Chemistry 543

Spring 1999 Final Exam
May 6, 1999 10:00 AM -1:00 PM

1. The laser excitation spectrum near the head of the (v′ = 0,v″ = 4) band of the $X\,{}^1\Sigma_g^+ \rightarrow A\,(0_u^+)$ system of the Bi_2 molecule is shown below. [*J. Mol. Spectrosc.* 194, 1-7 (***1999***)].

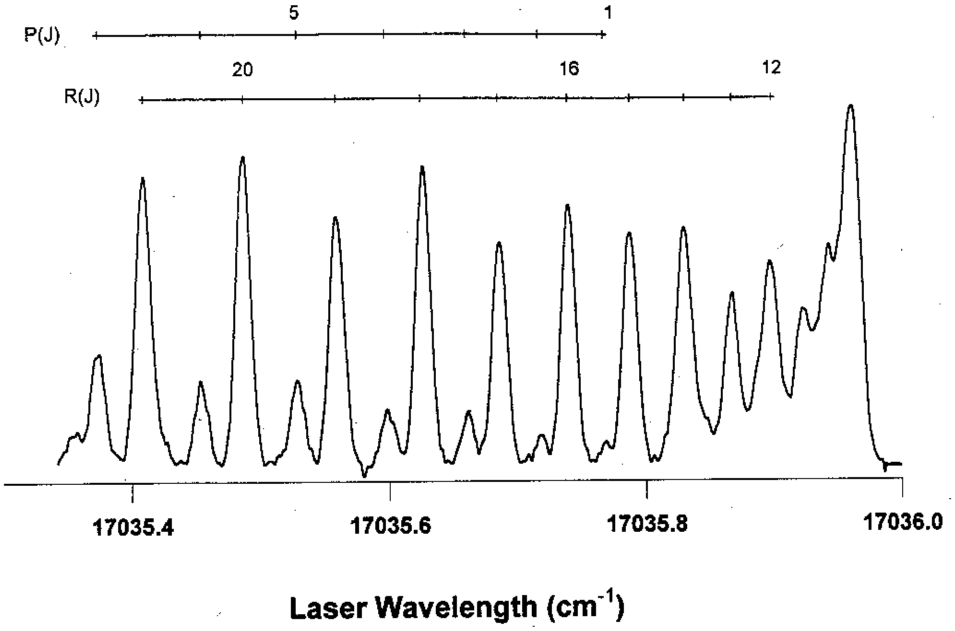


FIG. 2. Laser excitation spectrum near the head of the (v' = 0, v'' = 4) band. Rotational levels are assigned to the *P* and *R* branch.

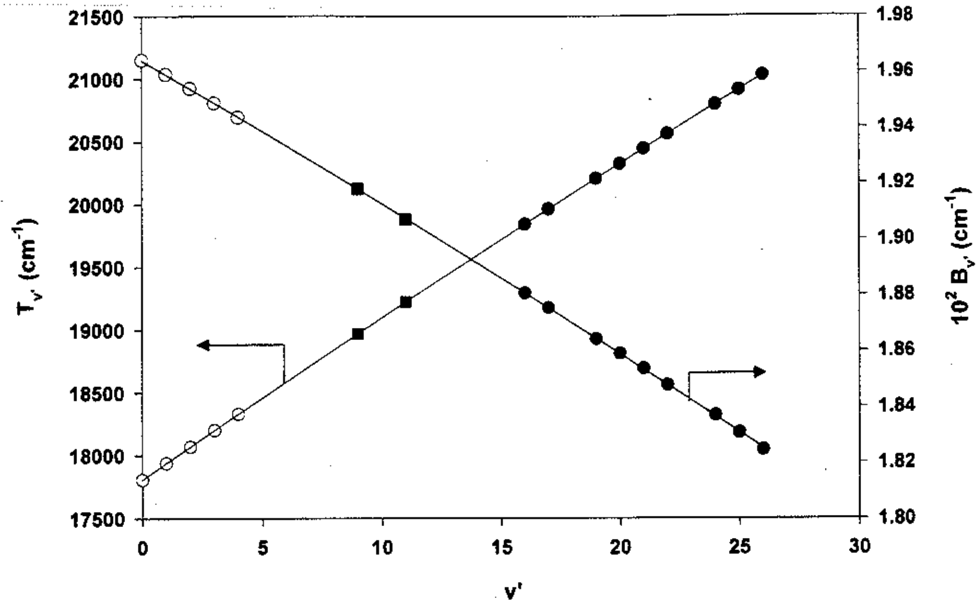
The bismuth dimer is the heaviest stable diatom. The Franck-Condon factors for the v″ = 2-5 and v′ = 0-4 have been reported in this paper. Answer the following questions:

Assign all the quantum numbers of the upper state and the lower state for the transition corresponding to the first tall peak on the left side of the spectrum.

UPPER STATE LOWER STATE

Write down an equation that would be used in the analysis of the peak frequencies in order to obtain the spectroscopic constants. You may use a running number m = (J+1) for one branch and -J for the other branch.

The vibrational and the rotational term values for the upper electronic state are plotted below, using data from the present paper and previous work.



Write down an equation that describes the vibrational term values in terms of the quantum number v'**.**

Write down an equation that describes the rotational term values in terms of the vibrational quantum number v′.

What spectroscopic constants can be obtained from the plot above? (First <u>derive</u> the equation for the plot, then define what intercept =, slope =).

The intensity observed in emission is related to the Franck Condon factors. As quoted from this 1999 paper,

$$I_{v,w} = \left(\frac{64\pi^4}{3}\right) c\,\nu_{vw} q_{vw} |R_e|^2 \left(\frac{S_J}{2J+1}\right) D(\nu_{vw})\, N_v \qquad [2]$$

v = vibrational level of emitting state, $A(0_u^+)$
w = vibrational level of ground state, $X^1\Sigma_g^+$
$I_{v,w}$ = observed LIF intensity for $v \rightarrow w$ emission band
$q_{v,w}$ = $|\langle v|w\rangle|^2$ = Franck–Condon factor for $v \rightarrow w$ emission band
ν_{vw} = frequency for $v \rightarrow w$ emission band
$|R_e|^2$ = electronic transition dipole moment
S_J = rotational linestrength
$D(\nu_{vw})$ = system spectral response (detectivity) as a function of emission frequency
N_v = concentration of emitting state, v

There is an error in this formula. What is it?

Give the formula for the rotational line strength S_J.

Give the formula for the concentration of emitting state, N_v.

Suppose you were asked to obtain $q_{v,w}$ ***from first principles, how would you do it?***

Show how $|R_e|^2$ ***is obtained theoretically.***

The paper states that Ehret and Gerber have measured $|R_e|^2 = (1.4\pm0.4\ \text{Debye})^2$, independent of internuclear separation. ***How could such a measurement be made?***

