\Sigma_u^- \rightleftarrows X^3\Sigma_g^-$ System (Schumann-Runge)

Band origins in absorption, λ (68.54, 66.45, 64.43, 64.42, 59.30, 54.23, 50.19):

v', v''	0	1	2	3	4	5	6	7	8
0	2026.01								
1	1998.17							2522.67	2614.67
2	1971.97	2034.29				2316.82	2396.80	2481.02	2569.95
3	1947.33	2008.11				2282.89	2360.52	2442.25	
4	1924.19	1983.60		2110.91	2179.36	2251.21	2326.53		
5	1902.23	1960.58	2021.28	2084.93	2151.61	2221.53	2295.03		
6	1882.43	1939.25	1998.63	2060.84	2125.94	2194.20			
7	1863.72	1919.37	1977.57	2038.35	2102.05	2168.78			
8	1846.51	1901.14	1958.21	2017.84	2080.22	2145.54			
9	1830.76	1884.47	1940.47	1999.05	2060.27	2124.31			
10	1816.50	1869.37	1924.48	1982.02	2042.23	2105.05			

IX. Partial Systems

$\alpha\,{}^1\Sigma_u^+ \leftarrow b\,{}^1\Sigma_g^+$ System

Band heads, λ (68.48):

(v', v'')	(0, 0)	(1, 1)	(1, 0)
λ	1583.9	1571.9	1537.9

$\alpha\,{}^1\Sigma_u^+ \leftarrow X\,{}^3\Sigma_g^-$ System

Band heads, λ (69.58, 68.48):

(v', v'')	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	1279.5	1250.0	1222.1	1196.4

$\beta\,{}^3\Sigma_u^+ \leftarrow X\,{}^3\Sigma_g^-$ System

Band origins, λ (69.58, 68.48):

(v', v'')	(2, 0)	(3, 0)
λ	1262.18	1233.47

${}^1\Delta_u \leftarrow a\,{}^1\Delta_g$ System

Band head, λ (68.48):

(v', v'')	(0, 0)
λ	1243.8

${}^1\Pi_u \leftarrow a\,{}^1\Delta_g$ System

Band head, λ (68.48):

(v', v'')	(0, 0)
λ	1229.0

O_2

$^3\Sigma_u^+ \leftarrow X^3\Sigma_g^-$ System

Double headed bands with 3 branches. Band head, λ (69.58):

(v', v'')	(0, 0)
λ	1144.6

X. Rydberg Series

$X^2\Pi_g(O_2^+) \leftarrow X^3\Sigma_g^-$ System

Single progression of doublets. Classification is doubtful (61.38, 52.21).

$b^4\Sigma_g^-(O_g^+) \leftarrow X^3\Sigma_g^-$ System

Many progressions with the proposed configuration $\cdots$ np σ_u $^3\Sigma_u$ have been observed (68.38, 62.40, 35.9).

Band head formula: $\nu = 146568 - \frac{R}{(n-1.679)^2}$ $(n = 5 \cdots \infty)$

Another weak, diffuse series has been observed with a proposed configuration of np π_u $^3\Pi_u$ (68.38).

$B^2\Sigma_g^-(O_2^+) \leftarrow X^3\Sigma_g^-$ System

Bands with simple heads (68.51, 68.50, 42.12).

Band head formula: $\nu = 163602 - \frac{R}{(n-0.658)^2}$ $(n = 4 \cdots \infty)$

$c^4\Sigma_u^-(0_2^+) \leftarrow X^3\Sigma_g^-$ System

Several series have been observed (69.61).

Π Series – probably excited to the nd $\pi_g\ ^3\Pi_u$ Rydberg state.

Band head formula: $\nu = 198125 - \frac{R}{(n-1.559)^2}$ $(n = 4 \cdots \infty)$

Σ Series – probably excited to the ns $\sigma_g\ ^3\Sigma_u^-$ Rydberg state.

Band head formula: $\nu = 198125 - \frac{R}{(n-0.955)^2}$ $(n = 4 \cdots \infty)$

Molecule O_2

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^2$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$^1\Pi_u$	89244.9[a]			(1.451)					(68.48)
$^1\Delta_u$	88278.4[a]			(1.446)					(68.48)
$^3\Sigma_u^+$	87369.1[a]			(1.706)	(2800)				(69.58)
$\alpha\,^1\Sigma_u^+$	76089	(1927)	(19)	1.599	1.6				(69.58, 68.48)
$\beta\,^3\Sigma_u^+$	75263	(1957)	(19.7)	(1.7)	(2)				(69.58, 68.48, 52.21)
$B\,^3\Sigma_u^-$	49794.33	709.058	10.6141	0.818975	1.19225		1.60428	(b, g)	(70.63, 66.45, 54.23, 34.7)
$A\,^3\Sigma_u^+$	35398.70	799.08	12.16	0.91053	1.416	4.79	1.52153	(c, h)	(54.24, 52.20)
$C\,^3\Delta_{u,i}$	34735	(750)	(14)				(1.5)		(53.22, 39.11, 32.5)
$c\,^1\Sigma_u^-$	33058.4	794.29	12.736	0.9155	1.391	(10.5)	1.5174	(d, i)	(68.49, 53.22)
$b\,^1\Sigma_g^+$	13195.314	1432.66	13.9336	1.4004796	1.8169303	5.356	1.22684	(e, j)	(n.p. 125, 48.15)
$a\,^1\Delta_g$	7918.11	(1509.3)	(12.9)	1.4263	1.71	(4.97)	1.21563		(47.14)

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^2$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$X^3\Sigma_g^-$	0	1580.19	11.981	1.445622	1.593268		1.20754	(f, k)	(n.p. 125, 66.45, 54.23, 34.7)

(a) T_o; (b) $y_e\omega_e = -0.059212435$, $z_e\omega_e = -0.023974994$; (c) $y_e\omega_e = -0.550$; (d) $y_e\omega_e = -0.2444$, $z_e\omega_e = 0.00055$;

(e) $y_e\omega_e = -0.0143$; (f) $y_e\omega_e = 0.047474736$, $z_e\omega_e = -0.00012727481$; (g) $\gamma_e = -6.30472 \times 10^{-4}$;

(h) $\gamma_e = -9.7 \times 10^{-4}$, $\beta_e = 3.0 \times 10^{-7}$; (i) $\gamma_e = -7.40 \times 10^{-4}$; (j) $\gamma_e = -4.2941920 \times 10^{-5}$, $\beta_e = 0.077$;

(k) $\gamma_e = 6.406456 \times 10^{-5}$

Dissociation energy = 5.12 ± 0.0019 eV, 117.97 kcal/mole, 41260 cm^{-1} (54.23).

Perturbations and General Information

Ionization potential (I_p) to $X^2\Pi_{g,i}\left(O_2^+\right)$ = 12.059 ± 0.001 eV (68.53, 66.44).

$A^3\Sigma_u^+ - X^3\Sigma_g$ has a strong perturbation in the (11,0) band for N > 11 (52.20).

$B^3\Sigma_u^-$ state is perturbed at v = 16, J = 8 and v = 19, J = 8 (54.23).

$B^3\Sigma_u^-$ state is predissociated, probably by a repulsive $^3\Pi_u$ state. The predissociation is characterized by an onset at v = 2 and broadening at v = 4, 8, and 11, with a minimum at v = 9. The interpretation of the predissociation is in question (72.73, 70.62, 69.60, 69.59, 61.36, 59.30, 58.28, 36.10).

Vibrational Raman effect has been observed (60.33, 30.3, 29.2).

Rotational Raman effect has been observed (74.114, 60.33, 30.3).

Potential energy curves – RKR potentials (72.73 and references cited therein):

State	v	V(cm^{-1})	r_{min}(Å)	r_{max}(Å)
$X^3\Sigma_g^-$	0	787.3818	1.1590417	1.2626908
	1	2343.7613	1.1272513	1.3078976
T_e = 0 cm^{-1}	2	3876.57	1.10700	1.34170
	3	5386.03	1.09146	1.37093
	4	6872.34	1.07864	1.39759
	5	8335.65	1.06767	1.42257
	6	9776.11	1.0580	1.4464
	7	11193.80	1.0494	1.4693
	8	12588.82	1.0417	1.4917
	9	13961.18	1.0346	1.5136
	10	15310.91	1.0280	1.5351
$a^1\Delta_g$	0	751.658	1.16619	1.27228
	1	2235.158	1.13396	1.31904
T_e = 7918.11 cm^{-1}	2	3692.86	1.11353	1.35422
	3	5124.76	1.0979	1.3848
$b^1\Sigma_g^+$	0	712.9766	1.176241	1.285186
	1	2117.7290	1.143442	1.333696
T_e = 13195.314 cm^{-1}	2	3494.4855	1.122734	1.370428
	3	4843.1603	1.106952	1.402561

State	v	V(cm^{-1})	r_{min}(Å)	r_{max}(Å)
$A^3\Sigma_u^+$	0	395.8	1.454	1.600
	1	1168.7	1.411	1.668
T_e = 35398.70 cm^{-1}	2	1912.5	1.385	1.722
	3	2623.5	1.366	1.772
	4	3298.9	1.350	1.822
	5	3934.9	1.337	1.872
	6	4527.2	1.326	1.925
	7	5070.0	1.317	1.982
	8	5555.6	1.310	2.050
	9	5973.4	1.304	2.131
	10	6309.1	1.298	2.245
$B^3\Sigma_u^-$	0	351.204	1.53266	1.68771
	1	1038.736	1.48649	1.75876
T_e = 49794.33 cm^{-1}	2	1703.961	1.45776	1.81426
	3	2345.774	1.43623	1.86450
	4	2962.845	1.41889	1.91257
	5	3553.643	1.40434	1.96005
	6	4118.425	1.39181	2.00806
	7	4649.207	1.38084	2.05761
	8	5149.746	1.37117	2.10976
	9	5615.548	1.36264	2.16578
	10	6043.932	1.35518	2.22722
	11	6432.167	1.34876	2.29602

Radiative lifetimes, Einstein coefficients and oscillator strengths:

Transition	Band	τ(sec)	$A_{v'}$ (sec^{-1})	$A_{v'v''}$ (sec^{-1})	Absorption f-Value	Reference
$a^1\Delta_g - X^3\Sigma_g^-$	0 - 0	$3.88(10^3)$		$2.58(10^{-4})$	$4.15(10^{-12})$	(68.55)
$b^1\Sigma_g^+ - X_3\Sigma_g^-$	0 - 0			0.085	$2.47(10^{-10})$	(67.46)
	1 - 0			(0.0069)		(32.4)
	2 - 0			$(0.1636)\ 10^{-3}$		(68.56)
	1 - 1			0.0704		(68.56)
$b^1\Sigma_g^+ - a^1\Delta_g$	0 - 0			$1.5(10^{-3})$		(61.34)
$A^3\Sigma_u^+ - X^3\Sigma_g^-$		$(1 - 10^3)$				(67.46, 64.41, 62.40)
	7 - 0				$1.24(10^{-10})$	(70.64)
$c^1\Sigma_u^- - X^3\Sigma_g^-$			$\sim 10^{-4}$			(62.40)
		$> 10^{-3}$				(64.41)
$C^3\Delta_u - X^3\Sigma_g^-$			$\leq 10^{-5}$			(62.40)
		$> 10^{-3}$				(64.41)

