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Energy Levels, Wave Functions, Dipole and Quadrupole Transitions of Fe^{+++} Ions in Sapphire*

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A computation is made of energy levels, wave functions and transition probabilities of the Fe^{3+} ion in Al_2O_3. The crystal field parameters used were those determined by Symmons and Bogle at 4 K. The magnetic field direction is described by the angles θ and φ indicating the directions with respect to and around the c axis of the crystal. The values of θ go from 0 to $\pi/2$ with $\pi/12$ intervals, the angles φ are 0 and $2\pi/3$ corresponding to the two nonequivalent sites of the crystal. The transition probabilities are given for dipole radiation in three polarization directions and for ultrasonic work the six components of the quadrupole transitions were computed.

Key words: Energy levels of Fe^{+++} in Al_2O_3; iron doped Al_2O_3; magneto elastic tensor; paramagnetic resonance; quadrupole transitions; spin hamiltonian; transition probabilities; ultrasonic (paramagnetic) resonance; ultrasonic transition probabilities; wave functions of Fe^{+++}

1. Introduction

As a result of recent work in ultrasonic paramagnetic resonance [1],[1] it became desirable to obtain a complete set of transition probabilities for quadrupole radiation, besides the known values for the dipolar transitions. We have programmed the calculations of these and related quantities in order to select *a priori* angles and field strengths that would enable us to observe specific components of the transition probabilities. There are some uncertainties with regard to the selection rules for ultrasonic absorption [2–4]. The first question is whether dipolar, quadrupolar, or a combination of these determines the line strength of the absorption. The next question is whether components of other multipoles are playing a role in the process.

In the available literature [5–8] the wave functions are never quoted. Consequently, it was necessary to recalculate these quantities in order to evaluate the transition probabilities. A new program was constructed for that purpose; the details are described in appendix I.

The physical properties and the spin hamiltonian are described in Sections 2 and 3.

The angle θ is the angle between the magnetic field and the c axis of the lattice which is a three-fold axis oriented along a body diagonal of the crystal field. There are two nonequivalent sites in the lattice. The angle φ depends on the ion in the unit cell. The crystal field is rotated over $\pi/3$ if one goes from one ion site to the other. Hence the spectrum is actually a superposition of two spectra. The differences are in general small, but noticeable.

The values for θ in which the calculation was performed are 0, $\pi/12$ . . . $\pi/2$ rad. for $\varphi=0$ and $\pi/3$. The field was varied from 0 to 0.5 Teslas (5000 Gauss) in steps of 0.025 T, but not all values are incorporated in

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[1] Figures in brackets indicate the literature references at the end of this paper.

the tables. At low field values and or near the crossing points, 10^{-3} T steps were used.

The crossing or non-crossing of the levels constitutes a certain practical difficulty in the labelling of the wave functions. We decided simply to list the levels in increasing order and label the wave functions accordingly.

2. Properties of the Crystal and Discussion of Previous Work

The free ion Fe^{3+} has the configuration $3d^5$. The $3d$ electron shell is half filled and the resultant orbital momentum L is equal to zero. The singlet ground state ^6S has a six-fold spin degeneracy. The first four excited states of the free ion are ^4G, ^4P, ^4D, and ^4F [9]. The optical spectrum has been studied by Moorjani and McAvoy [10].

The Al_2O_3 lattice, as described by Geschwind and Remeika [11] is shown in figure 1. It exhibits a three-fold symmetry around an axis perpendicular to the plane of the O^{2-}. The lattice presents the properties of the 3 m point group (D_{3d} in the Schoenflies notation) but each site has only a 3 (C_3) point of symmetry.

The specific directions for the propagation of sound waves have been studied by Borgnis [12]. The c axis and also the x axis (two-fold rotational symmetry often called "a" axis) are directions for purely compressional waves. There are two nonequivalent sites, which are identical except for a rotation of $\pi/6$ around the c axis. Consequently, the spectrum consists of the superposition of two slightly different spectra. The differences are large enough to be seen, i.e., the lines are clearly separated in certain directions and for certain fields. Ultrasonic propagation and absorption in Al_2O_3 were studied by Brian and Meister [13]. The velocity of sound for longitudinal waves is 10.9×10^5 cm/s, for shear waves, 6.41×10^5 cm/s. The Fe^{3+} ion, when introduced in the Al_2O_3 lattice occupies the sites of an Al ion. It is surrounded by 6 ions that are held responsible for the electric field: the O^{2-} ions. The positions of these ions determine the symmetry of the crystal field. Although deviations are known, the site symmetry can be considered bo be C_3 as mentioned above.

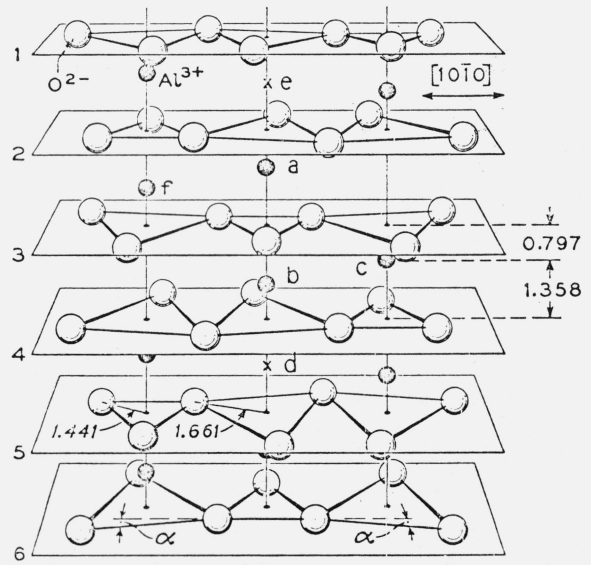

FIGURE 1. *Portion of the* Al_2O_3 *lattice, the two inequivalent sites are located in two adjacent planes for instance a and b (ref.* [10]).

The crystal field has a main component of trigonal symmetry and a smaller component of cubic symmetry. The total angular momemtum $J = S = 2\frac{1}{2}$ is split into three Kramers doublets whose degeneracy can be removed only by a magnetic field. For fields large compared to the zero field splitting the ion will be virtually free. Although the zero field splitting is small for S-state ions, most of the ultrasonic work was done in the low field region; hence we are mainly interested in the numerical values of the transition probabilities when magnetic field and crystal field are comparable.

This level structure is confirmed by many paramagnetic experiments [14–16]. The energy levels are most conveniently described by a spin hamiltonian with an effective spin $S = 5/2$. Abragam and Pryce proposed [7] the following expression:

$$\mathcal{H} = g\beta \mathbf{B} \cdot \mathbf{S} + D[S_z^2 - 35/12] + E[S_x^2 - S_y^2] + (a/6)[S_\xi^4 + S_\eta^4 + S_\zeta^4].$$

The D term corresponds to the trigonal or tetragonal crystalline field components and incorporates a part of the spin-spin interactions. A slight distortion from cylindrical symmetry around the z axis is described by the E term. The cubic field is described on a set of orthogonal axes such that the z axis (trigonal axis of the crystal) lies in the (111) direction. They considered the E term of no importance. Bleaney and Trenam [18] introduced another term for the fourth degree part of the trigonal field and wrote the spin hamiltonian

$$\mathcal{H} = g\beta \mathbf{B} \cdot \mathbf{S} + D[S_z^2 - (1/3)S(S+1)] + (F/180)[35S_z^4 - 30S(S+1)S_z^2 + 25S_z^2 - 6S(S+1) + 3S^2(S+1)^2] + (a/6)[S_\xi^4 + S_\eta^4 + S_\zeta^4 - (1/5)S(S+1)(3S^2 - 3S - 1)],$$

which became the generally accepted form. Basically, this is the most general form if one imposes the following conditions:

(1) The triangular rule requires that the main quantum number of the spin hamiltonian for d-electrons should be 4 or less.

(2) Inversion symmetry rules out even values for the main quantum number.

(3) The C_3 symmetry implies that the azimuthal quantum number can only take the values $0, \pm 3$.

For sufficiently high fields ($g\beta B \gg a$) the energy levels have been calculated. Bleaney and Ingram [19] obtained by perturbation calculation the matrix elements of the allowed transition in the absence of the

fourth order terms. This calculation was completed by Bleaney and Trenam [18]. The results are:

$$\pm 5/2 \leftrightarrow \pm 3/2: \quad g\beta B = g\beta B_0$$
$$\mp [2D(3\cos^2\theta - 1) + 2pa + 1/6Fq] - 32\delta_1 + 4\delta_2 + \epsilon_1$$
$$\pm 3/2 \leftrightarrow \pm 1/2: \quad g\beta B = g\beta B_0$$
$$\mp [D(3\cos^2\theta - 1) - 5/2pa - 5/24Fq] + 4\delta_1 - 5\delta_2 + \epsilon_2$$
$$+1/2 \leftrightarrow -1/2: \quad g\beta B = g\beta B_0 + 16\delta_1 - 8\delta_2 + \epsilon_3.$$

In these expressions B is the magnetic field corresponding to a transition at the frequency ν and $B_0 = h\nu/g\beta$.

Following Kronig and Bouwkamp [20] we introduced

$$p = (1 - 5\phi), \quad \phi = (l^2m^2 + m^2n^2 + n^2l^2),$$

where (l, m, n) are the directions cosines of H referred to the axes of the cubic crystalline field. θ is the angle between H and the trigonal axis and

$$\epsilon_1 = \frac{a^2}{g\beta H_0}\,[(5/3)\phi(1 - 7\phi)]$$

$$\epsilon_2 = -\frac{a^2}{g\beta H_0}\,[(5/4)\delta(3 + 16\delta\phi - 625\phi^2)]$$

$$\epsilon_3 = \frac{a^2}{g\beta H_0}\,[(10/3)\phi(7 - 25\phi)]$$

$$q = 35\cos^4\theta - 30\cos^2\theta + 3$$
$$\delta_1 = (D^2/g\beta H_0)\cos^2\theta \sin^2\theta$$
$$\delta_2 = (D^2/4g\beta H_0)\sin^4\theta.$$

3. Calculation of Eigenvalues and Eigenfunctions of the Spin Hamiltonian

The general expression for spin hamiltonians, using the conventions introduced by Stevens [21] as reviewed by Hutchings [22], is given by

$$\mathcal{H} = \sum_n \sum_{m=0}^{n} B_n^m O_n^m,$$

where n is the "length" of the vector, m the azimuthal quantum number of its projection. The three restrictions mentioned in section 2 lead to a spin hamiltonian with three undetermined parameters

$$\mathcal{H} = B_2^0\, O_2^0 + B_4^0\, O_4^0 + B_4^3\, O_4^3 \qquad (1)$$

On the basis of the description of the crystal some coefficients are dominant, in particular, the term representing the trigonal field called $D = 3\, B_2^0$. Next in importance is probably the field of cubic symmetry, oriented in such a way that a body diagonal of the cube coincides with the three-fold axis of the trigonal field.

This field can be described in a coordinate system with the axes along the four-fold axes of the cube or in a system with the axes along the three-fold axis (plus two orthogonal axes, to be defined) of the crystal.

