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RESONANCE TRANSITION PROBABILITIES IN INTERMEDIATE COUPLING FOR SOME NEUTRAL NON METALS*

George Lawrence

Princeton University Observatory
Princeton, New Jersey

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ABSTRACT

Intermediate coupling calculations are made for the ground configuration and 1st excited s configuration of neutral Si, Ge, Sn, Pb, P, As, S, Se, Cl, Br, and I. The similar calculations for Si, Ge, Sn, and Pb by Khokhlov are confirmed. Tables of wavelengths, line strengths, transition probabilities, and spin orbit parameters are given. Experimental radiative lifetime data are used to provide an absolute scale and thus values of σ^2. Some radiative lifetime measurements by the phase shift method in GeI, SiI, SnI, ClI, and I I are reported. The absolute scale accuracy is ± 20%. The relative scale accuracy is thought to be $\approx$ 10% for strong lines, 30-100% for intersystem lines.

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I. INTRODUCTION

The most prominent lines in the uv spectra of the neutral non-metals are in the transition array: ground state np^m to np^{m-1} $(n + 1)$ s. We tabulate here dipole transition probabilities in these arrays for neutral Si, Ge, Sn, Pb, P, As, S, Se, Cl, Br, and I, calculated using intermediate coupling theory (IC). This theory and some examples are given by Condon and Shortley (TAS), (1963), chap. 11, and by Edlén (1964). Garstang (1961) (1962) (1964) and Garstang and Blerkhom (1965) have published outstanding examples of IC and more general calculations for forbidden lines. Calculations by Lurio (1966) for PbI have been useful in finding a sign error made by Heliwell (1961).

The calculation assumes that the only deviation from LS coupling is caused by the spin orbit interaction. The matrices of this interaction are given in TAS, p. 268 except for some sign conventions mentioned in the appendix. The effect of the spin orbit interaction is to mix levels of the configuration which have the same J. Thus a classification assignment of a level to an LS coupling state simply names the largest component of the level. The coupling cases LS and JJ are limiting cases of IC. Essentially the same calculations have been done by Khokhlov (1961) for Si, Ge, Sn, and Pb. The inclusion of these transitions here is convenient, requires little extra effort, and allows examination of a change in the manner of determining the best fit. The present calculations yield the same line strengths within $\approx$ 1% for strong lines and $\approx$ 5% for weak lines. The elements B, C, N, O, and F are essentially in LS coupling in this context and are treated in the NBS tabulation for the first 10 elements by Glennon et al (1966a). In the s and p configurations of the boron column of the periodic table, there is no mixing of states due to the spin orbit interaction so that the theory gives LS coupling results. Some references to work on the neutral inert gas

resonance lines may be found in Anderson (1965) and Lincke and Griem (1966). The bibliography by Glennon and Wiese (1966) is recommended for other references.

II. PROCEDURE

Expansion in LS Coupling Basis

The eigen value calculations and matrix multiplications were done numerically and were made practical by use of the matrix subroutines at the Princeton Computer Center.*

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The Hamiltonian matrices used in the LS coupling basis are taken to be $\delta_{ij} E_j + \zeta \lambda_{ij}$, where λ_{ij} is the spin-orbit matrix from TAS, $\zeta \equiv \zeta_p$, the spin-orbit parameter, and E_j is the unperturbed energy of the jth LS coupling level. Following Garstang (1964), we treat the E_j's as independent parameters although in general the Slater integrals (TAS, p. 198) provide relations between them. Given a value of ζ_p, the E_j's were found, where possible, by means of trace relationships for each of the J values. The expressions for the diagonal elements are listed in appendix I and also the separate procedure used for the configurations p^2s and p^3s. Matrices involving more than half-filled shells, p^{6-m}, are formally the same as the corresponding partially filled shells but with $\zeta \rightarrow -\zeta$.

Given a value of ζ , the form of the Hamiltonian matrix, and the experimental energies, the eigen values were calculated numerically. The rms error $\Delta\zeta$,

between the experimental energies and the eigen values of the matrix was examined as a function of ζ and the minimum ζ value found. In the few cases where approximate energies had to be included in the calculation, the eigen values resulting from their perturbation were left out of the comparison. This allows the poorly known level to give an approximate contribution to the mixing of states but eliminates an undue contribution to the mean square error. Table 1 lists the values of ζ obtained in the fit process and the value of rms error divided by ζ .

Line Strengths

Given the "best" value of the spin orbit parameter from the energy fit, the eigen vectors of the energy matrix form the transformation matrix, $\underset{\sim}{U}$, between the LS coupling basis and the energy states. The matrix of square roots of strengths of transitions between an upper and lower configuration are given by the unitary transformation:

(1) $\underset{\sim}{L}^{\frac{1}{2}} = \underset{\sim}{U}^{+}_{lower} \; \underset{\sim}{R} \; \underset{\sim}{U}_{up}$, where $\underset{\sim}{R}$ is the matrix of the total dipole moment in the LS coupling basis. The $\underset{\sim}{R}$ matrices are obtainable (with the proper signs) from the tables of Shore and Menzel (1965) which were prepared specifically for use in transformations of the form of (1).

The absolute line strengths are

(3) $$\underset{\sim}{S}_{ij} = \sigma^2 \left(\underset{\sim}{L}^{1/2}_{ij} \right)^2 (4\ell_>^2 - 1)$$.

Where $(4\ell_>^2 - 1) = 3$, here, and is not used by Shore and Menzel but is included in the definition of the usual radial factor σ^2.

(4) $$\sigma^2 = \frac{1}{4\ell_>^2 - 1} \left(\int P_i \, P_f \, r \, dr \right)^2$$, where

P_i and P_f are the radial wavefunctions resulting from the choice of a (single) central potential.