Absolute *f*-values for the $B^3\Sigma_u^- - X^3\Sigma_g^-$ bands (72.73 and references cited therein):

v', v''	0	1	2
0	3.45-10		
1	3.90-9		
2	2.38-8	5.35-7	
3	9.90-8	2.08-6	
4	3.21-7	6.15-6	
5	8.52-7	1.53-5	
6	1.91-6	3.15-5	2.13-4
7	3.81-6	5.78-5	3.39-4
8	6.68-6	9.40-5	5.46-4
9	1.06-5	1.38-4	9.87-4
10	1.57-5	1.91-4	1.03-3
11	2.09-5	2.38-4	1.04-3
12	2.53-5	2.73-4	1.22-3
13	2.88-5	2.93-4	1.04-3
14	3.03-5	2.95-4	
15	2.92-5	2.77-4	
16	2.59-5	2.42-4	
17	2.23-5	2.01-4	
18	1.83-5		
19	1.44-5		

f-value followed by a factor of ten

Franck-Condon factors – RKR potentials (n.p. 125, 72.73):

$\underline{a^1\Delta_g - X^3\Sigma_g^-}$

v', v''	0	1	2	3	4
0	9.869-1	1.297-2	1.260-4		
1	1.303-2	9.586-1	2.791-2	4.296-4	1.735-6
2	6.795-5	2.814-2	9.258-1	4.497-2	9.802-4
3	2.591-4	4.548-2	8.881-1	6.423-2	1.867-3

Franck-Condon factors followed by a factor of ten

O_2

$b^1\Sigma_g^+ - X^3\Sigma_g^-$

v', v''	0	1	2	3	4	5	6
0	9.308-1	6.660-2	2.523-3	5.648-5			
1	6.647-2	7.928-1	1.322-1	8.284-3	2.736-4	6.417-6	
2	2.639-3	1.315-1	6.527-1	1.943-1	1.802-2	8.232-4	2.512-5
3	6.911-5	8.753-3	1.924-1	5.144-1	2.499-1	3.240-2	1.968-3

Franck-Condon factors followed by a factor of ten

$A^3\Sigma_u^+ - X^3\Sigma_g^-$

v', v''	6	7	8	9	10	11	12
0	4.260-2	7.935-2	1.214-1	1.546-1	1.654-1	1.495-1	1.140-1
1	8.985-2	1.052-1	8.298-2	3.500-2	1.510-3	1.512-2	6.765-2
2	8.158-2	4.457-2	4.492-3	1.049-2	5.486-2	7.589-2	4.343-2
3	3.593-2	1.434-3	1.700-2	5.478-2	4.681-2	6.822-3	9.761-3
4	3.900-3	1.162-2	4.595-2	3.559-2	1.700-3	1.847-2	5.157-2

Franck-Condon factors followed by a factor of ten

$B^3\Sigma_u^- - X^3\Sigma_g^-$

v', v''	12	13	14	15	16	17
0	1.192-1	1.443-1	1.514-1	1.378-1	1.087-1	7.417-2
1	6.350-2	2.328-2	3.441-4	1.553-2	6.165-2	1.087-1
2	5.507-5	1.853-2	5.696-2	6.930-2	3.928-2	3.934-3
3	3.150-2	5.446-2	3.492-2	2.823-3	1.221-2	5.283-2
4	4.503-2	1.900-2	1.904-4	2.620-2	4.910-2	2.392-2
5	1.579-2	6.553-4	2.667-2	3.844-2	9.388-3	5.262-3

Franck-Condon factors followed by a factor of ten

$b^1\Sigma_g^+ - a^1\Delta_g$

v', v''	0	1	2	3
0	9.770-1	2.283-2	2.136-4	
1	2.267-2	9.290-1	4.760-2	7.217-4
2	3.628-4	4.694-2	8.768-1	7.430-2
3	4.426-6	1.213-3	7.266-2	8.202-1

Franck-Condon factors followed by a factor of ten

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P_2

Methods of Production and Experimental Technique

Absorption in phosphorus vapor, flash photolysis of PH_3.

Emission from a discharge of He or H_2 with phosphorus, discharge in PH_3 or microwave discharge in PCl_3.

Fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Pi_g \rightarrow X^1\Sigma_g^+$	Emission	3110-2850	R	2970(0, 1)		(73.42, 58.21)
	II	$C^1\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$	Emission Absorption	3500-2000 2300-1800	R R	2953.6(6, 22) 2757.1(4, 17) 2456.9(3, 10) 2108.1(3, 1)		(67.31, 67.30, 66.24, 64.23, 61.22, 50.18, 50.17, 49.16, 46.14, 43.12, 43.11, 40.10, 35.9, 33.8, 32.7, 32.6, 32.5, 32.4, 31.3, 30.2, 07.1)
	III	$E^1\Pi_u \rightleftarrows X^1\Sigma_g^+$	Absorption, emission	1750-1600	R	1705.5(0, 1) 1728.1(0, 2)		(66.24, 55.20, 55.19)
	IV	$G^1\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+$	Absorption, emission	1530-1480	R	1508.7(0, 0)		(66.24, 55.19)
	V	$I^1\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	1480-1460	R	1460.7(0, 0)		(66.24)
	VI	$K^1\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	1400-1320	R	1384.0(0, 0)		(66.24)
	VII	$M^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Absorption	1350-1300	R	1355.1(0, 0)		(66.24)
	VIII	$N^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Absorption	1310-1290	R	1294.5(0, 0)		(66.24)

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	IX	$Q\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$	Absorption	~ 1250	R	1253.5(0, 0)		(66.24)
	X	$S\,^1\Sigma_u^+ \leftarrow X\,^1\Sigma_g^+$	Absorption	~ 1227	R	1227.6		(66.24)
	XI	$b'\,^3\Sigma_u^- \rightarrow X\,^1\Sigma_g^+$	Emission	4400-3500	R	3720.1(0, 2) 3828.8(0, 3)		(74.44, 67.29)
	XII	$B\,^1\Pi_u \rightarrow A\,^1\Pi_g$	Emission	6674-6270		6414.0(0, 0)		(72.42, 71.40)
	XIII	$c(^3\Pi_u) \rightarrow b(^3\Pi_g)$	Emission	10050-7700	V	8622.0(4, 2) 8738.9(4, 2) 8829.2(4, 2)		(68.32, 67.29, 67.27, 64.23)

Molecule P_2

I. $A\,^1\Pi_g \rightarrow X\,^1\Sigma_g^+$ System

Band heads, λ (58.21):

(v', v'')	(0, 3)	(0, 2)	(0, 1)	(0, 0)	(1, 0)
λ	3112.43	3039.29	2969.84	2902.99	2852.23

II. $C\,^1\Sigma_u^+ \rightleftarrows X\,^1\Sigma_g^+$ System

Band heads, λ

v', v''	0	1	2	3	4	5	6	7
0	2136.58				2286.36	2326.5	2367.6	2409.9
1	2115.23	2150.0	2186.4		2261.6	2301.0		
2	2094.38	2128.6		2164.3			2315.97	2356.3
3	2074.66	2108.1			2143.0	2253.24	2291.8	
4	2055.32	2088.3		2157.35		2122.6	2267.86	
5	2036.55	2069.0			2172.2		2245.4	2283.2
6	2018.08	2050.0					2223.0	
7	2000.26					2165.9		
8	1983.52					2145.31	2180.43	2216.1
9	1966.61		2027.52		2092.21		2159.89	2195.01
10	1950.15		2009.80			2073.56		

III. $E\,^1\Pi_u \rightleftarrows X\,^1\Sigma_g^+$ System

Band heads, λ (66.24, 55.19):

v', v''	0	1	2	3	4
0	1683.22	1705.47	1728.14	1751.23	
1	1663.76		1709.6	1732.24	1755.10
2	1644.92				
3	1626.65				
4	1608.89				

IV. $G\,^1\Sigma_u^+ \rightleftarrows X\,^1\Sigma_g^+$ System

Band heads, λ (66.24, 55.19):

v', v''	0	1	2	3	4	5
0	1508.68	1526.50				
1	1493.30	1510.75	1528.45			
2	1478.39	1495.51	1512.85	1530.54		
3		1480.74	1497.77	1515.07		
4				1500.12	1517.33	
5					1502.53	1519.67
6						

V. $I\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v', v'')	(0, 1)	(0, 0)
λ	1477.42	1460.69

VI. $K\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v', v'')	(0, 1)	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	1398.98	1383.98	1370.67	1357.81	1345.17	1333.16

VII. $M\,^1\Sigma_u^+ \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	1355.06	1342.82	1330.92	1319.33	1308.04

VIII. $N\,^1\Sigma_u^+ \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v, v'')	(1, 2)	(0, 1)	(2, 2)	(1, 1)	(0, 0)	(1, 0)	(2, 1)
λ	1309.82	1307.54	1299.96	1296.78	1294.47	1283.88	1287.09

IX. $Q\,^1\Pi_u \leftarrow X\,^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v', v'')	(1, 1)	(0, 0)
λ	1255.94	1253.45

XI. $b'\,^3\Sigma_u^- \rightarrow X\,^1\Sigma_g^+$ System

Band heads, λ (74.44, 67.29):

v', v''	0	1	2	3	4
0		3617.9	3721.5	3830.4	3944.9
1		3541.0	3640.2		
2					3767.2

XII. $B\,^1\Pi_g \rightarrow A\,^1\Pi_u$ System

Band heads, λ (73.42):

(v', v'')	(0, 2)	(1, 2)	(0, 0)	(1, 0)
λ	6674.0	6517.8	6414.0	6269.7

XIII. $c(^3\Pi_u) \rightarrow b(^3\Pi_g)$ System

Band heads, λ (67.29, 67.27, 64.23):

v', v''	λ			v', v''	λ		
0, 0	10047.5	9934.7	9784.9	2, 0	8924.6	8829.2	8716.8
1, 0	9449.2	9345.8	9218.3	3, 1	8875.4	8786.5	8673.6
2, 1	9389.7	9289.5	9159.1	4, 2	8829.2	8738.9	8622.0
3, 2	9325.8	9218.3	9105.0	5, 3	8786.5	8693.3	8585.7
4, 3	9269.6	9159.2	9047.3	6, 4	8738.9	8648.1	8537.4