On the first set of axes we have in operator polynomials

$$\frac{a}{6}\left[S_\xi^4 + S_\eta^4 + S_\zeta^4 - \frac{1}{5}\,S(S+1)(3S^2 + 3S - 1)\right]$$
$$= \frac{a}{120}\,[O_4^0 + 5O_4^4]$$

This expression can be transformed into the second set of axes [22]. In figure 2 the z axis is in the (111) direction. The x axis is in the zoζ plane (fig. 3) and y is in the $\eta\xi$ plane:

$$(O_4^0 + 5O_4^4)_{\xi\eta\zeta} = -\frac{2}{3}\,(O_4^0 - 20\sqrt{2}\,O_4^3)_{xyz}$$

Finally it is assumed that the cube is distorted (elongated or compressed) along the z axis. This is accom-

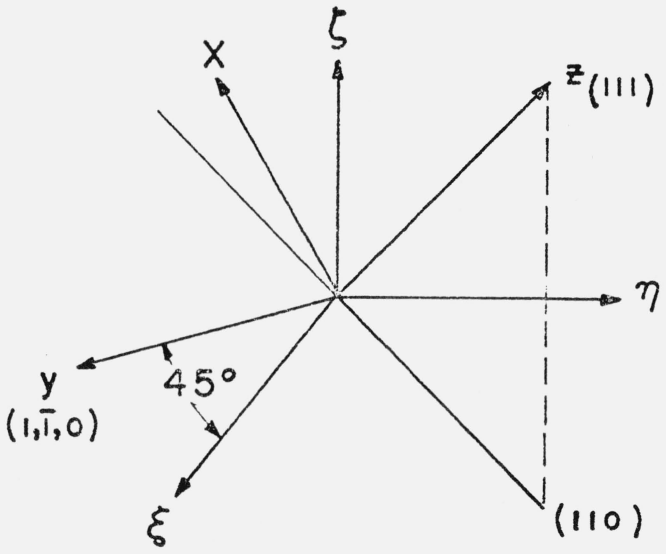

FIGURE 2. *Orientation of the* x y z *reference axes with respect to the* ξ, η, ζ *axes.*
The x axes is in the plane defined by ζ and (110) (see fig. 3).

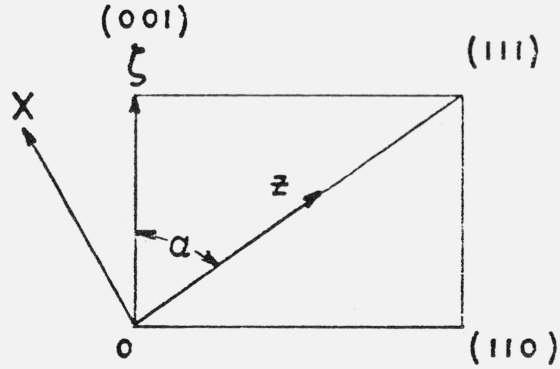

FIGURE 3. *Plane* $\zeta 0$ (110) *the angle* α *is defined by* $\mathrm{tg}\alpha = \sqrt{2}$.

plished by adding a term $F/180 = B_4^0$. Adding all contributions we have for the coefficients in eq (1)

$$B_2^0 = D/3,\ B_4^0 = (F-a)/180,\ B_4^3 = (\sqrt{2}/9)\ a.$$

$\|5/2\rangle$	$\|3/2\rangle$	$\|1/2\rangle$	$\|-1/2\rangle$	$\|-3/2\rangle$	$\|-5/2\rangle$
$10D/3-(a-F)/3$	0	0	$2\sqrt{5}\ a/3$	0	0
0	$-2D/3+(a-F)$	0	0	0	0
0	0	$-\pi\delta D/3-2(a-F)/3$	0	0	$-2\sqrt{5}\ a/3$
$2\sqrt{5}\ a/3$	0	0	$-8D/3-2(a-F)/3$	0	0
0	0	0	0	$-2D/3+(a-F)$	0
0	0	$-2\sqrt{5}\ a/3$	0	0	$10D/3-(a-F)/3$

To insert the magnetic field in this matrix we use polar coordinates:

$$B_z = B\cos\theta;\ B_x = B\sin\theta\cos\varphi;\ B_y = B\sin\theta\sin\varphi$$

where φ is the angle between the field and the xz plane as defined in figures 2 and 3. In the case of $\theta = 0$ the eigenvalues and eigenfunctions can be calculated directly:

$$E_{1,2} = \pm g\beta B + D/3 - (a-F)/2 - \Delta_\pm/2$$
$$E_{3,4} = \mp 3g\beta B/2 - 2D/3 + (a-F)$$
$$E_{5,6} = \mp g\beta B + D/3 - (a-F)/2 + \Delta_\mp/2$$

$$|\psi_{1,6}\rangle = 2\sqrt{5}/3\ aC_\pm\,|5/2\rangle \mp A_\pm/C_\pm\,|-1/2\rangle$$
$$|\psi_{2,5}\rangle = 2\sqrt{5}/3\ aD_\pm\,|1/2\rangle + B_\pm/D_\pm\,|-5/2\rangle$$
$$|\psi_{3,4}\rangle = |\mp 3/2\rangle$$

where

$$\Delta_\pm = [[3g\beta H \pm 6D \pm (a-F)/3]^2 + 80a^2/g]^{1/2}$$
$$A_\pm = [3g\beta H/2 + 3D + (a-F)/6 \pm \Delta_+]$$
$$B_\pm = [g\beta H/2 - 3D - (a-F)/6 \pm \Delta_-]$$
$$C_\pm = 20a^2/9 + A_\pm^2$$
$$D_\pm = 20a^2/9 + B_\pm^2$$

Note that for $\theta = 0$ (fig. 4) the levels $|-5/2\rangle$ and $|1/2\rangle$ do not cross, contrary to figures published elsewhere [5]. For θ different from zero the diagonalization cannot be accomplished by simple algebraic operations. The computation of these orientations is conveniently performed by computer. Moreover, each calculation has to be repeated for at least two different values of φ, differing by 60°, in order to obtain the spectra of both sites.

These coefficients can be easily translated in experimentally observable quantities with the exception of the sign of a.

The matrix describing the crystalline field expressed on the basis of the free spin eigenfunctions is:

4. Transition Probabilities

If the spin system previously described is placed in an rf magnetic field, B_{rf}, the time dependent interaction hamiltonian

$$\mathscr{H}_{int} = -\mu B_{rf} = g\beta B_{rf} \cdot S$$

will induce transitions between the energy levels.

The probability of a transition between the level E_i characterized by a wave function ψ_i and the level E_j characterized by ψ_j is proportional to the square of the matrix element of H_{int} between ψ_i and ψ_j:

$$W_{ij} \sim |\langle\psi_i|\mathscr{H}_{int}|\psi_j\rangle|^2$$

Since the ψ_i in most cases are not pure spin states, we have

$$|\psi_i\rangle = \sum_{n=-s}^{s} a_{in}|n\rangle$$

and

$$W_{ij} \sim |\sum_n \sum_m a_{in}^* a_{jm}\langle n|\mathscr{H}_{int}|m\rangle|^2 \qquad (2)$$

This expression was calculated for three polarizations of the magnetic field, along x, y, and z.

If an ultrasonic wave is applied to the lattice the periodic displacement of the ions will induce transitions between the energy levels, through the modulation of the crystalline electric field. This can be described assuming an interaction hamiltonian including two terms, one describing the modulation of the g-factor, the second one the modulation of the crystalline field parameters.

In the case of the Fe^{3+}, since the static spin hamiltonian includes, besides B_2^0, two other terms, B_4^0 and B_4^3, one would expect them to be also modulated by the ultrasonic wave. We have, however, neglected these

two terms on the basis that the ratios B_4^0/B_2^0 and B_4^3/B_2^0 are very small (of the order of 2 and 5%) provided that considerations about the static behavior can be carried over to the dynamic one. With these hypotheses the interaction hamiltonian can be written:

$$\mathcal{H}_{\text{int}} = \beta \mathbf{B} d g \mathbf{S} + \mathbf{S} \mathbf{d} \mathbf{S}$$

The first term is referred in the literature as the dipolar term, the second as the quadrupolar one. The relative importance of these two terms was discussed by Mattuck and Strandberg [3] who showed that in most cases the second one is dominant and experimental data seemed to confirm that fact [23–27] in the case of non-S state ions. In this expression δg and $d|$ are two second rank tensors related to the lattice strain ϵ as

$$dg_{ij} = \sum_{kl} F_{ijkl} \epsilon_{kl} \qquad \text{and} \qquad \mathbf{d}_{ij} = \sum_{kl} G_{ijkl} \epsilon_{kl}$$

where F_{ijkl} and G_{ijkl} are two fourth rank tensors (called the magnetoelastic tensors). Using the Voigt notation [28], they can be written as 6 by 6 matrices. Considering the fact that the point group symmetry at each Fe^{3+} site is C_3 the number of independent components of F or G is only 10. For the first site the G tensor can be written:

G_{11}	G_{12}	$-G_{33}/2$	G_{14}	$-G_{25}$	G_{16}
G_{12}	G_{11}	$-G_{33}/2$	$-G_{14}$	G_{25}	$-G_{16}$
$-(G_{11}+G_{12})$	$-(G_{11}+G_{12})$	G_{33}	0	0	0
G_{41}	$-G_{41}$	0	G_{44}	G_{45}	G_{52}
$-G_{52}$	G_{52}	0	$-G_{45}$	G_{44}	G_{41}
$-G_{16}$	G_{16}	0	G_{25}	G_{14}	$(G_{11}-G_{12})/2$

The tensor for the second site is similar except for the sign of G_{52}, G_{25}, G_{45}, and G_{16}. The interaction hamiltonian describing the "quadrupolar" term can now be written:

$$\mathcal{H}_{\text{quad}} = \mathbf{d}_{xx} S_x^2 + \mathbf{d}_{yy} S_y^2 + \mathbf{d}_{zz} S_z^2 + \mathbf{d}_{yz}(S_y S_z + S_z S_y) + \mathbf{d}_{zx}(S_z S_x + S_x S_z) + \mathbf{d}_{xy}(S_x S_y + S_y S_x).$$

Since the d's (or the G's) are not known for Fe^{3+} in Al_2O_3 and since we want to make it possible through a comparison with experimental data to evaluate the G's, we have calculated the matrix elements between the different wave functions of each term:

$$|\langle \psi_i | S_x^2 | \psi_j \rangle|^2, \ldots, |\langle \psi_i | S_x S_y + S_y S_x | \psi_j \rangle|^2, \ldots \quad (3)$$

the six (symmetrized) quadrupole moments.

5. Presentation of the Data

The energy level diagrams (figs. 4–10) were obtained by plotting the results of the calculation using steps of 0.025T (250G) except near crossover or noncrossover points, where the steps were decreased. The dotted lines represent the data for $\phi = 60°$.

The tables of numerical results use intervals for: θ, φ, and B (in 10^{-4} Tesla) larger than the ones computed in order to save space, but still maintain a representative sample. Each table consists of two parts:

(a) The normalized wave functions, where every other column gives the real part, alternated by the imaginary part. The first column is the corresponding energy in cm^{-1}. Note that the levels are arranged in ascending order. The lowest value is then called number one, the next lowest number two, etc. . . . This is

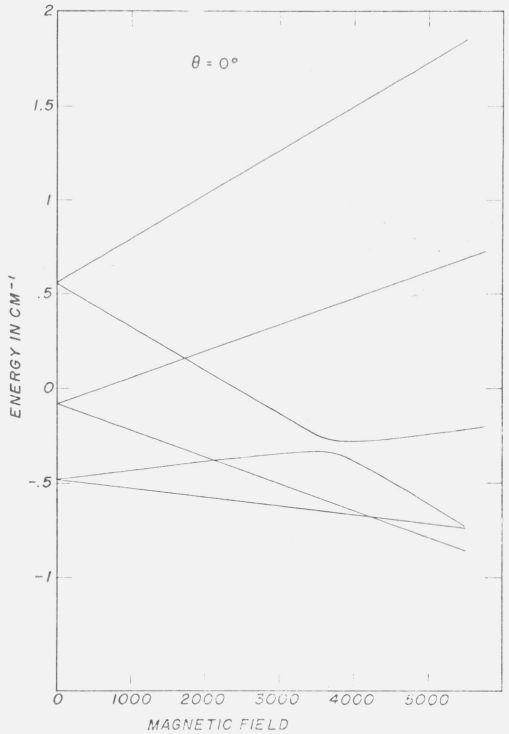

FIGURE 4. *Plot of the energy levels of* Fe^{3+} *in* Al_2O_3.
The solid line corresponds to $\varphi = 0$, the dotted line to $\varphi = 60°$. The Magnetic Field is in 10^{-4} Tesla.