III. TRANSITION PROBABILITY TABLES

From the line strengths, the experimental energies, and the statistical weights of the levels the quantities in Table 4 were calculated. The columns are labeled as follows: EV., upper level energy in ev; J, upper J value, NSEC, upper level mean lifetime; LAMBDA, wavelength in Angstroms - These are calculated from the energies given by Moore (1949-1958) and may differ slightly from measured values.; Lower state J; E, lower level energy; $L = S/\sigma^2$, the angular line strength, see Eq. (3); A, transition probability in sec^{-1}, uses Fortran E format; F = f, the absorption f value; BRANCH PERCENT, the percentage downward transition probability from the given upper level. The numerical form of the formulas connecting f's, A's, L's, etc., were taken from Allen (1963).

IV. THE ABSOLUTE SCALE

The value of σ^2 chosen for each element is given in Table 2 along with the experimental data used. The choice is meant to correspond to reality, as determined largely by radiative lifetime measurements. Those lifetimes marked phase have been measured in our laboratory using the phase shift method described in the references of the footnotes. Table 3 reports for the first time some phase shift determinations of lifetimes in Ge, Sn, Si, Cl and I. A liberal estimate of maximum systematic error in these values is ± 20%. The lifetime of the spin change line Iodine I, 1830A is somewhat more uncertain because it suffers from cascading with a lifetime similar to its own upper level. The measurements in Table 3, excepting SiI, are for resolved lines of multiplets, whereas our previously reported lifetimes are for unresolved multiplets. It

can be seen that as the spin orbit interaction causes an expected difference of lifetimes in a multiplet, the wavelength splitting becomes resolvable with our 10A monochrometer.

The experimental values available for comparison with the calculations are clearly limited. However general agreement is seen between calculated and measured relative lifetimes.

The lifetimes of the $^1P_1$ and $^3P_0$ states in PbI are well known from level crossing measurements as shown in Table 3. Comparing calculated and measured lifetimes, we find that

$$\left[\tau(^3P_1)/\tau(^1P_1)\right]_{calc} / \left[\tau(^3P_1)/\tau(^1P_1)\right]_{meas.} = 1.34 \pm 0.06.$$

Thus for heavy atoms, we may expect errors on the order of 30% or more, though this may be an overgeneralization.

We have been unable as yet to measure the appropriate radiative lifetimes as As, Br, and Se because of technical difficulties. Values of σ^2 were calculated for these transition arrays using numerical solutions of the radial Schroedinger equation as described by Lawrence (1967). For third and fourth row elements these central field σ^2 values agree quite well with the experimental values determined here.

V. ACCURACY

The $\Delta\zeta / \zeta$ values of Table 2 are the RMS percentage residual error in the fit and generally indicate a good fit. The excited states seem to fit less well than the ground configurations. The comparison of ζ values with those of other authors, who use different weighting procedures, shows that the discrepancies are generally on the order of $\Delta\zeta$. The strongest effect that

the value of ζ itself has on the calculated line strengths is on the inter-system lines. Typically, $S \propto \zeta^2$ for these lines. Thus $\approx$ 2% error is caused by the uncertainty in ζ, except for As, Se, and I.

However, several other perturbations on the central field, electrostatic, approximation have been neglected. The weak lines strengths are especially susceptible to admixture of "strong transition" states. The hook measurements of relative f-values in SiI and GeI by Slavenas (1964) allow examination of this problem. If we multiply the hook values of f rel by 1.57×10^{-3} for SiI and by 1.61×10^{-3} for GeI, the values for the non spin-change lines agree with the present calculation within ± 5%. On this scale, the measured f-values for the GeI inter-system lines 2590, 2534, 2499, 3126, and 3270 are factors of 1.9, 0.9, 1.3, 1.8, and 1.2, respectively, larger than the present calculations. Further, in these examples, the weaker the line the larger the deviation. Thus, weak lines, say line strengths $<$ 0.2, can be expected to have errors on the order of factors of two.

Since the level lifetimes and hence the σ^2 values used here are determined mostly by the strong transitions, the absolute scale calibration will not suffer from problems with the weak lines.

APPENDIX: Diagonal matrix elements

We denote the experimental energy of the " $(^{2s+1}L)_J$" level by $E\,(^{2s+1}L_J)$ and the sum of energies of levels with total ang. mom. J by E_J.

In the matrices for p^3 and p^3s, the spin orbit parameter ζ does not appear on the diagonal and hence the eigen values are functions of ζ^2. Using the matrices as given in TAS, it follows from Garstang (1961), Obi and Yanagawa

(1955), and Shore and Menzel (1965) that a consistent phase convention is obtained by using a negative ζ for these cases.

We list the diagonal matrix elements by the notation (term or level, expression giving the diagonal element including the spin-orbit parameter).

I. p^2 or p^4; call $E\,(^3P_1) = E$; $(^3P_1, E)$, $(^1D_2, E_2 - E - \zeta)$, $(^3P_2, E + \zeta)$, $(^3P_o, E - \frac{1}{2}\zeta)$, $(^1S_o, E_o - E + \frac{1}{2}\zeta)$.

II. ps; Note $\langle {}^3P_1 | \zeta\, L\cdot S | {}^1P_1 \rangle = -1/\sqrt{2}\,\zeta$ (TAS pg. 270).
$(^3P_1, E\,(^3P_o) + \frac{1}{2}\zeta)$, $(^1P_1, E_1 - E\,(^3P_o) - \frac{1}{2}\zeta)$, $(^3P_o, E\,(^3P_o))$
$(^3P_2, E\,(^3P_2))$.