Molecule P_2

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$S\,^1\Sigma_u^+$	81843.6[a]	-	-	0.2783[d]	-	-	1.978[e]		(66.24)
$Q\,^1\Pi_u$	80169.2[a]	618[b]	-	-	-	-	-		(66.24)
$N\,^1\Sigma_u^+$	77286.8	701.2	(29.70)	0.29845	5.11	3.1	1.910		(66.24)
$M\,^1\Sigma_u^+$	73845.7	678.5	3.0	0.2786	1.6	-	1.977		(66.24)
$K\,^1\Pi_u$	72288.5	713	5.5	0.2704[d]	-	-	2.006[e]		(66.24)
$I\,^1\Pi_u$	68849.4	-	-	0.2541[d]	-	2.5	2.070[e]		(66.24)
$G\,^1\Sigma_u^+$	66313.43	694.12	4.18	0.2973	1.95	2.25	1.913		(66.24, 55.19)
$E\,^1\Pi_u$	59446.28	700.66	2.92	0.2807[d]	-	1.84	1.969[e]		(66.24, 55.19)
$B\,^1\Pi_g$	50223.30	391.3	16.2	0.2300	6.0	3.3	2.176		(73.42)
$C\,^1\Sigma_u^+$	46941.33	473.93	2.340	0.24211	1.75	2.57	2.1204	(c)	(66.24)
$A\,^1\Pi_g$	34515.34	618.78	2.92	0.2752	1.70	2.2	1.9889		(73.42, 58.21)

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$c(^3\Pi_u)$	$10180 + x_1$ $10038 + x_2$ $9915 + x_3$	$640^{(f)}$	4.0						(67.29)
$b'\,^3\Sigma_u^-$	28507.74	604.48	2.2	0.2583	1.4	1.6			(74.44, 73.43, 67.29)
$b(^3\Pi_g)$	x_1, x_2, x_3	562	3.6						(67.29)
$X\,^1\Sigma_g^+$	0	780.89	2.820	0.30356	1.43	1.88	1.8937	(g)	(73.43, 67.31, 66.24)

(a) $T_e + G'(0)$; (b) $\Delta G_{1/2}$; (c) $y_e\omega_e = 0.0066\ cm^{-1}$; (d) B_o; (e) r_o; (f) v uncertain;

(g) $y_e\omega_e = -0.005511\ cm^{-1}$

Dissociation energy = 5.04 ± 0.11 eV, 147.5 kcal/mole, 40651 cm^{-1} (68.34).

Perturbations and General Information

Many of the vibrational levels of the $C\,^1\Sigma_u^+$ state are strongly perturbed (50.18, 50.17, 32.4).

Many of the levels of the $E\,^1\Pi_u$ state are perturbed (66.24).

Predissociation of the $C\,^1\Sigma_u^+$ state, by a $^3\Sigma_u^+$ state, is observed at v = 10, J = 58 and v = 11, J = 34. A second predissociation is observed at v = 19 (66.24).

A region of diffuse absorption at 1425Å probably belongs to the I - X system.

Levels of the $K\,^1\Pi_u$ state are diffuse (maximum at v = 3, 4), probably due to predissociation.

Potential energy curves – RKRV potentials (70.36):

State	v	$U+T_e$(cm^{-1})	r_{min}(Å)	r_{max}(Å)
$E\,^1\Pi_u$	0	59795.9	1.914	2.025
	1	60490.9	1.879	2.073
	2	61179.3	1.854	2.106
	3	61862.2	1.836	2.135
	4	62540.8	1.821	2.160
$G\,^1\Sigma_u^+$	0	66659.4	1.860	1.972
	1	67341.8	1.825	2.020
	2	68016.9	1.800	2.054
	3	68683.4	1.782	2.084
	4	69341.3	1.767	2.111
	5	69990.7	1.754	2.136
	6	70631.2	1.742	2.160
$K\,^1\Pi_u$	0	72643.6	1.966	2.076
	1	73345.3	1.932	2.125
	2	74036.0	1.911	2.161
	3	74728.1	1.895	2.193
	4	75398.1	1.864	2.194
	5	76078.2	1.857	2.232
$M\,^1\Sigma_u^+$	0	74184.2	1.922	2.035
	1	74856.4	1.886	2.083
	2	75523.5	1.862	2.118
	3	76182.5	1.842	2.146
	4	76836.6	1.828	2.173

State	v	$U+T_e(cm^{-1})$	$r_{min}(Å)$	$r_{max}(Å)$
$N\,^1\Sigma_u^+$	0	77286.8	1.858	1.972
	1	78264.0	1.828	2.032
	2	78844.0	1.805	2.079

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Pb_2

Methods of Production and Experimental Technique

Absorption.

Thermal emission.

Laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A \rightleftarrows X$	Absorption, fluorescence	7000-6200	R			(72.9, 67.8)
	II	$B \rightleftarrows X$	Absorption, fluorescence	5270-4200	R			(72.9, 67.8, 35.4)
	III	$C \leftarrow X$	Absorption	3000-2830	R			(n.p. 10, 67.8)
	IV	$D \leftarrow X$	Absorption	2780-2620	R			(n.p. 10, 67.8)
	V	$E \leftarrow X$	Absorption	2600-2460				(n.p. 10)
	VI	$F \leftarrow X$	Absorption	2450-2300	R			(n.p. 10, 67.8)
	VII	$G \leftarrow X$	Absorption	2167-2136				(n.p. 10)

II. B ⇄ X System

Band heads, λ (72.9):

(v', v'')	(3, 2)	(3, 1)	(3, 0)	(4, 1)	(4, 0)	(5, 0)
λ	5058.30	5030.56	5002.95	4991.79	4964.50	4927.56

III. C ← X System

Most intense band heads, λ (n.p. 10):

λ	3003.1	2942.3	2931.3	2920.4	2911.0	2901.0
Intensity	10	4	5	6	7	7

V. E ← X System

Most intense ultraviolet system, with several bands converging (n.p. 10).

VI. F ← X System

Most intense band heads, λ (Intensity) (n.p. 10):

λ	2435.7	2430.4	2417.4	2410.1	2403.4	2397.0	2390.7
Intensity	9	10	7	6	6	5	5

Molecule Pb_2

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
B	19490.3	161.64	1.036					(a)	(72.9)
A	14465.5	162.4	0.4						(72.9)
X	0	119.1	0.35						(72.9)

(a) $y_e\omega_e = 0.0055\ cm^{-1}$

Dissociation energy = 0.8 ± 0.2 eV, 18.5 kcal/mole, 6450 cm^{-1}

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Pd_2

Spectroscopic Constants

Dissociation energy = 1.13 ± 0.21 eV, 26 kcal/mole, 9114 cm^{-1} (69.3).

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Po_2

Methods of Production and Experimenta . Technique

Emission from an electrodeless discharge.

Band Systems

Emission, degrading R, has been observed in the region 5130-3600Å.

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
(0_u^+)	25149.3	108.532	0.4417						
$X(0_g^+)$	0	155.715	0.3353					(a)	

(a) $y_e\omega_e = -0.0003226\ cm^{-1}$

Dissociation energy = 1.89 ± 0.1 eV, 43.5 kcal/mole, 15244 cm^{-1}.

Po_2

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Pr_2

Spectroscopic Constants

Dissociation energy = 1.30 ± 0.30 eV, 30 kcal/mole, 10490 cm^{-1} (72.1).

Pr_2

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Rb_2

Methods of Production and Experimental Technique

Absorption.

Emission from a discharge in Rb vapor, from a discharge in a heat pipe.

Laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	Absorption, discharge	11000-8400	R	Max. ~ 10500		(71.20, 34.8)
	II	$B^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption, discharge	7350-6400	R	6824. 2(1, 1) 6797. 8(1, 0)		(71.20, 36.10)
	III	$C^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption, laser-induced fluorescence	5030-4690	R	4746. 5(10,2)		(71.20, 37.11)
	IV	$D \leftarrow X^1\Sigma_g^+$	Absorption	4550-4220	R	4326. 8(10,1) 4288. 2(14,0)		(37.11)
	V	$? \rightarrow X^1\Sigma_g^+$	Laser-induced fluorescence	6100-5400			Quasi-continuum	(71.20)
	VI	Bands associated with resonance lines (Van der Waals molecules)						(35.7, 32.6)

Molecule Rb_2

I. $A\,^1\Sigma_u^+ \rightleftarrows X\,^1\Sigma_g^+$ System

Bands are fragmentary, not analyzed (71.20, 34.8):

λ	10500	9033	8989	8941	8897	8852	8807	8762

II. $B\,^1\Pi_u \rightleftarrows X\,^1\Sigma_g^+$ System

Band heads of $^{85}Rb_2$ of greatest intensity, λ (Intensity) (36.10):

(v', v'')	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(6, 1)	(5, 0)
λ	6797.8	6775.7	6754.5	6734.0	6718.1	6713.2
(Intensity)	10	10	10	10	5	6

III. $C\,^1\Pi_u \rightleftarrows X\,^1\Sigma_g^+$ System

Band heads of greatest intensity, λ (Intensity) (71.20, 37.11):

(v', v'')	(2, 1)	(3, 0)	(4, 0)	(6, 1)	(9, 2)	(8, 1)	(10, 2)
λ	4797.1	4775.8	4767.7	4764.6	4754.1	4749.0	4746.5
(Intensity)	9	8	8	8	8	9	10

IV. $D \leftarrow X\,^1\Sigma_g^+$ System

Band heads of greatest intensity, λ (Intensity) (37.11):

(v', v'')	(7, 2)	(8, 2)	(8, 1)	(9, 1)	(10, 1)	(11, 1)	(11, 0)
λ	4359.3	4351.9	4341.1	4333.8	4326.8	4319.7	4309.2
(Intensity)	8	8	9	9	10	9	9

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
D	22777.5	40.42	0.745					(e)	(37.11)
$C^1\Pi_u$	20835.1	36.46	0.124						(37.11)
$B^1\Pi_u$	14662.1	48.05 [a]	0.191 [c]						(36.10)
$A^1\Sigma_u^+$	~11500	-	-						(34.8)
$X^1\Sigma_g^+$	0	57.31 [b]	0.105 [d]	~0.02					(71.20, 37.11, 36.10)

(a) $\omega_e \cdot 47.78$ for $^{85}Rb^{87}Rb$, (b) $\omega_e = 56.98$ for $^{85}Rb^{87}Rb$, (c) $x_e\omega_e = 9.188$ for $^{85}Rb^{87}Rb$,

(d) $x_e\omega_e = 0.103$ for $^{85}Rb^{87}Rb$, (e) $y_e\omega_e = -0.00144$

Dissociation energy = 0.47 ± 0.05 eV, 10.8 kcal/mole, 3790 cm^{-1}.

