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Radiation Transition Rates in a Uniform Longitudinal 6-kG Magnetic Field for the $(5p)^5(5d)$-$(5p)^5(6p)$ Terms in Xenon

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RADIATION TRANSITION RATES IN A UNIFORM LONGITUDINAL 6-kG MAGNETIC FIELD FOR THE $(5p)^5(5d)$-$(5p)^5(6p)$ TERMS IN XENON (U)

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ABSTRACT

Calculations are performed to predict the distribution of the $(5p)^5(5d)$- $(5p)^5(6p)$ emission cross section in Xe in a strong magnetic field. For isotopes with no nuclear magnetic moment, the question is the calculation of Lande g factors. This is done with wavefunctions obtained by diagonalizing the electrostatic interaction in jj coupling, leading to reasonable accurate Lande g factors. For levels discribed by quantum numbers J and M, the Zeeman interaction is always diagonal in M, and with a 6 kG magnetic field the Zeeman interaction is effectively diagonal in J (the non-diagonal matrix elements are negligible), so the resulting cross section calculations are simple. For the isotopes with non-zero magnetic moments, one must determine the dipole and quadrupole hyperfine splitting coefficients. To do this, and to improve the overall fit of the calculated and measured energy levels, it was necessary to include configuration interaction between terms of the $(5p)^5(5d)$ and $(5p)^5(6s)$ configurations. Comparisons are made between these calculated hyperfine parameters and experiment. Hyperfine splittings are tabulated as are the cross sections and energy shifts due to hyperfine interaction in each transition. When hyperfine interaction is included and levels are characterized by the quantum numbers F and M_F, the Zeeman interaction is diagonal in M_F, but there are large non-diagonal components between levels of the same M_F but different F. All these effects were included in the calculations leading to a particularly rich spectrum for Xe(131) with I = 3/2. For example, the $(5p)^5(5d)_{J=4}$- $(5p)^5(6p)_{J=3}$ transition is split into approximately 336 components.

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1) Introduction

Because of the large number of possible transitions, Xenon in a strong magnetic field is a messy system to model as an IR laser. Here I examine the effect of a moderate (5–10) kG longitudinal magnetic field on oscillator strengths and gain cross sections for the $(5p)^5(5d) - (5p)^5(6p)$ lasing transitions in Xe. At these moderate fields a linear analysis of the Zeeman effect should be sufficient, i.e., one needs megagauss fields to see quadratic Zeeman effects. But, before doing the Zeeman effect analysis, there are some other effects which need to be estimated.

First, at $\lambda = 2\mu$, corresponding to 0.45 eV or 3630 cm^{-1}, the Doppler width is $\Delta E_D = 0.024\ (kT(eV))^{1/2}\ cm^{-1}$, which is small even at kT = 1 eV (0.025 cm^{-1}). At room temperature (0.025 eV), the Doppler width is 0.004 cm^{-1}, which is comparable to the linewidth due to a level's natural lifetime corresponding to a decay rate (Einstein coefficient) of 55×10^6/sec.

Second, there are a number of stable isotopes with significant fractional concentrations, leading to isotope shifts in spectral lines. I list the isotopes in Table (1)[1].

Table (1)

Mass	Percent	Spin
128	1.92	0
129	26.44	1/2
130	4.08	0
131	21.18	3/2
132	26.89	0
134	10.44	0
136	8.87	0

Cowan[2] points out that the isotope effect is difficult to calculate. The easy part to calculate is that due to mass effects in the definition of the Rydberg where the reduced mass is replaced with the electron mass, i.e., the measured energy difference is $[M/(M + m_e)]\ \Delta E(M=\infty)$. Then in using $M + \delta M$ for a different isotope, one has for the isotope shift,

$$\delta(\Delta E) = m_e\ \delta M/[(M + m_e)(M + \delta M + m_e)]. \qquad (1)$$

For $M = 131$, $\delta M = 3$, and $\Delta E(M=\infty) = 10^4\ cm^{-1}$, then $\delta(\Delta E) = 0.001\ cm^{-1}$. Contributions to the isotope shift from the other effects may be larger, but unless they are larger than the above by a factor of 25, they can be neglected. Experimentally, Jackson et al[3] indicate that the isotope shifts are smaller than $0.006\ cm^{-1}$ for the levels studied here.

Third, two of the prominent isotopes, 129 and 131, have non-zero nuclear spin. This leads to a significant hyperfine splitting, and a considerable increase in the complexity of the analysis. If one is concerned over radiation trapping/detrapping the hyperfine splitting can be important since the mass 129 and 131 isotopes constitute 50 % of the Xenon. Hyperfine splitting effects will be discussed in secs.(5)–(8).

In secs.(2)–(4) the calculations of emission rates in a magnetic field are done neglecting hyperfine effects. The most useful results from secs.(2)–(4) are likely to be in Tables (4) and (8), which give the Lande g factors, and in Table (9a) which lists Einstein coefficients and room temperature emission cross sections. Tables (10a) and (11a) list the hyperfine splittings for Xe(129) and Xe(131), respectively, and the (extensive) Tables (12a) and (12b) list emission cross sections between hyperfine components for Xe(129) and Xe(131), respectively, without a magnetic field. Because the possible transitions between hyperfine components of Xe(129) and Xe(131) in a strong magnetic field are so numerous, they are not tabulated; a selection is shown in figs.(2a)–(3c).

2) The Case of Zero Magnetic Field

The excited terms of the noble gases are described by wavefunctions of the form $|(np)^5\ ^2P_{J_c},(n'\ell')\ ^2l'_j;LSJM\rangle = |^2P,^2\ell';LSJM\rangle$ and $|(np)^5J_c,\ell'j;JM\rangle$. There is a real difference between these wavefunctions as $|J_c,\ell'j;JM\rangle$ is obtained by adding J_c and j' directly, without introducing L and S, while $|^2P,^2\ell';LSJM\rangle$ does not involve J_c and j. However, one can find a linear relation between the wave functions,i.e.,

$$|J_c,\ell'j;JM\rangle = [(2J_c+1)(2j+1)]^{1/2} \sum_{L,S} [(2L+1)(2S+1)]^{1/2} \begin{Bmatrix} 1 & 1/2 & J_c \\ \ell' & 1/2 & j \\ L & S & J \end{Bmatrix} |^2P,^2\ell';LSJM\rangle, \tag{2}$$

where $\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix}$ is a 9-j symbol. The reason two wavefunctions are introduced is that the dominant effect in the spectrum of the noble gas atoms is the spin-orbit splitting of the core, i.e.,

$$\langle J_c",\ell'j";J"M"|H_{so}|J_c,\ell'j;JM\rangle = \delta_{J_c"J_c}\ \delta_{j"j}\ \delta_{J"J}\ \delta_{M"M}\ \ h(J_c,\ell'j). \tag{3}$$

For the noble gases Condon and Shortley[4] give the $h(J_c,\ell'j)$ values in Table (2)

Table (2)

J_c	j	$h(J_c,\ell'j)$
1/2	$\ell'-1/2$	$\zeta_{np} - (1/2)\ (\ell'+1)\ \zeta_{n'\ell'}$
1/2	$\ell'+1/2$	$\zeta_{np} + (1/2)\ \ell'\ \zeta_{n'\ell'}$
3/2	$\ell'-1/2$	$-\zeta_{np}/2 - (1/2)\ (\ell'+1)\ \zeta_{n'\ell'}$
3/2	$\ell'+1/2$	$-\zeta_{np}/2 + (1/2)\ P'\ \zeta_{n'\ell'}$

where ζ_{np} is the spin–orbit parameter for the subshell. For the noble gases the dominant effect on the level structure is the $3\zeta_{np}/2$ splitting due to the two J_c values. In the later numerical analysis I use $\zeta_{5p} = 7025\ cm^{-1}$ (from the $^2P_{3/2}$–$^2P_{1/2}$ splitting of the Xe ion), $\zeta_{6s} = 0$, $\zeta_{6p} = 369\ cm^{-1}$, and $\zeta_{5d} = 39\ cm^{-1}$ (from the splitting of the Cs neutral atom spectra), all data taken from Moore's Tables.[5]

The next largest effect on the spectrum is due to the electrostatic effect. Here the interaction matrix elements are

$$\langle J_c'',\ell'j'';J''M''|H_{el}|J_c,\ell'j;JM\rangle = [(2J_c+1)(2j+1)(2J_c''+1)(2j''+1)]^{1/2}$$

$$\sum_{L,S}[(2L+1)(2S+1)]^{1/2}\sum_{L',S'}[(2L'+1)(2S'+1)]^{1/2}\begin{Bmatrix} 1 & 1/2 & J_c \\ \ell' & 1/2 & j \\ L & S & J\end{Bmatrix}\begin{Bmatrix} 1 & 1/2 & J'' \\ \ell' & 1/2 & j'' \\ L' & S' & J''\end{Bmatrix}$$

$$\langle ^2P,^2\ell';LSJM|H_{el}|^2P,^2\ell';L'S'J''M''\rangle. \qquad (4a)$$

But the electrostatic matrix element is diagonal in LS coupling

$$\langle ^2P,^2\ell';LSJM||H_{el}||^2P,^2\ell';L'S'J''M''\rangle = \delta_{J''J}\,\delta_{M''M}\,\delta_{L''L}\,\delta_{S''S}\,h(\ell'LS), \qquad (4b)$$

so

$$\langle J_c'',\ell'j'';J''M''|H_{el}|J_c,\ell'j;JM\rangle = \delta_{J''J}\,\delta_{M''M}[(2J_c+1)(2j+1)(2J_c''+1)(2j''+1)]^{1/2}$$

$$\sum_{L,S}(2L+1)(2S+1)\,h(\ell'LS)\begin{Bmatrix} 1 & 1/2 & J_c \\ \ell' & 1/2 & j \\ L & S & J\end{Bmatrix}\begin{Bmatrix} 1 & 1/2 & J'' \\ \ell' & 1/2 & j'' \\ L & S & J\end{Bmatrix}. \qquad (4c)$$

The electrostatic interaction is diagonal in J and M but mixes terms of different J_c and j. This is discussed in detail in Ref.(6). In consequence, J_c and j are no longer good quantum numbers, while the new eigenvectors are $|i,JM\rangle$, where

$$|i,JM\rangle = \sum_{J_c,j} C(i,J_cj;J)\ |J_c,\ell'j;JM\rangle, \qquad (5a)$$

and the $C(i,J_c j;J)$ are mixing coefficients found by diagonalizing the interaction matrix. Tables (3), (4), and (5) (which are modifications of Tables (3a), (3b) and (3c) of Ref.(6)) list mixing parameters (relative energies, mixing coefficients, and Lande g factors with and without (in parenthesis) the interaction) calculated for the $(5p)^5(6s)$, $(5p)^5(6p)$, and $(5p)^5(5d)$ terms of Xe.

The measured level energies from Moore's Tables[5] are listed. The new levels resulting from the diagonalization of the electrostatic interaction are labeled (i,J). The calculated energy of the (1,2) level of $(5p)^5(6s)$, the (1,3) level of $(5p)^5(6p)$, and the (1,4) level of $(5p)^5(5d)$ have been adjusted to the experimental value. J is a good quantum number, and i increases with increasing binding energy. Moore's Tables[5] identify levels by specifying energy relative to the ground state, Paschen notation, e.g. $2p_{10}$, and a designation in jl coupling. The latter is a coupling scheme which first couples the core J_c to the valence electron l to determine another quantum number, k; this is then coupled to the spin of the valence electron to determine J. Thus, in place of the jj coupling notation ($J_c j$, J), one has the jl coupling expression (J_c,kJ). There is a slight advantage[6] to using jl coupling in place of jj coupling for the J = 1 level of $(5p)^5(6p)$ and the J = 2 level of $(5p)^5(5d)$. However, both the jj and jl designations are meaningless when significant configuration interaction occurs, while their use implies the sufficiency of a single configuration description. Thus it seems pointless to continue identifying levels with a jl coupling scheme. Thus, in addition to the (i,J) designation of levels, the tables herein also list the energy of the level relative to the ground state, and the Paschen notation (which orders rather than describes levels), e.g. $2p_{10}$/77270.

The Lande g factor is given by

$$g_L(iJ) = \sum_{L,S} (2L+1)(2S+1)\,[3J(J+1)+S(S+1)-L(L+1)]/[2J(J+1)]$$

$$\left| \sum_{J_c,j} C(i,J_c j;J)[(2J_c+1)(2j+1)]^{1/2} \begin{Bmatrix} l & 1/2 & J_c \\ L & S & J \end{Bmatrix} \right|^2, \qquad (5b)$$

and a comparison of $g_L(iJ)$ with $g_L(J_c j,J)$ is an additional measure of the mixing of the wavefunctions. If there are several configurations contributing to a term the Lande g factor is the sum of contributions, given by eq.(5b), from each configuration, that is there is no intererence.

Table (3) Results of the Matrix Diagonalization for the $(5p)^5(6s)$ Levels

Level	J_c	j	J	K_{ref}(calc)	K_{ref}(expl^5)	G_L(calc)	G_L(expl^5)	Comp. J_c,j	C(i,J_cj;J)
1,2 $1s_5$/67068	3/2	1/2	2	−4275	−4275	1.500 (3/2)	1.500	3/2,1/2	1.000
1,1 $1s_2$/77186	1/2	1/2	1	6822	5843	1.299(1.333)	1.321	1/2,1/2 3/2,1/2	−0.9975 0.0710
2,1 $1s_4$/68046	3/2	1/2	1	−3310	−3297	1.201(1.167)	1.204	3/2,1/2 1/2,1/2	0.9975 0.0710
1,0 $1s_3$/76197	3/2	1/2	0	6263	4857			3/2,1/2	1.000

Table (4) Results of the Matrix Diagonalization for the $(5p)^5(6p)$ Levels

Level	J_c	j	J	K_{rel}(calc)	K_{rel}(expl^5)	G_L(calc)	G_L(expl^5)	Comp. J_c,j	C(i,J_cj;J)
1,3	3/2	3/2	3	−3511	−3509	4/3 (4/3)	1.336	3/2,1/2	1.000
$2p_8$/78403									
1,2	1/2	3/2	2	7415	7520	1.173(1.167)	1.195	1/2,3/2	−0.9993
$2p_3$/89163								3/2,1/2	−0.0338
2,2	3/2	3/2	2	−2567	−2701	1.371(1.333)	1.379	3/2,3/2	0.9889
$2p_6$/79212								3/2,1/2	−0.1471
3,2	3/2	1/2	2	−3730	−3793	1.123(1.167)	1.106	3/2,1/2	0.9885
$2p_9$/78120								3/2,3/2	0.1477
1,1	1/2	3/2	1	7360	7366	1.462(1.500)	1.552	1/2,3/2	−0.9902
$2p_2$/89279								3/2,1/2	0.0868
2,1	1/2	1/2	1	6685	6467	0.640(0.667)	0.790	1/2,1/2	−0.9960
$2p_4$/88380								1/2,3/2	−0.0742
3,1	3/2	3/2	1	−3021	−2956	1.097(1.333)	1.022	3/2,3/2	0.7774
$2p_7$/78957								3/2,1/2	0.6155
4,1	3/2	1/2	1	−4551	−4645	1.800(1.500)	1.852	3/2,1/2	0.7833
$2p_{10}$/77270								3/2,3/2	−0.6205
1,0	1/2	1/2	0	8807	7948			1/2,1/2	0.9881
$2p_1$/89861								3/2,3/2	0.1539
2,0	3/2	3/2	0	−608	−1794			3/2,3/2	−0.9881
$2p_5$/80119								1/2,1/2	0.1539

Table (5) Results of the Matrix Diagonalization for the $(5p)^5(5d)$ Levels

Level	J_c	j	J	K_{rel}(calc)	K_{rel}(expl^5)	G_L(calc)	G_L(expl^5)	Comp. J_c,j	C(i,J_cj;J)
1,4 $3d_4'$/80197	3/2	5/2	4	−3826	−3826	5/4 (5/4)		3/2,5/2	1.000
1,3 $3s_1'''$/91747	1/2	5/2	3	7438	7724	1.121(1.111)	1.126	1/2,5/2 3/2,3/2	0.9978 −0.0563
2,3 $3d_1'$/82431	3/2	5/2	3	−2120	−1592	1.257(1.239)		3/2,5/2 3/2,3/2	0.8967 −0.4384
3,3 $3d_4$/80971	3/2	3/2	3	−3772	−3052	1.039(1.067)		3/2,3/2 3/2,5/2	0.8970 0.4410
1,2 $3s_1''''$/91448	1/2	5/2	2	7206	7425	1.256(1.289)	1.274	1/2,5/2 1/2,3/2	−0.9881 0.1023
2,2 $3s_1''$/91153	1/2	3/2	2	7014	7130	0.777(0.767)		1/2,3/2 1/2,5/2	0.9922 0.1036
3,2 $3d''$/81926	3/2	3/2	2	−2712	−2097	0.951(1.066)		3/2,3/2 3/2,5/2	0.8985 0.4336
4,2 $3d_3$/80323	3/2	5/2	2	−3635	−3700	1.348(1.211)	1.376	3/2,5/2 3/2,3/2	0.8944 −0.4321
1,1 $3s_1'$/93619	1/2	3/2	1	9548	9596	0.856(0.833)		1/2,3/2 3/2,5/2	0.9761 0.2165
2,1 $3d_2$/83890	3/2	5/2	1	− 236	− 133	0.764(1.067)		3/2,5/2 3/2,3/2	0.8533 0.4826
3,1 $3d_5$/79987	3/2	3/2	1	−4368	−4036	1.381(1.211)	1.395	3/2,3/2 3/2,5/2	0.8757 −0.4742
1,0 $3d_6$/79772	3/2	3/2	0	−4812	−4251			3/2,3/2	1.000

One should note that there is significant mixing of some of the level pairs of the $(5p)^5(6p)$ and $(5p)^5(5d)$ configurations.

In comparing the calculations in Tables (3)-(5) with experiment, it is seen that there are 3 major disagreements. First, the levels (1,1) and (1,0) of $(5p)^5(6s)$ are calculated to be higher than the measurements. Clearly some additional interaction is pushing these levels to lower energy. I will return to this point. The second major disagreement between the calculations and experiment are the energy of the J = 0 levels of the $(5p)^5(6p)$ configuration; this is expected since no configuration interaction with the ground state is included, and this point is not pursued further. The third major disagreement between calculation and measurement occurs for the Lande g factors for the two higher energy J = 1 levels of $(5p)^5(6p)$, even though their calculated relative energies are in excellent agreement with the measured values. The calculations indicate little mixing of the jj wavefunctions for the 2 higher levels, (1,1) and (2,1), but extensive mixing for the 2 lower levels, (3,1) and (4,1). But as listed in sec.(6^{13}) of Condon and Shortley[4] the electrostatic matrix element between the (1/2,3/2,1) and (1/2,1/2,1) levels of $(p)^5p'$ is zero. Thus, even though the levels (1,1) and (2,1) are close in energy, there is no significant mixing since the interaction matrix element is zero. The Lande g factors obey a sum rule, since

$$\sum_i C(i,J_c j;J)\, C(i,J_c' j';J) = \delta_{J_c,J_c'}\, \delta_{j,j'}, \tag{5c}$$

then

$$\sum_i g_L(iJ) = \sum_{L,S} \Delta(LSJ)\, [3J(J+1)+S(S+1)-L(L+1)]/[3J(J+1)], \tag{5d}$$

where $\Delta(LSJ)$ indicates that L, S and J satisfy triangular inequalities. For the excited states of the noble gases, the sum rule values for $g_L(iJ)$ are listed in Table (6).

Table (6) Sum Rule for Lande g factor for the noble gases

J	$\sum_i g_L(iJ)$
$\ell' + 2$	$(J + 1)/J$
$\ell' + 1$	$(3J^2 + 4J + 2)/J(J + 1)$
ℓ'	$2\,(2J^2 + 2J + 1)/J(J + 1)$
$\ell' - 1$	$(3J^2 + 2J + 3)/J(J + 1)$
$\ell' - 2$	$(J^2 + 1)/J(J + 1)$

For the J = 2 and J = 1 levels of $(5p)^5(6p)$ the sum rule values are 3.667 and 5. The calculations lead to 3.667 and 4.999, while the sums of experimental values are 3.680 and 5.216, with an excess of 0.216 for the J = 1 levels. The levels (1,1) and (2,1) of the $(5p)^5(6p)$ configuration are close in energy to levels (3,1) and (4,1) of the $(5p)^5(7p)$ configuration. For the latter 2 levels, the sum of the Lande g factors (0.903 and 1.728)^5 equals 2.631, lower than the sum rule value (for $J_c = 3/2$ only) of 2.833 by 0.202, so that weak configuration interaction (CI) between nearby levels could account for most of the increase for the J = 1 levels of $(5p)^5(6p)$. These calculations do not include CI effects on the $(5p)^5(6p)$ levels. This neglect of CI has interesting consequences, but they are not relevant to the important lasing transitions.

To account for the error in the calculated energy of the (1,1) and (1,0) levels of $(5p)^5(6s)$, and to have an accurate description of the $(5p)^5(5d)$ upper lasing level wavefunctions, one must include CI between adjacent $(5p)^5(5d)$ and $(5p)^5(6s)$ levels, with the former (latter) built on the $J_c = 3/2$ ($J_c = 1/2$) core. The CI matrix element in LS coupling is

$$\langle (n_1\ell_1)^m L_1 S_1, n_2\ell_2, LSM_L M_S | H_{CI} | (n_1\ell_1)^m P_1 Q_1, n_3\ell_3, L'S'M_{L'}, M_{S'} \rangle =$$

$$\delta_{L'L}\,\delta_{S'S}\,\delta_{M_L' M_L}\,\delta_{M_S' M_S}\; m \sum_{L_1', S_1'} (\ell_1^{m-1} L_1' S_1' | \} \ell_1^m L_1 S_1)\; (\ell_1^{m-1} L_1' S_1' | \} \ell_1^m P_1 Q_1)$$

$$(-1)^{-\ell_2-\ell_3}\,[(2L_1+1)(2P_1+1)]^{1/2}\;I(LS,\ell_1\ell_2\ell_3). \tag{6a}$$

where $(\ell_1^{m-1}L_1'S_1'|\}\ell_1^{m}L_1S_1)$ is a coefficient of fractional parentage.[2] In LSJM coupling it is

$$\langle(n_1\ell_1)^{m}L_1S_1,n_2\ell_2,LSJM|H_{CI}|(n_1\ell_1)^{m}P_1Q_1,n_3\ell_3,L'S'J'M'\rangle =$$

$$\delta_{L'L}\,\delta_{S'S}\,\delta_{J'J}\,\delta_{M'M}\sum_{L_1',S_1'}(\ell_1^{m-1}L_1'S_1'|\}\ell_1^{m}L_1S_1)\,(\ell_1^{m-1}L_1'S_1'|\}\ell_1^{m}P_1Q_1)$$

$$(-1)^{-\ell_2-\ell_3}\,[(2L_1+1)(2P_1+1)]^{1/2}\;I(LS,\ell_1\ell_2\ell_3). \tag{6b}$$

However, in JJ coupling the matrix element has the more imposing form

$$\langle(n_1\ell_1)^{m}L_1S_1J_1,n_2\ell_2j_2,JM|H_{CI}|(n_1\ell_1)^{m}P_1Q_1J_1',n_3\ell_3j_3,J'M'\rangle =$$

$$\delta_{J'J}\,\delta_{M'M}\sum_{L_1',S_1'}(\ell_1^{m-1}L_1'S_1'|\}\ell_1^{m}L_1S_1)\,(\ell_1^{m-1}L_1'S_1'|\}\ell_1^{m}P_1Q_1)\,(-1)^{-\ell_2-\ell_3}$$

$$[(2L_1+1)(2P_1+1)]^{1/2}\;[(2J_1+1)(2j_2+1)(2J_1'+1)(2j_3+1)]^{1/2}$$

$$\sum_{L,S}(2L+1)(2S+1)\,h(\ell'LS)\begin{Bmatrix} L_1 & S_1 & J_1 \\ \ell_2 & 1/2 & j_2 \\ L & S & J \end{Bmatrix}\begin{Bmatrix} P_1 & Q_1 & J_1' \\ \ell_3 & 1/2 & j_3 \\ L & S & J \end{Bmatrix} I(LS,\ell_1\ell_2\ell_3), \tag{6c}$$

where

$$I(LS,\ell_1\ell_2\ell_3) = (2\ell_1+1)\,[(2\ell_2+1)(2\ell_3+1)]^{1/2}$$

$$\Big[\delta_{S_1Q_1}\,(-1)^{-\ell_2-\ell_3-L_1'-L-L_1-P_1}\sum_k(-1)^k\,d_k\begin{Bmatrix} k & L_1 & P_1 \\ L_1' & \ell_1 & \ell_1 \end{Bmatrix}\begin{Bmatrix} k & L_1 & P_1 \\ L & \ell_3 & \ell_2 \end{Bmatrix}$$

$$+\,(-1)^{-S_1-Q_1}\,[(2S_1+1)(2Q_1+1)]^{1/2}\sum_k e_k\begin{Bmatrix} S_1' & 1/2 & Q_1 \\ S_1 & 1/2 & S_1 \end{Bmatrix}\begin{Bmatrix} \ell_1 & L_1 & L_1' \\ k & \ell_2 & \ell_1 \\ \ell_3 & L & P_1 \end{Bmatrix}\Big], \tag{6d}$$

with

$$d_k = \begin{pmatrix} \ell_1 & k & \ell_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \ell_2 & k & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} R_k(\ell_1\ell_2,\ell_1\ell_3)\;;\; e_k = \begin{pmatrix} \ell_1 & k & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \ell_1 & k & \ell_2 \\ 0 & 0 & 0 \end{pmatrix} R_k(\ell_1\ell_2,\ell_3\ell_1), \tag{6e}$$

where

$$R_k(\ell_a\ell_b,\ell_c\ell_d) = {}_0\int^{\infty} dx\ \phi_a(x)\ \phi_c(x)\ \ {}_0\int^{\infty} dy\ \phi_b(y)\ \phi_d(y)\ R^k_</R^{k+1}_>. \tag{6f}$$

For $\ell_1 = 1$, $\ell_2 = 2$, and $\ell_3 = 0$, the interaction matrix elements in JJ coupling are listed in Table (7).