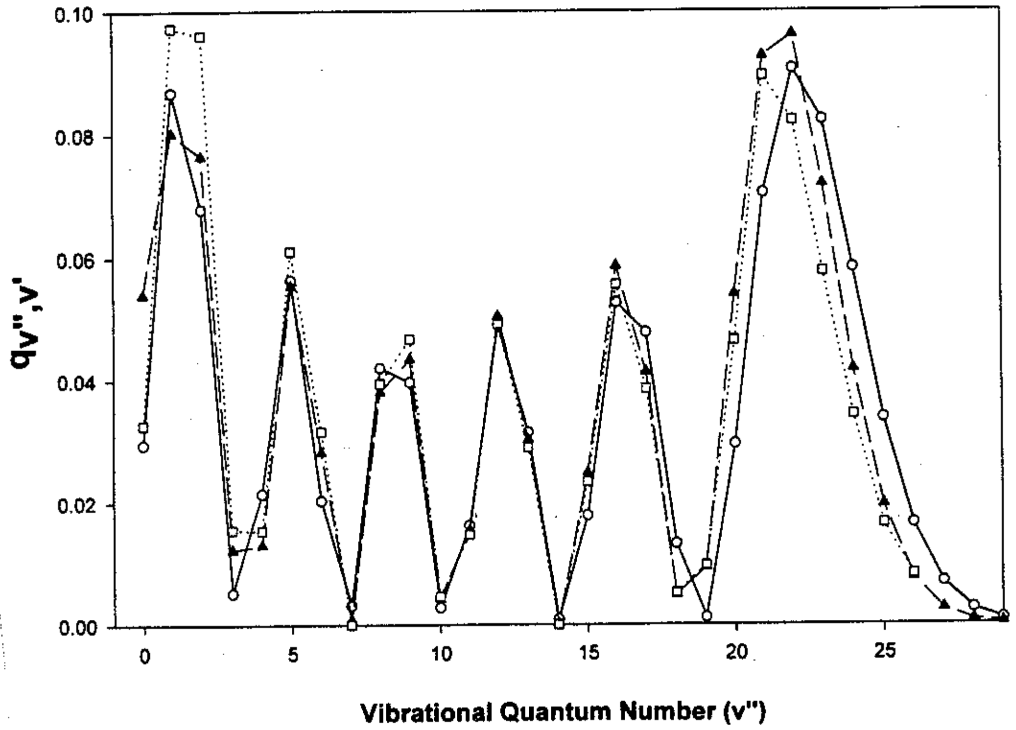
To obtain the experimental Franck Condon factors, the usual calibration procedures and forced normalization are carried out:

$$\frac{q_{vw'}}{q_{vu}} = \left(\frac{\nu_{vw'}}{\nu_{vu}}\right)^4 \left(\frac{D(\nu_{vw})}{D(\nu_{vu})}\right)\left(\frac{I_{vw'}}{I_{vu}}\right). \qquad [3]$$

The normalization

$$\sum_{w'} q_{vw'} = 1 \qquad [4]$$

These *experimental* values are shown as (···□···) in the figure below.
The Franck Condon factors were also *computed from the potential energy surfaces* using the spectroscopic constants for the upper A state and the lower X state; from the spectroscopic constants reported in this 1999 paper are shown as (– –▲– –) and from slightly different set of reported spectroscopic constants are shown as (—O—).



Explain how potential energy surfaces may be computed from spectroscopic constants.

Explain how Franck Condon factors may be computed from potential energy surfaces.

For which vibrational quantum number v′ ***in the upper state are the Franck Condon factors that are plotted in the above figure? Explain the variation of*** $q_{v''v'}$ ***versus*** v″ ***in the figure by using schematic drawings of the two surfaces and the transitions corresponding to the plotted FC factors.***

2. The visible transitions of the AuCl molecule were observed at high resolution for the first time [*J. Mol. Spectrosc.* 194, 124-7 (***1999***)]. The excited AuCl molecules were produced in a microwave discharge and the spectrum was recorded with a Fourier Transform emission spectrometer. A portion of the $B(\Omega=0^+) \rightarrow X\,^1\Sigma^+$ spectrum is shown in the figure below.

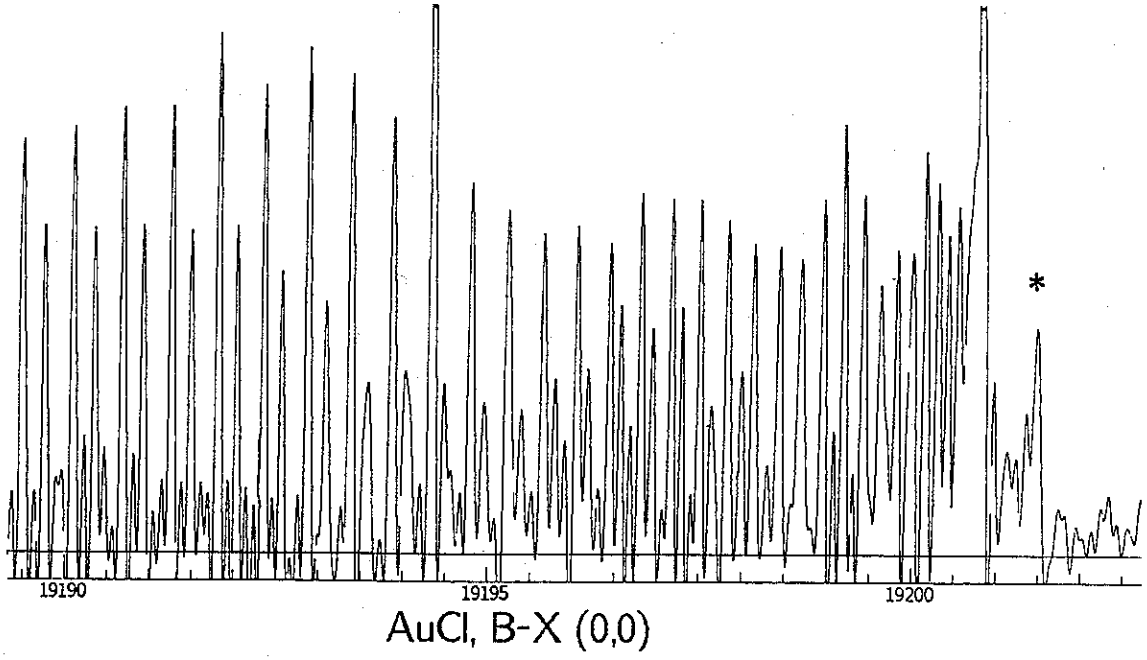


FIG. 1. A portion of the $B\ \Omega=0^+ - X\,^2\Sigma^+$ spectrum of $Au^{35}Cl$. The $Au^{37}Cl$ bandhead is marked with an asterisk.

Explain the intensity patterns of the peaks observed.

The spectroscopic constants for the $X\,^1\Sigma^+$ state and the $B(\Omega{=}0^+)$ state are shown in the table below, all values are in cm^{-1}.

	$X\,^1\Sigma^+$	$B(\Omega{=}0^+)$
T_0	0.0	19199.2549(14)
T_1	380.7018(16)	19512.8711(15)
B_0	0.1171165(64)	0.1089616(64)
B_1	0.1165734(66)	0.1082568(64)
D_0	$0.4419(75)\times10^{-7}$	$0.5424(73)\times10^{-7}$
D_1	$0.4430(77)\times10^{-7}$	$0.5542(74)\times10^{-7}$

From an earlier observation of the 43 vibrational bands of this electronic transition, the value of $\omega_e x_e$ for $X\,^1\Sigma^+$ and $B(\Omega{=}0^+)$ states are known to be respectively, 1.30 cm^{-1} and 1.45 cm^{-1}.[Ferguson, Phys. Rev. 31, 969-72 (***1928***)] ***Calculate*** ω_e ***and*** r_e ***for the ground state.*** (For comparison, relativistic density functional calculations by O. D. Häberlen and N. Rösch, *Chem. Phys. Lett.* 199, 491-6 (***1992***) give values that are 99.66% and 99.18% of the values reported in the 1999 paper.)