III. p^3; call $E\,(^2P_{\frac{1}{2}}) = Ep$ and $E\,(^2D_{5/2}) = E_D$. $(^2P, E_p)$, $(^4S, E_{3/2} - E_p - E_D)$, $(^2D, E_D)$.

IV. p^2s or p^4s; Two special problems occur with this matrix. There are four terms involved and only three trace relations. To solve this, the sign values of the 2 x 2 submatrix for J = 5/2 are expressed analytically, giving square root expressions for the unperturbed energies. For the elements studied, the experimental value of $E\,(^2S_{\frac{1}{2}})$ was generally not available. An approximate value was put into the calculation by means of the Slater relations.

Call $2E = E_{5/2} + \sqrt{\left[E(^2D_{5/2}) - E(^4P_{5/2})\right]^2 - 2\zeta^2}$

$^2D_{5/2}$	$^4P_{5/2}$	$^2D_{3/2}$	$^4P_{3/2}$
E	$E_{5/2} - E$	E	$E_{5/2} - E - 5/6\,\zeta$

$^2P_{3/2}$	$^4P_{\frac{1}{2}}$	$^2P_{\frac{1}{2}}$	$^2S_{\frac{1}{2}}$
$E_{3/2} - E_{5/2} + 5/6\,\zeta$	$E_{5/2} - E - 4/3\,\zeta$	$E_{3/2} - E_{5/2} - 1/6\,\zeta$	$7/2\,E - \frac{1}{2}E_{5/2} - \frac{1}{2}E_{3/2} + 1/4\,\zeta$

V. p^3s; Here, the diagonal elements do not depend on ζ. $E(^3D) = E(^3D_3)$ and $E(^3P) = E(^3P_0)$. The remaining term values, ^1D, ^5S, ^1P, and ^3S have only two trace relations to restrain them. An iterative process was used to obtain the "best" values of these terms. Starting with the respective experimental values, numerical trial values of the terms were fed into the program and the resulting error used to iterate, subject to the trace constraints. For S and Se the process converged in three trials.

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TABLE 1

SPIN ORBIT PARAMETERS

	Lower Config.	$\Delta\zeta/\zeta$ (%)	ζ (cm^{-1})	ζ Other	Upper Config.	$\Delta\zeta/\zeta$ (%)	ζ (cm^{-1})	ζ Other
Si	$3p^2$	0.12	148	148[a]	3p4s	2.2	214	178[c]
Ge	$4p^2$	0.7	920	921.5[b]	4p5s	0.06	1110	1110[c]
Sn	$5p^2$	1.1	2222	2247[b]	5p6s	0.3	2650	2648[c]
Pb	$6p^2$	1.4	7315	7355[b]	6p7s	0.85	8920	8908[c]
P	$3p^3$	0.5	-325	343[a]	$3p^24s$	0.2	298	
As	$4p^3$	0.5	-1448	1441[b]	$4p^25s$	5	1794	
S	$3p^4$	0.5	-387	-389[a]	$3p^34s$	0.4	-484	
Se	$4p^4$	0.9	-1812	1808[b]	$4p^35s$	3.2	-2015	
Cl	$3p^5$				$3p^44s$	0.1	-662	
Br	$4p^5$				$4p^45s$	0.6	-2714	
I	$5p^5$				$5p^46s$	8.7	-5253	

a. Pasternack (1940)

b. Garstang (1964)

c. Khokhlov (1961)

TABLE 2

Sources of Absolute Scale

Element	λ	Exper. τ nsec	σ^2 Exper.	σ^2 Adopted	σ^2 Other	τ Nominal
SiI	2505	6.1[a]	0.642	0.65		6.02
	2514-15	6.0[b]	0.646			6.02-6.08
GeI	3040	4.4[b]	0.913	0.8		5.02
	2593	6.0[b]	0.759			5.68
SnI	3176	6.0[b]	1.03	1.1	1.03[e]	6.28
	3035	6.0[b]	1.15		1.04[e]	5.62
	2707	4.7[b]	1.19		0.90[e]	5.09
PbI	2833	5.75[c]	1.47	1.25		6.80
	2022	4.99[d]	1.13			4.42
PI	1859	2.9[a]	0.605			2.89
	1775	4.0[a]	0.689	0.60		4.60
	2136	2.4[a]	0.594			2.38
AsI				0.42[f]		
SI	1807	1.5[a]	0.490	.50		1.47
	1666	1.5[a]	0.506			1.52
SeI				0.48		
Cl I	1335	2.0[b]	0.202	0.202		2.0
BrI				0.19[f]		
I I	1783	3.6[b]	0.407	.40		3.66
	1830	80±30[b]	0.31±.12			63

a. Phase/Life - Savage and Lawrence (1967)

b. Phase/Life - Table 3

c. Level Crossing - Saloman and Happer (1966)

d. Level Crossing - Saloman (1966)

e. Lawrence, Link, and King (1965)

f. Theoretical - Lawrence (1967)

TABLE 3

PHASE SHIFT LIFETIMES NOT REPORTED ELSEWHERE

El.	Gas	λ	τ (nsec) ± 15%	β/T	Nominal T
Si I	$Si\ Cl_4$	2514-15*	6.0	0.01	100
Ge I	$Ge\ Cl_4$	3040	4.4	0.014	100
		2593	6.0	0.01	100
Sn I	$Sn\ Cl_4$	3176	6.0	0.01	100
		3034	6.0	0.015	100
		2707	4.7	0.012	100
Cl I	$C\ Cl_4$	1335	2.0	0.013	50
		1390	1500	unknown	
I I	$I\ F_5$	1783	3.6		50
I I	$I\ F_5$	1830	90 ± 30	unknown	

