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Spectroscopic Constants for Selected Homonuclear Diatomic Molecules

Volume I. A Through I

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Interim Report

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FOR THE COMMANDER

Ronald C. Lawson
Ronald C. Lawson
2nd Lt, United States Air Force
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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 Franck-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 first volume, covers A through I.			

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19. KEY WORDS (Continued)

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

20. ABSTRACT (Continued)

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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

In recent years, the need for a complete collection of information relevant to diatomic molecules has become evident. Several excellent collections of this type of information have been available for many years (Refs. 1-3); however, the state of our collective knowledge has been considerably expanded since their publication. To this end, a comprehensive compendium of spectroscopic information relevant to selected heteronuclear diatomic molecules was compiled and disseminated by us during FY 74 (Ref. 4). At present, however, if recent information concerning a specific homonuclear species is desired, it is still necessary to institute a time-consuming library search to collect the required information from the large number of sources in which it may have been presented. If information concerning an entire isoelectric molecular series is required, the time involved in collecting the information can be considerable.

This compilation was assembled in the hopes of solving this time problem. We have attempted to gather a complete collection of spectroscopic information relevant to homonuclear diatomic systems. Unlike the compendium for heteronuclear molecules, where the decision was made to restrict our collection to molecules that, from thermodynamic reasoning, could be produced in an electronically excited state by a chemical reaction between a ground state atom and a ground state molecule, this collection includes information relevant to all homonuclear diatomic molecules.

The organization of the material has been patterned after our heteronuclear compendium (Ref. 4). We believe that this form of presentation displays the spectroscopic information in a manner that is amenable to efficient retrieval. The material itself was located with the help of several excellent earlier compendia (Refs. 1-3), a recent bibliography of spectroscopic data (Ref. 5), and from the continuously updated Berkeley Newsletters collected by J. G. Phillips and S. P. Davis of the University of California at Berkeley (Ref. 6).

II. ORGANIZATION OF THE SPECTROSCOPIC TABLE

The information that we are presenting deals primarily with the electronic spectra of homonuclear diatomic systems. In general, the spectroscopic constants have been derived from the interpretation of electronic spectra; however, when the amount of data was insufficient, the information was taken from alternative sources.

For simplicity, the molecules are presented in alphabetical order. The information for most of the molecules is broken into five separate sections, with several of the sections broken further into several subsections. Information is presented according to the following format.

METHODS OF PRODUCTION AND EXPERIMENTAL TECHNIQUE

The most favorable sources for the production of the molecule of interest and important experimental techniques used for studying the molecule.

BAND SYSTEMS

This section is broken into two subsections. In the first subsection, a general description of the molecular transition of each system or group is presented; the description is divided into eight headings.

1. System numbers or common designations for the system, or both (e.g., Swan bands of C_2).
2. Transition. Conventional or quantum designation for the states involved. The signs $\rightarrow$, $\leftarrow$, and $\rightleftharpoons$ refer to systems observed in emission, in absorption, or in both emission and absorption.
3. Sources. The most favorable sources for producing the particular system.
4. Wavelength Limits. Spectral range of the system ($\text{\AA}$).
5. Degradation. Direction of band head shading ($R \equiv$ red, $V \equiv$ violet).
6. Band Head $\nu_{0,0}$ or Characteristic Bands λ . Characteristic spectral bands free from overlapping bands or with sharp heads.

7. Remarks. Additional information that is useful in characterizing the particular system.
8. Bibliography. Listing of references that concern themselves with the particular system.

The second subsystem presents a more detailed analysis of the system. Wavelengths ($\text{\AA}$) of band heads or origins, intensities, and vibrational classifications are presented where available. Other available and relevant information is presented to characterize the system.

SPECTROSCOPIC CONSTANTS

The molecular constants that totally define the electronic states of the molecule are presented under ten headings. If not specifically mentioned, these constants refer to molecules made of the most abundant isotopes.

1. State. Quantum specification of the electronic state
2. T_e . Electronic energy above ground state (cm^{-1})
3. ω_e . Vibrational spacing (cm^{-1})
4. $x_e \omega_e$. Anharmonic correction to vibrational spacing (cm^{-1})
5. B_e . Rigid rotator rotational spacing (cm^{-1})
6. α_e . Nonrigid rotator correction to B_e (cm^{-1})
7. D_e . Anharmonic correction to rotational spacing (cm^{-1})
8. r_e . Equilibrium internuclear distance ($\text{\AA}$)
9. Remarks. Additional relevant information
10. Bibliography. Important references

Other molecular constants or information, if known, are given as footnotes. The dissociation energy D_0^0 or D_{298}^0 is given in cm^{-1} , kcal/mole, and eV. The greater majority of the values for the molecular dissociation energies have been adopted from the book, Dissociation Energies and Spectra of Diatomic Molecules, by Gaydon (Ref. 7). When molecular values that are more recent than Gaydon's for the dissociation energy exist, the appropriate reference is cited. Dissociation energies taken directly from Gaydon, it should be noted, are not followed by a reference.

PERTURBATIONS AND GENERAL INFORMATION

This section encompasses all other information that would be useful for a complete understanding of the specific molecule. The information, where available, includes predissociations, perturbations, dipole moments, ionization potentials, potential energy curves, Franck-Condon factors, spontaneous lifetimes, rates of production, and deactivation and branching ratios. We hope that this section, in conjunction with the other information set forth, presents a complete description of the physical parameters associated with each molecular species.

BIBLIOGRAPHY

Following the format of our heteronuclear compendium (Ref. 4), in addition to presenting the references used to gather information, a short description of the important points of the paper is given. The bibliography takes into account most papers published through 1974; however, during final preparation of the manuscript, numerous omissions were noted. It is our intention to update this report at suitable intervals; consequently, the omissions will be rectified in a supplement to this report.

Our referencing system is similar to that employed previously in that the references are presented in terms of two numbers. The first number refers to the year of publication, and the second number refers to a running count of the references for each specific molecule.

III. NOTATION AND NOTATIONAL CONVERSION FORMULAS

The total energy of a given state of a diatomic molecule is given by the formula

$$T = T_e + G + F \quad (1)$$

where T_e is electronic energy, G is vibrational energy, and F is rotational energy. Further breaking down these different forms of energy, the electronic energy T_e is given by

$$T_e = T_o + A\Lambda\Sigma \quad (2)$$

where T_o is the electronic energy if spin is neglected, A is spin-orbit coupling, Λ is the electronic orbital angular momentum quantum number about the internuclear axis, and Σ is the component of the resulting spin. The vibrational energy G is given by

$$G = \omega_e(v + 1/2) - x_e\omega_e(v + 1/2)^2 + y_e\omega_e(v + 1/2)^3 + \dots \quad (3)$$

where v is the vibrational quantum number, ω_e is the harmonic oscillator vibrational spacing, $x_e\omega_e$ is the first anharmonic correction to the vibrational spacing, and $y_e\omega_e$ is the second anharmonic correction. The rotational energy F is given by

$$F = B_v J(J + 1) - D_v J^2(J + 1)^2 + H_v J^3(J + 1)^3 + \dots \quad (4)$$

where J is the rotational quantum number, B_v is the rigid rotator rotational spacing, D_v is the first anharmonic correction to the rotational spacing, and H_v is the second anharmonic correction. In addition, there are nonrigid rotator corrections to both B_v and D_v . These corrections are given by

$$B_v = B_e - \alpha_e(v + 1/2) + \gamma_e(v + 1/2)^2 + \dots \quad (5)$$

and

$$D_v = D_e + \beta_e(v + 1/2)^2 + \dots \quad (6)$$

where B_e is $\hbar^2/2\mu r_e^2$, μ is the reduced mass, r_e is the equilibrium internuclear distance, α_e and β_e are the first anharmonic corrections, and γ_e is the second anharmonic correction.

Using these formulas, a transition from state 1 at energy T_1 to state 2 at energy T_2 will be at an energy (cm^{-1}) of

$$v = T_1 - T_2 = (T_{e1} - T_{e2}) + (G_1 - G_2) + (F_1 - F_2) \quad (7)$$

Since, in general, the rotational energy changes are much smaller than either the vibrational or electronic changes, neglecting rotation,

$$\begin{aligned} v_{v', v''} = & v_e + \omega_e'(v + 1/2) - x_e'\omega_e'(v + 1/2)^2 + y_e'\omega_e'(v + 1/2)^3 + \dots \\ & - [\omega_e''(v + 1/2) - x_e''\omega_e''(v + 1/2)^2 + y_e''\omega_e''(v + 1/2)^3 + \dots] \end{aligned} \quad (8)$$

Assuming, as is often the case in absorption, $v' = v'' = 0$, and substituting in Eq. (8),

$$\begin{aligned} v_{v', v''} = & v_{0,0} + \omega_o'v' - x_o'\omega_o'v'^2 + y_o'\omega_o'v'^3 + \dots \\ & - (\omega_o''v'' - x_o''\omega_o''v''^2 + y_o''\omega_o''v''^3 + \dots) \end{aligned} \quad (9)$$

where

$$\begin{aligned}\omega_o &= \omega_e - x_e \omega_e + 3/4 y_e \omega_e + \dots \\ x_o \omega_o &= x_e \omega_e - 3/2 y_e \omega_e + \dots \\ y_o \omega_o &= y_e \omega_e + \dots\end{aligned}$$

A final quantity that is also reported is $\Delta G_{1/2}$. This quantity corresponds to the energy difference between vibrational levels $v = 0$ and $v = 1$, neglecting $y_o \omega_o$, and is represented by

$$\Delta G_{1/2} = \omega_o - x_o \omega_o = \omega_e - 2 x_e \omega_e$$

Several other molecular constants that are reported for several molecules are represented in the following list:

- f = oscillator strength (f-value)
- λ, γ = spin-coupling constants for multiplet Σ states (cm^{-1})
- q, p = Λ doubling constants (cm^{-1})
- μ = electronic dipole moment (D)
- R_b^o = reactive branching ratio

IV. CONCLUSIONS ON THE AVAILABILITY OF SPECTROSCOPIC INFORMATION

It was our hope, when this search was initiated, to find sufficient information in the literature from which to draw definite conclusions regarding the feasibility of the production of an electronic transition chemical laser. As can be seen in the following table, our hopes were not fulfilled. At the present time, there does not appear to be sufficient information about any homonuclear diatomic molecule that would lead one to believe that molecule would definitely produce a chemically pumped electronic transition laser.

We have charted how much is known about the molecular systems we have researched. In general, very little information is available for any given system. The charts immediately precede the detailed information for the collected systems in each volume.

Sufficient information is available for the identification of the emitting species from potential laser systems. If, however, the experiment is to measure the partitioning of energy between the various accessible electronic levels of the molecule, molecular lifetimes and Franck-Condon factors must be known in order to interpret the data. To ascertain the feasibility of a specific molecule for a laser entails knowing not only the reactive branching ratio, but also the lifetime, pumping rates, and deactivation rates. We do not yet have all of this information for a single molecule.

Knowing that, at present, there is almost a complete lack of the necessary information for producing a chemically pumped electronic transition laser, we realize that we are in the same situation as experimenters who were trying to produce vibrational lasers during the early 1960s. At that time, pumping rates, vibrational distributions, and deactivation rates were all unknown, as is now the case for electronic transition lasers. Also in analogy with vibrational lasers, however, the ultimate demonstration of a chemically pumped electronic transition laser should be possible.

The question then arises: What information is required and is there any ordering in the importance of the information? The answer becomes obvious when you remember that an inversion must be created before laser action can occur. Therefore, a knowledge of the reactive branching ratio is absolutely necessary before predictions can be made as to the suitability of a molecule as a potential laser. Even if the lifetimes and pumping rates appear suitable, an inversion must exist before the system can lase. As previously mentioned, the interpretation of spectral intensities to determine the branching ratio for a particular transition requires a knowledge of both the Franck-Condon factors and radiative lifetime for the transition. The Franck-Condon factors, however, cannot be accurately calculated without accurate knowledge of the spectroscopic constants defining the two electronic states between which the transition takes place. So, at least from the experimental point of view, it is imperative that accurate spectroscopic constants and radiative lifetimes be known for the determination of reactive branching ratios. From a theoretical viewpoint, it may only be necessary to have accurate spectroscopic constants.

Whereas a sufficiently large reactive branching ratio may be a necessary condition for a system to reach threshold, it is not sufficient. Even with a sufficiently large reactive branching ratio, if the electronic state of interest is not produced in a time that is fast as compared to the rate at which it is being quenched, either by spontaneous emission or de-excitation, the required inversion cannot be produced. Consequently, once a particular set of reactants have been shown to produce a molecule with a sufficiently large reactive branching ratio, either by experiment, theory, or spin conservation rules, deactivation studies of the molecule should be actively pursued as well as similar studies on other molecules of the same family (e.g., Na_2 , K_2 , Rb_2 , and Cs_2 , or O_2 , S_2 , Se_2 , and Te_2). Once a suitable reactive branching ratio is found for a system and the important quenching rates measured, kinetic calculations can be made to determine proper operating conditions for the production of an inversion and laser action.

The above approach for determining the feasibility of chemically pumped electronic transition is sound. Whereas the actual production of the laser may prove to be quite difficult, the probability of finding one approaches unity. If one were to assign priorities to the information needed to assist the researcher, they would be as follows:

1. Reactive branching ratios. To ascertain the maximum possible inversion
2. Vibrational level distributions of the product molecules. A total inversion may not exist between the entire upper and lower electronic levels, but it still can exist between specific vibration-rotation levels of the two states.
3. Radiative lifetimes. Necessary for the experimental determination of reactive branching ratios and also for the dictation of minimum reaction rates
4. Spectroscopic constants and dissociation energies. Needed to calculate Franck-Condon factors
5. Pumping and quenching rates. Even if the inversion exists, it must do so on the proper time scale.

Lastly, while the straightforward research approach to the production of a laser may be aesthetically pleasing, the intuitive "shotgun" approach should not be discounted. The largest boost that could accelerate the discovery of new lasers is the discovery and understanding to the first chemically pumped electronic transition laser system.

Since the beginning of the keeping of sports statistics, no human being had run a four-minute mile. Once this record had been broken, however, it was not long before many had done so. Possibly this analogy will hold here.

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MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBU- TIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
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 I-1

MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBU- TIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
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 I-2

MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBU- TIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
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 I-3

MOLECULE	VIBRA-TIONAL CONSTANTS	ROTA-TIONAL CONSTANTS	VIBRA-TIONAL LEVEL DISTRIBU-TIONS	DISSO-CIATION ENERGY	LIFE-TIMES	FRANCK-CONDON FACTORS	BRANCH-ING RATIOS	QUENCH-ING	LASER ACTION OBSERVED	
									VIBRA-TIONAL	ELEC-TRONIC
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 I-4

MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBUTIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
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 I-5

Methods of Production and Experimental Technique

Absorption at 1700-1800°C }
 Emission at 2000°C } from a King furnace.

Absorption and emission in quartz discharge tube.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$A \approx X^1\Sigma_g^+$	Absorption and Emission	5050-4000	R	22984		(66.6, 59.2, 55.1)
	II		Absorption and Emission	3630-3150				(66.6)
	III	$B \approx X^1\Sigma_g^+$	Absorption and Emission	2880-2750	R	35631		(66.6, 59.2)
	IV	$C \approx X^1\Sigma_g^+$	Absorption and Emission	2710-2640	R	37618		(66.6, 63.4, 59.2)
	V	$D \approx X^1\Sigma_g^+$	Absorption and Emission	2620-2560	R	38995.5		(66.6, 59.2)
	VI	$E \approx X^1\Sigma_g^+$	Absorption and Emission	2560-2460	R	40137		(66.6, 63.4, 59.2)

Molecule Ag₂



I. $A \approx X^1\Sigma_g^+$ System

Intense bands in absorption, λ (55.1):

v', v''	0	1	2
0	4350.86	4387.34	4424.16
1	4322.08	4357.98	
2	4293.79		4365.30
3	4265.89		

II. Two strong bands and patches of weak continua have been seen at 3280.7 and 3382.9 Å. They probably arise from a transition between an unstable upper state and an unstable lower state of Ag_2 (66.6).

III. $B \approx X^1\Sigma_g^+$ System

Intense band heads in absorption, λ (intensity) (66.6, 59.2):

v', v''	0	1	2	3	4	5
0	2806.5(8)	2822.5(8)	2839.8(4)	2856.4(1)	2873.3(1)	
1	2792.6(10)	2809.6(7)	2825.4(8)	2842.7(5)		
2	2780.1(8)	2796.0(5)	2812.5(5)	2828.6(5)	2845.6(4)	2861.9(2)
3	2768.4(4)					2849.3(2)
4		2771.7(3)			2756.8(1)	
5		2761.4(2)				

IV. $C \approx X^1\Sigma_g^+$ System

Intense sequence with R and Q heads. Intense bands in absorption, λ (66.6, 59.2):

(v', v'')		(v', v'')	
(0, 0)	2657.49(Q)	(3, 3)	2661.7
	2656.79(R)	(4, 4)	2663.2
(1, 0)	2645.4	(5, 5)	2665.2
(1, 1)	2658.97(Q)	(6, 6)	2666.8
	2658.78(R)	(7, 7)	2668.7
(2, 2)	2660.45(Q)	(10, 10)	2674.9
	2660.03(R)		

V. D $\approx$ X¹ Σ_g^+ System

$\Delta v = 0$ sequence with intense Q and R heads. Intense bands in absorption, λ (66.6, 59.2):

(v', v'')		(v', v'')	
(0, 0)	2563.63(Q) 2562.64(R)	(2, 2)	2567.00(Q) 2566.25(R)
(1, 1)	2565.24(Q) 2564.38(R)	(3, 3)	2568.0
		(4, 4)	2570.0

VI. E $\approx$ X¹ Σ_g^+ System

Intense band heads in absorption, λ (66.6, 59.2):

v', v''	0	1	2	3
0	2490.72	2502.80	2514.61	
1	2481.9			2517.53
2		2485.2		
3			2488.1	

SPECTROSCOPIC CONSTANTS

Molecule <u>Ag₂</u>									
State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ³	D _e × 10 ⁶	r _e	Remarks	Bibliography
E	40159.1	146.08	1.54						(63.4, 59.2)
D(¹ Π _u) ^b	39023.7	166.7	1.134						(59.2)
C(¹ Π _u) ^b	37626.9	172.9	1.07						(63.4, 59.2)
B	35827.3	151.3	0.70						(59.2)
A	22996.4	154.6	0.587					y _e ω _e = 0.0022 ^a	(59.2, 55.1)
X ¹ Σ _g ⁺	0	207.0	0.643	0.496	0.19		2.5	y _e ω _e = 0.0003 ^a	(66.6, 59.2, 55.1)

^a Constants for ¹⁰⁷Ag¹⁰⁹Ag.

^b Ω = 1_u.

Dissociation energy = 1.68 ± 0.10 eV, 38.7 kcal/mole, 13550 cm⁻¹ (60.3).

Perturbations and General Information

Perturbations and predissociation have been observed in the $v = 4, 5, 6$, and 7 levels of the ground state (66.6).

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Methods of Production and Experimental Technique

Thermal emission from a King furnace.

Knudsen cell mass spectrometric method.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	I	$A^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$	Thermal Emission	6600-5650	R	17231.3		(65.4, 64.3, 54.1)

Molecule Al₂

Al₂

I. A³Σ_u⁻ → X³Σ_g⁻ System

Most intense bands, λ (54.1):

v', v''	0	1	2	3
0	5801	5709		
1	5920		5732	
2	6042	5943		5755
3		6064	5965	
4		6190	6086	5986

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_0 \times 10^6$	r_e	Remarks	Bibliography
$A^3\Sigma_u^-$	17269.3	278.80	0.831	0.1907	1.3	0.38	2.560	-0.010 ^a	(65.4, 64.3)
$X^3\Sigma_g^-$	0	350.01	2.022	0.2053	1.2	0.30	2.466	-0.010 ^a	(73.5, 65.4, 64.3)
$a y_e \omega_e$ Dissociation energy = 2.05 eV, 47.3 kcal/mole, 16544 cm^{-1} (73.5).									

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Methods of Production and Experimental Technique

Solid Ne at 6°K.

Discharge in helium continua.

Electron bombardment of high pressure Ar.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, ν	Remarks	Bibliography
	I	$^3\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Discharge	1083 - 1073	V	93124.2		(70.10)
	II	$^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Discharge	1073 - 1065	R	93703.9		(70.10)
	III		Discharge	1052 - 1047	V	95050.7		(70.10)
	IV		Discharge	944 - 941	R	106213.5		(70.10)
	V		Discharge	932 - 928	R	107667.7		(70.10)
	VI		Discharge	922 - 918	R	108884.8		(70.10)
	VII		Discharge	903 - 895	R	111722.4		(70.10)
	VIII		Discharge	893 - 883		113050.9		(70.10)
	IX		Discharge	851 - 846	R	118183		(70.10)
	X		Discharge	7000 - 2900		32258		(66.4)

Molecule Ar₂

Ar₂

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

Bands not classified completely, λ (Intensity) (70.10):

v' v''	0	1	2	3	4
v-7	1082.2(1)	1082.6(2)	1082.8(2)	1083.0(1)	
v-6	1080.7(2)	1081.0(3)	1081.3(2)	1081.4(1)	1081.6(1)
v-5	1079.2(4)	1079.5(4)	1079.8(3)	1080.0(1)	1080.1(1)
v-4	1077.9(6)	1078.2(4)	1078.4(3)	1078.6(1)	
v-3	1076.6(8)	1076.9(4)	1077.1(3)		
v-2	1075.5(9)	1075.8(3)	1076.0(2)		
v-1	1074.6(9)	1074.9(3)			
v	1073.8(10)	1074.1(5)			

II. $^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ System

Bands not classified completely, λ (Intensity) (70.10):

v' v''	0	1	2	3	4
v-3	1072.4(2)	1072.7(3)	1073.0(3)	1073.1(3)	1073.3(2)
v-2	1070.8(4)	1071.1(4)	1071.4(5)	1071.6(3)	1071.7(2)
v-1	1069.4(6)	1069.7(5)	1070.0(4)	1070.1(4)	1070.3(2)
v	1068.2(8)	1068.5(6)	1068.7(4)	1068.9(3)	1069.0(1)
v+1	1067.1(10)	1067.4(3)			
v+2	1066.3(3)	1066.5(6)			

Five other bands have been seen and not identified:

1065.1(3) 1065.2(3) 1065.3(3) 1065.4(3) 1065.4(3).

Probably all five originate with some upper level which is located on the potential hump and thus affected by dissociation through the hump (tunneling effect) (70.10).

III. SystemBand heads, λ (Intensity) (70.10):

v'	v''	0	1	2	3	4
0		1052.0(10)	1052.3(7)	1052.5(9)	1052.7(2)	1052.8(1)
1		1051.4(9)	1051.7(3)	1051.9(4)		
2		1050.8(7)	1051.4(8)			
3		1050.3(5)	1050.6(5)	1050.8(7)	1051.0(5)	1051.1(8)
4		1049.9(4)	1050.2(4)	1050.5(3)	1050.6(5)	
5		1049.7(3)	1049.9(4)	1050.2(3)	1050.4(4)	
6		1049.5(2)	1049.7(2)	1049.9(4)	1050.1(2)	1050.2(2)
7		1049.3(2)	1049.6(2)			
8		1049.2(2)	1049.5(2)			
9		1049.1(1)				

Four additional diffuse bands have also been seen but not positively identified:

1047.5(1) 1047.3(1) 1047.2(1) 1047.1(1).

IV. System

Band heads, λ (Intensity) (70.10). These are diffuse and have not been positively identified.

v'	v''	0	1	2	3
$v-1$		943.1(8)	943.3(5)	943.5(3)	943.6(1)
v		941.5(10)	941.7(3)		

V. System

Band heads, λ (Intensity) (70.10). These bands are diffuse and have not been positively identified.

v'	v''	0	1	2
$v-3$		931.7(7)		
$v-2$		930.2(3)		
$v-1$		929.2(6)	929.4(4)	929.6(2)
v		928.7(10)	929.0(6)	

Additional diffuse bands have been observed but not identified:

937.7(1) 936.8(10) 935.5(3) 924.2(9) 924.4(10) 924.6(4)

Ar₂

VI. System

Band heads, λ (Intensity) (70.10). These bands have not been positively identified.

v' v''	0	1	2	3	4
v-5	921.7(1)	921.9(1)			
v-4	920.5(3)	920.7(3)	920.9(3)	921.1(2)	921.1(1)
v-3	919.6(3)	919.8(4)	919.9(4)		
v-2	918.9(8)	919.1(5)	919.3(3)		
v-1	918.4(10)	918.6(3)	918.7(1)		
v	918.0(7)	918.2(5)			

VII. System

Band heads, λ (Intensity) (70.10). These bands have not been positively identified.

v' v''	0	1	2	3	4
v-5	901.4(1)	901.6(2)	901.8(2)	901.9(2)	902.0(1)
v-4	900.0(2)	900.2(3)	900.4(2)	900.5(2)	900.6(1)
v-3	898.7(4)	898.9(5)	899.1(5)	899.2(3)	899.3(2)
v-2	897.4(7)	897.6(5)	897.8(4)	897.9(2)	898.0(1)
v-1	896.2(8)	896.4(6)	896.5(4)	896.7(1)	
v	895.0(10)	895.2(7)	895.4(4)	895.5(1)	

VIII. System

Band heads, λ (Intensity) (70.10). These bands have not been positively identified.

v' v''	0	1	2
v-12	892.5(6)		
v-11	891.5(7)		
v-10	890.5(8)		
v-9	889.6(8)		
v-8	888.7(8)	888.9(1)	889.1(1)
v-7	887.9(8)	888.1(2)	888.2(2)
v-6	887.1(8)	887.3(4)	887.4(2)
v-5	886.3(7)	886.5(5)	886.7(2)
v-4	885.6(6)	885.8(6)	886.0(2)
v-3	884.9(2)	885.1(7)	
v-2	884.3(2)	884.5(10)	884.7(3)
v-1		884.0(5)	884.1(4)
v			883.7(4)

IX. System

Band heads, λ (Intensity) (70.10). These bands are very diffuse and have not been positively identified.

v'	v''	0	1
v-5		849.8(2)	850.0(1)
v-4		849.0(2)	
v-3		848.1(4)	
v-2		847.4(6)	847.5(4)
v-1		846.7(8)	846.9(1)
v		846.1(10)	846.3(5)

SPECTROSCOPIC CONSTANTS

Molecule <u>Ar₂</u>									
State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ³	D _e	r _e	Remarks	Bibliography
X ¹ Σ _g ⁺	0	30.68	2.56	0.060	4.0	91.6	3.8		(73.19, 70.10)
Dissociation energy = 9.53 × 10 ⁻³ eV, 220 cal/mole, 76.9 cm ⁻¹ (70.10).									

Perturbations and General Information

Laser action has been observed at 1261 Å from the $^3,1\Sigma_u \rightarrow X^1\Sigma_g^+$ transition (74.23).

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As₂As₂Methods of Production and Experimental Technique

Absorption.

Fluorescence.

Emission in a discharge tube containing arsenic

a. in the presence of hydrogen, neon, or helium

b. continuous flow.

Excitation by rf discharge in arsenic and neon.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$c(^3\Sigma_u^+) \rightarrow X(^1\Sigma_g^+)$	Discharge	8400-5380	R			(74.19, 72.17, 67.8)
	II	$e \rightarrow X(^1\Sigma_g^+)$	Discharge	6250-4440	R			(74.19, 72.17, 67.8)
	III	$a(^3\Sigma_u^+) \rightarrow X(^1\Sigma_g^+)$	Discharge	4500-3700	R	4317.9(2,5) 3870.5(5,1)		(74.19, 72.17, 70.14, 66.7, 37.4)
	IV	$A(^1\Sigma_u^+) \rightarrow X(^1\Sigma_g^+)$	Discharge	5555-2240	R	2506.9(5,4) 2449.9(7,3)		(74.19, 72.17, 70.15, 65.6, 37.4, 35.3, 34.2)
	V	$B(^1\Sigma_u^+) \rightarrow X(^1\Sigma_g^+)$	Discharge	5530-2350	R	3150.6(2,24) 2998.3(1,19) 2554.4(0,4)		(74.19, 72.17, 70.15, 37.4, 35.3)
	VI	$b(^3\Pi_u) \rightarrow X(^1\Sigma_g^+)$	Discharge	3840-2984	R	3235.9(0,18) 3198.2(0,2)	Single progression ($v' = 0$)	(74.19, 72.17, 37.4, 35.3)
	VII	$d(^3\Pi_g) \rightarrow X(^1\Sigma_g^+)$	Discharge	3390-2980	R	3180 (2,0)		(74.19, 72.17, 67.9)
	VIII	$F \leftarrow X(^1\Sigma_g^+)$	Absorption	2050-1800	V	1915.5(0,0)		(74.19, 72.17)
	IX	$G \leftarrow X(^1\Sigma_g^+)$	Absorption	1915-1775	V	1832.5(0,0)		(74.19, 72.17)

Molecule As₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	X	$a^3\Sigma_u^+ \rightarrow c(^3\Sigma_u^+)$	Discharge	10000-7400	V	8506		(74.19, 67.9)
	XI	$d(^3\Pi_g) \rightarrow c(^3\Sigma_u^+)$	Discharge	7000-5600	V	6051.3(1,0) 5992.6(1,0)		(74.19, 72.17, 67.9)

Molecule As₂

As₂

I. c(³Σ_u⁺) → X¹Σ_g⁺ System

Distinct bands, λ (70.14):

v', v''	0	1	2	3	4	5	6	7
0						8126	8410	8713
1				7428	7667			
2			7047	7263	7491	7733		
3		6702		7106	7324	7556	7803	
4		6567	6755				7620	
5		6439			7012	7226		
6	6152	6317					7283	
7	6040	6200						

II. e → X¹Σ_g⁺ System

Distinct bands, λ (70.14):

v', v''	0	1	2	3	4	5	6	7
0						5633	5768	5910
1			5170	5286	5406			
2		4977	5085	5196				
3		4893	5002					
4	4725	4822						
5	4654							
6	4586							
7	4520							

III. a³Σ_u⁺ → X¹Σ_g⁺ System

Partial vibrational scheme, λ (70.14, 66.7, 37.4):

v', v''	0	1	2	3	4	5
0				4286.7	4365.1	4446.3
1		4079.8	4151.5	4225.1	4302.1	4381.3
2	3957.1	4024.5	4094.5			4317.9
3	3905.5	3972.2	4040.0			4256.8
4					4126.7	

IV. $A^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ SystemPartial vibrational scheme, λ (72.17, 65.6, 37.4):

v', v''	0	1	2	3	4	5	6	7
0								
...								
4						2551.6	2578.9	
5		2430.3	2455.0	2480.7	2506.9	2533.4		2587.9
6		2415.1	2439.4	2464.7	2490.6			2570.4
7	2376.5	2400.7	2424.9	2449.9				

V. $B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ SystemBands of greatest intensity, λ (37.4):

v', v''	2,24	1,23	2,23	1,22	1,19	0,7	6,10	6,9	0,4
λ	3150.6	3141.8	3113.8	3105.1	2998.3	2638.6	2615.6	2588.0	2554.4

VII. $d(^3\Pi_g) \rightarrow X^1\Sigma_g^+$ SystemPartial vibrational scheme, λ (37.4):

v', v''	0	1	2	3	4	5
0	3248.9	3294.7	3341.4	3389.3	3438.2	3488.4
1	3214.1	3258.7		3351.2	3399.3	3448.3
2	3180.1		3268.7	3314.6		3409.2
3	3147.0		3233.8	3278.8	3324.6	3311.4
4	3114.8	3157.1			3288.5	

VIII. $F \leftarrow X^1\Sigma_g^+$ SystemPartial vibrational scheme, λ (72.17):

v', v''	0	1	2	3	4	5	6	7
0	1915	1931	1947	1963	1980			
1	1902				1965			
2	1887					1966	1982	1998
3	1874				1935			1983
4	1862							

IX. G ← X¹Σ_g⁺ System

Partial vibrational scheme, λ (72.17):

v', v''	0	1	2	3	4	5	6	7
0	1833	1847	1862	1876	1892	1907		
1	1820	1834		1863	1878	1983	1908	
2	1808		1836			1880	1894	1909
3	1796							
4	1784							1883
5	1775						1858	1872

X. a³Σ_u⁺ → c³Σ_u⁺ System

Many bands have been seen for this system but as yet remain unclassified. Some of the more intense bands are (67.9):

8794, 8759, 8738, 8507, 8318, 8256

XI. d³Π_g → c³Σ_g⁺ System

Partial vibrational scheme, λ (Intensity) (67.9):

v', v''	0	1	2	3	4	5	6
0	6118(3)	6236(3)	6359(2)	6486(1)	6616(0)	6748(0)	
	6180(3)	6299(4)	6425(3)	6554(2)		6824(1)	
1	5996(6)	6111(2)	6227(1)	6448(2)	6474(1)	6602(0)	6736(0)
	6054(6)	6171(2)	6289(2)	6313(3)	6541(2)	6673(1)	6809(1)
2	5879(7)	5988(0)	6101(3)	6217(2)		6462(1)	6588(0)
	5935(6)	6046(0)	6162(3)	6279(1)	6399(0)	6528(2)	6658(1)
3	5767(3)	5872(8)		6092(2)	6208(1)	6325(0)	
	5822(3)	5929(7)		6154(2)	6269(1)	6390(0)	
4		5762(3)		5974(0)		6199(0)	
		5816(3)		6031(0)		6260(0)	6380(0)
5			5756(2)				
			5810(0)				

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^8$	r_e	Remarks	Bibliography
G	54590	335.0	3.2						(72.17)
F	52220								(72.17)
$b(^3\Pi_u)$	42000								(70.14)
$B^1\Sigma_u^+$	40898	302	5.8	0.07112 ^a					(74.20, 70.15, 70.14, 69.12)
$A^1\Sigma_u^+$	40336	280	1.0	0.0797	0.31	2.6	2.374		(74.20, 74.19, 73.18, 72.17, 70.15, 70.14)
$d(^3\Pi_g)$	30818	336.7	1.36	0.09222	0.33	2.8	2.209		(70.14,
$a^3\Sigma_u^+$	24641	337.0	0.83	0.08666	0.30	2.3	2.279	d	(70.14)
e	19914	330.0	0.90						(70.14)
$c^3\Sigma_u^+(0_u^-)$	14643	314.3	1.09	0.08492	0.35		2.302	c	(70.14)
$c^3\Sigma_u^+(1_u)$	14479	314.3	1.09	0.08472	0.35	1.6	2.305	c	(70.14)
$X^1\Sigma_g^+$	0	429.55	1.117	0.10179	0.333	1.4	2.104	b	(70.14)

^a B_0 ; ^b $\gamma_e = -2.8 \times 10^{-7}$, $\gamma_e \omega_e = 1.39 \times 10^{-4}$, $z_e \omega_e = 1.958 \times 10^{-5}$; ^c $\lambda = -1.38$; ^d $\lambda = -0.55$
Dissociation energy = 3.96 eV, 91.3 kcal/mole, 31950 cm^{-1} .