Perturbations and General Information

Radiation in the region 6100-5400Å due to transfer from the C state into an unidentified state followed by transitions to high-lying and continuum levels of the ground state (71.20).

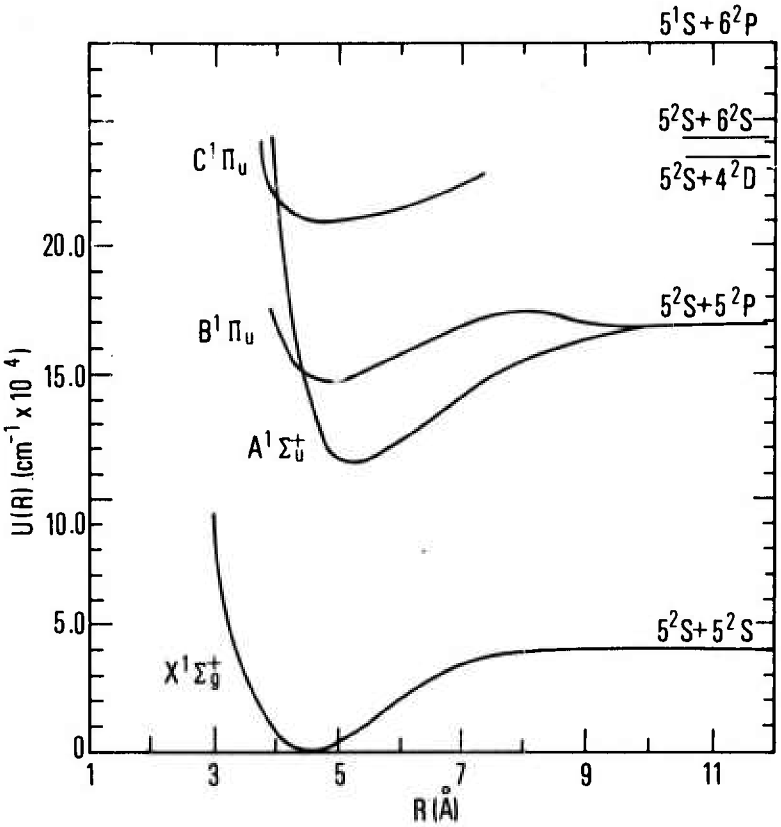
Predissociation of the C state caused by crossing of A state (71.20).

Radiative lifetimes (70.17):

$$B^1\Pi_u \quad - \quad \tau_r \sim 16 \text{ nsec}$$

$$C^1\Pi_u \quad - \quad \tau_r \sim 61 \text{ nsec}$$

Potential energy curves – empirical (71.20)



Average electric dipole polarizability (534°K) 68 ± 7 × 10^{-24} cm^3 (74.25).

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S_2

Methods of Production and Experimental Technique

Absorption: at elevated temperatures, in matrices, after flash photolysis.

Emission: high frequency discharge, microwave discharge, flames.

Fluorescence: excited by OH*, laser-induced.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$	Photolysis	11055-10920			Observation doubtful	(72.110)
	II	$B^3\Sigma_u^- \rightleftharpoons X^3\Sigma_g^-$	Absorption, discharge, fluorescence	7110-2400	R	31689	(a)	(72.104, 68.90, 63.73, 62.69, 60.67, 53.61, 48.54)
	III	$C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$	Absorption	1870-1650	V	55633.3		(65.83, 48.56, 48.55, 34.26)
	IV	$C'^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$	Microwave	1860-1760	V	56983.6	(b)	(62.71)
	V	$D^3\Pi_u \leftarrow X^3\Sigma_g^-$	Absorption	1750-1650	V	58750	(b)	(65.83, 48.55, 34.26)
	VI	$B'^3\Pi_{g,i} \rightarrow A^3\Sigma_u^+$	Discharge, microwaves	8083-7434	V	13447.7	(c)	(66.86, 64.76, 62.69, 35.28)
	VII	$B'^3\Pi_{g,i} \rightarrow A'^3\Delta_{u,i}$	Discharge, microwaves	7761-6984	V	$^3\Pi_1 - {}^3\Delta_2$ -14144.7 $^3\Pi_2 - {}^3\Delta_3$ -14318.0	(c)	(64.76, 62.69, 35.28)
	VIII	$f^1\Delta_u \rightleftharpoons a^1\Delta_g$	Absorption, discharge	3350-2400	R	36743		(70.103, 69.100, 64.78, 64.77, 64.76, 63.75)

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	IX	$g\,^1\Delta_u \rightarrow a\,^1\Delta_g$	Discharge, microwaves	2130-1880	V	52244.7		(68.93, 62.71)
	X	$h\,^1\Sigma_u^+ \rightarrow b\,^1\Sigma_g^+$	Discharge, microwaves	2130-1760	V	51401.3	(b)	(68.93, 67.89, 65.83, 62.71)
	XI	$i \rightarrow b\,^1\Sigma_g^+$	Discharge, microwaves	2130-1760	V	55448.3	(b)	(68.93, 65.83, 62.71)
	XII	$e\,^1\Pi_g \rightarrow c\,^1\Sigma_u$	Discharge	7430-7152	V	13452		(62.69)
	XIII	?	Microwaves	1850-1780	V	56077.7	(b)	(67.89)

(a) Numerous perturbations and predissociations. Several bands possess secondary heads.

(b) Analysis is uncertain.

(c) Predissociates.

Molecule S_2

I. $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$ System

Observed in laser emission only (75.L117. 72.110).

λ	11055	10975	10920

II. $B^3\Sigma_u^- \rightleftarrows X^3\Sigma_g^-$ System

Band heads of $^{32}S_2$, λ (Intensity) (36.30, 31.22, 31.21):

v', v''	0	1	2	3	4	5	6
0				3387.0(1)	3469.6(2)	3555.8(3)	3645.2(5)[a]
1			3259.9(2)	3336.7(2)	3417.0(4)	3500.5(5)	3587.4(5)
2		3143.7(1)	3216.1(2)	3290.7(3)	3369.6(4)	3451.0(2)	
3	3033.1(1)	3101.5(1)	3171.5(2)	3244.7(3)	3321.2(1)		
4	2997.0(1)	3063.6(3)	3132.4(3)	3203.2(2)			
5	2960.1(2)	3024.3(4)	3091.7(5)	3161.1(1)			
6	2926.6(2)	2989.7(4)[a]	3054.9(3)				

[a] Bands possessing weak secondary heads

Isotope studies of $^{34}S_2$ (70.105).

III. $C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ System

Each band possesses from 3 to 6 heads, with a maximum separation between extremes of 1 - 8Å. Isotope effect has been noted for several bands.

Most intense band heads, λ (Intensity) (65.83, 48.55):

v', v''	0	1	2	3	4	5
0	1796.93(9)	1820.46(4)	1844.43(3)	1868.82(1)	1894.50(1)	1919.81(1)
1	1770.75(9)		1816.88(1)	1840.51(1)	1864.65(1)	1889.93(1)
2	1745.57(8)	1768.99(2)				
3	1721.29(5)	1742.89(3)				
4	1697.97(4)	1718.90(2)				
5	1675.39(1)	1695.78(2)	1716.56(1)			
6	1653.60(1)	1673.52(1)	1693.72(1)			

IV. $C'^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$ System

Double-headed bands with separation of ~ 14 cm^{-1} are observed. Most intense band heads, λ (Intensity) (62.71):

(v', v'')	(0, 4)	(0, 3)	(0, 2)	(0, 1)	(0, 0)
λ	1859.49	1835.57	1811.94	1788.84	1766.11
(Intensity)	1	2	2	5	4

V. $D^3\Pi_u \leftarrow X^3\Sigma_g^-$ System

Each band has 9 heads. Most intense band heads of the a_3, b_3, and c_3 series, λ (Intensity) (65.83, 48.55):

v', v''		0	1	2	3	4
0	a_3	1709.95(10)	1729.18(1)	1750.93(1)		
	b_3	1702.37(8)	1723.44(1)			
	c_3	1694.60(10)	1715.83(1)	1737.02(0)		
1	a_3	1685.32(4)	1705.99(3)	1726.99(0)		
	b_3	1679.88(4)	1700.49(3)			
	c_3	1672.34(6)	1692.75(4)	1714.44(0)		
2	a_3	1663.49(2)	1683.63(2)	1704.08(1)	1724.91(0)	
	b_3	1658.23(2)	1678.25(2)	1698.63(0)		
	c_3	1650.85(2)	1670.87(6)		1711.34(0)	
3	a_3		1662.08(1)	1681.99(1)		
	b_3		1656.85(0)	1676.65(1)		1717.19(0)
	c_3		1649.49(1)	1669.16(1)		1709.36(0)

VI. $B'^3\Pi_{g,i} \rightarrow A^3\Sigma_u^+$ System

Two subsystems – because the $^3\Pi_0$ state is completely predissociated. Only 5 of the 9 possible heads are observed (65.83). Isotope shifts (66.86).

Most intense band heads, λ (66.86, 64.76):

$B'^3\Pi_2 \rightarrow A^3\Sigma_u^+$; (v', v'') λ | (0, 1) 7785.6 | (0, 0) 7506.8

$B'^3\Pi_1 \rightarrow A^3\Sigma_u^+$; (v', v'') λ | (0, 1) 7707.4 |

VII. $B'^3\Pi_{g,i} \rightarrow A^3\Delta_{u,i}$ System

Two subsystems – because the $^3\Pi_0$ state is completely predissociated.

λ (64.76, 62.69):

$B'^3\Pi_2 \rightarrow A'^3\Delta_{u,i}$; (v', v'') λ | | (0, 2) 7583 | (0, 1) 7328 | (0, 0) 7068

$B'^3\Pi_1 \rightarrow A'^3\Delta_{u,i}$; (v', v'') λ | (0, 3) 7759 | (0, 2) 7485 | (0, 1) 7228 | (0, 0) 6984

VIII. $f^1\Delta_u \rightleftarrows a^1\Delta_g$ System

Single-headed bands. Isotope studies (65.82, 65.80).