* Unresolved multiplet

TABLE 4 TRANSITION PROBABILITY

SILICON I

UPPER STATE EV.	J	NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
SING P	1.0		3906.6	SING S	0.	1.91	1.975273	0.145E 08	0.0991	7.368
5.08		5.07	2882.4	SING D	2.0	0.78	9.862839	0.181E 09	0.1342	91.590
			2452.9	TRIP P	2.0	0.03	0.020452	0.608E 06	0.0003	0.308
			2444.1	TRIP P	1.0	0.01	0.023316	0.700E 06	0.0006	0.355
			2439.5	TRIP P	0.	0.	0.024715	0.747E 06	0.0020	0.379
TRIP P	2.0		2967.7	SING D	2.0	0.78	0.002229	0.224E 05	0.0000	0.014
4.96		6.02	2514.3	TRIP P	2.0	0.03	7.497680	0.124E 09	0.1169	74.777
			2505.1	TRIP P	1.0	0.01	2.500006	0.418E 08	0.0652	25.209
TRIP P	1.0		4104.1	SING S	0.	1.91	0.024715	0.157E 06	0.0012	0.095
4.93		6.08	2988.5	SING D	2.0	0.78	0.134802	0.222E 07	0.0018	1.346
			2529.3	TRIP P	2.0	0.03	2.481782	0.673E 08	0.0385	40.877
			2520.0	TRIP P	1.0	0.01	1.476697	0.405E 08	0.0383	24.593
			2515.1	TRIP P	0.	0.	1.975273	0.545E 08	0.1540	33.089
TRIP P	0.		2524.9	TRIP P	1.0	0.01	1.999987	0.163E 09	0.0518	100.000
4.92		6.12								

GERMANIUM I

UPPER STATE EV.	J	NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
SING P	1.0		4227.7	SING S	0.	2.03	1.834415	0.131E 08	0.1047	6.579
4.96		5.02	3040.0	SING D	2.0	0.88	8.956236	0.172E 09	0.1422	86.399
			2590.0	TRIP P	2.0	0.17	0.054551	0.169E 07	0.0010	0.851
			2534.0	TRIP P	1.0	0.07	0.197822	0.656E 07	0.0063	3.295
			2498.7	TRIP P	0.	0.	0.165572	0.573E 07	0.0160	2.876
TRIP P	2.0		3125.7	SING D	2.0	0.88	0.098040	0.104E 07	0.0015	0.591
4.85		5.68	2652.0	TRIP P	2.0	0.17	7.401868	0.129E 09	0.1347	73.031
			2593.3	TRIP P	1.0	0.07	2.500006	0.464E 08	0.0775	26.378
TRIP P	1.0		4687.1	SING S	0.	2.03	0.165572	0.868E 06	0.0085	0.510
4.67		5.88	3270.4	SING D	2.0	0.88	0.945594	0.146E 08	0.0140	8.574
			2755.4	TRIP P	2.0	0.17	2.543495	0.656E 08	0.0445	38.565
			2692.1	TRIP P	1.0	0.07	1.302192	0.360E 08	0.0389	21.169
			2652.4	TRIP P	0.	0.	1.834415	0.531E 08	0.1669	31.183
TRIP P	0.		2710.4	TRIP P	1.0	0.07	1.999987	0.163E 09	0.0593	100.000
4.64		6.15								

TABLE 4 CONT.

TIN I

UPPER STATE EV.	J	NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
SING P	1.0		4526.0	SING S	0.	2.13	1.789242	0.143E 08	0.1312	5.732
4.87		4.70	3263.3	SING D	2.0	1.07	8.147502	0.174E 09	0.1657	81.783
			2791.0	TRIP P	2.0	0.42	0.015142	0.517E 06	0.0004	0.243
			2662.0	TRIP P	1.0	0.21	0.367455	0.145E 08	0.0153	6.795
			2547.3	TRIP P	0.	0.	0.210746	0.946E 07	0.0274	4.447
TRIP P	2.0		3331.6	SING D	2.0	1.07	0.744556	0.897E 07	0.0148	4.568
4.79		5.09	2840.8	TRIP P	2.0	0.42	6.755352	0.131E 09	0.1578	66.849
			2707.3	TRIP P	1.0	0.21	2.500006	0.561E 08	0.1021	28.583
TRIP P	1.0		5633.3	SING S	0.	2.13	0.210746	0.875E 06	0.0124	0.492
4.33		5.62	3802.1	SING D	2.0	1.07	1.107816	0.150E 08	0.0193	8.404
			3176.0	TRIP P	2.0	0.42	3.229416	0.748E 08	0.0675	42.035
			3010.0	TRIP P	1.0	0.21	1.132559	0.308E 08	0.0416	17.317
			2864.2	TRIP P	0.	0.	1.789242	0.565E 08	0.2073	31.753
TRIP P	0.		3035.0	TRIP P	1.0	0.21	1.999987	0.159E 09	0.0729	100.000
4.29		5.28								