Table(7) $(np)^5(n'd)-(np)^5(n"s)$ Interconfiguration Interaction in JJ Coupling

J_1	j_2	J_1'	j_3	J	Matrix Element
3/2	5/2	3/2	1/2	2	$[21/625]^{1/2}\ R_2(pd,ps)$
3/2	3/2	3/2	1/2	2	$-(2/25)\ R_2(pd,ps)$
1/2	5/2	3/2	1/2	2	$[24/625]^{1/2}\ R_2(pd,ps)$
1/2	3/2	3/2	1/2	2	$-(1/25)\ R_2(pd,ps)$
3/2	5/2	3/2	1/2	1	$[1/125]^{1/2}[R_2(pd,ps) - (20/3)\ R_1(pd,sp)]$
		1/2	1/2	1	$-[8/125]^{1/2}[R_2(pd,ps) - (5/3)\ R_1(pd,sp)]$
3/2	3/2	3/2	1/2	1	$[4/125]^{1/2}[R_2(pd,ps) - (10/9)\ R_1(pd,sp)]$
		1/2	1/2	1	$-[2/125]^{1/2}[R_2(pd,ps) + (10/9)\ R_1(pd,sp)]$
1/2	3/2	3/2	1/2	1	$(1/5)\ [R_2(pd,ps) - (20/9)\ R_1(pd,sp)]$
		1/2	1/2	1	$[8/81]^{1/2}\ R_1(pd,sp)]$
3/2	3/2	1/2	1/2	0	$-[2/25]^{1/2}\ R_2(pd,ps)$

As a consequence of the CI the Table (3) and (5) calculations are merged into Table (8).

Table (8) Results of the Matrix Diagonalization for the $(5p)^5(5d)+(5p)^5(6s)$

Level	J_c	j	J	K_{rel}(calc)	K_{rel}(expl)	G_L(calc)	G_L(expl)	Comp.	Coefficient
d,1,4	3/2	5/2	4	-3826	-3826	5/4 (5/4)		d,3/2,5/2	1.000
$3d_4'$/80197									
d,1,3	1/2	5/2	3	7438	7724	1.121(1.111)	1.126	d,1/2,5/2	0.9978
$3s_1''''$/91747								d,3/2,3/2	-0.0563
d,2,3	3/2	5/2	3	-2120	-1592	1.257(1.239)		d,3/2,5/2	0.8967
$3d_1'$/82431								d,3/2,3/2	-0.4384
d,3,3	3/2	3/2	3	-3772	-3052	1.039(1.067)		d,3/2,3/2	0.8970
$3d_4$/80971								d,3/2,5/2	0.4410
d,1,2	1/2	5/2	2	7239	7425	1.258(1.289)	1.274	d,1/2,5/2	-0.9863
$3d_1''''$/91448				(7206)		(1.256)		d,1/2,3/2	0.1165
d,2,2	1/2	3/2	2	7014	7130	0.777(0.767)		d,1/2,3/2	0.9906
$3s_1''$/91153				(7014)		(0.777)		d,1/2,5/2	0.1178
d,3,2	3/2	3/2	2	-2712	-2097	0.951(1.066)		d,3/2,3/2	0.8967
3d''/81926				(-2712)		(0.951)		d,3/2,5/2	0.4373
d,4,2	3/2	5/2	2	-3540	-3700	1.347(1.211)	1.376	d,3/2,5/2	0.8901
$3d_3$/80323				(-3635)		(1.348)		d,3/2,3/2	-0.4348
s,5,2	3/2	1/2	2	-16957	-16955	1.4999(3/2)	1.500	s,3/2,1/2	0.9958
$1s_5$/67068				(-16828)		(1.500)		d,3/2,5/2	0.0727
d,1,1	1/2	3/2	1	9556	9596	0.856(0.833)		d,1/2,3/2	0.9763
$3s_1'$/93619				(9548)		(0.856)		d,3/2,5/2	0.2145
d,2,1	3/2	5/2	1	- 227	- 133	0.777(1.067)		d,3/2,5/2	0.8592
$3d_2$/83890				(-236)		(0.764)		d,3/2,3/2	0.4703
d,3,1	3/2	3/2	1	-3762	-4036	1.358(1.211)	1.395	d,3/2,3/2	0.7899
$3d_5$/79987				(-4368)		(1.381)		s,1/2,1/2	-0.4658
								d,3/2,5/2	-0.3929
s,4,1	1/2	1/2	1	-6292	-6837	1.307(1.333)	1.321	s,1/2,1/2	-0.8799
$1s_2$/77186				(-5733)		(1.299)		d,3/2,5/2	0.2445
s,5,1	3/2	1/2	1	-15933	-15977	1.206(1.167)	1.204	s,3/2,1/2	0.9940
$1s_4$/68046				(-15868)		(1.201)		s,1/2,1/2	0.0789

Table (8) continued

d,1,0	3/2	3/2	0	−3863	−4251	d,3/2,3/2	0.8603
$3d_6$/79772				(−4812)		s,1/2,1/2	0.5097
s,2,0	1/2	1/2	0	−7143	−7826	s,1/2,1/2	0.8603
$1s_3$/76197				(−6292)		d,3/2,3/2	−0.5097

To complete this section Table (9a) lists some calculated Einstein emission coefficients and emission cross sections and compares the Einstein coefficients with the dipole length calculations of Aymar and Coulombe,[6] while Table (9b) lists calculated radiative lifetimes and compares them with calculations of Ref.(6) and measurements. The cross sections are calculated from

$$\sigma_{ij}(cm^2) = 8x10^{-18}\ f_{ij}/\Gamma_{Dopp}(Ry)$$

where f_{ij} is the emission oscillator strength and $\Gamma_{Dopp}(Ry)$ is the Doppler width in Rydbergs, calculated at room temperature. It is assumed that the Doppler width is the dominant broadening mechanism; if it is not dominant, then the Doppler width should be replaced by the appropriate width. The above formula is obtained from oscillator density continuity, and a factor connecting continuum oscillator strength and cross section.

Table (9a) Some Einstein Coefficients

$(5p)^5(5d)$ Term	$(5p)^5(6p)$ Term	λ(microns)	$A(10^6/sec)$	$A(10^6/sec)$ Ref.(7)	$\sigma(10^{-12}cm^2)$
1,4	1,3	5.571	0.348	0.207	90.0
1,3	3,2	0.7338	0.0303	0.554	0.0179
1,3	1,3	0.7495	0.191	0.166	0.120
1,3	2,2	0.7978	0.0076	0.0214	0.0058
1,3	1,2	3.869	1.03	0.699	89.1
2,3	3,2	2.320	0.400	0.192	7.45
2,3	1,3	2.483	1.24	0.479	28.4
2,3	2,2	3.107	1.20	1.14	53.6
3,3	3,2	3.508	1.11	0.737	71.5
3,3	1,3	3.897	0.0173	0.102	1.53
3,3	2,2	5.69	0.0613	0.00051	16.8
1,2	4,1	0.7053	1.10	0.00087	0.576
1,2	3,2	0.7503	0.144	0.0034	0.091
1,2	1,3	0.7666	0.0819	0.00006	0.055
1,2	3,1	0.8006	0.749	0.114	0.574
1,2	2,2	0.8173	0.777	0.0044	0.633
1,2	2,1	3.258	0.0030	0.101	0.153
1,2	1,1	4.610	0.524	0.0024	76.8
1,2	1,2	4.373	0.0906	0.044	11.3
2,2	4,1	0.7203	0.217	0.00087	0.121
2,2	3,2	0.7673	0.102	0.0034	0.069
2,2	1,3	0.7843	0.0071	0.00006	0.0051
2,2	3,1	0.8199	0.195	0.114	0.161
2,2	2,2	0.8375	0.0076	0.0044	0.0067
2,2	2,1	3.605	1.09	0.101	76.5
2,2	1,1	5.336	0.0112	0.0024	2.53
2,2	1,2	5.023	0.057	0.044	10.9
3,2	4,1	2.148	0.070	0.0526	1.04
3,2	3,2	2.627	1.11	0.742	30.1
3,2	1,3	2.839	0.0460	0.0343	1.57
3,2	3,1	3.368	0.983	0.681	56.1
3,2	2,2	3.685	0.0042	0.0068	0.312

Table (9a) continued

4,2	4,1	3.275	0.609	0.287	31.9
4,2	3,2	4.54	0.0214	0.0153	2.99
4,2	1,3	5.21	0.0207	0.0030	4.36
4,2	3,1	7.32	0.0149	0.0098	8.72
4,2	2,2	9.00	0.0374	0.0274	40.8
1,1	4,1	0.6117	1.29	0.624	0.442
1,1	3,2	0.6452	0.014	0.0436	0.0057
1,1	3,1	0.6820	0.825	0.0180	0.391
1,1	2,2	0.6941	0.193	0.0433	0.097
1,1	2,0	0.7407	0.174	0.252	0.106
1,1	2,1	1.908	2.20	0.746	22.9
1,1	1,1	2.304	0.869	0.418	15.9
1,1	1,2	2.244	0.112	0.0813	1.90
1,1	1,0	2.660	1.73	0.764	48.7
1,1	(5p)**6	0.1068	1370.	3370.	2.49
2,1	4,1	1.511	0.00045	0.0396	0.0023
2,1	3,2	1.733	0.626	0.304	4.87
2,1	3,1	2.027	2.42	2.46	30.1
2,1	2,2	2.138	0.0104	0.0060	0.153
2,1	2,0	2.652	1.99	1.27	55.5
2,1	(5p)**6	0.1192	915.	1710.	2.32
3,1	4,1	3.68	0.553	0.279	41.2
3,1	3,2	5.36	0.0038	0.0077	0.86
3,1	3,1	9.71	0.0095	0.0004	13.0
3,1	2,2	12.90	0.0119	0.0016	38.2
3,1	(5p)**6	0.1250	14.5	11.0	0.042
1,0	4,1	4.00	0.717	0.232	68.4
1,0	3,1	12.27	0.0027	0.0006	7.48

Table (9b) Lifetimes (ns)

Level	Calc.	Ref.(7) (calc)	Ref.(8) (exp)	Ref.(9) (exp)	Ref.(10) (exp)	Ref.(11) (exp)
$(5p)^5(5d)$						
(1,4)	2865.	4820.	1200.	1330.		
(1,3)	787.					
(2,3)	349.	551.				
(3,3)	837.	1190.	1000.	1170.		
(1,2)	288.					
(2,2)	592.					
(3,2)	452.	659.	1700.	1010±50		
(4,2)	1423.	2920.	2900.	2100,1020		
B (1,1)	0.87			<350.		
(2,1)	1.02	0.6		<350.		
(3,1)	4.59	88.9				
(4,1)	0.92					
(5,1)	6.21					
(1,0)	1389.	4300.				
$(5p)^5(6p)$						
(1,3)	29.9	25.5				
(1,2)	26.4	27.7			29.0±1.5	30.5±3
(2,2)	27.6	28.1			33 ±20	
(3,2)	35.7	33.0				
(1,1)	23.1	27.2			43.5±1.5	29.5±3
(2,1)	28.0	37.4				
(3,1)	32.3	29.9				
(4,1)	38.0	29.7				
(1,0)	21.9	28.4			38.5±1.5	30.7±3
(2,0)	28.7	22.4			40 ±12	

The present calculations of Einstein coefficients are generally larger than those of Ref.(6) for the $(5p)^5(5d)$ levels, though the difference is generally less than a factor of 2.

3) Non-zero Magnetic Field and No Hyperfine Interaction

If next we include the effect of a uniform longitudinal magnetic field (in the z direction) with the interaction[12]

$$H_Z = (e\ h/4\pi m_e c)\ (\vec{L} + 2\ \vec{S}) \cdot \vec{H} = (e\ h/4\pi m_e c)\ (L_z + 2\ S_z)\ H = \beta H\ (L_z + 2S_z), \tag{7a}$$

where β is the Bohr magneton whose value is listed in Ref.(12) as 0.927×10^{-20} erg/Gauss, which is 0.579×10^{-8} eV/Gauss or

$$\beta H(cm^{-1}) = H(Gauss)/21400. \tag{7b}$$

The matrix element is

$$\langle i',J'M'|H_Z|i,JM\rangle = {}_{J_c}\Sigma_{,j}\ {}_{J_c'}\Sigma_{,j'}\ C(i,J_c j;J)\ C(i',J_c' j';J')$$

$$\langle J_c',l'j';J'M'|H_Z|J_c,l'j;JM\rangle$$

$$= {}_{J_c}\Sigma_{,j}\ {}_{J_c'}\Sigma_{,j'}\ C(i,J_c j;J)\ C(i',J_c' j';J')\ [(2J_c+1)(2j+1)(2J_c'+1)(2j'+1)]^{1/2}$$

$$\sum_{L,S} [(2L+1)(2S+1)]^{1/2} \sum_{L',S'} [(2L'+1)(2S'+1)]^{1/2} \begin{Bmatrix} 1 & 1/2 & J_c \\ \ell' & 1/2 & j \\ L & S & J \end{Bmatrix} \begin{Bmatrix} 1 & 1/2 & J_c' \\ \ell' & 1/2 & j' \\ L' & S' & J' \end{Bmatrix}$$

$$\langle {}^2P,{}^2\ell';LSJM||H_Z||{}^2P,{}^2\ell';L'S'J'M'\rangle. \tag{7c}$$

As discussed in Ref.(13), the matrix element in eq.(7c) is diagonal in L, S, and M, but not in J. It is given by

$$\langle {}^2P,{}^2\ell';LSJM||H_Z||{}^2P,{}^2\ell';L'S'J'M'\rangle = \beta H\ \ \delta_{M'M}\ \delta_{L'L}\ \delta_{S'S}$$

$$[M\ (1 + g_{LO})\ \delta_{J'J}\ \ -\ \ \delta_{J',J+1}\ F_+ -\ \ \delta_{J',J-1}\ F_-], \tag{8a}$$

where g_{LO} is given by

$$g_{LO} = [J(J+1) + S(S+1) - L(L+1)]/[2J(J+1)], \tag{8b}$$

$$F_+ = (1/2J+2)$$

$$\{[(J+M+1)(J-M+1)(L+S+J+2)(S+J+1-L)(L+J+1-S)(L+S-J)/(2J+1)(2J+3)]\}^{1/2}, \tag{8c}$$

and

$$F_- = (1/2J)$$

$$\{[(J+M)(J-M)(L+S+J+1)(S+J-L)(L+J-S)(L+S+1-J)]/[(2J+1)(2J-1)]\}^{1/2}. \tag{8d}$$

Note that g_{LO} is independent of M, while F_+ and F_- are symmetric in M, so that we have to evaluate explictly only the case $M \geq 0$. Then

$$\langle i',J'M'|H_Z|i,JM\rangle = \beta H\, M\, g_L\, \delta_{J'J}\, \delta_{M'M} - \beta H\, \delta_{M'M} \sum_{J_c,j} \sum_{J_c',j'} C(i,J_c j;J)$$

$$C(i',J_c'j';J')\, [(2J_c+1)(2j+1)(2J_c'+1)(2j'+1)]^{1/2}\, [\delta_{J',J+1} B(\ell') + \delta_{J',J-1}\, C(\ell')], \tag{9a}$$

where the diagonal term is written in terms of the Lande g factor, and

$$\begin{Bmatrix} B(\ell') \\ C(\ell') \end{Bmatrix} = \sum_{L,S} (2L+1)(2S+1) \begin{Bmatrix} 1 & 1/2 & J_c \\ \ell' & 1/2 & j \\ L & S & J \end{Bmatrix} \begin{Bmatrix} 1 & 1/2 & J' \\ \ell' & 1/2 & j' \\ L & S & J' \end{Bmatrix} \begin{Bmatrix} F_+ \\ F_- \end{Bmatrix}. \tag{9b}$$

Preliminary calculations, without including 6s–5d CI, indicated that the effect of the non-diagonal matrix elements $B(\ell')$ and $C(\ell')$ were small even at 20 kG. For any level one can consider a 2x2 interaction with the nearest level with the same M value. If the energy difference is ΔE and the non-diagonal interaction is $V = \beta H$, the mixing coefficient is $V/\Delta E$. For 20 kG, $V \approx 1\ cm^{-1}$, but as Tables (4) and (8) show, the level splitting is always greater than 100 cm^{-1}. Thus for the magnetic fields studied here, the non-diagonal effects can be neglected.

On the other hand, the new eigenvalues increased linearly with magnetic field, i.e. the new eigenvalues are approximately the diagonal matrix elements, $E(i,J) + g_L(iJ)\, M\, \beta H$, where $g_L(iJ)$ is the Lande g factor. That is, for for 1–10 kG magnetic fields only the diagonal component of the interaction is significant,

$$\langle i',J'M'|H_Z|i,JM\rangle = \delta_{i'i}\, \delta_{J'J}\, \delta_{M'M}\, g_L(iJ)\, M\, \beta H. \tag{10}$$

Then the effect of the magnetic field is to split a transition at energy $E(i,JM) - E(i',J'M')$ into a M and M' dependent multiplet at energies $E(i,J)$

$- E(i',J') + [\, g_L(iJ)M - g_L(i'J')M']\, \beta H$. In addition, for each (M,M') term in the multiplet there is a strength factor, $D(i,\ell M;i'\ell'M')$, which is discussed in the next section.

4) Radiative Transition Rates

In most treatments of radiative transition rates one averages over initial state M_J values and sums over final state $M_{J'}$ values. However, with a magnetic field present the M_J values must be retained. The squared dipole matrix element is

$$D(k,dM;k',pM') = |\langle k,dM|\vec{r}|k',pM'\rangle|^2$$

$$= \Big|\sum_{i,J}\sum_{i',J'} C_2(i,J;H,k,dM)\, C_2(i',J';H,k',pM')\, \langle i,dJM|\vec{r}|i',pJ'M'\rangle\Big|^2$$

$$= \Big|\sum_{i,J}\sum_{i',J'} C_2(i,J;H,k,dM)\, C_2(i',J';H,k',pM')$$

$$\sum_{j_1,j_2}\sum_{j_1',j_2'} C_1(i,dJ;j_1,j_2)\, C_1(i',pJ';j_1',j_2')\, \langle j_1 j_2 JM|\vec{r}|j_1' j_2' J'M'\rangle\Big|^2, \tag{11a}$$

where the Zeeman coefficients $C_2(i,J;H,k,lM)$ are those found in the preceeding section, while the $C_1(i,dJ;j_1,j_2)$ are intermediate coupling coefficients and are independent of M. The radiative transition matrix element in jj coupling is

$$\langle j_1 \ell_2 j_2 JM|\vec{r}|j_1' \ell_3 j_3 J'M'\rangle = \delta_{j_1,j_1'}\, (A_{\ell_2,\ell_3}/2)\, (-1)^{\ell_3-1/2+j_1-J'} \begin{Bmatrix} 1/2 & j_3 & \ell_3 \\ 1 & \ell_2 & j_2 \end{Bmatrix}$$

$$\begin{Bmatrix} j_1 & J' & j_3 \\ 1 & j_2 & J \end{Bmatrix} [(2j_2+1)(2j_3+1)(2J+1)]^{1/2} \sum_{\beta=-1}^{1} (-1)^{\beta}\, \vec{a}_{\beta}\, C(J1J',M\beta M'), \tag{11b}$$

where C(ABC,abc) is a Clebsch–Gordan coefficient,

$$A_{\ell_2,\ell_3} = (r_{\ell_2,\ell_3})\, [(2\ell_2+1)(2\ell_3+1)]^{1/2} \begin{pmatrix} \ell_2 & 1 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}, \tag{11c}$$

with $\begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix}$ a 3j symbol and $(r_{p,q})$ the radial matrix element. The vectors are

$$\vec{a}_1 = (2)^{1/2}\, (\vec{I}_x + i\vec{I}_y),$$

$$\vec{a}_0 = 2\ \vec{I}_z, \tag{12a}$$

(12b)

$$\vec{a}_{-1} = (2)^{1/2} (-\vec{I}_x + i\vec{I}_y).$$

(12c)

At the level of intermediate coupling, one may take the factor $C(J1J',M\beta M')$ outside the absolute value sign and sum and average the squared quantity over M and M'. In the present case this is not possible. However, one can write eq.(11a) as

$$D(k,dM;k',pM') = \left| {}_{i,\Sigma_J}\, {}_{i',\Sigma_{J'}} \cdots \sum_{\beta=-1}^{1} (-1)^{\beta} \vec{a}_{\beta}\ C(J1J',M\beta M') \right|^2$$

$$= {}_{i,\Sigma_J}\, {}_{i',\Sigma_{J'}}\, {}_{i'',\Sigma_{J''}}\, {}_{i''',\Sigma_{J'''}} \cdots \sum_{\beta=-1}^{1} \sum_{\beta'=-1}^{1} (-1)^{\beta+\beta'} C(J1J',M\beta M')$$

$$C(J''1J''',M\beta'M')\ \vec{a}_{\beta} \cdot \vec{a}^{*}_{\beta'}.$$

(13a)

But $\vec{a}_{\beta} \cdot \vec{a}^{*}_{\beta'} = 4\ \delta_{\beta,\beta'}$, so that the squared matrix element is

$$D(k,dM;k',pM') = 4\ (A_{5d,6p}/2)^2 \sum_{\beta=-1}^{1} \left| {}_{i,\Sigma_J}\ (2J+1)^{1/2}\ {}_{i',\Sigma_{J'}}\ C_2(i,J;H,k,dM) \right.$$

$$\left. C_2(i',J';H,k',pM')\ (-1)^{-J'} C(J1J',M\beta M')\ W(\ell_2 iJ,\ell_3 i'J') \right|^2,$$

(13b)

where

$$W(\ell_2 iJ,\ell_3 i'J') = {}_{j_1,\Sigma_{j_2}}\ {}_{j_2',\Sigma}\ (-1)^{\ell_3 - 1/2 + j_1} C_1(i,dJM;j_1,j_2)$$

$$C_1(i',pJ'M';j_1,j_2')[(2j_2+1)(2j_3+1)]^{1/2} \begin{Bmatrix} 1/2 & j_3 & \ell_3 \\ 1 & \ell_2 & j_2 \end{Bmatrix} \begin{Bmatrix} j_1 & J' & j_3 \\ 1 & j_2 & J \end{Bmatrix}.$$

(13c)

However, if for each [i,lM] eigenstate one and only one of the Zeeman mixing coefficients were close to unity, then there is a unique relation between k and i,J. For such a case the matrix element becomes

$$D(k,dM;k',pM') = D(iJ,dM;i'J',pM')$$

$$= 4\ (A_{5d,6p}/2)^2\ (2J+1) \sum_{\beta=-1}^{1} C(J1J',M\beta M')^2\ |W(\ell_2 iJ,\ell_3 i'J')|^2.$$

(13d)

When magnetic fields are neglected one sums over M' and averages over M to find a term dependent squared matrix element, oscillator strength, Einstein coefficient, and cross section. The sum and average operation is

$$[1/(2J+1)] \sum_{M=-J}^{J} \sum_{M'=-J'}^{J'} \sum_{\beta=-1}^{1} C(J1J',M\beta M')^2 = [1/(2J+1)] \sum_{M'=-J'}^{J'} = [(2J'+1)/(2J+1)]. \tag{14a}$$

If $S(iJ,i'J')$ is the strength calculated by summing and averaging,

$$S(iJ,i'J') = [1/(2J+1)] \sum_{M=-J}^{J} \sum_{M'=-J'}^{J'} D(iJ,dM;i'J',pM')$$

$$= (2J'+1)\ (A_{5d,6p})^2\ |W(l_2 iJ, l_3 i'J')|^2, \tag{14b}$$

then the multiplet strength with a non-zero magnetic field is

$$D(iJ,dM;i'J',pM') = z(idJM,i'pJ'M')\ S(iJ,i'J'), \tag{14c}$$

where

$$z(idJM,i'pJ'M') = [(2J+1)/(2J'+1)] \sum_{\beta=-1}^{1} C(J1J',M\beta M')^2 = (2J+1)\ \begin{pmatrix} J & 1 & J' \\ M', & -M+M', & -M' \end{pmatrix}^2. \tag{14d}$$

The line strengths $S(iJ,i'J')$ are given as Einstein coefficients and cross sections at the end of sec.(2).