Calculate T_e ***for the*** $B(\Omega{=}0^+)$ ***state.***

3. The emission spectra of the AsI molecule radical were measured in the near-infrared spectral region with a Fourier transform spectrometer [*J. Mol. Spectrosc.* 194, 250-255 (***1999***)]. The most prominent features in the spectrum are the six band sequences in the range 800-900 nm of the transition $b^1\Sigma^+$ ($b0^+$) $\rightarrow X^3\Sigma^-$ (X_10^+), shown in the figures below:

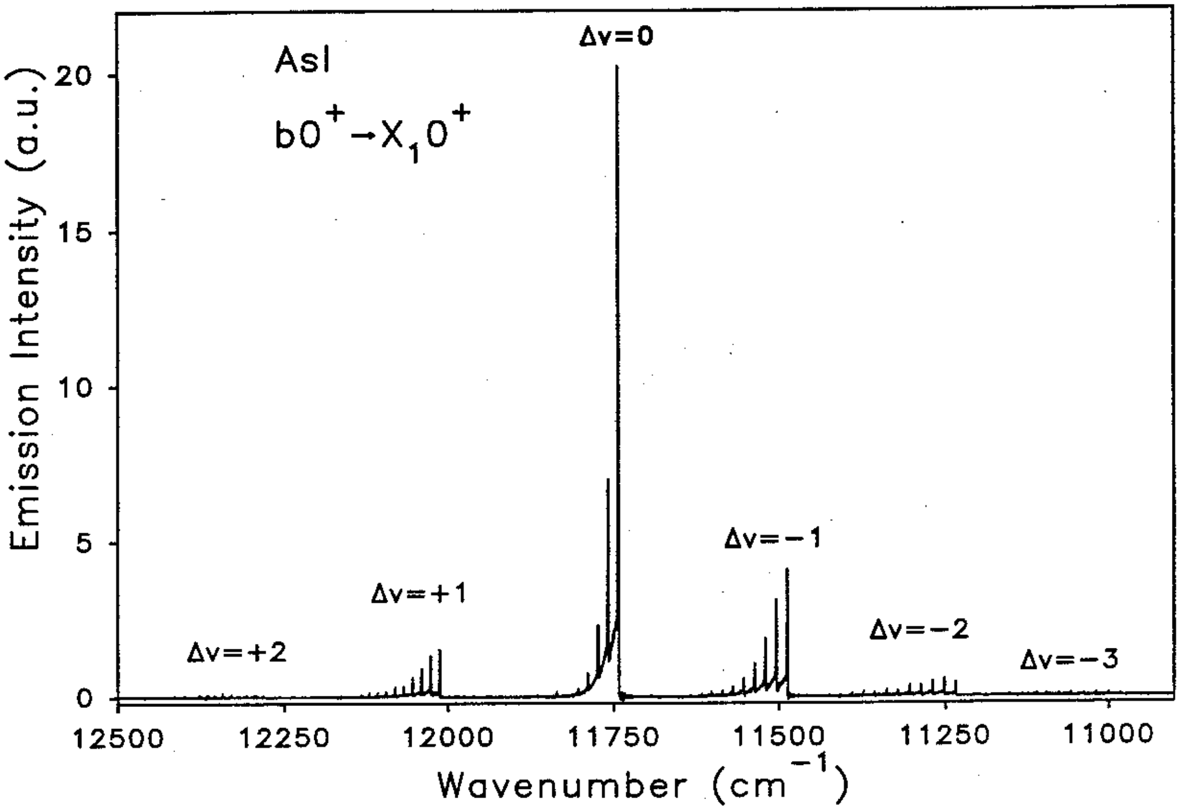
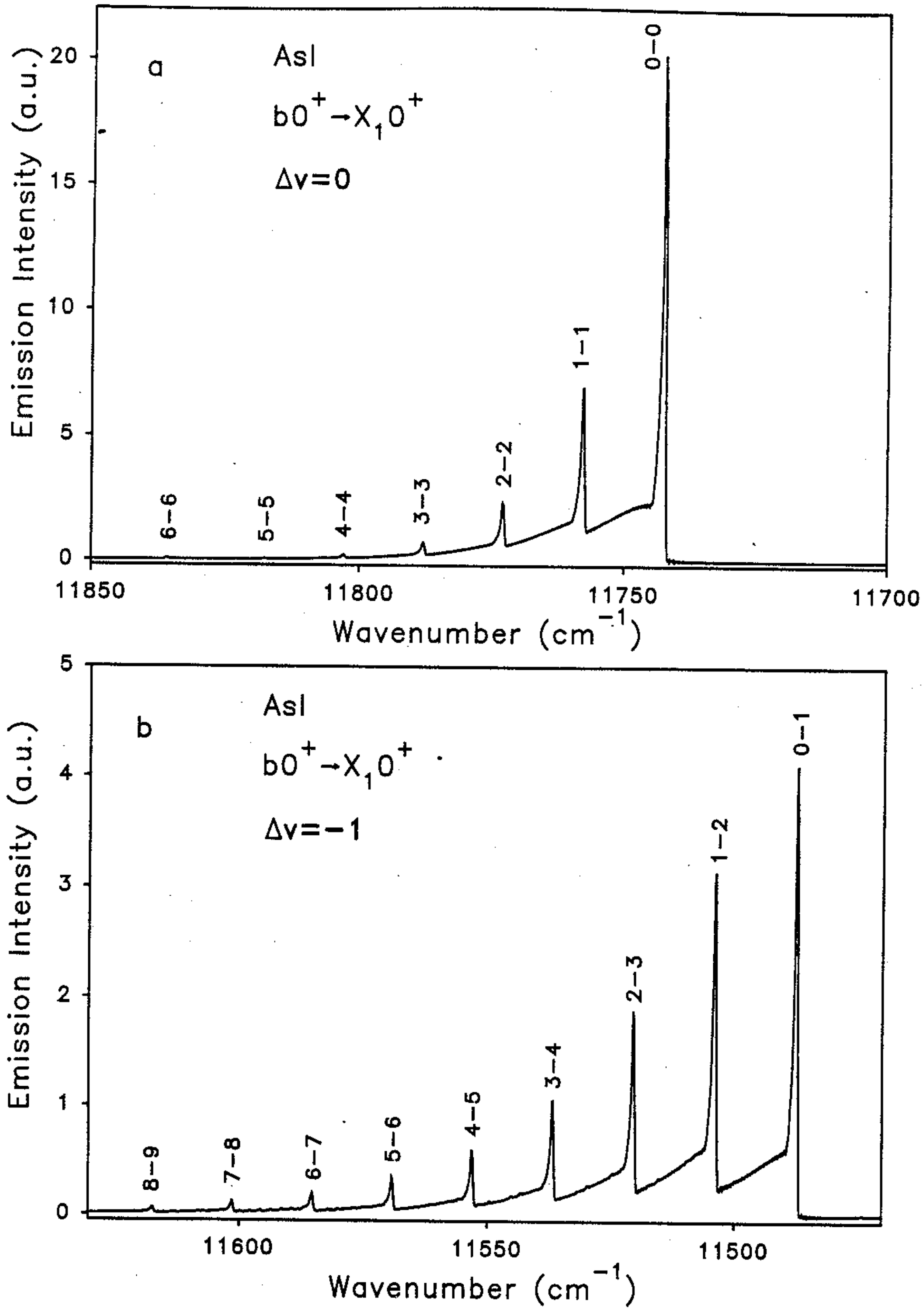


FIG. 1. Survey spectrum of the $b0^+ \rightarrow X_10^+$ transition of AsI at a spectral resolution of 0.5 cm^{-1}.



IG. 2. Spectra of the $\Delta v = 0$ and $\Delta v = -1$ sequences of the $b0^+ \rightarrow X_1 0^+$ system of AsI with assignments of the *P*-branch maxima. The r
cm^{-1}.