LEAD I

UPPER STATE EV.	J	NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
SING P	1.0		5006.8	SING S	0.	3.65	1.940525	0.130E 08	0.1461	5.769
6.13		4.42	3573.8	SING D	2.0	2.66	6.723227	0.124E 09	0.1419	54.958
			2578.0	TRIP P	2.0	1.32	1.156709	0.569E 08	0.0338	25.187
			2402.7	TRIP P	1.0	0.97	0.423998	0.258E 08	0.0222	11.405
			2022.7	TRIP P	0.	0.	0.059462	0.606E 07	0.0111	2.681
TRIP P	2.0		3741.0	SING D	2.0	2.66	3.092765	0.299E 08	0.0623	12.936
5.97		4.33	2664.0	TRIP P	2.0	1.32	4.407144	0.118E 09	0.1247	51.048
			2477.1	TRIP P	1.0	0.97	2.500006	0.832E 08	0.1268	36.016
TRIP P	1.0		17180.8	SING S	0.	3.65	0.059462	0.989E 04	0.0013	0.007
4.37		6.80	7231.0	SING D	2.0	2.66	0.183897	0.410E 06	0.0019	0.279
			4059.0	TRIP P	2.0	1.32	4.436043	0.560E 08	0.0824	38.037
			3640.6	TRIP P	1.0	0.97	1.076015	0.188E 08	0.0371	12.786
			2833.9	TRIP P	0.	0.	1.940525	0.719E 08	0.2582	48.891
TRIP P	0.		3684.5	TRIP P	1.0	0.97	1.999987	0.101E 09	0.0682	100.000
4.33		9.88								

TABLE 4 CONT.

PHOSPHORUS I

UPPER STATE EV.	J	NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
DOUB S	0.5		1951.1	DOUB P	1.5	2.32	2.624322	0.215E 09	0.0609	65.549
8.68		3.06	1950.2	DOUB P	0.5	2.32	1.373028	0.112E 09	0.0637	34.346
			1705.4	DOUB D	1.5	1.41	0.002738	0.335E 06	0.0001	0.102
			1428.6	QUAR S	1.5	0.	0.000033	0.689E 04	0.0000	0.002
DOUB D	1.5		2154.8	DOUB P	1.5	2.32	0.568380	0.173E 08	0.0119	5.045
8.08		2.92	2153.6	DOUB P	0.5	2.32	1.594644	0.485E 08	0.0670	14.179
			1859.4	DOUB D	2.5	1.41	0.477903	0.226E 08	0.0078	6.602
			1858.9	DOUB D	1.5	1.41	5.364644	0.254E 09	0.1306	74.171
			1534.8	QUAR S	1.5	0.	0.000097	0.815E 04	0.0000	0.002
DOUB D	2.5		2154.8	DOUB P	1.5	2.32	2.863414	0.579E 08	0.0601	16.765
8.08		2.89	1859.4	DOUB D	2.5	1.41	8.395211	0.264E 09	0.1362	76.499
			1858.9	DOUB D	1.5	1.41	0.737132	0.232E 08	0.0179	6.722
			1534.8	QUAR S	1.5	0.	0.000785	0.440E 05	0.0000	0.013
DOUB P	1.5		2536.4	DOUB P	1.5	2.32	5.110009	0.951E 08	0.0912	22.664
7.21		2.38	2534.7	DOUB P	0.5	2.32	1.070272	0.200E 08	0.0382	4.756
			2136.8	DOUB D	2.5	1.41	9.099360	0.283E 09	0.1284	67.491
			2136.2	DOUB D	1.5	1.41	0.676917	0.211E 08	0.0143	5.026
			1719.0	QUAR S	1.5	0.	0.004405	0.263E 06	0.0001	0.063
DOUB P	0.5		2555.7	DOUB P	1.5	2.32	0.824286	0.300E 08	0.0146	7.145
7.18		2.38	2554.0	DOUB P	0.5	2.32	1.959040	0.714E 08	0.0694	17.014
			2149.8	DOUB D	1.5	1.41	5.205934	0.318E 09	0.1096	75.806
			1727.8	QUAR S	1.5	0.	0.001257	0.148E 06	0.0000	0.035
QUAR P	2.5		2660.2	DOUB P	1.5	2.32	0.000004	0.409E 02	0.0000	0.000
6.98		4.60	2224.0	DOUB D	2.5	1.41	0.004789	0.881E 05	0.0001	0.041
			2223.3	DOUB D	1.5	1.41	0.000291	0.536E 04	0.0000	0.002
			1774.9	QUAR S	1.5	0.	5.998337	0.217E 09	0.1529	99.957
QUAR P	1.5		2677.9	DOUB P	1.5	2.32	0.008249	0.130E 06	0.0001	0.061
6.95		4.65	2676.1	DOUB P	0.5	2.32	0.001731	0.274E 05	0.0001	0.013
			2236.4	DOUB D	2.5	1.41	0.022717	0.617E 06	0.0003	0.287
			2235.7	DOUB D	1.5	1.41	0.004698	0.128E 06	0.0001	0.059
			1782.8	QUAR S	1.5	0.	3.995827	0.214E 09	0.1014	99.580
QUAR P	0.5		2688.8	DOUB P	1.5	2.32	0.001300	0.406E 05	0.0000	0.019
6.94		4.69	2687.0	DOUB P	0.5	2.32	0.001247	0.391E 05	0.0000	0.018
			2243.3	DOUB D	1.5	1.41	0.007500	0.403E 06	0.0002	0.189
			1787.7	QUAR S	1.5	0.	1.999271	0.213E 09	0.0506	99.773

TABLE 4 CONT.