The multiplet emission cross sections with a 6 kG field are shown in figs.(1a) and (1b) for the 9 transitions with the largest cross sections. They show that at 6kG the Zeeman effect splits the emission pattern into triplets. This occurs because in the energy difference

$$\Delta E = E(i,J) - E(i',J') + [\ g_L(iJ)M - g_L(i'J')M'\ ]\ \beta H, \tag{15a}$$

$M = M' + \epsilon$, where $\epsilon = 0, \pm 1$. Then

$$\Delta E = E(i,J) - E(i',J') + \epsilon\ g_L(iJ)\ \beta H + [g_L(iJ) - g_L(i'J')]\ \beta H\ M'. \tag{15b}$$

If $2J_s[g_L(iJ) - g_L(i'J')]$ is small compared to $g_L(iJ)$, where J_s is the smaller of J or J', one has a triplet structure with individual components of the triplet separated by $[g_L(iJ) - g_L(i'J')]\ \beta H$. Since $\sum_{M=-J_s}^{J_s} M' = 0$, the average energy of each component of the triplet is

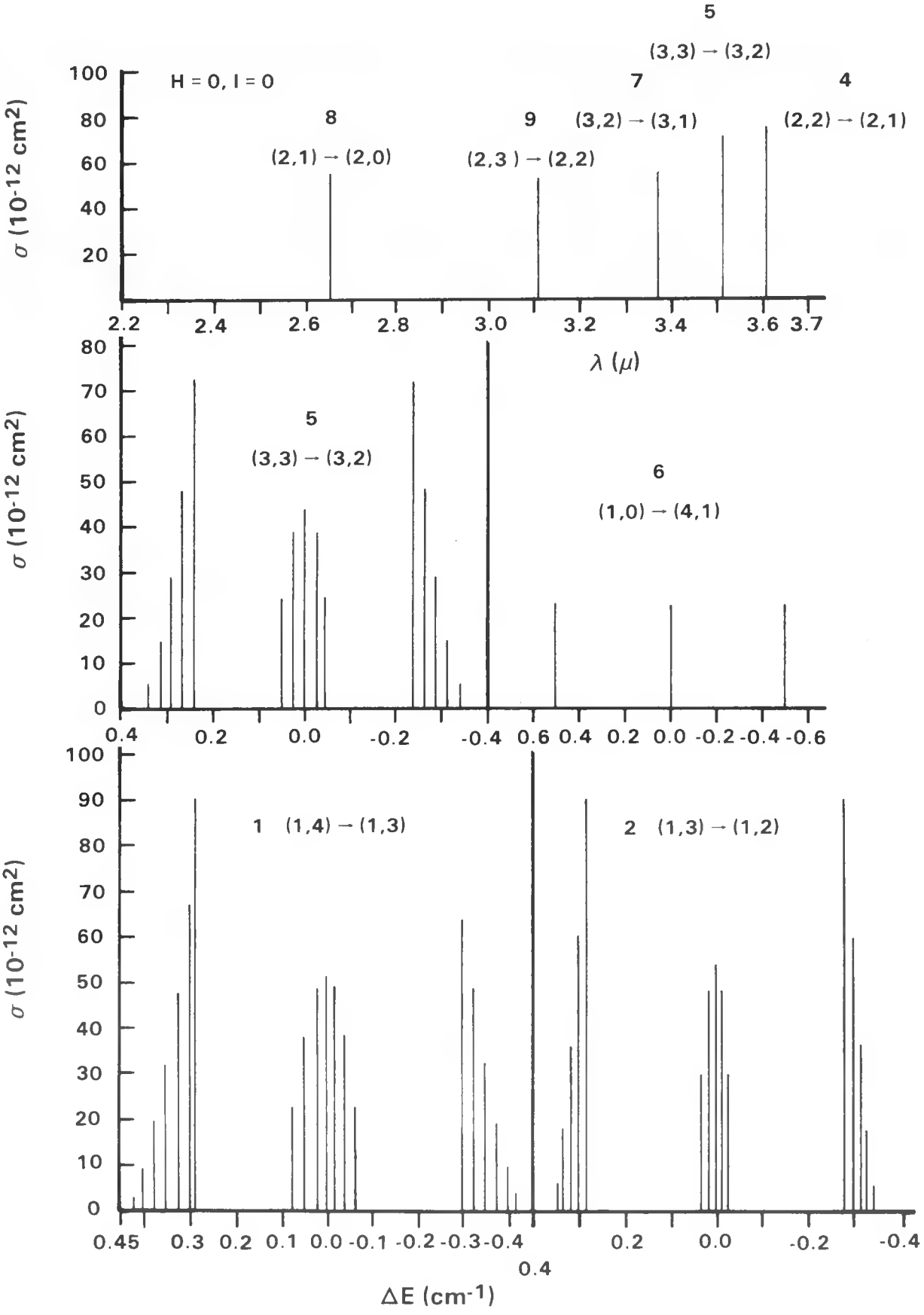
$$\bar{E}(iJ,i'J',H) = E(i,J) - E(i',J') + \epsilon\ g_L(iJ)\ \beta H.$$

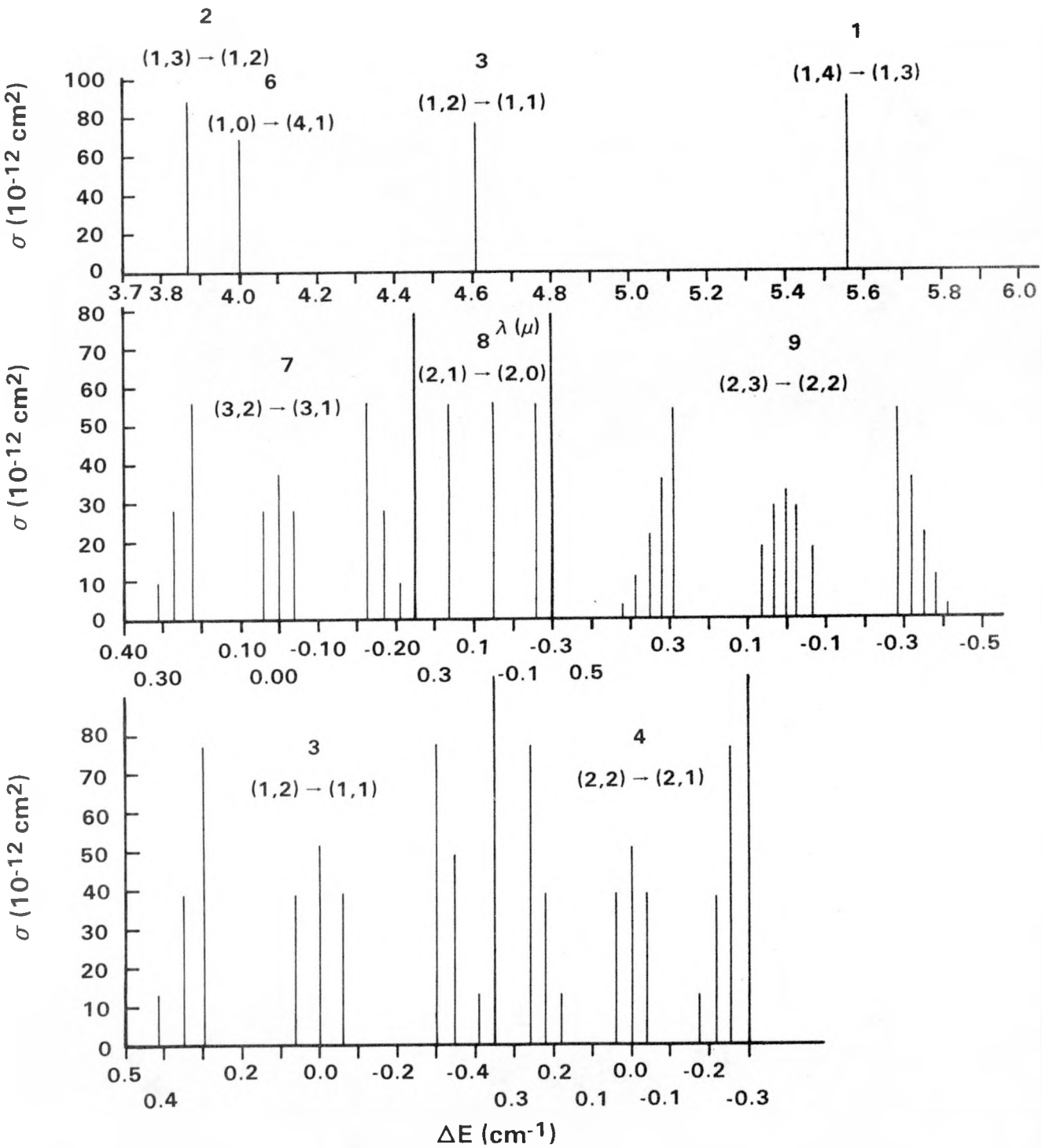
(15c)

A width for each component of the triplet may be defined by

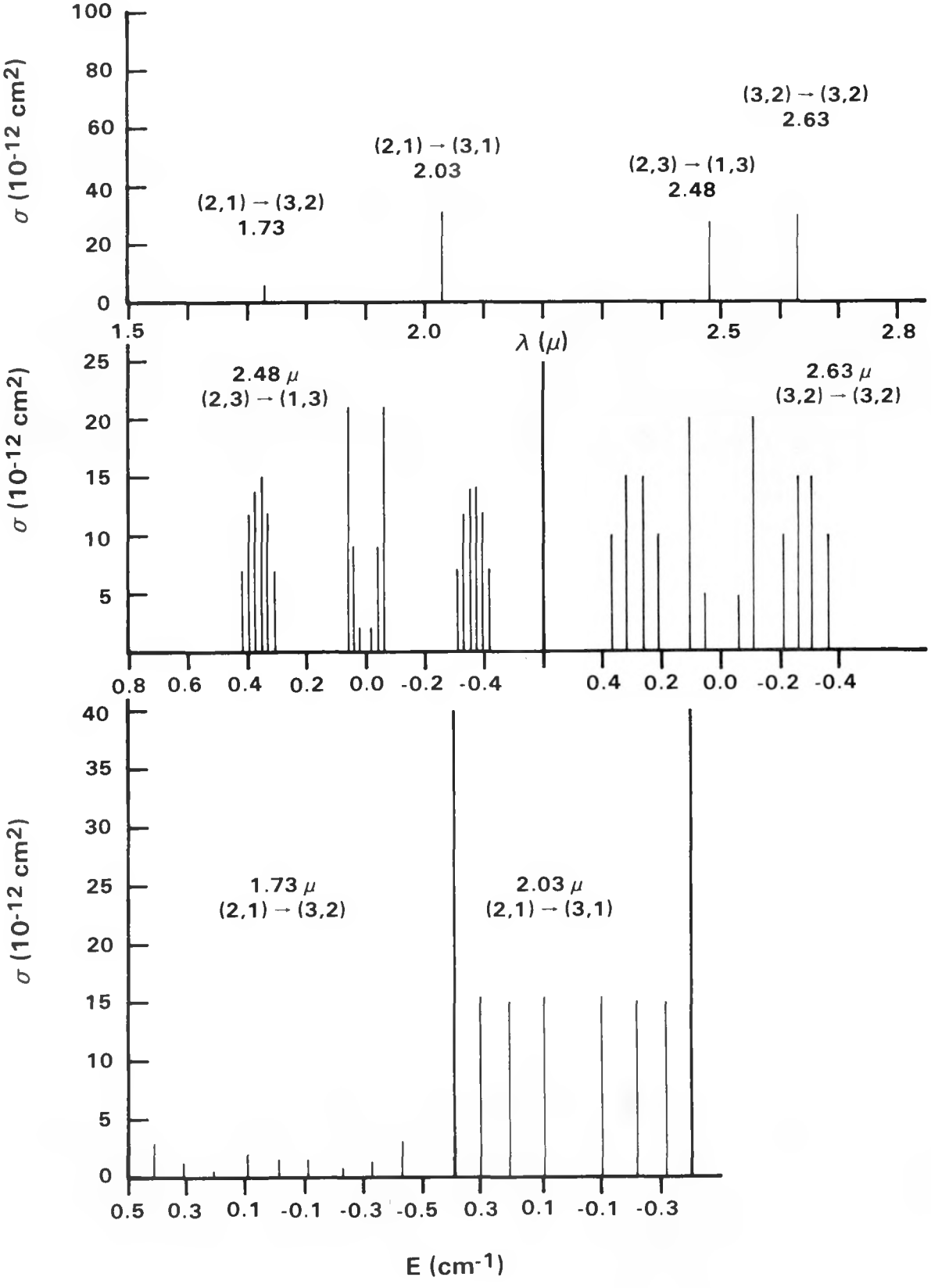
$$\Gamma_Z = [1/(2J_s+1) \sum_{M'=-J_s}^{J_s} (E - \bar{E})^2]^{1/2} = [g_L(iJ) - g_L(i'J')]\, \beta H\, [J_s(J_s+1)/3]^{1/2}$$

(15d)


H = 0, I = 0
5
(3,3) → (3,2)
7
(3,2) → (3,1)
4
(2,2) → (2,1)
8
(2,1) → (2,0)
9
(2,3) → (2,2)
σ (10-12 cm2)
λ (μ)
5
(3,3) → (3,2)
6
(1,0) → (4,1)
σ (10-12 cm2)
1 (1,4) → (1,3)
2 (1,3) → (1,2)
σ (10-12 cm2)
ΔE (cm-1)


2
(1,3) → (1,2)
6
(1,0) → (4,1)
3
(1,2) → (1,1)
1
(1,4) → (1,3)
σ (10-12 cm2)
100
80
60
40
20
0
3.7 3.8 4.0 4.2 4.4 4.6 4.8 5.0 5.2 5.4 5.6 5.8 6.0
λ (μ)
7
(3,2) → (3,1)
8
(2,1) → (2,0)
9
(2,3) → (2,2)
0.40 0.10 -0.10 -0.20 0.1 -0.3 0.3 0.1 -0.1 -0.3 -0.5
0.30 0.00 0.3 -0.1 0.5
3
(1,2) → (1,1)
4
(2,2) → (2,1)
0.5 0.2 0.0 -0.2 -0.4 0.2 0.0 -0.2
0.4 0.3 0.1 -0.1 -0.3
ΔE (cm-1)

Of the nine strongest transitions shown in figs.(1a) and (1b), only the (2,1)→(2,0) transition at 2.65 μ, the (3,2)→(3,1) transition at 3.37 μ, and the (3,3)→(3,2) transition at 3.51 μ are observed at high pressure.[14] In fig.(1c) some additional multiplet cross sections are shown for transitions that are significant in lasing at high pressure.[14] Note that for the transitions at 1.73 μ and 2.03 μ, the triplet pattern is not manifested clearly; however, the central 3(2) lines for the transition at 1.73 μ(2.03μ) arise from $\Delta M = 0$ transitions.


σ (10-12 cm2)
100
80
60
40
20
0
(2,1) → (3,2)
1.73
(2,1) → (3,1)
2.03
(2,3) → (1,3)
2.48
(3,2) → (3,2)
2.63
1.5
2.0
2.5
2.8
λ (μ)
σ (10-12 cm2)
25
20
15
10
5
2.48 μ
(2,3) → (1,3)
2.63 μ
(3,2) → (3,2)
0.8 0.6 0.4 0.2 0.0 -0.2 -0.4
0.4 0.2 0.0 -0.2 -0.4
σ (10-12 cm2)
40
35
30
25
20
15
10
5
0
1.73 μ
(2,1) → (3,2)
2.03 μ
(2,1) → (3,1)
0.5 0.3 0.1 -0.1 -0.3 -0.5
0.3 0.1 -0.1 -0.3
E (cm-1)

For lasing transitions with the direction of the laser axis parallel to the magnetic field, one should not see the $\Delta M = 0$ transitions, i.e. the central peaks of the triplets. Condon and Shortley[4] (p.90) show that the far field Poynting vector due to a dipole source of radiation at the origin is

$$\vec{S} = (c^2k^4/8\pi r^2)\ |\vec{P}\cdot\vec{P} - (\vec{I}_r\cdot\vec{P})^2|^2\ \vec{I}_r, \tag{15e}$$

where $\vec{I}_r$ is a unit vector in the direction of the field point at a distance r from the origin and $\vec{P} = e\,\vec{r}$. Then for the laser axis in the direction of the magnetic field (along the z axis), $\vec{I}_r = \vec{I}_z$ and $\vec{P}\cdot\vec{P} - P_z^2 = P_x^2 + P_y^2$. Thus $\vec{S}$ depends on P_x^2 and P_y^2 but not P_z^2. But in eq.(14d) $\beta = 0 = \Delta M$ corresponds to P_z, so the central peak will not be seen for laser and magnetic field axes parallel.

5) The Hyperfine Splitting without an External Magnetic Field

The hyperfine splitting arises from both the interaction of the nuclear spin with the magnetic field at the nucleus generated by the currents associated with the atomic electrons, and from a correction to the electron Schrodinger equation due to the finite size of the nucleus. The hyperfine splitting is comparable to the Zeeman splitting, i.e., much smaller than the splitting due to the electrostatic interaction. Therefore the wavefunction for the atom including the nuclear spin, I, is written

$$|iJITt> = \sum_{M,M_I} C(JIT,MM_It)\ |iJM>\ |IM_I> \tag{16a}$$

When two subshells are partially filled the hyperfine interaction is complicated. I begin with the magnetic dipole hyperfine interaction. A detailed evaluation for excited states of the noble gases is found in eq.(49) of Ref.(15). Unfortunately, the calculation in Ref.(15) is done in LS coupling. In Appendix (A) the desired hyperfine matrix element in intermediate coupling $<iJIF'M_{F'}|H^1_{HF}|iJIFM_F>$ is obtained. It is

$$<iJIF'M_{F'}|H^1_{HF}|iJIFM_F> = \delta_{FF'}\ \delta_{M_FM_{F'}}(\mu_0/4\pi)\ 2\ g_n m_{ep}\ (\mu_B)^2\ (1/a_0)^3$$

$$(-1)^{I+F+l_1+l_2}\ \begin{Bmatrix} F & I & J \\ 1 & J & I \end{Bmatrix}\ (2J+1)\ [I(I+1)(2I+1)]^{1/2}\ (W_1 + W_2) = (0.00321\ cm^{-1})$$

$$g_n\ \delta_{FF'}\ \delta_{M_FM_{F'}}(-1)^{I+F+l_1+l_2}\ \begin{Bmatrix} F & I & J \\ 1 & J & I \end{Bmatrix}\ (2J+1)\ [I(I+1)(2I+1)]^{1/2}\ (W_1 + W_2)$$

$$= \delta_{FF'}\ \delta_{M_FM_{F'}}[F(F+1)-J(J+1)-I(I+1)]\ (1/2)\ (0.00321\ cm^{-1})\ (-1)^{-J+l_1+l_2}\ g_n$$

$$\{(2J+1)/[J(J+1)]\}^{1/2}\ (W_1 + W_2) = \delta_{FF'}\delta_{M_FM_{F'}}[F(F+1)-J(J+1)-I(I+1)]\ (1/2)\ A_{iJ}, \tag{16b}$$

where W_1 and W_2 are given by eqs.(A4-b) and (A4-c), respectively, A_{iJ} is a parameter used to describe the magnetic hyperfine interaction,[16] and the calculations are done in atomic units. μ_n is the nuclear magnetic moment in nuclear magnetons; g_n is defined by $\mu_n = g_n\ m_{ep}\mu_B\ I$, where μ_B is the Bohr magneton, and m_{ep} is the ratio of electron to proton mass, 1/1836. For

Xe(129) $\mu_n/m_{ep}\mu_B = -0.777$[1] and I =1/2, so that $g_n = -1.554$, while for Xe(131) $\mu_n/m_{ep}\mu_B = 0.691$[1] and I =3/2, so that $g_n = 0.461$. The ratio $\mu_n(129)/\mu_n(131) = -1.124$, while $g_n(129)/g_n(131) = -3.372$.