Perturbations and General Information

Potential energy curves (67.10):

State	v	T(v)(cm ⁻¹)	r _{min} (Å)	r _{max} (Å)
X ¹ Σ _g ⁺	0	214.3	2.243	2.332
	1	641.7	2.211	2.371
	2	1067.0	2.192	2.397
	3	1489.7	2.175	2.417
	4	1910.2	2.163	2.440
	5	2328.4	2.152	2.458
	6	2744.6	2.141	2.475
	7	3158.4	2.131	2.489
	8	3570.4	2.122	2.507
	9	3979.4	2.115	2.525
	10	4386.5	2.107	2.540
	11	4791.5	2.100	2.554
	12	5194.0	2.094	2.568
	13	5594.4	2.087	2.581
	14	5992.5	2.081	2.594
	15	6388.4	2.075	2.608
	16	6782.0	2.070	2.622
	17	7170.3	2.064	2.635
	18	7562.5	2.060	2.646
	19	7949.1	2.055	2.659
	20	8333.7	2.051	2.671
a ³ Σ _u ⁺	0	24810.9	2.464	2.568
	1	25146.3	2.430	2.610
	2	25480.7	2.408	2.640
	3	25812.9	2.391	2.668
	4	26143.1	2.376	2.691
	5	26471.5	2.362	2.712
	6	26798.1	2.351	2.731
	7	27122.7	2.340	2.751
A ¹ Σ _u ⁺	0	40474.3	2.745	2.858
	1	40736.7	2.710	2.918
	2	40989.4	2.687	2.958
	3	41205.0	2.672	3.010

Franck-Condon factors for a ${}^3\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ (68.11):

v', v''	0	1	2	3	4	5	6	7	8
0	0.0029	0.0149	0.0459	0.1015	0.1394	0.1941	0.1653	0.1674	0.0853
1	0.0160	0.0582	0.1181	0.1460	0.0916	0.0318	0.0086	0.0901	0.1508
2	0.0437	0.1151	0.1321	0.0558	0.0011	0.0317	0.1012	0.0438	0.0017
3	0.0685	0.1206	0.0590	0.0000	0.0447	0.0818	0.0139	0.0147	0.0836
4	0.1086	0.1093	0.0089	0.0332	0.0638	0.0184	0.0248	0.0604	0.0145
5	0.1464	0.0471	0.0088	0.0626	0.0140	0.0160	0.0576	0.0053	0.0383
6	0.1498	0.0157	0.0362	0.0446	0.0004	0.0471	0.0102	0.0144	0.0425
7	0.1326	0.0000	0.0635	0.0071	0.0291	0.0337	0.0103	0.0468	0.0010

The perturbations that appear in (2,14) and (2,15) bands of $A^1\Sigma_u^+ \approx X^1\Sigma_g^+$ system as well as in the (0,5) and (0,6) bands of $B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ system have been shown to be due to a mutual interaction between $A(v=2)$ and $B(v=0)$ levels, although this has been shown to be relatively weak (74.20, 70.15).

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Au₂

Au₂

Methods of Production and Experimental Technique

Emission at ~2100° C.

Absorption in a King furnace at ~2000° C.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$AO_u^+ \approx X^1\Sigma_g^+$	Absorption	6500-4300	R	19643.8		(67. 8, 54. 1)
	II	$BO_u^+ \approx X^1\Sigma_g^+$	Absorption	4100-3800	R	25679.9		(67. 8, 59. 5, 54. 2)

Molecule Au₂

I. AO⁺ ≈ X¹Σ_g⁺ System

Intense bands, λ (72.9, 54.1):

v', v''	0	1	2	3	4	5
0	5089.2	5138.9	5189.5	5240.7	5292.9	5345.8
1	5052.8	5112.2		5202.2	5253.4	5305.4
2	5017.2		5114.5	5164.5		
3	4982.3		5078.2		5177.2	5227.6
4	4947.0	4995.1				

II. BO_u⁺ ≈ X¹Σ_g⁺ System

Intense bands, λ (59.5):

v', v''	0	1	2	3	4
0	3892.9	3921.9			
1	3866.0		3923.6	3952.8	
2	3839.7	3868.0			3954.5
3		3841.8			

SPECTROSCOPIC CONSTANTS

Molecule An₂

State	T _e	ω _e	x _e ω _e	B _e × 10 ²	α _e × 10 ⁵	D _e × 10 ⁴	r _e	Remarks	Bibliography
BO _u ⁺	25679.87	179.85	0.680	2.7000	9.6		2.5174	y _e w _e = +0.003	(67.8, 59.5)
AO _u ⁺	19668.1	142.3	0.445	2.5958	9.0		2.5678	y _e w _e = -0.0015	(72.9, 67.8, 54.1)
X ¹ Σ _g ⁺	0	190.9	0.420	2.8013	7.2	1.68	2.4719	y _e w _e = -0.0001	(67.8, 65.7, 54.1)
Dissociation energy = 2.34 ± 0.1 eV, 53.9 kcal/mole, 18850 cm ⁻¹ (60.6).									

Perturbations and General Information

Potential energy curves (72.9):

State	v	U+Te(cm ⁻¹)	r _{max} (Å)	r _{min} (Å)
XO _g ⁺	0	95.4	2.515	2.430
	2	475.3	2.573	2.384
	4	852.0	2.612	2.356
	6	1225.5	2.645	2.336
	8	1594.0	2.673	2.320
	10	1959.4	2.700	2.304
	12	2321.9	2.724	2.291
	14	2680.6	2.747	2.280
	16	3037.0	2.770	2.268
	18	3389.5	2.793	2.259
	20	3738.3	2.814	2.249
AO _u ⁺	0	19739.1	2.618	2.520
	2	20021.2	2.687	2.466
	4	20299.3	2.734	2.436
	6	20574.0	2.774	2.414
	8	20844.6	2.807	2.393
	10	21111.3	2.842	2.380
	12	21374.2	2.872	2.364
	14	21633.3	2.902	2.352
	16	21870.3	2.928	2.340
	18	22136.5	2.958	2.328
	20	22385.5	2.987	2.318

Au₂

Franck-Condon Factors and r-Centroids of the $\text{AO}_u^+ - \text{XO}_g^+$ System (72. 9):

v', v''	0	1	2	3	4	5	6
0	0. 107 2. 518 2	0. 237 2. 542 3	0. 266 2. 564 4	0. 300 2. 587 5	0. 117 2. 610 2	0. 057 2. 632 1	0. 016
1	0. 234 2. 500 3	0. 161 2. 523 2	0. 008 2. 547	0. 009 2. 570 1	2. 592	2. 615	
2	0. 261 2. 482 3	0. 012 2. 506	0. 120 2. 529 2	0. 096 2. 552 2	2. 576	2. 599	
3	0. 198 2. 464 2	0. 042 2. 488	0. 236 2. 512 3	2. 535	2. 558	2. 580	
4	0. 114 2. 446 2	0. 147 2. 571 2	2. 494	2. 518	2. 542	2. 564	
5	0. 065 1						

Top line = Franck-Condon factor
 Middle line = r-Centroids
 Bottom line = Intensity

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Methods of Production and Experimental Technique

Emission from a high voltage ac discharge in He + BCl₃.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$^3\Sigma_u^- - X^3\Sigma_g^-$	Discharge	3300-3170	R	3272.8(0,0)		(74.7, 40.2, 40.1)

Molecule B₂

B₂

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

Band heads, λ (40.1):

(v', v'')	(3, 3)	(2, 2)	(1, 1)	(0, 0)	(4, 3)	(3, 2)	(2, 1)	(1, 0)
λ	3300.5	3292.7	3283.4	3272.8	3204.2	3196.3	3178.1	3176.4
Intensity	2	8	9	10	0	1	2	3

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^4$	r_e	Remarks	Bibliography
$3\Sigma_u^-$	30573.4	937.4	2.6	1.160	11		1.625		(67.5, 59.3, 40.1)
$X^3\Sigma_g^-$	0	1051.3	9.4	1.212	14	5.13	1.589		(74.7, 67.5, 59.3, 40.1)
Dissociation energy = 2.9 ± 0.4 eV, 67 kcal/mole, 23400 cm^{-1} .									

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J. Chem. Phys. 60, 1288-96

Be₂

It has been calculated that the ground state ($^1\Sigma_g^+$) is repulsive (74.9).

Dissociation energy = <0.7 eV, <16 kcal/mole, <5600 cm⁻¹.

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J. Chem. Phys. 60, 1288-96

Methods of Production and Experimental Technique

Absorption.

Thermal Emission.

Fluorescence.

Microwave Discharge.

Mass Spectrometric Methods.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$AO_u^+ \rightarrow X^1\Sigma_g^+$	Absorption $T > 850^\circ\text{C}$	7900-4500	R	5587(4, 2) 5725(2, 3) 5883(1, 5)		(70.23, 65.19, 35.13, 33.11)
	II	$C \rightarrow X^1\Sigma_g^+$	Absorption $T > 900^\circ\text{C}$	4000-2600		Continuous	Superimposed on System III	(70.23, 33.12)
	III	$D \rightarrow X^1\Sigma_g^+$	Absorption $T > 1000^\circ\text{C}$	2900-2600	R	2731.6(1, 0)		(70.23, 35.13, 33.12)
	IV	$F \rightarrow X^1\Sigma_g^+$	Absorption $T > 825^\circ\text{C}$	2270-2060	R	2188.8(0, 0)		(70.23, 33.12)
	V	$G \rightarrow X^1\Sigma_g^+$	Absorption	1930-1840	R	1857.2(0, 0)		(74.26)
	VI	$E \rightarrow A$	Absorption $T > 1000^\circ\text{C}$	4200-4000	R	4128.0(0, 2) 4105.5(0, 1)		(70.23, 33.12)
	VII	$G \rightarrow A$	Discharge	8820-8030	R	8528(0, 1) 8451(1, 1) 8359(1, 0)		(70.23)
	VIII	$H \rightarrow A$	Discharge	7050-6730	V	6733(0, 0) 6794(0, 1)		(70.23)
	IX	$I \rightarrow A$	Discharge	6570-6290	V	6457(0, 0) 6452(1, 1)		(70.23)
	X	?	Absorption	2500-2470		2492 2482 2470	3 continuous bands	(33.12)

Molecule Bi₂

Bi₂

I. AO_u⁺ ← X¹Σ_g⁺ System

Band heads, λ (Intensity) (70.23):

v',v''	0	1	2	3	4	5	6	7	8
0					5871(4)	5929(4)	5989(6)	6049(6)	6111(8)
1			5712(4)	5768(4)	5823(6)	5883(8)	5942(6)	6002(6)	
2			5669(4)	5725(6)	5780(6)	5837(6)		5955(4)	6015(6)
3	5521(4)		5628(4)	5682(6)	5738(4)			5909(4)	
4	5482(4)	5533(4)	5587(6)				5807(4)	5864(4)	
5	5443(2)	5494(4)	5547(6)	5599(2)		5708(4)	5763(4)		
6	5405(2)	5456(4)	5508(4)						5833(4)
7	5368(2)	5418(4)						5734(4)	
8	5332(4)	5381(4)					5639(4)		

II. C ← X¹Σ_g⁺ System

This system appears continuous with the upper state being a repulsive state in the region 4000-2600Å (70.23, 33.12).

III. D ← X¹Σ_g⁺ System

Band heads, λ (Intensity):

v',v''	0	1	2	3	4	5	6
0		2755.9(4)	2768.9(7)	2782.2(4)			
1	2731.6(9)	2744.5(6)			2783.7(5)	2796.7(7)	2810.2(5)
2	2720.7(7)						
3	2710.3(5)						

IV. F ← X¹Σ_g⁺ System

Bands unclassified, λ (Intensity):

2205.4(1) 2197.2(1) 2188.8(2) 2180.5(1) 2172.7(1) 2148.8(1) 2142.9(1) 2135.8(1)

V. G ← X¹Σ_g⁺ System

Band heads, λ (Intensity) (74.26):

v', v''	0	1	2	3	4	5
0	1857.1	1866.5	1876.0	1885.5	1895.0	1904.6
1	1850.8	1860.1		1879.0	1888.4	1897.9
2	1844.1					

VI. E ← A System

Band heads, λ (Intensity):

v', v''	0	1	2	3
0	4083.0(1)	4105.5(4)	4128.0(5)	4150.7(4)
1	4065.5(2)	4086.8(1)		
2	4049.3(1)			

VII. G → A System

Band heads, λ (Intensity) (70.23):

v', v''	0	1	2	3	4
0		8528(4)	8623(6)	8720(8)	8818(4)
1	8359(6)	8451(4)	8545(4)		
2	8286(6)				
3	8214(2)	8303(6)			
4					
5		8161(2)			
6		8091(2)			
7			8110(6)	8194(4)	
8			8041(6)		8209(4)

VIII. H → A System

Band heads, λ (Intensity) (70.23):

v', v''	0	1	2	3	4	5
0	6733(6)	6794(8)	6856(8)	6919(8)	6982(8)	7046(6)

Bi₂

IX. I → A System

Band heads, λ (Intensity) (70.23):

v', v''	0	1	2
0	6457(6)	6512(6)	6568(6)
1	6397(10)	6452(10)	6507(6)
2	6343(10)		
3	6295(6)		

In addition, three more bands have been seen but not identified:

6341(6) 6402(4) 6302(4)

X. System

Three continuous bands have been observed (33.12) in the region 2500-2470Å and not identified. They are:

2492 2482 2470

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^4$	$D_e \times 10^4$	r_e	Remarks	Bibliography
F	46000								(70.23, 33.12)
E	42252	129	9.7						(70.23, 33.12)
D	36457	157	4.6						(70.23, 33.12)
I	33216.9	156.4	6.1						(70.23)
H	32591								(70.23)
C	32000							Repulsive state	(70.23, 33.12)
G	29609.0	107.0	0.2						(70.23)
AO_u^+	17742.3	132.49	0.302	0.01968	0.53	1.452267	2.8629		(70.24, 70.23, 65.9, 35.13, 33.12)
X	0	172.71	0.341	0.022806	0.50	2.310872	2.6594		(70.24, 70.23, 65.19, 35.13, 33.12)
Dissociation energy = 1.85 ± 0.1 eV, 43 kcal/mole, 15040 cm^{-1} .									

Bi₂

Perturbations and General Information.

Potential energy curves (70.24):

State	v	Te+U(cm ⁻¹)	r _{min} (Å)	r _{max} (Å)
X ¹ Σ _g ⁺	0	86.3	2.617	2.704
	1	258.3	2.587	2.737
	2	430.5	2.568	2.762
	3	601.0	2.553	2.783
	4	771.5	2.540	2.801
	5	941.2	2.529	2.818
	6	1110.1	2.518	2.833
	7	1277.9	2.509	2.848
	8	1443.4	2.500	2.862
	9	1610.5	2.492	2.876
	10	1775.4	2.484	2.889
	11	1939.2	2.478	2.901
	12	2103.0	2.470	2.911
	13	2266.1	2.464	2.923
	14	2428.4	2.458	2.935
	15	2590.2	2.452	2.946
	16	2750.6	2.447	2.959
	17	2910.2	2.442	2.971
	18	3069.0	2.437	2.982
	19	3227.6	2.432	2.992
	20	3385.1	2.427	3.003
AO _u ⁺	0	17808.3	2.813	2.912
	1	17939.3	2.781	2.953
	2	18070.3	2.760	2.982
	3	18200.5	2.742	3.006
	4	18329.5	2.728	3.027
	5	18458.5	2.715	3.047
	6	18587.1	2.704	3.065
	7	18715.2	2.694	3.082
	8	18842.6	2.685	3.099
	9	18969.8	2.676	3.114
	10	19095.8	2.668	3.129
	11	19221.1	2.661	3.144
	12	19345.3	2.653	3.159
	13	19470.6	2.646	3.173
	14	19594.1	2.639	3.186
	15	19716.6	2.633	3.200
	16	19838.4	2.627	3.214
	17	19960.0	2.621	3.227
	18	20080.8	2.615	3.240
	19	20201.1	2.610	3.253
	20	20321.7	2.606	3.264

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Br₂Br₂Methods of Production and Experimental Technique

Absorption

Emission from a discharge, thermoluminescence, chemiluminescence, and flames

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$A^3\Pi_u \approx X^1\Sigma_g^+$ (1_u) (0_g^+)	Absorption, Emission, Chemilumi- nescence	8180-6450	R	13815		(67.58)
	II	$B^3\Pi_u \approx X^1\Sigma_g^+$ (0_u^+) (0_g^+)	Absorption, Emission	8672-5510	R	15814.3	Converges at $\lambda \sim$ 5110Å	(67.60, 47.39, 47.42, 37.22, 26.1)
	III	?	Discharge	6700-5100	R	16105		(28.2)
	IV	?	Discharge	6700-5100	R	17325.80		(28.2)
	V	?	Absorption	<5100	Continuum		Maximum at λ : 4950/4150	(47.40, 47.39, 34.16)
	VI	$C^3\Sigma^+ \rightarrow$ dissociation (1_u)	Emission	-	Continuum	31104.4	Dissoci- ates to $2p + 2p$ atoms	(67.63)
	VII	$D^3\Sigma_g^- \approx B^3\Pi_u$ (1_g or 0_g^+)	Emission	2950-2670	R	32620.70		(57.51)

Molecule Br₂

BAND SYSTEMS

	System	Transition	Sources	Wave.length Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	VIII	$E^1\Sigma_g^+ \rightarrow B^3\Pi_u$ (0_g^+)	Emission	3150-2970	R	35900.7		(57.52)
	IX	$H^3\Pi_g \rightarrow B^3\Pi_u$ (1_g or 0_g^+)	Emission	3150-2970		40854.7		(57.52, 57.51)
	X	$F^3\Sigma^- \rightarrow X^1\Sigma_g^+$ (1_u)	Emission	2100-1850	R	52090		(58.53)
	XI	$a\Pi_g \rightarrow$ dissociation	Emission	-	Continuum	39638.4	Dissociates to $2P + 2P$ atoms	(47.40)
	XII	$G^3\Sigma^- \rightarrow X^1\Sigma_g^+$ (0_u^+)	Emission	1850-1700	R	56303		(58.53)
	XIII	$J^1\Pi_g \rightarrow$ dissociation (1_g)	Emission	-	Continuum	45548.4	Dissociates to $2P + 2P$ atoms	(47.40)
	XIV	$d\Pi \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1510-1485	-	66227		(67.63)

Molecule Br₂

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	XV	$e\Delta \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1505	-	66473		(67.63)
	XVI	$f\Pi \rightarrow$ dissociation ($2_g, 1_g$)	Emission	-	Continuum	50604.4	Dissociates to $2P + 2P$ atoms	(67.63, 47.40)
	XVII	$K(^1\Sigma_u^+) \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1700-1500	R	(62500)		(67.63)
	XVIII	$g\Sigma^- \leftarrow X^1\Sigma_g^+$ (0_u^-)	Absorption	1458	-	68608		(67.63)
	XIX	$h\Sigma^+ \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1465-1410	-	68651		(67.63)
	XX	$i\Pi \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1460-1445	-	68814		(67.63)
	XXI	$j\Pi \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1442-1400		69396		(67.63)

Molecule Br₂



BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	XXII	$k\Pi \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1425-1410		70913		(67.63)
	XXIII	$i\Sigma^+ \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	(1399)		(71481)		(67.63)
	XXIV	$m\Pi \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1408-1380		71705		(67.63)
	XXV	$n\Sigma^- \leftarrow X^1\Sigma_g^+$ (0_u^+ or 1_u)	Absorption	1398-1367		71876		(67.63)
	XXVI	$L^3\Pi_u \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1383-1368		72674		(67.63)
	XXVII	$o\Delta \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	(1365)		(73240)		(67.63)
	XXVIII	$p\Sigma^+ \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1374-1360		73459		(67.63)

 Molecule Br_2

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{1/2}, 0$	Remarks	Bibliography
	XXIX	$M^3\Pi_u \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1369-1325		74018		(67.63)
	XXX	$q\Pi \leftarrow X^1\Sigma_g^+$ ($0_u^+, 1_u$)	Absorption	1355-1329		74161		(67.63)
	XXXI	$r\Pi \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1349-1330		74455		(67.63)
	XXXII	$s\Pi \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1352-1328		74651		(67.63)
	XXXIII	$t\Pi \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1344-1320		74768		(67.63)
	XXXIV	$N^1\Pi_u \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1325-1270		76491		(67.63)
	XXXV	$u\Sigma^+ \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1296-1278		77491		(67.63)

 Molecule Br_2

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	XXXVI	$\nu\Sigma^- \leftarrow X^1\Sigma_g^+$ ($0_u^+, 1_u$)	Absorption	1294-1283		77639		(67.63)

Molecule Br₂

Br₂

I. A³Π(1_u) ← X¹Σ_g⁺ System

Band heads of ⁷⁹Br₂, λ (72.73):

v', v''	3	4	5
7		7430	
8	7202	7370	
9	7149	7315	
10	7101	7264	7434
11	7056	7215	7385
12	7016	7175	
13	6979	7137	
14	6946	7103	

II. B³Π(0_u⁺) ← X¹Σ_g⁺ System

Band heads of ⁷⁹Br₂, λ (71.70):

v', v''	4	5	6	7	8	9	10
1						7599	
2					7339	7508	7682
3				7097	7255	7420	7591
4		6727	6871	7020	7175	7336	
5	6523	6659	6800	6947	7099		
6	6461	6595	6733	6877			
7		6533	6669	6810			
8		6465	6607				
9	6290		6549				

III. and IV. 6700-5100 Å Systems — the two systems are superimposed on one another (28.2).

a. $v = 17325.80 + 191.45 u' - 1.05 u'^2 - 360.65 u'' + 0.65 u''^2$

b. $v = 16105.00 + 152.40 u' - 0.40 u'^2 - 361.70 u'' + 1.62 u''^2$

u', u''	System	λ	u', u''	System	λ	u', u''	System	λ
		6664	1, 4	a	} 6217.0	7, 3	a	5699.9
		6646	7, 3	b		10, 0	b	5684.7
3, 4	b	6604.1	5, 2	b	6194.4			5661.1
0, 6	a	6579.0	2, 4	a	6144.8	8, 3	a	5644.7
4, 4	b	6540.7	1, 3	a	} 6083.1	7, 2	a	5586.1
2, 3	b	6519.7	7, 2	b		8, 2	a	5532.4
0, 2	b	6499.4	3, 4	a	6074.6	6, 1	a	5529.2
5, 4	b	6475.6	8, 2	b	6027.8	7, 1	a	5476.5
3, 3	b	6455.1	4, 4	a	6004.6			5463.9
1, 2	b	6435.9	9, 2	b	5975.8	10, 2	a	5428.6
2, 6	a	6421.2	3, 3	a	5945.7			5382.6
4, 3	b	6392.8	10, 2	b	5924.3	10, 1	a	5324.9
2, 2	b	6372.1	8, 1	b	5905.0	11, 1	a	5277.1
5, 3	b	6332.8	6, 4	a	5880.6	12, 1	a	5230.7
		6315.4	9, 1	b	5852.1		a	5205.6
2, 5	a	6282.0	5, 3	a	5819.7		a	5168.8
		6260.0	10, 1	b	5804.5	12, 0	a	5134.2
			6, 3	a	5758.3	15, 1	a	5100.7
			9, 0	b	5731.6			

V., VI., XI., XIII., and XVI. Dissociative Systems

The transitions have not been positively identified, λ (Intensity)
(67.63, 47.40):

3549.4(10)	2900.4(10)	2732.4(7)	2526.9(6)
3366.8(6)	2872.5(8)	2709.8(7)	2510.9(6)
3336.6(10)	2780.6(7)	2638.8(6)	2494.2(6)
2923.8(8)	2753.6(8)	2623.1(6)	2478.8(7)

VII. $D^3\Sigma_g^- \rightarrow B^3\Pi_u$ System

Band heads, λ (67.63, 57.51):

2813.3(0, 2) | 2800.3(0, 1) | 2792.1(0, 0) | 2788.9(1, 1) | 2777.6(2, 1)

VIII. $E^1\Sigma_g^+ \rightarrow B^3\Pi_u$ System

Band heads, λ (72.71, 57.52):

3098.4(0, 2) | 3083.6(0, 1) | 3067.9(1, 1) | 3067.9(0, 0) | 3053.0(2, 1)

Br₂

XIV. $d\Pi(1_u) \leftarrow X^1\Sigma_g^+$ System

First member of a Rydberg Series represented by:

$$\nu = 85165 - R/(n - 2.593)^2, \quad n = 5, 6, 7, \dots 20 \quad (67.63)$$

(ν' , ν''), λ (Intensity) for $n = 5$ level

(0, 0)	1505.96(10)	
(1, 0)	1502.43(10)	
(2, 0)	1495.10(8)	
(3, 0)	1488.12	(4)
	1488.03	
	1487.96	
	1487.90	

XV. $e\Delta(1_u) \leftarrow X^1\Sigma_g^+$ System

Weak system, probably a forbidden transition.

ν', ν''	0	1
0	1504.37(4)	1511.53
1	1495.82(4)	1503.08(4)
2	1487.01(4)	

XVIII. $g\Sigma^-(0_u^-) \leftarrow X^1\Sigma_g^+$ System

Weak system, probably a forbidden transition (67.63):

(ν' , ν'')	λ (Intensity)
0, 1	1464.43(2)
0, 0	1457.56(2)
1, 0	1450.43
	1450.49
	1450.39

XIX. $h\Sigma^+(0_u^+) \leftarrow X^1\Sigma_g^+$ System

First member of a Rydberg Series represented by:

$$\nu = 35165 - R/(n - 2.422)^2, \quad n = 5, 6, 7, \dots 20 \quad (67.63)$$

(ν' , ν''), λ (Intensity) for $n = 5$ level

ν', ν''	0	1	2
0	1456.64(10)	1463.49(4)	
1	1445.63(8)	1456.41(6)	1463.25(4)
2	1441.82(8)		
3	1438.25(8)		
4	1430.98(8)		
5		1430.45(6)	
		1430.35(6)	
		1430.27(6)	
6	1417.25(6)	1423.95(6)*	
	1417.13(6)	1423.81(6)*	
	1416.99(6)	1423.69(6)*	
7	1410.89(6)	1417.07(4)	1423.55(4)
	1410.76(6)		1423.45(4)
	1410.66(6)		
	1410.48(6)		

*Has also tentatively been classified as part of the (5, 0) system.

XX. $i\Pi(1_u) \leftarrow X^1\Sigma_g^+$ System

First member of a Rydberg Series represented by:

$$\nu = 88306 - R/(n - 2.629)^2, \quad n = 5, 6, 7 \quad (67.63)$$

(ν' , ν''), λ (Intensity) for $n = 5$ level

ν', ν''	0	1	
0	1453.28(8) } 1453.21(8) } 1433.17(8) }	1460.05(2)	(a) Has also tentatively been identified as the (1,1) level.
1	1446.55(6) } 1446.51(6) } 1446.47(6) }		(b) Has also tentatively been identified as the (2,1) level.
2	1435.76(2)		

Br₂

XXI. $j\Pi(0_u^+) \leftarrow X^1\Sigma_g^+$ System

First member of a Rydberg Series represented by:

$$v = 88306 - R/(n - 2.591)^2, \quad n = 5, 6, 7 \quad (67.63)$$

(v', v''), λ (Intensity) for n = 5 level

v', v''	0	1	2
0	1441.05(6) 1441.01(6) 1440.97(6)		
1	1434.37(6) 1434.33(6) 1434.29(6) 1434.25(6)		
2	1427.51(8) 1427.39(8) 1427.33(8) 1427.27(8)	1434.04(6) 1433.96(6) 1433.88(6)	1440.55(2)
3	1420.64(4) 1420.54(4) 1420.47(4) 1420.41(4)	1427.21(6) 1427.13(6) 1427.06(6)	1433.75(4) 1433.65(4) 1433.57(4)
4	1414.23(4) 1414.09(6) 1413.59(4) 1413.83(6)	1420.35(4) 1420.31(4) 1420.29(4)	1426.90(4) 1426.84(4) 1426.80(4)
5	1407.36(2)* 1407.28(2)* 1407.20(2)*	1413.67(4) 1413.61(4) 1413.55(4)	1420.15(2)
6	1400.62(2)		

*Has also been tentatively identified as part of the m₅(0,2) level.