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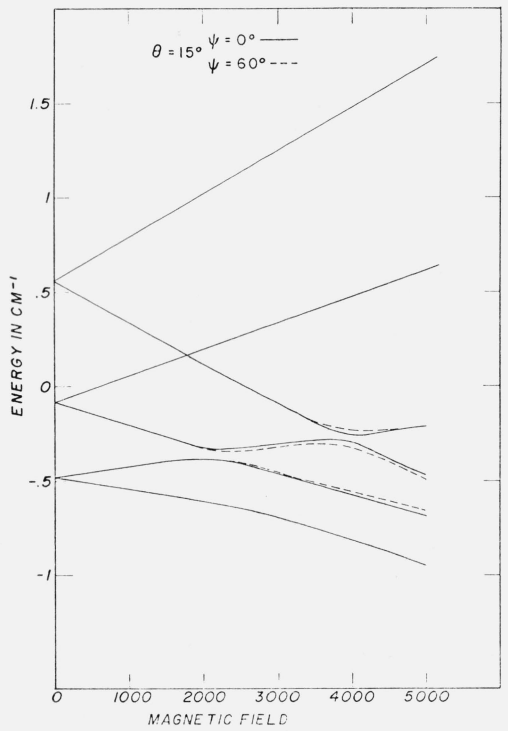

FIGURE 5. *Plot of the energy levels of* Fe^{3+} *in* Al_2O_3.

The solid line corresponds to $\varphi = 0$, the dotted line to $\varphi = 60°$. The Magnetic Field is in 10^{-4} · Tesla.

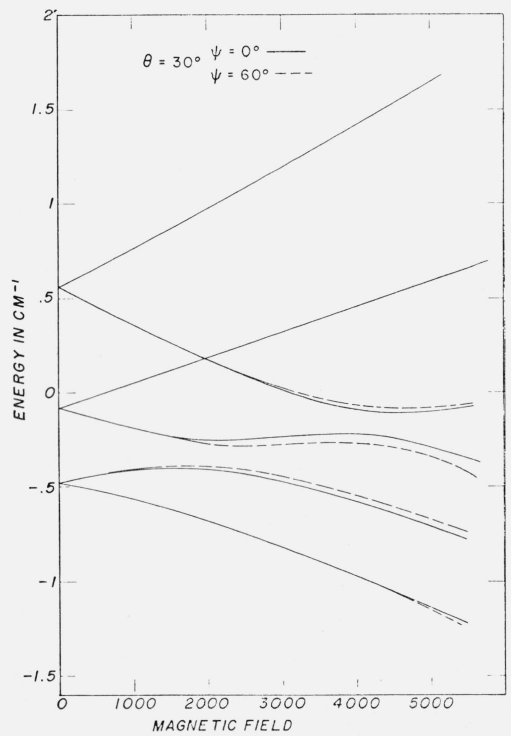

FIGURE 6. *Plot of the energy levels of* Fe^{3+} *in* Al_2O_3.

The solid line corresponds to $\varphi = 0$, the dotted line to $\varphi = 60°$. The Magnetic Field is in 10^{-4} · Tesla.

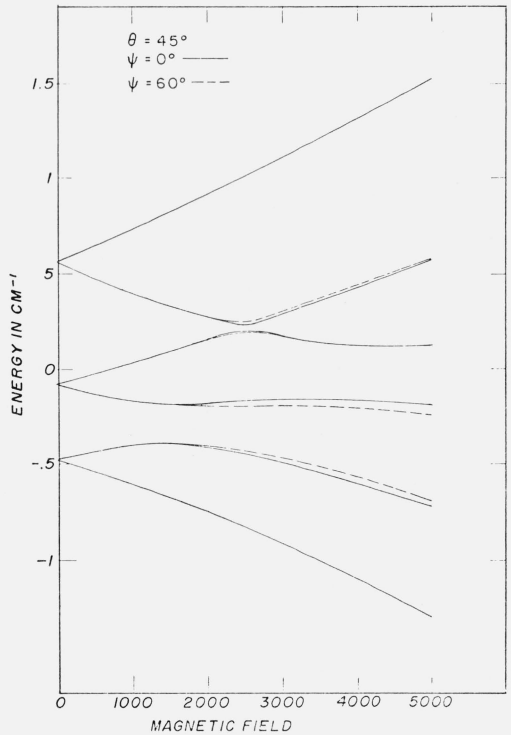

FIGURE 7. *Plot of the energy levels of* Fe^{3+} *in* Al_2O_3.

The solid line corresponds to $\varphi = 0$, the dotted line to $\varphi = 60°$. The Magnetic Field is in 10^{-4} · Tesla.

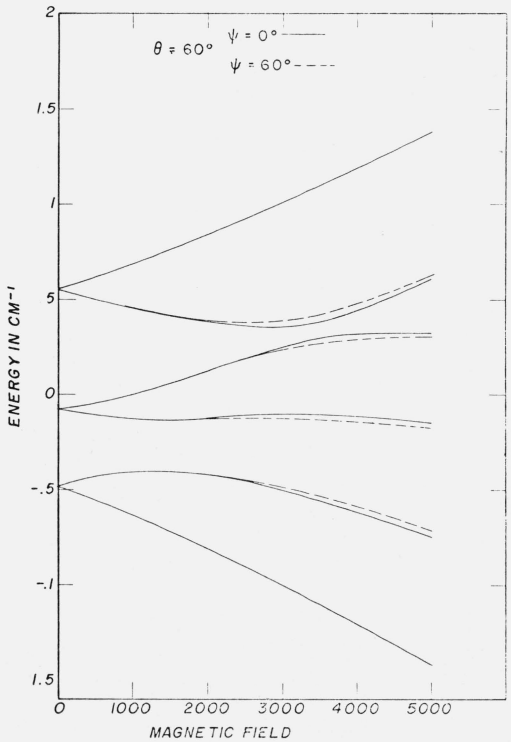

FIGURE 8. *Plot of the energy levels of* Fe^{3+} *in* Al_2O_3.

The solid line corresponds to $\varphi = 0$, the dotted line to $\varphi = 60°$. The Magnetic Field is in 10^{-4} · Tesla.

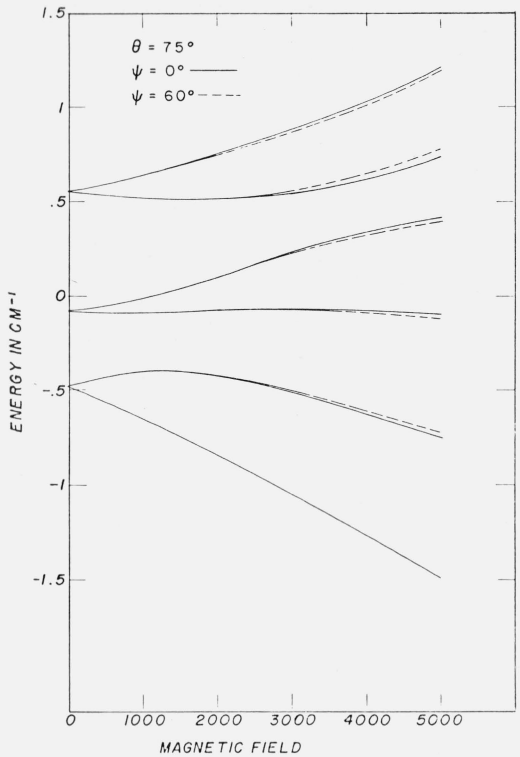

FIGURE 9. *Plot of the energy levels of* Fe^{3+} *in* Al_2O_3.

The solid line corresponds to $\varphi = 0$, the dotted line to $\varphi = 60°$. The Magnetic Field is in 10^{-4} · Tesla.

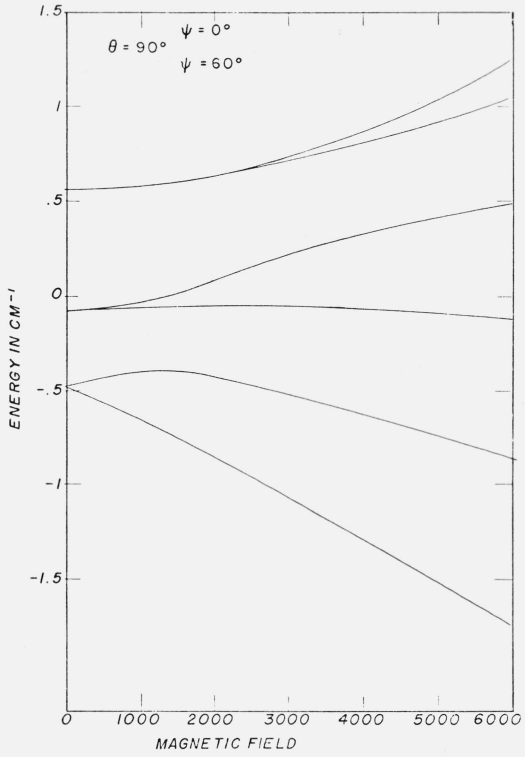

FIGURE 10. *Plot of the energy levels of* Fe^{3+} *in* Al_2O_3.

The solid line corresponds to $\varphi = 0$, the dotted line to $\varphi = 60°$. The Magnetic Field is in 10^{-4} · Tesla.

to establish the correspondence with the next part of each table.

(b) Tables that give the probabilities, i.e., absolute square of the matrix elements for dipole and quadrupole transitions between the energy level differences indicated. The column on the left gives the initial value i and the final value j which are of course interchangeable. The next column gives the positive energy difference in Gigahertz. The multiplication factor is 28.05 GHz/Tesla. The next three columns indicate the probabilities for a dipole transition in the x direction, the y direction, and the z direction. For $\theta = 0$, the first two are equal. The last six columns are the quadrupolar transition probabilities. The symbol PSXSX stands for the probability corresponding to an $S_X S_X$ transition. Similarly, PSXSY corresponds to $\frac{1}{2}(S_x S_y + S_y S_x)$. The tables are for $\varphi = 0$, except for $\theta = 45°$, where $\varphi = 0, 30, 60, 90$ is used to indicate the variation with φ.

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*

THETA = .00 PHI = .00 B = .0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.4823	.000	.000	.000	.000	.999	.000	.000	.000	.000	.000	.033	.000
−.4823	.033	.000	.000	.000	.000	.000	.999	.000	.000	.000	.000	.000
−.0805	.000	.000	.000	.000	.000	.000	.000	.000	1.000	.000	.000	.000
−.0805	.000	.000	1.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.5628	.999	.000	.000	.000	.000	.000	.033	.000	.000	.000	.000	.000
.5628	.000	.000	.000	.000	−.033	.000	.000	.000	.000	.000	.999	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	.00	2.245	2.245	.000	.000	.000	.000	.000	.000	.000
1–3	12.06	.001	.001	.000	4.495	4.495	.000	.005	.005	4.495
1–4	12.06	1.998	1.998	.000	.000	.000	.000	1.998	1.998	.000
1–5	31.35	.002	.002	.000	2.500	2.500	.000	.000	.000	2.500
1–6	31.35	.000	.000	.010	.010	.010	.039	.000	.000	.000
2–3	12.06	1.998	1.998	.000	.000	.000	.000	1.998	1.998	.000
2–4	12.06	.001	.001	.000	4.495	4.495	.000	.005	.005	4.495
2–5	31.35	.000	.000	.010	.010	.010	.039	.000	.000	.000
2–6	31.35	.002	.002	.000	2.500	2.500	.000	.000	.000	2.500
3–4	.00	.000	.000	.000	.000	.000	.000	.000	.000	.000
3–5	19.30	.002	.002	.000	.000	.000	.000	.002	.002	.000
3–6	19.30	1.249	1.249	.000	.005	.005	.000	4.995	4.995	.005
4–5	19.30	1.249	1.249	.000	.005	.005	.000	4.995	4.995	.005
4–6	19.30	.002	.002	.000	.000	.000	.000	.002	.002	.000
5–6	−.00	.000	.000	.000	.000	.000	.000	.000	.000	.000