For the 5p, 6p, and 5d orbitals of Xe I calculate $\langle(1/r)^3\rangle = 19.947$, 1.086, and 0.07077, respectively. Because of the 6s–5d configuration interaction one requires the additional parameter, $\langle(1/r)^3\rangle_{6s,5d} = 0.0562$. The 6s orbital density at the origin was calculated to be $R_{6s}(0)^2 = 22/(BR^3)$. The results for the magnetic hyperfine splitting are listed in Table (10a) for I = 1/2 (mass 129). In Table (10b) I compare the calculated A_{iJ} values with measurements from Jackson and Coulombe,[17] and Liberman.[18]

Table (10a) Hyperfine splitting in Xe for I = 1/2

Config	i,J	$E(cm^{-1})$	W_1	W_2	W_2'/W_2''	F	$\Delta E_{HF}(cm^{-1})$
$(5p)^5(6p)$	1,3	$2p_8$/78403	-6.964	0.379	-	5/2	0.0560
						7/2	-0.0420
	1,2	$2p_3$/89163	14.49	0.476		3/2	0.1022
						5/2	-0.0682
	2,2	$2p_6$/79212	5.978	0.298		3/2	0.0429
						5/2	-0.0286
	3,2	$2p_9$/78120	8.665	0.811		3/2	0.0647
						5/2	-0.0432
	1,1	$2p_2$/89279	9.942	-0.571		1/2	-0.0573
						3/2	0.0286
	2,1	$2p_4$/88380	-21.48	-1.19		1/2	0.1385
						3/2	-0.0693
	3,1	$2p_7$/78957	-6.192	-0.087		1/2	0.0384
						3/2	-0.0192
	4,1	$2p_{10}$/77270	-8.324	0.431		1/2	0.0482
						3/2	-0.0241
	1,0	$2p_1$/89861	0	0		1/2	0
	2,0	$2p_5$/80119	0	0		5/2	0
$(5p)^5$	1,4	$3d_4'$/80197	-5.947	-0.0450		7/2	0.0501
(5d+6s)						9/2	-0.0401
	1,3	$3s_1'''$/91747	11.46	0.0530		5/2	0.0877
						7/2	-0.0658
	2,3	$3d_4'$/82431	4.814	0.0477		5/2	0.0370
						7/2	-0.0278
	3,3	$3d_4$/80971	6.360	0.0714		5/2	0.0490
						7/2	-0.0368
	1,2	$3s_1''''$/91448	8.744	-0.0614	-0.00006	3/2	-0.0593
						5/2	0.0395

Table (10a) continued

2,2	$3s_1''$/91153	−13.95	−0.0931	0.000006	3/2	0.0959
					5/2	−0.0640
3,2	3d''/81926	−5.177	−0.0643	0.00009	3/2	0.0358
					5/2	−0.0239
4,2	$3d_4$/80323	−1.369	−0.0465	0.00112	3/2	0.0097
					5/2	−0.0064
5,2	$1s_5$/67068	−8.643	−0.0004	−0.0010	3/2	0.0590
					5/2	−0.0394
1,1	$3s_1'$/93619	−10.74	0.1134	0.0007	1/2	−0.0649
				0.0023	3/2	0.0325
2,1	$3d_2$/83890	−3.661	0.0729	0.00012	1/2	−0.0218
				0.0127	3/2	0.0109
3,1	$3d_5$/79987	6.034	0.0346	0.0021	1/2	0.0450
				1.297	3/2	−0.0225
4,1	$1s_2$/77186	17.35	0.0100	0.00025	1/2	0.1342
				4.603	3/2	−0.0671
5,1	$1s_4$/68046	10.56	0.0003	−0.0031	1/2	0.0466
				−2.921	3/2	−0.0233
1,0	$3d_6$/79772	0	0		1/2	0
2,0	$1s_3$/76197	0	0		1/2	0

Table (10b) Comparison of Calculated A_{iJ} with Measurements for Xe(129)

Mass	I	config	i,J	$A_{iJ}(mK)_{calc}$	$A_{iJ}(mK)_{exp}$
129	1/2	$(5p)^5 6p$	1,3	-28.0	-29.06*
			1,2	-68.2	-96.45*
			2,2	-28.6	-29.76*
			3,2	-43.2	-45.52*
			1,1	57.3	66.20*
			2,1	-138.5	-147.6*
			3,1	-38.4	-43.73*
			4,1	-48.2	-46.77*
129	1/2	$(5p)^5 5d$	1,4	-20.1	-19.4
			1,3	-43.9	-56.88*
			2,3	-18.5	-15.8
			3,3	-24.5	-26.6
			1,2	39.5	33.96*
			2,2	-64.0	-88.7
			3,2	-23.9	-27.6
			4,2	- 6.57(-6.44)[-4.83]	- 0.
			5,2	-57.7(-39.4)	-79.56*
			1,1	64.9	
			2,1	21.8(21.9)	
			3,1	-45.0(-37.1)[-0.94]	-80.7
			4,1	-134.2(-106.1)	-193.65*
			5,1	-46.6(-64.7)	-32.15*

* Values obtained from Ref.(17)

The values listed in Table (10b) include both 6s-5d configuration interaction and the Fermi contact term. The values in parenthesis are calculations including the 6s-5d CI, but neglecting the Fermi contact term. The values in brackets are obtained with both the 6s-5d and Fermi contact

term neglected. In general, for those terms involving the Fermi contact term, the calculated effect of the Fermi contact term is too small. This may be a consequence of determining the 6s electron density at the origin with non-relativistic wavefunctions. However these effects occur for levels that that are not involved in lasing transitions in high pressure Xe. Thus we use the calculated A_{iJ} in calculating the hyperfine splitting for Xe(129).

For the I = 3/2 (mass 131) isotope one needs in addition to the magnetic dipole contribution to the hyperfine splitting there is a quadrupole contribution. An expression for the splitting due to the electric quadrupole interaction is obtained in Appendix (B). It is

$$<iJIF'M_{F'}|H^2_{Hy}|iJIFM_F> = \delta_{F,F'}\,\delta_{M_F,M_{F'}}(-e^2\,Q/2)\;\;(-1)^{F-I}\;(2J+1)\;\begin{Bmatrix}2 & I & I\\ F & J & J\end{Bmatrix}$$

$$\{(2I+1)(2I+3)(I+1)/[I(2I-1)]\}^{1/2}[W_3 - W_4] = -\,(0.00393\ \mathrm{cm}^{-1}]\ Q(\mathrm{barns}^2)\ \delta_{F,F'}$$

$$\delta_{M_F,M_{F'}}(-1)^{F-I+j+1/2}\;(2J+1)\;\begin{Bmatrix}2 & I & I\\ F & J & J\end{Bmatrix}\;\{(2I+1)(2I+3)(I+1)/[I(2I-1)]\}^{1/2}[W_3 - W_4]$$

$$= \delta_{F,F'}\,\delta_{M_F,M_{F'}}[A(A+1)-(4/3)I(I+1)J(J+1)]\;B_{iJ}, \qquad (17a)$$

where Q is the nuclear quadrupole moment in barns, W_3 and W_4 are given in eqs.(C14-b) and (C14-c), and B_{iJ} is a coefficient[16] used in describing the quadrupole contribution to hyperfine splitting. An alternative parameter is often used, with B'_{ij} in place of B_{iJ}. They are related by

$$B'_{iJ} = (8/3)\;I\;(2I-1)\;J\;(2J-1)\;B_{iJ}. \qquad (17b)$$

The quadrupole contribution to hyperfine splitting is relevant for the mass 131 (I = 3/2) isotope only, and is included in Table (11a) as ΔE^2_{HF}. The quadrupole moment used was $Q(b^2) = -0.12$.[1] Since W_1, W_2, W'_2, and W''_2 are independent of I and were tabulated in Table (10a), the parameters W_3, W_4, and W'_4 are tabulated in Table (11a). In Table (11b) the calculated A_{iJ} and B_{iJ} values are compared with the measurements of Refs.(17) and (19).

Table (11a) Hyperfine splitting in Xe for I = 3/2

Config	i,J	$E(cm^{-1})$	W_3	W_4	W_4'	F	$\Delta E^1_{HF}(cm^{-1})$	$\Delta E^2_{HF}(cm^{-1})$
$(5p)^5(6p)$	1,3	$2p_8$/78403	−2.34	−0.127		3/2	−0.0498	0.0042
						5/2	−0.0290	−0.0011
						7/2	0	−0.0036
						9/2	0.0373	0.0018
	1,2	$2p_3$/89163	−0.118	0.181		1/2	−0.0909	−0.0005
						3/2	−0.0607	0
						5/2	−0.0101	0.0004
						7/2	0.0606	−0.0002
	2,2	$2p_6$/79212	0.224	−0.053		1/2	−0.0381	0.0005
						3/2	−0.0254	0
						5/2	−0.0042	−0.0004
						7/2	0.0254	0.0002
	3,2	$2p_9$/78120	3.231	0.053		1/2	−0.0576	0.0063
						3/2	−0.0384	0
						5/2	−0.0064	−0.0045
						7/2	0.0384	−0.0018
	1,1	$2p_2$/89279	0.329	−0.153		1/2	0.0425	−0.0006
						3/2	0.0170	0.0005
						5/2	−0.0255	−0.0001
	2,1	$2p_4$/88380	−0.0304	−0.0421		1/2	−0.1027	−0.00002
						3/2	−0.0411	0.00001
						5/2	0.0616	−0.000003
	3,1	$2p_7$/78957	−0.211	0.181		1/2	−0.0284	0.0005
						3/2	−0.0114	−0.0004
						5/2	0.0171	0.0001
	4,1	$2p_{10}$/77270	−0.819	−0.0255		1/2	−0.0358	0.0010
						3/2	−0.0143	−0.0008
						5/2	0.0215	0.0002
	1,0	$2p_1$/89861	0	0		3/2	0	0
	2,0	$2p_5$/80119	0	0		3/2	0	0

Table (11a) continued

$(5p)^5$	1,4 $3d_4'$/80197	1.86	0.0094	5/2	−0.0446	0.00368
(5d+6s)				7/2	−0.0237	−0.00147
				9/2	0.0030	−0.00328
				11/2	0.0357	0.00187
	1,3 $3s_1'''$/91747	0.191	−0.0118	3/2	−0.0781	−0.00039
				5/2	−0.0455	0.00010
				7/2	0	0.00032
				9/2	0.0586	−0.00016
	2,3 $3d_1'$/82431	−0.250	−0.0034	3/2	−0.0330	0.00048
				5/2	−0.0192	−0.00012
				7/2	0	−0.00040
				9/2	0.0247	0.00020
	3,3 $3d_4$/80971	−1.69	−0.0114	3/2	−0.0436	0.00325
				5/2	−0.0254	−0.00081
				7/2	0	−0.00271
				9/2	0.0327	0.00135
	1,2 $3s_1''''$/91448	−0.332	0.012 −0.00004	1/2	0.0528	−0.00068
				3/2	0.0351	0
				5/2	0.0059	0.00048
				7/2	−0.0352	−0.00019
	2,2 $3s_1''$/91153	−0.375	0.013 0.000001	1/2	−0.0854	−0.0008
				3/2	−0.0569	0
				5/2	−0.0095	0.0008
				7/2	0.0569	−0.0002
	3,2 3d''/81926	−0.062	0.0053 −0.00002	1/2	−0.0319	0.00013
				3/2	−0.0212	0
				5/2	−0.0035	0.00010
				7/2	0.0212	−0.00004
	4,2 $3d_3$/80323	−1.58	−0.0003 0.0008	1/2	−0.0088	−0.0031
				3/2	−0.0058	0
				5/2	−0.0010	0.0022
				7/2	0.0058	−0.0009

Table (11a) continued (2)

5,2	$1s_5$/67068	3.31	0.00003	−0.0007	1/2	−0.0767	0.0065
					3/2	−0.0512	0
					5/2	−0.0085	−0.0047
					7/2	0.0512	0.0019
1,1	$3s_1'$/93619	−0.086	−0.013	0.0003	1/2	0.0481	−0.000095
					3/2	0.0193	−0.000076
					5/2	−0.0288	0.000019
2,1	$3d_2$/83890	0.410	−0.012	0.0002	1/2	0.0162	−0.00055
					3/2	0.0065	0.00043
					5/2	−0.0097	−0.00011
3,1	$3d_2$/79987	1.68	0.0096	0.0005	1/2	−0.0334	−0.00216
					3/2	−0.0135	0.00172
					5/2	0.0200	−0.00043
4,1	$1s_2$/77186	−0.675	0.0024	−0.0007	1/2	−0.0995	0.00087
					3/2	−0.0398	0.00070
					5/2	0.0597	0.00017
5,1	$1s_4$/68046	−2.79	0.00005	−0.0003	1/2	−0.0346	0.0036
					3/2	−0.0138	−0.0027
					5/2	0.0207	0.00072
1,0	$3d_6$/79772	0	0		3/2	0	
2,0	$1s_3$/76197	0	0		3/2	0	

Table (11b) Comparison of Calculated A_{iJ} and B_{iJ} Values with Measurements

Mass	I	config	i,J	$A_{iJ}(mK)_{calc}$	$A_{iJ}(mK)_{exp}$	$B_{iJ}(mK)_{calc}$	$B_{iJ}(mK)_{exp}$
131	3/2	$(5p)^5 6p$	1,3	8.30		−0.059	
			1,2	20.2		−0.014	
			2,2	8.48	8.83	0.013	0.020
			3,2	12.8	13.31	0.149	0.17
			1,1	−17.0		−0.062	−0.02±0.025*
			2,1	41.1		−0.0015	−0.10±0.025*
			3,1	11.4	12.96	0.051	0.16±0.06*
			4,1	14.3	13.99	0.101	0.14±0.025*
			1,0				
			2,0				
131	3/2	$(5p)^5 5d$	1,4	5.95		0.0334	
			1,3	13.0		−0.0054	
			2,3	5.50		0.0066	
			3,3	7.27		0.0452	
			1,2	−11.7		−0.016	
			2,2	19.0		−0.014	
			3,2	7.08	8.18	−0.0032	−0.027±0.010
			4,2	1.95(1.91)	−0.04	−0.074	−0.058
			5,2	17.1 (11.6)		0.155	
			1,1	−19.3		0.010	
			2,1	−6.48(6.50)		−0.0545	
			3,1	13.35(11.02)	23.89	−0.216	−0.14±0.08
			4,1	39.8 (31.4)	57.12*	0.087	0.13±0.025*
			5,1	13.8 (19.1)		0.360	0.36±0.075*

* Values obtained from Ref.(17)

Again the calculations include both 6s–5d CI and the Fermi contact term. Results with the Fermi contact term neglected are shown in parenthesis. Again the calculated effect of the Fermi contact term appears to be underestimated, possibly showing the need for a relativistic calculation of

the 6s charge density at the nucleus. These effects are not important for the levels involved in lasing transitions in high pressure Xe, and the calculated A_{iJ} and B_{iJ} values are used to determine hyperfine splitting in the radiative transitions.

6) Radiative Transition Rates between Hyperfine Terms with no Magnetic Field

The quantity we wish to calculate here is

$$D(l_2,iJIFM_F;l_3,i'J'IF'M_{F'}) = \sum_{M_F,M_{F'}} |\langle l_2,iJIFM_F|\vec{r}|i'J'IF'M_{F'}\rangle|^2/(2F+1). \tag{18a}$$

In a later section an expression is obtained for the radiative transition rate including both Zeeman and hyperfine splitting. For the present I use the limit of that expression when the magnetic field is zero, i.e.

$$D(l_2,iJIFM_F;l_3,i'J'IF'M_{F'}) = S(iJ,i'J')\,(2J+1)\,(2F'+1)\,\begin{Bmatrix} I & F' & J' \\ 1 & J & F \end{Bmatrix}^2, \tag{18b}$$

where S(iJ,i'J') is the line strength for a transition from iJ to i'J', defined in eq.(14b). Note that if one multiplies eq.(18b) by (2F + 1), then sums over F' and sums over F, to remove the hyperfine structure, one has

$$\begin{aligned} \bar{D} &= 1/[(2J+1)(2I+1)] \sum_F \sum_{F'} S(iJ,i'J')\,(2J+1)\,(2F'+1)\,(2F+1)\,\begin{Bmatrix} I & F' & J' \\ 1 & J & F \end{Bmatrix}^2 \\ &= 1/[(2J+1)(2I+1)]\; S(iJ,i'J')\,(2J+1) \sum_{F'} (2F'+1) \sum_F (2F+1)\,\begin{Bmatrix} I & F' & J' \\ 1 & J & F \end{Bmatrix}^2 \\ &= 1/(2I+1)\; S(iJ,i'J') \sum_{F'} (2F'+1)\; 1/(2J'+1) = S(iJ,i'J'), \end{aligned} \tag{18c}$$

which is as one expects. For various hyperfine transitions the energy shift and emission cross sections are listed in Table (12a) for Xe(129) and in Table (12b) for Xe(131).

Table (12a) Emission Cross Sections for Xe(129)

5d Term	5p Term	λ(μ)	F	F'	ΔE(mK)	$\sigma(10^{-12}cm^2)$	F'	ΔE(mK)	$\sigma(10^{-12}cm^2)$
1,4	1,3	5.571	9/2	7/2	1.9	90.3			
			7/2	7/2	92.1	3.2	5/2	-5.8	87.1
1,3	3,2	0.7338	7/2	5/2	-22.6	0.0179			
			5/2	5/2	131.	0.0012	3/2	23.0	0.0167
1,3	1,3	0.7495	7/2	7/2	-23.8	0.116	5/2	-12.2	0.004
			5/2	7/2	130.	0.006	5/2	31.8	0.114
1,3	2,2	0.7978	7/2	5/2	-37.2	0.0058			
			5/2	5/2	116.	0.0004	3/2	44.9	0.0054
1,3	1,2	3.864	7/2	5/2	2.4	90.2			
			5/2	5/2	156.	6.0	3/2	-14.5	84.2
2,3	3,2	2.320	7/2	5/2	15.4	7.66			
			5/2	5/2	80.2	0.51	3/2	-27.7	7.15
2,3	1,3	2.483	7/2	7/2	14.2	27.4	5/2	-83.7	1.01
			5/2	7/2	79.0	1.36	5/2	-18.9	27.1
2,3	2,2	3.107	7/2	5/2	0.80	54.1			
			5/2	5/2	65.6	3.61	3/2	-5.8	50.5
3,3	3,2	3.508	7/2	5/2	6.4	72.0			
			5/2	5/2	92.1	4.8	3/2	-15.7	67.2
3,3	1,3	3.897	7/2	7/2	5.2	1.48	5/2	-92.7	0.055
			5/2	7/2	91.0	0.073	5/2	-6.9	1.46
3,3	2,2	5.69	7/2	5/2	-8.2	16.8			
			5/2	5/2	77.6	1.12	3/2	6.1	15.6
1,2	4,1	0.7053	5/2	3/2	63.6	0.576			
			3/2	3/2	-35.1	0.096	1/2	-107.	0.480
1,2	3,2	0.7503	5/2	5/2	82.7	0.0849	3/2	-25.2	0.0061
			3/2	5/2	-16.1	0.0091	3/2	-124.	0.0819
1,2	1,3	0.7666	5/2	7/2	81.5	0.0525	5/2	-16.4	0.0026
			3/2				5/2	-115.	0.0551
1,2	3,1	0.8006	5/2	3/2	58.7	0.574			
			3/2	3/2	-40.0	0.096	1/2	-97.6	0.479
1,2	2,2	0.8173	5/2	5/2	68.1	0.591	3/2	-3.4	0.042
			3/2	5/2	-30.7	0.063	3/2	-102.	0.570
1,2	2,1	3.258	5/2	3/2	109.	0.152			
			3/2	3/2	0.01	0.025	1/2	-198.	0.127

Table (12a) continued (1)

1,2	1,1	4.610	5/2	3/2	11.0	76.8			
			3/2	3/2	-87.9	12.8	1/2	-2.0	64.0
1,2	1,2	4.373	5/2	5/2	108.	10.6	3/2	-62.7	7.56
			3/2	5/2	0.009	1.13	3/2	-162.	10.2
2,2	4,1	0.7208	5/2	3/2	-39.8	0.121			
			3/2	3/2	120.	0.020	1/2	47.7	0.101
2,2	3,2	0.7673	5/2	5/2	-20.8	0.0645	3/2	-129.	0.0046
			3/2	5/2	139.	0.0069	3/2	31.1	0.0622
2,2	1,3	0.7843	5/2	7/2	-22.0	0.00489	5/2	-120.	0.00024
			3/2				5/2	40.0	0.00513
2,2	3,1	0.8199	5/2	3/2	-44.8	0.161			
			3/2	3/2	115.	0.027	1/2	57.6	0.134
2,2	2,2	0.8375	5/2	5/2	-35.4	0.0063	3/2	-107.	0.0004
			3/2	5/2	124.5	0.0007	3/2	53.1	0.0060
2,2	2,1	3.605	5/2	3/2	5.3	76.5			
			3/2	3/2	165.	12.7	1/2	-42.6	63.8
2,2	1,1	5.336	5/2	3/2	-92.6	2.53			
			3/2	3/2	67.3	0.42	1/2	153.	2.11
2,2	1,2	5.023	5/2	5/2	42.1	10.17	3/2	-166.	0.72
			3/2	5/2	164.	1.09	3/2	-6.3	9.81
2,2	4,1	2.148	5/2	3/2	0.0002	1.04			
			3/2	3/2	59.9	0.173	3/2	-12.4	0.866
3,2	3,2	2.627	5/2	5/2	19.3	28.1	3/2	-88.6	2.00
			3/2	5/2	79.0	3.00	3/2	-28.9	27.1
3,2	1,3	2.839	5/2	7/2	18.1	1.495	5/2	-79.8	0.075
			3/2				5/2	-20.2	1.57
3,2	3,1	3.368	5/2	3/2	-46.9	56.1			
			3/2	3/2	55.0	9.35	1/2	-2.6	46.7
3,2	2,2	3.685	5/2	5/2	4.72	0.292	3/2	-66.7	0.021
			3/2	5/2	64.4	0.031	3/2	-7.1	0.281
4,2	4,1	3.275	5/2	3/2	17.5	31.9			
			3/2	3/2	34.0	5.32	1/2	-38.4	26.6
4,2	3,2	4.54	5/2	5/2	36.6	2.77	3/2	-71.2	0.20
			3/2	5/2	53.0	0.30	3/2	-54.9	2.69

Table (12a) continued (2)

4,2	1,3	5.21	5/2	7/2	35.4	4.16	5/2	−62.5	0.21
			3/2				5/2	−46.1	4.36
4,2	3,1	7.32	5/2	3/2	12.6	8.72			
			3/2	3/2	29.0	1.45	1/2	−28.5	7.27
4,2	2,2	9.00	5/2	5/2	22.0	38.1	3/2	−49.4	2.72
			3/2	5/2	38.4	4.08	3/2	−33.0	36.7
1,1	4,1	0.6117	3/2	3/2	56.6	0.369	1/2	−15.8	0.074
			1/2	3/2	−40.8	0.147	1/2	−113.	0.295
1,1	3,2	0.6452	3/2	5/2	75.6	0.00514	3/2	−32.3	0.00057
			1/2				3/2	−139.	0.00571
1,1	3,1	0.6820	3/2	3/2	51.6	0.325	1/2	−5.9	0.065
			1/2	3/2	−45.7	0.130	1/2	−103.	0.260
1,1	2,2	0.6941	3/2	5/2	61.0	0.0870	3/2	−10.4	0.0097
			1/2				3/2	−108.	0.0966
1,1	2,0	0.7407	3/2	1/2	32.5	0.106			
			1/2	1/2	−64.9	0.106			
1,1	2,1	1.908	3/2	3/2	102.	19.1	1/2	−106.	3.8
			1/2	3/2	4.3	7.6	1/2	−203.	15.3
1,1	1,1	2.304	3/2	3/2	3.8	13.2	1/2	89.7	2.65
			1/2	3/2	−93.5	5.3	1/2	−7.7	10.6
1,1	1,2	2.244	3/2	5/2	101.	1.71	3/2	−69.8	0.19
			1/2				3/2	−167.	1.90
1,1	1,0	2.660	3/2	1/2	32.5	48.7			
			1/2	1/2	−64.9	48.7			
2,1	4,1	1.511	3/2	3/2	35.0	0.00194	1/2	−37.3	0.00039
			1/2	3/2	2.2	0.00078	1/2	−70.0	0.00155
2,1	3,2	1.733	3/2	5/2	54.1	4.39	3/2	−53.8	0.49
			1/2				3/2	−86.6	4.87
2,1	3,1	2.027	3/2	3/2	30.1	25.1	1/2	−27.4	5.01
			1/2	3/2	−2.7	10.0	1/2	−60.2	20.1
2,1	2,2	2.138	3/2	5/2	39.5	0.137	3/2	−32.0	0.015
			1/2				3/2	−64.7	0.153
2,1	2,0	2.652	3/2	1/2	10.9	55.5			
			1/2	1/2	−21.8	55.5			

Table (12a) continued (3)

3,1	4,1	3.68	3/2	3/2	1.6	34.4	1/2	−70.7	6.87

			1/2	3/2	69.1	13.7	1/2	-3.2	27.5
3,1	3,2	5.36	3/2	5/2	20.6	0.777	3/2	-87.3	0.086
			1/2				3/2	-19.7	0.863
3,1	3,1	9.71	3/2	3/2	-3.3	10.8	1/2	-60.9	2.16
			1/2	3/2	64.2	4.33	1/2	6.7	8.65
3,1	2,2	12.90	3/2	5/2	60.8	34.4	3/2	-65.4	3.8
			1/2				3/2	2.1	38.2
1,0	4,1	4.00	1/2	3/2	24.1	45.6	1/2	-48.2	22.8
1,0	3,1	12.25	1/2	3/2	19.2	4.99	1/2	-38.4	2.49

Table (12b) Emission Cross Sections in $10^{-12}cm^2$ for Xe(131)