XXII. $k\Pi(1_u) \leftarrow X^1\Sigma_g^+$ System

Bands with $v' \geq 1$ have not been observed. First member of a Rydberg Series represented by:

$$v = 85165 - R/(n - 2.225)^2, \quad n = 5, 6, 7, \dots 20 \quad (67.63)$$

(v', v''), λ (Intensity) for $n = 5$ level

v', v''	0	1	2
0	1410.18(10)	1416.71(6)	1423.04(4)
	1410.04(10)	1416.61(6)	1422.96(4)
		1416.51(6)	1422.88(4)
		1416.45(6)	1422.80(4)
		1416.35(6)	

XXIII. $1\Sigma^+(1_u) \leftarrow X^1\Sigma_g^+$ System

First member of a Rydberg Series represented by:

$$v = 88306 - R/(n - 2.446)^2, \quad n = 5, 6, 7 \quad (67.63)$$

(v', v''), λ (Intensity) for $n = 5$ level

v', v''	0	1
0	1399.15(6)	1405.46(4)
	1399.09(6)	1405.32(4)
	1398.97(6)	1405.24(4)
	1398.88(6)	1405.15(4)
	1398.62(6)	1405.05(4)
	1398.58(6)	1404.93(4)
	1398.52(6)	

Br₂

XXIV. $m\Pi(1_u) \leftarrow X^1\Sigma_g^+$ System

Member of a Rydberg Series (67.63)

(v', v''), λ (Intensity) for n = 5 level

v', v''	0	1	2
0	1394.64(8) 1394.60(8) 1394.56(8) 1394.51(8) 1394.41(8)	1400.89(4)	1407.36(2)* 1407.28(2)* 1407.20(2)*
1	1388.45(6) 1388.35(6) 1388.19(6) 1388.12(6)		

*Has also been tentatively described as the (5,0) level of the j₅ state.

XXV. $n\Sigma^-(0_g^+ \text{ or } 1_u) \leftarrow X^1\Sigma_g^+$ System

First member of a Rydberg Series represented by:

$$\nu = 88306 - R/(n - 2.416)^2, \quad n = 5, 6, 7 \quad (67.63)$$

(v', v''), λ (Intensity) for n = 5 level

v', v''	0	1
0	1391.28(4)	1397.57(4)
1	1385.33(4)* 1385.20(4)* 1385.06(4)*	1391.36(4)
2	1379.12(4) 1379.06(4) 1378.99(4)	
3	1373.19(4) 1373.14(4) 1373.08(4)	
4	1367.41(4)	1373.44(2)

*May also be tentatively assigned to the (2,1) level.

XXVI. $L^3\Pi_u(1_u) \leftarrow X^1\Sigma_g^+$ SystemBand heads, λ (Intensity) (67.63):

v', v''	0	1
0	1376.01(6)	1382.15(4)
1	1372.01(6)	1378.11(4)
2	1368.14(4)	1374.04(2)

XXVII. $o\Delta(1_u) \leftarrow X^1\Sigma_g^+$ System

Represents a forbidden transition. Only the (0,0) and (0,1) bands have been identified (67.63).

v', v''	λ (Intensity)
(0, 0)	1365.37(2)
(0, 1)	1371.38(3)

XXVIII. $p\Sigma^+(0_u^+) \leftarrow X^1\Sigma_g^+$ System

First member of a Rydberg Series represented by:

$$v = 85165 - R/(n - 1.938)^2, \quad n = 5, 6, 7 \cdots 18 \quad (67.63)$$

v', v''	λ (Intensity) for $n = 5$ level
(0, 0)	1361.30(6)
	1361.10(6)
(0, 1)	1367.28(4)

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XXIX. $M^3\Pi_u(0_u^+) \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (Intensity) (67.63):

v', v''	0	1	2	3
0	1351.00(8)	1356.96(6)	1363.97(6) 1362.90(6) 1362.82(6)	1368.85(2)
1	1346.64(10)	1352.52(6)	1358.44(4)	
2	1342.35(8) 1342.30(8) 1342.26(8)	1348.29(6) 1348.20(6) 1348.11(6)		
3	1338.01(8)			
4	1333.87(4) 1333.80(4) 1333.74(4)			
5	1329.58(6) 1329.50(6) 1329.43(6)			
6	1325.26(2)			

XXX. $q\Pi(0_u^+ \text{ or } 1_u^+) \leftarrow X^1\Sigma_g^+$ System

First member of a Rydberg Series represented by:

$$v = 85165 - R/(n - 1.843)^2, \quad n = 5, 6, 7 \dots 12 \quad (67.63):$$

(v', v''), λ (Intensity) for $n = 5$ level

v', v''	0	1
0	1348.47(4) 1348.42(4) 1348.36(4)	1354.30(2)
1	1342.16(2)	
2	1336.01(4) 1335.95(4) 1335.86(4)	
3	1329.80(4)	1335.61(6) 1335.54(6) 1335.43(6) 1334.94(6)

XXXI. $r\Pi(0_u^+) \leftarrow X^1\Sigma_g^+$ System

Probably a Rydberg transition. Assignment is tentative (67.63).

(v', v''), λ (Intensity) for $n = 5$ level

v', v''	0	1
0	1343.09(4)	
1	1337.15(6) 1337.08(6) 1336.97(6)	1342.82(4)
2	1331.01(2)	1336.72(2)

XXXII. $s\Pi(1_u) \leftarrow X^1\Sigma_g^+$ System

Represents a Rydberg transition (67.63).

(v', v''), λ (Intensity) for $n = 5$ level

v', v''	0	1	2
0	1339.33(6) 1339.62(6) 1339.75(6)	1345.35(2)	1351.22(4)
1	1334.19(6)	1340.14(6) 1339.98(6) 1339.94(6)	
2	1328.69(4)	1334.43(6) 1334.40(6)	
3		1328.96(6) 1328.78(6)	

XXXIII. $t\Pi(0_u^+) \leftarrow X^1\Sigma_g^+$ System

Represents a Rydberg transition (67.63).

(v', v''), λ (Intensity) for $n = 5$ level

v', v''	0	1
0	1337.52(6) 1337.47(6) 1337.43(6) 1337.33(6) 1337.29(6)	1343.27(2)
1	1332.16(8)	1337.94(8) 1337.86(8)
2	1326.96(4)	1332.69(8)
3	1321.56(4)	

XXXIV. $N^1\Pi_u(1_u) \leftarrow X^1\Sigma_g^+$ SystemBand heads, λ (Intensity) (67.63):

v', v''	0	1	2
0	1307.34(6)	1312.85(4)	1318.37(4)
1	1303.51(10)	1308.97(8)	1314.47(6) 1314.44(6)
2	1299.60(8) 1299.49(8) 1299.41(8)	1304.94(8)	1310.39(6)
3	1295.44(8)	1300.83(6)	1306.25(4)
4	1291.61(8) 1291.46(8) 1291.32(8)	1296.97(4) 1296.83(4)	
5	1287.55(8)	1292.96(4)	
6	1283.61(6)	1288.93(2)	
7	1279.84(6) 1279.59(6) 1279.30(6)	1285.08(4)	1290.42(6)
8	1276.54(6)	1278.42(4)	1287.13(4)
9	1273.25(6)		1283.75(4)
10	1270.00(4)	1275.17(4)	1280.39(4)

XXXV. $u\Sigma^+(1_u) \leftarrow X^1\Sigma_g^+$ System

Represents a Rydberg transition. Assignment is tentative (67.63).

 (v', v'') , λ (Intensity) for $n = 5$ level

v', v''	0	1
0	1295.87(6) 1295.82(6) 1295.76(6) 1290.47(6)	
1	1284.27(6)	1289.64(2)
2	1278.43(6) 1278.20(6) 1278.13(6)	1283.43(4)

XXXVI. $\nu\Sigma^-(0_u^+, 1_u) \leftarrow X^1\Sigma_g^+$ System

Represents a Rydberg transition. Assignment is tentative (67.63).

(v' , v''), λ (Intensity) for $n = 5$ level

v', v''	0	1
0	1288.08(8) 1288.01(8) 1287.95(8)	1293.16(2)
1	1283.01(2)	1288.36(6)

SPECTROSCOPIC CONSTANTS

Molecule Br₂

State	T ₀	ω ₀	x ₀ ω ₀	B _e	α _e × 10 ³	D _e × 10 ⁸	r _e	Remarks	Bibliography
vΣ ⁺ (0 ⁺ , 1 _u)	77639	303						Rydberg	(67.63)
uΣ ⁺ (1 _u)	77491	374						Rydberg	(67.63)
N ¹ Π _u (1 _u)	76491	230							(67.63)
tΠ(0 ⁺)	74768	299	~1					Rydberg	(67.63)
sΠ(1 _u)	74651	303						Rydberg	(67.63)
rΠ(0 ⁺)	74455	341	(1.0)					Rydberg	(67.63)
qΠ(0 ⁺ , 1 _u)	74161	346						Rydberg	(67.63)
m ³ Π _u (0 ⁺)	74018	241	(0.3)						(67.63)
pΣ ⁺ (0 ⁺)	73459							Rydberg	(67.63)
oΔ(1 _u)	(73240)								(67.63)
L ³ Π _u (1 _u)	72674	215	~3						(67.63)

SPECTROSCOPIC CONSTANTS

Molecule Br_2									
State	T_0	ω_0	$\times \omega_0$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^8$	r_e	Remarks	Bibliography
$n\Sigma^-(0_u^+, 1_u)$	71876	313						Rydberg	(67.63)
$m\Pi(1_u)$	71705	323	(1.0)					Rydberg	(67.63)
$1\Sigma^+(1_u)$	(71481)							Rydberg	(67.63)
$k\Pi(1_u)$	70913							Rydberg	(67.63)
$j\Pi(0_u^+)$	69396	338	(1.0)					Rydberg	(67.63)
$i\Pi(1_u)$	68814	324						Rydberg	(67.63)
$h\Sigma^+(0_u^+)$	68651	330						Rydberg Perturbed, possibly predissoci- ated	(67.63)
$g\Sigma^-(0_u^-)$	68608	339							(67.63)
$K(1\Sigma_u^+)(0_u^+)$	(62500)	(293)							(67.63, 58.53)
$f\Pi(2, 1_g)$	66500	480							(67.63, 47.40)
$e\Delta(1_u)$	66473	381							(67.63)

SPECTROSCOPIC CONSTANTS

State	T_0	ω_0	$\times \omega_0$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^8$	r_e	Remarks	Bibliography
$d\Pi(1_u)$	66227	335	3.0					Rydberg	(67.63)
$J^1\Pi(1_g)$	61444	220							(67.63, 47.40)
$H^3\Pi_g$	56669	106.5	1.5						(67.63, 57.51)
$(1_g, 0^+)$									
$G^3\Sigma^-(0_u^+)$	56303	255							(67.63, 58.53)
$a\Pi(1_g)$	55534	330							(67.63, 47.40)
$F^3\Sigma^-$	52090	120							(67.63, 58.53)
$E^1\Sigma^+(0_g^+)$	51715	149.2	1.15						(67.63, 57.51)
$D^3\Sigma_g^-$	48435	161.7	0.29						(67.63, 63.55, 57.52, 57.51)
$(1_g, 0^+)$									
$C^3\Sigma^+(1_u)$	(47000)								(67.63, 47.40)

SPECTROSCOPIC CONSTANTS

State	T_0	ω_0	$\times \omega_0$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^8$	r_e	Remarks	Bibliography
$B^3\Pi_u(0^+)$	15840	166.1	1.84	0.0585	0.41	2.8	2.686		(67.63, 67.60, 37.22, 32.11)
$A^3\Pi_u(1_-)$	13815	150	2.7						(67.63, 67.59, 67.58, 37.22, 32.11)
$X^1\Sigma_g^+(0^+)$	0	323.07	1.167	0.081101	0.321	2.05	2.2809		(67.63, 67.60)
Dissociation energy = 1.970 eV, 45.44 kcal/mole, $15893 \pm 2 \text{ cm}^{-1}$.									

Br₂

Perturbations and General Information

The B³Π(0_u⁺) state appears to be predissociated (73.75).

The hΣ⁺(0_u⁺) state appears to be perturbed and possibly predissociated in the region v'' = 1 to 4 (67.63).

Lifetimes — B³Π(0_u⁺) state v = 1, 3, 5 τ = 0.28 ± 0.1 μsec (71.69)

A³Π(1_u) state τ = 1 msec (72.74)

Potential energy curve for the X¹Σ_g⁺ state using RKR potential (71.70):

T_e = 0

v	E(v)(cm ⁻¹)	r _{min}	r _{max}
0	162.38	2.2316	2.3342
1	485.52	2.1979	2.3762
2	806.49	2.1759	2.4067
3	1125.28	2.1586	2.4325
4	1441.87	2.1441	2.4555
5	1756.25	2.1315	2.4768
6	2068.39	2.1202	2.4967
7	2378.28	2.1101	2.5157
8	2685.93	2.1007	2.5339
9	2991.31	2.0921	2.5515
10	3294.38	2.0841	2.5685

Potential energy curve for the A³Π(1_u) state (⁷⁹Br₂) using RKR potential (72.71):

$$T_e = 13901 \text{ cm}^{-1}$$

v	E(v)	r _{min}	r _{max}
0	76.2	2.627	2.777
1	224.3	2.503	2.848
2	367.0	2.556	2.903
3	504.0	2.535	2.952
4	635.5	2.518	3.000
5	761.4	2.504	3.046
6	881.7	2.492	3.092
7	996.4	2.482	3.139
8	1105.23	2.473	3.188
9	1207.65	2.465	3.239
10	1303.43	2.457	3.293
11	1392.31	2.451	3.351
12	1474.07	2.445	3.414
13	1548.61	2.440	3.483
14	1615.98	2.436	3.558
15	1676.44	2.432	3.641
16	1730.50	2.428	3.730
17	1778.84	2.425	3.825
18	1822.21	2.423	3.925
19	1861.31	2.420	4.029
20	1896.72	2.418	4.138

Br₂

Potential energy curve for the B³Π(0_u⁺) state of (⁷⁹Br₂) using RKR potentials (71.70):

T_e = 15902.51

v	E(v')(cm ⁻¹)	r _{min}	r _{max}
0	83.37	2.6107	2.7541
1	247.63	2.5667	2.8172
2	408.58	2.5386	2.8648
3	566.11	2.5171	2.9065
4	720.17	2.4994	2.9450
5	870.71	2.4842	2.9816
6	1017.67	2.4710	3.0171
7	1160.99	2.4592	3.0519
8	1300.62	2.4485	3.0863
9	1436.47	2.4388	3.1206
10	1568.51	2.4299	3.1550
11	1696.70	2.4218	3.1898
12	1820.99	2.4143	3.2250
13	1941.34	2.4074	3.2608
14	2057.69	2.4012	3.2976
15	2169.99	2.3954	3.3351
16	2278.21	2.3897	3.3734
17	2382.33	2.3846	3.4131
18	2482.33	2.3796	3.4539
19	2578.20	2.3751	3.4962

Franck-Condon factors and r-Centroids for the $A^3\Pi - X^1\Sigma_g^+$ system of $^{79}\text{Br}^{81}\text{Br}$ using RKR potential (72. 74):

v', v''	0	1	2	3	4	5	6	7
0	- 2.456	- 2.467	- 2.479	- 2.491	- 2.503	- 2.515	0.00005 2.527	0.00017 2.540
1	- 2.451	- 2.462	- 2.474	- 2.485	0.00002 2.497	0.00009 2.509	0.00035 2.521	0.0011 2.533
2	- 2.445	- 2.457	- 2.468	- 2.480	0.00008 2.492	0.00038 2.504	0.0013 2.516	0.0040 2.528
3	- 2.441	- 2.452	- 2.463	0.00005 2.475	0.00028 2.486	0.0011 2.498	0.0036 2.510	0.0093 2.522
4	- 2.436	- 2.447	0.00002 2.459	0.00015 2.470	0.00072 2.481	0.0026 2.493	0.0075 2.505	0.0171 2.517
5	- 2.432	- 2.443	0.00005 2.454	0.00034 2.465	0.0015 2.477	0.0051 2.488	0.0129 2.500	0.0254 2.512
6	- 2.428	- 2.439	0.00012 2.450	0.00069 2.461	0.0028 2.472	0.0084 2.484	0.0189 2.495	0.0320 2.507
7	- 2.424	0.00003 2.434	0.00022 2.446	0.0012 2.457	0.0045 2.468	0.0122 2.479	0.0242 2.491	0.0350 2.502
8	- 2.420	0.00005 2.431	0.00039 2.442	0.0019 2.453	0.0066 2.464	0.0160 2.475	0.0279 2.487	0.0338 2.498
9	- 2.416	0.00008 2.427	0.00061 2.438	0.0023 2.449	0.0088 2.460	0.0193 2.471	0.0292 2.483	0.0290 2.494
10	- 2.413	0.00012 2.424	0.00088 2.435	0.0038 2.446	0.0110 2.457	0.0215 2.468	0.0282 2.479	0.0224 2.490

Top line = Franck-Condon factor
Bottom line = r-Centroid

Br₂

Franck-Condon factors and r-Centroids for the B³Π - X¹Σ_g⁺ system of ⁷⁹Br⁸¹Br (72.71) using exact Morse potentials.

v', v''	0	1	2	3	4	5	6	7
0	3. -10 2.4511	8. -9 2.4629	1. -7 2.4747	1. -6 2.4867	0.00001 2.4989	0.00003 2.5112	0.00013 2.5236	0.00046 2.5362
1	4. -9 2.4451	1. -7 2.4568	1. -6 2.4685	0.00001 2.4804	0.00006 2.4925	0.00028 2.5046	0.00102 2.5169	0.00307 2.5294
2	3. -8 2.4394	7. -7 2.4509	8. -6 2.4625	0.00006 2.4743	0.00030 2.4862	0.00122 2.4982	0.00391 2.5104	0.01017 2.5227
3	1. -7 2.4337	3. -6 2.4451	0.00003 2.4567	0.00022 2.4683	0.00102 2.4801	0.00364 2.4920	0.01015 2.5041	0.02243 2.5163
4	6. -7 2.4283	0.00001 2.4396	0.00011 2.4510	0.00063 2.4626	0.00265 2.4742	0.00832 2.4860	0.01992 2.4979	0.03672 2.5100
5	2. -6 2.4320	0.00003 2.4342	0.00028 2.4455	0.00151 2.4570	0.00564 2.4685	0.01542 2.4802	0.03131 2.4920	0.04690 2.5038
6	5. -6 2.4178	0.00008 2.4290	0.00064 2.4402	0.00309 2.4515	0.01022 2.4630	0.02411 2.4745	0.04075 2.4862	0.04775 2.4979
7	0.00001 2.4129	0.00018 2.4239	0.00128 2.4351	0.00557 2.4463	0.01617 2.4576	0.03257 2.4690	0.04470 2.4805	0.03852 2.4920
8	0.00003 2.4081	0.00036 2.4190	0.00232 2.4301	0.00899 2.4412	0.02281 2.4525	0.03863 2.4637	0.04153 2.4751	0.02350 2.4862
9	0.00005 2.4034	0.00065 2.4143	0.00383 2.4253	0.01322 2.4363	0.02906 2.4474	0.04059 2.4586	0.03243 2.4697	0.00930 2.4802

Top line = Franck-Condon factor followed by factor of ten
Bottom line = r-Centroid

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Methods of Production and Experimental Technique

Absorption in a King furnace.

Absorption from flash-photolysis or flash-discharge into mixtures of hydrocarbons and rare gases.

Emission from flames, arcs, and discharges with C, CO, CO₂, or hydrocarbon shock waves with and without rare gases.

Astrophysics: Absorption in stellar (type R and N) atmospheres.

Emission from comets.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Molecule C ₂	I	$b^3\Sigma_g^- \rightarrow a^3\Pi_u$	King furnace	27000-11000	R	17675(0,0)	Perturbed	(63.41, 63.40)
	II	$A^1\Pi_u \rightarrow X^1\Sigma_g^+$	Discharge	15490-6720	R	8750.8(2,0)	Perturbed	(70.126, 63.41)
	III	$d^3\Pi_g \rightarrow a^3\Pi_u$	Numerous sources	7850-3400	V	5635.5(0,1) 5165.2(0,0) 4737.1(1,0)	Perturbed	(73.135, 69.112, 63.43)
	IV	$C^1\Pi_g \rightarrow A^1\Pi_u$	Discharge	4110-3390	V	4102.3(0,1) 3852.2(0,0) 3607.3(0)	Perturbed	(67.80, 40.6, 30.4)
	V	$C^1\Pi_g \rightarrow A^1\Pi_u$	Discharge	3780-3390	V	(a)	Perturbed	(67.80)
	VI	$e^3\Pi_g \rightarrow a^3\Pi_u$	Discharge	3285-2370	R	2987(0,4) 2855(0,3)		(68.100, 49.8)

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Mulliken Freyemark Ultraviolet Region	VII	$D^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Discharge, Flames	2415-2310	R	2312.7(0,0)		(68.100, 39.5)
	VIII	$E^1\Sigma_g^+ \rightarrow A^1\Pi_u$	Discharge in C_2H_2	2220-2070	V	2218.2(0,1) 2142.9(0,0) 2072.4(1,0)	Perturbed	(51.10)
	IX	$f^3\Sigma_g^- \rightarrow a^3\Pi_u$	Absorption from flash discharge into mixtures of hydrocarbons and rare gases	1425-1370	R	1424.34(0,0) 1397.8(1,0) 1372.87(2,0)		(69.109)
	X	$g^3\Delta_g \rightarrow a^3\Pi_u$		1400-1365	R	1395.21(0,0) 1367.47(1,0)		(69.109)
	XI	$F^1\Pi_u \rightarrow X^1\Sigma_g^+$		1345-1310	R	1341.38(0,0) 1313.97(1,0)		(69.109)
(a) This band system has been observed by analysis of the perturbations of the $C^1\Pi_g \rightarrow A^1\Pi_u$ System.								

Molecule
C₂

Redesignation of the electronic states of C₂ based on work by Herzberg et al. (69.109). In assigning the new designation, the letter B has been left out since two predicted low lying singlet states have not yet been found.

<u>Old</u>	<u>New</u>	
$a^1\Sigma_g^+, x^1\Sigma_g^+$	$X^1\Sigma_g^+$	Lower state of Mulliken and Phillips bands
$X^3\Pi_u, X'^3\Pi_u$	$a^3\Pi_u$	Lower state of Swan bands
$A'^3\Sigma_g^-$	$b^3\Sigma_g^-$	Upper state of Ballik-Ramsay bands
$b^1\Pi_u$	$A^1\Pi_u$	Lower state of Deslandres-d'Azambuja bands
$A''^3\Sigma_g^+$	$c^3\Sigma_u^+$	From perturbations in upper state of Phillips bands
$A^3\Pi_g$	$d^3\Pi_g$	Upper state of Swan bands
$c^1\Pi_g$	$C^1\Pi_g$	Upper state of Deslandres-d'Azambuja bands
$c'^1\Pi_g$	$C'^1\Pi_g$	State perturbing $C^1\Pi_g$
$B^3\Pi_g$	$e^3\Pi_g$	Upper state of Fox-Herzberg bands
$d^1\Sigma_u^+$	$D^1\Sigma_u^+$	Upper state of Mulliken bands
$e^1\Sigma_u^+$	$E^1\Sigma_g^+$	Upper state of Freymark bands
	$f^3\Sigma_g^-$	Upper state of ultraviolet bands
	$g^3\Delta_g$	Upper state of ultraviolet bands
	$F^1\Pi_u$	Upper state of ultraviolet bands

C₂

I. $b^3\Sigma_g^- \rightarrow a^3\Pi_u$ System (Ballik-Ramsay)

Band heads, λ (Intensity) (63.41, 63.40, 62.36):

(v', v'')	(0, 1)	(0, 0)	(1, 0)	(2, 0)
λ (Intensity)	24745(2)	17675(4)	14075(3)	11726(1)

II. $A^1\Pi_u \rightleftharpoons X^1\Pi_g$ System (Phillips)

Band heads, λ (70.126, 67.76, 66.56, 64.45, 63.41):

(v', v'')	(0, 1)	(0, 0)	(2, 0)	(6, 3)	(5, 2)	(4, 1)
λ	15484.06	12070.21	8750.86	8315.86	8108.17	7907.69

(v', v'')	(3, 0)	(8, 4)	(7, 3)	(6, 2)	(5, 1)	(4, 1)	(8, 3)
λ	7714.58	7612.97	7428.12	7249.03	7076.79	6909.37	6722.59

III. $d^3\Pi_g \rightleftharpoons a^3\Pi_u$ System (Swan)

Band heads, λ (74.141, 74.140, 73.135, 71.130, 70.123, 69.112, 69.108, 67.83, 66.67, 66.58, 65.53):

v', v''	0	1	2	3	4	5	6
0	5165.2	5635.5	6191.3				
1	4737.1	5129.4	5585.5	6122.2	6762.4		
2	4382.2	4715.4	5097.7	5540.7	6059.7	6675.9	
3		4371.4	4697.6	5070.9	5501.9	6004.8	6599.1
4			4364.9	4684.9		5470.3	5959.0
5					4678.6		5447.7
6	3419	3619.5		4093	4368.8	4680.2	5030

IV. C¹Π_g → A¹Π_u System (Deslandres-d'Azambuja)

Band heads, λ (Intensity) (67.80, 40.6, 30.4):

v', v''		1	2	3	4	5
0	3852.2(10)	4102.3(9)				
1	3607.3(8)	3825.6(5)	4068.1(6)			
2	3399.8(5)	3592.9(7)		4041.9(3)		
3		3398.1(5)	3587.6(7)		4026.9(1)	
4			3405.1	3599.3		
5				3431.9	3617.9	
6						3689.0

Isotope shift studies (69.107).

V. C¹Π_g → A¹Π_u System (Messerle-Krauss)

Band heads determined by perturbations in C¹Π_g → A¹Π_u System, λ (67.80):

v', v''	(4, 6)	(3, 5)	(5, 6)	(2, 4)	(0, 2)	(1, 2)	(0, 1)
λ	3779.64	3691.54	3672.73	3627.03	3586.02	3405.66	3396.09

VI. e³Π_g → a³Π_u System (Fox-Herzberg)

Band heads, λ (49.8):

v', v''	0	1	2	3	4	5	6
0			2731.6	2855	2987	3129	3283
1			2656.3	2772.1	2896.4		
2		2486.3	2589.0	2698.8			
3		2429.9	2527.9				
4		2378.2					

VII. D¹Σ_u⁺ → X¹Σ_g⁺ System (Mulliken)

Band heads, λ (68.100, 39.5):

(v', v'')	(0, 1)	(3, 3)	(2, 2)	(1, 1)	(0, 0)
λ	2414.8	2316.8	2315.4	2314.0	2312.7

VIII. $E^1\Sigma_g^+ \rightarrow A^1\Pi_u$ System (Freymark)Band heads, λ (Intensity) (51.10):

v', v''	0	1	2	3	4
0	2142.6(10)	2218.2(7)			
1	2072.4(6)	2142.9(1)	2216.6(9)		
2		2075.6(6)			
3			2081.2(5)		
4				2087.1(5)	
5					2096.9(4)

IX. $f^3\Sigma_g^- \leftarrow a^3\Pi_u$ System (Ultraviolet)Band heads, λ (69.109):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	1424.34	1397.86	1372.87

X. $g^3\Delta_g \leftarrow a^3\Pi_u$ System (Ultraviolet)Band heads, λ (69.109):

(v', v'')	(0, 0)	(1, 0)
λ	1395.21	1367.47

XI. $F^1\Pi_u \leftarrow X^1\Sigma_g^+$ System (Ultraviolet)Band heads, λ (69.109):

(v', v'')	(0, 0)	(1, 0)
λ	1341.38	1313.97

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
$F^1\Pi_u$	74532.9 ^(a)	1557.5 ^(b)		1.645	19		1.307	Rydberg	(69.109)
$g^3\Delta_g$	71649.6 ^(a)	1458.06 ^(b)		1.5238	17.0		1.358	Rydberg	(69.109)
$f^3\Sigma_g^-$	70188.4 ^(a)	1360.5	14.8	1.448	40		1.393	Rydberg	(69.109)
$E^1\Sigma_g^+$	55034.6	1671.5	40.02	1.7930	42.1	8.3	1.2517	$y_e \omega_e = +0.248$ $\beta_e = 0.6 \times 10^{-6}$	(69.109, 51.10)
$D^1\Sigma_u^+$	43240.23	1829.57	13.97	1.8334	20.4		1.2378	Rydberg	(39.5)
$e^3\Pi_g$	40797.65	1106.56	39.26	1.1922	24.2	6.3	1.5350	$y_e \omega_e = +2.805$ $z_e \omega_e = -0.1271$	(49.8)
$C'^1\Pi_g$	(37450) ^(c)	(1697) ^(c)		(1.7113) ^(c)		(11.25) ^(c)	(1.2813) ^(c)	Perturbed	(67.80)
$C^1\Pi_g$	34261.9	1809.1	15.81	1.7834	18.0	7.1	1.2552	$y_e \omega_e = -4.02$	(63.41, 40.6)
$d^3\Pi_g$	20022.50	1788.22	16.440	1.7527	16.08		1.2660	$y_e \omega_e = -0.5067$ $\gamma_e = -1.274$ $\times 10^{-3}$	(68.97, 63.43, 63.42, 63.41)
								Perturbed	

Molecule C_2

SPECTROSCOPIC CONSTANTS

Molecule C₂

State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ³	D _e × 10 ⁶	r _e	Remarks	Bibliography
c ³ Σ _u ⁺	13312.1(d)	(d) 1961.6	(d) 13.65	1.87(d)			1.23(d)		(63.41)
A ¹ Π _u	9391.00	1608.35	12.078	1.6163	16.86	6.44	1.3184	y _e ω _e = -0.01 β _e = 3.6 × 10 ⁻⁸ γ _e = -5.4 × 10 ⁻⁵ q = -2.3 × 10 ⁻⁴	(63.41)
b ³ Σ _g ⁻	6434.27	1470.45	11.19	1.4985	16.34	6.22	1.3692	y _e ω _e = +0.02	(63.41, 63.40)
a ³ Π _u	714.24	1641.35	11.67	1.6324	16.61	6.44	1.3119		(63.40)
X ¹ Σ _g ⁺	0	1854.71	13.34	1.8198	17.65	6.92	1.2425	y _e ω _e = -1.17 β _e = 8.1 × 10 ⁻⁸ γ _e = -2.3 × 10 ⁻⁴	(74.138, 63.41)

(a) Values of ν₀(0,0); (b) Values of ΔG_{1/2}; (c) Approximate values determined by the study of the perturbations between the C and C' states; (d) Values determined starting with the perturbations between the C and A states.

Dissociation energy = 6.25 ± 0.2 eV, 144 kcal/mole, 50400 cm⁻¹.

Perturbations and General Information

The $e^3\Pi_g$ state is perturbed (64.44, 62.33).

The $C^1\Pi_g$ state has been identified by study of the perturbation of the $C^1\Pi_g$ state (67.80).

The $d^3\Pi_g$ state is perturbed (68.97, 63.43, 63.42).

The $A^1\Pi_u$ state is perturbed by the $c^3\Sigma_u^+$ state (63.41).

The $X^1\Sigma_g^+$ state is perturbed by the $b^3\Sigma_g^-$ state (63.40).