THETA = .00 PHI = .00 B = 1000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.5289	.026	.000	.000	.000	.000	.000	1.000	.000	.000	.000	.000	.000
−.4360	.000	.000	.000	.000	.999	.000	.000	.000	.000	.000	.045	.000
−.2207	.000	.000	.000	.000	.000	.000	.000	.000	1.000	.000	.000	.000
.0598	.000	.000	1.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.3294	.000	.000	.000	.000	−.045	.000	.000	.000	.000	.000	.999	.000
.7964	1.000	.000	.000	.000	.000	.000	.026	.000	.000	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	2.79	2.244	2.244	.000	.001	.001	.000	.000	.000	.001
1–3	9.24	1.999	1.999	.000	.000	.000	.000	1.999	1.999	.000
1–4	17.66	.001	.001	.000	4.497	4.497	.000	.003	.003	4.497
1–5	25.75	.004	.004	.000	2.499	2.499	.000	.000	.000	2.499
1–6	39.76	.000	.000	.006	.006	.006	.024	.000	.000	.000
2–3	6.46	.003	.003	.000	4.491	4.491	.000	.010	.010	4.491
2–4	14.87	1.996	1.996	.000	.000	.000	.000	1.996	1.996	.000
2–5	22.96	.000	.000	.018	.018	.018	.072	.000	.000	.000
2–6	36.97	.001	.001	.000	2.499	2.499	.000	.000	.000	2.499
3–4	8.42	.000	.000	.000	.000	.000	.000	.000	.000	.000
3–5	16.50	1.247	1.247	.000	.009	.009	.000	4.990	4.990	.009
3–6	30.51	.001	.001	.000	.000	.000	.000	.001	.001	.000
4–5	8.09	.004	.004	.000	.000	.000	.000	.004	.004	.000
4–6	22.10	1.249	1.249	.000	.003	.003	.000	4.997	4.997	.003
5–6	14.01	.000	.000	.000	.001	.001	.000	.000	.000	.001

THETA = .00 PHI = .00 B = 2000.0

Energy levels and wave functions

E(CM-1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.5755	.021	.000	.000	.000	.000	.000	−1.000	.000	.000	.000	.000	.000
−.3901	.000	.000	.000	.000	.998	.000	.000	.000	.000	.000	.070	.000
−.3610	.000	.000	.000	.000	.000	.000	.000	.000	1.000	.000	.000	.000
.0965	.000	.000	.000	.000	−.070	.000	.000	.000	.000	.000	.998	.000
.2001	.000	.000	1.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
1.0300	1.000	.000	.000	.000	.000	.000	.021	.000	.000	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	5.56	2.238	2.238	.000	.006	.006	.000	.000	.000	.006
1–3	6.43	1.999	1.999	.000	.000	.000	.000	1.999	1.999	.000
1–4	20.16	.011	.011	.000	2.494	2.494	.000	.000	.000	2.494
1–5	23.27	.001	.001	.000	4.498	4.498	.000	.002	.002	4.498
1–6	48.16	.000	.000	.004	.004	.004	.016	.000	.000	.000
2–3	.87	.006	.006	.000	4.478	4.478	.000	.025	.025	4.478
2–4	14.60	.000	.000	.044	.044	.044	.178	.000	.000	.000
2–5	17.71	1.990	1.990	.000	.000	.000	.000	1.990	1.990	.000
2–6	42.60	.001	.001	.000	2.494	2.494	.000	.000	.000	2.494
3–4	13.73	1.244	1.244	.000	.022	.022	.000	4.975	4.975	.022
3–5	16.83	.000	.000	.000	.000	.000	.000	.000	.000	.000
3–6	41.73	.001	.001	.000	.000	.000	.000	.001	.001	.000
4–5	3.11	.010	.010	.000	.000	.000	.000	.010	.010	.000
4–6	28.00	.000	.000	.000	.006	.006	.000	.000	.000	.006
5–6	24.90	1.249	1.249	.000	.002	.002	.000	4.998	4.998	.002

THETA = .00 PHI = .00 B = 3000.0

Energy levels and wave functions

E(CM-1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.6221	.018	.000	.000	.000	.000	.000	−1.000	.000	.000	.000	.000	.000
−.5013	.000	.000	.000	.000	.000	.000	.000	.000	1.000	.000	.000	.000
−.3466	.000	.000	.000	.000	.987	.000	.000	.000	.000	.000	.163	−.000
−.1340	.000	.000	.000	.000	−.163	.000	.000	.000	.000	.000	.987	.000
.3404	.000	.000	1.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
1.2637	1.000	.000	.000	.000	.000	.000	.018	.000	.000	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	3.63	1.999	1.999	.000	.000	.000	.000	1.999	1.999	.000
1–3	8.27	2.189	2.189	.000	.053	.053	.000	.000	.000	.053
1–4	14.64	.060	.060	.000	2.447	2.447	.000	.000	.000	2.447
1–5	28.87	.000	.000	.000	4.499	4.499	.000	.002	.002	4.499
1–6	56.57	.000	.000	.003	.003	.003	.012	.000	.000	.000
2–3	4.64	.033	.033	.000	4.380	4.380	.000	.133	.133	4.380
2–4	11.02	1.217	1.217	.000	.120	.120	.000	4.867	4.867	.120
2–5	25.25	.000	.000	.000	.000	.000	.000	.000	.000	.000
2–6	52.95	.001	.001	.000	.000	.000	.000	.001	.001	.000
3–4	6.38	.000	.000	.233	.233	.223	.932	.000	.000	.000
3–5	20.61	1.947	1.947	.000	.000	.000	.000	1.947	1.947	.000
3–6	48.31	.001	.001	.000	2.447	2.447	.000	.000	.000	2.447
4–5	14.23	.053	.053	.000	.000	.000	.000	.053	.053	.000
4–6	41.93	.000	.000	.000	.053	.053	.000	.000	.000	.053
5–6	27.70	1.250	1.250	.000	.001	.001	.000	4.998	4.998	.001

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = .00 PHI = .00 B = 4000.0

Energy levels and wave functions

E(CM-1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.6688	.016	.000	.000	.000	.000	.000	−1.000	.000	.000	.000	.000	.000
−.6416	.000	.000	.000	.000	.000	.000	.000	.000	1.000	.000	.000	.000
−.3862	.000	.000	.000	.000	.348	.000	.000	.000	.000	.000	.937	.000
−.2815	.000	.000	.000	.000	−.937	.000	.000	.000	.000	.000	.348	.000
.4806	.000	.000	1.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
1.4974	1.000	.000	.000	.000	.000	.000	.016	.000	.000	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	.82	2.000	2.000	.000	.000	.000	.000	2.000	2.000	.000
1–3	8.48	.273	.273	.000	2.170	2.170	.000	.000	.000	2.170
1–4	11.62	1.976	1.976	.000	.330	.330	.000	.000	.000	.330
1–5	34.48	.000	.000	.000	4.499	4.499	.000	.001	.001	4.499
1–6	64.98	.000	.000	.002	.002	.002	.009	.000	.000	.000
2–3	7.66	1.098	1.098	.000	.546	.546	.000	4.393	4.393	.546
2–4	10.80	.152	.152	.000	3.954	3.954	.000	.607	.607	3.954
2–5	33.67	.000	.000	.000	.000	.000	.000	.000	.000	.000
2–6	64.17	.000	.000	.000	.000	.000	.000	.000	.000	.000
3–4	3.14	.000	.000	.960	.960	.960	3.841	.000	.000	.000
3–5	26.00	.243	.243	.000	.000	.000	.000	.243	.243	.000
3–6	56.51	.000	.000	.000	.330	.330	.000	.000	.000	.330
4–5	22.86	1.757	1.757	.000	.000	.000	.000	1.757	1.757	.000
4–6	53.37	.000	.000	.000	2.170	2.170	.000	.000	.000	2.170
5–6	30.50	1.250	1.250	.000	.001	.001	.000	4.999	4.999	.001

THETA = .00 PHI = .00 B = 5000.0

Energy levels and wave functions

E(CM-1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.7818	.000	.000	.000	.000	.000	.000	.000	.000	1.000	.000	.000	.000
−.7155	.014	.000	.000	.000	.000	.000	−1.000	.000	.000	.000	.000	.000
−.6105	.000	.000	.000	.000	.094	.000	.000	.000	.000	.000	.996	.000
−.2442	.000	.000	.000	.000	−.996	.000	.000	.000	.000	.000	.094	.000
.6209	.000	.000	1.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
1.7311	1.000	.000	.000	.000	.000	.000	.014	.000	.000	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	1.99	2.000	2.000	.000	.000	.000	.000	2.000	2.000	.000
1–3	5.14	1.239	1.239	.000	.040	.040	.000	4.956	4.956	.040
1–4	16.13	.011	.011	.000	4.460	4.460	.000	.044	.044	4.460
1–5	42.08	.000	.000	.000	.000	.000	.000	.000	.000	.000
1–6	75.39	.000	.000	.000	.000	.000	.000	.000	.000	.000
2–3	3.15	.020	.020	.000	2.471	2.471	.000	.000	.000	2.471
2–4	14.14	2.230	2.230	.000	.029	.029	.000	.000	.000	.029
2–5	40.09	.000	.000	.000	4.499	4.499	.000	.001	.001	4.499
2–6	73.40	.000	.000	.002	.002	.002	.007	.000	.000	.000
3–4	10.99	.000	.000	.078	.078	.078	.314	.000	.000	.000
3–5	36.94	.018	.018	.000	.000	.000	.000	.018	.018	.000
3–6	70.25	.000	.000	.000	.029	.029	.000	.000	.000	.029
4–5	25.95	1.982	1.982	.000	.000	.000	.000	1.982	1.982	.000
4–6	59.26	.000	.000	.000	2.471	2.471	.000	.000	.000	2.471
5–6	33.31	1.250	1.250	.000	.001	.001	.000	4.999	4.999	.001

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 15.00 PHI = .00 B = 1000.0

Energy levels and wave functions

E(CM-1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.5435	.025	.000	−.020	.000	.327	.000	−.939	.000	.097	.000	.010	.000
−.4276	.008	.000	.066	.000	−.941	.000	−.323	.000	.058	.000	−.044	.000
−.2134	−.004	.000	−.003	.000	.025	.000	.111	.000	.992	.000	−.047	.000
.0564	−.037	.000	.997	.000	.069	.000	.002	.000	.001	.000	.008	.000
.3387	.000	.000	−.005	.000	−.044	.000	.000	.000	.049	.000	.998	.000
.7894	−.999	.000	−.037	.000	−.002	.000	−.026	.000	−.001	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	3.48	1.212	2.326	.099	.062	.058	.000	.002	.036	.169
1–3	9.90	1.639	1.586	.008	.449	.740	.036	1.866	1.664	.554
1–4	18.00	.153	.115	.000	3.914	4.091	.002	.168	.265	3.930
1–5	26.46	.011	.000	.001	2.198	2.001	.005	.022	.024	2.108
1–6	39.99	.000	.000	.005	.137	.267	.021	.001	.001	.197
2–3	6.43	.435	.316	.007	4.008	3.515	.016	.137	.307	3.779
2–4	14.52	1.825	1.890	.005	.476	.315	.017	1.837	1.715	.378
2–5	22.99	.004	.000	.016	.230	.547	.067	.015	.010	.366
2–6	36.51	.000	.004	.001	2.362	2.209	.003	.009	.010	2.297
3–4	8.09	.003	.002	.000	.146	.142	.000	.004	.000	.142
3–5	16.56	1.221	1.266	.002	.031	.000	.035	4.957	4.914	.074
3–6	30.08	.001	.001	.000	.004	.002	.000	.002	.002	.003
4–5	8.47	.004	.004	.001	.000	.001	.002	.004	.004	.000
4–6	21.99	1.256	1.240	.001	.057	.008	.022	4.977	4.972	.003
5–6	13.52	.000	.000	.000	.001	.001	.000	.000	.000	.001