Most intense band heads, λ (70.103, 64.77)

v', v''	0	1	2	3	4	5	6
0					2940.49	2999.74	3060.77
1				2847.52	2903.53		
2			2760.14	2813.24			
3		2677.92	2728.33				
4		2648.34	2697.64				
5		2619.78	2668.02				
6	2546.28	2592.52					
7	2520.56	2565.59					
8	2495.77						
9	2471.77						
10	2448.98						

IX. $g^1\Delta_u \rightarrow a^1\Delta_g$ System

Single-headed bands. Most intense band heads, λ (Intensity) (68.90, 62.71):

v', v''	0	1	2	3	4	5	6	7
0	1914.06 (9)	1939.89 (9)	1966.08 (9)	1992.63 (7)	2019.68 (6)	2047.24 (4)	2075.24 (3)	2103.73 (2)
1	1884.80 (6)		1934.96 (0)	1960.85 (3)	1987.12 (3)	2013.79 (4)	2040.90 (3)	2068.49 (2)
2			1905.09 (2)			1981.57 (2)	2007.91 (2)	2034.59 (1)
3							1976.15 (0)	2002.01 (1)

X. $h^1\Sigma_u^+ \rightarrow b^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (68.90, 67.89, 65.83):

v', v''	0	1	2	3	4	5	6	7
0	1943.25 (4)	1969.75 (5)	1996.80 (5)	2024.18 (5)	2052.04 (3)	2080.47 (2)		
1				1991.44 (9)	2018.27 (4)	2045.87 (4)	2073.77 (3)	
2			1934.20 (5)		1985.95 (1)	2012.44 (3)	2039.66 (3)	2067.19 (2)
3			1905.09 (2)	1929.42 (1)			2006.75 (1)	2033.33 (1)

XI. $i \rightarrow b^1\Sigma_g^+$ System

Only a single head is observed. Most intense band heads, λ (Intensity) (68.93, 65.83, 62.71):

(v', v'')	(0, 7)	(1, 8)	(0, 6)	(1, 7)	(0, 5)
λ	1984.52	1979.18	1959.15	1954.07	1934.20
(Intensity)	3	2	0	2	5

(v', v'')	(1, 6)	(0, 4)	(1, 5)	(0, 2)	(1, 1)
λ	1929.44	1909.57	1905.09	1861.73	1811.94
(Intensity)	1	1	2	0	2

Molecule S_2

SPECTROSCOPIC CONSTANTS

State	T_o (Observed)	T_o (Calculated)	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^8$	r_e	Remarks	Bibliography
$i ?\ ^1\Sigma_u^+,\ ^1\Delta_u$	{55448 + b {55448 + a	~64000 ? ~59900 ?	- -	- -	>0.29 -	- -	- -	<1.9 - }		(68.93, 65.83, 62.71)
$h^1\Sigma_u^+$	51401.3+b	~59900 ?	819.6	2.70	>0.29	-	~14.52	<1.89		(65.83, 62.71)
$D^3\Pi_u$	58750	58750	793.9	4.0	0.3066	-	~16.293	(1.854)	(a)	(69.100, 65.83, 48.55)
$C' ?\ ^3\Sigma_u^-$	56983.6	56984	-	-	>0.295	-	-	<1.89		(65.83)
$g^1\Delta_u$	52244.7+a	~56700	816.4	2.7	0.3217	1.44	20.0	1.811		(68.83)
$C^3\Sigma_u^-$	55633.3	55633.3	829.15	3.34	0.32196	1.4	22.0	1.810	(b)	(69.99, 65.83, 48.55)
$f^1\Delta_u$	36743.5+a	~41200	438.32	2.70	0.22704	1.78	24.5	2.155	(d)	(70.103, 68.93, 65.83)
$e^1\Pi_g$	13451.8+a	~37000	533.7 (c)	-	~0.25	-	-	~2.08		(65.83)
$B'^3\Pi_{g,i}$	14144.7+A'	~36000	-	-	0.244	-	-	2.08	(e)	(65.83, 62.69)
$B^3\Sigma_u^-$	31689	31689	434	2.75	0.2244	1.8	23.1	2.168		(63.73)
$B''^3\Pi_u$	≤31700	≤31700	-	-	>0.2029	-	-	<2.280		(65.83, 63.73)
$A^3\Sigma_u^+$	697 + A'	~22550	477 (c)	-	-	-	-	-		(65.83, 62.69)
$c^1\Sigma_u^-$	c	~23550	533.6 (c)	-	~0.235	-	-	2.122		(62.69)
$A'^3\Delta_{u,i}$	A'	~21855	488.6	2.63	0.2284	1.40	19.96	2.148	(f)	(62.69)

Molecule S_2

SPECTROSCOPIC CONSTANTS

State	T_o (Observed)	T_o (Calculated)	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^8$	r_e	Remarks	Bibliography
$b^1\Sigma_g^+$	b	~ 8500	700.8?	3.4?	-	-	-	-		(65.83)
$a^1\Delta_g$	a	~ 4500	702.35	3.09	0.29262	1.73	20.4	1.8987		(70.103, 68.93)
$X^3\Sigma_g^-$ $^{32}S_2$	0	0	725.668	2.844	0.29541	1.58	21.48	1.889	(g)	(n.p. 115)
$X^3\Sigma_g^-$ $^{34}S_2$	0	0	704.026	2.677	0.27813	1.45	19.59	1.889	(h)	(n.p. 115)

(a) $^3\Pi_2 - {}^3\Pi_1 \approx 462$ cm^{-1}; (b) $\lambda_o = -11.61$ cm^{-1}, $\gamma_o = 0.033$ cm^{-1}; (c) $\Delta G_{1/2}$; (d) $\gamma_e\omega_e = -0.005$ cm^{-1};

(e) $^3\Pi_1 - {}^3\Pi_2 \approx 130$ cm^{-1}; (f) $^3\Delta_2 - {}^3\Delta_1 \approx 303.5$ cm^{-1}; (g) $\lambda_e = 11.82$ cm^{-1}, $\gamma_e = -0.0066$ cm^{-1}; (h) $\lambda_e = 11.73$ cm^{-1},

$\gamma_e = -0.0062$ cm^{-1}

Dissociation energy = 4.4 ± 0.1 eV, 10 . 5 kcal/mole, 35300 cm^{-1} (71.107).

Perturbations and General Information

Perturbations by a $B''{}^3\Pi_u$ state are observed for all vibrational levels. There are three perturbations within each branch.

In emission, the predissociation of the $v'' = 0$ series stops with the (9, 0) band at 2828Å (31.21).

Higher rotational levels of $v' = 17$ of the B - X system and all rotational levels of $v' \geq 18$ are extremely diffuse.

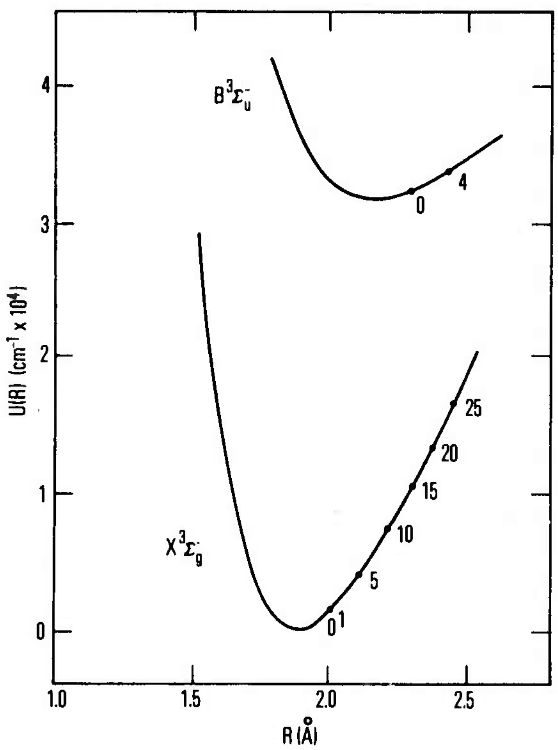
The $B'{}^3\Pi_g$ and $e{}^1\Pi_g$ states are predissociated at $v' = 0$ ($B'{}^3\Pi_2$ for $J \geq 34$ and $B'{}^3\Pi_2$ for $J \geq 16$) (65.80).

$f{}^1\Delta_u - a'\Delta_g$ systems predissociates for $v' \geq 10$ (65.80).

Radiative lifetimes (73.111):

	v'	τ(nsec)
$B^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$	3	20.7
	4	18.3

Potential energy curves - RKR potential (73. 112)



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Sb_2

Methods of Production and Experimental Technique

Absorption at elevated temperatures (800-1600° C).

Thermal emission and microwave discharge.

Fluorescence excited by Hg.

BAND SYSTEMS

System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
I	$A \rightleftarrows X^1\Sigma_g^+$	Absorption	7500-6000	R			(49.6)
II	$B \rightleftarrows X^1\Sigma_g^+$	Absorption	6000-4500	R			(72.9, 49.6)
III	$D \rightleftarrows X^1\Sigma_g^+$	Absorption	3400-2830	R	3049.2(6, 2)		(67.8, 35.4)
IV	$F \leftarrow X^1\Sigma_g^+$	Absorption	2340-2150	R	2222.8(2, 1)		(35.4)
V	?	Microwaves	8400-7200	V	8315.5, 7788.1		(67.8)
VI	?	Microwaves	4200-3600	R			(67.8)
VII	?	Microwaves	3000-2900	R		Triplet structure	(67.8)
VIII	?	Absorption	< 2170	R	2138.6		(35.4)

II. $B \rightleftarrows X^1\Sigma_g^+$ System

Band heads of $^{121}Sb_2$, λ (72.9):

(v', v'')	(5, 0)	(4, 0)	(4, 1)	(3, 0)	(3, 1)
λ	5644.6	5562.0	5496.1	5481.4	5417.5

III. $D \rightleftarrows X^1\Sigma_g^+$ System

Most intense bands, λ (Intensity):

(v', v'')	(3, 3)	(4, 3)	(7, 4)	(5, 2)	(8, 4)	(6, 2)
λ	3134.7	3114.5	3079.0	3068.9	3059.2	3049.2
(Intensity)	4	4	4	4	4	6

IV. $F \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (35.4):

(v', v'')	(0, 2)	(2, 3)	(0, 1)	(1, 1)	(2, 1)	(2, 0)
λ	2258.5	2249.7	2244.9	2233.4	2222.8	2209.4
(Intensity)	4	2	5	3	7	5

VIII. Band Groups at 2170A

Most intense bands, λ (Intensity) (35.4):

λ	2138.6	2126.8	2115.0	2104.3
(Intensity)	3	2	2	2

Molecule Sb_2

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^9$	r_e	Remarks	Bibliography
F	44780	226.0	1.17						(35.4)
D	31605	212	0.2						(35.4)
B	19068.9	218.08	0.537	0.044481[a]		9.1[b]			(72.9, 37.5)
A	14991.5	217.0	0.45						(37.5)
$X^1\Sigma_g^+$	0	269.98	0.588	0.050039[a]		9.4[b]			(72.9, 37.5)

[a] B_2, [b] D_2

Dissociation energy = 2.37 ± 0.10 eV, 54.7 kcal/mole, 19120 cm^{-1} (73.10).

Perturbations and General Information

D state is vibrationally perturbed (35.4).

D - X system displays predissociation with a peak at 2842Å. Shorter wavelengths are very diffuse.