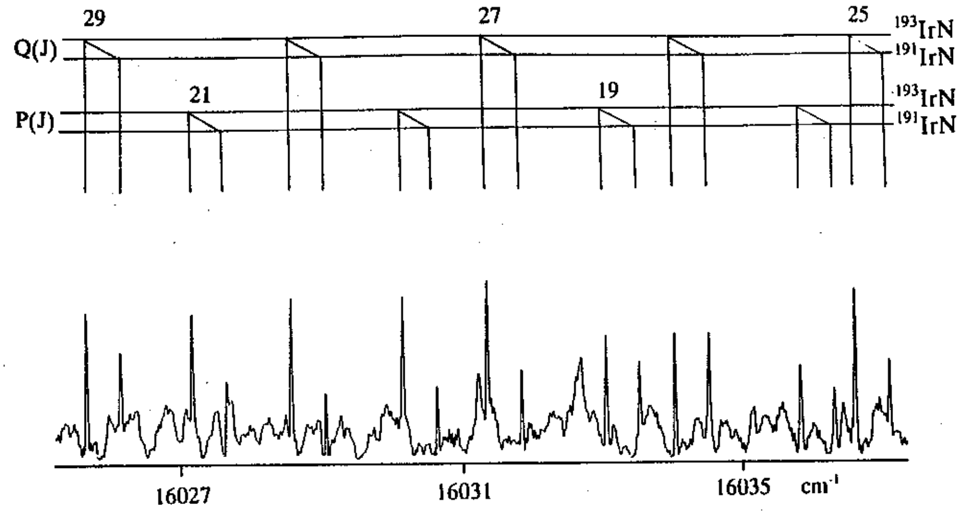
Draw a schematic of the potential surfaces and draw the transitions in Fig. 2a in the diagram. Be sure your drawing is consistent with everything in the figures on the previous page (intensity patterns, frequency differences, narrow P branches with sharp heads and broad R brances).

The identification of the transitions and the assignment of the bands observed in this paper is unambiguous. Therefore the spectroscopic constants derived represent a first complete and reliable set of molecular constants for the low-lying states of AsI. ***From the spectra shown in the figures, which spectroscopic constants for which states would have been obtained and reported by the authors?***

Identify the atomic states that are the dissociation limits of AsI molecule radical.

Draw a schematic molecular orbital diagram for this molecule, identifying the As and I orbitals involved in the bonding.

4. Transition metal atoms have relatively high abundances in many stars and several transition metal hydrides and oxides have been detected. There is a strong possibility that metal nitrides can also be found, but without precise spectroscopic data, a meaningful search for these in the complex stellar spectra can not be made. The high resolution emission spectrum of IrN has been recently investigated in the 10,000-20,000 cm^{-1} region [*J. Mol. Spectrosc.* 193, 363-375 (***1999***)]. In spite of overlapping with strong N_2 bands present in the same region, the IrN rotational lines were easily distinguished because of their narrow linewidths and the relatively small separation between consecutive rotational lines in a branch. see for example the expanded portion of the 1- 0 band of the $A\ ^1\Pi \rightarrow X\ ^1\Sigma^+$ system of IrN.



An expanded portion of the 1–0 band of the $A\,^1\Pi$–$X\,^1\Sigma^+$ system of IrN with the lines of the ^{191}IrN and ^{193}IrN isotopomers marked.

Why is there a Q branch?

Why the Q branch overlapping the regions of the P branch? Which has the larger rotational constant, the $A\,^1\Pi$ ***or the*** $X\,^1\Sigma^+$ ***state? Explain.***

The molecular constants were determined by fitting the observed line positions with the customary energy level expressions for $^1\Sigma^+$ and $^1\Pi$ states. ***Derive these expressions for*** $F_v(J)$ ***in the*** $^1\Sigma^+$ ***case and add the required term for the*** $^1\Pi$ ***case.***

The ground state $X\,^1\Sigma^+$ of IrN arises from the electron configuration $(1\sigma)^2\,(2\sigma)^2\,(1\pi)^4\,(3\sigma)^2\,(1\delta)^4$, whereas the $A\,^1\Pi$ state arises from the configuration $(1\sigma)^2\,(2\sigma)^2\,(1\pi)^4\,(3\sigma)^2\,(1\delta)^3\,(2\pi)^1$, where only the atomic valence shells have been included. ***Identify which of these molecular orbitals are the bonding, nonbonding, and antibonding ones.***

5. Ab initio configuration interaction calculations have resulted in the theoretically calculated potential energy curves of CuN [*J. Mol. Spectrosc.* 194, 8-16 (*1999*)] shown below.

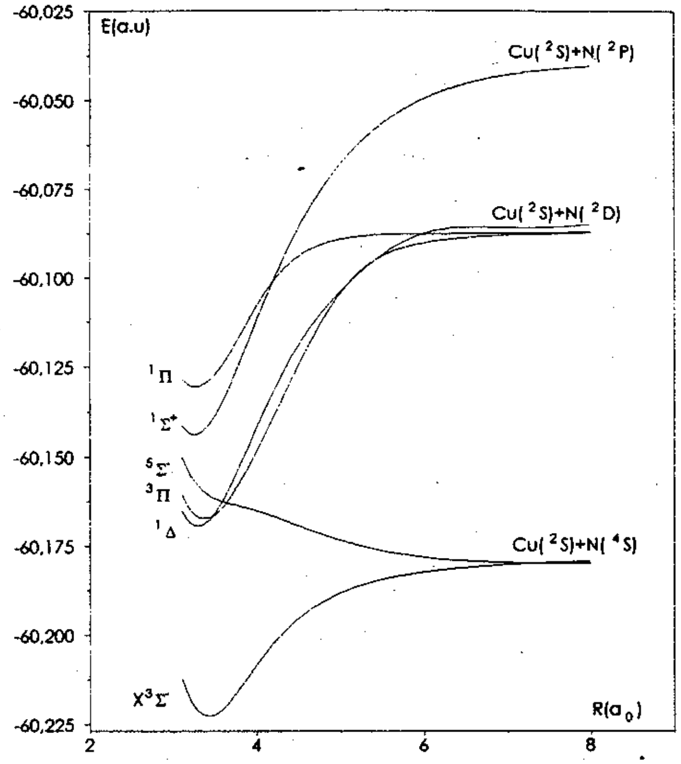


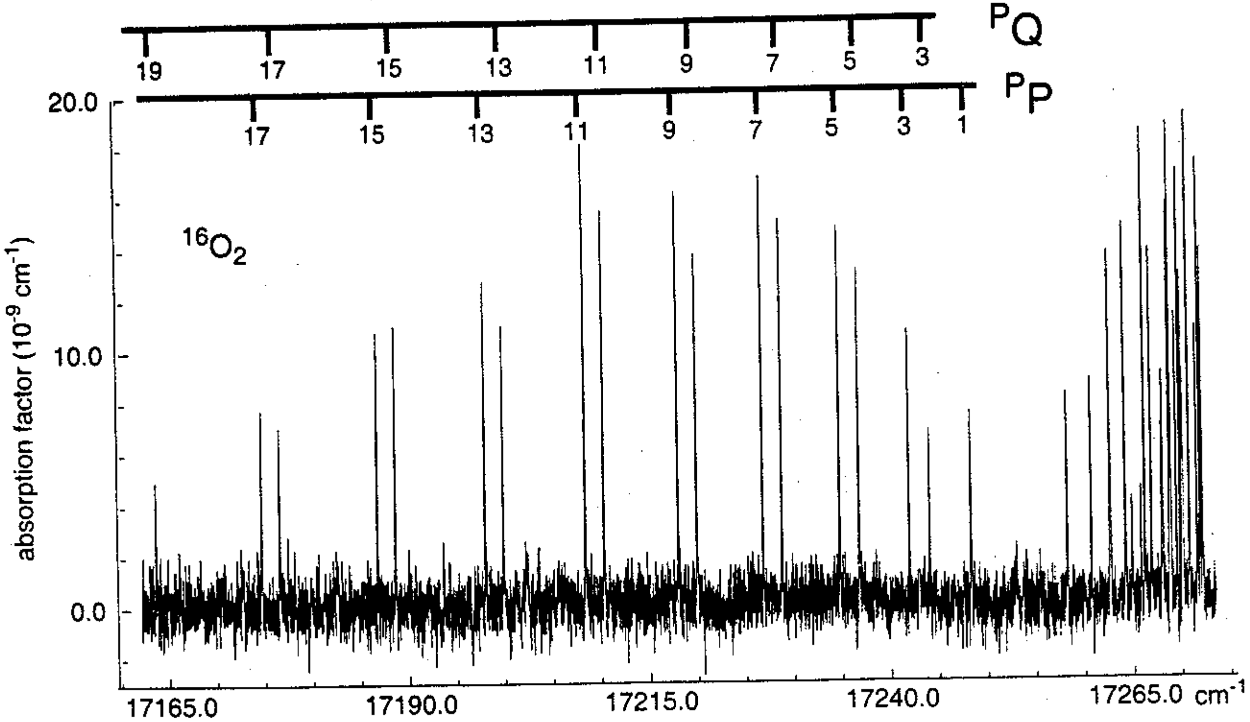
FIG. 2. CIPSI potential energy curves for the ground and excited states of CuN.