THETA = 15.00 PHI = .00 B = 2000.0

Energy levels and wave functions

E(CM-1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.6144	.021	.000	−.027	.000	.307	.000	−.920	.000	.240	.000	−.003	.000
−.3891	.000	.000	.101	.000	−.858	.000	−.168	.000	.462	.000	−.109	.000
−.3277	−.007	.000	−.051	.000	.390	.000	.353	.000	.846	.000	−.074	.000
.1183	−.004	.000	.058	.000	−.058	.000	.005	.000	.115	.000	.990	.000
.1952	−.066	.000	.989	.000	.120	.000	.008	.000	−.004	.000	−.051	.000
1.0176	.998	.000	.066	.000	.004	.000	.022	.000	.001	.000	−.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	6.76	.247	3.392	.145	.092	.007	.048	.352	.644	1.155
1–3	8.60	2.012	.282	.007	.546	1.319	.168	1.583	.977	.128
1–4	21.98	.052	.000	.002	2.334	2.240	.001	.162	.125	1.498
1–5	24.29	.080	.065	.000	3.226	3.458	.004	.134	.245	3.908
1–6	48.96	.000	.000	.004	.088	.175	.015	.002	.001	.128
2–3	1.84	.299	.529	.565	2.265	.469	.672	.089	.136	3.215
2–4	15.22	.162	.287	.050	.078	.654	.280	.917	1.103	.158
2–5	17.53	1.564	1.474	.008	.058	.000	.053	1.665	1.329	.029
2–6	42.20	.000	.006	.000	1.907	1.865	.000	.017	.018	1.904
3–4	13.38	.997	1.004	.000	.503	.209	.063	3.888	3.539	.505
3–5	15.69	.315	.468	.003	.847	.703	.007	.220	.380	.896
3–6	40.36	.000	.000	.001	.477	.414	.002	.010	.011	.450
4–5	2.31	.008	.007	.044	.023	.001	.034	.009	.005	.003
4–6	26.98	.004	.004	.000	.002	.004	.000	.014	.014	.003
5–6	24.67	1.253	1.231	.004	.134	.011	.070	4.938	4.902	.020

THETA = 15.00 PHI = .00 B = 3000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.7021	.016	.000	−.028	.000	.267	.000	−.862	.000	.428	.000	−.044	.000
−.4709	−.009	.000	.049	.000	−.374	.000	.312	.000	.842	.000	−.228	.000
−.3138	.002	.000	.139	.000	−.868	.000	−.399	.000	−.258	.000	−.044	.000
−.0946	.002	.000	−.028	.000	.114	.000	−.017	.000	−.205	.000	−.972	.000
.3345	−.089	.000	.984	.000	.151	.000	.014	.000	.001	.000	−.011	.000
1.2470	.996	.000	.089	.000	.007	.000	.019	.000	.001	.000	−.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	6.93	.119	2.702	.233	.007	.483	.603	1.818	1.377	1.474
1–3	11.65	1.243	.602	.018	.979	1.454	.047	.251	.001	.863
1–4	18.22	.147	.005	.001	1.763	1.982	.006	.482	.426	1.112
1–5	31.10	.040	.031	.000	2.727	2.930	.004	.107	.169	2.957
1–6	58.47	.000	.000	.002	.047	.096	.009	.002	.001	.070
2–3	4.71	.777	.802	.286	.964	1.799	.129	.019	.164	2.152
2–4	11.29	.786	1.184	.100	.386	.130	.966	3.990	3.450	.258
2–5	24.16	.207	.177	.001	.815	1.042	.014	.313	.285	.951
2–6	51.54	.001	.002	.000	.253	.295	.002	.002	.002	.276
3–4	6.58	.179	.208	.060	.591	1.265	.127	.438	.415	1.054
3–5	19.45	1.695	1.778	.020	.851	.419	.076	1.581	1.448	.649
3–6	46.83	.000	.003	.001	2.131	2.035	.001	.042	.044	2.102
4–5	12.87	.024	.023	.004	.020	.018	.000	.031	.027	.019
4–6	40.25	.000	.001	.000	.019	.022	.000	.002	.002	.021
5–6	27.38	1.255	1.232	.008	.209	.010	.127	4.923	4.853	.041

THETA = 15.00 PHI = .00 B = 4000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.8139	.013	.000	−.024	.000	.211	.000	−.754	.000	.609	.000	−.124	.000
−.5767	−.011	.000	.046	.000	−.342	.000	.520	.000	.689	.000	−.367	.000
−.3012	−.002	.000	−.040	.000	.225	.000	.239	.000	.391	.000	.859	.000
−.2598	.004	.000	−.166	.000	.870	.000	.322	.000	.021	.000	−.335	.000
.4744	.108	.000	−.978	.000	−.177	.000	−.020	.000	−.002	.000	.007	.000
1.4772	.994	.000	.107	.000	.010	.000	.017	.000	.001	.001	−.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	7.11	.003	2.437	.344	.216	.418	1.234	2.220	1.010	1.784
1–3	15.38	.015	.123	.001	.218	.396	.026	.426	.758	1.352
1–4	16.62	.882	.334	.009	2.543	3.531	.081	.587	.016	.842
1–5	38.65	.014	.011	.000	1.794	1.923	.002	.062	.099	1.923
1–6	68.73	.000	.000	.001	.018	.042	.005	.001	.001	.029
2–3	8.26	1.232	.331	.078	1.606	.008	1.838	2.901	2.216	.087
2–4	9.51	.512	1.995	.329	.062	1.002	.565	.604	.120	1.380
2–5	31.53	.114	.095	.001	1.739	2.059	.013	.249	.255	1.942
2–6	61.62	.000	.001	.001	.150	.195	.003	.001	.001	.173
3–4	1.24	.143	.288	.602	3.159	.007	2.876	.260	.001	1.495
3–5	23.27	.147	.160	.001	.467	.325	.013	.100	.089	.403
3–6	53.35	.000	.000	.000	.201	.182	.000	.004	.005	.193
4–5	22.02	1.683	1.740	.031	.445	.126	.097	1.630	1.465	.274
4–6	52.11	.001	.005	.000	2.055	2.022	.000	.055	.057	2.061
5–6	30.09	1.252	1.231	.012	.282	.010	.186	4.899	4.789	.062

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 15.00 PHI = .00 B = 5000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.9509	.009	.000	−.018	.000	.156	.000	−.626	.000	.725	.000	−.242	.000
−.6870	−.011	.000	.045	.000	−.326	.000	.625	.000	.421	.000	−.570	.000
−.4692	−.006	.000	.022	.000	−.133	.000	.283	.000	.535	.000	.784	.000
−.2154	.007	.000	−.191	.000	.902	.000	.370	.000	.105	.000	−.047	.000
.6145	.123	.000	−.972	.000	−.197	.000	−.024	.000	−.002	.000	.005	.000
1.7080	.992	.000	.123	.000	.012	.000	.015	.000	.001	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	7.92	.027	2.315	.401	.713	.348	2.056	2.914	.814	2.178
1–3	14.45	.256	.002	.001	.598	1.290	.131	.635	.622	.072
1–4	22.06	.369	.220	.002	2.151	2.872	.052	.258	.049	2.017
1–5	46.96	.004	.003	.000	1.010	1.072	.001	.029	.049	1.074
1–6	79.77	.000	.000	.001	.005	.014	.003	.001	.001	.009
2–3	6.53	.151	1.005	.509	1.454	1.042	4.957	2.968	.515	.601
2–4	14.15	1.073	1.295	.167	.000	.053	.054	.000	.000	.100
2–5	39.04	.072	.060	.000	2.073	2.420	.013	.213	.231	2.293
2–6	71.85	.000	.000	.001	.104	.143	.003	.001	.001	.123
3–4	7.62	.579	.676	.012	1.916	1.602	.014	.224	.146	1.984
3–5	32.51	.008	.006	.001	.718	.760	.001	.044	.045	.752
3–6	65.32	.000	.000	.000	.008	.014	.001	.000	.000	.010
4–5	24.90	1.868	1.936	.039	.658	.190	.141	1.762	1.566	.404
4–6	57.70	.001	.004	.000	2.284	2.268	.000	.072	.074	2.301
5–6	32.81	1.249	1.230	.016	.349	.009	.244	4.879	4.728	.082

THETA = 30.00 PHI = .00 B = 1000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.5737	.024	.000	−.054	.000	.483	.000	−.860	.000	.152	.000	.009	.000
−.4144	.008	.000	.124	.000	−.862	.000	−.464	.000	.156	.000	−.049	.000
−.1925	−.007	.000	−.017	.000	.066	.000	.209	.000	.972	.000	−.088	.000
.0462	−.073	.000	.988	.000	.135	.000	.013	.000	.006	.000	.014	.000
.3655	.001	.000	−.009	.000	−.043	.000	.004	.000	.092	.000	.995	.000
.7689	.997	.000	.072	.000	.005	.000	.027	.000	.002	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	4.78	.400	2.445	.204	.075	.058	.001	.010	.211	.565
1–3	11.44	1.197	1.018	.013	.999	1.665	.085	1.643	1.277	1.087
1–4	18.60	.279	.238	.002	3.118	3.537	.013	.403	.528	3.263
1–5	28.18	.013	.000	.003	1.691	1.480	.007	.046	.054	1.597
1–6	40.28	.000	.001	.004	.317	.490	.019	.007	.005	.400
2–3	6.66	.891	.772	.049	3.189	2.134	.106	.361	.576	2.847
2–4	13.82	1.668	1.741	.016	.934	.528	.058	1.605	1.405	.662
2–5	23.40	.019	.004	.014	.598	1.075	.070	.099	.076	.794
2–6	35.50	.000	.008	.001	2.127	1.938	.004	.032	.035	2.055
3–4	7.16	.026	.021	.001	.523	.485	.001	.016	.001	.494
3–5	16.74	1.190	1.272	.007	.178	.006	.120	4.839	4.730	.188
3–6	28.84	.001	.001	.001	.026	.015	.001	.005	.005	.021
4–5	9.58	.002	.002	.003	.001	.008	.004	.005	.006	.004
4–6	21.68	1.261	1.228	.005	.174	.016	.085	4.929	4.893	.025
5–6	12.10	.000	.000	.000	.001	.001	.000	.001	.001	.001

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 30.00 PHI = .00 B = 2000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.6862	.022	.000	−.072	.000	.442	.000	−.838	.000	.311	.000	−.021	.000
−.4005	−.009	.000	.181	.000	−.765	.000	−.207	.000	.561	.000	−.152	.000
−.2551	−.003	.000	−.128	.000	.405	.000	.502	.000	.737	.000	−.154	.000
.1738	.096	.000	−.712	.000	−.137	.000	−.049	.000	−.152	.000	−.663	.000
.1870	.087	.000	−.650	.000	−.189	.000	−.006	.000	.145	.000	.716	.000
.9810	.991	.000	.129	.000	.015	.000	.023	.000	.002	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	8.57	.039	3.046	.298	.070	.006	.117	.391	1.187	2.434
1–3	12.93	1.047	.064	.002	1.122	2.420	.246	1.438	.445	.127
1–4	25.80	.148	.045	.005	3.729	4.134	.010	.498	.034	.256
1–5	26.20	.011	.066	.000	.048	.106	.011	.005	.562	3.646
1–6	50.02	.000	.000	.003	.173	.278	.012	.009	.006	.223
2–3	4.36	.248	1.141	.668	.997	.006	.850	.276	.254	1.907
2–4	17.23	.227	1.353	.074	.166	.334	.029	.001	2.443	.162
2–5	17.62	1.259	.143	.002	.022	.775	.536	2.841	.010	.180
2–6	41.45	.002	.010	.000	1.533	1.538	.000	.059	.061	1.560
3–4	12.87	1.457	.012	.001	3.332	1.587	.320	2.782	.631	.065
3–5	13.26	.028	1.652	.040	.009	.141	.079	.817	2.518	2.649
3–6	37.08	.000	.002	.001	.656	.580	.002	.052	.056	.632
4–5	.40	.002	.001	3.796	.918	.923	3.681	.011	.256	.054
4–6	24.22	.685	.666	.010	.234	.009	.150	2.583	2.501	.050
5–6	23.82	.571	.548	.008	.225	.015	.124	2.235	2.166	.056