5d Term	5p Term	λ(μ)	F	F'	ΔE(mK)	σ	F'	ΔE(mK)	σ	F'	ΔE(mK)	σ
1,4	1,3	5.571	11/2	9/2	-1.6	90.3						
			9/2	9/2	-39.4	7.5	7/2	3.3	82.8			
			7/2	9/2	-64.4	0.27	7/2	-21.7	12.3	5/2	4.9	77.8
			5/2	7/2	-37.4	0.46	5/2	-10.8	12.4	3/2	4.6	77.4
1,3	3,2	0.7338	9/2	7/2	18.2	0.018						
			7/2	7/2	-39.9	0.003	5/2	11.2	0.015			
			5/2	7/2	-85.6	0.000	5/2	-34.6	0.004	3/2	-7.0	0.013
			3/2	5/2	-67.6	0.000	3/2	-40.1	0.005	1/2	-27.1	0.013
1,3	1,3	0.7495	9/2	9/2	19.3	0.110	7/2	61.9	0.010			
			7/2	9/2	-38.8	0.013	7/2	-3.9	0.092	5/2	30.4	0.016
			5/2	7/2	-41.9	0.021	5/2	-15.3	0.083	3/2	0.000	0.016
			3/2	5/2	-48.3	0.024	3/2	-32.9	0.096			
1,3	2,2	0.7978	9/2	7/2	32.8	0.006						
			7/2	7/2	-25.3	0.001	5/2	5.0	0.005			
			5/2	7/2	-71.0	0.000	5/2	-40.8	0.001	3/2	20.0	0.004
			3/2	5/2	-73.8	0.000	3/2	-53.0	0.002	1/2	-40.9	0.004
1,3	1,2	3.864	9/2	7/2	-2.1	90.2						
			7/2	7/2	-60.2	12.9	5/2	100.2	77.3			
			5/2	7/2	-106.	0.86	5/2	-35.8	22.0	3/2	15.2	67.3
			3/2	5/2	-68.8	1.8	3/2	-17.8	25.3	1/2	13.1	63.1
2,3	3,2	2.320	9/2	7/2	-15.3	7.66						
			7/2	7/2	-40.6	1.09	5/2	10.5	6.57			
			5/2	7/2	-59.5	0.072	5/2	-8.5	1.87	3/2	19.1	5.72
			3/2	5/2	-21.6	0.15	3/2	5.9	2.14	1/2	18.8	5.36
2,3	1,3	2.483	9/2	9/2	-14.2	26.1	7/2	28.5	2.3			
			7/2	9/2	-39.5	3.0	7/2	3.2	21.7	5/2	29.7	3.8
			5/2	7/2	-15.8	5.08	5/2	10.8	19.6	3/2	26.2	3.8
			3/2	5/2	-2.4	5.69	3/2	13.0	22.8			
2,3	2,2	3.107	9/2	7/2	-0.001	54.1						
			7/2	7/2	-26.0	7.7	5/2	4.2	46.4			
			5/2	7/2	-44.9	0.52	5/2	-14.7	13.2	3/2	6.1	40.4
			3/2	5/2	-27.9	1.1	3/2	-7.1	15.2	1/2	5.1	37.9
3,3	3,2	3.508	9/2	7/2	- 6.1	72.0						
			7/2	7/2	-42.9	10.3	5/2	8.2	61.7			

Table (12b) continued (1)

			5/2	7/2	-15.4	17.6	5/2	12.1	53.8	3/2	-66.4	0.69
			3/2	5/2	- 2.0	20.2	3/2	11.0	50.4	1/2	-29.5	1.4
3,3	1,3	3.897	9/2	9/2	- 5.1	1.41	7/2	37.6	0.13			
			7/2	9/2	-41.8	0.16	7/2	0.001	1.17	5/2	27.4	0.21
			5/2	7/2	-22.7	0.27	5/2	3.9	1.06	3/2	19.3	0.20
			3/2	5/2	-10.2	0.31	3/2	5.2	1.23			
3,3	2,2	5.69	9/2	7/2	8.5	16.8						
			7/2	7/2	-28.3	2.4	5/2	1.9	14.4			
			5/2	7/2	-51.8	0.16	5/2	-21.6	4.1	3/2	0.001	12.5
			3/2	5/2	-35.7	0.34	3/2	-14.9	4.7	1/2	- 2.8	11.7
1,2	4,1	0.7053	7/2	5/2	-57.0	0.576						
			5/2	5/2	-15.3	0.173	3/2	21.5	0.403			
			3/2	5/2	13.5	0.029	3/2	50.3	0.307	1/2	70.0	0.240
			1/2	3/2	67.2	0.096	1/2	86.8	0.480			
1,2	3,2	0.7503	7/2	7/2	-75.6	0.078	5/2	-24.5	0.013			
			5/2	7/2	-33.8	0.017	5/2	17.2	0.052	3/2	44.7	0.021
			3/2	5/2	46.0	0.032	3/2	73.6	0.036	1/2	86.5	0.023
			1/2	3/2	90.5	0.046	1/2	103.	0.046			
1,2	1,3	0.7666	7/2	9/2	-74.5	0.049	7/2	-31.8	0.006	5/2	-5.2	0.000
			5/2	7/2	9.9	0.045	5/2	36.5	0.010	3/2	51.9	0.001
			3/2	5/2	65.2	0.044	3/2	80.7	0.011			
			1/2	3/2	97.6	0.055						
1,2	3,1	0.8006	7/2	5/2	-52.5	0.574						
			5/2	5/2	-10.8	0.172	3/2	18.1	0.402			
			3/2	5/2	18.0	0.029	3/2	47.0	0.306	1/2	63.1	0.239
			1/2	3/2	63.9	0.095	1/2	8.0	0.478			
1,2	2,2	0.8173	7/2	7/2	-61.0	0.543	7/2	-30.7	0.090			
			5/2	7/2	-19.2	0.120	5/2	11.0	0.365	3/2	31.8	0.148
			3/2	5/2	39.8	0.221	3/2	60.6	0.253	1/2	72.8	0.158
			1/2	3/2	77.5	0.317	1/2	89.7	0.317			
1,2	2,1	3.258	7/2	5/2	-97.0	0.153						
			5/2	5/2	-55.3	0.046	3/2	47.4	0.107			
			3/2	5/2	-26.5	0.008	3/2	76.2	0.081	1/2	138.	0.064
			1/2	3/2	93.1	0.025	1/2	155.	0.127			

Table (12b) continued (2)

1,2	1,1	4.610	7/2	5/2	-9.8	76.8						
			5/2	5/2	31.9	23.0	3/2	-11.1	53.7			
			3/2	5/2	60.8	3.84	3/2	17.7	40.9	1/2	-6.7	32.0
			1/2	3/2	34.6	12.8	1/2	10.2	64.0			
1,2	1,2	4.373	7/2	7/2	-95.9	9.72	5/2	-25.7	1.62			
			5/2	7/2	-54.1	2.16	5/2	16.0	6.53	3/2	67.0	2.65
			3/2	5/2	44.9	3.97	3/2	95.8	4.54	1/2	127.	2.84
			1/2	3/2	113.	5.67	1/2	144.	5.67			
2,2	4,1	0.7208	7/2	5/2	35.0	0.121						
			5/2	5/2	-30.6	0.036	3/2	6.2	0.085			
			3/2	5/2	-78.6	0.006	3/2	-41.8	0.065	1/2	-22.2	0.050
			1/2	3/2	-71.0	0.020	1/2	-51.4	0.101			
2,2	3,2	0.7673	7/2	7/2	16.5	0.059	7/2	67.6	0.010			
			5/2	7/2	-49.1	0.013	5/2	19.4	0.040	3/2	29.5	0.016
			3/2	5/2	-46.0	0.024	3/2	-18.5	0.028	1/2	-5.6	0.017
			1/2	3/2	-47.7	0.035	1/2	-34.8	0.035			
2,2	1,3	0.7843	7/2	9/2	17.6	0.005	7/2	60.3	0.001	5/2	86.8	0.000
			5/2	7/2	-53.8	0.004	5/2	21.1	0.001	3/2	36.6	0.000
			3/2	5/2	-26.8	0.004	3/2	-11.3	0.001			
			1/2	3/2	-40.6	0.005						
2,2	3,1	0.8199	7/2	5/2	39.5	0.161						
			5/2	5/2	-26.1	0.048	3/2	2.8	0.113			
			3/2	5/2	-74.1	0.008	3/2	-45.1	0.086	1/2	-29.0	0.067
			1/2	3/2	-74.4	0.027	1/2	-58.2	0.134			
2,2	2,2	0.8375	7/2	7/2	31.1	0.006	5/2	61.3	0.001			
			5/2	7/2	-34.5	0.001	5/2	- 4.3	0.004	3/2	16.5	0.002
			3/2	5/2	-52.3	0.002	3/2	-31.5	0.003	1/2	-19.3	0.002
			1/2	3/2	-60.7	0.003	1/2	-48.5	0.003			
2,2	2,1	3.605	7/2	5/2	- 4.9	76.5						
			5/2	5/2	-70.6	23.0	3/2	32.1	53.6			
			3/2	5/2	-119.	3.8	3/2	-15.8	40.8	1/2	45.8	31.9
			1/2	3/2	-45.1	12.8	1/2	16.6	63.8			
2,2	1,1	5.336	7/2	5/2	82.3	2.53						
			5/2	5/2	16.7	0.76	3/2	-26.4	1.77			

Table (12b) continued (3)

			3/2	5/2	-31.3	0.13	3/2	-74.3	1.35	1/2	-98.8	1.05
			1/2	3/2	-104.	0.42	1/2	-128.	2.11			
2,2	1,2	5.023	7/2	7/2	- 3.8	9.34	5/2	66.4	1.56			
			5/2	7/2	-69.4	2.08	5/2	0.001	6.28	3/2	51.7	2.54
			3/2	5/2	-47.2	3.81	3/2	3.7	4.36	1/2	34.7	2.72
			1/2	3/2	-25.5	5.45	1/2	5.4	5.45			
3,2	4,1	2.148	7/2	5/2	0.001	1.04						
			5/2	5/2	-25.1	0.312	3/2	11.7	0.727			
			3/2	5/2	-42.9	0.052	3/2	-6.1	0.554	1/2	13.5	0.433
			1/2	3/2	-16.9	0.173	1/2	2.7	0.866			
3,2	3,2	2.627	7/2	7/2	-19.0	25.8	5/2	32.1	4.3			
			5/2	7/2	-43.6	5.7	5/2	7.4	17.3	3/2	35.0	7.0
			3/2	5/2	-10.4	10.5	3/2	17.1	12.0	1/2	30.1	7.5
			1/2	3/2	6.4	15.0	1/2	19.3	15.0			
3,2	1,3	2.839	7/2	9/2	-17.9	1.40	7/2	24.8	0.160	5/2	51.3	0.008
			5/2	7/2	0.000	1.28	5/2	26.7	0.27	3/2	42.1	0.015
			3/2	5/2	8.9	1.26	3/2	24.3	0.31			
			1/2	3/2	13.5	1.57						
3,2	3,1	3.368	7/2	5/2	4.0	56.1						
			5/2	5/2	-20.6	16.8	3/2	8.3	39.3			
			3/2	5/2	-38.4	2.8	3/2	-9.5	29.9	1/2	6.7	23.4
			1/2	3/2	-20.2	9.35	1/2	-4.1	46.7			
3,2	2,2	3.685	7/2	7/2	- 4.4	0.268	5/2	25.8	0.045			
			5/2	7/2	-29.0	0.059	5/2	1.2	0.180	3/2	22.0	0.073
			3/2	5/2	-16.6	0.109	3/2	4.2	0.125	1/2	16.4	0.078
			1/2	3/2	- 6.6	0.156	1/2	5.6	0.156			
4,2	4,1	3.275	7/2	5/2	-16.7	31.9						
			5/2	5/2	-20.4	9.6	3/2	16.4	22.4			
			3/2	5/2	-27.5	1.6	3/2	9.3	17.0	1/2	28.9	13.3
			1/2	3/2	3.2	5.32	1/2	22.8	26.6			
4,2	3,2	4.54	7/2	7/2	-35.2	2.56	5/2	15.8	0.43			
			5/2	7/2	-39.0	0.57	5/2	12.1	1.72	3/2	39.7	0.70
			3/2	5/2	5.0	1.05	3/2	32.6	1.19	1/2	45.5	0.75
			1/2	3/2	26.5	1.49	1/2	39.4	1.49			

Table (12b) continued (4)

4,2	1,3	5.21	7/2	9/2	-34.2	3.90	7/2	8.5	0.44	5/2	35.1	0.022
			5/2	7/2	4.8	3.56	5/2	31.4	0.76	3/2	46.8	0.042
			3/2	5/2	24.3	3.49	3/2	39.7	0.87			
			1/2	3/2	33.6	4.36						
4,2	3,1	7.32	7/2	5/2	-12.2	8.72						
			5/2	5/2	-15.9	2.62	3/2	13.0	6.11			
			3/2	5/2	-23.0	0.44	3/2	5.9	4.65	1/2	22.1	3.63
			1/2	3/2	0.000	1.45	1/2	16.0	7.27			
4,2	2,2	9.00	7/2	7/2	-20.6	35.0	5/2	9.6	5.8			
			5/2	7/2	-24.3	7.8	5/2	5.9	23.5	3/2	27.0	9.5
			3/2	5/2	- 1.2	14.3	3/2	19.6	16.3	1/2	31.8	10.2
			1/2	3/2	13.5	20.4	1/2	25.7	20.4			
1,1	4,1	0.6117	5/2	5/2	-50.5	0.310	3/2	-13.7	0.133			
			3/2	5/2	- 2.5	0.199	3/2	34.3	0.059	1/2	53.9	0.184
			1/2	3/2	63.4	0.368	1/2	83.0	0.074			
1,1	3,2	0.6452	5/2	7/2	-69.1	0.005	5/2	-18.0	0.001	3/2	9.5	0.000
			3/2	5/2	30.1	0.004	3/2	57.6	0.008	1/2	70.5	0.000
			1/2	3/2	86.6	0.003	1/2	99.6	0.003			
1,1	3,1	0.6820	5/2	5/2	-46.0	0.274	3/2	-17.1	0.117			
			3/2	5/2	2.0	0.176	3/2	31.0	0.052	1/2	47.1	0.163
			1/2	3/2	60.0	0.325	1/2	76.2	0.065			
1,1	2,2	0.6941	5/2	7/2	-54.5	0.077	5/2	-24.2	0.017	3/2	-3.4	0.002
			3/2	5/2	23.8	0.061	3/2	44.6	0.031	1/2	56.8	0.005
			1/2	3/2	73.7	0.048	1/2	85.8	0.048			
1,1	2,0	0.7407	5/2	3/2	-28.9	0.106						
			3/2	3/2	19.2	0.106						
			1/2	3/2	48.2	0.106						
1,1	2,1	1.908	5/2	5/2	-90.5	16.0	3/2	12.2	6.87			
			3/2	5/2	-42.5	10.3	3/2	60.3	3.05	1/2	122.	9.54
			1/2	3/2	89.3	19.1	1/2	151.	3.81			
1,1	1,1	2.304	5/2	5/2	- 3.2	11.1	3/2	-46.3	4.77			
			3/2	5/2	44.8	7.15	3/2	1.7	2.12	1/2	-22.7	6.62
			1/2	3/2	30.8	13.2	1/2	64.0	2.65			

Table (12b) continued (5)

1,1	1,2	2.244	5/2	7/2	-89.4	1.52	5/2	-19.2	0.341	3/2	31.8	0.038
			3/2	5/2	28.9	1.19	3/2	79.8	0.607	1/2	111.	0.095
			1/2	3/2	109.	0.948	1/2	140.	0.948			
1,1	1,0	2.660	5/2	3/2	-28.9	48.7						
			3/2	3/2	19.2	48.7						
			1/2	3/2	48.2	48.7						
2,1	4,1	1.511	5/2	5/2	-31.5	0.002	3/2	5.3	0.001			
			3/2	5/2	-14.7	0.001	3/2	22.0	0.000	1/2	41.7	0.001
			1/2	3/2	30.8	0.002	1/2	50.4	0.000			
2,1	3,2	1.733	5/2	7/2	-50.0	3.90	5/2	1.1	0.88	3/2	28.6	0.097
			3/2	5/2	17.8	3.07	3/2	45.3	1.56	1/2	58.3	0.243
			1/2	3/2	54.1	2.44	1/2	67.0	2.44			
2,1	3,1	2.027	5/2	5/2	-27.0	21.1	3/2	2.0	9.03			
			3/2	5/2	-10.3	13.5	3/2	18.7	4.01	1/2	34.9	12.5
			1/2	3/2	27.4	25.1	1/2	43.6	5.01			
2,1	2,2	2.138	5/2	7/2	-35.4	0.122	5/2	- 5.2	0.027	3/2	15.6	0.003
			3/2	5/2	11.5	0.096	3/2	32.3	0.049	1/2	44.5	0.008
			1/2	3/2	41.1	0.076	1/2	53.3	0.076			
2,1	2,0	2.652	5/2	3/2	- 9.8	55.5						
			3/2	3/2	6.9	55.5						
			1/2	3/2	15.7	55.5						
3,1	4,1	3.68	5/2	5/2	- 2.1	28.9	3/2	34.7	12.4			
			3/2	5/2	-33.3	18.6	3/2	3.5	5.50	1/2	23.1	17.2
			1/2	3/2	-20.4	34.4	1/2	-0.001	6.87			
3,1	3,2	5.36	5/2	7/2	-20.6	0.69	5/2	30.5	0.155	3/2	58.0	0.017
			3/2	5/2	-0.001	0.54	3/2	26.8	0.28	1/2	39.7	0.043
			1/2	3/2	2.9	0.43	1/2	15.8	0.43			
3,1	3,1	9.71	5/2	5/2	2.4	9.09	3/2	31.4	3.89			
			3/2	5/2	-28.8	5.84	3/2	0.000	1.73	1/2	16.3	5.41
			1/2	3/2	-23.8	10.8	1/2	- 7.6	2.16			
3,1	2,2	12.90	5/2	7/2	- 6.0	30.6	5/2	24.2	6.88	3/2	45.0	0.76
			3/2	5/2	- 7.0	24.1	3/2	13.8	12.2	1/2	26.0	1.91
			1/2	3/2	-10.1	19.1	1/2	2.1	19.1			
1,0	4,1	4.00	3/2	5/2	-21.7	34.2	3/2	15.1	22.8	1/2	34.7	11.4
1,0	3,1	12.25	3/2	5/2	-17.2	3.74	3/2	11.8	2.49	1/2	27.9	1.25

7) The Hyperfine Splitting with an External Magnetic Field

We now want to calculate the Zeeman splitting with wavefunctions

$$|iJIFM_F\rangle = \sum_{M,M_I} C(JIF,MM_IM_F)\ |iJM\rangle\ |IM_I\rangle. \tag{19a}$$

But this is

$$\langle iJIFM_F|H_Z|iJIF'M_F'\rangle = \sum_{M,M_I}\sum_{M',M_I'} \delta_{M_IM_I'} C(JIF,MM_IM_F)C(JIF',MM_IM_F')\langle iJM|H_Z|iJM'\rangle. \tag{19b}$$

But as shown at the end of sec.(3)

$$\langle iJM|H_Z|iJM'\rangle = \beta H\ g_L(i,J)\ M\ \delta_{M'M}, \tag{20a}$$

so that

$$\langle iJIFM_F|H_Z|iJIF'M_F'\rangle = \beta H\ g_L(i,J) \sum_{M,M_I} M\ C(JIF,MM_IM_F)\ C(JIF',MM_IM_F'). \tag{20b}$$

In Appendix (C) I show

$$\sum_{M,M_I} M\ C(JIF,MM_IM_F)\ C(JIF',MM_IM_F') = [(2F'+1)(2J+1)J(J+1)]^{1/2}\ (-1)^{+I+1+J+F'} \begin{Bmatrix} I & F & J \\ 1 & J & F' \end{Bmatrix}\ C(F'1F,M_F'0M_F), \tag{20c}$$

so that

$$\langle iJIFM_F|H_Z|iJIF'M_F'\rangle = \beta H\ g_L(i,J)\ \delta_{M_F,M_F'}[(2F'+1)(2J+1)J(J+1)]^{1/2}\ (-1)^{+I+1+J+F'} \begin{Bmatrix} I & F & J \\ 1 & J & F' \end{Bmatrix}\ C(F'1F,M_F0M_F)$$

$$=\beta H g_L(i,J)\delta_{M_F,M_F'}[(2F'+1)(2F+1)(2J+1)J(J+1)]^{1/2}(-1)^{I+J-M_F} \begin{pmatrix} F' & 1 & F \\ M_F & 0 & -M_F \end{pmatrix} \begin{Bmatrix} I & F & J \\ 1 & J & F' \end{Bmatrix}. \tag{20d}$$

The diagonal matrix element is

$$\langle iJIFM_F|H_Z|iJIFM_F\rangle = \beta H\ g_L(i,J)\ (1/2)M_F\ [F(F+1)+J(J+1)-I(I+1)]/F(F+1), \tag{21a}$$

which, with I = 0, reduces to the diagonal matrix element for Zeeman splitting in the absence of hyperfine splitting. The non-diagonal matrix element is

$$\langle iJI(F+1)M_F|H_Z|iJIFM_F\rangle = \beta H\, g_L(i,J)\ (1/2)$$

$$\{(I+J+F+2)(J+F+1-I)(I+F+1-J)\ [(F+1)^2 - M_F^2]/[(2F+1)(2F+3)(F+1)^2]\}^{1/2}. \tag{21b}$$

For I = 1/2, one has a sequence of 1x1 and 2x2 matrices to diagonalize, and for I = 3/2 a sequence of up to 4x4 matrices. The final eigenfunctions can be written, $|iJIkM_F\rangle$, where k is an index, i.e.

$$|iJIkM_F\rangle = \sum_{F\equiv F_s}^{J+I} C_3(k;\beta H;iJIFM_F)\ |iJIFM_F\rangle$$

$$= \sum_{F\equiv F_s}^{J+I} C_3(k;\beta H;iJIFM_F) \sum_{M,M_I} C(JIF,MM_IM_F)\ |iJM\rangle\ |IM_I\rangle, \tag{22}$$

where F_s is the greater of $|M_F|$ or $|J - I|$. Therefore the number of allowed B values is $J + I + 1 - F_s$. The new energies and mixing coefficients are too extensive to tabulate entirely. In Table (13) I compare the level energies for the case of no hyperfine splitting and a 6 kG magnetic field, with that for I = 3/2 in Xe for the level (1,4). In the absence of hyperfine splitting this level is split by the Zeeman effect into 9 components labelled by M. The Zeeman splitting is shown as the first entry in Table (13). With hyperfine splitting included there are 4 hyperfine levels with F = 11/2, 9/2, 7/2, and 5/2. The magnetic field splits these 4 levels into 36 components with 12 different M_F values, from -11/2 to 11/2. But we expect these 36 components to be clustered around the 9 Zeeman components occuring when I = 0, if the Zeeman splitting dominates the hyperfine splitting. This is illustrated in Table (13) where the (k,M_F) components are ordered in energy. The entry in parenthesis is the diagonal matrix element for the initial (F,M_F) level. It is also ordered in energy. As expected, with a 6 kG field the non-diagonal matrix element is so large that all the energies are changed from their initial diagonal values, and all the mixing coefficients are significant. On the other hand, with no magnetic field, the mixing coefficients are of the form δ_{F,F_k} and one regains the eigenfunctions for the case of hyperfine splitting.