Franck-Condon factors, r-Centroids for the $d^3\Pi_g \rightleftharpoons a^3\Pi_u$ System using Klein-Dunham potentials (74.140):

v', v''	0	1	2	3	4	5	6	7
0	1.294 7.22-1	1.225 2.21-1	1.169 4.69-2	1.120 8.55-3	1.076 1.48-3			
1	1.368 2.48-1	1.307 3.33-1	1.232 2.84-1	1.177 1.02-1	1.127 2.62-2	1.083 5.78-3		
2	1.462 2.84-2	1.378 3.75-1	1.328 1.30-1	1.239 2.61-1	1.184 1.40-1	1.134 4.78-2	1.089 1.31-2	
3		1.475 6.89-2	1.390 4.23-1	1.371 3.86-2	1.245 2.08-1	1.190 1.60-1	1.140 6.90-2	1.096 2.28-2
4			1.488 1.12-1	1.402 4.31-1	1.520 5.72-3	1.250 1.51-1	1.196 1.62-1	1.145 8.61-2
5				1.502 1.52-1	1.416 4.25-1		1.252 9.99-2	1.202 1.52-1
6					1.518 1.86-1	1.432 4.22-1	0.839 2.92-3	1.246 6.02-2
7						1.538 2.08-1	1.450 4.35-1	0.725 3.66-3
8							1.564 2.08-1	1.470 4.77-1
9								1.601 1.72-1

Top line = r-Centroid

Bottom line = Franck-Condon factor followed by factor of ten

C₂

Franck-Condon factors for the C₂ Phillips Band System $A^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$ using Morse potentials (64.45):

v', v''	0	1	2	3	4	5	6	7	8	9
0	0.41016	39989	15563	03084	00328	00018	00000	00000	00000	00000
1	0.33151	00532	29010	27207	08728	01232	00089	00003	00000	00000
2	0.16304	17104	05749	11769	30490	15320	03001	00255	00008	00000
3	0.06365	19934	03208	14143	01919	27053	21337	05462	00559	00021
4	0.02181	12600	13824	00094	15649	00156	20131	25764	08521	01035
5	0.00690	06017	14519	05926	03421	11767	03163	12594	28149	
6	0.00208	02452	09555	12105	01024	07766	06307	07500		
7	0.00061	00905	04937	11202	07554	00092	10081			
8	0.00017	00314	02205	07326	10511	03236				
9	0.00005	00104	00896	03932	08809					
10	0.00001	00034	00342	01861						
11	0.00000	00011	00125							
12	0.00000	00003								

Lifetimes

$$d^3\Pi_g \rightleftharpoons a^3\Pi_u \quad 185 \pm 70 \text{ nsec (73.135)}$$

$$D^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+ \quad 14.6 \pm 1.5 \text{ nsec (69.108)}$$

Oscillator strengths

$$A^1\Pi_u \rightleftharpoons X^1\Sigma_g^+ \quad f_{(0,0)} = 0.8931 \quad (70.127)$$

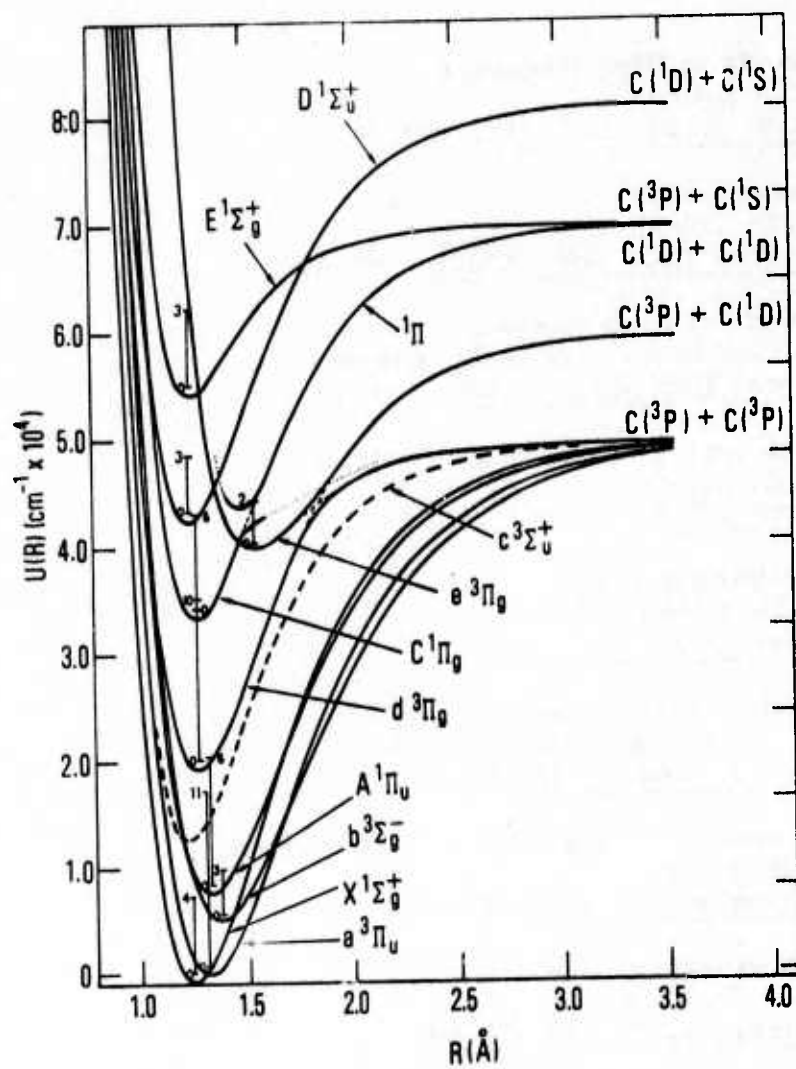
$$e^3\Pi_g \rightarrow a^3\Pi_u \quad f_{(0,0)} = 0.0995 \quad (70.127)$$

$$D^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+ \quad f_{(0,0)} = 0.1206 \quad (70.127)$$

$$C^1\Pi_g \rightarrow A^1\Pi_u \quad f_{(0,0)} = 0.2016 \quad (70.127)$$

$$d^3\Pi_g \rightleftharpoons a^3\Pi_u \quad f_{(0,0)} = 0.017 \pm .007 \quad (73.135)$$

Potential energy curves (69.109, 63.41):



Isotope effects (69.107)

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Methods of Production and Experimental Technique

Emission from a hollow cathode discharge.

Absorption in a King furnace, T > 2300° K.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	I	$^1\Sigma - X^1\Sigma_g^+$	Absorption	6500-5900		16395.6(0,0)		(68.5, 67.4)
	II	$A^1\Sigma_u^+ - X^1\Sigma_g^+$	Absorption	5300-4300		19401.0(v,0)		(71.7)
	III	Continuum		5100-3980				(31.1)

Molecule Ca₂

Ca₂

I. $1\Sigma^+ - X^1\Sigma_g^+$ System

Band heads, λ (67.4):

v', v''	λ
0, 0	6099.2
0, 1	6180.2
0, 2	6259.1
1, 0	6014.5
1, 1	6093.4
2, 1	6013.1

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

Band heads of the $v', 0$ progression, λ (71.7):

v''	v	$v+1$	$v+2$	$v+3$	$v+4$	$v+5$	$v+6$
λ	5154.4	5119.9	5086.2	5053.4	5021.5	4990.3	4960.0

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
$^1\Sigma$	16395.59								(71.7)
$X^1\Sigma_g^+$	0.0	65.0	1.11	0.046			4.28		(71.7)
Dissociation energy = 0.12 ± 0.1 eV, 2.69 kcal/mole, 940 cm^{-1} (71.7).									

Molecule Ca_2

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Cd₂

Methods of Production and Experimental Technique

Absorption.

Emission from normal and hollow cathode discharges.

Fluorescence when excited by Cu, Zn, or Al sparks.

BAND SYSTEMS

System	Absorption (33.10, 29.2, 29.1)	Emission (35.14, 34.12, 32.6, 31.4, 31.3, 29.1)	Fluorescence (34.12, 32.7)
I		Continuum: 5400-4058 Bands: 4463 4439 4416 4392 4369 4343	Continuum: 5000-3800 max. at 4000
II	Broad line: 3261 Band: 3178	Continuum: 4044-3178 max. at 3939 and 3261 min. at 3370 Bands: 4044-3936, 3186-3148	Broad line: 3261 Band: 3178
III	Continuum: 2800-2212 Band: 2212	6 Bands: 2870-2780 Continuum: 3000-2191 max. at 2980 and 2288 min. at 2450 Band: 2214	Continuum: 3050-2260 max. at 2288 Bands: 3050-2700, 2560-2288
IV	Band: 2114	Bands: 2140-2110 max. at 2114	Bands: 2140-2110 max. at 2125

Spectroscopic Constants

Dissociation energy = 0.07 ± 0.01 eV, 1.63 kcal/mole, 940 cm^{-1} .

Perturbations and General Information

Potential energy curves (35.18).



Spectroscopic Constants

Dissociation energy = $D_0^0 = 0.07 \pm 0.01 \text{ eV}$, 1.63 kcal/mole , 940 cm^{-1} .

Perturbations and General Information

Potential energy curves (35.18).

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Cd₂

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Ce₂

Ce₂

Spectroscopic Constants

Dissociation energy = 2.83 ± 0.01 eV, 65.3 kcal/mole, 22840 cm^{-1} (72.4).

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Methods of Production and Experimental Technique

Absorption.

Emission in many different discharges, flames, thermoluminescence, and "active" nitrogen flames.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	I	$A^3\Pi(0_u^+) \rightarrow X^1\Sigma_g^+$	Discharge Absorption	6500-5400 6000-4780	R	17651.5		(63.50, 62.49, 36.22)
	II	(a)	Absorption Discharge Discharge Discharge Discharge Absorption	<4785 3063-2715 2565-2097 1997-1855 <3400 <1950	Continuum Continuum Continuum Continuum Continuum Continuum	- (58000) (67700) (75000) - - -	(b) $\lambda_{\max.}$ 3300 - - - - <1560	(59.46, 47.38, 47.37, 38.28, 37.26, 37.24, 30.14)
	III	$? \rightarrow A^3\Pi(0_u^+)$	Discharge	2600-2390	R	40119		(59.45)
	IV	$? \rightarrow A^3\Pi(0_u^+)$	Discharge	2365-2239	V	43632		(59.44)
	V	?	Discharge	1870-1070			Rydberg transitions	(59.46)
(a) Attributed to $1.3\Sigma_u^+ \rightarrow 1\Sigma_g^+$ transitions, discussed in (59.46). (b) Analysis is difficult.								

Molecule Cl₂

Cl₂

I. A³Π(0_u⁺) → X¹Σ_g⁺ System

Bands in emission, λ (37.25, 36.22, 28.8); isotope effect (63.50, 43.36); numbering of v' (62.49).

v', v''	0	1
15	4932.8	5070.6
16	4911.7	5048.8
17	4892.7	5030.0
18	4875.7	5013.4
19	4859.6	4995.6

II. Continuum Spectra

3063-1855Å System

Three groups of continuum bands due to transitions to the unstable lower states:

$$(^2P_{3/2} + ^2P_{3/2}), \quad (^2P_{3/2} + ^2P_{1/2}), \quad (^2P_{1/2} + ^2P_{1/2})$$

<3400Å System

Principal maxima (37.24): λ|3063|2564

Secondary maxima: λ|2957|2881|2819|2758|2714|2432

When produced using "active" nitrogen two series of diffuse bands are observed. These bands are interpreted as arising from a ¹Σ_u⁺ → ¹Π_g transition with a pronounced minimum in the ¹Π_g state.

<1950Å System

Corresponds to a transition from the ground state to the ³Σ_g⁺ state, which dissociates to two ²P_{1/2} atoms (47.37).

III. 2600-2390Å SystemBand heads, λ (59.45):

v', v''	0	1	2
0	2492.6	2519.8	2523.5
1	2477.6	2493.5	
2	2462.6	2477.9	

IV. 2365-2239Å SystemBand heads, λ (59.44):

v', v''	0	1	2
0	2291.9	2305.1	
1	2278.7		
2		2277.6	2290.4

V. 1870-1070Å Systems

Many Rydberg transitions. Molecular orbital discussion (59.46).

SPECTROSCOPIC CONSTANTS

Molecule Cl_2

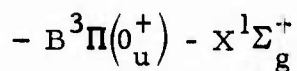
State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
?	61433	261.5 ^a	0.812 ^b	-	-	-	-		(59.44)
?	57916	246.6 ^a	0.615 ^b	-	-	-	-		(59.45)
$A^3\Pi(0_u^+)$	17301.2	261.9	5.45	0.1680	3.7	-	2.396		(63.50, 62.49)
$X^1\Sigma_g^+$	0	559.71	2.70	0.24407	1.53	-	1.9878		(63.50, 62.49)
$a \omega_0; b x_0 \omega_0$ Dissociation energy = 2.4795 ± 0.0003 eV, 57.2 kcal/mole, 19999 cm^{-1} (63.50).									

Perturbations and General Information

Ionization potential = $92590 \pm 80 \text{ cm}^{-1}$, 11.48 eV (57.42).

Potential energy curves (47.16).

Franck-Condon factors - RKR potential for $^{35}\text{Cl}_2$ (71.58)



v', v''	0	1	2	3	4	5	6
0	2. -9	6. -8	7. -7	6. -6	0.00003	0.00016	0.00061
1	3. -8	6. -7	7. -6	0.00005	0.00027	0.00112	0.00363
2	2. -7	3. -6	0.00003	0.00023	0.00110	0.00371	0.01089
3	6. -7	0.00001	0.00012	0.00072	0.00300	0.00930	0.02202
4	2. -6	0.00004	0.00032	0.00170	0.00631	0.01698	0.03380
5	5. -6	0.00009	0.00069	0.00333	0.01030 ^(a)	0.02425 ^(a)	0.04075 ^(a)
6	0.00001	0.00018	0.00129	0.00560	0.01623	0.03227	0.04337
7	0.00002	0.00032	0.00213	0.00836	0.02134	0.03607	0.03842
8	0.00004	0.00053	0.00319	0.01129	0.03611	0.03611	0.02935
9	0.00006	0.00079	0.00439	0.01406	0.02778	0.03287	0.01924
10	0.00009	0.00109	0.00563	0.01635	0.02835	0.02749	0.01054

(a) $q_{v', v''}$ for $J' = 25$, $J'' = 26$. All others rotationless.

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Cl₂

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Can. J. Phys. 52, 246-56

Co₂Spectroscopic Constants

Dissociation energy = 1.69 ± 0.26 eV, 39 kcal/mole, 13600 cm^{-1} (64.1).

Co₂

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Cr₂Methods of Production and Experimental Technique

Single band at 4600Å, attributed to Cr₂, has been observed by photolysis of Cr(CO)₆ (74.4).

Spectroscopic Constants

Dissociation energy = 1.56 ± 0.31 eV, 36.0 kcal/mole, 12600 cm^{-1} (62.1, 64.2, 68.3).

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Methods of Production and Experimental Technique

Heat pipe.

Absorption.

Laser Fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, v ₀ , 0	Remarks	Bibliography
7667 Å 6250 Å	I	$^3\Pi_u \rightarrow X^1\Sigma_g^+$	Heat pipe	11900				(71.23, 68.15)
	II	$^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Heat pipe	11300				(71.23, 68.15)
	III	$A \leftarrow X^1\Sigma_g^+$	Absorption	11300-8800	R			(38.13, 34.7)
	IV	$B \leftarrow X^1\Sigma_g^+$	Absorption	8350-6950	R			(69.18, 38.13, 34.7)
	V	$C \leftarrow X^1\Sigma_g^+$	Absorption, fluorescence	6443-6340	R, V		Spectra not fully analyzed	(68.16, 36.11)
	VI	$D \leftarrow X$	Absorption	6360-6260	R, V		Spectra not fully analyzed	(68.16, 36.11)
	VII	$E \leftarrow X$	Absorption	5230-4450			55 bands of which 16 are provisionally classified	(34.7)
	VIII			Ultraviolet and visible				(35.9, 32.4, 32.3)

Molecule Cs₂

Cs₂

IV. B ← X¹Σ_g⁺ System (7667Å)

Bands of greatest intensity (38. 13):

v', v''	1, 3	0, 2	0, 1	0, 0	1, 0	3, 1	2, 0
λ	7720. 4	7716. 0	7691. 2	7666. 6	7646. 6	7631. 4	7626. 7
(Intensity)	2	4	5	3	5	2	4

V. C ← X¹Σ_g⁺ System (6250Å)

Band heads (Q). There are 3 bands degrading R and 1 degrading V (68. 16):

v', v''	0	1	2	3	4
0	6265. 4	6281. 3		6313. 1	
1	6255. 1	6271. 0	6286. 9	6302. 8	6318. 6
2	6244. 8	6260. 7	6276. 6	6292. 5	6308. 3
3		6250. 4	6266. 3	6282. 1	6298. 0
4			6255. 8		6287. 6

VI. D ← X¹Σ_g⁺ System

Observed bands (v' numbering uncertain):

v', v''	9, 17	7, 13	8, 13	7, 12	5, 9	8, 10
λ	6359. 8	6317. 5	6307. 1	6301. 7	6274. 9	6259. 6
(Intensity)	7	10	7	9	9	8

VIII. Ultraviolet and Visible Bands

- Diffuse bands, λ|7185|7128
- Bands degrading V, λ|7078|7075|7072
- System at ~ 5600, intensified by Ar at 300° C
- Bands degrading R, λ|3959|3953|3947|3941
- Bands degrading V, λ|3920

Perturbations and General Information

Maximum photoionization cross-section = 21.6 Mb at 3214Å (73.24).

Recombination rate constant $3\text{Cs} \rightarrow \text{Cs}_2 + \text{Cs}$ (71.22):

$$k \approx 3 \times 10^{-30} \text{ cm}^6/\text{sec at } 600^\circ\text{K}$$

Radiative lifetimes (70.19):

$\lambda_{\text{exc}}(\text{\AA})$	Upper State	Lifetime (nsec)
4879.86	?, above D state	27.0 ± 2
4764.86		12.0 ± 1.5
4726.86		12.0 ± 1.5
4579.35		6.4 ± 0.8

SPECTROSCOPIC CONSTANTS

Molecule Cs₂

State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ³	D _e × 10 ⁶	r _e	Remarks	Bibliography
E	(20500)	(31)	-	-	-	-	-	-	(34.7)
D	(16175.8)	(27.34)	(0.0733)	-	-	-	-	-	(36.11)
C	15948.6	29.7030	0.05756	-	-	-	-	y _e ω _e = 1.608 × 10 ⁻³	(68.16)
B	13043.88	34.3293	0.07996	-	-	-	-	y _e ω _e = -1.511 × 10 ⁻⁴	(69.18)
A	(10000)	-	-	-	-	-	-	-	(38.13, 34.7)
1Σ _u ⁺	(8850)	-	-	-	-	-	-	-	(71.23, 68.15)
3Π	(8403)	-	-	-	-	-	-	-	(71.23, 68.15)
X ¹ Σ _g ⁺	0	42.0267	0.08348	-	-	-	-	y _e ω _e = -2.361 × 10 ⁻⁵	(69.18, 69.16)
Dissociation energy = 0.40 ± 0.01 eV, 9.13 kcal/mole, 3197 cm ⁻¹ (69.18).									

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Cu₂

Cu₂

Methods of Production and Experimental Technique

Absorption.

Emission: thermal, discharges, exploding wires, "active" nitrogen.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	I	$A^1\Pi_u - X^1\Sigma_g^+$	Absorption	5750-4850	R	20401.79		(71.8, 65.5, 54.2)
	II	$B^1\Sigma_u^+ - X^1\Sigma_g^+$	Absorption	4720-4490	R	21748.48		(71.7, 65.5, 54.2)
	III			Ultraviolet			3 or 4 bands not analyzed	(71.7, 65.5, 54.2)

Molecule Cu₂

I. A¹Π_u ← X¹Σ_g⁺ SystemBand heads for ⁶³Cu₂, λ (71.8):

v', v''	1, 0	0, 0	0, 1
λ	4856.3	4901.5	4966.0

II. B¹Σ_u⁺ ← X¹Σ_g⁺ SystemBand heads for ⁶³Cu₂, isotope shifts, λ (71.7):

v', v''	0	1	2
0	4598.1	4654.7	4712.3
1	4547.4	4603.0	4659.7
2	4498.8		4608.1

III. Ultraviolet SystemsBands observed in the regions: 2900 > λ > 2700, 2560 > λ > 2490,
2460 > λ > 2330

SPECTROSCOPIC CONSTANTS

Molecule Cu₂

State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ³	D _e × 10 ⁸	r _e	Remarks	Bibliography
B ¹ Σ _u ⁺	21760.4	245.2	1.90						(71.7, 65.5, 54.2)
A ¹ Π _u	20434.2	191.9	0.348	0.08185	0.62	3.81	2.559		(71.8, 54.2)
X ¹ Σ _g ⁺	0	268.9	1.63	0.10867	0.56	5.11	2.22		(71.7, 65.5, 54.2)
Dissociation energy = 2.05 ± 0.09 eV, 47.3 kcal/mole, 16550 cm ⁻¹ (60.4).									

Perturbations and General Information

Franck-Condon factors, $B^1\Sigma_u^+ - X^1\Sigma_g^+$, RKR potentials (71.9):

v', v''	0	1	2	3
0	0.237	0.283	0.261	0.104
1	0.251	0.051	0.078	
2	0.227	0.010	0.156	
3	0.149			

Potential energy curves (71.9):

State	v	$U+T_e(\text{cm}^{-1})$	$r_{\text{max}}(\text{\AA})$	$r_{\text{min}}(\text{\AA})$
$X^1\Sigma_g^+$	0	132.3	2.286	2.158
	1	396.9	2.338	2.117
	2	659.8	2.376	2.091
	3	919.6	2.409	2.070
	4	1177.7	2.439	2.053
	5	1433.7	2.467	2.038
	6	1687.7	2.492	2.024
	7	1939.1	2.517	2.013
	8	2188.8	2.541	2.002
	9	2436.9	2.563	1.992
	10	2682.7	2.585	1.983
	11	2926.6	2.607	1.975
	12	3169.5	2.628	1.967
	13	3409.5	2.649	1.959
	14	3647.5	2.670	1.952
	15	3883.4	2.689	1.945
	16	4117.3	2.708	1.939
	17	4349.5	2.728	1.933
	18	4579.3	2.747	1.927
	19	4807.5	2.767	1.921
	20	5033.7	2.786	1.916
	21	5257.9	2.806	1.911
	22	5479.9	2.826	1.906
	23	5700.5	2.842	1.901
$B^1\Sigma_u^+$	0	21869.3	2.396	2.263
	1	22109.0	2.453	2.221
	2	22344.6	2.495	2.193
	3	22575.9	2.531	2.171
	4	22802.7	2.563	2.152

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Dy₂

Dy₂

Spectroscopic Constants

Dissociation energy = 0.78 ± 0.17 eV, 18 kcal/mole, 6291 cm^{-1} (71.1).

Dy₂

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Er₂

E₂

Spectroscopic Constants

Dissociation energy = 0.78 ± 0.17 eV, 18 kcal/mole, 6291 cm^{-1} (71.1).

E-1

Er₂

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Eu₂

Eu₂

Spectroscopic Constants

Dissociation energy = 0.43 ± 0.17 eV, 10 kcal/mole, 3500 cm^{-1} (72.1).

Eu₂

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Methods of Production and Experimental Technique

Absorption.

Emission in a discharge.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Pi_u - X^1\Sigma_g^+$	Absorption	4400-2200	Continuum	-	Peaks, $\lambda = 2845\text{\AA}$	(56.25, 37.5, 31.3)
	II	$C^1\Sigma^+ - B^1\Pi$	Discharge	7510-4220	R	6517.2(0, 5) 5398.0(0, 2) 5388.5(1, 3)	Perturbed	(68.39, 66.36, 29.2)
	III	$C^1\Sigma^+ - B^1\Pi$	Discharge	Z bands	R	5852.6(0, ?) 5495.7(1, ?)	3 heads	(68.39)
	IV		Absorption	Far ultraviolet	R V	1935 952	Rydberg series	(59.29)

Molecule F₂

F₂

II. C¹Σ⁺ → B¹Π System

Band heads, λ (Intensity) (68.39, 32.4, 29.2, 24.1):

v', v''	0	1	2	3	4	5	6
0			5398(10) ^a	5731.5(25)	6102.8(70)	6517.2(100) ^b	6982.5(4)
1		4823(1) ^a	5092.3(3) ^a	5388.5(10)	5715.6(4) ^a		6480.4(25)

^aNo rotational analysis; ^bpartial rotational analysis

III. C¹Σ⁺ → B'¹Π System

Two bands have been attributed to this system (68.39):

(v', v'')	(0, ?)	(1, ?)
λ	5852.6	5495.7
(Intensity)	8	1

IV. Rydberg Series

Band series have been reported for a number of systems (59.29):

System	Degrades	Intensity	λ	System	Degrades	Intensity	λ
V	R	2	1035.8	B ₂ ''		7	946.6
			1031.1				937.0
			1026.6				927.7
			1021.2				918.8
			1017.4				910.3
			1012.4	C ₂ '	R	10	874.2
			1008.2				867.2
			1003.5				861.2
V'	R	5	998.4	B ₃ '		12	859.8
			969.1				850.2
			962.8	B ₃ ''		15	855.6
B ₂ '		7	952.3				848.7
			942.7	B ₄ '		18	830.7
			933.7	B ₄ ''		18	828.3
			924.8	B ₅ '		18	814.7
				B ₅ ''		18	813.8
				B ₆ '		18	807.0

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
$C^1\Sigma^+{}^a$	$x+(20900)^b$	(1110)	-	0.804	8.0	-	1.485		(68.39, 29.2)
$B'^1\Pi^a$	-	-	-	(1.005)	-	-	(1.329)		(68.39)
$B^1\Pi^a$	x	(1100)	-	(1.047)	(12.0)	-	(1.302)		(68.39, 29.2)
$A^1\Pi_u$	-	-	-	-	-	-	-		(56.25, 37.5, 31.3)
$X^1\Sigma_g^+$	0	891.85^c	-	0.8828^d	-	-	1.417^e		(51.18)

^a Possibly a Rydberg series; ^b position uncertain because of perturbations; ^c $\Delta G_{1/2}$; ^d B_0 ; ^e r_0

Dissociation energy = 1.61 ± 0.05 eV, 37.1 kcal/mole, 12976 cm^{-1} (72.45).

F₂

Perturbations and General Information

Intense perturbations are noted in the positions and intensities of the C¹Σ state (32.4).

Potential curve of the repulsive A¹Π_u state (57.27).

Molecular orbital wavefunctions of the X¹Σ_g⁺ state (66.35, 64.34).

Calculated energies of the X¹Σ_g⁺ state using Hartree-Fock method (64.33).

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Fe₂

Fe₂

Spectroscopic Constants

Dissociation energy = 1.30 ± 0.22 eV, 30 kcal/mole, 10500 cm^{-1} (69.1).

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Emission from a King furnace.

Band Systems

The spectra of gallium has been observed in emission and consists primarily of red-degraded bands in the region 4600-5500Å (65.3).

Spectroscopic Constants

Dissociation energy = 1.39 ± 0.22 eV, 32 kcal/mole, 11200 cm^{-1} (58.2, 57.1).

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Gd₂

Gd₂

Spectroscopic Constants

Dissociation energy = 1.78 ± 0.35 eV, 41 kcal/mole, 14340 cm^{-1} (72.1).

Gd₂

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Ge₂

Ge₂

Spectroscopic Constants

Dissociation energy = 2.81 ± 0.12 eV, 64.9 kcal/mole, 22700 cm^{-1} (66.2, 66.1).

Ge₂

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Methods of Production and Experimental Technique

Absorption.

Emission from discharge into H₂ gas.