THETA = 30.00 PHI = .00 B = 3000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.8195	.019	.000	−.073	.000	.390	.000	−.795	.000	.452	.000	−.074	.000
−.4764	−.018	.000	.159	.000	−.593	.000	.130	.000	.715	.000	−.307	.000
−.2352	−.014	.000	.248	.000	−.639	.000	−.578	.000	−.391	.000	.208	.000
.0162	−.005	.000	.014	.000	−.015	.000	.111	.000	.361	.000	.925	.000
.3172	.175	.000	−.937	.000	−.295	.000	−.064	.000	−.012	.000	.023	.000
1.1976	.984	.000	.174	.000	.025	.000	.022	.000	.003	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	10.29	.000	2.686	.390	.092	.208	.576	1.116	1.714	3.428
1–3	17.53	.707	.081	.006	1.550	2.991	.235	1.035	.017	.208
1–4	25.07	.037	.004	.001	.794	.959	.008	.275	.279	.684
1–5	34.10	.048	.046	.002	1.707	2.081	.018	.211	.305	2.101
1–6	60.51	.000	.000	.002	.083	.144	.008	.007	.005	.112
2–3	7.24	.105	1.553	.750	.034	.462	.745	.267	.097	.931
2–4	14.78	.457	.535	.105	.087	.789	1.401	2.799	2.033	.026
2–5	23.81	.525	.455	.012	.416	1.039	.140	.935	.708	.715
2–6	50.22	.001	.005	.000	.675	.752	.002	.034	.033	.724
3–4	7.54	.625	.696	.052	2.827	.641	.776	1.495	.954	1.728
3–5	16.57	1.333	1.468	.088	1.918	.890	.195	.958	.720	1.507
3–6	42.99	.004	.010	.001	1.477	1.468	.000	.155	.164	1.510
4–5	9.03	.004	.006	.004	.339	.247	.007	.009	.005	.302
4–6	35.44	.001	.001	.000	.007	.003	.001	.000	.000	.005
5–6	26.41	1.244	1.203	0.33	.765	.028	.499	4.704	4.405	.198

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 30.00 PHI = .00 B = 4000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.9716	.017	.000	−.068	.000	.338	.000	−.740	.000	.558	.000	−.145	.000
−.5848	−.021	.000	.146	.000	−.530	.000	.310	.000	.633	.000	−.447	.000
−.2160	.028	.000	−.290	.000	.659	.000	.451	.000	.027	.000	−.526	.000
−.1014	−.009	.000	.123	.000	−.229	.000	−.380	.000	−.535	.000	−.708	.000
.4563	.211	.000	−.911	.000	−.342	.000	−.086	.000	−.020	.000	.011	.000
1.4175	.977	.000	.211	.000	.036	.000	.021	.000	.003	.000	−.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	11.60	.005	2.352	.467	.311	.268	1.157	1.545	1.722	3.456
1–3	22.67	.513	.105	.009	2.158	4.000	.282	1.214	.014	.312
1–4	26.11	.002	.023	.000	.012	.013	.000	.027	.289	.767
1–5	42.84	.019	.018	.001	1.163	1.419	.013	.137	.196	1.397
1–6	71.67	.000	.000	.001	.037	.070	.005	.005	.003	.052
2–3	11.06	.117	2.238	.853	.247	.741	1.844	1.069	.536	.271
2–4	14.50	.573	.044	.019	.191	.679	1.590	2.173	.801	.009
2–5	31.23	.260	.225	.006	.978	1.784	.120	.712	.600	1.410
2–6	60.07	.000	.002	.000	.380	.453	.003	.022	.020	.422
3–4	3.44	.143	.815	.910	2.838	.202	4.557	.961	.000	2.078
3–5	20.17	1.268	1.334	.111	.720	.102	.280	1.211	.831	.382
3–6	49.01	.007	.012	.000	1.375	1.484	.002	.186	.191	1.467
4–5	16.73	.340	.380	.022	1.582	.997	.067	.088	.047	1.338
4–6	45.57	.001	.001	.000	.341	.341	.000	.047	.050	.351
5–6	28.84	1.231	1.199	.050	1.053	.030	.729	4.603	4.151	.288

THETA = 30.00 PHI = .00 B = 5000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.1395	.014	.000	−.060	.000	.292	.000	−.682	.000	.629	.000	−.224	.000
−.7079	−.022	.000	.136	.000	−.492	.000	.418	.000	.493	.000	−.567	.000
−.2889	−.027	.000	.208	.000	−.492	.000	−.110	.000	.393	.000	.740	.000
−.1000	.034	.000	−.297	.000	.535	.000	.580	.000	.454	.000	.286	.000
.5964	−.241	.000	.888	.000	.377	.000	.103	.000	.025	.000	−.006	.000
1.6398	−.969	.000	−.241	.000	−.046	.000	−.022	.000	−.003	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	12.95	.026	2.120	.526	.708	.273	1.861	1.916	1.571	3.473
1–3	25.52	.284	.066	.007	1.485	3.047	.278	.993	.052	.145
1–4	31.19	.091	.056	.001	.565	.954	.051	.157	.190	1.087
1–5	52.08	.007	.007	.001	.753	.913	.008	.084	.122	.896
1–6	83.38	.000	.000	.001	.015	.033	.003	.003	.002	.023
2–3	12.57	.026	1.974	.892	.785	1.392	4.268	2.482	.535	.075
2–4	18.24	.597	.310	.061	.006	.475	.372	.726	.006	.013
2–5	39.13	.141	.121	.003	1.218	2.024	.102	.565	.504	1.665
2–6	70.43	.000	.001	.000	.232	.290	.003	.015	.013	.263
3–4	5.67	.381	1.062	.982	.017	2.645	2.239	.714	.733	2.125
3–5	26.56	.431	.434	.041	.048	.386	.162	.802	.583	.170
3–6	57.86	.003	.006	.000	.510	.594	.003	.071	.071	.565
4–5	20.89	1.280	1.388	.128	2.432	.992	.318	.730	.416	1.743
4–6	52.19	.006	.009	.000	1.284	1.421	.003	.224	.229	1.389
5–6	31.30	1.217	1.196	.065	1.312	.030	.947	4.516	3.916	.369

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 45.00 PHI = .00 B = 1000.0

Energy levels and wave functions

E(CM−1)	(5/2)	(3/2)	(1/2)	(−1/2)	(−3/2)	(−5/2)
−.6051	.025 .000	−.087 .000	.561 .000	−.804 .000	.176 .000	.006 .000
−.4058	.004 .000	.175 .000	−.797 .000	−.525 .000	.235 .000	−.056 .000
−.1616	.007 .000	.047 .000	−.095 .000	−.277 .000	−.947 .000	.120 .000
.0296	.105 .000	−.974 .000	−.196 .000	−.033 .000	−.020 .000	−.014 .000
.4072	−.001 .000	.009 .000	.040 .000	−.009 .000	−.126 .000	−.991 .000
.7357	.994 .000	.104 .000	.011 .000	.028 .000	.003 .000	−.000 .000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	5.98	.125	2.520	.269	.042	.024	.003	.018	.439	1.024
1–3	13.30	.913	.647	.011	1.384	2.285	.112	1.505	.984	1.257
1–4	19.04	.321	.295	.005	2.509	3.106	.032	.544	.694	2.847
1–5	30.37	.011	.000	.003	1.326	1.142	.007	.053	.064	1.242
1–6	40.22	.000	.002	.004	.411	.602	.018	.016	.012	.504
2–3	7.32	1.068	1.107	.108	2.405	1.170	.220	.509	.747	2.199
2–4	13.06	1.588	1.606	.032	1.123	.515	.117	1.471	1.172	.681
2–5	24.39	.034	.012	.012	.823	1.397	.076	.213	.171	1.043
2–6	34.24	.002	.012	.002	1.938	1.763	.004	.066	.072	1.883
3–4	5.74	.071	.063	.007	.961	.848	.004	.029	.001	.885
3–5	17.06	1.166	1.269	.013	.371	.019	.223	4.697	4.517	.298
3–6	26.92	.000	.000	.001	.061	.041	.002	.015	.017	.052
4–5	11.33	.001	.001	.003	.008	.026	.005	.010	.011	.017
4–6	21.18	1.263	1.214	.012	.344	.027	.179	4.854	4.767	.067
5–6	9.86	.000	.000	.000	.000	.000	.000	.001	.001	.000

THETA = 45.00 PHI = .00 B = 2000.0

Energy levels and wave functions

E(CM−1)	(5/2)	(3/2)	(1/2)	(−1/2)	(−3/2)	(−5/2)
−.7552	.027−.000	−.116−.000	.518−.000	−.785−.000	.317−.000	−.030−.000
−.4139	−.022−.000	.257−.000	−.714−.000	−.276−.000	.565−.000	−.167−.000
−.1827	−.012−.000	.210−.000	−.328−.000	−.543−.000	−.709−.000	.226−.000
.1554	−.188−.000	.916−.000	.333−.000	.100−.000	.057−.000	.040−.000
.2748	.008 .000	−.046 .000	−.045 .000	.052 .000	.273 .000	.958 .000
.9215	.981 .000	.188 .000	.030 .000	.027 .000	.004 .000	−.001 .000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	10.24	.013	2.776	.385	.044	.013	.106	.273	1.520	3.170
1–3	17.17	.681	.034	.000	1.500	3.114	.292	1.524	.278	.149
1–4	27.32	.122	.119	.005	1.826	2.447	.045	.415	.510	2.138
1–5	30.90	.013	.003	.002	.740	.713	.000	.110	.171	.909
1–6	50.30	.000	.001	.002	.205	.324	.014	.019	.014	.261
2–3	6.94	.246	1.581	.671	.625	.016	.843	.412	.550	1.101
2–4	17.08	1.109	1.087	.052	.073	.062	.270	1.300	1.091	.012
2–5	20.66	.236	.137	.030	.263	1.419	.460	1.514	1.012	.566
2–6	40.06	.006	.016	.000	1.363	1.427	.001	.123	.129	1.432
3–4	10.14	.745	.622	.092	2.699	1.617	.138	.388	.068	1.923
3–5	13.73	.865	1.177	.060	1.691	.166	.797	3.160	2.739	1.264
3–6	33.13	.007	.010	.001	.568	.562	.000	.154	.164	.593
4–5	3.58	.005	.006	.038	.135	.285	.028	.027	.054	.217
4–6	22.98	1.242	1.180	.040	.982	.051	.586	4.563	4.225	.264
5–6	19.40	.002	.002	.000	.000	.000	.001	.018	.017	.000

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 45.00 PHI = .00 B = 3000.0

Energy levels and wave functions

E(CM−1)	(5/2)	(3/2)	(1/2)	(−1/2)	(−3/2)	(−5/2)
−.9238	.027 .000	−.122 .000	.475 .000	−.758 .000	.422 .000	−.078 .000
−.4953	−.036 .000	.260 .000	−.632 .000	−.039 .000	.663 .000	−.301 .000
−.1643	−.046 .000	.349 .000	−.438 .000	−.609 .000	−.434 .000	.353 .000
.1754	−.009 .000	.062 .000	−.002 .000	−.163 .000	−.436 .000	−.883 .000
.2908	−.254 .000	.853 .000	.424 .000	.156 .000	.065 .000	.000 .000
1.1172	−.965 .000	−.254 .000	−.054 .000	−.030 .000	−.005 .000	.001 .000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	12.86	.003	2.501	.480	.096	.103	.398	.632	2.082	4.072
1–3	22.79	.486	.017	.003	1.749	3.787	.389	1.528	.028	.037
1–4	32.98	.006	.002	.001	.312	.345	.001	.092	.187	.560
1–5	36.44	.042	.048	.003	1.127	1.575	.037	.262	.369	1.550
1–6	61.23	.000	.000	.001	.097	.167	.010	.015	.009	.128
2–3	9.93	.001	1.998	.928	.201	.326	1.039	.459	.634	.311
2–4	20.12	.294	.172	.043	.011	1.329	1.097	2.188	1.161	.222
2–5	23.58	.588	.499	.025	.149	.944	.343	1.216	.849	.534
2–6	48.37	.003	.009	.000	.781	.909	.005	.096	.096	.866
3–4	10.19	.632	1.039	.229	2.873	.063	2.088	2.068	1.082	1.685
3–5	13.65	1.164	1.192	.224	2.282	.812	.371	.740	.254	1.571
3–6	38.44	.021	.027	.001	.938	1.134	.009	.367	.377	1.089
4–5	3.46	.074	.088	.020	.851	.740	.004	.024	.050	.845
4–6	28.25	.001	.001	.000	.028	.036	.001	.026	.026	.034
5–6	24.79	1.211	1.157	.077	1.673	.068	1.068	4.288	3.644	.493