Starting from the electronic configurations of the atoms, <u>derive</u> the atomic states of Cu and N to which the CuN molecules dissociate.

Starting from the atomic states of the separated atoms, derive the molecular states of the CuN molecule that can result from these combinations.

Starting from the ground molecular electronic configuration, $(1\sigma)^2 (2\sigma)^2 (1\pi)^4 (1\delta)^4 (2\pi)^2 (3\sigma)^1 (4\sigma)^1$, where only the atomic valence shells have been included, that is, N: $(1s)^2$ and Cu: $(1s)^2 (2p)^6 (3s)^2 (3p)^6$ are not included, ***derive the molecular electronic states that can result.***

6. The $b\,^1\Sigma_g^+ \rightarrow X\,^3\Sigma_g^-$ red atmospheric system of the O_2 molecule is, despite its small oscillator strength, of importance for light scattering and extinction studies of the Earth's atmosphere. For this reason this band system has been the subject of many studies, the latest of which was the high resolution study of reported in [*J. Mol. Spectrosc.* 193, 442-445 (***1999***)] . The (3,0) bands of this system for the $^{16}O_2$ and the $^{18}O_2$ molecules are shown below.



The molecular constants of the $X\,^3\Sigma_g^-$ v = 0 ground state are very accurately known from previous work, these can be kept constant in the analysis to find the molecular constants for the $b\,^1\Sigma_g^+$ state. ***Why is the oscillator strength so small for this band system?***

Explain the meaning of the labels ^PP and ^PQ in the P branches of $^{16}O_2$ and ^RR and ^RQ in the R branches of $^{16}O_2$ spectra shown.

Provide the quantum numbers of the upper and lower state of the first marked line (19) on the left side of the top spectrum

UPPER STATE	LOWER STATE

7. The cyanogen (NCCN) molecule is an important constituent of flames. For this reason this molecule has been the subject of many studies, the latest of which was the high resolution infrared spectra of various isotopomers of cyanogen reported in [*J. Mol. Spectrosc.* 193, 183-194 (***1999***)] . The table summarizing the nuclear spin statistical weights in this paper is reproduced below. Parity *e* is (+) and *f* is (–)

TABLE 1

Relative Nuclear Spin Statistical Weights for Cyanogen[a]

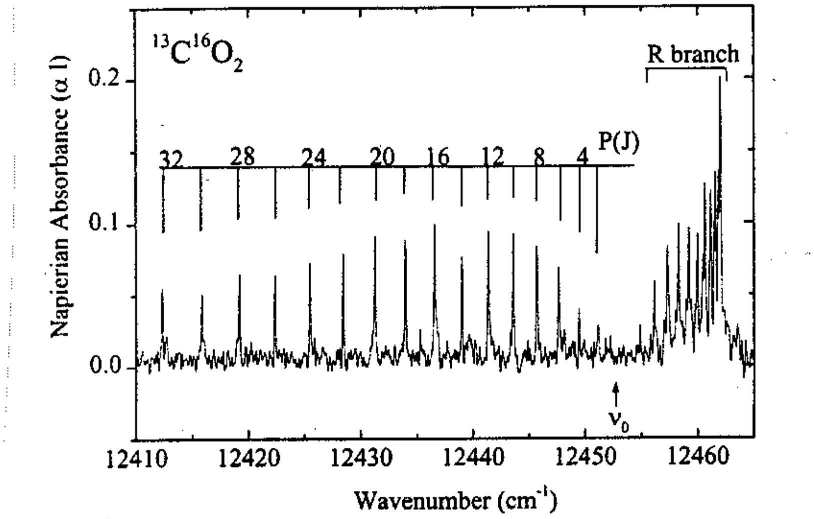
State	Parity	*J*	$^{12}C_2{}^{14}N_2$	$^{12}C_2{}^{15}N_2$	$^{13}C_2{}^{15}N_2$	$^{13}C_2{}^{14}N_2$
g	*e*	Even	2	1	5	5
		Odd	1	3	3	7
	f	Even	1	3	3	7
		Odd	2	1	5	5
u	*e*	Even	1	3	3	7
		Odd	2	1	5	5
	f	Even	2	1	5	5
		Odd	1	3	3	7

[a] For the non-centrosymmetric isotopomers there is no *g*-*u* distinction and all rovibrational levels have the same nuclear spin statistical weight.

Derive the entries for the $^{13}C_2{}^{15}N_2$ ***isotopomer in this table, defining all the symmetry terms used.***

Given that the equilibrium bond length of the N-C bond is 1.157Å ***and that for the C-C bond is*** 1.380Å ***, calculate the moments of inertia of the various isotopomers given in the table.***

8. The $(1\ 0^0\ 5)_{\text{1st or 2nd}} \rightarrow (0\ 0^0\ 0)$ band of $^{13}C^{16}O_2$ molecule has been reported in [*J. Mol. Spectrosc.* 193, 204-212 (***1999***)] . The figure below, taken from this paper shows the intracavity laser spectrum taken of 200 Torr of gas in the cell under conditions which gives an equivalent path length of 13.5 km.



The 1st or 2nd (subscript 1 or 2) notation refer to the first or second member of the Fermi dyad that result from coupling of the nearly degenerate $(1\ 0^0\ 5)$ and the $(0\ 2^0\ 5)$ vibrational states. The Fermi dyad resulting from the near degeneracy of $(1\ 0^0\ 0)$ and $(0\ 2^0\ 0)$ of $^{12}C^{16}O_2$ is the most well known case. ***Explain the notation used for the upper combination state in the figure.***

Derive the expression for G_v ***in this case.***

Given the experimental numerical values in cm^{-1} ***in Table 7 below ,***

show how to determine G_v, B_v, D_v.

9. The high resolution infrared study of the ν_{14}, ν_{17}, and ν_{18} of $^{11}B_2H_6$ and $^{10}B^{11}BH_6$ molecules has been reported in [*J. Mol. Spectrosc.* 191, 331-342 (***1998***)]. The figure below, taken from this paper shows the diborane molecule and the symmetry species of the normal modes.