Table (13) Splitting of the (1,4) component of $(5p)^5(5d)$ in a 6 kG field without and with (I = 3/2) hyperfine splitting

M_F\	E(M=4)	E(M=3)	E(M=2)	E(M=1)	E(M=0)	E(M=−1)	E(M=−2)	E(M=−3)	E(M=−4)
	1.40	1.05	0.70	0.35	0.0	−0.35	−0.70	−1.05	−1.40
11/2	1.439								
9/2	1.413	1.079							
	(1.306)	(1.185)							
7/2	1.333	1.095	0.738						
	(1.221)	(1.016)	(0.930)						
5/2	1.271	1.035	0.760	0.410					
	(1.2111	(0.865)	(0.725)	(0.675)					
3/2		0.877	0.698	0.411	0.088				
		(0.710)	(0.509)	(0.435)	(0.420)				
1/2			0.545	0.316	0.043	−0.233			
			(0.209)	(0.165)	(0.153)	(0.145)			
−1/2				0.237	−0.062	−0.341	−0.563		
				−(0.090)	−(0.145)	−(0.203)	−(0.291)		
−3/2					−0.070	−0.419	−0.714	−0.929	
					−(0.345)	−(0.436)	−(0.559)	−(0.792)	
−5/2						−0.380	−0.758	−1.049	−1.346
						−(0.600)	−(0.726)	−(0.915)	−(1.293)
−7/2							−0.697	−1.084	−1.362
							−(0.855)	−(1.016)	−(1.271)
−9/2								−1.023	−1.393
								−(1.109)	−(1.307)
−11/2									−1.364

8) The Radiative Transition Rate with Both a 6 kG Magnetic Field and Hyperfine Splitting

The squared dipole matrix element is more complicated in this case than with zero hyperfine splitting. In this case

$$D(\ell_2,iJIkM_F;\ell_3,i'J'Ik'M_{F'}) = |\langle \ell_2,iJIkM_F|\vec{r}|\ell_3 i'J'Ik'M_{F'}\rangle|^2$$

$$= \Big|\sum_{F\equiv F_s}^{J+I}\sum_{F'\equiv F_s'}^{J'+I} C_3(k;\beta H;iJIFM_F)C_3(k';\beta H;i'J'IF'M_{F'})\langle \ell_2,iJIFM_F|\vec{r}|\ell_3,i'J'IF'M_{F'}\rangle\Big|^2$$

$$= \Big|\sum_{F\equiv F_s}^{J+I}\sum_{F'\equiv F_s'}^{J'+I} C_3(k;\beta H;iJIFM_F)\, C_3(k';\beta H;i'J'IF'M_{F'}) \sum_{M,M_I}\sum_{M} C(JIF,MM_IM_F)$$

$$C(J'IF',M'M_IM_{F'})\ \langle \ell_2,iJM|\vec{r}|\ell_3,i'J'M'\rangle\Big|^2. \tag{23a}$$

But the last matrix element is given in eqs.(11) of sec.(4), so that

$$D(l_2,iJIkM_F;l_3,i'J'Ik'M_{F'}) = \Big|\sum_{F\equiv F_s}^{J+I}\sum_{F'\equiv F_s'}^{J'+I} C_3(k;\beta H;iJIFM_F)\, C_3(k';\beta H;i'J'IF'M_{F'})$$

$$\sum_{M,M_I}\sum_{M'} C(JIF,MM_IM_F)\, C(J'IF',M'M_IM_{F'}) \sum_{j_1,j_2}\sum_{j_1',j_2'} C_1(l_2,iJ;j_1,j_2)$$

$$C_1(l_3,i'J';j_1',j_2')\,\delta_{j_1,j_1'}(A_{\ell_2,\ell_3}/2)(-1)^{\ell_3-1/2+j_1-J'}\,[(2j_2+1)(2j_2'+1)(2J+1)]^{1/2}$$

$$\begin{Bmatrix} 1/2 & j_2' & \ell_3 \\ 1 & \ell_2 & j_2 \end{Bmatrix}\begin{Bmatrix} j_1 & J' & j_2' \\ 1 & j_2 & J \end{Bmatrix}\sum_{\beta\equiv -1}^{1}(-1)^{\beta}\,\vec{a}_{\beta}\ C(F1F',M_F\beta M_{F'})\Big|^2$$

$$= (A_{\ell_2,\ell_3}/2)^2\,(2J+1)|W(\ell_2 iJ,\ell_3 i'J')|^2\Big|\sum_{F\equiv F_s}^{J+I}\sum_{F'\equiv F_s'}^{J'+I}\sum_{\beta\equiv -1}^{1}(-1)^{\beta}\,\vec{a}_{\beta}\ C_3(k;\beta H;iJIFM_F)$$

$$C_3(k';\beta H;i'J'IF'M_{F'})\sum_{M,M_I}\sum_{M'} C(JIF,MM_IM_F)\, C(J'IF',M'M_IM_{F'})\, C(J1J',M\beta M')\Big|^2, \tag{23b}$$

where W is defined in eq.(13c). The sums over M, M', and M_I, which were not present in sec.(4) are readily done leading to

$$D(\ell_2,iJIkM_F;\ell_3,i'J'Ik'M_{F'}) = (A_{\ell_2,\ell_3}/2)^2\,(2J+1)(2J'+1)\,|W(\ell_2 iJ,\ell_3 i'J')|^2$$

$$\Big|\sum_{F\equiv F_s}^{J+I}\sum_{F'\equiv F_s'}^{J'+I} C_3(k;\beta H;iJIFM_F)\, C_3(k';\beta H;i'J'IF'M_{F'})\,(-1)^{F+I}\,(2F+1)^{1/2}\begin{Bmatrix} I & F' & J' \\ 1 & J & F \end{Bmatrix}$$

$$\sum_{\beta=-1}^{1} (-1)^{\beta} \vec{a}_{\beta} \, C(F1F', M_F \beta M_{F'}) \Big|^2 .$$

(23c)

Note that the result in eq.(23c) does not depend on M and M', which were good quantum numbers for the case of Zeeman splitting with hyperfine effects neglected. As discussed in sec.(4), one can take the sum over β outside the absolute value sign and use $\vec{a}_{\beta} \cdot \vec{a}^{\,*}_{\beta'} = 4\,\delta_{\beta,\beta'}$ to arrive at

$$D(\ell_2, iJIkM_F; \ell_3, i'J'Ik'M_{F'}) = (A_{\ell_2,\ell_3})^2 \, (2J+1)(2J'+1) \, |W(\ell_2 iJ, \ell_3 i'J')|^2$$

$$Z(\ell_2 iJM_F, \ell_3 i'J'M_{F'}) = (2J+1) \; S(iJ, i'J') \;\; Z(\ell_2 iJM_F, \ell_3 i'J'M_{F'}),$$

(24a)

where S(iJ,i'J') is the level strength defined in eq.(14b), and

$$Z(\ell_2 iJkM_F, \ell_3 i'J'k'M_{F'}) = \Big| \sum_{F=F_s}^{J+I} \sum_{F'=F_s}^{J'+I} C_3(k;\beta H;iJIFM_F) \; C_3(k';\beta H;i'J'IF'M_{F'})$$

$$(-1)^{F+I} \, (2F+1)^{1/2} \begin{Bmatrix} I & F' & J' \\ 1 & J & F \end{Bmatrix} C(F1F';M_F, -M_F+M_{F'}, M_{F'}) \Big|^2 .$$

(24b)

For this case proof of sum rules requires special care. Consider the sum of eq.(24b) over final state parameters k' and M_F'. One has

$$\sum_{k', M_F'} Z(\ell_2 iJkM_F, \ell_3 i'J'k'M_{F'}) = \sum_{k', M_F'} \sum_{\beta=-1}^{1} \Big| \sum_{F=F_s}^{J+I} \sum_{F'=F_s}^{J'+I} C_3(k;\beta H;iJIFM_F)$$

$$C_3(k';\beta H;i'J'IF'M_{F'}) \; (-1)^{F+I} \, (2F+1)^{1/2} \begin{Bmatrix} I & F' & J' \\ 1 & J & F \end{Bmatrix} C(F1F';M_F, \beta, M_{F'}) \Big|^2$$

$$= \sum_{M_F} \sum_{\beta=-1}^{1} \sum_{F'=F_s}^{J'+I} \Big| \sum_{F=F_s}^{J+I} C_3(k;\beta H;iJIFM_F) (-1)^{F+I} \, (2F+1)^{1/2} \begin{Bmatrix} IF' & J' \\ 1J & F \end{Bmatrix} C(F1F';M_F, \beta, M_F') \Big|^2 .$$

(25)

Consider the sum over $M_F' = m$ and $F' = M$, which is

$$T = \sum_{m=-|J^{\Sigma}_{=}I|}^{|J-I|} \sum_{M=|J^{\Sigma}_{=}I|}^{J+I} U(M,m) + \sum_{m=|J^{\Sigma}_{=}I|+1}^{J+I} \sum_{M\overset{\Sigma}{=}m}^{J+I} U(M,m) + \sum_{m=-J^{\Sigma}_{=}I}^{-|J+I|-1} \sum_{M\overset{\Sigma}{=}|m|}^{J+I} U(M,m)$$

$$= \sum_{m=-|J^{\Sigma}_{=}I|}^{|J-I|} \sum_{M=|J^{\Sigma}_{=}I|}^{J+I} U(M,m) + \sum_{m=|J^{\Sigma}_{=}I|+1}^{J+I} \sum_{M\overset{\Sigma}{=}m}^{J+I} [U(M,m) + U(M,-m)].$$

(26a)

But interchanging the order of the summations in the second term leads to

$$T = \sum_{M=|J\pm I|}^{J+I} \sum_{m=-|J\pm I|}^{|J-I|} U(M,m) + \sum_{M=|J\pm I|+1}^{J+I} \sum_{m=|J\pm I|+1}^{M} [U(M,m) + U(M,-m)]$$

$$= \sum_{m=-|J\pm I|}^{|J-I|} U(|J-I|,m) + \sum_{M=|J\pm I|+1}^{J+I} \sum_{m\equiv -M}^{M}.$$

(26b)

Then

$$\sum_{k',M_F'} Z(\ell_2 iJkM_F, \ell_3 i'J'k'M_{F'}) = \sum_{M_F'=-|J'-I|}^{|J'-I|} \sum_{\beta\equiv -1}^{1} \Big| \sum_{F\equiv F_s}^{J+I} C_3(k;\beta H;iJIFM_F)(-1)^{F+I}$$

$$(2F+1)^{1/2} \begin{Bmatrix} I & |J'-I| & J' \\ 1 & J & F \end{Bmatrix} C(F1|J'-I|;M_F,\beta,M_F') \Big|^2 + \sum_{F'=|J'\pm I|+1}^{J'+I} \sum_{M_F'\equiv -F'}^{F'} \sum_{\beta\equiv -1}^{1}$$

$$\Big| \sum_{F\equiv F_s}^{J+I} C_3(k;\beta H;iJIFM_F)(-1)^{F+I} (2F+1)^{1/2} \begin{Bmatrix} IF'J' \\ 1J\ F \end{Bmatrix} C(F1F';M_F,\beta,M_F') \Big|^2.$$

(27a)

Now the sum over β and M_F' can be done, leading to

$$\sum_{k',M_F'} Z(\ell_2 iJkM_F, \ell_3 i'J'k'M_{F'}) = (2|J'-I|+1) \sum_{F\equiv F_s}^{J+I} |C_3(k;\beta H;iJIFM_F) \begin{Bmatrix} I & |J'-I| & J' \\ 1 & J & F \end{Bmatrix}|^2$$

$$+ \sum_{F'=|J'\pm I|+1}^{J'+I} (2F'+1) \sum_{F\equiv F_s}^{J+I} |C_3(k;\beta H;iJIFM_F) \begin{Bmatrix} I & F' & J' \\ 1 & J & F \end{Bmatrix}|^2$$

$$= \sum_{F'=|J'\pm I|}^{J'+I} (2F'+1) \sum_{F\equiv F_s}^{J+I} |C_3(k;\beta H;iJIFM_F) \begin{Bmatrix} I & F' & J' \\ 1 & J & F \end{Bmatrix}|^2$$

$$= 1/(2J+1) \sum_{F\equiv F_s}^{J+I} |C_3(k;\beta H;iJIFM_F)|^2 = 1/(2J+1),$$

(27b)

so that

$$\sum_{k',M_F'} D(\ell_2, iJIkM_F; \ell_3, i'J'Ik'M_{F'}) = S(iJ, i'J').$$

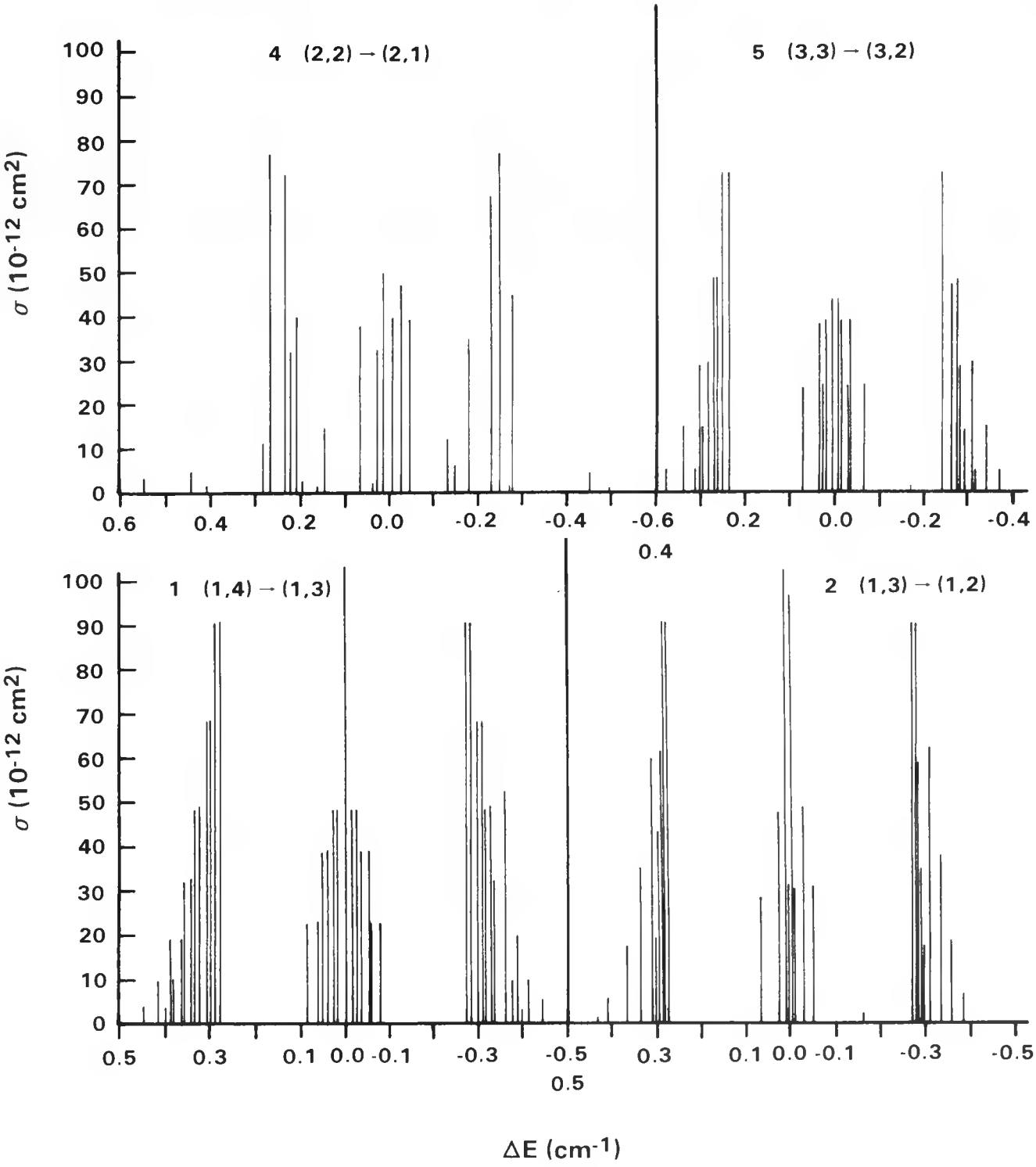
(27c)

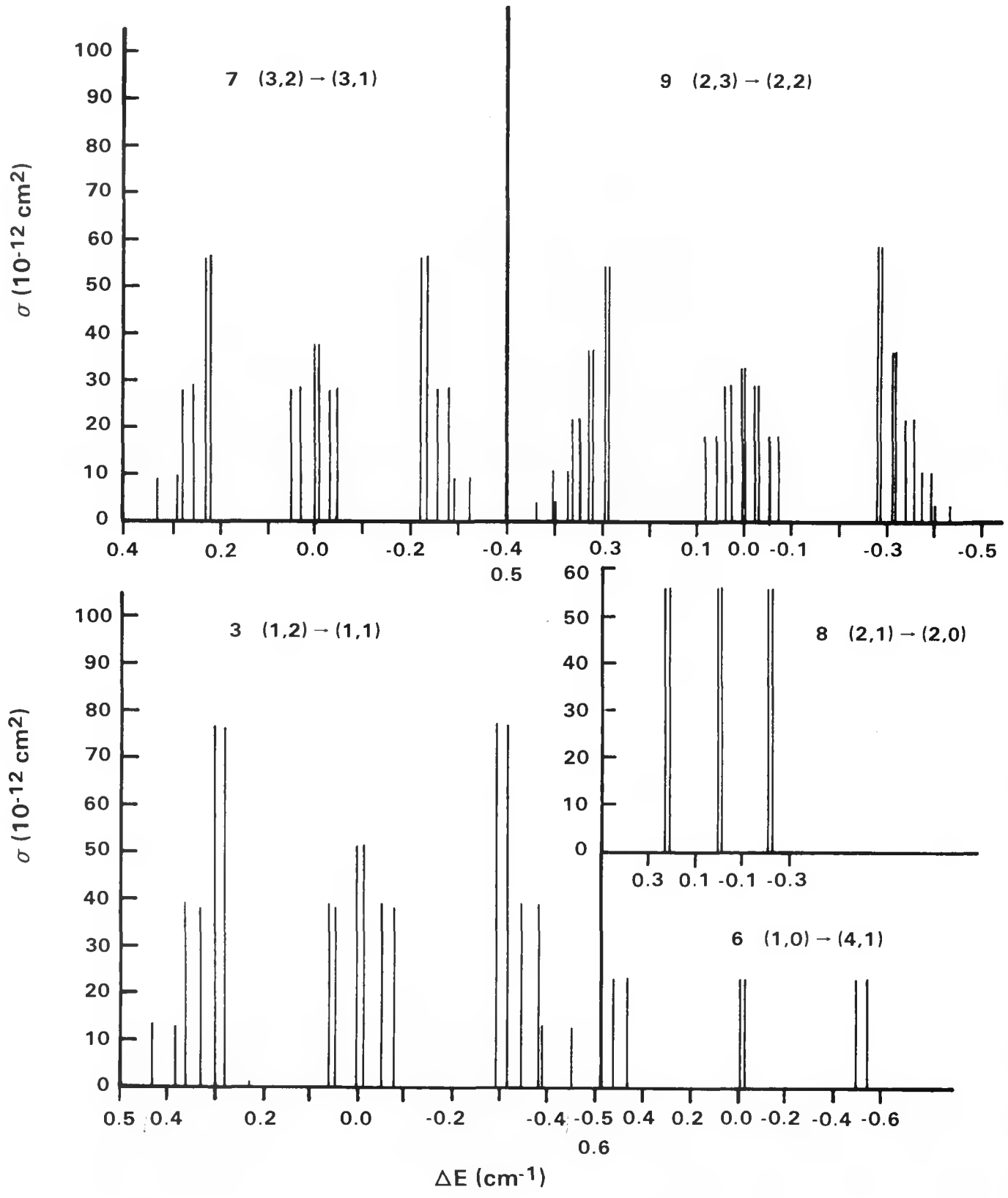
Thus, summing over k' and M_F' reduces the radiative transition rate to its value in the absence of hyperfine splitting and Zeemann splitting. This is useful is checking that the programming is correct. Note that each initial state with quantum numbers k and M_F has the entire radiative transition rate, S(iJ,i'J'). For each iJ, the total number of (k,M_F) states is

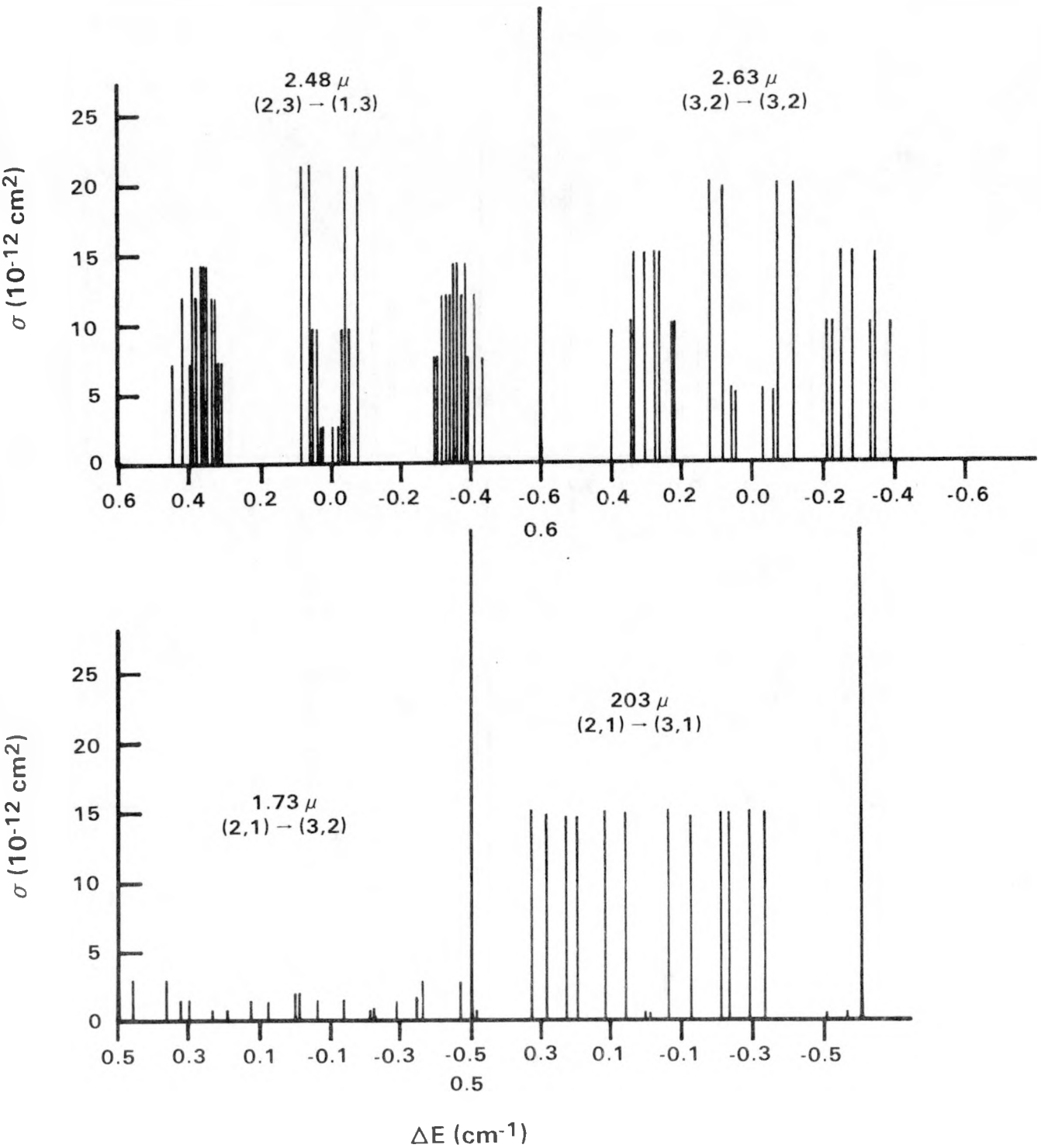
(2J+1)(2I+1). Since all the levels have the same rate, an average over k and M_F leads to S(iJ,i'J').