ARSENIC I

UPPER STATE EV.	J NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
DOUB S	0.5	1860.4	DOUB P	1.5	2.31	2.418845	0.160E 09	0.0412	59.622
8.98	3.73	1844.6	DOUB P	0.5	2.25	1.558164	0.106E 09	0.0535	39.405
		1617.9	DOUB D	1.5	1.31	0.025781	0.259E 07	0.0005	0.966
		1381.2	QUAR S	1.5	0.	0.000106	0.172E 05	0.0000	0.006
DOUB D	1.5	2371.5	DOUB P	1.5	2.31	2.172920	0.346E 08	0.0290	18.568
7.54	5.36	2345.8	DOUB P	0.5	2.25	1.162552	0.191E 08	0.0314	10.264
		2004.0	DOUB D	2.5	1.35	0.039421	0.104E 07	0.0004	0.558
		1991.1	DOUB D	1.5	1.31	4.876524	0.131E 09	0.0776	70.403
		1644.3	QUAR S	1.5	0.	0.008100	0.387E 06	0.0002	0.208
DOUB D	2.5	2370.4	DOUB P	1.5	2.31	2.376877	0.253E 08	0.0318	13.078
7.54	5.17	2003.2	DOUB D	2.5	1.35	8.165541	0.144E 09	0.0861	74.440
		1990.4	DOUB D	1.5	1.31	1.221766	0.220E 08	0.0194	11.355
		1643.8	QUAR S	1.5	0.	0.068309	0.218E 07	0.0013	1.127
DOUB P	1.5	2781.0	DOUB P	1.5	2.31	4.466795	0.441E 08	0.0509	19.698
6.77	4.46	2745.8	DOUB P	0.5	2.25	1.471869	0.151E 08	0.0340	6.744
		2288.8	DOUB D	2.5	1.35	9.167459	0.163E 09	0.0846	72.521
		2272.1	DOUB D	1.5	1.31	0.004322	0.783E 05	0.0001	0.035
		1831.3	QUAR S	1.5	0.	0.064890	0.225E 07	0.0011	1.002
QUAR P	2.5	2899.6	DOUB P	1.5	2.31	0.005129	0.298E 05	0.0001	0.023
6.59	7.79	2368.5	DOUB D	2.5	1.35	0.234458	0.250E 07	0.0021	1.947
		2350.6	DOUB D	1.5	1.31	0.013801	0.151E 06	0.0002	0.117
		1882.0	QUAR S	1.5	0.	5.914081	0.126E 09	0.0995	97.912
DOUB P	0.5	2919.7	DOUB P	1.5	2.31	0.358330	0.612E 07	0.0039	2.841
6.56	4.64	2880.9	DOUB P	0.5	2.25	1.715414	0.305E 08	0.0377	14.160
		2363.8	DOUB D	1.5	1.31	5.411808	0.174E 09	0.0725	80.869
		1890.4	QUAR S	1.5	0.	0.072916	0.459E 07	0.0012	2.130
QUAR P	1.5	3033.7	DOUB P	1.5	2.31	0.157631	0.120E 07	0.0016	0.978
6.40	8.15	2991.9	DOUB P	0.5	2.25	0.032225	0.256E 06	0.0007	0.208
		2457.3	DOUB D	2.5	1.35	0.393101	0.563E 07	0.0034	4.591
		2438.0	DOUB D	1.5	1.31	0.052942	0.777E 06	0.0007	0.633
		1937.6	QUAR S	1.5	0.	3.929100	0.115E 09	0.0642	93.590
QUAR P	0.5	3120.5	DOUB P	1.5	2.31	0.043449	0.608E 06	0.0004	0.507
6.28	8.35	3076.2	DOUB P	0.5	2.25	0.059737	0.872E 06	0.0012	0.728
		2493.7	DOUB D	1.5	1.31	0.392896	0.108E 08	0.0050	8.988
		1972.6	QUAR S	1.5	0.	1.942509	0.108E 09	0.0312	89.776

TABLE 7 CONT.

SULFUR I

UPPER STATE EV.	J	NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
SING P	1.0		1782.2	SING S	0.	2.75	11.979724	0.714E 09	1.0137	56.294
9.71		0.79	1448.2	SING D	2.0	1.15	4.988924	0.554E 09	0.1039	43.696
			1286.7	TRIP P	0.	0.07	0.000011	0.169E 04	0.0000	0.000
			1283.8	TRIP P	1.0	0.05	0.000000	0.777E 02	0.0000	0.000
			1277.3	TRIP P	2.0	0.	0.000711	0.115E 06	0.0000	0.009
TRIP P	2.0		1471.8	SING D	2.0	1.15	0.049635	0.315E 07	0.0010	0.680
9.57		2.16	1302.3	TRIP P	1.0	0.05	1.445948	0.133E 09	0.0558	28.597
			1295.6	TRIP P	2.0	0.	3.521039	0.328E 09	0.0820	70.723
TRIP P	1.0		1819.2	SING S	0.	2.75	0.001125	0.630E 05	0.0001	0.014
9.56		2.18	1472.5	SING D	2.0	1.15	0.005020	0.530E 06	0.0001	0.115
			1305.9	TRIP P	0.	0.07	1.117520	0.169E 09	0.1291	36.826
			1302.9	TRIP P	1.0	0.05	0.728887	0.111E 09	0.0281	24.186
			1296.2	TRIP P	2.0	0.	1.153113	0.179E 09	0.0268	38.859
TRIP P	0.		1303.1	TRIP P	1.0	0.05	0.999999	0.457E 09	0.0386	100.000
9.56		2.19								
SING D	2.0		1666.7	SING D	2.0	1.15	14.941411	0.653E 09	0.2704	99.605
8.58		1.52	1452.6	TRIP P	1.0	0.05	0.005239	0.346E 06	0.0002	0.053
			1444.3	TRIP P	2.0	0.	0.033456	0.225E 07	0.0007	0.343
TRIP D	3.0		1706.4	SING D	2.0	1.15	0.006163	0.179E 06	0.0001	0.057
8.41		3.16	1474.0	TRIP P	2.0	0.	6.993834	0.316E 09	0.1431	99.943
TRIP D	2.0		1706.9	SING D	2.0	1.15	0.000040	0.162E 04	0.0000	0.001
8.41		3.21	1483.0	TRIP P	1.0	0.05	3.548401	0.220E 09	0.1203	70.587
			1474.4	TRIP P	2.0	0.	1.452758	0.918E 08	0.0297	29.412
TRIP D	1.0		2191.3	SING S	0.	2.75	0.013052	0.419E 06	0.0009	0.135
8.41		3.22	1707.1	SING D	2.0	1.15	0.007184	0.487E 06	0.0001	0.157
			1487.1	TRIP P	0.	0.07	1.578989	0.162E 09	0.1601	52.170
			1483.2	TRIP P	1.0	0.05	1.321426	0.137E 09	0.0448	44.005
			1474.6	TRIP P	2.0	0.	0.104266	0.110E 08	0.0021	3.534
TRIP S	1.0		3016.6	SING S	0.	2.75	0.000947	0.116E 05	0.0000	0.002
6.86		1.47	2169.6	SING D	2.0	1.15	0.001479	0.489E 05	0.0000	0.007
			1826.2	TRIP P	0.	0.07	1.308616	0.725E 08	0.1081	10.682
			1820.4	TRIP P	1.0	0.05	3.949673	0.221E 09	0.1091	32.553
			1807.3	TRIP P	2.0	0.	6.739226	0.385E 09	0.1125	56.756
QUIN S	2.0		2304.9	SING D	2.0	1.15	0.000000	0.295E 01	0.0000	0.005
6.52		17,396.	1914.7	TRIP P	1.0	0.05	0.000443	0.128E 05	0.0000	22.230
			1900.3	TRIP P	2.0	0.	0.001515	0.447E 05	0.0000	77.765