SINGLET SYSTEMS

BAND SYSTEMS

	System	Transition	Sources	Electronic Configuration	Degrades	Band Head, $\nu_0, 0$	Remarks	Bibliography
Lyman Werner Hopfield- Beutler	I	$B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Absorption, emission	$2p\sigma \rightarrow 1s\sigma$	R	90203.55	Perturbed	(73.92, 68.30, 68.26, 64.23, 61.17, 60.16, 59.15)
	II	$C^1\Pi \rightarrow X^1\Sigma_g^+$	Absorption, emission	$2p\pi \rightarrow 1s\sigma$	R	99081.72	Perturbed	(64.23, 62.21, 62.20, 58.14, 33.1)
	III	$B'^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Absorption	$2p\sigma \rightarrow 1s\sigma$	R	110478.54	Perturbed	(68.28, 64.24, 61.18, 34.5)
	IV	$D^1\Pi_u^- \rightarrow X^1\Sigma_g^+$	Absorption	$2p\pi \rightarrow 1s\sigma$	R	112871.74	Perturbed, predis-sociated	(68.28, 64.24)
	V	$B''^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Absorption	$2p\sigma \rightarrow 1s\sigma$	R	116882.00	Perturbed	(68.28, 64.24, 61.18)
	VI	$D'^1\Pi_u^- \rightarrow X^1\Sigma_g^+$	Absorption	$2p\pi \rightarrow 1s\sigma$	R	117834.65	Perturbed	(68.28, 64.24)
	VII	$D''^1\Pi_u^- \rightarrow X^1\Sigma_g^+$	Absorption	$2p\pi \rightarrow 1s\sigma$	R	120172.21		(68.28, 62.22)
	VIII	$E^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$2s\sigma \rightarrow 2p\sigma$	V	8961.2		(36.7)
	IX	$F^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$(2p\sigma)^2 \rightarrow 2p\sigma$	R	~14000	Perturbed	(49.13)

Molecule H₂

H₂

SINGLET SYSTEMS

BAND SYSTEMS

	System	Transition	Sources	Electronic Configuration	Degrades	Band Head, $\nu_0, 0$	Remarks	Bibliography
	X	$Q \rightarrow B^1\Sigma_g^+$	Emission	$\rightarrow 2p\sigma$	R	21151		(34.4, 34.3, 34.2)
	XI	$K \rightarrow B^1\Sigma_g^+$	Emission	$\rightarrow 2p\sigma$	R	21425.4		(34.5)
	XII	$G^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$3d\sigma \rightarrow 2p\sigma$	V	(21609)	Perturbed	(34.5)
	XIII	$I^1\Pi_g \rightarrow B^1\Sigma_g^+$	Emission	$3d\pi \rightarrow 2p\sigma$	V	21813		(34.5)
	XIV	$J^1\Delta_g \rightarrow B^1\Sigma_g^+$	Emission	$3d\delta \rightarrow 2p\sigma$	V	22150		(34.5)
	XV	$H^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$3s\sigma \rightarrow 2p\sigma$	V	22754.1		(34.5)
	XVI	$L^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$\rightarrow 2p\sigma$		23054.8		(34.5)
	XVII	$M^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$\rightarrow 2p\sigma$		23190		(34.5)
	XVIII	$N^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$\rightarrow 2p\sigma$		24896		(34.5)
	XIX	$T^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$\rightarrow 2p\sigma$		27130		(34.5)
	XX	$P^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$4d\sigma \rightarrow 2p\sigma$		27148		(34.5)

Molecule H₂

	System	Transition	Sources	Electronic Configuration	Degrades	Band Head, $\nu_0, 0$	Remarks	Bibliography
	XXI	$R^1\Pi_g \rightarrow B^1\Sigma_g^+$	Emission	$4d\pi \rightarrow 2p\sigma$		~27400	Perturbed	(34.5)
	XXII	$S^1\Delta_g \rightarrow B^1\Sigma_g^+$	Emission	$4d\delta \rightarrow 2p\sigma$		27460		(34.5)
	XXIII	$O^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$	Emission	$4s\sigma \rightarrow 2p\sigma$		27487		(34.5)
	XXIV	$K \rightarrow C^1\Pi_u^-$	Emission	$\rightarrow 2p\pi$	R	12541.2		(34.5)
	XXV	$G^1\Sigma_g^+ \rightarrow C^1\Pi_u^-$	Emission	$3d\sigma \rightarrow 2p\pi$	R	12725	Perturbed	(34.5)
	XXVI	$I^1\Pi_g \rightarrow C^1\Pi_u^-$	Emission	$3d\pi \rightarrow 2p\pi$	R	12925		(34.5)
	XXVII	$J^1\Delta_g \rightarrow C^1\Pi_u^-$	Emission	$3d\delta \rightarrow 2p\pi$	R	13264		(34.5)
	XXVIII	$H^1\Sigma_g^+ \rightarrow C^1\Pi_u^-$	Emission	$3s\sigma \rightarrow 2p\pi$	R	13866.6		(34.5)
	XXIX	$P^1\Sigma_g^+ \rightarrow C^1\Pi_u^-$	Emission	$4d\sigma \rightarrow 2p\pi$		18260		(34.5)
	XXX	$E^1\Pi_g \rightarrow C^1\Pi_u^-$	Emission	$4d\pi \rightarrow 2p\pi$		~18400	Perturbed	(34.5)
	XXXI	$D^1\Pi_u^- \rightarrow E^1\Sigma_g^+$	Emission	$2p\pi \rightarrow 2s\sigma$	R	13713.3		(38.11, 37.10)

Molecule H₂

TRIPLET SYSTEMS

BAND SYSTEMS

	System	Transition	Sources	Electronic Configuration	Degrades	Band Head, $\nu_0, 0$	Remarks	Bibliography
(β)	I'	$e^3\Sigma_u^+ \rightarrow a^3\Sigma_g^+$	Emission	$3p\sigma \rightarrow 2s\sigma$	R	11605.7		(34.5)
		$d^3\Pi_u \rightarrow a^3\Sigma_g^+$	Emission	$3p\pi \rightarrow 2s\sigma$	R	16619.0	Perturbed	(35.6)
	III'	$f^3\Sigma_u^+ \rightarrow a^3\Sigma_g^+$	Emission	$4p\sigma \rightarrow 2s\sigma$	R	20526.0		(34.5)
	IV'	$k^3\Pi_u \rightarrow a^3\Sigma_g^+$	Emission	$4p\pi \rightarrow 2s\sigma$	R	22271.5		(34.5)
	V'	$m^3\Sigma_u^+ \rightarrow a^3\Sigma_g^+$	Emission	$4f\sigma \rightarrow 2s\sigma$		23295.1		(34.4, 34.3, 34.2)
	VI'	$n^3\Pi_u \rightarrow a^3\Sigma_g^+$	Emission	$5p\pi \rightarrow 2s\sigma$	R	24847.5		(34.5)
	VII'	$t^3\Sigma_u \rightarrow a^3\Sigma_g^+$	Emission	$5f\sigma \rightarrow 2s\sigma$	R	25343		(34.4)
	VIII'	$u^3\Pi_u \rightarrow a^3\Sigma_g^+$	Emission	$6p\pi \rightarrow 2s\sigma$	R	26232.5		(34.5)
	IX'	$a^3\Sigma_g^+ \rightarrow b^3\Sigma_u^+$	Emission	$2s\sigma \rightarrow 2p\sigma$		Continuum 20000 < ν < 62500		(44.12)
	X'	$g^3\Sigma_g^+ \rightarrow c^3\Pi_u$	Emission	$3d\sigma \rightarrow 2p\pi$		16926		(34.5, 34.4, 34.3, 34.2)

Molecule H₂

	System	Transition	Sources	Electronic Configuration	Degrades	Band Head, $\nu_0, 0$	Remarks	Bibliography
	XI'	$l^3\Sigma_g^+ \rightarrow c^3\Pi_u$	Emission	$3s\sigma \rightarrow 2p\pi$	R	16990	Predissociated	(34.4, 34.3, 34.2)
	XII'	$i^3\Pi_g \rightarrow c^3\Pi_u$	Emission	$3d\pi \rightarrow 2p\pi$		17162		(34.5)
	XIII'	$j^3\Delta_g \rightarrow c^3\Pi_u$	Emission	$3d\delta \rightarrow 2p\pi$		17355	Preionized	(34.5)
	XIV'	$p^3\Sigma_g^+ \rightarrow c^3\Pi_u$	Emission	$4d\sigma \rightarrow 2p\pi$		22588	Perturbed	(34.5)
	XV'	$s^3\Delta_g \rightarrow c^3\Pi_u$	Emission	$4d\delta \rightarrow 2p\pi$		22626	Perturbed	(34.5)
	XVI'	$r^3\Pi_g \rightarrow c^3\Pi_u$	Emission	$4d\pi \rightarrow 2p\pi$		22699	Perturbed	(34.5)
	XVII'	$v \rightarrow c^3\Pi_u$	Emission	$\rightarrow 2p\pi$	R	22487		(34.5)
	XVIII'	$q \rightarrow c^3\Pi_u$	Emission	$\rightarrow 2p\pi$	R	25220		(34.4, 34.3, 34.2)

Molecule H₂

H₂

SINGLET SYSTEMS

I. B¹Σ_u⁺ ⇌ X¹Σ_g⁺ System (Lyman)

Band heads, λ (59.15):

v', v''	0	1	2	3	4	5	6	7	8
0	1108.6			1275.2	1334.2	1394.5	1455.7	1517.1	1578.0
1	1092.6		(1198.5)	1254.1	1311.1	1369.3	1428.2	1487.3	1545.8
2	1077.5		(1180.3)	1234.3	1289.4	1345.7	1402.6	1459.5	1515.8
3	1063.3	(1112.4)		1215.5	1269.0	1323.5	1378.5	1433.4	1487.7
4	1049.7			1197.9	1249.8	1302.6	1355.8	1408.9	1461.3
5	1036.9			1181.2	1231.6	1282.9	1334.4	1385.9	1436.5
6	1024.7	(1070.3)				1264.2	1314.3	1364.2	1413.2
7	1013.1					1246.7	1295.3	1343.8	1391.3
8	1002.1						1268.6	1324.5	1370.6
9	991.6						1260.4	1306.3	1351.1
10	981.7						1244.4	1289.0	1332.7
11	972.2							1272.8	1315.3
12	963.2							1257.4	1298.9
13	954.6							1242.8	1283.3

II. C¹Π_u⁻ ⇌ X¹Σ_g⁺ System (Werner)

Band heads, λ (33.1):

v', v''	1	2	3	4	5	6	7	8
0		1098.9	1145.4	1192.7				
1	1028.4		1115.8	1160.8	1206.2			
2		1047.3	1089.4	1132.2	1175.4	1218.5		
3				1106.6		1188.9	1229.6	
4					1123.1		1201.3	1239.2

Absorption series, $v'' = 0$ (58.14):C¹Π_u⁺ ← X¹Σ_g⁺ System

v'	λ	v'	λ	v'	λ
0	1009.3	6	901.2	12	848.5
1	986.3	7	889.0	13	845.0
2	965.6	8	878.2		
3		9			
4	930.0	10	860.5		
5	914.8	11	853.8		

C¹Π_u⁻ ← X¹Σ_g⁺ System

v'	λ	v'	λ	v'	λ
0	1009.3	5	914.8	10	860.5
1	986.3	6	901.2	11	853.8
2	965.6	7	889.0	12	848.6
3	946.9	8	878.1	13	845.0
4	930.0	9	868.7		

III. B¹Σ_u⁺ ← X¹Σ_g⁺ SystemBand heads, λ (68.28):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)	(6, 0)
λ	905.2	890.0	876.6	865.0	855.4	848.5	845.1

IV. D¹Π_u⁻ ← X¹Σ_g⁺ SystemBand heads, λ for $v'' = 0$ (68.28):

v'	λ	v'	λ	v'	λ
0	886.0	6	804.2	12	760.7
1	868.8	7	794.7	13	756.5
2	853.3	8	786.1	14	753.1
3	839.2	9	778.4	15	750.7
4	826.3	10	771.6		
5	814.7	11	765.7		

H₂

D¹Π_u⁺ ← X¹Σ_g⁺ System

Band heads, λ for v'' = 0 (68.28):

v'	λ	v'	λ	v'	λ
0	886.0	6	804.2	12	760.7
1	868.8	7	794.7	13	756.5
2	853.3	8	786.1	14	753.1
3	839.2	9	778.4	15	750.7
4	826.4	10	771.6		
5	814.7	11	765.7		

V. B''¹Σ_u⁺ ← X¹Σ_g⁺ System

Band heads, λ (68.28):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)	(6, 0)
λ	855.6	840.7	827.3	815.3	804.4	794.7	786.1

VI. D'¹Π_u⁻ ← X¹Σ_g⁺ System

Band heads, λ (68.28):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)
λ	848.65	833.06	818.94	806.02

D'¹Π_u⁺ ← X¹Σ_g⁺ System

Band heads, λ (68.28):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)
λ	848.64	833.06	818.89	806.00

VII. D''¹Π_u⁻ ← X¹Σ_g⁺ System

Band heads, λ (68.28):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	832.14	817.18	803.56

D''¹Π_u⁺ ← X¹Σ_g⁺ System

Band heads, λ (68.28):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	832.09	817.21	803.67

XI. K → B¹Σ_g⁺ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4	5
0	4662.7	4968.2	5305.9	5681.8		6515.9
1	4223.9	4472.2	4744.7	5043.1		5735.3
2	3871.8	4080.0	4305.1	4549.2	4814.9	5707.3

XII. G¹Σ_g⁺ → B¹Σ_g⁺ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4	5
0	4629.4	4930.2	5262.6	5632.2		
1	4196.9	4442.7	4710.8	5004.8	5328.2	5685.7
2	3861.0	4068.0	4291.8	4534.3	4798.2	5086.5
3	3617.4	3798.5	3993.0	4202.2	4427.9	4672.0

XIII. I¹Π_a → B¹Σ_g⁺ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4	5	6
0	4559.5	4851.3		5529.4			
1	4163.0	4404.9	4668.3	4956.9	5274.0	5624.0	6012.1
2	3841.6	4046.6					5363.9
3		3785.3	3978.2				

H₂

I¹Π_b → B¹Σ_g⁺ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4	5	6
0	4580.6	4874.7	5198.9	5559.0			
1	4178.9	4422.2	4687.6	4978.1	5297.5	5650.4	
2	3865.2	4072.3	4296.3	4539.1	4803.3	5091.6	5407.2
3	3617.3	3798.2	3992.3				

XIV. J¹Δ_g → B¹Σ_g⁺ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4
0	4503.3	4786.1	5097.6	5442.2	
1	4098.5	4335.0	4585.3	4854.4	5165.8

XV. H¹Σ_g⁺ → B¹Σ_g⁺ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4	5	6
0	4383.5	4652.2	4947.1				
1	3985.2	4206.1		4706.5	4991.5		5647.8
2	3685.3	3873.4	4075.8	4293.9	4512.6		

XVI. L¹Σ_g⁺ → B¹Σ_g⁺ System.

Band heads, λ (34.5):

v', v''	0	1	2	3	4
0	4333.9	4596.4	4884.2	5202.4	5550.9
1					
2	3741.4	3935.5	4666.6	4370.2	4614.9

XVII. $M^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4	5
0	4307.6	4566.8		5162.9	5507.8	5890.7
1	3941.0	4157.0		4645.1		
2	3634.9	3817.8	4014.3			4701.2

XVIII. $N^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4	5	6
0	4010.7	4234.6	4477.7	4742.3	5031.7		5686.0
1	3717.1	3908.5	4114.7	4334.1	4577.9	4839.3	5124.0

XX. $P^1\Sigma_g^+ \rightarrow B^1\Sigma_g^+$ System

Band heads, λ (34.5):

(v', v'')	(0, 0)	(0, 1)	(0, 2)	(0, 3)	(0, 4)	(0, 5)
λ	3675.4	3862.6	4072.8	4280.6	4515.1	4769.2

XXI. $R^1\Pi_a \rightarrow B^1\Sigma_g^+$ System

Band heads, λ (34.5):

(v', v'')	(0, 1)	(0, 2)	(0, 4)
λ	3640.6	3824.1	4462.5

$R^1\Pi_b \rightarrow B^1\Sigma_g^+$ System

Band heads, λ (34.5):

v', v''	0	1	2	3	4	5
0	3656.7	3841.6	4040.2	4264.0	4485.5	4736.0
1	3391.1		3718.4	3898.9	4092.2	4299.6

H₂

XXII. S¹Δ_a → B¹Σ_g⁺ System

Band heads, λ (34.5):^p

(v', v'')	(0, 0)	(0, 1)	(0, 2)	(0, 3)	(0, 4)	(0, 5)
λ	3636.1	3817.5	4012.5	4198.5	2387.9	4623.6

S¹Δ_b → B¹Σ_g⁺ System

(v', v'')	(0, 0)	(0, 1)	(0, 2)	(0, 3)	(0, 4)	(0, 5)
λ	3634.4	3816.4	4011.9	4222.3	4421.8	4695.3

TRIPLET SYSTEMS

II'. d³Π_u → a³Σ_g⁺ System (Fulcher α)

Band heads, λ (35.6):

v', v''	0	1	2	3	4
0	6020.1	7097.2			
1	5304.5	6123.3	7170.5		
2	4769.4	5421.5	6226.7	7242.7	
3	4355.4	4892.6	5538.9	6328.7	7311.5
4		4481.5	5017.8	5657.4	6430.0
5		4153.9	4610.6	5145.1	5776.3

IV'. k³Π_u → a³Σ_g⁺ System (β)

Band heads, λ (34.5):

v', v''	0	1	2	3	4
0	4491.8	5065.3			
1	4086.1	4555.4	5110.6		
2	3765.5	4160.4	4618.7	5155.4	5789.0
3		3846.4	4235.0	4681.6	5198.6
4			3928.3	4309.8	4744.1
5				4011.1	4384.8

VI'. $n^3\Pi_u \rightarrow a^3\Sigma_g^+$ System (γ)

Band heads, λ (34.5):

v', v''	0	1	2	3	4
0	4025.9	4480.7			
1		3934.8	4519.0		
2			4134.4	4556.6	
3				4185.0	4593.3

TRIPLET STATES

SPECTROSCOPIC CONSTANTS

Molecule		H_2									
State	T_o	(a) ω_e	(b) $\times \omega_e$	(c) B_e	(d) α	D_o	r_e	Remarks	Configuration		
$^3\Pi_u$	121316.7			~ 29.3 (f)			1.07 ^(g)		1s σ 6p π		
$^3\Sigma_u$	120427	~ 2661.4	~ 121.9	~ 31.5 (f)			1.03 ^(g)		1s σ 5f σ		
q	120017	2172.6 ^(e)		~ 30 (f)			~ 1.06 (g)				
$^3\Pi_u$	119931.7	2322	62.9	29.03	1.3		1.057		1s σ 5p π		
$^3\Sigma_u^+$	118379.3	2457.1 ^(e)		~ 36 (f)			~ 0.96 (g)		1s σ 4f σ		
$^3\Pi_g$	117492	2170 ^(e)						(h)	1s σ 4d π		
$^3\Delta_g$	117419	2170 ^(e)						(h)	1s σ 4d δ		
$^3\Sigma_g^+$	117381	2147.7 ^(e)						(h)	1s σ 4d σ		
$^3\Pi_u$	117356	2336	60	29.40	1.58		1.067		1s σ 4p π		
v	117280	~ 2339	~ 57	~ 29.1 (f)			1.07 ^(g)				
$^3\Sigma_u^+$	115610	2140.1 ^(e)		29.61	2.18	~ 2.2	1.063		1s σ 4p σ		
$^3\Delta_g$	112148	2265	58						1s σ 3s δ		

SPECTROSCOPIC CONSTANTS

TRIPLET STATES

State	T_o	(a) ω_e	(b) $x_e \omega_e$	(c) B_e	(d) α	D_o	r_e	Remarks	Configuration
$i^3\Pi_g$	111955	2268	~75						$1s\sigma\ 3d\pi$
$h^3\Sigma_g^+$	111783	2395.2	64.2	30.6	1.26	2.0	1.04		$1s\sigma\ 3s\sigma$
$g^3\Sigma_g^+$	111719	2265.5	89						$1s\sigma\ 3d\sigma$
$d^3\Pi_u$	111703	2371.58	66.27	30.364	1.545	2.0	1.0496		$1s\sigma\ 3p\pi$
$e^3\Sigma_u^+$	106690	2195.8	65.80	27.30	1.515	1.65	1.107		$1s\sigma\ 3p\sigma$
$a^3\Sigma_g^+$	95084	2664.83	71.65	34.216	1.671	2.21	0.9887		$1s\sigma\ 2s\sigma$
$c^3\Pi_u$	94793	2465.0	61.4	31.07	1.425	1.9	1.038		$1s\sigma\ 2p\pi$
$b^3\Sigma_u^+$	Unstable								$1s\sigma\ 2p\sigma$

SINGLET STATES

SPECTROSCOPIC CONSTANTS

State	T_o	(a) ω_e	(b) $\times_e \omega_e$	(c) B_e	(d) α	D_o	r_e	Remarks	Configuration
$D''^1\Pi_u^-$	120172.21	2323.56	62.15	30.76	1.45	21232.48	1.043		$1s\sigma 2p\pi$
$D'^1\Pi_u^-$	117834.65	2330.19	63.26	29.89	1.11	21102.27	1.058		$1s\sigma 2p\pi$
$O^1\Sigma_g^+$	117680			~32 (f)			~1.0 (g)		$1s\sigma 4s\sigma$
$S^1\Delta_g$	117656			~28.8 (f)			~1.08 (g)		$1s\sigma 4d\delta$
$R^1\Pi_g$	~117600	2142(e)		~30 (f)			~1.1 (g)		$1s\sigma 4d\pi$
$P^1\Sigma_g^+$	117342			~30 (f)			~1.1 (g)		$1s\sigma 4d\sigma$
$T^1\Sigma_g^+$	117330			~19			~1.3		
$B''^1\Sigma_u^+$	116882.00	2197.50	68.14	27.13	1.30	16723.31	1.111		$1s\sigma 2p\sigma$
$N^1\Sigma_g^+$	115090	1983.3 (e)		~17.5 (f)			~1.38 (g)		
$M^1\Sigma_g^+$	113390	2176(e)		~13 (f)			~1.6 (g)		
$L^1\Sigma_g^+$	113250	1835(e)		~10 (f)			~1.8 (g)		

SINGLET STATES

SPECTROSCOPIC CONSTANTS

State	T_o	(a) ω_e	(b) $x_e \omega_e$	(c) B_e	α (d)	D_o	r_e	Remarks	Configuration
$H^1\Sigma_g^+$	112949	2538	124	~ 29.5 (f)			~ 1.07 (g)		$1s\sigma\ 3s\sigma$
$D^1\Pi_u^-$	112871.74	2361.59	69.15	30.81	0.102	20733.57	1.042		$1s\sigma\ 2p\pi$
$J^1\Delta_g$	112345	2220 (e)		~ 28.8 (f)			~ 1.07 (g)		$1s\sigma\ 3d\delta$
$I^1\Pi_g$	112007	2265.2	78.47	29.79			1.060		$1s\sigma\ 3d\pi$
$G^1\Sigma_g^+$	111805.3	2404.3	88.6	28.4 (f)			~ 1.08 (g)		$1s\sigma\ 3d\sigma$
K	111621.5	2293	30	~ 11 (f)			~ 1.7 (g)		
Q	111347.2	742 (e)		16.3 (f)			~ 1.43 (g)		
$B'^1\Sigma_u^+$	110478.54	2074.93	113.39	26.78	0.380	7893.55	1.118		$1s\sigma\ 2p\sigma$
$F^1\Sigma_g^+$	~ 100400	~ 1000 (e)		~ 6.24 (f)			~ 2.32 (g)	(h)	$(2p\sigma)^2$
$E^1\Sigma_g^+$	99157.3	2588.9		32.68	1.82	(16938)	1.012		$1s\sigma\ 2p\sigma$
$C^1\Pi_u^-$	99081.72	2431.22	60.88	31.50	1.83	19290.37	1.031		$1s\sigma\ 2p\pi$

Molecule H_2

SINGLET STATES

SPECTROSCOPIC CONSTANTS

Molecule H₂

State	T ₀	(a) ω_e	(b) $x_e \omega_e$	(c) B_e	(d) α	D ₀	r _e	Remarks	Configuration
B ¹ Σ_u^+	90203.55	1357.39	20.42	20.035	1.2312	28168.54	1.29253		1s σ 2p σ
X ¹ Σ_g^+	0	4401.21	121.34	60.8530	3.0622	36113.05	0.74116		(1s σ) ²
(a) Actual value of $Y_{10}(\sim \omega_e)$; (b) Actual value of $-Y_{20}(\sim x_e \omega_e)$; (c) Actual value of $Y_{01}(\sim B_e)$; (d) Actual value of $-Y_{11}(\sim \alpha)$; (e) $\Delta G_{1/2}$; (f) B_0; (g) r_0; (h) Observed in perturbation. Dissociation energy = 4.47733 eV, 103.251 kcal/mole, 36118.62 cm⁻¹.									

Perturbations and General Information

Strong heterogeneous perturbations are observed in the $B^1\Sigma_u^+$, $B'^1\Sigma_g^+$, $D^1\Pi_u^-$, and $C^1\Pi_u^-$ states (73.93, 64.24, 61.17).

Homogeneous perturbations of the $C^1\Pi_u$ ($v = 3$) state by the $B^1\Sigma_u^+$ ($v = 14$) state are observed (73.110).

Weak heterogeneous perturbations are observed in the $B'^1\Sigma_g^+$ and $D'^1\Pi_u$ state (64.24).

Weak homogeneous perturbations are observed in the $B'^1\Sigma_g^+$ and $B''^1\Sigma_g^+$ state (64.24).

Strong vibrational and rotational perturbations are seen in the $F^1\Sigma_g^+$ state.

Strong vibrational perturbations are observed in the $G^1\Sigma_g^+$ state (37.9).

The $R^1\Pi_g^+$ and $d^3\Pi_u^+$ states are perturbed (73.106).

The $p^3\Sigma_g^+$, $p^3\Pi_g$, and $s^3\Delta_g$ states are perturbed.

The $h^3\Sigma_g^+$ state is predissociated at level $v = 3$ (36.8).

The $D^1\Pi_u$ state is predissociated at level $v = 3$ by $B'^1\Sigma_u^+$ state (72.48, 61.19).

The $j^3\Delta_g$ state is preionized at the $v = 3$ level.

The E and F states have been shown to represent a single state, the E, $F^1\Sigma_g^+$ state with a double minimum (74.134, 74.125, 71.41, 69.33).

Isotope shifts (68.26).

Lasing has been observed from the Werner and Lyman bands (74.115, 74.114, 73.95, 73.91, 70.37).

H₂

Franck-Condon factors for the B¹Σ_u⁺ - X¹Σ_g⁺ system (69.32):

v', v''	0	1	2	3	4	5	6	7	8
0	0.0037	0.0273	0.0903	0.1799	0.2403	0.2248	0.1474	0.0654	0.0181
1	0.0133	0.0689	0.1384	0.1220	0.0269	0.0139	0.1367	0.2294	0.1754
2	0.0273	0.0984	0.1066	0.0186	0.0235	0.1081	0.0559	0.0065	0.1613
3	0.0427	0.1036	0.0471	0.0047	0.0787	0.0392	0.0126	0.1041	0.0272
4	0.0563	0.0878	0.0080	0.0394	0.0571	0.0007	0.0715	0.0213	0.0438
5	0.0663	0.0624	0.0007	0.0599	0.0129	0.0342	0.0422	0.0112	0.0676
6	0.0723	0.0371	0.0130	0.0509	0.0005	0.0534	0.0022	0.0517	0.0073
7	0.0740	0.0175	0.0294	0.0278	0.0160	0.0352	0.0101	0.0394	0.0110
8	0.0725	0.0055	0.0402	0.0084	0.0337	0.0096	0.0334	0.0074	0.0392
9	0.0688	0.0005	0.0426	0.0003	0.0289	0.0000	0.0379	0.0014	0.0338
10	0.0634	0.0005	0.0382	0.0024	0.0315	0.0067	0.0239	0.0163	0.0106

Franck-Condon factors for the I¹Π_g - B¹Σ_g⁺ system (69.32):

v', v''	0	1	2	3	4	5	6	7	8
0	0.4663	0.3126	0.1397	0.0528	0.0185	0.0064	0.0023	0.0008	0.0003
1	0.3902	0.0248	0.1893	0.1849	0.1117	0.0551	0.0247	0.0106	0.0046
2	0.1263	0.3604	0.0264	0.0482	0.1303	0.1254	0.0845	0.0478	0.0248
3	0.0167	0.2551	0.2285	0.0988	0.0008	0.0589	0.0981	0.0895	0.0630
4	0.0005	0.0461	0.3440	0.1319	0.1267	0.0099	0.0160	0.0592	0.0746
5	0.0000	0.0009	0.0716	0.4042	0.0905	0.1156	0.0284	0.0015	0.0296
6	0.0000	0.0001	0.0002	0.0775	0.4576	0.0941	0.0856	0.0390	0.0002
7		0.0000	0.0004	0.0009	0.0539	0.4970	0.1494	0.0465	0.0440
8			0.0000	0.0005	0.0094	0.0114	0.4678	0.2763	0.0086
9			0.0000	0.0002	0.0000	0.0222	0.0109	0.2883	0.4363
10				0.0000	0.0003	0.0034	0.0126	0.1093	0.0371

Franck-Condon factors for the $d^3\Pi_u - a^3\Sigma_g^+$ system (69.32):

v', v''	0	1	2	3	4	5	6	7
0	0.93058	0.06863	0.00078	0.00000	0.00000			
1	0.06414	0.79842	0.13516	0.00226	0.00001	0.00000		
2	0.00485	0.11577	0.67463	0.19937	0.00433	0.00003	0.00000	
3	0.00039	0.01423	0.15683	0.56046	0.26113	0.00687	0.00008	0.00000
4	0.00003	0.00171	0.02725	0.18385	0.45689	0.32038	0.00972	0.00017
5	0.00000	0.00020	0.00448	0.04251	0.19799	0.36464	0.37715	0.01269
6	0.00000	0.00002	0.00073	0.00910	0.05825	0.20006	0.28411	0.43155
7		0.00000	0.00011	0.00193	0.01566	0.07249	0.19146	0.21539
8		0.00000	0.00002	0.00041	0.00417	0.02378	0.08332	0.17411
9			0.00000	0.00009	0.00113	0.00772	0.03259	0.08913
10			0.00000	0.00002	0.00032	0.00257	0.01258	0.04071

Franck-Condon factors for the $E, F^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ System (74.125):

v', v''	0	1	2	3	4	5	7	9
0	0.341	0.313	0.187	0.910-1	0.403-1	0.166-1	0.266-2	0.428-3
0*	0.825-4	0.207-2	0.180-1	0.843-1	0.216	0.314	0.994-1	0.451-3
1	0.424	0.497-3	0.794-1	0.174	0.138	0.818-1	0.260-1	0.102-1
1*	0.615-3	0.842-2	0.482-1	0.130	0.132	0.143-1	0.290	0.597-1
2	0.186	0.333	0.190-1	0.439-2	0.122-1	0.103	0.226-1	0.557-1
2*	0.874-4	0.232-1	0.877-1	0.958-1	0.338-1	0.373-1	0.405-2	0.317
3	0.129-1	0.129	0.193-1	0.172	0.120-2	0.549-1	0.177-2	0.112
3*	0.743-2	0.618-1	0.932-1	0.496-1	0.189-3	0.836-1	0.481-1	0.532-1
4	0.291-4	0.870-2	0.242-1	0.212-1	0.382-1	0.105	0.501-1	0.167-2
4*	0.184-1	0.802-4	0.199	0.132-1	0.579-1	0.169-2	0.130	0.343-1
5								
5*	0.227-2	0.905-1	0.137	0.244-1	0.496-1	0.381-2	0.296-1	0.199-2
6								
6*	0.637-2	0.196-1	0.254-1	0.786-1	0.102	0.642-2	0.114-1	0.356-1
7								
7*	0.699-3	0.107-2	0.509-1	0.495-3	0.115	0.325-1	0.562-1	0.300-6
8								
8*	0.326-3	0.661-2	0.175-2	0.347-1	0.184-5	0.778-1	0.166-2	0.360-1

v' with an asterisk refers to the outer minimum. v' without an asterisk refers to the inner minimum.

Franck-Condon factors followed by a factor of ten.

Franck-Condon factors for the $C^1\Pi_u \rightarrow E, F^1\Sigma_g^+$ system (74.125):

v', v''	0	0*	1	1*	2
0	0.993	0.672-6	0.706-2	0.101-9	0.232-3
1	0.678-2	0.122-5	0.981	0.323-4	0.500-2
2	0.555-3	0.146-4	0.662-2	0.145-3	0.794
3	0.256-4	0.201-3	0.283-2	0.133-2	0.725-2
4	0.738-5	0.203-2	0.483-4	0.929-2	0.326-1
5	0.190-6	0.143-1	0.536-3	0.435-1	0.594-2
6	0.503-6	0.673-1	0.191-3	0.118	0.229-3
7	0.578-7	0.200	0.190-4	0.142	0.115-1
8	0.259-6	0.347	0.158-3	0.185-1	0.172-2
9	0.119-6	0.292	0.136-3	0.121	0.835-2
10	0.205-7	0.748-1	0.222-3	0.413	0.120-2

v', v''	2*	3	3*	4*	5*
0	0.255-4	0.548-6	0.921-5	0.370-4	0.181-5
1	0.244-2	0.105-2	0.284-4	0.245-2	0.108-2
2	0.146-2	0.459-5	0.131-1	0.164	0.974-2
3	0.482-2	0.463	0.169-1	0.444-1	0.206
4	0.248-1	0.159-3	0.516-1	0.425-1	0.674-1
5	0.745-1	0.523-2	0.909-1	0.710-1	0.311-1
6	0.111	0.343-1	0.598-1	0.152-1	0.470-2
7	0.354-1	0.727-3	0.284-3	0.151-1	0.388-1
8	0.237-1	0.212-1	0.645-1	0.364-1	0.615-3
9	0.847-1	0.896-3	0.691-2	0.704-2	0.345-1
10	0.335-1	0.204-1	0.510-1	0.301-1	0.112-2

v'' with an asterisk refers to the outer minimum. v'' without an asterisk refers to the inner minimum.

Franck-Condon factors followed by a factor of ten.

Oscillator strengths (74.127, 74.126):

System	Band	$f_{v',0} \times 10^3$
$B^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	(0,0)	1.75
	(1,0)	5.19
	(2,0)	11.5
	(3,0)	17.6
	(4,0)	24.5
	(5,0)	25.8
$C^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	(1,0)	59.2
	(2,0)	64.2
	(3,0)	44.2
	(4,0)	31.7
	(5,0)	22.4
	(6,0)	17.0
$B^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	(1,0)	2.84
	(3,0)	4.84
$D^1\Pi_u^- \leftarrow X^1\Sigma_g^+$	(0,0)	6.14
	(2,0)	10.9

Radiative lifetimes:

$d^3\Pi_u$ state	τ_1	= 29.4 ± 3.2 nsec	(73.75, 73.74)
$a^3\Sigma_g^+$ state	τ_0	= 11.9 ± 1.2 nsec	(72.65)
	τ_1	= 10.8 ± 1.1 nsec	
	$\tau_{2,3}$	= 10 ± 2 nsec	
$B^1\Sigma_u^+$ state	τ_{8-11}	= 1 ± 0.2 nsec	(72.65)
$c^3\Pi_a$ state	τ_0	= 3.15 msec	(69.35)

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He₂He₂Methods of Production and Experimental Technique

Absorption in He discharges.

Emission - A condensed discharge in He at pressures of 20-50 Torr produces the continuum systems.