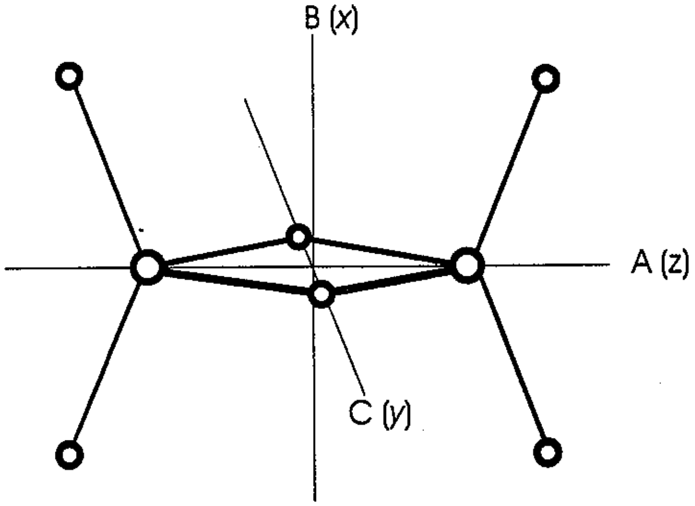


FIG. 1. Model of the diborane molecule showing the position of the atoms and the inertial axes.

TABLE 1
D_{2h} Point Group for $^{11}B_2H_6$ and $^{10}B_2H_6$

	I	C_2^z	C_2^x	C_2^y	i	σ_{xy}	σ_{yz}	σ_{xz}		
A_g	1	1	1	1	1	1	1	1		ν_1,ν_2,ν_3,ν_4
A_u	1	1	1	1	-1	-1	-1	-1		ν_5
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	ν_{15}
B_{1u}	1	1	-1	-1	-1	-1	1	1	T_z	$\nu_{16},\nu_{17},\nu_{18}$
B_{2g}	1	-1	-1	1	1	-1	-1	1	R_y	ν_{11},ν_{12}
B_{2u}	1	-1	-1	1	-1	1	1	-1	T_y	ν_{13},ν_{14}
B_{3g}	1	-1	1	-1	1	-1	1	-1	R_x	ν_6,ν_7
B_{3u}	1	-1	1	-1	-1	1	-1	1	T_x	ν_8,ν_9,ν_{10}

Derive these results, i.e., derive the irreducible representations of the normal vibrations of the diborane molecule.

$$E = U_\alpha(R_e) + (v+\tfrac{1}{2})\nu_e - x_e\nu_e\,(v+\tfrac{1}{2})^2 + y_e\nu_e\,(v+\tfrac{1}{2})^3 + B_eJ(J+1) - D_e[J(J+1)]^2 - \alpha_e(v+\tfrac{1}{2})J(J+1) + Y_{00}$$

where all spectroscopic quantities are expressed in energy units (or the corresponding frequency or wavenumbers). In energy units,

$$B_e \equiv \hbar^2 / 2\mu\, R_e^{\,2}$$
$$h x_e\nu_e \equiv \tfrac{1}{4}\, B_e^{\,2}/(h\nu_e)^2 \cdot \{\, (^{10}/_3)B_e[U'''(R_e)R_e^{\,3}]^2/(h\nu_e)^2 - U^{iv}(R_e)R_e^{\,4} \,\}$$
$$D_e \equiv 4\, B_e^{\,3}/(h\nu_e)^2$$
$$\alpha_e \equiv -\,2\, B_e^{\,2}/h\nu_e \cdot \{3 \;+\; 2\, B_e[U'''(R_e)R_e^{\,3}]^2/(h\nu_e)^2 \,\}$$
$$Y_{00} \equiv B_e^{\,2}/16(h\nu_e)^2 \cdot \{\, U^{iv}(R_e)R_e^{\,4} - (^{14}/_9)B_e[U'''(R_e)R_e^{\,3}]^2/(h\nu_e)^2 \,\}$$
$$h\nu_e \equiv (h/2\pi)[\, U''(R_e)/\mu\,]^{\frac{1}{2}}$$

Energy Conversion Factors 300 MHz = 0.01 cm^{-1}, 208.5 cm^{-1} = 300 K

		erg	eV	cm^{-1}
1 erg	=	1	6.2415×10^{11}	5.0340×10^{15}
1 eV	=	1.6022×10^{-12}	1	8065.5
1 cm^{-1}	=	1.9865×10^{-16}	1.23985×10^{-4}	1
1 kcal/mole	=	6.9478×10^{-14}	4.3364×10^{-2}	349.75
1 hartree	=	4.3598×10^{-11}	27.212	219,474.6

		kcal/mole	hartree
1 erg	=	1.4393×10^{13}	2.2937×10^{10}
1 eV	=	23.060	3.6749×10^{-2}
1 cm^{-1}	=	2.8591×10^{-3}	4.55634×10^{-6}
1 kcal/mole	=	1	1.5936×10^{-3}
1 hartree	=	627.51	1

PERIODIC TABLE OF THE ELEMENTS

Table of Radioactive Isotopes

Ac 227(22y)β^-,α
Ag 110(24s)β^-,γ
111(7.5d)β^-,γ
Am 241(458y)α,γ,e^-
242(16.0h)β^-,K,α,γ
243(8000y)α,γ
As 76(26.7h)β^-,γ
77(39h)β^-,γ
At 210(8.3h)K,α,γ
211(7.2h),$K\alpha,\gamma$
Au 198(2.69d)β^-,γ
Ba 131(12d)K,γ
133(7.2y)K,γ,e^-
Bi 210(5d)β^-,α
Bk 245(4.9d)K,α,γ
249(314d)β^-,α,SF
Br 82(36h)β^-,γ
C 14(5700y)β^-
Ca 41(8×10^4y)K
45(165d)β^-
47(4.5d)β^-,γ

Cd 115(43d)β^-,γ
Ce 141(32d)β^-,γ
143(33h)β^-,γ
144(285d)β^-,γ
Cf 246(35h)α,γ,SF
249(360y)α,γ,SF
251(800y)γ
Cl 36(3×10^5y)β^-
Cm 243(35y),α,γ
245(9300y),α,γ
247(10^7y)
Co 58(71d),K,β^+,γ
60(5.27y)β^-,γ
Cr 51(27d),K,γ
Cs 134(2.0y)β^-,γ
135(3×10^6y)β^-
137(30y)β^-,γ
Cu 64(12.8h)K,β^-,β^+,γ
Es 253(20d)α,γ,SF
254(1y)α,SF
Eu 154(16y)β^-,γ
155(1.8y)β^-,γ

Fe 55(2.6y)K
59(45d)β^-,γ
Fm 255(20h)α
Fr 223(22m)β^-,γ,α
Ga 72(14.1h),β^-,γ
Gd 153(236d)K,γ,e^-
159(18h)β^-,γ
Ge 71(11d)K
H 3(12.3y)β^-
Hf 181(45d)β^-,γ,e^-
Hg 197(65h)K,γ,e^-
203(47d)β^-,γ,e^-
Ho 166(27.3h)β^-,γ
I 129(10^7y)β^+,γ,e
131(8.05d)β^-,γ
In 114(50d)γ
Ir 192(74.4d)β^-,γ
K 40(10^9y)β^+,K,γ
42(12.4h),β^-,γ

La 140(40.2h)β^-,γ
Lu 176(10^{10}y)β^-,K,γ
177(6.8d)β^-,γ
Md 256(90m)K,SF
Mo 99(67h)β^-,γ
Na 22(2.6y)β^+,K,γ
24(15h)β^-,γ
Nd 147(11.1d)β^-,γ
Ni 63(125y)β^-
59(8×10^4y),K
Np 237(2.2×10^6y)α,γ
239(2.33d)β^-,γ
Os 191(15d)β^-,γ,e^-
P 32(14.2d)β^-
Pa 231(34000y)α,γ
Pb 210(19.4y)β^-,γ,e^-
202(10^5y)L
Pd 103(17d)K,γ
Pm 147(2.6y)β^-