TABLE 4 CONT.

SELENIUM I

UPPER STATE EV.	J	NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
SING P	1.0		1995.1	SING S	0.	2.78	11.174498	0.456E 09	0.8109	54.935
9.00		1.21	1587.5	SING D	2.0	1.19	4.461933	0.361E 09	0.0814	43.542
			1427.9	TRIP P	0.	0.31	0.019279	0.214E 07	0.0020	0.259
			1416.8	TRIP P	1.0	0.25	0.019934	0.227E 07	0.0007	0.274
			1378.0	TRIP P	2.0	0.	0.066410	0.822E 07	0.0014	0.991
TRIP P	2.0		1610.7	SING D	2.0	1.19	0.773961	0.360E 08	0.0139	10.440
8.88		2.90	1435.3	TRIP P	1.0	0.25	2.026021	0.133E 09	0.0681	38.621
			1395.5	TRIP P	2.0	0.	2.455726	0.176E 09	0.0510	50.939
TRIP P	1.0		2051.1	SING S	0.	2.78	0.484995	0.182E 08	0.0342	4.931
8.83		2.71	1622.8	SING D	2.0	1.19	0.453017	0.343E 08	0.0081	9.300
			1456.3	TRIP P	0.	0.31	1.496988	0.157E 09	0.1488	42.518
			1444.9	TRIP P	1.0	0.25	0.650520	0.698E 08	0.0217	18.920
			1404.5	TRIP P	2.0	0.	0.768422	0.898E 08	0.0158	24.332
TRIP P	0.		1449.2	TRIP P	1.0	0.25	0.999999	0.319E 09	0.0333	100.000
8.80		3.13								
SING D	2.0		1855.2	SING D	2.0	1.19	13.864148	0.422E 09	0.2164	93.861
7.87		2.22	1626.3	TRIP P	1.0	0.25	0.273318	0.123E 08	0.0081	2.747
			1575.3	TRIP P	2.0	0.	0.306777	0.152E 08	0.0056	3.392
TRIP D	3.0		1898.6	SING D	2.0	1.19	0.127771	0.259E 07	0.0019	1.114
7.72		4.30	1606.5	TRIP P	2.0	0.	6.872227	0.230E 09	0.1239	98.886
TRIP D	2.0		1913.8	SING D	2.0	1.19	0.179211	0.497E 07	0.0027	2.192
7.67		4.41	1671.2	TRIP P	1.0	0.25	2.694544	0.112E 09	0.0778	49.492
			1617.4	TRIP P	2.0	0.	2.384660	0.110E 09	0.0427	48.316
TRIP D	1.0		2548.7	SING S	0.	2.78	0.188843	0.369E 07	0.0107	1.668
7.65		4.52	1919.2	SING D	2.0	1.19	0.107035	0.490E 07	0.0016	2.214
			1690.7	TRIP P	0.	0.31	1.316090	0.882E 08	0.1127	39.825
			1675.3	TRIP P	1.0	0.25	1.656889	0.114E 09	0.0477	51.536
			1621.2	TRIP P	2.0	0.	0.138628	0.105E 08	0.0025	4.758
TRIP S	1.0		3502.5	SING S	0.	2.78	0.016250	0.122E 06	0.0007	0.025
6.32		2.05	2414.2	SING D	2.0	1.19	0.032738	0.754E 06	0.0004	0.154
			2063.4	TRIP P	0.	0.31	1.303040	0.480E 08	0.0914	9.835
			2040.5	TRIP P	1.0	0.25	3.672644	0.140E 09	0.0869	28.667
			1960.9	TRIP P	2.0	0.	6.971737	0.299E 09	0.1029	61.318
QUIN S	2.0		2590.3	SING D	2.0	1.19	0.000042	0.472E 03	0.0000	0.053
5.97		1128.45	2164.8	TRIP P	1.0	0.25	0.006147	0.118E 06	0.0001	13.287
			2075.5	TRIP P	2.0	0.	0.035329	0.768E 06	0.0005	86.659

TABLE 4 CONT.