Radio frequency, microwave, and hollow cathode discharges.

SINGLET SYSTEMS

BAND SYSTEMS

	System	Transition	Sources	Electronic Configuration ^(a)	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography ^(b)
	I	$A^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Emission	Hopfield Continuum 600Å Bands		Max. intensity ~ 810Å	Continuum	(66.48, 65.41, 65.37, 62.29, 58.24)
	II	$D^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Emission			Max. intensity ~ 680Å	Continuum	(65.41, 58.24)
	III	$A^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Absorption			Max. intensity ~ 600-625Å	Continuum	(70.68, 69.67, 68.63, 66.46, 63.32)
	IV	$C^1\Sigma_g^+ \rightarrow A^1\Sigma_u^+$	Emission	$3p\sigma \rightarrow 2s\sigma$	R	10945.50		(65.36)
	V	$D^1\Sigma_u^+ \rightarrow B^1\Pi_g$	Emission	$3s\sigma \rightarrow 2p\pi$	R, V	15161.81		(65.38, 28.6)
	VI	$E^1\Pi_g \rightarrow A^1\Sigma_u^+$	Emission	$3p\pi \rightarrow 2s\sigma$	R	19476.4		(71.76, 29.18, 29.17, 29.11)
	VII	$F^1\Sigma_u^+ \rightarrow B^1\Pi_g$	Emission	$3d\sigma \rightarrow 2p\pi$	R	15837	(c)	(65.38, 28.6, 28.5)
	VIII	$F^1\Pi_u \rightarrow B^1\Pi_g$	Emission	$3d\pi \rightarrow 2d\pi$	R, V	16360	(c)	(65.38, 29.18, 29.17, 29.14)
	IX	$F^1\Delta_u \rightarrow B^1\Pi_g$	Emission	$3d\delta \rightarrow 2p\pi$	V	16360	(c)	(65.38, 29.18, 29.17, 29.14)
	X	$H^1\Sigma_u^+ \rightarrow C^1\Sigma_g^+$	Emission	$4s\sigma \rightarrow 3p\sigma$	V	13719.6	Perturbed $N > 5$	(73.84)

Molecule He₂

SINGLET SYSTEMS

BAND SYSTEMS

	System	Transition	Sources	Electronic ^(a) Configuration	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography ^(b)
	XI	$H^1\Sigma_u^+ \rightarrow B^1\Pi_g$	Emission	$4s\sigma \rightarrow 2p\pi$	R	21163	Perturbed N > 6	(73.84, 28.7)
	XII	$I^1\Pi_g \rightarrow A^1\Sigma_u^+$	Emission	$4p\pi \rightarrow 2s\sigma$	R	24979.6		(28.6, 27.3, 25.2)
	XIII	$J^1\Sigma_u^+ \rightarrow B^1\Pi_g$	Emission	$4d\sigma \rightarrow 2p\pi$		21416.11	(c)	(73.84)
	XIV	$J^1\Pi_u \rightarrow B^1\Pi_u$	Emission	$4d\pi \rightarrow 2p\pi$		21523.76	(c)	(73.84)
	XV	$J^1\Delta_u \rightarrow B^1\Pi_u$	Emission	$4d\delta \rightarrow 2p\pi$		21661.60	(c)	(73.84, 29.9)
	XVI	$L^1\Pi_g \rightarrow A^1\Sigma_u^+$	Emission	$5p\pi \rightarrow 2s\sigma$	R	27507		(29.18, 29.11, 25.2)
	XVII	$M^1\Sigma_u^+ \rightarrow B^1\Pi_g$	Emission	$5d\sigma \rightarrow 2p\pi$		(23960)	(c, d)	(29.18, 29.14)
	XVIII	$M^1\Pi_u \rightarrow B^1\Pi_g$	Emission	$5d\pi \rightarrow 2p\pi$		(24000)	(c, d)	(29.18, 29.14)
	XIX	$M^1\Delta_u \rightarrow B^1\Pi_g$	Emission	$5d\delta \rightarrow 2p\pi$		(24050)	(c, d)	(29.18, 29.14)
	XX	$P^1\Pi_g \rightarrow A^1\Sigma_u^+$	Emission	$6p\pi \rightarrow 2s\sigma$	R	28873		(29.18, 25.2)
	XXI	$R^1\Pi_g \rightarrow A^1\Sigma_u^+$	Emission	$7p\pi \rightarrow 2s\sigma$	R	29616		(29.10)

Molecule He₂

	System	Transition	Sources	Electronic ^(a) Configuration	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography ^(b)
	XXII	$S^1\Pi_g \rightarrow A^1\Sigma_u^+$	Emission	$8p\pi \rightarrow 2s\sigma$	R	30228		(29.10)

Molecule He₂

He₂

TRIPLET SYSTEMS

BAND SYSTEMS

	System	Transition	Sources	Electronic ^(a) Configuration	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography ^(b)
	I	$b^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$2p\pi \rightarrow 2s\sigma$	R	4768.2		(65.40, 56.23)
	II	$c^3\Sigma_g^+ \rightarrow a^3\Sigma_u^+$	Emission	$3p\sigma \rightarrow 2s\sigma$	R	10889.48		(65.36, 53.22, 32.20)
	III	$d^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$	Emission	$3s\sigma \rightarrow 3p\sigma$	V	9502.66		(65.39, 32.20)
	IV	$d^3\Sigma_u^+ \rightarrow b^3\Pi_g$	Emission	$3s\sigma \rightarrow 2p\pi$	R, V	15623.1		(65.39, 29.15, 29.8, 28.6, 28.4, 22.1)
	V	$e^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$3p\pi \rightarrow 2s\sigma$	R	21507.24		(71.76, 50.21, 28.6, 27.3, 25.2)
	VI	$f^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$	Emission	$3d\sigma \rightarrow 3p\sigma$	R	10658	(c)	(66.43, 32.20)
	VII	$f^3\Pi_u \rightarrow c^3\Sigma_g^+$	Emission	$3d\pi \rightarrow 3p\sigma$	V	10865	(c)	(66.43, 32.20)
	VIII	$f^3\Delta_u \rightarrow c^3\Sigma_g^+$	Emission	$3d\delta \rightarrow 3p\sigma$	V	11315	(c)	(66.43)
	IX	$f^3\Sigma_u^+ \rightarrow b^3\Pi_g$	Emission	$3d\sigma \rightarrow 2p\pi$	R	16779	(c)	(65.39, 29.17, 29.14, 28.6, 28.5)

Molecule He₂

	System	Transition	Sources	Electronic ^(a) Configuration	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography ^(b)
	X	$f^3\Pi_u \rightarrow b^3\Pi_g$	Emission	$3d\pi \rightarrow 2p\pi$		16986	(c)	(65.39, 29.17, 29.14, 28.6, 28.5)
	XI	$f^3\Delta_u \rightarrow b^3\Pi_g$	Emission	$3d\delta \rightarrow 2p\pi$	R, V	17437	(c)	(65.39, 28.6, 28.5, 22.1)
	XII	$h^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$	Emission	$4s\sigma \rightarrow 3p\sigma$	V	15870.7	Perturbed for large N	(29.9)
	XIII	$h^3\Sigma_u^+ \rightarrow b^3\Pi_g$	Emission	$4s\sigma \rightarrow 2p\pi$	R	21992.2	Perturbed for large N	(73.84, 29.15, 28.6, 28.5, 22.1)
	XIV	$i^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$4p\pi \rightarrow 2s\sigma$	R	27193.0		(29.18, 28.6, 27.3, 25.2)
	XV	$j^3\Sigma_u^+ \rightarrow b^3\Pi_g$	Emission	$4d\sigma \rightarrow 2p\pi$	R	22434	(c)	(73.84, 29.18, 29.16, 29.14, 28.6, 28.5)
	XVI	$j^3\Pi_u \rightarrow b^3\Pi_g$	Emission	$4d\pi \rightarrow 2p\pi$	R, V	22524	(c)	(73.84, 29.18, 29.16, 29.14, 28.6, 28.5)
	XVII	$j^3\Delta_u \rightarrow b^3\Pi_g$	Emission	$4d\delta \rightarrow 2p\pi$	V	22702	(c)	(73.84, 29.18, 29.16, 29.14, 28.6, 28.5)
	XVIII	$j^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$	Emission	$4d\sigma \rightarrow 3p\sigma$	R	(16313)	(c)	(29.15, 29.9)

Molecule He₂

TRIPLET SYSTEMS

BAND SYSTEMS

	System	Transition	Sources	Electronic ^(a) Configuration	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography ^(b)
	XIX	$j^3\Pi_u \rightarrow c^3\Sigma_g^+$	Emission	$4d\pi \rightarrow 3p\sigma$	R	16402	(c)	(29.15, 29.9)
	XX	$j^3\Delta_u \rightarrow c^3\Sigma_g^+$	Emission	$4d\delta \rightarrow 3p\sigma$	V	16581	(c)	(29.15)
	XXI	$k^3\Sigma_u^+ \rightarrow b^3\Pi_g$	Emission	$5s\sigma \rightarrow 2p\pi$	R	24804		(29.16, 29.15, 27.3)
	XXII	$k^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$	Emission	$5s\sigma \rightarrow 3p\sigma$	V	16683.5		(29.15, 29.11)
	XXIII	$l^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$5p\pi \rightarrow 2s\sigma$	R	29785.3		(68.62, 29.18, 29.11, 29.10, 25.2)
	XXIV	$l^3\Pi_g \rightarrow d^3\Sigma_u^+$	Emission	$5p\pi \rightarrow 3s\sigma$	R	9393.9		(73.84)
	XXV	$m^3\Sigma_u^+ \rightarrow b^3\Pi_g$	Emission	$5d\sigma \rightarrow 2p\pi$	R	25019	(c)	(29.15, 29.9)
	XXVI	$m^3\Pi_u \rightarrow b^3\Pi_g$	Emission	$5d\pi \rightarrow 2p\pi$	R	(25070)	(c, d)	(29.15, 29.9)
	XXVII	$m^3\Delta_u \rightarrow b^3\Pi_g$	Emission	$5d\delta \rightarrow 2p\pi$	V	25152	(c)	(29.16, 29.15)
	XXVIII	$m^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$	Emission	$5d\sigma \rightarrow 3p\sigma$	R	18899	(c)	(29.15)
	XXIX	$m^3\Pi_u \rightarrow c^3\Sigma_g^+$	Emission	$5d\pi \rightarrow 3p\sigma$	R	(18944)	(c, d)	(29.15)

Molecule He₂

	System	Transition	Sources	Electronic ^(a) Configuration	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography ^(b)
	XXX	$m^3\Delta_u \rightarrow c^3\Sigma_g^+$	Emission	$5d\delta \rightarrow 3p\sigma$	V	(19039)	(c)	(29.15)
	XXXI	$o^3\Sigma_u^+ \rightarrow b^3\Pi_g$	Emission	$6s\sigma \rightarrow 2p\pi$	R	26290.3		(29.15)
	XXXII	$o^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$	Emission	$6s\sigma \rightarrow 3p\sigma$	V	20168.8		(29.15, 29.11)
	XXXIII	$p^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$6p\pi \rightarrow 2s\sigma$	R	31179.93		(68.62, 29.18, 29.12, 27.3, 25.2)
	XXXIV	$p^3\Pi_g \rightarrow d^3\Sigma_u^+$	Emission	$6p\pi \rightarrow 3s\sigma$	R	10788.6		(n.p. 95)
	XXXV	$q^3\Sigma_u^+ \rightarrow b^3\Pi_g$	Emission	$6d\sigma \rightarrow 2p\pi$	R	26409	(c)	(29.16)
	XXXVI	$q^3\Pi_u \rightarrow b^3\Pi_g$	Emission	$6d\pi \rightarrow 2p\pi$	R	(26466)	(c, d)	(29.14)
	XXXVII	$q^3\Delta_u \rightarrow b^3\Pi_g$	Emission	$6d\delta \rightarrow 2p\pi$	V	(26483)	(c, d)	(29.15)
	XXXVIII	$q^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$	Emission	$6d\sigma \rightarrow 3p\sigma$	R	20288	(c)	(29.15)
	XXXIX	$q^3\Pi_u \rightarrow c^3\Sigma_g^+$	Emission	$6d\pi \rightarrow 3p\sigma$	R	(20330)	(c, d)	(29.15)
	XL	$q^3\Delta_u \rightarrow c^3\Sigma_g^+$	Emission	$6d\delta \rightarrow 3p\sigma$	V	20365	(c, d)	(29.15)

Molecule He₂

	System	Transition	Sources	Electronic ^(a) Configuration	Degrading	Band Head, v ₀ , 0	Remarks	Bibliography ^(b)
	XLI	$r^3\Sigma_g^+ \rightarrow a^3\Sigma_u^+$	Emission	$7p\sigma \rightarrow 2s\sigma$	V	31478.62		(68.62)
	XLII	$r^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$7p\pi \rightarrow 2s\sigma$	R	32016.56	(e)	(68.62, 29.18, 29.12, 27.3, 25.2)
	XLIII	$r^3\Pi_g \rightarrow d^3\Sigma_u^+$	Emission	$7p\pi \rightarrow 3s\sigma$	R	11625.3	(e)	(68.62)
	XLIV	$s^3\Sigma_g^+ \rightarrow a^3\Sigma_u^+$	Emission	$8p\sigma \rightarrow 2s\sigma$	V	32211.70	(e)	(68.62)
	XLV	$s^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$8p\pi \rightarrow 2s\sigma$	R	32556.66	(e)	(68.62, 29.12, 25.2)
	XLVI	$t^3\Sigma_g^+ \rightarrow a^3\Sigma_u^+$	Emission	$9p\sigma \rightarrow 2s\sigma$	V	32693.18	(e)	(68.62)
	XLVII	$t^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$9p\pi \rightarrow 2s\sigma$	R	32925.96	(e)	(68.62, 29.12, 25.2)
	XLVIII	$u^3\Sigma_g^+ \rightarrow a^3\Sigma_u^+$	Emission	$10p\sigma \rightarrow 2s\sigma$	V	33026.5	(e)	(68.62)
	XLIX	$u^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$10p\pi \rightarrow 2s\sigma$	R	33189.16	(e)	(68.62, 29.12, 25.2)
	L	$v^3\Sigma_g^+ \rightarrow a^3\Sigma_u^+$	Emission	$11p\sigma \rightarrow 2s\sigma$	V	33266.5	(e)	(68.62)
	LI	$v^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$11p\pi \rightarrow 2s\sigma$	R	33383.51	(e)	(68.62)

Molecule He₂

	System	Transition	Sources	Electronic ^(a) Configuration	Degrading	Band Head, v ₀ , 0	Remarks	Bibliography ^(b)
	LII	$w^3\Sigma_g^+ \rightarrow a^3\Sigma_u^+$	Emission	$12p\sigma \rightarrow 2s\sigma$	V	33445.1	(e)	(68.62)
	LIII	$w^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$12p\pi \rightarrow 2s\sigma$	R	33531.04	(e)	(68.62)
	LIV	$y^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$13p\pi \rightarrow 2s\sigma$	R	33645.7	(e)	(68.62)
	LV	$z^3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$14p\pi \rightarrow 2s\sigma$	R	33736.65	(e)	(68.62)
	LVI	$3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$15p\pi \rightarrow 2s\sigma$	R	33809.8	(e)	(68.62)
	LVII	$3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$16p\pi \rightarrow 2s\sigma$	R	33869.8	(e)	(68.62)
	LVIII	$3\Pi_g \rightarrow a^3\Sigma_u^+$	Emission	$17p\pi \rightarrow 2s\sigma$	P	33919.2	(e)	(68.62)

(a) These are the United Atom Orgital Rydberg symbols. Except for the ground state $X^1\Sigma_g^+$ ($\sigma_g 1s^2 \sigma_u 1s^2$), the inner shell configurations ($\sigma_g 1s^2 \sigma_u 1s^2 n\lambda$) will be designated by their $n\lambda$ value since all of these states converge to the He₂⁺ $X^2\Sigma_u^+$ state.

(b) For publications before 1925, see (29.13).

(c) States associated with the $nd\lambda$ configuration are strongly affected by l-decoupling (large Δ splitting), hence the band structures do not follow the usual intensity scheme of Hund's case b. See (66.43) for discussion.

(d) Data is fragmentary and may be in error. (e) l-decoupling affects $np\pi \Pi_g^+$ and $np\sigma \Sigma_g^+$ levels. As a result, branches using these terms become diffuse for $N \geq 7$ (68.62).

Molecule He₂

SINGLET SYSTEMSIV. C¹Σ_g⁺ → A¹Σ_g⁺ System

Band origins, λ (65.36):

v', v''	0	1	2	3
0	9136.2	10923.4		
1	7989.1	9322.3	11102.5	
2	7139.5	8186.0	9527.4	11302.0
3		7343.3	8404.8	9756.1

V. D¹Σ_u⁺ → B¹Π_g System

Band origins, λ (65.38, 28.6):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(1, 2)	(0, 1)
λ	6595.4	6605.0	6615.1	7400.8	7426.7

VI. E¹Π_g → A¹Σ_u⁺ System

Band origins, λ (71.76):

(v', v'')	(1, 0)	(2, 1)	(0, 0)	(1, 1)	(2, 2)	(0, 1)
λ	4733.1	4780.1	5134.3	5171.4	5208.3	5654.2

VII. F¹Σ_u⁺ → B¹Π_u System

Band origins, λ (65.38, 29.18):

(v', v'')	(0, 0)	(1, 1)	(0, 1)	(1, 2)
λ	6314.3	6367.8	7072.1	7104.8

VIII. F¹Π_u → B¹Π_u System

Band origins, λ (65.38, 29.18):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(0, 1)	(1, 2)	(2, 3)
λ	6246.9	6288.5	6335.5	6987.6	7005.7	7029.9

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IX. F¹Δ_u → B¹Π_g System

Band origins, λ (65.38, 29.18):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(1, 2)	(0, 1)
λ	6112.5	6135.0	6158.4	6815.7	6819.4

TRIPLET SYSTEMS

II. c³Σ_g⁺ → a³Σ_u⁺ System

Band origins, λ (65.36, 53.22):

v', v''	0	1	2	3
0	9183.6	10920.6		
1	8084.1	9401.1	11132.1	
2	7277.5	8326.4	9657.2	11389.7
3		7543.2	8619.2	9973.1
4			7875.3	8990.4

III. d³Σ_u⁺ → c³Σ_g⁺ System

Band origins, λ (65.39):

(v', v'')	(3, 2)	(2, 1)	(1, 0)	(3, 3)	(2, 2)	(1, 1)
λ	8775.0	8881.0	8962.2	9854.2	10113.3	10332.7

IV. d³Σ_u⁺ → b³Π_g System

Band origins, λ (65.39):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(3, 3)	(0, 1)	(1, 2)
λ	6400.8	6418.1	6437.5	6458.3	7181.3	7167.4

V. e³Π_g → a³Σ_u⁺ System

Band origins, λ (71.76, 50.21):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(0, 1)	(1, 2)
λ	4649.6	4667.2	4683.2	5056.9	5057.7

VI. $f^3\Sigma_u^+ \rightarrow c^3\Sigma_g^+$ System

Band origins, λ (66.43, 32.20):

(v', v'')	(1, 0)	(2, 1)	(2, 2)	(1, 1)	(0, 0)	(0, 1)	(1, 2)
λ	8192.0	8206.8	9248.1	9322.3	9382.6	10895.6	10689.5

VII. $f^3\Pi_u \rightarrow c^3\Sigma_g^+$ System

Band origins, λ (66.43, 32.20):

(v', v'')	(3, 2)	(2, 1)	(1, 0)	(2, 2)	(1, 1)	(0, 0)	(1, 2)
λ	8034.7	8039.2	8040.5	9035.1	9126.6	9203.9	10433.0

VIII. $f^3\Delta_u \rightarrow c^3\Sigma_g^+$ System

Band origins, λ (66.43):

(v', v'')	(2, 1)	(1, 0)	(2, 2)	(1, 1)	(0, 0)
λ	7669.3	7720.8	8571.2	8716.9	8837.8

IX. $f^3\Sigma_u^+ \rightarrow b^3\Pi_g$ System

Band origins, λ (65.39, 29.14):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(0, 1)	(1, 2)	(2, 3)
λ	5959.8	6014.0	6076.1	6630.9	6666.7	6711.4

X. $f^3\Pi_u \rightarrow b^3\Pi_g$ System

Band origins, λ (65.39, 29.14):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(0, 1)	(1, 2)	(2, 3)
λ	5887.2	5931.5	5983.0	6541.5	6564.3	6598.0

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XI. $f^3\Delta_u \rightarrow b^3\Pi_g$ System

Band origins, λ (65.39, 29.14):

(v', v'')	(0, 0)	(1, 1)	(2, 2)
λ	5734.9	5755.4	5775.7

XIV. $i^3\Pi_g \rightarrow a^3\Sigma_u^+$ System

Band origins, λ (29.18, 28.6):

(v', v'')	(1, 0)	(0, 0)	(1, 1)	(0, 1)	(1, 2)
λ	3468.5	3677.4	3690.2	3927.6	3930.2

XXIII. $l^3\Pi_g \rightarrow a^3\Sigma_u^+$ System

Band origins, λ (68.62, 29.10):

(v', v'')	(1, 0)	(0, 0)	(1, 1)	(2, 2)	(0, 1)
λ	3182.8	3357.4	3368.5	3378.8	3564.7

XXXIII. $p^3\Pi_g \rightarrow a^3\Sigma_u^+$ System

Band origins, λ (68.62, 29.12):

(v', v'')	(1, 0)	(2, 1)	(0, 0)	(1, 1)	(2, 2)
λ	3047.9	3063.8	3207.2	3217.7	3227.4

XLII. $r^3\Pi_g \rightarrow a^3\Sigma_u^+$ System

Band origins, λ (68.62, 29.12):

(v', v'')	(1, 0)	(0, 0)	(1, 1)	(0, 1)
λ	2972.1	3123.3	3133.4	3302.1

XLV. $\underline{s^3\Pi_g \rightarrow a^3\Sigma_u^+ \text{ System}}$

Band origins, λ (68.62, 29.12):

(v', v'')	(1, 0)	(0, 0)	(1, 1)	(0, 1)
λ	2925.2	3071.5	3081.3	3244.1

XLVII. $\underline{t^3\Pi_g \rightarrow a^3\Sigma_u^+ \text{ System}}$

Band origins, λ (68.62, 29.12):

(v', v'')	(1, 0)	(0, 0)	(1, 1)	(0, 1)
λ	2893.9	3037.1	3046.6	3205.7

SINGLET STATES

SPECTROSCOPIC CONSTANTS

State	$T_0 - A^{(a)}$	ω_e	$\times_e \omega_e$	B_e	α_e	$D_e \times 10^6$	r_e	Remarks	Configuration
$S^1\Pi_g$	30228			(7.21)	(0.22)		(1.08)		$8p\pi$
$R^1\Pi_g$	29696			(7.22)	(0.22)		(1.07)		$7p\pi$
$P^1\Pi_g$	28873			(7.22)	(0.22)		(1.07)		$6p\pi$
$M^1\Delta_u$	(27551)								$5d\delta$
$M^1\Pi_u$	(27501)								$5d\pi$
$M^1\Sigma_u^+$	(27461)								$5d\sigma$
$L^1\Pi_g$	27507			(7.23)	(0.22)		(1.079)		$5p\pi$
$J^1\Delta_u$	25129.4			7.097 ^(b)					$4d\delta$
$J^1\Pi_u$	25003.87			7.080 ^(b)					$4d\pi$
$I^1\Pi_g$	24979.6			(7.24)	(0.22)		(1.078)		$4p\pi$
$H^1\Sigma_u^+$	24665.0			(7.26)	(0.23)		(1.07)		$4s\sigma$

SPECTROSCOPIC CONSTANTS

SINGLET STATES

State	$T_0 - A(a)$	ω_e	$x_e \omega_e$	B_e	α_e	$D_e \times 10^6$	r_e	Remarks	Configuration
$F^1\Delta_u$	19862.4	1706.59	35.06	7.230	0.225		1.079		3d δ
$F^1\Pi_u$	19509.8	1670.57	40.03	7.156	0.235		1.085		3d π
$F^1\Sigma_u^+$	19339.0	(1644)	(40)	7.098	0.246		1.089		3d σ
$E^1\Pi_g$	19476.4	1721.2	34.9	7.270	0.215		1.076	$y_e \omega_e = -0.04$ $\gamma_e = -0.0022$	3p π
$D^1\Sigma_u^+$	18663.3	1746.43	35.54	7.365	0.218		1.069	$\gamma_e = -0.0059$	3s σ
$C^1\Sigma_g^+$	10945.5	1653.43	41.04	7.052	0.215		1.093	$y_e \omega_e = 0.355$ $z_e \omega_e = -0.131$	3p σ
$B^1\Pi_g$	3501.5	1765.76	34.39	7.403	0.216		1.068	$y_e \omega_e = -0.0267$ $\gamma_e = -0.0015$	2p π
$A^1\Sigma_u^+$	0	1861.27	35.0	7.787	0.228		1.040	$y_e \omega_e = -0.105$	2s σ
$X^1\Sigma_g^+$	$-A(c)$								

TRIPLET STATES

SPECTROSCOPIC CONSTANTS

State	$T_0 - a^{(a)}$	ω_e	$x_e \omega_e$	B_e	α_e	$D_e \times 10^6$	r_e	Remarks	Configuration
$3\Pi_g$	33919.2	1698	(35)	(7.211)	(0.224)		(1.080)		17p π
$3\Pi_g$	33869.8	1698	(35)	(7.211)	(0.224)		(1.080)		16p π
$3\Pi_g$	33809.8	1698	(35)	(7.211)	(0.224)		(1.080)		15p π
$3^3\Pi_g$	33736.65	1698	(35)	(7.211)	(0.224)		(1.080)		14p π
$3^3\Pi_g$	(33645.7)	1698	(35)	(7.211)	(0.224)		(1.080)		13p π
$3^3\Pi_g$	33531.04	1698	(35)	(7.211)	(0.224)		(1.080)		12p π
$3^3\Sigma_g^+$	33445.2								12p σ
$3^3\Pi_g$	33383.51	(1698.95)	(35)	7.21	0.22		1.080		11p π
$3^3\Sigma_g^+$	33266.6								11p σ
$3^3\Pi_g$	33189.16	(1699.19)	(35.2)	7.21	0.22		1.080		10p π
$3^3\Sigma_g^+$	33026.58								10p σ

Molecule He₂

SPECTROSCOPIC CONSTANTS

TRIPLET STATES

State	$T_0 - a$ (a)	ω_e	$x_e \omega_e$	B_e	α_e	$D_e \times 10^6$	r_e	Remarks	Configuration
$t^3\Pi_g$	32925.96	(1699.65)	(35.2)	7.21	0.23		1.080		$9p\pi$
$t^3\Sigma_g^+$	32693.1								$9p\sigma$
$s^3\Pi_g$	32556.60	(1699.80)	(35.2)	7.213	0.224		1.080		$8p\pi$
$s^3\Sigma_g^+$	32211.70								$8p\sigma$
$r^3\Pi_g$	32016.56	(1700.5)	(35.2)	(7.216)	(0.224)		1.080		$7p\pi$
$r^3\Sigma_g^+$	31478.6								$7p\sigma$
$q^3\Delta_u$	31255								$6d\delta$
$q^3\Pi_u$	(31234)								$6d\pi$
$q^3\Sigma_u^+$	31177								$6d\sigma$
$p^3\Pi_g$	31179.9	1701.18	35.3	7.220	0.224		1.079		$6p\pi$
$o^3\Sigma_u^+$	31058.4			(7.22)	(0.23)		1.07		$6s\sigma$

TRIPLET STATES

SPECTROSCOPIC CONSTANTS

Molecule He₂

State	$T_0 - a$ (a)	ω_e	$x_e \omega_e$	B_e	α_e	$D_e \times 10^6$	r_e	Remarks	Configuration
$^3m\Delta_u$	29920								5d δ
$^3m\Pi_u$	(29835)								5d π
$^3m\Sigma_u^+$	29788								5d σ
$^1^3\Pi_g$	29785.3	(1704.46)	(35.2)	7.226	0.222		1.079		5p π
$^3k\Sigma_u^+$	29573	1635.3 ^(d)		7.23	0.23		1.079		5s σ
$^3j\Delta_u$	27470	1633 ^(d)							4d δ
$^3j\Pi_u$	27292	1598 ^(d)							4d π
$^3j\Sigma_u^+$	27202	1592 ^(d)							4d σ
$^3i\Pi_g$	27193.0	(1708.4)	(35.2)	7.242	0.223		1.078		4p π
$^3h\Sigma_u^+$	26760.4	1637.9 ^(d)		7.26	0.23		1.077		4s σ
$^3f\Delta_u$	22205.5	1706.82	35.10	7.230	0.229		1.079		3d δ

SPECTROSCOPIC CONSTANTS

TRIPLET STATES

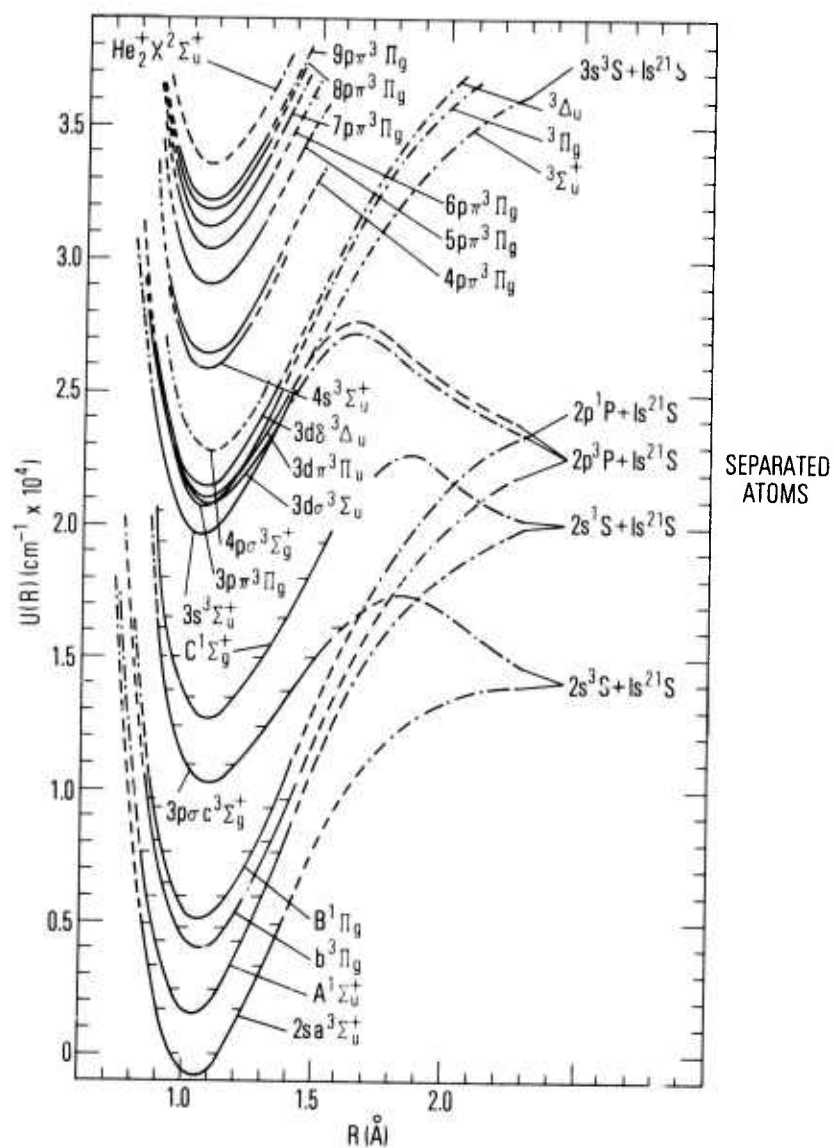
State	$T_0 - a$ ^(a)	ω_e	$x_e \omega_e$	B_e	α_e	$D_e \times 10^6$	r_e	Remarks	Configuration
$f^3\Pi_u$	21754.0	1661.48	44.79	7.136	0.233		1.086		3d π
$f^3\Sigma_u^+$	21548.8	1635.77	44.41	7.071	0.246		1.091		3d σ
$e^3\Pi_g$	21507.2	1721.1	34.7	7.283	0.221		1.075	$y_e^w = -0.02$ $\gamma_e = -0.0013$	3p π
$d^3\Sigma_u^+$	20391.3	1728.01	36.13	7.341	0.224		1.071	$y_e^w = -0.127$ $\gamma_e = 0.0027$	3s σ
$c^3\Sigma_g^+$	10889.5	1583.85	52.74	7.005	0.310		1.096	$y_e^w = -1.257$ $z_e^w = -0.488$ $\gamma_e = 0.0016$	3p σ
$b^3\Pi_g$	4768.2	1769.07	35.02	7.447	0.219		1.063	$y_e^w = -0.048$ $\gamma_e = -0.0017$	2p π
$a^3\Sigma_u^+$	0	1808.5	38.2	7.703	0.228		1.045	$y_e^w = -0.3$ $\gamma_e = -0.0046$	2s σ

(a) A and a represent the energies of the $A^1\Sigma_u^+$ and $a^3\Sigma_u^+$ states ($v=0$, $N=0$ levels) above the $X^1\Sigma_g^+$ state.The $A^1\Sigma_u^+$ state is 2344.1 cm^{-1} above the $a^3\Sigma_u^+$ state.(b) B_0 ; (c) $X^1\Sigma_g^+$ state is unstable; (d) $\Delta G_{1/2}$

He₂

Perturbations and General Information

Potential energy curves (70.70)



Stimulated emission has been observed on the $d^3\Sigma_u^+ \rightarrow b^3\Pi_g$ transition at $6400\text{\AA}$ (74.90).