THETA = 45.00 PHI = 30.00 B = 3000.0

Energy levels and wave functions

E(CM−1)	(5/2)	(3/2)	(1/2)	(−1/2)	(−3/2)	(−5/2)
−.9262	.013 −.013	−.067 .099	.422 −.219	−.754 −.043	.351 .239	−.027 −.093
−.4840	.003 .039	.124 −.238	−.540 .342	−.040 −.029	.596 .294	−.182 −.202
−.1776	−.060 .014	.281 .183	−.181 −.384	−.003 −.609	.183 −.388	−.347 .168
.1743	.058 −.004	−.186 −.112	−.009 −.009	−.091 .123	−.387 .174	−.859 −.086
.2970	.203 −.130	−.828 .067	−.383 −.189	−.080 −.162	.037 −.112	.141 −.047
1.1166	.030 .965	−.119 .224	−.039 .030	−.008 .021	−.004 .003	.000 −.001

Transition probabilities

I, J	D(GC)	PX1SX	PY1SY	PZ1SZ	P2SXX	P2SYY	P2SZZ	PSXSY	PSXSZ	PSYSZ
1–2	13.27	.600	1.860	.492	3.211	2.991	.422	1.068	1.705	.886
1–3	22.46	.387	.083	.003	.283	1.449	.451	1.884	.387	1.245
1–4	33.02	.021	.012	.004	.976	.946	.011	.122	.168	.151
1–5	36.70	.038	.044	.001	.995	1.215	.038	1.592	.351	.245
1–6	61.28	.000	.000	.001	.107	.161	.006	.131	.007	.011
2–3	9.19	.480	1.632	.897	.470	.422	.985	.098	.662	.569
2–4	19.75	.246	.322	.026	.084	.835	.890	.380	1.521	1.791
2–5	23.43	.572	.448	.032	.394	.987	.277	.393	.801	1.271
2–6	48.02	.002	.007	.000	.833	.892	.008	.881	.118	.117
3–4	10.56	.834	.790	.388	3.213	1.781	2.242	.728	1.183	1.829
3–5	14.24	.984	1.222	.146	1.519	.897	.684	1.855	.511	.560
3–6	38.83	.023	.028	.003	1.011	1.025	.039	1.054	.342	.323
4–5	3.68	.123	.133	.504	1.010	.752	.184	.795	.095	.088
4–6	28.27	.056	.055	.003	.050	.013	.053	.019	.217	.224
5–6	24.59	1.158	1.104	.066	1.263	.462	.952	.528	3.644	3.958

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 45.00 PHI = 60.00 B = 3000.0

Energy levels and wave functions

E(CM-1)	(5/2)	(3/2)	(1/2)	(−1/2)	(−3/2)	(−5/2)
−.9286	.000 .000	.097 −.064	−.425 −.214	.042 .750	.358 −.234	−.100 −.050
−.4720	−.025 .033	.275 .036	−.248 −.598	.023 −.031	−.662 −.087	.090 .216
−.1917	.062 −.039	−.282 −.151	.014 .408	−.518 .323	−.372 −.199	.014 .418
.1734	.049 .060	.102 −.270	.017 −.003	−.091 −.111	.146 −.387	.836 −.137
.3029	−.133 .187	.809 .075	.180 .391	−.116 .164	−.147 −.014	−.084 −.182
1.1160	−.966 −.028	−.120 −.222	.024 −.038	−.012 −.000	−.001 −.002	−.001 .001

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	13.70	1.820	.610	.505	3.126	3.188	.440	1.634	.829	1.021
1–3	22.11	.111	.317	.000	1.342	.197	.513	.469	1.247	1.919
1–4	33.06	.038	.017	.005	.934	.913	.022	.248	.102	.320
1–5	36.95	.036	.040	.000	1.237	.990	.039	.229	.339	1.[illegible]1
1–6	61.34	.000	.001	.001	.125	.147	.004	.007	.005	.135
2–3	8.41	1.715	.572	.861	.475	.398	.912	.685	.713	.074
2–4	19.36	.177	.479	.001	.672	.126	.667	1.167	2.130	.375
2–5	23.25	.535	.428	.038	.766	.522	.179	1.233	.839	.422
2–6	47.64	.002	.004	.000	.933	.836	.010	.140	.145	.896
3–4	10.95	1.052	.525	.531	1.921	2.920	2.419	1.346	1.533	.881
3–5	14.84	.822	1.255	.084	.675	2.065	.997	.321	.814	1.666
3–6	39.23	.026	.029	.005	1.134	.871	.068	.281	.304	1.011
4–5	3.88	.159	.170	.868	1.164	.673	.318	.202	.067	.785
4–6	28.28	.102	.100	.006	.043	.015	.096	.369	.400	.007
5–6	24.39	1.108	1.064	.056	.505	1.183	.848	3.516	3.813	.572

THETA = 45.00 PHI = 90.00 B = 3000.0

Energy levels and wave functions

E(CM-1)	(5/2)	(3/2)	(1/2)	(−1/2)	(−3/2)	(−5/2)
−.9262	.013 −.013	−.001 −.119	−.475 −.007	−.002 .755	.425 −.006	−.018 −.095
−.4840	.000 .039	.268 −.006	−.016 −.639	.038 −.032	−.001 −.665	−.269 −.039
−.1776	.015 −.060	−.335 .012	.028 .424	−.609 −.014	.043 −.427	−.385 .021
.1743	.046 .036	.119 −.181	.009 .010	−.006 −.153	.424 −.012	.021 .863
.2970	−.002 −.241	−.831 −.022	.005 −.427	.180 −.022	.043 .110	−.106 .105
1.1166	−.966 .001	.001 −.254	.049 .004	−.021 .009	−.002 −.004	−.001 −.001

Transition probabilities

I, J	D(GC)	PX1SX	PY1SY	PZ1SZ	P2SXX	P2SYY	P2SZZ	PSXSY	PSXSZ	PSYSZ
1–2	13.27	2.455	.004	.492	.083	.133	.422	4.060	.528	2.064
1–3	22.46	.018	.452	.003	3.807	1.653	.451	.020	1.580	.051
1–4	33.02	.026	.006	.004	.189	.148	.011	.914	.057	.261
1–5	36.70	.040	.042	.001	1.706	1.236	.038	1.226	.331	.265
1–6	61.28	.000	.000	.001	.140	.128	.007	.132	.009	.008
2–3	9.19	2.110	.002	.897	.328	.178	.985	.291	.573	.657
2–4	19.75	.110	.458	.026	1.260	.054	.890	.182	2.391	.920
2–5	23.43	.536	.484	.032	.767	.139	.277	.630	.933	1.139
2–6	48.02	.006	.004	.000	.957	.789	.008	.870	.121	.114
3–4	10.56	1.176	.449	.388	.028	2.398	2.242	2.011	1.856	1.156
3–5	14.24	.888	1.317	.146	.812	2.976	.684	1.169	.892	.179
3–6	38.83	.025	.025	.003	1.220	.863	.039	1.030	.342	.324
4–5	3.68	.121	.134	.504	1.096	.600	.184	.827	.013	.170
4–6	28.27	.056	.055	.003	.044	.015	.053	.021	.236	.205
5–6	24.59	1.140	1.121	.066	.075	1.556	.952	.575	4.110	3.492

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 45.00 PHI = .00 B = 4000.0

Energy levels and wave functions

E(CM−1)	(5/2)	(3/2)	(1/2)	(−1/2)	(−3/2)	(−5/2)
−1.1058	.026 .000	−.120 .000	.436 .000	−.729 .000	.496 .000	−.131 .000
−.6053	−.043 .000	.254 .000	−.592 .000	.108 .000	.634 .000	−.411 .000
−.1639	−.073 .000	.407 .000	−.465 .000	−.556 .000	−.168 .000	.525 .000
.1237	−.041 .000	.192 .000	−.066 .000	−.322 .000	−.561 .000	−.734 .000
.4311	−.304 .000	.790 .000	.483 .000	.206 .000	.091 .000	.020 .000
1.3202	.948 .000	.308 .000	.077 .000	.034 .000	.007 .000	−.000 .000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	15.02	.008	2.240	.554	.251	.147	.781	.896	2.261	4.315
1–3	28.26	.355	.045	.007	1.817	4.144	.473	1.598	.002	.174
1–4	36.89	.001	.005	.000	.009	.004	.001	.004	.200	.538
1–5	46.11	.015	.019	.002	.734	1.038	.026	.173	.236	.989
1–6	72.78	.000	.000	.001	.046	.086	.006	.010	.006	.062
2–3	13.24	.042	2.286	1.060	.324	.506	1.641	.788	.929	.018
2–4	21.87	.321	.019	.011	.000	1.480	1.451	2.233	.453	.043
2–5	31.09	.298	.257	.013	.454	1.491	.299	.981	.774	1.027
2–6	57.77	.001	.005	.000	.478	.594	.006	.068	.065	.545
3–4	8.63	.166	1.195	.760	2.136	.236	3.793	1.451	.135	1.869
3–5	17.85	1.126	1.102	.230	1.206	.084	.654	1.170	.392	.523
3–6	44.52	.023	.029	.000	.925	1.277	.028	.436	.435	1.150
4–5	9.22	.348	.397	.151	1.924	1.437	.035	.000	.055	1.827
4–6	35.89	.011	.011	.000	.137	.244	.015	.177	.170	.201
5–6	26.67	1.174	1.138	.116	2.312	.079	1.538	4.015	3.076	.718

THETA = 45.00 PHI = .00 B = 5000.0

Energy levels and wave functions

E(CM−1)	(5/2)	(3/2)	(1/2)	(−1/2)	(−3/2)	(−5/2)
−1.2979	.025 .000	−.115 .000	.402 .000	−.701 .000	.548 .000	−.183 .000
−.7289	−.046 .000	.247 .000	−.569 .000	.206 .000	.570 .000	−.496 .000
−.1989	−.085 .000	.405 .000	−.465 .000	−.447 .000	.071 .000	.638 .000
.1229	−.080 .000	.315 .000	−.134 .000	−.454 .000	−.599 .000	−.559 .000
.5738	.344 .000	−.735 .000	−.521 .000	−.243 .000	−.107 .000	−.026 .000
1.5290	−.930 .000	−.351 .000	−.099 .000	−.039 .000	−.009 .000	.000 .000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	17.07	.020	2.051	.612	.498	.159	1.219	1.108	2.263	4.329
1–3	32.97	.256	.054	.009	1.584	3.944	.529	1.540	.000	.261
1–4	42.63	.012	.009	.000	.070	.154	.016	.031	.191	.573
1–5	56.15	.005	.008	.001	.472	.669	.017	.110	.154	.640
1–6	84.81	.000	.000	.001	.021	.044	.005	.006	.003	.030
2–3	15.90	.071	2.305	1.143	.579	.695	2.544	1.224	.945	.014
2–4	25.56	.310	.020	.001	.018	1.675	1.342	1.968	.045	.008
2–5	39.08	.163	.139	.006	.617	1.663	.254	.809	.667	1.211
2–6	67.74	.000	.002	.000	.306	.395	.006	.046	.043	.356
3–4	9.65	.007	1.370	1.196	.742	1.144	3.728	1.097	.038	1.775
3–5	23.18	.799	.775	.160	.300	.113	.782	1.426	.561	.018
3–6	51.84	.016	.020	.000	.733	1.090	.035	.359	.350	.949
4–5	13.53	.732	.843	.323	2.783	1.580	.169	.060	.027	2.427
4–6	42.18	.024	.024	.000	.321	.642	.055	.416	.384	.499
5–6	28.65	1.138	1.129	.155	2.849	.082	1.964	3.799	2.595	.910