CHLORINE I

UPPER STATE EV.	J NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
DOUB S	0.5	1122.1	DOUB P	0.5	0.11	0.263322	0.381E 08	0.0071	38.687
11.16	10.15	1111.1	DOUB P	1.5	0.	0.405196	0.604E 08	0.0056	61.313
DOUB D	1.5	1201.4	DOUB P	0.5	0.11	3.550043	0.209E 09	0.0900	88.125
10.43	4.21	1188.8	DOUB P	1.5	0.	0.463506	0.282E 08	0.0059	11.875
DOUB D	2.5	1188.8	DOUB P	1.5	0.	5.991076	0.243E 09	0.0768	100.000
10.43	4.12								
DOUB P	0.5	1351.7	DOUB P	0.5	0.11	3.936107	0.326E 09	0.0887	65.142
9.28	2.00	1335.8	DOUB P	1.5	0.	2.032713	0.174E 09	0.0232	34.858
DOUB P	1.5	1363.5	DOUB P	0.5	0.11	1.754837	0.708E 08	0.0392	14.517
9.20	2.05	1347.3	DOUB P	1.5	0.	9.969636	0.417E 09	0.1127	85.483
QUAR P	0.5	1390.0	DOUB P	0.5	0.11	0.022790	0.173E 07	0.0005	77.100
9.03	444.40	1373.2	DOUB P	1.5	0.	0.006526	0.515E 06	0.0001	22.900
QUAR P	1.5	1396.6	DOUB P	0.5	0.11	0.028429	0.107E 07	0.0006	10.504
8.99	98.46	1379.6	DOUB P	1.5	0.	0.233490	0.909E 07	0.0026	89.496
QUAR P	2.5	1389.8	DOUB P	1.5	0.	0.008894	0.226E 06	0.0001	100.000
8.92	4428.8								

[redacted] I

UPPER STATE EV.	J NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
DOUB S	0.5	1384.7	DOUB P	0.5	0.46	0.416330	0.302E 08	0.0086	55.804
9.41	18.51	1317.5	DOUB P	1.5	0.	0.284001	0.239E 08	0.0031	44.196
DOUB D	1.5	1358.0	DOUB P	0.5	0.46	4.071402	0.156E 09	0.0859	97.133
9.59	6.21	1293.3	DOUB P	1.5	0.	0.103795	0.461E 07	0.0011	2.867
DOUB D	2.5	1293.6	DOUB P	1.5	0.	5.882957	0.174E 09	0.0652	100.000
9.58	5.74								
DOUB P	0.5	1531.9	DOUB P	0.5	0.46	3.636961	0.195E 09	0.0680	59.226
8.55	3.04	1450.0	DOUB P	1.5	0.	2.123561	0.134E 09	0.0210	40.774
DOUB P	1.5	1575.0	DOUB P	0.5	0.46	0.806914	0.199E 08	0.0147	10.704
8.33	5.39	1488.6	DOUB P	1.5	0.	5.683382	0.166E 09	0.0547	89.296
QUAR P	0.5	1582.5	DOUB P	0.5	0.46	0.168928	0.820E 07	0.0031	79.445
8.29	96.91	1495.3	DOUB P	1.5	0.	0.036873	0.212E 07	0.0004	20.555
QUAR P	1.5	1633.6	DOUB P	0.5	0.46	0.454992	0.100E 08	0.0080	7.257
8.05	7.23	1540.8	DOUB P	1.5	0.	4.879454	0.128E 09	0.0454	92.743
QUAR P	2.5	1576.5	DOUB P	1.5	0.	0.117013	0.191E 07	0.0011	100.000
7.86	522.4								

TABLE 4 CONT.

IODINE I

UPPER STATE EV.	J NSEC	LAMBDA	LOWER STATE	J	E (EV.)	L	A (/SEC)	F	BRANCH PERCENT
DOUB S	0.5	1593.6	DOUB P	0.5	0.94	1.140384	0.114E 09	0.0432	98.808
8.72	8.66	1421.4	DOUB P	1.5	0.	0.009764	0.138E 07	0.0002	1.192
DOUB D	1.5	1702.1	DOUB P	0.5	0.94	4.990320	0.205E 09	0.1769	92.059
8.23	4.49	1507.0	DOUB P	1.5	0.	0.298811	0.177E 08	0.0060	7.941
DOUB D	2.5	1514.7	DOUB P	1.5	0.	5.273707	0.205E 09	0.1050	100.000
8.19	4.88								
DOUB P	0.5	1799.1	DOUB P	0.5	0.94	3.034920	0.211E 09	0.1018	50.445
7.83	2.39	1582.6	DOUB P	1.5	0.	2.029481	0.207E 09	0.0387	49.555
QUAR P	1.5	1844.5	DOUB P	0.5	0.94	0.214634	0.692E 07	0.0070	4.928
7.66	7.12	1617.6	DOUB P	1.5	0.	2.793041	0.134E 09	0.0521	95.072
QUAR P	0.5	1876.4	DOUB P	0.5	0.94	0.046915	0.287E 07	0.0015	7.202
7.55	25.05	1642.1	DOUB P	1.5	0.	0.405191	0.370E 08	0.0074	92.798
DOUB P	1.5	2062.3	DOUB P	0.5	0.94	0.128355	0.296E 07	0.0038	1.083
6.95	3.66	1782.8	DOUB P	1.5	0.	7.574779	0.271E 09	0.1282	98.917
QUAR P	2.5	1830.4	DOUB P	1.5	0.	0.726263	0.160E 08	0.0120	100.000
6.77	62.57								