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Hg₂

Hg₂

Methods of Production and Experimental Technique

Absorption in mercury vapor.

Emission from a Tesla discharge, hollow cathode discharge, argon and mercury discharge, electrodeless glow discharge.

Fluorescence (primarily from 2537Å mercury resonance line), resonance irradiation at low temperatures.

Band SystemsA. Continuous SpectraI. $A^3\sigma_u^- \rightarrow X^1\Sigma_g^+$ System

Visible region - "4850Å continuum" (73.33, 73.32, 73.31, 52.23, 49.21, 44.20, 31.9, 31.8)

Emission: 6000-3800Å, maximum at ~ 5200Å
 Fluorescence: 5300-4000Å, maximum at ~ 4850Å

II. $A^3\pi_u \rightarrow X^1\Sigma_g^+$ System

Near ultraviolet region - "3350Å continuum" (73.34, 73.31, 52.23, 49.21, 44.20, 31.9)

Emission and fluorescence: 3700-3000Å region, maximum at 3350Å
 Absorption (32.14)

III. ~ 2650Å

Emission at ~ 2650 ± 30Å (27.1)

IV. Ultraviolet Region

Emission and Absorption: 2345-1808Å region (31.12, 31.10, 31.8, 30.4)

V. Far Ultraviolet Region

Absorption: Three continua at 1403, 1692, and 1800Å (31.12, 31.10)
 Emission: 1692Å only

B. Band SpectraI. $B^3\pi_u \rightarrow A^3\sigma_u^-$ System

Triplet: 5461, 4358 and 4047Å (73.34, 73.31, 68.27, 33.15)

Emission (λ): 5492.7 | 5483.6 | 5473.5 | 4364.8 | 4061.1 | 4060.8 | 4050.4 |
 4023.8

II. Takeyama Bands

Emission

a. 5411-5369Å - group of 9 weak bands (52.23)

b. 5313-4988Å - group of 47 bands. Band heads of high intensity (λ)

v', v''	0	1	2	3	4	5	6	7
0	5096.8	5133.7	5170.2	5208.3	5246.4			
1	5066.0		5138.6	5175.3	5213.2	5250.5		
2	5036.2	5071.7	5108.5	5144.5	5180.5	5218.0	5254.5	5292.0
3	5006.5	5041.5	5076.5	5112.5	5149.5	5186	5223.2	5259.0
4		5012.3	5047	5082.0		5154.1		5227.2
5			5017.6		5087		5159	
6			4987.7			5092		5164

c. 4962-4926Å - 3 weak bands at 4962, 4938, and 4926Å

d. 4905-4768Å - 12 bands, (λ)

|4905|4890|4874|4855|4839|4834|4817|4811|4788|4782|4773|
4768|

e. 4751-4400Å - group of 61 bands. Band heads of high intensity (λ)

v', v''	0	1	2	3	4	5	6
0	4513.0	4541.9	4571.7	4601.3	4631.5	4662.0	
1	4488.4	4517.5	4546.5	4576.0	4605.6	4635.3	4666.0
2	4464.4	4493	4522.9	4551	4580.5	4610.0	4639.4
3	4441	4470.0	4498.2	4527	4555.7		4614.0
4	4417.8	4446	4475	4503		4560.3	
5		4423.0			4507.5		4564.5

f. 4321-3680Å - group of 117 bands (33.16). Bands of highest intensity (λ)

|4281.7|4277.6|4252.8|4251.0|4227.6|4225.5|4202.3|4200.2|
4181.6|4179.0|

g. 4310-4298Å - 2 large intense sets of bands; one at 4309 and 4305Å, the other at 4302 and 4298Å

h. 4133-4120Å - bands between 4132.3-4130.0 and 4122.4-4120.4Å

i. 4011-3685Å - diffuse bands (30.3). Bands of highest intensity at 3984 and 3946Å

j. 3663-3342Å - group of 26 bands partially superimposed on the continuum at 3350Å. Bands of highest intensity (λ)

|3497|3486|3474|3455|3443|

- k. 3342-3014Å - heads of intense bands distinct at 3135.9, 3134.4, and 3112.3Å
- l. 3014-2537Å - several structures discovered by (52.23) superimposed on continuous bands

III. Rayleigh Bands

- a. 3014-2857Å "Core Bands" - the bands form a convergent series up to a point near the 2537Å resonance line

Fluorescence (λ)	3012.0	Emission (λ)	3014.3
(32.13, 31.11)	2993.8	(31.11, 27.1)	2994.4
	2977.6		2976.1
	2959.4		2960.2
	2944.4		2945.4
	2930.1		2929.7
	2911.1		2913.2
	--		2896.9
	2883.3		2884.1
	2871.6		2871.6
	2857.4		2860.8

- b. 2930-2782Å "Wing Bands" - the bands converge at ~ 2645Å

Fluorescence (λ)	2931.1	Absorption (λ)	2930.7
(32.13, 31.11)	2917.4	(27.1)	2918.2
	2904.7		2907.0
	2892.9		2894.8
	2882.7		2883.8
	2871.2		2873.6
	2860.6		2863.6
	2851.5		2853.1
	2841.8		2843.2
	2832.3		2833.2
	2823.6		2825.3
	2814.9		2815.3
	2806.4		2807.4
	2798.6		2799.2
	2790.2		2790.8
	2781.9		2784.3

IV. 2540Å Bands

Emission (49.22) at high dispersion

 λ | 2540.467 | 2540.453 | 2540.424 | 2540.378 | 2540.345 | 2540.290 | 2540.235 |
 bordered by 2540.524 and 2539.823Å

Absorption (49.22, 32.14). Very weak bands apparently of the same system

 λ | 2542.5 | 2541.5 | 2539.6 | 2538.5 |
V. Wood Bands 2345-2311Å

Emission (31.8)

Fluorescence (32.13)

Absorption (32.14, 29.2)

Band heads:

Absorption (λ)	Emission (λ)
2341.50	2345.5
2340.48	
2339.48	
2338.47	2338.6
2337.38	
2336.40	
2335.38	
2334.37	
2333.33	2333.8
2331.33	
2329.35	2329.0
2328.41	
2327.36	
2326.44	
2325.39	
2324.50	2324.4
2323.54	
2322.58	
2321.59	
2320.66	2320.8
2319.76	
2318.87	
2317.87	2318.0
2316.89	
2316.03	
2315.03	2315.1
2314.23	
2313.25	
2312.51	2312.2
2311.54	

VI. Steubing-Kremenevsky Bands 2167-2038Å

Emission (31.8)

Absorption (31.12)

Very diffuse bands

Hg₂

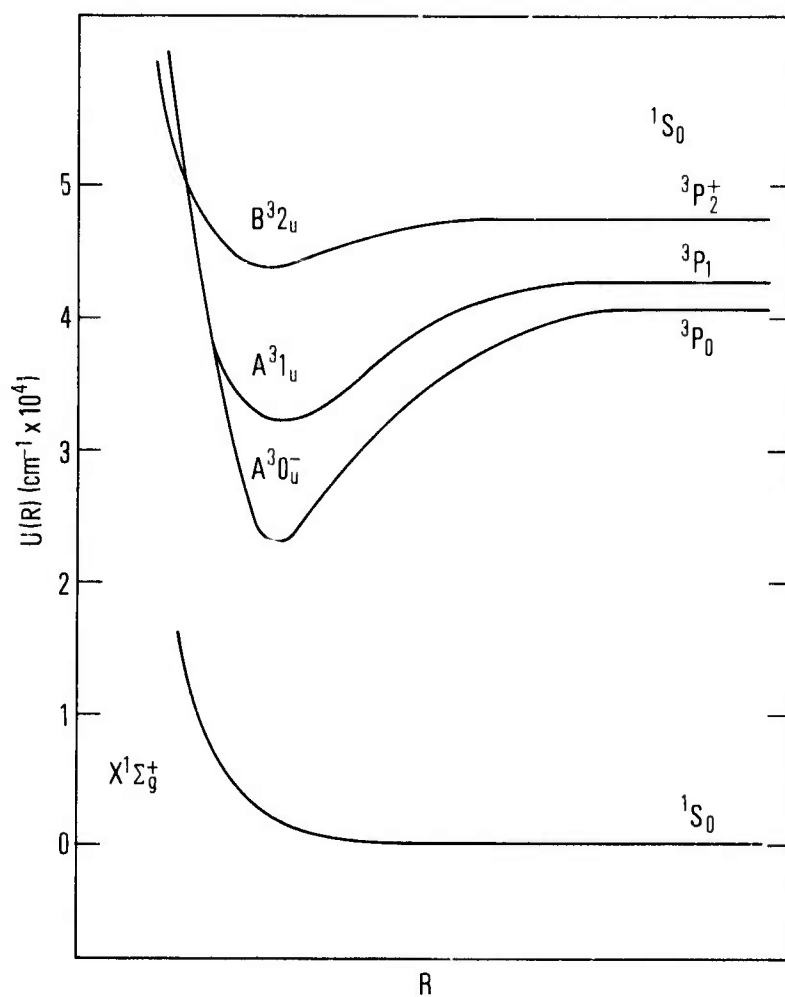
Spectroscopic Constants

Dissociation energy = 0.14 ± 0.02 eV, 3.2 kcal/mole, 1120 cm^{-1} .

Perturbations and General Information

The ground state has been shown to be a repulsive state.

Potential energy curves (73.34)



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Hg₂

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Ho₂

Ho₂

Spectroscopic Constants

Dissociation energy = 1.98 ± 0.74 eV, 16 kcal/mole, 15970 cm^{-1} (72.2, 71.1).

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Methods of Production and Experimental Technique

Absorption (between 0 and 1100° C).

Emission from discharge into I₂ in the presence of foreign gases.

Resonance and laser-excited fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	I	$A^3\Pi_u - X^1\Sigma_g^+$ (1 _u) (0 _g ⁺)	Absorption	9300-8300	R	11803		(70.73, 64.49, 31.11)
	II	$1\Pi = X^1\Sigma_g^+$ (1 _u)		6000-4500			Continuum	(73.118)
	III	$B^3\Pi_u = X^1\Sigma_g^+$ (0 _u ⁺)	Absorption, emission, and fluorescence	8600-4300	R	15724.95		(73.119, 73.111, 73.107, 73.105, 72.87, 72.86, 72.85, 72.81, 70.74, 70.73, 70.67, 67.58, 65.53)
	IV	$C^3\Sigma_u^+ - X^1\Sigma_g^+$ (1 _u)	Emission, photofragment spectroscopy	2500-2400				(73.113)
	V	$D^3\Sigma_g^- = X^1\Sigma_g^+$ (1 _g , 0 _g ⁺)	Absorption, fluorescence	3460-3100	R			(72.87, 71.80)
	VI	$E^3\Sigma_u^- - X^1\Sigma_g^+$ (1 _u)	Discharge, emission	2400-2240	R	45170		(58.39)

Molecule I₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	VII	$F^1\Sigma_g^+ - X^1\Sigma_g^+$ (0_g^+)	Absorption	2740-2530	R	47158.6		(72.87, 35.17, 34.15, 29.8, 29.7, 28.6)
	VIII	$G^3\Sigma_u^- - X^1\Sigma_g^+$ (0_u^+)	Emission	2730-2486	R	47148	Absorption superim- posed on D-X and F-X systems	(58.40, 51.30, 47.27, 40.21, 35.17, 29.8, 29.7, 28.6)
	IX	$H^1\Sigma_u^+ - X^1\Sigma_g^+$ (0_u^+)	Discharge, absorption	2240-1950	R	45543(0, 12) 45030(1, 15)		(58.39, 46.23, 35.19, 29.8, 29.7)
	X	$I^1\Sigma_u^+ - X^1\Sigma_g^+$ (0_u^+)	Resonance fluores- cence	2370-1770				(70.73, 56.37)
	XI	$c\Pi - X^1\Sigma_g^+$ (1_u)	Absorption	1770-1723	V			(70.73)
	XII	$d\Delta - X^1\Sigma_g^+$ (1_u)	Absorption	1736-1707	V			(70.73)
	XIII	$e\Sigma_u^+ - X^1\Sigma_g^+$ (0_u^+)	Absorption	1703-1688	V			(70.73)

Molecule I₂

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	XIV	$f^3\Pi - X^1\Sigma_g^+$ (1_u)	Absorption	1625-1611	R			(70.73)
	XV	$g\Sigma_u^- - X^1\Sigma_g^+$ ($1_u, 0_u^+$)	Absorption	1625-1593	R			(70.73)
	XVI	$f\Pi - X^1\Sigma_g^+$ (0_u^+)	Absorption	1600-1590	R			(70.73)
	XVII	$M^3\Pi_u - X^1\Sigma_g^+$ (0_u^+)	Absorption	1602-1574	R			(70.73)
	XVIII	$g\Pi - X^1\Sigma_g^+$ (1_u)	Absorption	1592-1564	R			(70.73)
	XIX	$h\Pi - X^1\Sigma_g^+$ (1_u)	Absorption	1579-1556	V			(70.73)
	XX	$i\Sigma_u^+ - X^1\Sigma_g^+$ (1_u)	Absorption	1578-1561	V			(70.73)

Molecule I₂

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	XXI	$j\Sigma_u^- \leftarrow X^1\Sigma_g^+$ ($1_u, 0_u^+$)	Absorption	~ 1555	V			(70.73)
	XXII	$k\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1558-1539	R			(70.73)
	XXIII	$1\Pi \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	~ 1540	V			(70.73)
	XXIV	$N^1\Pi_u \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1539-1533	R			(70.73)
	XXV	$m\Pi \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1504-1495	V			(70.73)
	XXVI	$\beta\Sigma^- \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1488-1464	R			(70.73)
	XXVII	$\beta'\Sigma^- \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1495-1480	R			(70.73)

Molecule I₂

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	XXVIII	$o\Pi \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1491-1477	R			(70.73)
	XXIX	$p\Sigma^+ \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1480-1472	R			(70.73)
	XXX	$o'\Pi \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	1486-1467	V			(70.73)
	XXXI	$q\Sigma^+ \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	~ 1472	V			(70.73)
	XXXII	$\gamma\Sigma^+ \leftarrow X^1\Sigma_g^+$ (1_u)	Absorption	1467-1459	R			(70.73)
	XXXIII	$\gamma'\Sigma^+ \leftarrow X^1\Sigma_g^+$ (0_u^+)	Absorption	~ 1445	R			(70.73)
	XXXIV	$r\Sigma^- \leftarrow X^1\Sigma_g^+$ ($1_u, 0_u^+$)	Absorption	1445-1428	R			(70.73)

Molecule I₂

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	XXXV	$\delta\Sigma^- - X^1\Sigma_g^+$ (1 _u)	Absorption	~ 1436	R			(70.73)
	XXXVI	$\delta'\Sigma^- - X^1\Sigma_g^+$ (0 _u ⁺)	Absorption	~ 1434				(70.73)
	XXXVII	$\zeta\Pi - X^1\Sigma_g^+$ (1 _u)	Absorption	1442-1423	R			(70.73)
	XXXVIII	$\zeta'\Pi - X^1\Sigma_g^+$ (0 _u ⁺)	Absorption	1439-1427				(70.73)
	XXXIX	$\eta'\Pi - X^1\Sigma_g^+$ (1 _u)	Absorption	~ 1427	V			(70.73)
	XL	$\theta\Pi - X^1\Sigma_g^+$ (0 _u ⁺)	Absorption	1425-1407	V			(70.73)
	XLI	$\iota\Pi - X^1\Sigma_g^+$ (1 _u)	Absorption	1418-1397	R			(70.73)

Molecule I₂

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	XLII	$\iota'\Pi - X^1\Sigma_g^+$ (0 _u ⁺)	Absorption	1423-1397	R			(70.73)
	XLIII	$\eta\Sigma^+ - X^1\Sigma_g^+$ (1 _u)	Absorption	1401-1388	R			(70.73)
	XLIV	$\eta'\Sigma^+ - X^1\Sigma_g^+$ (0 _u ⁺)	Absorption	1398-1381	R			(70.73)
	XLV	$\theta\Pi - X^1\Sigma_g^+$ (1 _u , 0 _u ⁺)	Absorption	1390-1369	R			(70.73)
	XLVI	$u\Pi - X^1\Sigma_g^+$ (1 _u)	Absorption	1382-1364	V			(70.73)
	XLVII	$u'\Pi - X^1\Sigma_g^+$ (0 _u ⁺)	Absorption	1385-1367	V			(70.73)
	XLVIII	$v - X^1\Sigma_g^+$	Absorption	1374-1365			Very weak	(70.73)

Molecule I₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	XLIX	$\omega\Sigma^+ \rightarrow X^1\Sigma_g^+$ (1 _u)	Absorption	1370-1349				(70.73)
	L	Repulsive states $\rightarrow X^1\Sigma_g^+$	Absorption	1461-1447				(70.73)
	LI	$D^3\Sigma_g^- \rightarrow B^3\Pi_u$ (1 _g , 0 _g ⁺) (0 _u ⁺)	Emission	4420-4000	R			(70.73, 51.30, 47.27)
	LII	$E^3\Sigma_u^- \rightarrow B^3\Pi_u$ (1 _u)	Emission	4360-4000	R			(72.87)
	LIII	$F^1\Sigma_g^+ \rightarrow B^3\Pi_u$ (0 _g ⁺)	Emission	3460-3015	R			(58.40, 33.14)
	LIV	$J^3\Pi_g \rightarrow B^3\Pi_u$ (1 _g , 0 _g ⁺)	Emission	2785-2731				(58.40)

Molecule I₂

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	LV	$a\Pi(2, 1_g) \rightarrow$ Repulsive states	Emission	4520-2910			5 groups of bands	(70.73)
	LVI	$b\Pi(1, 0_g) \rightarrow$ Repulsive states	Emission	3775-2730			5 groups of bands	(70.73)
	LVII	$H^1\Sigma_u^+(0_u^+) \rightarrow$ Repulsive states	Emission	2730-2486			5 groups of bands	(70.73, 46.24, 15.1)
	LVIII	$I^1\Sigma_u^+(0_u^+) \rightarrow$ Repulsive states	Emission	4155-2687			5 groups of bands	(70.73, 46.24)
	LIX	$K^1\Pi(1_g) \rightarrow$ Repulsive states	Emission	2672-2448			3 groups of bands	(70.73, 47.26, 47.25)

Molecule I₂

I₂

I. A³Π_u(1_u) ← X¹Σ_g⁺(0_g⁺) System

Band heads, λ (31.11):

v', v''	2	3	4	5
0		8950	9124	9299
1		8917	9084	9265
2		8887	9055	9230
3			9024	9197
4	8667	8828	8994	9168
5	8641	8801	8967	9137
...				
21	8384	8534		
22	8376			

III. B³Π_u(0_u⁺) ⇌ X¹Σ_g⁺(0_g⁺) System

Band heads, λ (n.p. 136, 74.125, 73.119, 73.118, 65.53, 65.51, 23.2):

v', v''	4	5	6	7	8	9	10	11	12
0	6721.0	6816.4	6914.0	7013.9	7115.9	7220.4	7327.2	7436.5	7548.4
1	6665.4	6759.2	6855.2	6953.3	7053.6	7156.2	7261.2	7368.5	7478.3
2	6611.3	6703.7	6798.1	6894.5	6993.1	7094.0	7197.1	7312.5	7410.4
3	6558.9	6649.7	6742.6	6837.5	6934.4	7033.6	7134.9	7238.5	7344.5
4	6505.3	6597.3	6688.7	6782.0	6877.5	6975.0	7074.6	7176.5	7280.6
5	6458.3	6546.4	6636.4	6728.3	6822.1	6918.1	7016.1	7116.3	7218.7
6	6410.2	6496.9	6585.5	6676.0	6768.4	6862.9	6959.3	7057.9	7158.6
7	6363.4	6448.9	6536.2	6625.3	6716.3	6809.3	6904.2	7001.2	7100.3
8	6318.0	6402.2	6488.3	6576.1	6665.7	6757.3	6850.8	6946.3	7043.8
9	6273.8	6356.9	6441.7	6528.3	6616.6	6706.8	6798.9	6893.0	6989.0
10	6231.0	6312.9	6396.6	6481.9	6569.0	6657.9	6748.6	6841.3	6935.8
11	6189.4	6270.2	6352.7	6436.9	6522.7	6610.4	6699.8	6791.1	6884.3
12	6149.0	6228.8	6310.1	6393.2	6477.9	6564.3	6652.5	6742.5	6834.3
13	6109.7	6188.5	6268.8	6350.8	6434.4	6519.6	6606.6	6695.4	6785.9
14	6071.6	6149.4	6228.6	6309.6	6392.1	6476.3	6562.1	6649.7	6739.0
15	6034.7	6111.5	6189.9	6269.7	6351.2	6434.3	6519.0	6605.4	6693.5

VI. $E^3\Sigma_u^-(1_u) \rightarrow X^1\Sigma_g^+(0_g)$ System

Band heads, λ (58.39):

v', v''	6	7	8	9	10	11	12	13	14
0		2287.9	2298.7		2320.2	2330.7	2341.4	2352.1	2362.6
1		2283.1	2293.9	2304.0	2315.2	2325.6	2336.2	2347.0	2357.5
2	2267.4		2289.0	2299.3	2310.2	2320.9		2342.0	2352.6
3	2262.7	2276.2	2284.3	2294.8	2305.4	2316.2	2326.7	2337.2	2347.6
4	2258.4	2269.1		2290.2	2300.6	2311.6			2342.9
5	2254.3	2264.9	2275.5	2285.9		2306.4			2338.3
6	2250.0	2260.7	2271.3	2281.6			2312.5	2323.2	2333.6
7	2247.9	2256.5	2267.0			2297.4	2308.1		2329.3
8	2241.9								
9	2237.7								

VII. $F^1\Sigma_g^+(0_g) \leftarrow X^1\Sigma_g^+(0_g)$ System

Band heads, λ (72.87, 51.30):

v', v''	43	44	45	46	47	48	49	50	51
0			2568.6	2577.9	2587.3	2597.3	2606.3	2615.6	2624.8
1				2571.6	2581.0	2590.4	2599.8	2609.0	2618.2
2		2546.3	2555.8	2565.3	2574.8	2584.1	2593.4	2602.6	2611.8
3	2530.6	2540.2	2549.7	2559.1	2568.5				
4	2524.7	2534.2	2543.7	2553.1	2562.4				2599.2
5	2518.8	2528.3							
6	2512.9				2550.6	2559.6			
7					2544.6				
8									
9			2514.7						

VIII. $G^3\Sigma_u^-(0_u^+) \rightleftharpoons X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (58.40, 51.30, 40.21):

v', v''	λ	Intensity	v', v''	λ	Intensity
5, 69	2735.6	3	0, 58	2685.8	4
4, 66	2721.0	5	1, 58	2678.9	3
3, 65	2720.5	5	0, 57	2677.4	4
4, 65	2713.8	6	0, 56	2668.7	4
3, 64	2713.1	6	0, 55	2660.0	4
3, 63	2705.3	5	0, 54	2651.2	4
2, 62	2704.5	5	0, 53	2642.2	3
1, 61	2703.5	5	1, 53	2635.5	3
1, 60	2695.5	4	0, 52	2633.1	3
0, 59	2694.1	3	1, 52	2626.5	2
1, 59	2687.3	4			

IX. $H^1\Sigma_u^+(0_u^+) \rightleftharpoons X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (58.39):

v', v''	5	6	7	8	9	10	11	12	13
0								2195.0	
1						2172.2	2181.8	2191.3	
2						2168.8	2178.4	2187.7	2197.2
3						2165.2	2174.6	2184.2	2193.7
4						2161.6	2171.0	2180.3	2190.0
5						2158.3	2167.4	2176.7	
6					2146.3	2165.0	2164.1		
7					2142.6	2151.8	2160.9		
8					2193.3	2148.6	2167.5		
9					2136.1	2145.2			
10					2132.7				
11			2111.2	2120.4	2129.7	2139.3			
12					2126.6	2136.1			
13			2105.5	2114.3	2123.4	2132.7			
14			2102.4	2111.2	2120.4				
15	2081.7	2090.5	2099.3	2108.1	2117.1				
16	2078.8	2087.6	2096.3	2105.0					
17	2075.7	2084.6	2093.3						
18	2072.9	2081.7							
19	2069.9	2078.8							
20	2066.7	2075.7							

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

Band heads, λ (70.73, 58.40, 46.23, 35.19, 29.8):

"Cordes Bands"

(3, 4)	1948.1	(6, 2)	1914.7	(10, 1)	1885.2
(2, 3)	1945.9	(10, 2)	1892.3	(21, 3)	1845.0
(1, 2)	1944.7	(9, 1)	1890.8	(23, 4)	1843.5
(5, 2)	1920.7	(8, 0)	1888.6	(18, 1)	
(4, 1)	1918.6	(12, 3)		(17, 0)	1841.8
(3, 0)	1916.6	(11, 2)	1887.0	(22, 3)	1840.4
				(20, 0)	1794.3

XI. $c\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{00} = 75814 - [R/(n-3.588)^2]$ where
 $n = 6, 7, 8, \dots 36$

λ (Intensity) for $n = 6$

ν', ν''	0	1	2
0	1756.1(10)	1762.7(6)	1769.3(4)
1	1749.4(8)		
2	1743.9(8)		
3	1738.1(6)	1744.6(6)	
4	1731.7(4)		
5	1725.4(4)		

XII. $d\Delta(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73):

ν', ν''	0	1
0	1730.0(2)	1736.3(4)
1	1722.5(2)	
2	1723.1(4)	1721.3(4)
3	1707.3(4)	1713.6(4)

XIII. $e\Sigma^+(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{\infty} = 75814 - [R/(n-3.449)^2]$ where $n = 6, 7, 8, \dots 34$ λ (Intensity) for $n = 6$

ν', ν''	0	1
0	1696.3(10)	
1	1688.1(8)	1694.2(4)
2	1682.1(8)	
3	1676.1(6)	

XIV. $L^3\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73):

ν', ν''	0	1	2
0	1616.9(8)	1622.5(4)	
1	1614.0(8)	1619.6(6)	1625.2(2)
2	1611.3(8)		
3			
4	1605.8(4)		

XV. $\alpha\Sigma_u^-(1_u, 0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73)

Probably represents a Rydberg state

ν', ν''	0	1	2	3	4
0	1613.6(6)	1619.2(4)	1624.9(2)		
1	1609.2(5)	1614.7(4)	1620.2(2)		
2	1604.9(4)	1610.5(2)	1616.0(4)	1621.4(2)	1626.9(2)
3				1614.5(4)	
4	1596.6(6)			1610.3(2)	
5	1592.6(4)	1597.9(4)			

XVI. $f\Pi(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (90.73)

Represents a Rydberg Series $\nu_{oo} = 80895 - [R/(n-3.544)^2]$ where $n = 6, 7, 8$

λ (Intensity) for $n = 6$

v', v''	0	1
0	1594.9(8)	1600.4(6)
1	1589.5(4)	1595.0(6)

XVII. $M^3\Pi_u(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73):

v', v''	0	1	2
0	1591.2(8)	1596.7(8)	1602.1(2)
1		1593.3(4)	1598.7(2)
2	1584.2(8)	1589.6(6)	
3			
4	1577.3(6)		
5	1574.0(6)		

XVIII. $g\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{oo} = 75814 - [R/(n-1.048)^2]$ where $n = 4, 5, 6, \dots 33$

v', v''	0	1	2	3	4
0	1581.9(8)	1587.2(2)	1592.6(4)		
1	1577.2(8)	1582.6(8)			
2		1577.7(8)	1583.0(4)		
3		1573.1(6)			
4		1568.5(6)	1573.8(4)		
5		1564.1(6)	1569.3(4)	1574.6(4)	
6					1575.3(4)

I₂

XIX. $h\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Represents a Rydberg Series although only $n = 6$ has been observed

v', v''	0	1	2	3
0	1573.9(6)	1579.2(6)	1584.5(8)	
1	1567.3(8)	1572.6(6)		
2	1561.4(6)	1566.6(6)		
3		1560.7(8)	1566.0(6)	1571.3(6)

XX. $i\Sigma_u^+(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{oo} = 80895 - \left[R/(n-3.484)^2 \right]$ where $n = 6, 7, 8$

λ (Intensity) for $n = 6$

v', v''	0	1
0	1573.0(8)	
1	1566.9(8)	1572.1(4)
2	1561.1(8)	1566.4(6)

XXI. $j\Sigma_u^-(1_u, 0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band head (70.73)

Represents a Rydberg Series $\nu_{oo} = 80895 - \left[R/(n-3.343)^2 \right]$ where $n = 6, 7, 8$

The existence of this is uncertain

For $n = 6$, (0,0) 1555.6(2)

XXII. $\underline{k\Sigma_u^+(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+) \text{ System}}$

Band heads (70.73)

Represents a Rydberg Series $\nu_{oo} = 75814 - [R/(n-0.900)^2]$ where $n = 4, 5, 6, \dots 16$ λ (Intensity) for $n = 4$

ν', ν''	0	1	2
0	1552.9(4)	1558.0(4)	
1	1548.3(6)	1553.4(4)	
2	1543.6(4)		1548.7(4)
3	1539.2(4)		
4			
5	1530.8(4)		

XXIII. $\underline{1\Pi_u(1_u) \leftarrow X^1\Sigma_g^+(0_g^+) \text{ System}}$ Band heads, λ (Intensity) (70.73)Represents a Rydberg Series $\nu_{oo} = 75814 - [R/(n-0.843)^2]$ Only two bands of the $n = 4$ system have been identified