Po 210(138.4d)α,γ
209(103y)α,K,γ
Pr 143(13.8d)β^-
Pt 197(18h)β^-,γ
Pu 242(3.8×10^5y)α,SF
241(13y)β^-,α,γ
239(24300y)α,γ,SF
Ra 226(1620y)α,γ
Rb 86(18.6d)β^-,γ
Re 188(16.7h)β^-,γ
186(3.7d)β^-,γ
Rn 222(3.82d)α
Ru 103(40d)β^-,γ
97(2.9d),K,γ,e^-
S 35(88d)β^-
Sb 122(2.8d)β^-,K,β^+,γ
124(60d)β^-,γ
Sc 46(84d)β^-,γ
Se 75(120d)K,γ
Sm 153(47h)β^-,γ
145(340d)K,γ
Sn 113(119d)K,L,γ,e^-

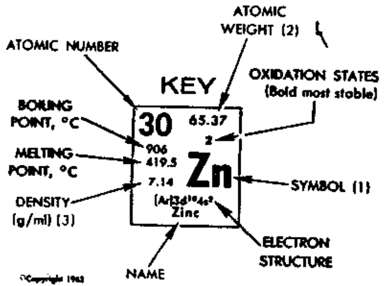
Sr 90(28y)β^-
89(51d)β^-,γ
85(64d)K,γ
Ta 182(115d)β^-,γ
Tb 160(73d)β^-,γ
Tc 99(2×10^5y)β^-
97(10^6y)K
Te 127(9.3h)β^-
Th 232(1.4×10^{10}y)α,γ,SF
228(1.91y)β^-
Tl 204(3.81y)β^-,K
Tm 170(134d)β^-,γ,e^-
U 238(4.5×10^9y)α,γ,SF
234(2.5×10^5y)α,γ,SF
235(7.1×10^8y)α,γ,SF
233(1.6×10^5y)α,γ
W 185(75d)β^-
Y 90(64h)β^-,e^-
Yb 175(4.2d)β^-,γ
169(31d)K,γ,e^-
Zn 65(245d)K,β^+,γ
Zr 95(65d)β^-,γ,e^-
93(9×10^5y)β^-,γ

Naturally occurring radioactive isotopes are indicated by a blue mass number. Half lives are in parentheses where s, m, h, d and y stand for seconds, minutes, hours, days and years respectively. The symbols describing the mode of decay and resulting radiation are defined as follows:

α	alpha particle	L	L-electron capture
β^-	beta particle	SF	spontaneous fission
β^+	positron	γ	gamma ray
K	K-electron capture	e^-	internal electron conversion

GROUP IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1 1.00797 1 −252.7 −259.2 0.071 **H** $1s^1$ Hydrogen																	2 4.0026 −268.9 −269.7 0.126 **He** $1s^2$ Helium
3 6.939 1 1330 180.5 0.53 **Li** $1s^2 2s^1$ Lithium	4 9.0122 2 2770 1277 1.85 **Be** $1s^2 2s^2$ Beryllium											5 10.811 3 — (2030) 2.34 **B** $1s^2 2s^2 2p^1$ Boron	6 12.01115 ±4,2 4830 3727? 2.26 **C** $1s^2 2s^2 2p^2$ Carbon	7 14.0067 ±3,5,4,2 −195.8 −210 0.81 **N** $1s^2 2s^2 2p^3$ Nitrogen	8 15.9994 −2 −183 −218.8 1.14 **O** $1s^2 2s^2 2p^4$ Oxygen	9 18.9984 −1 −188.2 −219.6 1.505 **F** $1s^2 2s^2 2p^5$ Fluorine	10 20.183 −246 −248.6 1.20 **Ne** $1s^2 2s^2 2p^6$ Neon
11 22.9898 1 892 97.8 0.97 **Na** $[Ne]3s^1$ Sodium	12 24.312 2 1107 650 1.74 **Mg** $[Ne]3s^2$ Magnesium											13 26.9815 3 2450 660 2.70 **Al** $[Ne]3s^2 3p^1$ Aluminum	14 28.086 4 2680 1410 2.33 **Si** $[Ne]3s^2 3p^2$ Silicon	15 30.9738 ±3,5,4 280w 44.2w 1.82w **P** $[Ne]3s^2 3p^3$ Phosphorus	16 32.064 ±2,4,6 444.6 119.0 2.07 **S** $[Ne]3s^2 3p^4$ Sulfur	17 35.453 ±1,3,5,7 −34.7 −101.0 1.56 **Cl** $[Ne]3s^2 3p^5$ Chlorine	18 39.948 −185.8 −189.4 1.40 **Ar** $[Ne]3s^2 3p^6$ Argon
19 39.102 1 760 63.7 0.86 **K** $[Ar]4s^1$ Potassium	20 40.08 2 1440 838 1.55 **Ca** $[Ar]4s^2$ Calcium	21 44.956 3 2730 1539 3.0 **Sc** $[Ar]3d^1 4s^2$ Scandium	22 47.90 4,3 3260 1668 4.51 **Ti** $[Ar]3d^2 4s^2$ Titanium	23 50.942 5,4,3,2, 3450 1900 6.1 **V** $[Ar]3d^3 4s^2$ Vanadium	24 51.996 6,3,2 2665 1875 7.19 **Cr** $[Ar]3d^5 4s^1$ Chromium	25 54.938 7,6,4,2,3 2150 1245 7.43 **Mn** $[Ar]3d^5 4s^2$ Manganese	26 55.847 2,3 3000 1536 7.86 **Fe** $[Ar]3d^6 4s^2$ Iron	27 58.933 2,3 2900 1495 8.9 **Co** $[Ar]3d^7 4s^2$ Cobalt	28 58.71 2,3 2730 1453 8.9 **Ni** $[Ar]3d^8 4s^2$ Nickel	29 63.54 2,1 2595 1083 8.96 **Cu** $[Ar]3d^{10} 4s^1$ Copper	30 65.37 2 906 419.5 7.14 **Zn** $[Ar]3d^{10} 4s^2$ Zinc	31 69.72 3 2237 29.8 5.91 **Ga** $[Ar]3d^{10} 4s^2 4p^1$ Gallium	32 72.59 4 2830 937.4 5.32 **Ge** $[Ar]3d^{10} 4s^2 4p^2$ Germanium	33 74.922 ±3,5 613* 817 5.72 **As** $[Ar]3d^{10} 4s^2 4p^3$ Arsenic	34 78.96 −2,4,6 685 217 4.79 **Se** $[Ar]3d^{10} 4s^2 4p^4$ Selenium	35 79.909 ±1,5 58 −7.2 3.12 **Br** $[Ar]3d^{10} 4s^2 4p^5$ Bromine	36 83.80 −152 −157.3 2.6 **Kr** $[Ar]3d^{10} 4s^2 4p^6$ Krypton
37 85.47 1 688 38.9 1.53 **Rb** $[Kr]5s^1$ Rubidium	38 87.62 2 1380 768 2.6 **Sr** $[Kr]5s^2$ Strontium	39 88.905 3 2927 1509 4.47 **Y** $[Kr]4d^1 5s^2$ Yttrium	40 91.22 4 3580 1852 6.49 **Zr** $[Kr]4d^2 5s^2$ Zirconium	41 92.906 5,3 3300 2468 8.4 **Nb** $[Kr]4d^4 5s^1$ Niobium	42 95.94 6,5,4,3,2 5560 2610 10.2 **Mo** $[Kr]4d^5 5s^1$ Molybdenum	43 (98) 7 — 2140 11.5 **Tc** $[Kr]4d^5 5s^2$ Technetium	44 101.07 2,3,4,6,8 4900 2500 12.2 **Ru** $[Kr]4d^7 5s^1$ Ruthenium	45 102.905 2,3,4 4500 1966 12.4 **Rh** $[Kr]4d^8 5s^1$ Rhodium	46 106.4 2,4 3980 1552 12.0 **Pd** $[Kr]4d^{10} 5s^0$ Palladium	47 107.870 1 2210 960.8 10.5 **Ag** $[Kr]4d^{10} 5s^1$ Silver	48 112.40 2 765 320.9 8.65 **Cd** $[Kr]4d^{10} 5s^2$ Cadmium	49 114.82 3 2000 156.2 7.31 **In** $[Kr]4d^{10} 5s^2 5p^1$ Indium	50 118.69 4,2 2270 231.9 7.30 **Sn** $[Kr]4d^{10} 5s^2 5p^2$ Tin	51 121.75 ±3,5 1380 630.5 6.62 **Sb** $[Kr]4d^{10} 5s^2 5p^3$ Antimony	52 127.60 −2,4,6 989.8 449.5 6.24 **Te** $[Kr]4d^{10} 5s^2 5p^4$ Tellurium	53 126.904 ±1,5,7 183 113.7 4.94 **I** $[Kr]4d^{10} 5s^2 5p^5$ Iodine	54 131.30 −108.0 −111.9 3.06 **Xe** $[Kr]4d^{10} 5s^2 5p^6$ Xenon
55 132.905 1 690 28.7 1.90 **Cs** $[Xe]6s^1$ Cesium	56 137.34 2 1640 714 3.5 **Ba** $[Xe]6s^2$ Barium	57 138.91 3 3470 920 6.17 **La** ★ $[Xe]5d^1 6s^2$ Lanthanum	72 178.49 4 5400 2222 13.1 **Hf** $[Xe]4f^{14} 5d^2 6s^2$ Hafnium	73 180.948 5 5425 2996 16.6 **Ta** $[Xe]4f^{14} 5d^3 6s^2$ Tantalum	74 183.85 6,5,4,3,2 5930 3410 19.3 **W** $[Xe]4f^{14} 5d^4 6s^2$ Wolfram	75 186.2 7,6,4,2,−1 5900 3180 21.0 **Re** $[Xe]4f^{14} 5d^5 6s^2$ Rhenium	76 190.2 2,3,4,6,8 5500 3000 22.6 **Os** $[Xe] 4f^{14} 5d^6 6s^2$ Osmium	77 192.2 2,3,4,6 5300 2454 22.5 **Ir** $[Xe]4f^{14} 5d^7 6s^2$ Iridium	78 195.09 2,4 4530 1769 21.4 **Pt** $[Xe] 4f^{14} 5d^9 6s^1$ Platinum	79 196.967 3,1 2970 1063 19.3 **Au** $[Xe]4f^{14} 5d^{10} 6s^1$ Gold	80 200.59 2,1 357 −38.4 13.6 **Hg** $[Xe]4f^{14} 5d^{10} 6s^2$ Mercury	81 204.37 3,1 1457 303 11.85 **Tl** $[Xe]4f^{14} 5d^{10} 6s^2 6p^1$ Thallium	82 207.19 4,2 1725 327.4 11.4 **Pb** $[Xe]4f^{14} 5d^{10} 6s^2 6p^2$ Lead	83 208.980 3,5 1560 271.3 9.8 **Bi** $[Xe]4f^{14} 5d^{10} 6s^2 6p^3$ Bismuth	84 (210) 2,4 — 254 (9.2) **Po** $[Xe]4f^{14} 5d^{10} 6s^2 6p^4$ Polonium	85 (210) ±1,3,5,7 — (302) — **At** $[Xe]4f^{14} 5d^{10} 6s^2 6p^5$ Astatine	86 (222) (−61.8) (−71) — **Rn** $[Xe]4f^{14} 5d^{10} 6s^2 6p^6$ Radon
87 (223) 1 — (27) — **Fr** $[Rn]7s^1$ Francium	88 (226) 2 — 700 5.0 **Ra** $[Rn]7s^2$ Radium	89 (227) 3 — 1050 — **Ac** ★★ $[Rn]6d^1 7s^2$ Actinium	104														