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Sc_2

Spectroscopic Constants

Dissociation energy = 1.12 ± 0.2 eV, 25.9 kcal/mole, 9275 cm^{-1}.

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Se_2

Methods of Production and Experimental Technique

Absorption at elevated temperatures.

Emission from a microwave discharge in Se vapor.

Laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$B^3\Sigma_u^- \rightleftarrows X^3\Sigma_g^-$ $\begin{pmatrix} 0_u^+ - 0_g^+ \\ 1_u - 1_g \end{pmatrix}$	Absorption, fluorescence	6700-3250	R			(72.21, 71.19, 66.11)
	II	$C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ $\begin{pmatrix} 0_u^+ - 0_g^+ \\ 1_u - 1_g \\ 1_u - 0_g^+ \end{pmatrix}$	Absorption	1960-1868	V			(70.17)
	III	?	Absorption	1856-1843				(72.20)
	IV	$? \leftarrow X^3\Sigma_g^-$ $(1_u - 1_g)$	Absorption	1845-1820				(70.17)
	V	$? \leftarrow X^3\Sigma_g^-$ $(0_u^+ - 0_g^+)$	Absorption	1826-1812				(70.17)

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	VI	$n \rightarrow a^1\Delta_g$ $(1_u \rightarrow 2_g)$	oures-nce					(72.20)

Molecule Se_2

I. $B^3\Sigma_u^- \rightleftarrows X^3\Sigma_g^- \left(0_u^+ - 0_g^+,\ 1_u - 1_g\right)$ Systems

Origins of bands with greatest intensity, λ (66.11):

(v', v'')	(12, 0)	(13, 0)	(14, 0)	(15, 0)	(16, 0)	(17, 0)	(18, 0)
$\lambda(^{80}Se_2)$	3483.4	3457.5	3432.1	3407.3	3383.3	3360.0	3337.3
$\lambda(^{78}Se_2)$	3479.8	3453.4	3427.8	3402.9	3378.6	3355.1	3332.4

II. $C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ Systems

a. $C(0_u^+) \leftarrow X(0_g^+)$

Strong, diffuse bands with no rotational structure, λ (70.17):

(v', v'')	(0, 2)	(0, 1)	(0, 0)	(1, 0)
λ	1902.04	1888.43	1874.80	1860.36

b. $C(1_u) \leftarrow X(1_g)$

Strong bands with sharp rotational structure, λ (70.17):

v', v''	0	1	2	3
0	1896.49	1910.43	1924.50	1938.7
1	1881.29			1922.87
2	1866.45	1879.96	1893.6	
3	1851.97	1865.25		

c. $C(1_u) \leftarrow X(0_g^+)$

Weak bands with sharp structure, λ (70.17):

(v', v'')	(0, 1)	(0, 0)	(1, 0)
λ	1897.18	1883.38	1868.38

III. <u>? System</u>

Overlaps a continuum centered at ~ 1845A. Weak bands with sharp structure, λ (70.17):

(v', v'')	(0, 1)	(1, 2)	(0, 0)
λ	1856.53	1855.88	1843.35

IV. <u>$? \leftarrow X^3\Sigma_g^- \ (1_u \leftarrow 1_g)$ System</u>

Strong bands, λ (70.17):

(v', v'')	(0, 2)	(1, 3)	(0, 1)	(1, 2)	(0, 0)
λ	1846.23	1844.61	1833.26	1831.69	1820.41

V. <u>$? \leftarrow X^3\Sigma_g^- \left(0_u^+ \leftarrow 0_g^+\right)$ System</u>

Band heads, λ (70.17):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(3, 3)	(1, 0)	(1, 2)
λ	1826.09	1825.47	1824.85	1824.38	1812.81	1812.28

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^4$	$D_e \times 10^8$	r_e	Remarks	Bibliography
1_u	55276.81	430							(70.17)
0_u^+	54752.48	403.9	1.3	0.0924[a]	3.3		2.133[b]		(70.17)
?	54239.41	404							(70.17)
$C(0_u^+)$	53339[c]								(70.17)
$C(1_u)$	52709.61	428.0	1.22	0.09647[a]	3.33		2.0893		(70.17)
$q(1_u)$[d]	26991	155	2	0.055[e]					(72.20)
$n(1_u)$	~25985.2	183	~0.75						(72.20)
$B(0_u^+)$	25980.36	246.291	1.016	0.07048	3.45	4[f]	2.4464		(66.11)
$B(1_u)$	25912.45	246.42	1.225	0.07086	5.53	2[f]	2.4398		(66.11)
$m(1_u)$	~24000	>154[g]	0.99						(72.20)
$a(2_g)$	~4000	319	0.81						(72.20)
$X(1_g)$	366.7	387.156	0.964	0.09016	2.98	2	2.1630		(71.19, 66.11)

Molecule Se_2

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^4$	$D_e \times 10^8$	r_e	Remarks	Bibliography
$X(0_g^+)$	0	385.302	0.96363	0.08992	2.88	2.4	2.1659		(71.19, 66.11)

(a) B_o, (b) r_o, (c) T_o, (d) analyzed through perturbation of the B state, (e) B_2, (f) D_o, (g) $\Delta G_{1/2}$

Dissociation energy = 3.164 ± 0.002 eV, 72.9 kcal/mole, 25518 cm^{-1} (72.20).

Perturbations and General Information

$B(0_u^+)$ state is perturbed for all vibrational levels, $v \leq 15$ by m, n, and q states. Perturbations for levels of low v are weak (72.20, 63.9).

Both $B(0_u^+)$ and $B(1_u)$ states predissociate (63.9).

Ionization potential (I_p) = 8.88 ± 0.03 eV (69.15).

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Si_2

Methods of Production and Experimental Technique

Absorption by flash-photolysis in $C_6H_5SiH_3$ or $BrSiH_3$.

Emission from discharge in SiH_4 and Xe.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$H^3\Sigma_u^- - X^3\Sigma_g^-$	Flash-photolysis	4526-3863	R	3979.6(4,1)		(71.6, 63.3, 55.2)
	II	$L^3\Pi_g - D^3\Pi_u$	Discharge and flash-photolysis	3695-3489	R	3568.7(0,1) 3496.0(1,1)		(71.6, 55.2)
	III	$K^3\Sigma_u^- - X^3\Sigma_g^-$	Flash-photolysis	3275-3067	R	3202.0(1,0)		(71.6, 63.3)
	IV	$D^3\Pi_u - X^3\Sigma_g^-$	Flash-photolysis	2900-2700		2882.84 2795.80		(70.5)
	V	$N^3\Sigma_u^- - X^3\Sigma_g^-$	Flash-photolysis	2166-2097	R	2138.35(0,0)		(70.4, 63.3)
	VI	$O^3\Sigma_u^- - X^3\Sigma_g^-$	Flash discharge	2200-1800		1874.28(0,0) 1892.21(0,1)		(70.4)
	VII	$P^3\Pi_g - D^3\Pi_u$	Flash discharge	1870-1900	R	1879.9(0,0) 1898.4(0,1)		(70.4)

Molecule Si_2

I. $H^3\Sigma_u^- - X^3\Sigma_g^-$ System

Band heads, λ (63.3, 55.2):

v', v''	0	1	2	3	4	5	6
0					4427.6	4526.0	
1				4283.1	4375.8	4471.9	
2					4326.0		
3	3942.1						
4	3900.8	3979.6	4060.9				4414.4
5	3863.4						

II. $L^3\Pi_g - D^3\Pi_u$ System

Band heads, λ (71.6, 55.2):

v', v''	0	1	2	3	4
0		3568.7	3634.4	3710.4	3772.3
1		3496.0	3563.1	3632.2	

III. $K^3\Sigma_u^- - X^3\Sigma_g^-$ System

Band heads, λ (63.3):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	3248.9	3202.0	3157.8	3115.8	3076.1

IV. $D^3\Pi_u - X^3\Sigma_g^-$ System

Several lines have been observed in absorption but have not been identified (70.5):

λ	2882.8	2838.8	2795.8	2758.8

V. $N^3\Sigma_u^- - X^3\Sigma_g^-$ System

Band heads, λ (70.4):

v', v''	0	1
0	2138.35	2161.78
1	2117.92	
2	2098.53	
3	2079.75	2101.92
4		2083.53

VI. $O^3\Sigma_g^- - X^3\Sigma_g^-$ System

Band heads, λ (70.4):

v', v''	0	1	2
0	1874.28	1892.21	
1	1860.53		189.32
2	1847.22	1864.63	

VII. $P^3\Pi_g - D^3\Pi_u$ System

Two red shaded bands have been observed overlapping the O - X system. They are tentatively assigned as follows:

1879.0(0, 0)
1898.4(0, 1)

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$P^3\Pi_g$	88219								(70.4)
$L^3\Pi_g$	63059.1			0.2370			2.255		(70.4, 55.2)
$O^3\Sigma_u^-$	53341.94	404.2	3.0	0.2225	3		2.327		
$N^3\Sigma_u^-$	46762.21	458.6	4.8	0.2193	2.5		2.344		(70.4, 63.3)
$D^3\Pi_u$	~35000	547.94	2.43	0.2596	1.55		2.155		(70.4, 55.2)
$K^3\Sigma_u^-$	30768.77	462.6	5.95	0.2185	3.16		2.349		(70.4, 63.4)
$H^3\Sigma_u^-$	24311.15 [(a)]	275.30	1.99	0.1712			2.6536		(71.6, 70.4) 63.3, 55.2)
$X^3\Sigma_g^-$	0	510.98	2.02	0.2390	1.3		2.246		(70.4, 63.3)

(a) T_o

Dissociation energy = 3.35 ± 0.2 eV, 75 kcal/mole, 26168 cm^{-1}.

Perturbations and General Information

The bands of the K - X and H - X systems exhibit the presence of perturbations. In the H - X system, the (4, 0) band is sharp, but the (5, 0) band is diffuse and does not appear in emission. All the bands of the K - X system are diffuse.

All the levels above v' = 0, J' = 51 of the L state are predissociated.

The position of the (2, 0) band in the N - X system is displaced somewhat to the red, indicating a perturbation (70. 4).

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Sm_2

Spectroscopic Constants

Dissociation energy = 0.52 ± 0.22 eV, 12 kcal/mole, 4200 cm^{-1} (72.1).

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Sn_2

Band Systems

Bands in the region 4780-4350Å have been attributed to Sn_2 but may possibly arise from $SnCl_2$ (62.2).

Spectroscopic Constants

Dissociation energy = 1.99 ±0.18 eV, 45.8 kcal/mole, 16000 cm^{-1} (62.1).

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Tb_2

Spectroscopic Constants

Dissociation energy = 1.34 ± 0.35 eV, 31 kcal/mole, 11000 cm^{-1} (72.1).

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Monatshefte für Chemie 103, 757-63

Te_2

Methods of Production and Experimental Technique

Absorption.