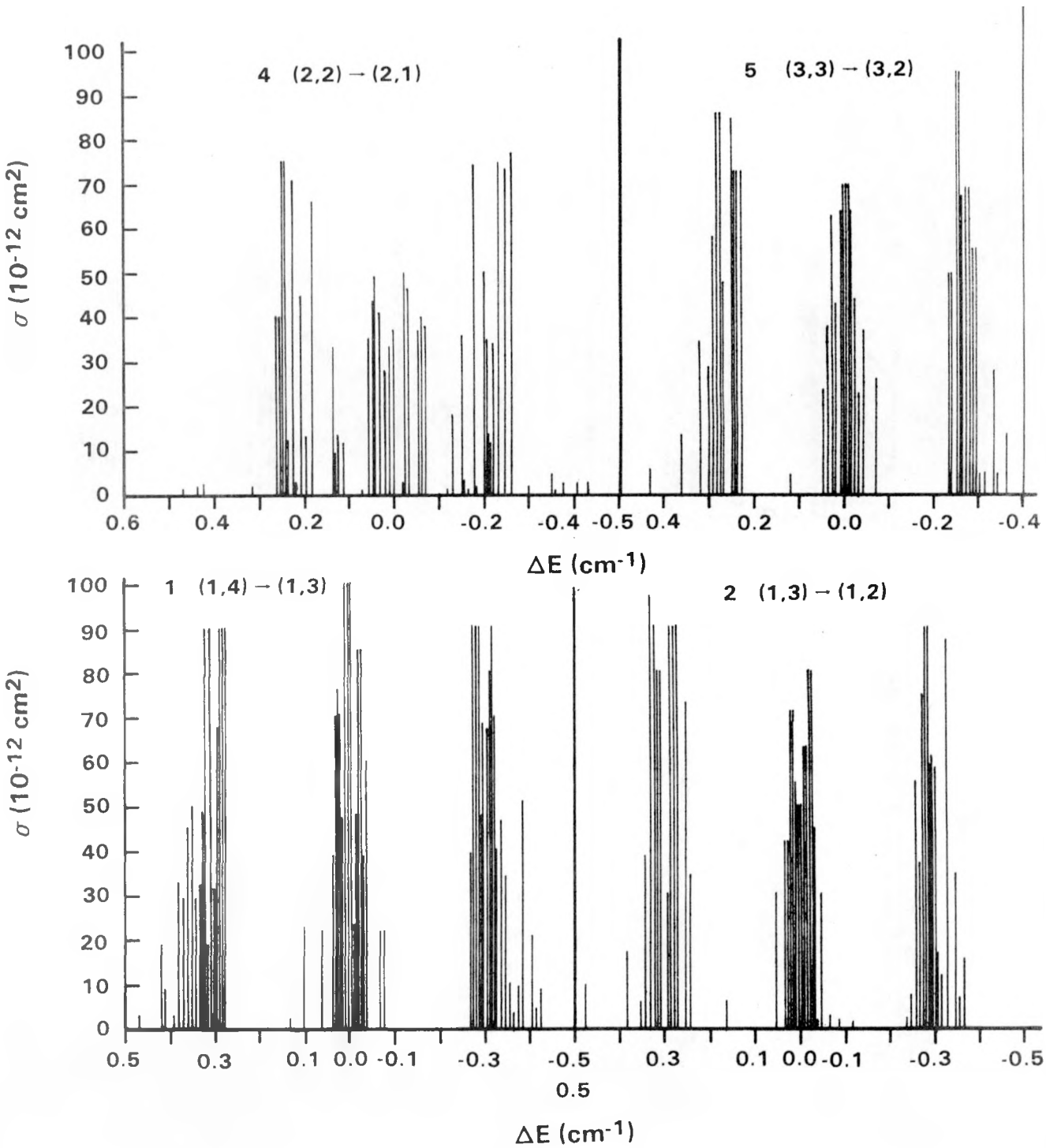
In figs.(2a)–(2c) I show the emission cross sections for Xe(129) for the same transitions as shown in figs.(1a)–(1c). The triplet shape is retained though the cross section density is increased. As a crude generalization, when Zeeman spliting is significant the number of components in each iJ–i'J' transition is $3\ (2I + 1)^2\ (2J_s + 1)$, where J_s is the smaller of J or J'. When these components are distributed over a triplet, there are $(2I + 1)^2\ (2J_s + 1)$ components in each member of the triplet. In the absence of a magnetic field there are roughly $(2I + 1)^2$ components in a single peak. For these transitions and a 6kG magnetic field the width of the members of the triplet seem slightly larger for the case I = 1/2 than for I = 0.

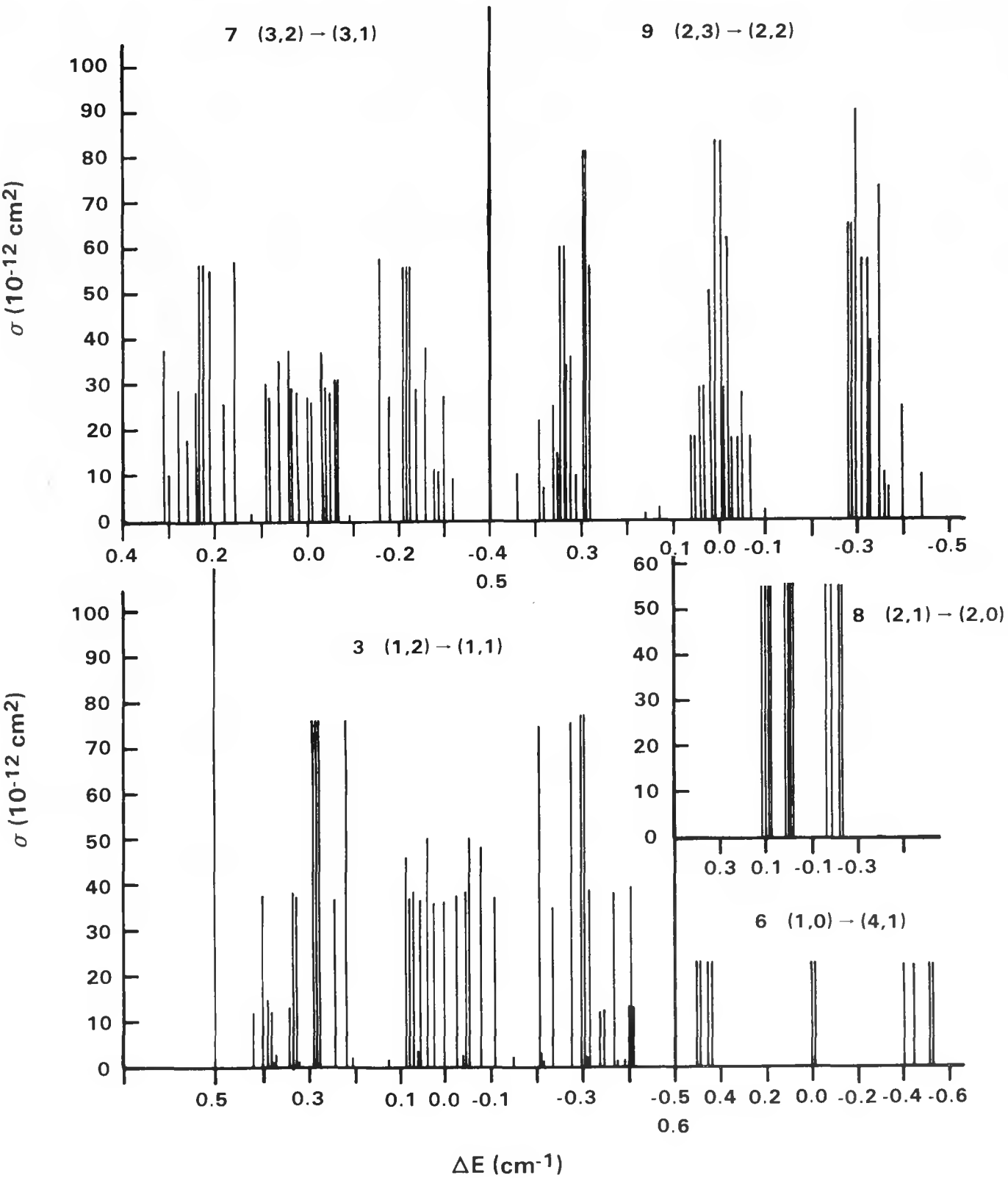
In figs.(3a)–(3c) I show the emission cross sections for Xe(131). Here the number of components is so large for some transitions (112 components for each member of the (1,4)–(1,3) triplet) that for transitions with J = 2,3 and 4, I have added all cross sections in a 0.01 cm^{-1} interval, except where such an addition would produce unrealistically large summed cross sections. One must remember that with $I \geq 1/2$ there will be more components than with I = 0, but that the individual cross sections are smaller than in the case I = 0. The Doppler width at room temperature in each transition is $\leq 0.004\ cm^{-1}$, while the scale size in the figures is 0.01 cm^{-1}. Thus while each component may be isolated from all the others, the scale size may imply an overlap. Again for I = 3/2 one sees the triplet pattern, with a barely discernable increase in width over I = 0 and I = 1/2.

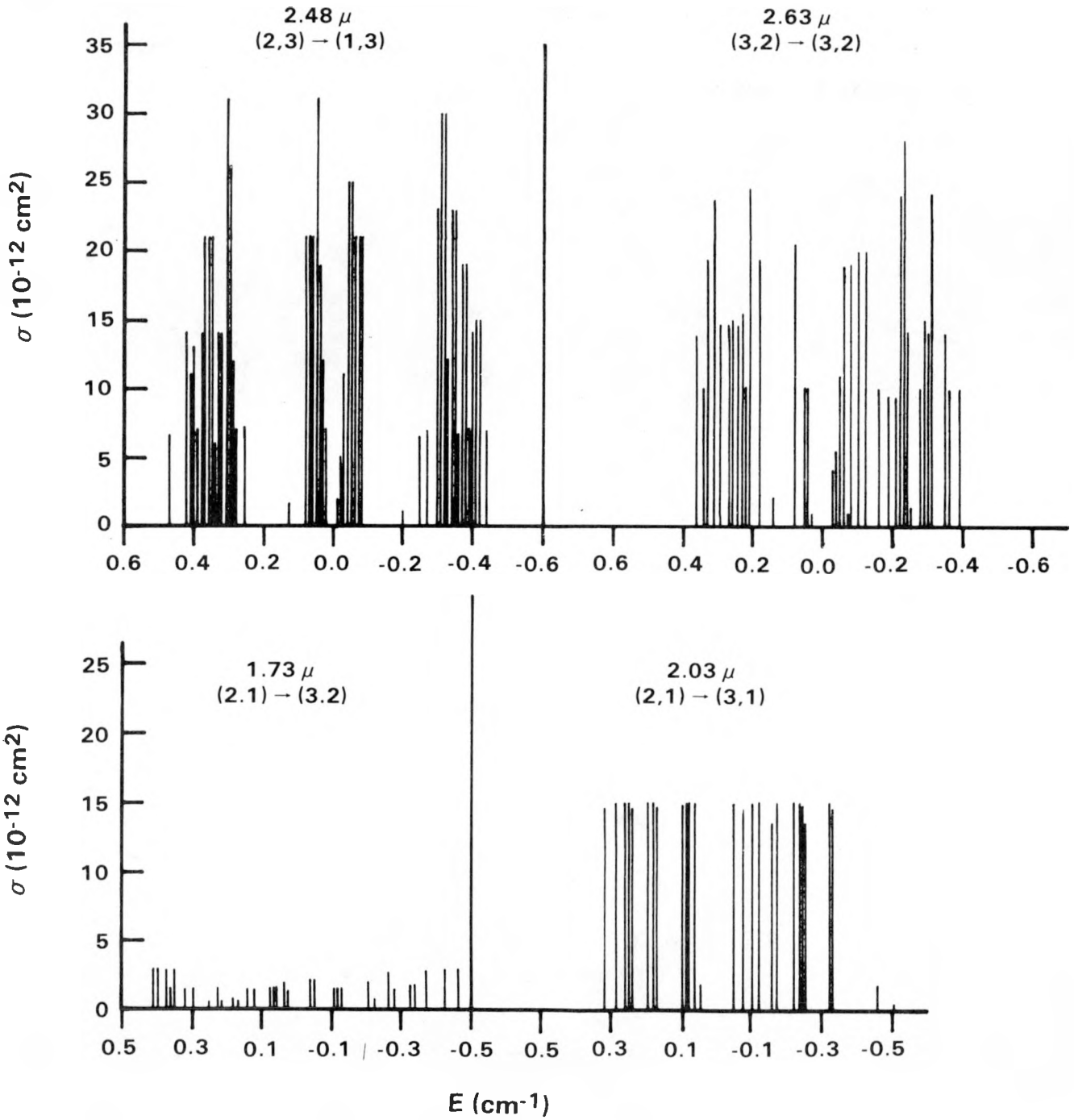

4 (2,2) → (2,1)
5 (3,3) → (3,2)
1 (1,4) → (1,3)
2 (1,3) → (1,2)
σ (10-12 cm2)
ΔE (cm-1)


7 (3,2) → (3,1)
9 (2,3) → (2,2)
3 (1,2) → (1,1)
8 (2,1) → (2,0)
6 (1,0) → (4,1)
σ (10-12 cm2)
ΔE (cm-1)


2.48 μ
(2,3) → (1,3)
2.63 μ
(3,2) → (3,2)
σ (10-12 cm2)
25
20
15
10
5
0
0.6 0.4 0.2 0.0 -0.2 -0.4 -0.6 0.4 0.2 0.0 -0.2 -0.4 -0.6
0.6
203 μ
(2,1) → (3,1)
1.73 μ
(2,1) → (3,2)
σ (10-12 cm2)
25
20
15
10
5
0
0.5 0.3 0.1 -0.1 -0.3 -0.5 0.3 0.1 -0.1 -0.3 -0.5
0.5
ΔE (cm-1)


4 (2,2) → (2,1)
5 (3,3) → (3,2)
σ (10-12 cm2)
ΔE (cm-1)
1 (1,4) → (1,3)
2 (1,3) → (1,2)
σ (10-12 cm2)
ΔE (cm-1)


7 (3,2) → (3,1)
9 (2,3) → (2,2)
3 (1,2) → (1,1)
8 (2,1) → (2,0)
6 (1,0) → (4,1)
σ (10-12 cm2)
σ (10-12 cm2)
ΔE (cm-1)


2.48 μ
(2,3) → (1,3)
2.63 μ
(3,2) → (3,2)
σ (10-12 cm2)
35
30
25
20
15
10
5
0
0.6 0.4 0.2 0.0 -0.2 -0.4 -0.6 0.6 0.4 0.2 0.0 -0.2 -0.4 -0.6
1.73 μ
(2.1) → (3.2)
2.03 μ
(2,1) → (3,1)
σ (10-12 cm2)
25
20
15
10
5
0
0.5 0.3 0.1 -0.1 -0.3 -0.5 0.5 0.3 0.1 -0.1 -0.3 -0.5
E (cm-1)

9) Conclusions

These calculations are done with as simple a set of wavefunctions as will produce reasonable agreement with Lande g factors and dipole and quadrupole hyperfine splitting paramaters. Since the distribution of oscillator strength is dominated by the 6 kG magnetic field it did not seem necessary to use more accurate hyperfine splitting parameters. Comparison with experiment (such as Ref.(20)) can be made if Doppler and instrumental line widths are available.

References

1) "American Institute of Physics Handbook, Third Ed.", (McGraw-Hill, New York, (1972))

2) R. D. Cowan, "The Theory of Atomic Structure and Spectra", (Univ. Of California Press, Berkeley, (1981))

3) D. A. Jackson, M.-C. Coulombe, and J. Bauche, Proc. Roy. Soc. Lond. A 343, 443 (1975)

4) E. U. Condon and G. H. Shortley, "The Theory of Atomic Spectra", (Cambridge Univ. Press, Cambridge, (1935))

5) C. E. Moore, "Atomic Energy Levels, Vol. III", NBS Circular No. 467 (U. S. Gov. Printing Office, Washington, D. C. 1958)

6) E. J. McGuire, "Radiative Transitions in Atomic Xenon", (Sandia Report, SAND76-0196)

7) M. Aymar and M. Coulombe, Atomic Data Tables, 21, 537 (1978)

8) H. R. Schlossberg and A. Javan, Phys. Rev. Lett. 17, 1242 (1966)

9) C. C. Davis and T. A. King, J. Quant. Spectrosc. Radiat. Transfer 13, 825 (1973)

10) L. Allen, D. Jones, and D. Schofield, J. Opt. Soc. Amer. 59, 842 (1969)

11) E. Jiminez, J. Campos, and C. Sanchez del Rio, J. Opt. Soc. Amer. 64, 1009 (1974)

12) L. D. Landau and E. M. Lifshitz, "Quantum Mechanics", (Addison-Wesley, Reading, Mass., (1958))

13) E. J. McGuire, "Magnetic Field Effects in the Oxygen Auroral Line", (Sandia Report, SAND77-0177)

14) M. Ohwa, T. J. Moratz, and M. J. Kushner, J. Appl. Phys. 66, 5131 (1989)

15) E. J. McGuire, "The Magnetic Hyperfine Interaction for Partially Filled Shells", (Sandia Report, SAND77-1431)

16) I. I. Sobelman, "Introduction to the Theory Of Atomic Spectra", (Pergamon Press, New York, 1972)

17) D. A. Jackson and M. C. Coulombe, Proc. Roy. Soc. Lond. A 335, 127 (1973)

18) S. Liberman, C. R. Acad. Sci. Paris, B 266, 236, (1968), and J. de Physique, 30, 53, (1969)

19) S. Liberman, J. de Physique, 32, 867, (1971)

20) P. J. Brannon, R. W. Morris, and E. L. Patterson, (to be published)

21) L. C. Biedenharn, J. M. Blatt, and M. E. Rose, Rev. Mod. Phys. 24, 249 (1952)

Appendix A

The wave function including nuclear spin is

$$|iJITt\rangle = \sum_{M,M_I} C(JIT,MM_It)\ |iJM\rangle\ |IM_I\rangle \tag{A1-a}$$

$$= \sum_{J_c,j}\ \sum_{M,M_I} C(JIT,MM_It)\ C(J_cj,iJ)\ |J_cjJM\rangle\ |IM_I\rangle$$

$$= \sum_{J_c,j} C(J_cj,iJ)\ [(2J_c+1)(2j+1)]^{1/2} \sum_{L,S} [(2L+1)(2S+1)]^{1/2} \begin{Bmatrix} l & 1/2 & J_c \\ l' & 1/2 & j \\ L & S & J \end{Bmatrix}$$

$$\sum_{M,M_I} C(JIT,MM_It)\ |^2P,^2l';LSJM\rangle\ |IM_I\rangle = \sum_{J_c,j} C(J_cj,iJ)\ [(2J_c+1)(2j+1)]^{1/2}$$

$$\sum_{L,S} [(2L+1)(2S+1)]^{1/2} \begin{Bmatrix} l & 1/2 & J_c \\ l' & 1/2 & j \\ L & S & J \end{Bmatrix}\ |^2P,^2l';LSJIFM_F\rangle \tag{A1-b}$$

which is the wavefunction in an LS coupling basis. Then the hyperfine interaction matrix element is

$$\langle iJIF'M_F,|H_{HF}|iJIFM_F\rangle = \sum_{J_c,j}\ \sum_{J_c',j'} [(2J_c+1)(2j+1)(2J_c'+1)(2j'+1)]^{1/2} C(J_cj,iJ)$$

$$C(J_c'j',iJ) \sum_{L,S}\ \sum_{P,Q} [(2L+1)(2S+1)(2P+1)(2Q+1)]^{1/2} \begin{Bmatrix} l & 1/2 & J_c \\ l' & 1/2 & j \\ L & S & J \end{Bmatrix} \begin{Bmatrix} l & 1/2 & J_c' \\ l' & 1/2 & j' \\ P & Q & J \end{Bmatrix}$$

$$\langle^2P,^2l';PQJIF'M_F,|H_{HF}|^2P,^2l';LSJIFM_F\rangle. \tag{A2-a}$$

The last matrix element is given in eq.(49) of Ref.(15) and is

$$\langle^2P,^2l';PQJIF'M_F,|H_{HF}|^2P,^2l';LSJIFM_F\rangle = \delta_{FF'}\ \delta_{M_FM_F'}\ A(F)\ [(2L+1)(2P+1)]^{1/2}$$

$$[(-1)^S\ \delta_{SQ} \begin{Bmatrix} P & S & J \\ J & 1 & L \end{Bmatrix} [(-1)^{L+P}\ B \begin{Bmatrix} L & 1 & P \\ l_1 & l_2 & l_1 \end{Bmatrix} + C \begin{Bmatrix} L & 1 & P \\ l_2 & l_1 & l_2 \end{Bmatrix}] - [45(2S+1)(2Q+1)]^{1/2}$$

$$(-1)^{-S-J} \begin{Bmatrix} Q & S & 1 \\ 1/2 & 1/2 & 1/2 \end{Bmatrix} \begin{Bmatrix} P & L & 2 \\ Q & S & 1 \\ J & J & 1 \end{Bmatrix} [(-1)^L\ D \begin{Bmatrix} L & 2 & P \\ l_1 & l_2 & l_1 \end{Bmatrix} + (-1)^{P+S-Q}\ E \begin{Bmatrix} L & 2 & P \\ l_2 & l_1 & l_2 \end{Bmatrix}]], \tag{A2-b}$$

where

$$A(F) = (\mu_0/4\pi)\ 2\ g_n m_{ep}\ (\mu_B)^2\ (-1)^{I+F+l_1+l_2} \begin{Bmatrix} F & I & J \\ 1 & J & I \end{Bmatrix} (2J+1)\ [I(I+1)(2I+1)]^{1/2}, \tag{A2-c}$$

$$B = [(1/r_1)^3]_{5p}\ [\ell_1(\ell_1+1)(2\ell_1+1)]^{1/2},$$

(A2-d)

$$C = [(1/r_2)^3]_{n\ell_2}\ [\ell_2(\ell_2+1)(2\ell_2+1)]^{1/2},$$

(A2-e)

$$D = [(1/r_1)^3]_{5p}\ (-1)^{\ell_1}\ (2\ell_1+1)\ \begin{pmatrix} \ell_1 & \ell_1 & 2 \\ 0 & 0 & 0 \end{pmatrix},$$

(A2-e)

$$E = [(1/r_2)^3]_{n\ell_2}\ (-1)^{\ell_2}\ (2\ell_2+1)\ \begin{pmatrix} \ell_2 & \ell_2 & 2 \\ 0 & 0 & 0 \end{pmatrix},$$

(A2-f)

where $[(1/r_2)^3]_{n\ell_2}$ is the expectation value of $(1/r)^3$ for the $n\ell_2$ orbital.