★	58 140.12 3,4 3468 795 6.67 **Ce** $[Xe]4f^2 5d^0 6s^2$ Cerium	59 140.907 3,4 3127 935 6.77 **Pr** $[Xe] 4f^3 5d^0 6s^2$ Praseodymium	60 144.24 3 3027 1024 7.00 **Nd** $[Xe] 4f^4 5d^0 6s^2$ Neodymium	61 (147) 3 — (1027) — **Pm** $[Xe] 4f^5 5d^0 6s^2$ Promethium	62 150.35 3,2 1900 1072 7.54 **Sm** $[Xe] 4f^6 5d^0 6s^2$ Samarium	63 151.96 3,2 1439 826 5.26 **Eu** $[Xe] 4f^7 5d^0 6s^2$ Europium	64 157.25 3 3000 1312 7.89 **Gd** $[Xe]4f^7 5d^1 6s^2$ Gadolinium	65 158.924 3,4 2800 1356 8.27 **Tb** $[Xe]4f^9 5d^0 6s^2$ Terbium	66 162.50 3 2600 1407 8.54 **Dy** $[Xe] 4f^{10} 5d^0 6s^2$ Dysprosium	67 164.930 3 2600 1461 8.80 **Ho** $[Xe]4f^{11} 5d^0 6s^2$ Holmium	68 167.26 3 2900 1497 9.05 **Er** $[Xe] 4f^{12} 5d^0 6s^2$ Erbium	69 168.934 3,2 1727 1545 9.33 **Tm** $[Xe]4f^{13} 5d^0 6s^2$ Thulium	70 173.04 3,2 1427 824 6.98 **Yb** $[Xe]4f^{14} 5d^0 6s^2$ Ytterbium	71 174.97 3 3327 1652 9.84 **Lu** $[Xe] 4f^{14} 5d^1 6s^2$ Lutetium
★★	90 232.038 4 3850 1750 11.7 **Th** $[Rn] 5f^0 6d^2 7s^2$ Thorium	91 (231) 5,4 — (1230) 15.4 **Pa** $[Rn]5f^2 6d^1 7s^2$ Protactinium	92 238.03 6,5,4,3 3818 1132 19.07 **U** $[Rn]5f^3 6d^1 7s^2$ Uranium	93 (237) 6,5,4,3 — 637 19.5 **Np** $[Rn] 5f^4 6d^1 7s^2$ Neptunium	94 (242) 6,5,4,3 3235 640 — **Pu** $[Rn]5f^6 6d^0 7s^2$ Plutonium	95 (243) 6,5,4,3 — — 11.7 **Am** $[Rn]5f^7 6d^0 7s^2$ Americium	96 (247) 3 — — — **Cm** $[Rn]5f^7 6d^1 7s^2$ Curium	97 (247) 4,3 — — — **Bk** $[Rn] 5f^9 6d^0 7s^2$ Berkelium	98 (249) 3 — — — **Cf** $[Rn] 5f^{10} 6d^0 7s^2$ Californium	99 (254) — — — — **Es** $[Rn] 5f^{11} 6d^0 7s^2$ Einsteinium	100 (253) — — — — **Fm** $[Rn] 5f^{12} 6d^0 7s^2$ Fermium	101 (256) — — — — **Md** $[Rn] 5f^{13} 6d^0 7s^2$ Mendelevium	102 (254) — — — — **No** $[Rn] 5f^{14} 6d^0 7s^2$ Nobelium	103 (257) — — — — **Lw** $[Rn] 5f^{14} 6d^1 7s^2$ Lawrencium



NOTES:

(1) Black — solid.
Red — gas.
Blue — liquid.
Outline — synthetically prepared.

(2) Based upon carbon – 12. ( ) indicates most stable or best known isotope.

(3) Values for gaseous elements are for liquids at the boiling point.

SIDE 1

SARGENT-WELCH
SARGENT-WELCH SCIENTIFIC COMPANY
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