Emission from microwave discharge.

Fluorescence, laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$A\ 0_u^+ \leftarrow X\ 0_g^+$	Absorption	5190-4250	R			(69.45, 69.43)
	II	$B\ 0_u^+ \rightleftharpoons X\ 0_g^+$	Absorption from discharge	6320-3836	R			(69.43, 69.41, 66.36, 42.31, 38.28, 35.16, 27.1)
	III	$B\ 0_u^+ \rightarrow X\ 1_g$	Laser fluorescence	5300-6050	R			(72.49)

Molecule Te_2

Te_2

I. $A\ 0_u^+ \leftarrow X\ 0_g^+$ System $\left(^{130}Te_2\right)$

Band origins, λ (69.43):

v', v''	0	1	2	3	4
0					
...					
6					5190.0
7				5089.7	5153.4
8				5054.8	5117.7
9				5020.7	5082.6
10		4868.5		4987.2	5048.4
11		4837.4			5015.0
12		4806.9	4864.2		
13		4777.1	4833.7		
14			4803.8		
15	4665.2		4774.9		
16	4637.9				
17	4611.3		4664.2		
18	4585.1		4637.5		
19	4559.6		4611.4		
20			4585.8		

II. $B\ 0_u^+ \rightleftarrows X\ 0_g^+$ System $\left(^{130}Te_2\right)$

Band origins, λ (69.45, 69.41):

v', v''	0	1	2	3
0				
...				
5			4449.1	
6			4418.5	4466.6
7		4341.8	4388.5	4436.0
8		4313.2	4359.3	4406.2
9	4240.5	4285.2	4330.7	
10	4213.7	4257.8	4302.7	
11	4187.5	4231.1		
12	4162.0	4205.0		
13	4137.0	4179.6		
14	4112.6			
15	4088.8			
16	4065.7			
17	4043.1			
18	4021.2			
19	3999.8			
20	3979.1			

$B\,0_u^+ \rightleftarrows X\,0_g^+$ System $^{128}Te_2$

Band origins, λ (69.45, 69.41):

v', v''	0	1	2	...	30	31	32	33
0								
...								
5					6248.7			
6					6188.6	6271.3		
7			4388.8			6210.7	6294.3	
8		4312.9	4359.4				6233.8	6317.7
9		4284.7	4330.2					
10		4257.1						
11	4186.4	4230.3						
12	4160.7	4204.0						
13	4135.6	4178.6						
14	4110.9							
15	4087.2							
16	4064.0							
17	4041.3							
18	4019.2							
19	3997.8							
20	3977.0							

III. $B\,0_u^+ - X\,1_g$ System

Band heads, λ (72.58):

	$^{128}Te_2$	$^{130}Te_2$
v'', v'	0	0
0		
...		
5	5350.0	
6	5421.1	
7	5493.6	5492.7
8	5567.9	5566.1
9	5643.8	5641.6
10	5721.6	5718.8
11	5800.9	5797.8
12	5882.3	5878.7
13	5965.6	5961.1
14	6050.8	6045.5
15	6138.2	
16	6227.7	

Molecule Te_2

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	$B_e \times 10^2$	$\alpha_e \times 10^4$	$D_e \times 10^9$	r_e	Remarks	Bibliography
$^{130}Te_2$									
$B\ 0_u^+$	22207.4	162.3	0.45	3.254	1.25		2.8244	$y_e\omega_e = -11.09 \times 10^{-3}$	(72.48, 69.45, 69.43)
$A\ 0_u^+$	19450.8	143.6	0.45	3.124	1.30		2.8824	$y_e\omega_e = -3.892 \times 10^{-3}$	(72.48, 69.43)
$X\ 1_g$	2234	250.00	0.547	3.968[(a)]	1.06[(a)]				(72.49, 69.43)
$X\ 0_g^+$	0	247.07	0.515	3.968	1.06	4.4	2.5774	$y_e\omega_e = -0.55 \times 10^3$	(72.48, 69.43)
$^{128}Te_2$									
$B\ 0_u^+$	22285.6[(b)]			3.3121	1.41		2.82442		(72.48, 69.45, 69.43)
$A\ 0_u^+$	19450			3.1740	1.32		2.88226		(72.48, 69.45, 69.43)
$X\ 1_g$	2228.5	251.26	0.536	4.0299[(a)]	1.03[(a)]				(72.48, 69.45, 69.43)
$X\ 0_g^+$	0			4.0299	1.03	4.1	2.55766		(72.48, 69.45, 69.43)

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	$B_e \times 10^2$	$\alpha_e \times 10^4$	$D_e \times 10^9$	r_e	Remarks	Bibliography

(a) It is assumed that the rotational constants for this state are the same as those of the X 0_g^+ state (72.49).

(b) T_o

Dissociation energy = 2.5 ± 0.4 eV, 57.7 kcal/mole, 20200 cm^{-1} (71.47).

Perturbations and General Information

RKR potential energy curve (n.p. 50) for $^{128}Te_2$ X 0_g^+ state:

T_e = 0 cm^{-1}	v	T_e+E(v)cm^{-1}	r_{min}(Å)	r_{max}(Å)
	0	124.35	2.51335	2.60548
	1	372.26	2.48249	2.64234
	2	619.12	2.46205	2.66878
	3	864.92	2.44591	2.69096
	4	1109.65	2.43229	2.71065
	5	1353.33	2.42037	2.72867
	6	1595.94	2.40971	2.74547
	7	1837.49	2.40000	2.76133
	8	2077.96	2.39108	2.77646
	9	2317.36	2.38286	2.79084
	10	2555.68	2.37513	2.80484
	11	2792.92	2.36782	2.81846
	12	3029.09	2.36095	2.83165
	13	3264.16	2.35441	2.84456
	14	3498.15	2.34819	2.85715
	15	3731.05	2.34227	2.86953

RKR potential energy curve (n.p. 50) for $^{128}Te_2$ A 0_u^+ state:

T_e = 19450 cm^{-1}	v	T_e+E(v)cm^{-1}	r_{min}(Å)	r_{max}(Å)
	0	72.24	2.82474	2.94564
	1	216.01	2.78550	2.99546
	2	358.83	2.75988	3.03171
	3	500.67	2.73987	3.06242
	4	641.50	2.72311	3.08994
	5	781.30	2.70854	3.11533
	6	920.05	2.69557	3.13918
	7	1057.72	2.68383	3.16188
	8	1194.28	2.67307	3.18367
	9	1329.73	2.66317	3.20455
	10	1464.02	2.65389	3.22501
	11	1597.14	2.64511	3.24506
	12	1729.07	2.63686	3.26464
	13	1859.78	2.62900	3.28393
	14	1989.24	2.62153	3.30290
	15	2117.43	2.61435	3.32167

RKR potential energy curve (n.p. 50) for $^{128}Te_2$ B 0_u^+ state:

T_e = 22285.5 cm^{-1}	v	T_e+E(v)cm^{-1}	r_{min}(Å)	r_{max}(Å)
	0	81.68	2.77021	2.88390
	1	244.31	2.73361	2.93102
	2	405.92	2.70967	2.96521
	3	566.44	2.69099	2.99420
	4	725.80	2.67543	3.02028
	5	883.93	2.66201	3.04448
	6	1040.77	2.65009	3.06729
	7	1196.24	2.63915	3.08889
	8	1350.28	2.62870	3.10929
	9	1502.76	2.61904	3.12893
	10	1653.68	2.60899	3.14728
	11	1803.11	2.60141	3.16717
	12	1950.68	2.59302	3.18565
	13	2096.49	2.58499	3.20395
	14	2240.49	2.57882	3.22345
	15	2382.58	2.57212	3.24213

Franck-Condon factors for $^{128}Te_2$ $\left(A\ 0_u^+ - X\ 0_g^+\right)$ (n.p. 50):

	12	13	14	15	16	17	18	19
0	4.985-2	6.959-2	8.846-2	1.032-1	1.110-1	1.102-1	1.014-1	8.679-2
1	7.975-2	7.178-3	5.109-2	2.559-2	5.839-3	2.330-4	1.094-2	3.319-2
2	3.035-2	7.032-3	4.068-4	1.415-2	3.767-2	5.356-2	5.064-2	3.155-2
3	4.838-4	1.598-2	3.871-2	4.614-2	3.100-2	8.307-3	2.854-4	1.440-2
4	2.969-2	4.213-2	2.891-2	6.186-3	1.449-3	1.988-2	3.861-2	3.526-2
5	3.601-2	1.414-2	2.368-6	1.316-2	3.354-2	3.128-2	9.981-3	2.531-4
6	7.044-3	1.933-3	2.217-2	3.304-2	1.643-2	2.123-4	1.101-2	3.076-2
7	3.998-3	2.552-2	2.833-2	7.349-3	1.782-3	2.138-2	2.942-2	1.135-2
8	2.536-2	2.501-2	3.738-3	5.140-3	2.536-2	2.256-2	2.672-3	5.871-3
9	2.428-2	3.104-3	6.396-3	2.556-2	1.740-2	2.713-4	1.184-2	2.638-2
10	4.517-3	5.263-3	2.444-2	1.540-2	2.557-6	1.458-2	2.409-2	6.246-3

Franck-Condon factor followed by factor of ten

Franck-Condon factors for $^{128}Te_2\left(B\ 0_u^+ - X\ 0_g^+\right)$ (n.p. 50):

	9	10	11	12	13	14	15	16
0	8.506-2	1.101-1	1.267-1	1.305-1	1.208-1	1.001-1	7.702-2	5.374-2
1	8.231-2	5.196-2	1.833-2	5.264-4	8.427-3	3.676-2	7.006-2	9.305-2
2	7.989-3	1.866-3	2.622-2	5.616-2	6.270-2	4.059-2	1.115-2	1.710-4
3	1.719-2	4.769-2	5.101-2	2.326-2	6.824-4	1.165-2	4.208-2	5.623-2
4	4.911-2	3.233-2	3.279-3	7.950-3	3.754-2	4.508-2	1.981-2	1.478-4
5	2.209-2	1.318-5	1.961-2	4.190-2	2.498-2	8.072-4	1.316-2	4.003-2
6	1.247-4	2.365-2	3.789-2	1.228-2	1.716-3	2.766-2	3.619-2	1.062-2
7	2.161-2	3.507-2	8.070-3	5.026-3	3.186-2	2.546-2	1.000-3	1.360-2
8	3.429-2	8.942-3	5.096-3	3.117-2	1.933-2	4.950-5	2.135-2	3.063-2
9	1.396-2	2.415-3	2.848-2	1.842-2	2.691-4	2.322-2	2.494-2	1.082-3
10	3.614-5	2.312-2	2.132-2	3.220-6	2.129-2	2.269-2	2.589-4	1.739-2

Franck-Condon factor followed by factor of ten

Perturbations of the v = 0 level of the B 0_u^+ state have been observed.