The quantities in A(F) are m_{ep}= 1/1836, $\mu_0 = 4\pi\ 10^{-7}$ Henrys/meter, μ_B is the Bohr magneton, while g_n is defined in terms of the nuclear magnetic moment, μ_N via $\mu_N = g_n\ m_{ep}\ \mu_B$. Since we seek the hyperfine interaction matrix element in intermediate coupling we want to sum over LSPQ and $J_c j J_c' j'$. The sum over LSPQ is straightforward but tedious. It leads to

$$\langle iJIF'M_{F'}|H_{HF}|iJIFM_F\rangle = \delta_{FF'}\ \delta_{M_F M_{F'}}\ A(F)\ {}_{J_c,\Sigma_j}\ {}_{J_c',\Sigma_j'}\ C(J_c j, iJ)\ C(J_c' j', iJ)$$

$$[(2J_c+1)(2j+1)(2J_c'+1)(2j'+1)]^{1/2}\ [T_1 + T_2 + T_3 + T_4],$$

(A3-a)

where

$$T_1 = (-1)^{\ell_2-1/2-j-J_c-J_c'}\ B\ [\delta_{jj'}/(2j+1)]\ \begin{Bmatrix} 1 & J_c & J_c' \\ 1/2 & \ell_1 & \ell_1 \end{Bmatrix}\ \begin{Bmatrix} 1 & J_c & J_c' \\ j & J & J_c \end{Bmatrix},$$

(A3-b)

$$T_2 = (-1)^{\ell_1-1/2+J_c-2J}\ C\ [\delta_{J_c J_c'}/(2J_c+1)]\ \begin{Bmatrix} 1 & j & j' \\ 1/2 & \ell_2 & \ell_2 \end{Bmatrix}\ \begin{Bmatrix} 1 & j & j' \\ J_c & J & J \end{Bmatrix},$$

(A3-c)

$$T_3 = (-1)^{-\ell_1-\ell_2-j-J_c'-2J}\ D\ (45)^{1/2}\ [\delta_{jj'}/(2j+1)]\ \begin{Bmatrix} 1 & J_c & J_c' \\ j & J & J_c \end{Bmatrix}\ \begin{Bmatrix} J_c' & J_c & 1 \\ \ell_1 & \ell_1 & 2 \\ 1/2 & 1/2 & 1 \end{Bmatrix},$$

(A3-d)

$$T_4 = (-1)^{-\ell_1-\ell_2+j+J_c} E\,(45)^{1/2} [\delta_{J_cJ_c'}/(2J_c+1)] \{{}^{1}_{J_c}\ {}^{j}_{J}\ {}^{j'}_{J}\} \begin{Bmatrix} j' & j & 1 \\ \ell_2 & \ell_2 & 2 \\ 1/2 & 1/2 & 1 \end{Bmatrix}.$$

(A3-e)

Then the interaction becomes

$$\langle iJIF'M_F'|H_{HF}|iJIFM_F\rangle = \delta_{FF'}\,\delta_{M_FM_F'}\,A(F)\,(W_1 + W_2),$$

(A4-a)

where

$$W_1 = \sum_j (-1)^{\ell_2-1/2-j} \sum_{J_c,J_c'} (-1)^{-J_c-J_c'} [(2J_c+1)(2J_c'+1)]^{1/2} C(J_cj,iJ)\, C(J_c'j,iJ)$$

$$\{{}^{1}_{j}\ {}^{J_c}_{J_c}\ {}^{J_c'}_{J_c}\} [B \{{}^{1}_{1/2}\ {}^{J_c}_{\ell_1}\ {}^{J_c'}_{\ell_1}\} + (-1)^{-\ell_1+1/2+J_c-2J} D\,(45)^{1/2} \begin{Bmatrix} J_c' & J_c & 1 \\ \ell_1 & \ell_1 & 2 \\ 1/2 & 1/2 & 1 \end{Bmatrix}],$$

(A4-b)

and

$$W_2 = \sum_{J_c} (-1)^{\ell_1-1/2+J_c-2J} \sum_{j,j'} [(2j+1)(2j'+1)]^{1/2} C(J_cj,iJ)\, C(J_cj',iJ)$$

$$\{{}^{1}_{J_c}\ {}^{j}_{J}\ {}^{j'}_{J}\} [C \{{}^{1}_{1/2}\ {}^{j}_{\ell_2}\ {}^{j'}_{\ell_2}\} + (-1)^{-\ell_2+1/2+j+2J} E\,(45)^{1/2} \begin{Bmatrix} j' & j & 1 \\ \ell_2 & \ell_2 & 2 \\ 1/2 & 1/2 & 1 \end{Bmatrix}].$$

(A4-c)

When configuration interaction effects are included, the hyperfine splitting is further complicated. For the simple case of 6s,5d mixing in the excited states of the noble gases, the modification to the $(5p)^5(5d)$ results is a reduction in the contributions of the W_1 and W_2 terms since if $S > C$, then $S^2 > C^2 + (S - C)^2$, an increase due to an additional cross-term, given by $W_2 \rightarrow W_2 + W_2'$, where

$$W_2' = -6\,\langle 5d|1/r^3|6s\rangle \sum_{J_c} (-1)^{J_c+1/2} \sum_{j_d} (2j_d+1)^{1/2} \{{}^{1}_{J_c}\ {}^{j_d}_{J}\ {}^{1/2}_{J}\} \{{}^{1/2}_{1}\ {}^{1}_{j_d}\ {}^{1/2}_{2}\}$$
$$C(dJ_cj_d,iJ)\, C(sJ_c1/2,iJ),$$

(A5)

and the need to include the Fermi contact term due to s electrons, which is given by $W_2 \rightarrow W_2 + W_2''$, where

$$W_2'' = (2/3)^{1/2} R_{ns}(0)^2 \sum_{J_c} (-1)^{-J_c-1/2} \begin{Bmatrix} J_c & J & 1/2 \\ 1 & 1/2 & J \end{Bmatrix} C(sJ_c1/2,iJ)^2, \quad \text{(A5)}$$

where $R_{ns}(0)^2$ is the ns electron density at the origin.

Appendix B

The textbook formulation of the electric quadrupole contribution to hyperfine splitting seems unduly complicated. As an illustration see Ref.(15). This effect arises as the lowest order correction to the assumption of a point nucleus in atomic physics calculations. That is, the potential $-Ze^2 \sum_i (1/|r_i|)$ is actually $-e^2 \sum_{N=1}^{Z} \sum_i (1/|\vec{r}_i - \vec{r}_N|)$, where $\vec{r}_N$ are the coordinates of the Z protons. The interaction contributing to the hyperfine effect is the difference of these two potentials

$$H^2_{Hy} = -e^2 \left[\sum_{N=1}^{Z} \sum_i (1/|\vec{r}_i - \vec{r}_N|) - Ze^2 \sum_i (1/|r_i|) \right]$$

$$= -e^2 \left[\sum_{N=1}^{Z} \sum_i \sum_K (r_<)^K/(r_<)^{K+1} P_K(\cos(\Theta)) - Ze^2 \sum_i (1/|r_i|) \right]. \quad \text{(B1-a)}$$

If we assume that the smaller radius ($r_<$) is always the nuclear coordinate, then

$$H^2_{Hy} = -e^2 \left[\sum_{N=1}^{Z} \sum_i \sum_K (r_N)^K/(r_i)^{K+1} P_K(\cos(\Theta)) - Ze^2 \sum_i (1/|r_i|) \right]. \quad \text{(B1-b)}$$

The K = 0 term is $-e^2 \sum_{N=1}^{Z} \sum_i 1/(r_i)^1 = -Ze^2 \sum_i (1/|r_i|)$, which cancels the potential due to the assumption of a point mass nucleus. Then, using the spherical harmonic addition theorem, the interaction can be written

$$H^2_{Hy} = -e^2 \left[\sum_{N=1}^{Z} \sum_i \sum_{K,p} (r_N)^K/(r_i)^{K+1} [4\pi/(2K+1)] Y^p_K(\theta_i,\phi_i) [Y^p_K(\theta_N,\phi_N)]^* \right]. \quad \text{(B1-c)}$$

Parity considerations eliminate the K = 1 term, i.e. diagonal matrix element calculations lead to 3j symbols of the form $\begin{pmatrix} \ell & \ell & K \\ 0 & 0 & 0 \end{pmatrix}$, which require K even. Thus the lowest order correction is the quadrupole, and if all higher interactions are neglected

$$H^2_{Hy} = -e^2 \left[\sum_{N=1}^{Z} \sum_i \sum_p (r_N)^2/(r_i)^3 [4\pi/5] Y^p_2(\theta_i,\phi_i) [Y^p_2(\theta_N,\phi_N)]^* \right]. \quad \text{(B1-d)}$$

For the general case of n ℓ_1 electrons with quantum numbers $L_1S_1J_1$, and m ℓ_2 electrons with quantum numbers $L_2S_2J_2$, forming a term in intermediate coupling with quantum numbers iJM, which is then coupled to a nuclear

moment, I, to produce a term of the form $\langle iJIFM_F|$, the matrix element of the quadrupole hyperfine interaction is

$$\langle iJIF'M_{F'}|H^2_{Hy}|iJIFM_F\rangle = \sum_{J_1,J_2}\sum_{J_1',J_2'} C(J_1J_2,iJ)\, C(J_1'J_2',iJ) \sum_{M,M_I} C(JIF,MM_IM_F)$$

$$\sum_{M',M_I'} C(JIF',M'M_I'M_{F'}) \left[-(4\pi/5)e^2\right] \sum_{p=-2}^{2} \sum_{N=1}^{Z} \langle IM_I|r_N^2\,[Y_2^p(\theta_N,\phi_N)]^*|IM_I'\rangle\, H_a, \tag{C2-a}$$

where

$$H_a=\langle(\ell_1)^nL_1S_1J_1(\ell_2)^mL_2S_2J_2,JM|\sum_i(1/r_i)^3Y_2^p(\theta_i,\phi_i)|(\ell_1)^nP_1Q_1J_1'(\ell_2)^mP_2Q_2J_2',J'M'\rangle \tag{C2-b}$$

The last matrix element, H_a, is a standard atomic physics calculation, which, after extensive tedious algebra can be reduced to

$$H_a = (5/4\pi)^{1/2}C(J2J',MpM')\,\delta_{S_1Q_1}\,\delta_{S_2Q_2}[\delta_{L_2P_2}\,\delta_{J_2J_2'}\,F_1V_1 + \delta_{L_1P_1}\,\delta_{J_1J_1'}\,F_2V_2]. \tag{B3-a}$$

where

$$F_1 = n \sum_{L_1',S_1'} (\ell_1^{n-1}L_1'S_1'|\}\ell_1^nL_1S_1)\,(\ell_1^{n-1}L_1'S_1'|\}\ell_1^nP_1Q_1), \tag{B3-b}$$

$$F_2 = m \sum_{L_2',S_2'} (\ell_2^{m-1}L_2'S_2'|\}\ell_2^mL_2S_2)\,(\ell_2^{m-1}L_2'S_2'|\}\ell^mP_2Q_2), \tag{B3-c}$$

$$V_1=(-1)^{-L_1'-S_1-\ell_1-J'+J_1'+J_1-J_2}\,[(2L_1+1)(2P_1+1)(2J_1+1)(2J_1'+1)(2J+1)(2\ell_1+1)\,]^{1/2}$$

$$a(\ell_1)\,\begin{Bmatrix} 2 & J_1 & J_1' \\ J_2 & J' & J \end{Bmatrix}\begin{Bmatrix} 2 & J_1 & J_1' \\ S_1 & P_1 & L_1 \end{Bmatrix}\begin{Bmatrix} 2 & P_1 & L_1 \\ L_1' & \ell_1 & \ell_1 \end{Bmatrix}, \tag{B3-d}$$

$$V_2=(-1)^{-L_2'-S_2-\ell_2+J_1+J}\,[(2L_2+1)(2P_2+1)(2J_2+1)(2J_2'+1)(2J+1)(2\ell_2+1)\,]^{1/2}$$

$$a(\ell_2)\,\begin{Bmatrix} 2 & J_2 & J_2' \\ J_1 & J' & J \end{Bmatrix}\begin{Bmatrix} 2 & J_2 & J_2' \\ S_2 & P_2 & L_2 \end{Bmatrix}\begin{Bmatrix} 2 & P_2 & L_2 \\ L_2' & \ell_2 & \ell_2 \end{Bmatrix}, \tag{B3-e}$$

$$a(\ell) = (-1)^{\ell} \begin{pmatrix} 2 & \ell & \ell \\ 0 & 0 & 0 \end{pmatrix} \langle 1 | 1/r^3 | 1 \rangle \, (2\ell+1)^{1/2},$$

(B3-f)

where $(\ell_1^{n-1} L_1' S_1' | \} \ell_1^n L_1 S_1)$ is a fractional parentage coefficient.

Next consider the nuclear matrix element in eq.(B2-a). Since we do not have a complete theory of the nucleus we cannot explicitly calculate $\langle IM_I | r_N^2 \, [Y_2^p(\theta_N,\phi_N)]^* | IM_I' \rangle$. Assuming a spherical harmonic description is valid for the nuclear wavefunctions then the matrix element is of the form

$$\sum_N \langle IM_I | r_N^2 \, [Y_2^p(\theta_N,\phi_N)]^* | IM_I' \rangle = (-1)^{-p} \, C(I2I; M_I, -p, M_I') \sum_N \langle I | r_N^2 | I \rangle,$$

(B4-a)

with all other coefficients lumped in $\sum_N$. Note that the Clebsch-Gordan coefficient requires $I \geq 1$, so there is no effect for isotopes with $I \leq 1/2$. The nuclear quadrupole moment is defined by[16] (I use the traditional spherical harmonics, Y_K^m, rather than $Q_{Km} = [4\pi/(2K+1)]^{1/2} \, Y_K^m$)

$$Q = [16\pi/5]^{1/2} \sum_N \langle IM_I | r_N^2 \, Y_2^0(\theta_N,\phi_N)]^* | IM_I \rangle_{M_I=I}$$

(B4-b)

$$= [16\pi/5]^{1/2} \, C(I2I, M_I, -p, M_I)_{M_I=I} \sum_N \langle I | r_N^2 | I \rangle$$

$$= (-1)^{2I} \, [16\pi/5]^{1/2} \, \{I(2I-1)/[(2I+3)(I+1)]\}^{1/2} \sum_N \langle I | r_N^2 | I \rangle,$$

(B4-c)

which defines the unknown integral $\sum_N \langle I | r_N^2 | I \rangle$ in terms of the nuclear quadrupole moment,

$$\sum_N \langle I | r_N^2 | I \rangle = Q \, (-1)^{2I} \, [5/16\pi]^{1/2} \, \{(2I+3)(I+1)/[I(2I-1)]\}^{1/2}.$$

(B4-d)

Then the nuclear matrix element in eq.(B2-a) is

$$\langle IM_I | r_N^2 \, [Y_2^p(\theta_N,\phi_N)]^* | IM_I' \rangle = (-1)^{-p} \, C(I2I, M_I, -p, M_I') \, Q \, (-1)^{2I} \, [5/16\pi]^{1/2}$$

$$\{(2I+3)(I+1)/[I(2I-1)]\}^{1/2} = (-1)^{-p} \, C(I2I, M_I, -p, M_I') \, F_N,$$

(B4-e)

where

$$F_N = Q\ (-1)^{2I}\ [5/16\pi]^{1/2}\ \{(2I+3)(I+1)/[I(2I-1)]\}^{1/2}\ .$$

(B4-f)

The eq.(B2-a) becomes

$$\langle iJIF'M_{F'}|H^2_{Hy}|iJIFM_F\rangle = \sum_{J_1,J_2;J_1',J_2'} C(J_1J_2,iJ)\ C(J_1'J_2',iJ)\ [-(4\pi/5)e^2]\ F_N\ F_a$$

$$(5/4\pi)^{1/2}\ \delta_{S_1Q_1}\ \delta_{S_2Q_2}[\delta_{L_2P_2}\ \delta_{J_2J_2'}\ V_1 + \delta_{L_1P_1}\ \delta_{J_1J_1'}\ V_2]$$

$$\sum_{M,M_I} C(JIF,MM_IM_F)\ \sum_{M',M_I'} C(JIF',M'M_I'M_{F'}) \sum_{p=-2}^{2}(-1)^{-p}\ C(I2I,M_I,-p,M_I')C(J2J',MpM').$$

(B5-a)

Some tedious but straightforward algebra reduces the last line of eq.(B5-a) to

$$\delta_{F,F'}\ \delta_{M_F,M_{F'}}\ (-1)^{-F-I-J}\ [(2I+1)(2J+1)]^{1/2}\ \begin{Bmatrix} 2 & I & I \\ F & J & J \end{Bmatrix}.$$

(B5-b)

Thus one has the selection rules $F = F'$, $M_F = M_{F'}$. Then the matrix element is

$$\langle iJIF'M_{F'}|H^2_{Hy}|iJIFM_F\rangle = \delta_{F,F'}\ \delta_{M_F,M_{F'}}\delta_{S_1Q_1}\ \delta_{S_2Q_2}(-1)^{-F-I-J}\ [(2I+1)(2J+1)]^{1/2}$$

$$\begin{Bmatrix} 2 & I & I \\ F & J & J \end{Bmatrix}\ (5/4\pi)^{1/2}\ [-(4\pi/5)e^2]\ F_N\ F_a$$

$$\sum_{J_1,J_2;J_1',J_2'} C(J_1J_2,iJ)\ C(J_1'J_2',iJ)\ [\delta_{L_2P_2}\ \delta_{J_2J_2'}\ V_1 + \delta_{L_1P_1}\ \delta_{J_1J_1'}\ V_2]$$

(B6-a)

$$= \delta_{F,F'}\ \delta_{M_F,M_{F'}}\delta_{S_1Q_1}\ \delta_{S_2Q_2}(-1)^{-F+I-J}\ [(2I+1)(2J+1)]^{1/2}\ \begin{Bmatrix} 2 & I & I \\ F & J & J \end{Bmatrix}\ Q\ (-e^2/2)$$

$$[(2I+3)(I+1)/(I(2I-1)]^{1/2}\ F_a\ \sum_{J_1,J_2;J_1',J_2'} C(J_1J_2,iJ)\ C(J_1'J_2',iJ)$$

$$[\delta_{L_2P_2}\ \delta_{J_2J_2'}\ V_1 + \delta_{L_1P_1}\ \delta_{J_1J_1'}\ V_2].$$

(B6-b)

For the excited states of closed shell atoms including the noble gases, $F_2 = 1$, and

$$F_1 = (1/3)\ \sum_{L_1',S_1'} (2L_1' + 1)\ (2S_1' + 1),$$

(B7-a)

$$F_1\ V_1 = (-1)^{-1-S_1-\ell_1-J'+J_1'+J_1-J_2}\ [(2\ell_1+1)/3]\ [(2J_1+1)(2J_1'+1)(2J+1)(2\ell_1+1)]^{1/2}$$

$$a(\ell_1)\ \begin{Bmatrix} 2 & J_1 & J_1' \\ J_2 & J' & J \end{Bmatrix} \begin{Bmatrix} 2 & J_1 & J_1' \\ 1/2 & \ell_1 & \ell_1 \end{Bmatrix},$$

(B7-b)

$$F_2\ V_2 = (-1)^{-1/2-\ell_2+J_1+J}\ [(2J_2+1)(2J_2'+1)(2J+1)(2\ell_2+1)\ ]^{1/2}$$

$$a(\ell_2)\ \begin{Bmatrix} 2 & J_2 & J_2' \\ J_1 & J' & J \end{Bmatrix} \begin{Bmatrix} 2 & J_2 & J_2' \\ 1/2 & \ell_2 & \ell_2 \end{Bmatrix},$$

(B7-c)

so that

$$\langle iJIF'M_{F'}|H^2_{Hy}|iJIFM_F\rangle = \delta_{F,F'}\ \delta_{M_F,M_{F'}}(-e^2\ Q/2)\ \ (-1)^{F-I}\ (2J+1)\ \begin{Bmatrix} 2 & I & I \\ F & J & J \end{Bmatrix}$$

$$\{(2I+1)(2I+3)(I+1)/[I(2I-1)]\}^{1/2}[W_3 - W_4]\ ,$$

(B8-a)

where

$$W_3 = (2\ell_1+1)\ \begin{pmatrix} \ell_1 & \ell_1 & 2 \\ 0 & 0 & 0 \end{pmatrix} \langle(1/r)^3\rangle_{\ell_1}\ \ J_c,\Sigma_{j,J_c'}$$

$$(-1)^{-j+1/2-J_c'-J_c}[(2J_c+1)(2J_c'+1)]^{1/2}C(J_cj,iJ)\ C(J_c'j,iJ) \begin{Bmatrix} 2 & J_c & J_c' \\ j & J & J \end{Bmatrix} \begin{Bmatrix} 2 & J_c & J_c' \\ 1/2 & \ell_1 & \ell_1 \end{Bmatrix},$$

(B8-b)

$$W_4 = (2\ell_2+1)\ \begin{pmatrix} \ell_2 & \ell_2 & 2 \\ 0 & 0 & 0 \end{pmatrix} \langle(1/r)^3\rangle_{\ell_2}\ \ J_c,\Sigma_{j,j'}$$

$$(-1)^{J_c+1/2+2J}\ [(2j+1)(2j'+1)]^{1/2}C(J_cj,iJ)\ C(J_cj',iJ) \begin{Bmatrix} 2 & j & j' \\ J_c & J & J \end{Bmatrix} \begin{Bmatrix} 2 & j & j' \\ 1/2 & \ell_2 & \ell_2 \end{Bmatrix}],$$

(B8-c)

where J_c and j have been substituted for J_1 and J_2.

Biedenharn et al[21] give the relation

$$\begin{Bmatrix} 2 & I & I \\ F & J & J \end{Bmatrix} = (-1)^{F+I+J}\ 6\ [A(A+1) - (4/3)\ I(I+1)J(J+1)]$$

$$\{(2I-2)!(2J-2)!/[(2I+3)!\ (2J+3)!]\}^{1/2},$$

(B9-a)

where

$$A = F(F+1) - I(I+1) - J(J+1), \tag{B9-b}$$

so that

$$\langle iJIF'M_{F'}|H^2_{Hy}|iJIFM_F\rangle = \delta_{F,F'}\,\delta_{M_F,M_{F'}}(-e^2\,Q/2)\;\;(-1)^{2I-J}\;[W_3 - W_4]\;6$$

$$\{[A(A+1)-(4/3)I(I+1)J(J+1)]/[2I(2I-1)]\}\;\{(2J+1)/[(2J+3)(2J+2)(2J)(2J-1)]\}^{1/2}$$

$$= \delta_{F,F'}\,\delta_{M_F,M_{F'}}[A(A+1)-(4/3)I(I+1)J(J+1)]\;B_{iJ}, \tag{B9-c}$$

with

$$B_{iJ}=(-3e^2Q)(-1)^{2I-J}\{[W_3-W_4]/[2I(2I-1)]\}\;\{(2J+1)/[(2J+3)(2J+2)(2J)(2J-1)]\}^{1/2} \tag{B9-d}$$

where B_{iJ} is a coefficient used to describe the quadrupole contribution to hyperfine splitting. In studies of hyperfine splitting the second term in brackets in eq.(B9-c) is neglected as an irrelevant constant, but it must be included when one studies transitions between levels with different iJ.

When configuration interaction (CI) effects are included in the wavefunction the calculation of the quadrupole contribution to the hyperfine splitting is complicated. For the simple case of 5d-6s mixing considered here, the effect of CI is to add a cross term which may be described by $W_4 \rightarrow W_4 + W_4'$, where

$$W_4' = -(1/5)^{1/2}\,\langle 5d|1/r^3|6s\rangle \sum_{J_c}\sum_{j_d}(2j_d+1)^{1/2}(-1)^{J_c+j_d}$$

$$C(dJ_cj_d,iJ)\;C(sJ_c1/2,iJ)\;\begin{Bmatrix} 2 & j_d & 1/2 \\ J_c & J & J \end{Bmatrix}. \tag{B10}$$

Appendix (C)

To evaluate

$$I = \sum_{M,M_I} {}_{M} \; C(JIF,MM_IM_F)\; C(JIF',MM_IM_{F'}),$$

(C1-a)

I use

$$M = \sum_{M'} [L(L+1)]^{1/2} \; C(L1L,M'0M).$$

(C1-b)

Then

$$I = [J(J+1)]^{1/2} \sum_{q} \sum_{M,M_I} C(J1J,q0M)\; C(JIF,MM_IM_F)\; C(JIF',MM_IM_{F'}).$$

(C1-c)

But since C(J1J,q0M) is non-zero only when M = q

$$I = [J(J+1)]^{1/2} \sum_{q} \sum_{M,M_I} C(J1J,q0M)\; C(JIF,MM_IM_F)\; C(JIF',qM_IM_{F'})$$

$$= [J(J+1)]^{1/2}\; (-1)^{2F+1} \sum_{A,a} \sum_{q,M_I} [(2A+1)(2J+1)]^{1/2} \begin{Bmatrix} I & F & J \\ 1 & J & A \end{Bmatrix} C(A1F,a0M_F)$$

$$C(IJA,M_Iqa)\; C(JIF',qM_IM_{F'})$$

$$= [J(J+1)]^{1/2}\; (-1)^{2F+1-J-I+F'} \sum_{A,a} [(2A+1)(2J+1)]^{1/2} \begin{Bmatrix} I & F & J \\ 1 & J & A \end{Bmatrix} C(A1F,a0M_F)$$

$$\sum_{q,M_I} C(IJA,M_Iqa)\; C(IJF',M_IqM_{F'}).$$

(C1-d)

But the last sum is $\delta_{A,F'}\; \delta_{a,M_{F'}}$, so that

$$I = [(2F'+1)(2J+1)J(J+1)]^{1/2}\; (-1)^{+I+1+J+F'} \begin{Bmatrix} I & F & J \\ 1 & J & F' \end{Bmatrix} C(F'1F,M_{F'}0M_F).$$

(C1-e)

HISTORY: started originally as a memo to E. patterson in august 1989 for the Xe laser in the falcon program. Recast as a report end of Oct 1989 because it had grown so large.

1) calculations complete for isotopes with no hyperfine effect

2) need for mass 129 with spin 1/2 and 131 with spin 3/2

3) puzzling feature is the dominance by the transition at 1.73 ξ. Is this due to dominance of the laser medium by radiation trapping?

completed 1/31/90