(ν', ν'')	(0,0)	(1,0)
λ	1543.1	1538.1
Intensity	2	2

XXIV. $\underline{N^1\Pi_u(1_u) \leftarrow X^1\Sigma_g^+(0_g^+) \text{ System}}$ Band heads, λ (Intensity) (70.73):

ν', ν''	0	1
0	1539.5(4)	1544.6(2)
1	1536.1(6)	1541.0(2)
2	1532.7(4)	

XXV. $m\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73)Represents a Rydberg Series, although only $n = 5$ has been observed

(v', v'')	$(0, 1)$	$(0, 0)$	$(1, 0)$
λ	1505.0	1500.2	1495.3
Intensity	6	6	4

XXVI. $\beta\Sigma^-(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

v', v''	0	1	2
0	1484.3(2)	1489.0(2)	1493.7(2)
1	1480.7(4)		1490.0(6)

XXVII. $\beta'\Sigma^-(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

v', v''	0	1
0	1483.5(2)	
1	1479.9(2)	
2	1476.4(8)	
3	1472.8(2)	
4	1469.3(4)	1474.0(2)
5		1470.5(2)

XXVIII. $\text{o}\Pi(1_u) \leftarrow \text{X}^1\Sigma_g^+(0_g^+)$ System

Band heads (λ J.73)

Represents a Rydberg Series $\nu_{00} = 80895 - \left[R/(n-1.139)^2 \right]$ where $n = 4, 5$

λ (Intensity) for $n = 4$

ν', ν''	0	1	2
0	1481.9(6)	1486.5(6)	1491.2(6)
1	1477.2(6)	1481.9(6)	1486.6(4)

XXIX. $\text{p}\Sigma^+(0_u^+) \leftarrow \text{X}^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Only four bands have been identified for $n = 5$

(ν', ν'')	(1, 1)	(0, 0)	(1, 0)	(2, 0)
λ	1480.7	1480.2	1476.1	1472.0
Intensity	4	6	6	10

XXX. $\text{o}'\Pi(0_u^+) \leftarrow \text{X}^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{00} = 80895 - \left[R/(n-1.113)^2 \right]$ where $n = 4, 5$

λ (Intensity) for $n = 4$

ν', ν''	0	1	2
0	1476.6(10)	1481.2(8)	1485.9(2)
1	1471.7(4)	1476.3(6)	1481.0(2)
2	1467.0(10)	1471.6(6)	

XXXI. $q\Sigma^+(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{\infty} = 80895 - [R/(n-1.093)^2]$ where $n = 4, 5$ λ (Intensity) for $n = 4$

ν', ν''	0	1
0	1472.1(8)	1476.7(6)
1	1471.8(8)	1467.2(4)

XXXII. $\gamma\Sigma^+(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

(ν', ν'')	(1, 1)	(0, 0)	(1, 0)
λ	1463.6	1462.5	1459.0
Intensity	4	8	8

XXXIII. $\gamma'\Sigma^+(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

(ν', ν'')	(1, 1)	(0, 0)	(1, 0)	(2, 0)
λ	1446.3	1445.4	1441.8	1438.4
Intensity	4	8	4	2

XXXIV. $r\Sigma^-(1_u^+, 0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{00} = 80895 - [R/(n-0.909)^2]$ where $n = 4, 5$

λ (Intensity) for $n = 4$

v', v''	0	1	2
0	1440.7(8)	1445.2(6)	
1		1440.8(8)	1446.4(6)
2	1432.3(6)	1436.7(4)	1441.0(2)
3	1428.0(10)		

XXXV. $\delta\Sigma^-(1_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

(v', v'')	(0, 1)	(0, 0)	(1, 0)
λ	1440.2	1435.8	1432.3
Intensity	4	4	6

XXXVI. $\delta^1\Sigma^-(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

(v', v'')	(0, 1)	(1, 1)	(0, 0)	(1, 0)
λ	1438.7	1435.3	1434.4	1431.0
Intensity	4	2	2	4

XXXVII. $\zeta\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

v', v''	0	1	2
0	1433. 3(6)	1437. 6(4)	1442. 0(2)
1	1429. 7(2)	1434. 0(2)	
2		1430. 4(4)	1434. 9(2)
3	1422. 5(2)	1426. 9(4)	1431. 2(6)

XXXVIII. $\zeta\Pi(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

(v', v'')	(3, 3)	(0, 0)	(1, 0)
λ	1435. 5	1430. 5	1427. 2
Intensity	2	4	4

XXXIX. $s'\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{00} = 80895 - [R/(n-0.814)^2]$ where $n = 4, 5$ λ (Intensity) for $n = 4$

(v', v'')	(0, 1)	(0, 2)	(0, 0)
λ	1431. 6	1436. 0	1427. 3
Intensity	4	2	6

XL. $s\Pi(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads (70.73)

Represents a Rydberg Series $\nu_{00} = 80895 - \left[R/(n-0.768)^2 \right]$ where $n = 4, 5$

λ (Intensity) for $n = 4$

ν', ν''	0	1	2	3
0	1420.7(6)	1425.0(6)	1429.3(2)	
1	1416.0(6)	1420.3(4)	1424.6(2)	1429.0(4)
2	1411.4(4)	1415.7(2)	1420.0(4)	1415.3(4)
3	1406.9(2)	1411.1(2)		

XLI. $t\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Represents a Rydberg Series, although only $n = 6$ has been observed

ν', ν''	0	1
0	1413.8(6)	1418.1(6)
1	1409.6(8)	
2	1405.4(8)	1409.6(8)
3	1401.3(8)	1405.6(8)
4	1397.4(2)	

XLII. $t'\Pi(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Represents a Rydberg Series, although only $n = 6$ has been observed

ν', ν''	0	1
0	1409.3(6)	1413.6(4)
1	1405.2(6)	
2	1401.1(6)	1405.3(6)
3	1397.0(2)	1401.2(6)

XLIII. $\eta\Sigma^+(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	1401.1	1397.8	1394.6	1391.3	1388.2
Intensity	8	6	6	4	4

XLIV. $\eta\Sigma(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

(v', v'')	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)
λ	1394.7	1391.2	1387.8	1384.5	1381.3
Intensity	6	4	4	8	2

XLV. $\theta\Pi(1_u, 0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Probably represents a Rydberg Series

v', v''	0	1	2
0	1385.9(6)	1390.0(4)	
1	1382.5(4)		
2		1383.3(4)	1387.4(4)
3	1376.0(6)	1380.0(6)	

XLVI. $u\Pi(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Represents a Rydberg Series, although only $n = 5$ has been observed

v', v''	0	1	2
0	1378. 1(6)	1382. 1(4)	
1	1373. 5(4)	1377. 5(4)	1381. 5(2)
2	1369. 1(2)	1373. 0(2)	
3	1364. 6(4)	1368. 6(2)	
4			1368. 4(2)

XLVII. $u'\Pi(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Represents a Rydberg Series, although only $n = 5$ has been observed

v', v''	0	1	2	3
0	1376. 5(10)	1380. 6(8)	1384. 6(6)	1388. 7(2)
1	1372. 2(10)	1376. 2(4)	1380. 2(2)	
2	1367. 9(6)	1371. 9(6)		

XLVIII. $v \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (Intensity) (70.73)

Probably a forbidden transition

v', v''	0	1
0	1374. 4(2)	1378. 5(2)
1	1369. 9(2)	
2	1365. 4(2)	

XLIX. $\omega\Sigma^+(1_u) \leftarrow X^1\Sigma_g^+(0_g^+)$ System

Band heads, λ (Intensity) (70.73)

Represents a Rydberg Series, although only $n = 5$ has been observed

v', v''	0	1	2	3
0	1361.8(6)			
1	1357.8(2)			
2	1353.8(2)		1365.7(2)	1369.7(2)
3	1349.9(2)	1353.7(2)		1365.6(4)

L. Repulsive State $\leftarrow X^1\Sigma_g^+(0_g^+)$ Systems (70.73)

The bands at 1447.1, 1451.9, 1456.6, and 1461.3 Å are due to a transition from the $v'' = 0, 1, 2$, and 3 of the ground state to a repulsive state dissociating into $p^5 2P_{3/2} + p^4 s^2 P_{3/2}$ atoms at 68545 cm^{-1} . Also, the bands at 1446.9, 1450.9, 1449.5, and 1454.4 Å could be explained as due to transitions from the ground state with $v'' = 0$ and $v'' = 1$ to two different repulsive states dissociating again into $p^5 2P_{3/2} + p^4 s^2 P_{3/2}$ atoms at 68545 cm^{-1} .

LI. $D^3\Sigma_g^-(1_g, 0_g^+) \rightarrow B^3\Pi_u(0_u^+)$ System

Band heads, λ (70.73, 51.30, 47.27):

v', v''	16	17	18	19	20	21	22	23	24
0	4177.3	4194.6	4211.4	4229.0	4245.9	4262.8	4279.0	4295.2	4310.2
1	4159.7	4177.3	4193.9			4242.9	4259.9	4275.9	4291.7
2	4143.5							4256.9	4273.5
3					4191.1	4207.3		4239.1	4254.8
4	4108.5					4189.7	4205.2		
5						4173.6		4204.2	4333.7
6							4170.8	4186.7	
7							4154.9		
8									
9	4110.3		4060.4						4167.7
10			4044.7						4151.6
							4105.4	4119.3	

LII. $E^3\Sigma_u^-(1_u) \rightarrow B^3\Pi_u(0_u^+)$ System

Band heads, λ (Intensity) for $^{127}I_2$ (72.87):

v', v''	16	17	18	19	20	21	22
0	4194.6(4)	4211.9(9)	4228.8(9)	4245.6(9)	4262.1(9)	4278.4(9)	4294.4(10)
1	4177.0(7)	4194.0(8)	4210.9(6)	4227.5(3)		4260.1(4)	4276.1(3)
2	4159.6(8)	4176.2(1)		4209.6(1)	4225.8(4)	4242.1(3)	4257.3(1)
3			4175.4(1)	4191.9(3)	4208.2(2)		4239.6(3)
4			4158.5(1)	4174.1(2)	4190.0(2)	4206.5(2)	
5					4173.1(2)		4203.6(2)

LIII. $F^1\Sigma_g^+(0_g^+) \rightarrow B^3\Pi_u(0_u^+)$ System

Band heads, λ (70.73, 58.40, 34.15, 33.14):

v', v''	0	1	2	3	4	5	6	7	8
0	3301.2	3315.3	3329.0	3342.4	3355.8	3369.4	3382.8	3396.0	3409.7
1	3289.7	3303.8	3317.5	3331.1	3344.5	3357.7	3371.3	3385.0	3397.8
2	3278.8	3292.3	3305.6	3319.9	3333.3	3346.2	3359.7	3373.0	3385.6
3	3268.2	3281.5	3294.9	3308.0	3321.7	3334.7	3347.9	3360.9	3374.3
4	3257.1	3270.0	3283.9	3297.0	3310.5	3323.5	3336.3	3349.6	3362.2
5	3246.0	3259.6	3272.9	3286.0	3299.0	3311.8	3325.0	3337.9	3350.4
6	3234.8	3248.5	3261.8	3274.6	3287.8	3301.2	3313.7	3326.7	3338.6
7	3224.3	3237.6	3250.7	3263.5	3276.8	3289.7	3302.9	3315.3	3328.0
8	3214.3	3227.9	3239.8	3252.5	3265.8	3278.6	3290.9	3303.8	3316.2
9	3203.6	3216.8	3229.5	3242.2	3254.9	3267.6	3280.0	3292.5	3304.6
10	3192.8	3206.0	3219.2	3231.3	3244.1	3257.5	3269.6	3281.9	3294.2

LIV. $J^3\Pi_g(1_g, 0_g^+) \rightarrow B^3\Pi_u(0_u^+)$ System

Band heads, λ (70.73, 58.40):

v', v''	0	1	2	3	4	5	6	7	8
0	2762.5	2772.0	2782.0						
1	2753.8	2763.8	2773.0						
2	2745.8	2755.1	2765.1	2774.4					
3	2737.5	2747.3	2756.7	2766.1	2775.4	2784.2			
4		2739.7	2748.9	2758.3	2767.6	2776.6			
5		2731.7	2740.9	2750.0	2759.4	2768.6		2785.7	
6			2733.1	2742.1		2760.1	2769.3	2778.2	
7				2734.0	2743.4	2752.4	2760.8	2770.2	2779.2
8					2736.4	2745.2		2762.5	2771.2
9						2737.5	2746.1		2763.2
10							2738.4	2747.3	2755.9

I₂

LV. aΠ(2, 1_g) → Repulsive States

Five groups of diffuse semicontinuous emission bands arise in this level and have for their lower levels different repulsive states dissociating into 2P + 2P iodine atoms (70.73)

Group	λ	Transition
I	4519.0	$a\Pi(2, 1_g) \rightarrow {}^3\Sigma_u^+(1_u)$
	4473.5	
	4431.8	
	4391.4	
II	4357.4	$a\Pi(2, 1_g) \rightarrow {}^3\Sigma_u^+(0_u^-)$
	4319.1	
	4283.4	
	4243.8	
	4202.9	
III	3332.7	$a\Pi(2, 1_g) \rightarrow {}^3\Delta_u(1_u^-)$
	3307.9	
	3282.3	
	3258.3	
	3234.8	
	3211.4	
	3189.5	
IV	3169.7	$a\Pi(2, 1_g) \rightarrow {}^3\Delta_u(2_u)$
	3143.1	
	3123.4	
	3103.6	
V	3085.5	$a\Pi(2, 1_g) \rightarrow {}^1\Pi_u(1_u)$
	3062.8	
	3043.8	
	3025.8	
	3007.2	
	2987.9	
	2970.5	
	2953.6	
	2940.7	
	2919.5	

LVI. $b\Pi(1, 0_g) \rightarrow$ Repulsive States

Five groups of semicontinuous bands arise in this level (70.73)

Group	λ	Transition
I	3774.3	$b\Pi(1, 0_g) \rightarrow {}^3\Sigma_u^+(1_u^-)$
	3721.5	
	3671.9	
	3624.4	
	3579.6	
	3537.6	
	3500.4	
II	3741.0	$b\Pi(1, 0_g) \rightarrow {}^3\Sigma_u^+(0_u^-)$
	3687.6	
	3641.8	
	3601.8	
	3516.7	
	3480.0	
III	2904.3	$b\Pi(1, 0_g) \rightarrow {}^3\Delta_u(1_u)$
	2875.1	
	2847.0	
IV	2821.0	$b\Pi(1, 0_g) \rightarrow {}^3\Delta_u(2_u)$
	2793.5	
	2769.0	
	2745.9	
V	2754.8	$b\Pi(1, 0_g) \rightarrow {}^1\Pi_u(1_u)$
	2732.0	

LVII. $H^1\Sigma_u^+(0_u^+) \rightarrow \text{Repulsive States}$

"MacLennan Bands" are observed due probably to transitions from the $H^1\Sigma_u^+(0_u^+)$ to lower unstable states (70.73, 46.25, 15.1)

λ	Intensity	λ	Intensity
4154.4	6	3919.4	3
4124.2	5	3879.9	6
4094.6	8	3855.8	6
4067.6	7	3821.8	3
4044.6	8	3798.0	4
4018.0	8	2712.0	4
3991.1	3	2699.6	3
3945.6	8	2687.5	4

LVIII. $I^1\Sigma_u^+(0_u^+) \rightarrow \text{Repulsive States}$

Five groups of diffuse emission bands arise in this level and have for their lower levels different repulsive states dissociating into $^2P + ^2P$ iodine atoms

Bands seen in emission, λ (Intensity) (70.73, 46.25)

Group		Transition
I	4154.4(6) 4124.2(5) 4094.6(8) 4067.6(7) 4044.6(8) 4018.0(8) 3991.1(3)	$I^1\Sigma_u^+(0_u^+) \rightarrow ^1\Sigma_g^+(0_g^+)$
II	3945.6(8) 3919.4(3)	$I^1\Sigma_u^+(0_u^+) \rightarrow ^3\Sigma_g^-(0_g^+)$
III	3879.9(6) 3855.8(6)	$I^1\Sigma_u^+(0_u^+) \rightarrow ^3\Sigma_g^-(1_g)$

Bands seen in emission, λ (Intensity) (70.73, 46.25)

Group		Transition
IV	3821.8(3)	$I^1\Sigma_u^+(0_u^+) \rightarrow I^1\Pi_g(1_g)$
	3798.0(4)	
V	2712.0(4)	$I^1\Sigma_u^+(0_u^+) \rightarrow I^3\Pi_g(0_g^+)$
	2699.6(3)	
	2687.5(4)	

LIX. $K^1\Pi(1_g) \rightarrow$ Repulsive States

Three groups of diffuse emission bands arise in this level and have for their lower level three different repulsive states dissociating into $2P_{3/2} + 2P_{1/2}$ iodine atoms (70.73)

Group	λ	Transition
I	2671.1	$K^1\Pi(1_g) \rightarrow I^3\Delta_u(1_u)$
	2661.1	
	2652.5	
	2642.6	
	2633.3	
	2623.6	
	2616.6	
	2607.5	
II	2593.3	$K^1\Pi(1_g) \rightarrow I^3\Delta_u(2_u)$
	2584.4	
	2575.9	
	2569.2	
	2562.2	
	2555.1	
	2548.9	
	2541.6	
	2534.1	
	2526.7	

I_2

Group	λ	Transition
III	2522.7	$K^1\Pi(1_g) \rightarrow ^1\Pi_u(1_u)$
	2516.0	
	2508.6	
	2501.4	
	2494.1	
	2487.2	
	2481.0	
	2474.1	
	2467.9	
	2461.8	
	2454.9	
	2448.8	

SPECTROSCOPIC CONSTANTS

Molecule I_2									
State	T_0	ω_0	$\times \omega_0$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$w\Sigma^+(1_u)$	73432	218						Rydberg	(73.101, 70.73)
v	72757	241						Rydberg	(73.101, 70.73)
$u'\Pi(0_u^+)$	72647	230						Rydberg	(73.101, 70.73)
$u\Pi(1_u)$	72565	240						Rydberg	(73.101, 70.73)
$\theta\Pi(1_u \text{ or } 0_u^+)$	72157	174						Possibly Rydberg	(73.101, 70.73)
$\eta'\Sigma^+(0_u^+)$	71522	179						Possibly Rydberg	(73.101, 70.73)
$\eta\Sigma^+(1_u)$	71372	168						Possibly Rydberg	(73.101, 70.73)
$t'\Pi(0_u^+)$	70955	211						Rydberg	(73.101, 70.73)
$t\Pi(1_u)$	70730	212						Rydberg	(73.101, 70.73)

SPECTROSCOPIC CONSTANTS

State	T_o	ω_o	$\times \omega_o$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$s\Pi(0_u^+)$	70388	233						Rydberg	(73.101, 70.73)
$s'\Pi(1_u)$	70064							Rydberg	(73.101, 70.73)
$\zeta'\Pi(0_u^+)$	69904	164						Possibly Rydberg	(73.101, 70.73)
$\zeta\Pi(1_u)$	69771	175						Possibly Rydberg	(73.101, 70.73)
$\delta'\Sigma^-(0_u^+)$	69717	166						Possibly Rydberg	(73.101, 70.73)
$\delta\Sigma^-(1_u)$	69649	171						Possibly Rydberg	(73.101, 70.73)
$r\Sigma^-(1_u, 0_u^+)$	69410	209						Rydberg	(73.101, 70.73)
$\gamma'\Sigma^+(0_u^+)$	69184	172						Possibly Rydberg	(73.101, 70.73)
$\gamma\Sigma^+(1_u)$	68375	164						Possibly Rydberg	(73.101, 70.73)
$q\Sigma^+(1_u)$	67930	229						Rydberg	(73.101, 70.73)

SPECTROSCOPIC CONSTANTS

State	T_c	ω_0	$\times \omega_0$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$o\Pi(0_u^+)$	67723	226						Rydberg	(73.101, 70.73)
$p\Sigma^+(0_u^+)$	67559	188						Rydberg	(73.101, 70.73)
$o\Pi(1_u)$	67483	212						Rydberg	(73.101, 70.73)
$\beta'\Sigma^-(0_u^+)$	67410	164						Possibly Rydberg	(73.101, 70.73)
$\beta\Sigma^-(1_u)$	67373	164						Possibly Rydberg	(73.101, 70.73)
$m\Pi(1_u)$	66660	214						Rydberg	(73.101, 70.73)
$N^1\Pi_u(1_u)$	64956	145							(73.101, 70.73)
$1\Pi(1_u)$	64803	214						Rydberg	(73.101, 70.73)
$k\Sigma_u^+(0_u^+)$	64395	195						Rydberg	(73.101, 70.73)
$j\Sigma_u^-(1_u, 0_u^+)$	64282							Rydberg	(73.101, 70.73)

SPECTROSCOPIC CONSTANTS

Molecule		I_2							
State	T_o	ω_o	$\times \omega_o$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$i\Sigma_u^+(1_u)$	63574	248						Rydberg	(73.101, 70.73)
$h\Pi(1_u)$	63538	265						Rydberg	(73.101, 70.73)
$g\Pi(1_u)$	63216	190						Rydberg	(73.101, 70.73)
$M^3\Pi_u$ (0_u^+)	62844	144							(73.101, 70.73)
$f\Pi(0_u^+)$	62700	211						Rydberg	(73.101, 70.73)
$\alpha\Sigma_u^-$ $(1_u, 0_u^+)$	61972	173	1.5					Possibly Rydberg	(73.101, 70.73)
$L^3\Pi$ (1_u)	61847	110	1.9						(73.101, 70.73)
$e\Sigma_u^+$ (0_u^+)	58953	284						Rydberg	(73.101, 70.73)
$K^1\Pi$ (1_g)	58578	120							(73.101, 70.73)

SPECTROSCOPIC CONSTANTS

State	T_0	ω_0	$\times \omega_0$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$d\Delta(1_u)$	57805	250							(73.101, 70.73)
$c\Pi(1_u)$	56944	219						Rydberg	(73.101, 70.73)
$b\Pi(1, 0_g)$	56000	360							(73.101, 70.73)
$J^3\Pi_g(1_g, 0_g^+)$	51923	111.7	0.705						(73.101, 70.73)
$a\Pi(2, 1_g)$	51528	215						Rydberg	(73.101, 70.73)
$I^1\Sigma_u^+(0_u^+)$	51405	168.47	0.938						(73.101, 70.73)
$H^1\Sigma_u^+(0_u^+)$	48072	79							(73.101, 70.73)
$G^3\Sigma_u^-(0_u^+)$	47148	96.0	0.505						(73.101, 70.73)

Molecule I_2

SPECTROSCOPIC CONSTANTS

State	T_o	ω_o	$\times \omega_o$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$F^1\Sigma_g^+$ (0_g^+)	46009	103.6	0.095				3.6		(73.101, 72.87, 70.73)
$E^3\Sigma_u^-$ (1_u)	45230	93.4	0.6				3.7		(73.101, 72.87, 70.73)
$D^3\Sigma_g^-$ ($1_g, 0_g^+$)	41483.1	101.88	0.3				4.1		(73.101, 70.73, 70.70)
$C^3\Sigma_u^+$ (1_u)	40473.5	203.49	0.42						(73.101, 70.73)
$B^3\Pi_u$ (0_u^+)	15770.45 (a)	124.97 (b)	0.693		289.944	0.004381	3.0309		(74.125, 73.118, 73.101, 70.73)
$A^3\Pi_u$ (1_u)	11803	43	1.0						(73.118, 70.73)
$X^1\Sigma_g^+$ (0_g^+)	0	214.50 (b)	0.615 (c)	0.037389	11.298	0.00425	2.6663	$y_e \omega_e = -1.30 \times 10^{-3}$	(73.105, 73.101, 70.73, 52.33)

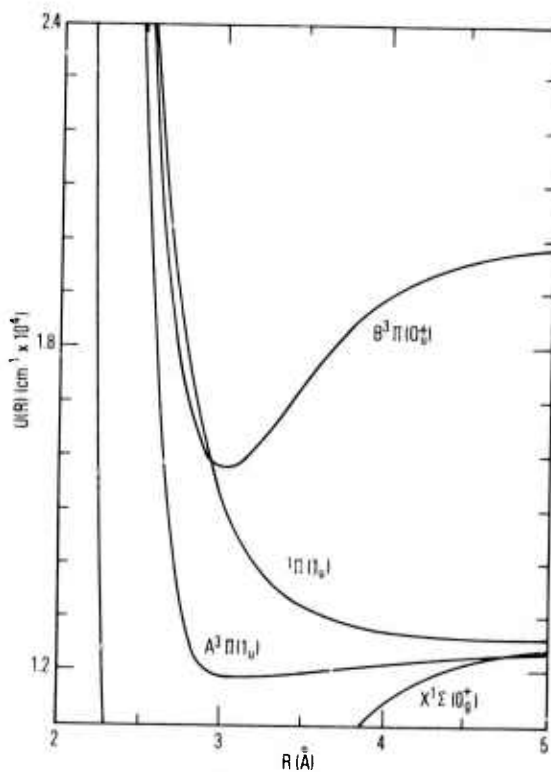
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Perturbations and General Information

Potential energy curves - RKR potential (73.105):

	State	v	E(v) cm ⁻¹	r _{min} (Å)	r _{max} (Å)
T _e = 15770.45	B ³ Π(0 ⁺ _u)	0	62.66	2.963	3.093
		1	186.82	2.921	3.148
		2	309.44	2.895	3.189
		3	430.49	2.874	3.224
		4	549.97	2.856	3.256
		5	667.88	2.842	3.286
		6	784.18	2.828	3.314
		7	898.83	2.816	3.341
		8	1011.82	2.806	3.367
		9	1123.17	2.796	3.393
		10	1232.80	2.786	3.418
		11	1340.72	2.778	3.444
		12	1446.90	2.770	3.469
		13	1551.33	2.762	3.493
		14	1653.97	2.755	3.518
		15	1754.80	2.749	3.543

Potential energy curves for low-lying systems (73.118):



Predissociation of the $B^3\Pi(0_u^+)$ state is observed from the crossing by the $^1\Pi(1_u)$ repulsive state at low v' values ($v' < 6$) (74.135, 73.106, 72.88, 72.83).

Vibrational deactivation and quenching rates of the $B^3\Pi(0_u^+)$ state by various gases (73.110).

Z_o^k - rate constant for vibrational deactivation between first and zeroth vibrational levels

Z_o^T - rate of electronic quenching by collision with gas reservoir (independent of vibrational level)

System	Z_o^k , cm ³ /mole sec	σ_k^2 , (Å) ²	Z_o^T , cm ³ /mole sec	σ_T^2 , (Å) ²
I ₂ - He	1.058×10^{-12}	0.0839	0.745×10^{-12}	0.0593
I ₂ - Ar	1.493×10^{-12}	0.3480	4.870×10^{-12}	1.1310
I ₂ - N ₂	2.260×10^{-12}	0.4480	6.360×10^{-12}	1.0730

Radiative lifetimes of the $B^3\Pi(0_u^+)$ state have been studied and are found to be strongly dependent on v' , varying from less than 0.4 μsec for $v' = 6$ to greater than 7 μsec for $v' = 56$ (73.103).

Self quenching cross sections are also given in (73.103) varying from 47 to 90×10^{-16} cm².

Foreign gas quenching cross sections have been measured for Ar, Br₂, CO₂, H₂, He, Kr, N₂, NO, Ne, O₂, SF₆ and Xe showing a dependence on v' and the particular gas used (73.103).

A study of the photo dissociation quantum yields for the $^1\Pi(1u) \rightleftharpoons X^1\Sigma^+g$ and the $B^3\Pi_u(0_u^+) \rightleftharpoons X^1\Sigma^+g$ systems is given in (72.88a).

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Franck-Condon factors for $B^3\Pi(0_u^+) \rightleftharpoons X^1\Sigma_g^+(0_g^+)$ system (n.p. 136):

v', v''	4	5	6	7	8	9	10
0	.2831-04	.1308-03	.4903-03	.1532-02	.4087-02	.9419-02	.1900-01
1	.2585-03	.1043-02	.3364-02	.8899-02	.1961-01	.3639-01	.5704-01
2	.1201-02	.4196-02	.1150-01	.2523-01	.4465-01	.6353-01	.7131-01
3	.3778-02	.1131-01	.2590-01	.4582-01	.6205-01	.6187-01	.4086-01
4	.9864-02	.2284-01	.4270-01	.5841-01	.5551-01	.3282-01	.5151-02
5	.1740-01	.3656-01	.5395-01	.5310-01	.2919-01	.3617-02	.4642-02
6	.2807-01	.4779-01	.5282-01	.3242-01	.5198-02	.3638-02	.2664-01
7	.3872-01	.5163-01	.3901-01	.1015-01	.1142-02	.2192-01	.3393-01
8	.4628-01	.4584-01	.1958-01	.9323-04	.1438-01	.3240-01	.1797-01
9	.4814-01	.3240-01	.4448-02	.5548-02	.2799-01	.2372-01	.1669-02
10	.4338-01	.1666-01	.1021-03	.1849-01	.2864-01	.7278-02	.3315-02
11	.3326-01	.4600-02	.6177-02	.2740-01	.1713-01	.1380-05	.1651-01
12	.2076-01	.1539-04	.1674-01	.2601-01	.4356-02	.6391-02	.2365-01
13	.9433-02	.3049-02	.2461-01	.1638-01	.6198-04	.1740-01	.1748-01
14	.2106-02	.1071-01	.2552-01	.5625-02	.5504-02	.2189-01	.5783-04
15	.2616-04	.1868-01	.1971-01	.1862-03	.1457-01	.1667-01	.2146-04

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In_2 In_2 Methods of Production and Experimental Technique

Absorption.

Emission from a King furnace, Tesla discharge in (Hg + In).

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I		Emission	> 5500	R		Feature-less	(65.5)
	II		Emission	5460-5500	V		Line-like bands	(65.5)
	III		Emission	5370-5480	R, V			(65.5)
	IV		Emission	5320-5350	V		Q-like bands	(65.5)
	V		Emission	5100-5310	(V)		Line-like bands	(65.5)
	VI		Emission	4950-5100	R, V		Diffuse	(65.5)
	VII		Absorption	3680-3818				(37.2, 37.1)
	VIII		Absorption	2336-2339				(37.2, 37.1)

Molecule In_2

I. 5500Å System

No apparent Q branches. Bands exhibit much overlapped rotational structure. λ (65.5).

$v' \mid v''$	m	$m+1$	$m+2$	$m+3$
n	5552.1	5596.5	5641.6	5687.1
$n+1$			5605.2	5650.2
$\vdots$				
$n+3$	5447.3			
$n+4$	5412.9			
$n+5$	5379.6	5421.3	5463.6	

VII., VIII. Absorption Bands (37.2, 37.1)

Continuum bands: $\lambda \sim 3818 \mid 3734 \mid 3680$

Line-like bands: $\lambda_{\max} \sim 3548 \mid 3544 \mid 3541 \mid 3536 \mid 3534 \mid 3526 \mid 3523 \mid$
 $3290 \mid 3280 \mid 3262 \mid 3259$

Bands: $\lambda \sim 2339 \mid 2337.5 \mid 2336$

SPECTROSCOPIC CONSTANTS

Molecule In₂

State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ³	D _e × 10 ⁶	r _e	Remarks	Bibliography
X(³ Σ _g ⁻)	18025.1	115.0 ^a							(65.5)
	0.0	143.1	0.1						(65.5)
^a ω ₀ Dissociation energy = 0.88 ± 0.15 eV, 20.3 kcal/mole, 7100 cm ⁻¹ if the ground state is ³ Σ _g ⁻ , or: 1.00 ± 0.11 eV, 23.2 kcal/mole, 8100 cm ⁻¹ if the ground state is Ω=0 (⁵ Σ _g ⁻).									

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