Ionization cross sections = 17.46 ± 0.48 × 10^{-6} cm^2 (66.37).

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Th_2

Spectroscopic Constants

Dissociation energy = 2.95 ± 0.35 eV, 68 kcal/mole, 24000 cm^{-1} (69.1).

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Ti_2

Spectroscopic Constants

Dissociation energy = 1.15 ± 0.17 eV, 28.3 kcal/r[illegible] 9000 cm^{-1} (69.2).

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Tl_2

Methods of Production and Experimental Technique

Absorption.

Emission from a hollow chathode and a King furnace.

Band Systems

Five groups of bands have been observed in emission and absorption (65.5, 65.4, 31.2, 31. 1).

I. "Red System" - 6500-4900Å

λ in emission (65.5):

v', v''	0	1	2	3	4
0	6320. 3	6375. 5	6428. 4	6483. 0	6537. 2
1	6285. 4	6339. 1	6393. 0		
2	6252. 0				

The conclusions on the origin of this band system are uncertain. Initial investigation gives $\omega' \sim 88\ cm^{-1}$ and $\omega'' \approx 136\ cm^{-1}$ (65.5).

II. 4635-3680Å System

Emission

In emission, the band head appears to be at $\lambda \sim 3770.7$Å, with band maxima at:

λ = 4635|4405|4308|4237|4187|4133|4047|4004

diffuse and weak maxima at:

λ = 3923|3857|3800

Absorption

Extensive tables of lines seen in absorption (4400-4200Å) are given in (65.5). There are two tentative assignments given to some of them.

Assignment I:

v', v''	0	1	2	3	4	5	6	7	8
0	4269.9	4287.1	4302.2	4322.2	4340.3				
1		4263.7		4299.1	4360.2	4335.4	4354.2	4372.4	4390.3
2			4251.6	4276.8	4293.9				
3				4255.3	4271.9				
4					4250.8				

Assignment II:

v', v''	0	1	2	3	4	5	6	7
0	4400.2	4419.0						
1		4394.3	4412.6	4431.9				
2		4370.2		4406.5	4425.1			
3					4401.9	4420.4		
4						4396.0	4414.2	
5						4372.4	4390.3	4408.7

III. 3776-3260Å System

Bands are symmetrical around the lines at 3529 and 3519Å. Maxima at ~ 3600Å.

IV. 2850-2740Å System

Bands are asymmetrical around the 2768Å line with an apparent head at 2766.3Å.

V. Visible Continua - 2768Å System

This system arises from the broadening of the lines 3230, 3092, 2922-2919Å. Maxima at $\lambda \sim 3446 | 3156 | 3050$Å.

Spectroscopic Constants

Dissociation energy = <0.9 eV, <21 kcal/mole, <7300 cm^{-1} (57.3).

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Tm_2

Spectroscopic Constants

Dissociation energy = 0.52 ± 0.17 eV, 12 kcal/mole, 4200 cm^{-1} (72.2).

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U_2

Spectroscopic Constants

Dissociation energy = 1.73 ± 0.43 eV, 40 kcal/mole, 14000 cm^{-1} (69.1).

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High Temp. Sci. 1, 258-67

V_2

Spectroscopic Constants

Dissociation energy = 2.49 ± 0.13 eV, 57.5 kcal/mole, 20100 cm^{-1} (69.1).

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Xe_2

Methods of Production and Experimental Technique

Absorption.

Emission from electron beam discharge, laser pumping, α particles, x rays.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	?	Electron beam, X rays	5000–2600			Continuum	(67.7)
	II	$^{1,3}\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$ $\begin{pmatrix} 0_u^+ - 0_g^+ \\ 1_u - 0_g^+ \end{pmatrix}$	Electron beam	2250–1470			Continuum	(74.33, 72.14, 65.4, 55.3, 55.2)
	III	$^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ $(0_u^+ - 0_g^+)$	Electron beam	1305–1295				(74.33, 72.14)
	IV	$^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ $(0_u^+ - 0_g^+)$	Electron beam	1207–1192				(74.33, 72.14)
	V	$^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ $(1_u - 0_g^+)$	Electron beam	1192–1191				(74.33, 72.14)

II. $^{1,3}\Sigma_u^+ \rightleftarrows X^1\Sigma_g^+ \left(0_u^+, 1_u - 0_g^+\right)$ Systems

Upper state correlated to $5p^6\ ^1S_0 + 6s(3/2)_1^0$ (74.33, 72.14).

III. $^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+ \left(0_u^+ - 0_g^+\right)$ System

Upper state correlated to $5p^6\ ^1S_0 + 6s'(1/2)_1^0$ (74.33, 72.14).

IV. $^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+ \left(0_u^+ - 0_g^+\right)$ System

Upper state correlated to $5p^6\ ^1S_0 + 5d(3/2)_1^0$ (74.33, 72.14).

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e\omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$X^1\Sigma_g^+$ (0_g^+)	0	~ 21.26	~ 0.75	~ 0.013	~ 0.4		~ 4.45	$y_e\omega_e \sim 0.008$	(70.9)

Dissociation energy $\sim 2.4 \times 10^{-2}$ eV, 0.55 kcal/mole, 192.02 cm^{-1} (70. 9).

Perturbations and General Information

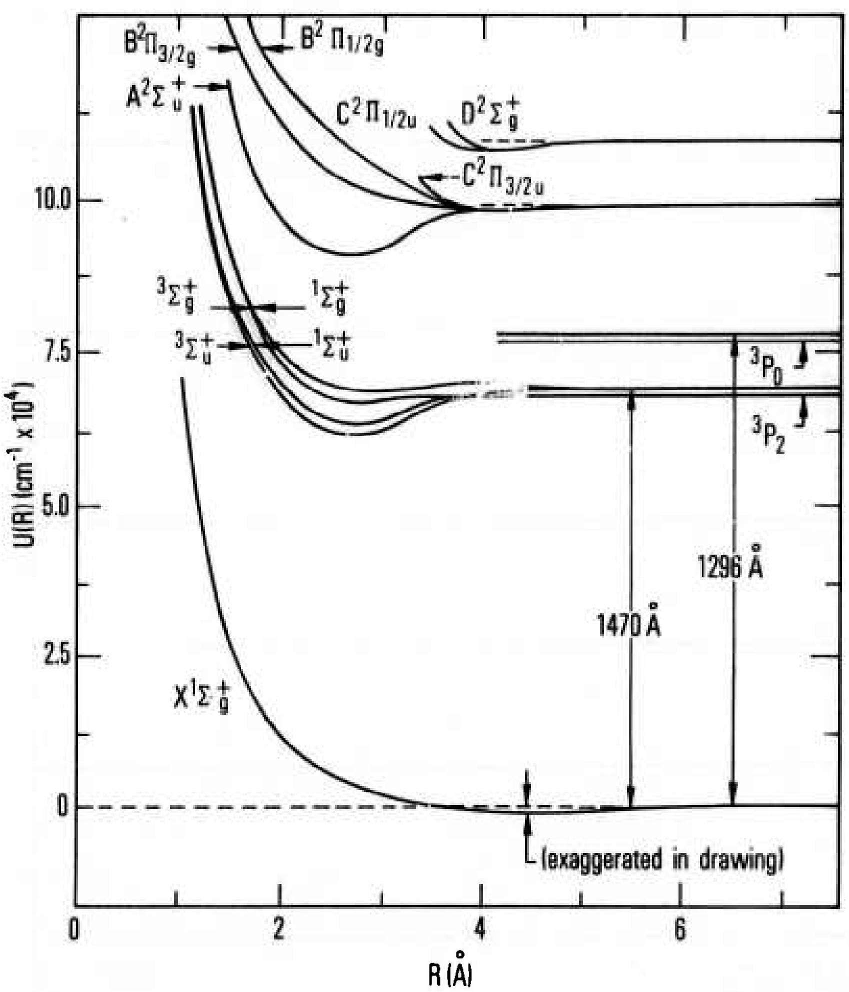
Quenching of $Xe_2\ {}^{1,3}\Sigma_u^+$ by Xe: $\sigma \approx 10^{-17}$ cm^2 (73.25).

Laser action observed on the ${}^{1,3}\Sigma_u^+ \rightarrow X\,{}^1\Sigma_g^+$ transition at 1720 ± 10Å (74.36, 74.31, 74.30, 73.28, 73.23, 73.22, 73.21, 73.20, 73.19, 73.18).

Radiative lifetime of ${}^{1,3}\Sigma_u^+ - X\,{}^1\Sigma_g^+$

$$\tau = 23 \text{ nsec } (74.32)$$
$$= 130 \text{ nsec } (73.18).$$

Potential energy curves - estimated (70.10):



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Y_2

Spectroscopic Constants

Dissociation energy = 1.62 ± 0.22 eV, 37.3 kcal/mole, 13050 cm^{-1}.

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Yb_2

Methods of Production and Experimental Technique

Knudsen cell effusion.

Spectroscopic Constants

Dissociation energy = 4 ± 4 eV, 92 kcal/mole, 32000 cm^{-1} (72.3).

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Zn_2

Methods of Production and Experimental Technique

Absorption.

Emission (Tesla coil, hollow cathode).

Fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Maximum (λ) in Emission	Remarks	Bibliography
	I		Emission	5350-3890		4450	Continuum	(31.6, 31.5)
	II		Emission	3893-3776		3787	Continuum	(31.6, 31.5)
	III		Emission Absorption	3763-2936		3688	Continuum	(31.6, 31.5, 29.2)
	IV		Absorption Emission Fluorescence	3073-2002		2550	Continuum	(31.6, 31.5, 31.4, 29.2)

Molecule Zn_2

Zn_2

III. 3763-2936Å System

Emission

In emission maximum is at λ = 3688Å (31.6, 31.5) and line broadens at 3076A (31.6, 31.5).

Bands superimposed λ | 3749 | 3724 | 3706 | 3688 | 3575 | 3522 | 3483 | 3454 | 3431 | 3411 | 3052 |

Absorption

In absorption bands are without structure and maxima is at ~3050Å (31.6, 29.2).

IV. 3073-2002Å System

Emission (31.6, 31.5)

In emission continuous bands are 2826-2035Å, maximum is at 2550Å, line broadens at 2139Å, and diffuse bands are at λ ~ 2002Å.

Absorption (31.6, 29.2)

In absorption continuous bands are at 2550-2002Å, maxima are at λ = 2139, 2064, and 2002Å, and the line broadens at 2139Å.

Fluorescence (31.3)

Numerous bands in the region 3073-2456Å.

Spectroscopic Constants

Dissociation energy = 0.25 eV(?), 6 kcal/mole(/), 2100 cm^{-1}.

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