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 60.00 PHI = .00 B = 1000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.6309	.028	.000	−.117	.000	.612	.000	−.760	.000	.181	.000	.004	.000
−.4016	−.001	.000	.217	.000	−.743	.000	−.565	.000	.279	.000	−.060	.000
−.1260	−.003	.000	−.093	.000	.097	.000	.312	.000	.930	.000	−.142	.000
.0072	−.132	.000	.956	.000	.251	.000	.062	.000	.050	.000	.009	.000
.4597	−.001	.000	.009	.000	.036	.000	−.013	.000	−.149	.000	−.988	.000
.6915	.991	.000	.131	.000	.016	.000	.030	.000	.004	.000	−.001	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	6.88	.036	2.542	.309	.015	.005	.002	.017	.626	1.398
1–3	15.15	.752	.428	.007	1.730	2.785	.125	1.449	.751	1.248
1–4	19.14	.322	.338	.008	1.986	2.679	.052	.604	.836	2.633
1–5	32.72	.009	.000	.003	1.078	.916	.007	.049	.060	1.001
1–6	39.67	.000	.003	.004	.470	.677	.019	.027	.021	.571
2–3	8.27	1.059	1.397	.151	1.734	.619	.281	.582	.922	1.787
2–4	12.27	1.580	1.434	.047	1.271	.472	.194	1.430	.951	.623
2–5	25.84	.040	.017	.010	.976	1.600	.077	.285	.235	1.205
2–6	32.80	.005	.018	.002	1.776	1.630	.003	.105	.117	1.747
3–4	4.00	.116	.109	.039	1.300	1.101	.008	.030	.000	1.192
3–5	17.57	1.155	1.264	.019	.513	.024	.315	4.596	4.354	.355
3–6	24.53	.001	.002	.001	.074	.058	.001	.050	.053	.072
4–5	13.57	.001	.001	.003	.032	.054	.003	.028	.030	.046
4–6	20.53	1.260	1.198	.019	.547	.042	.286	4.746	4.598	.124
5–6	6.96	.000	.000	.000	.000	.000	.000	.002	.002	.000

THETA = 60.00 PHI = .00 B = 2000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.8096	.034	.000	−.159	.000	.576	.000	−.743	.000	.298	.000	−.030	.000
−.4246	−.039	.000	.328	.000	−.662	.000	−.358	.000	.546	.000	−.162	.000
−.1198	.042	.000	−.311	.000	.211	.000	.528	.000	.711	.000	−.271	.000
.1249	−.238	.000	.845	.000	.428	.000	.185	.000	.109	.000	−.025	.000
.3877	−.001	.000	.015	.000	.023	.000	−.071	.000	−.309	.000	−.948	.000
.8413	.969	.000	.239	.000	.049	.000	.034	.000	.007	.000	−.001	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	11.55	.004	2.619	.438	.018	.012	.059	.150	1.752	3.593
1–3	20.69	.544	.021	.000	1.867	3.790	.337	1.690	.172	.147
1–4	28.04	.090	.126	.006	1.080	1.652	.061	.362	.641	1.988
1–5	35.92	.008	.001	.002	.583	.557	.000	.079	.106	.592
1–6	49.53	.000	.001	.002	.224	.357	.016	.032	.022	.285
2–3	9.14	.218	1.992	.679	.362	.050	.683	.417	.974	.628
2–4	16.49	1.161	.795	.053	.128	.156	.566	1.639	.734	.008
2–5	24.37	.135	.100	.020	.433	1.561	.350	1.171	.882	.786
2–6	37.98	.011	.024	.000	1.226	1.360	.003	.207	.220	1.343
3–4	7.34	.635	.730	.309	2.434	1.374	.150	.200	.022	2.245
3–5	15.23	.942	1.125	.090	1.813	.063	1.198	3.383	2.618	.926
3–6	28.83	.036	.040	.000	.337	.471	.011	.395	.404	.445
4–5	7.88	.043	.054	.000	.537	.395	.011	.109	.111	.501
4–6	21.49	1.206	1.122	.071	1.681	.103	.952	4.162	3.613	.505
5–6	13.61	.000	.000	.000	.007	.007	.000	.005	.005	.008

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 60.00 PHI = .00 B = 3000.0

Energy levels and wave functions

E(CM-1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.0038	.037	.000	−.174	.000	.543	.000	−.726	.000	.376	.000	−.069	.000
−.5105	.063	.000	−.353	.000	.608	.000	.192	.000	−.628	.000	.265	.000
−.1069	.100	.000	−.449	.000	.230	.000	.578	.000	.494	.000	−.397	.000
.2553	.313	.000	−.727	.000	−.513	.000	−.229	.000	−.026	.000	.238	.000
.3576	.058	.000	−.091	.000	−.106	.000	−.217	.000	−.468	.000	−.843	.000
1.0082	.940	.000	.326	.000	.090	.000	.044	.000	.012	.000	.000	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	14.80	.002	2.384	.537	.049	.050	.199	.306	2.375	4.515
1–3	26.91	.389	.005	.003	1.868	4.328	.509	1.855	.017	.005
1–4	37.77	.021	.047	.003	.427	.737	.042	.160	.524	1.573
1–5	40.84	.005	.000	.002	.373	.424	.002	.087	.039	.139
1–6	60.36	.000	.001	.001	.104	.183	.011	.024	.014	.137
2–3	12.11	.004	2.310	.993	.164	.243	.806	.391	1.240	.066
2–4	22.97	.773	.272	.014	0.53	1.621	1.088	2.423	.319	.186
2–5	26.04	.056	.153	.027	.093	.944	.445	.955	1.116	.603
2–6	45.56	.006	.015	.000	.758	.960	.012	.182	.186	.889
3–4	10.87	.506	1.594	.691	.907	.497	.061	.111	.243	2.292
3–5	13.94	.923	.594	.132	2.909	.002	2.763	2.932	1.017	.552
3–6	33.45	.066	.071	.000	.416	.863	.081	.746	.726	.690
4–5	3.07	.129	.233	.399	2.217	.301	.884	.135	.003	1.385
4–6	22.59	1.097	1.027	.131	2.527	.090	1.661	3.644	2.661	.761
5–6	19.52	.047	.046	.010	.346	.110	.066	.050	.024	.206

THETA = 60.00 PHI = .00 B = 4000.0

Energy levels and wave functions

E(CM-1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.2072	.040	.000	−.178	.000	.516	.000	−.710	.000	.430	.000	−.106	.000
−.6209	.077	.000	−.359	.000	.582	.000	.083	.000	−.631	.000	.348	.000
−.1147	.142	.000	−.501	.000	.232	.000	.567	.000	.313	.000	−.505	.000
.3181	.238	.000	−.471	.000	−.309	.000	.043	.000	.394	.000	.685	.000
.4361	.304	.000	−.460	.000	−.477	.000	−.402	.000	−.404	.000	−.380	.000
1.1887	.907	.000	.394	.000	.133	.000	.059	.000	.018	.000	.002	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	17.59	.005	2.175	.613	.124	.071	.382	.427	2.689	4.826
1–3	32.78	.283	.018	.005	1.677	4.402	.645	1.931	.000	.077
1–4	45.76	.003	.011	.000	.032	.093	.016	.021	.357	.974
1–5	49.30	.005	.009	.002	.377	.555	.017	.121	.072	.218
1–6	71.88	.000	.000	.001	.047	.094	.008	.015	.008	.065
2–3	15.19	.010	2.412	1.158	.222	.305	1.047	.478	1.480	.016
2–4	28.17	.476	.015	.000	.153	3.130	1.900	3.395	.022	.005
2–5	31.71	.082	.185	.017	.049	.168	.035	.117	.987	.841
2–6	54.29	.002	.008	.000	.482	.659	.014	.134	.133	.586
3–4	12.98	.002	2.161	1.144	.303	.363	1.329	.533	.519	1.996
3–5	16.52	1.018	.120	.049	2.147	.023	2.615	2.407	.000	.048
3–6	39.10	.061	.065	.000	.403	1.035	.146	.826	.771	.758
4–5	3.54	.111	.508	2.180	.003	1.143	1.023	.084	1.335	2.208
4–6	26.12	.365	.344	.051	.528	.048	.893	1.707	1.144	.045
5–6	22.58	.737	.719	.168	3.308	.297	1.623	1.804	.916	1.337

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TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 60.00 PHI = .00 B = 5000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.4170	.041	.000	−.178	.000	.494	.000	−.695	.000	.468	.000	−.140	.000
−.7431	.086	.000	−.360	.000	.568	.000	.008	.000	−.610	.000	.410	.000
−.1413	−.167	.000	.514	.000	−.238	.000	−.540	.000	−.168	.000	.575	.000
.3401	−.232	.000	.425	.000	.235	.000	−.165	.000	−.506	.000	−.653	.000
.5813	.380	.000	−.441	.000	−.540	.000	−.438	.000	−.352	.000	−.233	.000
1.3799	.875	.000	.446	.000	.173	.000	.075	.000	.025	.000	.004	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	20.22	.010	2.020	.672	.237	.078	.587	.524	2.846	4.916
1–3	38.27	.211	.025	.007	1.424	4.237	.748	1.938	.005	.149
1–4	52.71	.004	.006	.000	.042	.115	.018	.031	.257	.646
1–5	59.95	.002	.005	.001	.219	.342	.014	.075	.081	.239
1–6	83.91	.000	.000	.001	.022	.049	.006	.009	.004	.031
2–3	18.05	.033	2.403	1.261	.340	.340	1.359	.593	1.544	.135
2–4	32.50	.323	.016	.000	.133	3.173	2.008	3.145	.005	.023
2–5	39.73	.080	.097	.007	.158	.586	.135	.348	.705	.836
2–6	63.69	.001	.004	.000	.313	.449	.012	.093	.090	.388
3–4	14.44	.009	1.998	1.355	.415	.593	2.002	.674	.175	1.453
3–5	21.68	.707	.274	.094	.916	.316	2.310	2.306	.121	.013
3–6	45.63	.043	.046	.000	.368	1.036	.169	.744	.676	.730
4–5	7.23	.345	.790	1.560	.692	1.436	.134	.029	1.112	2.688
4–6	31.19	.208	.196	.029	.131	.267	.770	1.411	.908	.012
5–6	23.96	.855	.870	.271	4.426	.277	2.489	2.079	.745	1.741

THETA = 75.00 PHI = .00 B = 1000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.6476	.031	.000	−.143	.000	.652	.000	−.723	.000	.173	.000	.004	.000
−.3999	−.005	.000	.250	.000	−.694	.000	−.605	.000	.294	.000	−.059	.000
−.0902	.013	.000	−.194	.000	.060	.000	.311	.000	.916	.000	−.153	.000
−.0197	−.152	.000	.926	.000	.297	.000	.112	.000	.139	.000	−.007	.000
.5187	.002	.000	−.007	.000	−.033	.000	.016	.000	.160	.000	.986	.000
.6387	−.988	.000	−.150	.000	−.021	.000	−.033	.000	−.005	.000	.001	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	7.43	.007	2.536	.331	.001	.000	.001	.011	.739	1.620
1–3	16.72	.714	.266	.004	2.246	3.496	.138	1.532	.494	1.033
1–4	18.84	.271	.418	.012	1.351	1.981	.060	.526	1.045	2.715
1–5	34.99	.007	.000	.003	.909	.758	.007	.040	.051	.835
1–6	38.59	.000	.004	.004	.527	.752	.020	.039	.030	.634
2–3	9.29	.861	1.805	.182	1.084	.297	.246	.517	1.202	1.636
2–4	11.41	1.743	1.094	.047	1.597	.506	305	1.538	.642	.499
2–5	27.56	.037	.016	.008	1.113	1.732	.068	.298	.251	1.336
2–6	31.16	.008	.024	.002	1.640	1.512	.003	.145	.163	1.629
3–4	2.12	.134	.141	.226	1.382	1.140	.012	.022	.003	1.377
3–5	18.27	1.139	1.241	.024	.534	.015	.371	4.470	4.196	.326
3–6	21.87	.022	.022	.001	.040	.051	.001	.206	.209	.057
4–5	16.15	.019	.022	.001	.096	.088	.000	.139	.139	.105
4–6	19.75	1.239	1.161	.027	.770	.067	.383	4.515	4.318	.197
5–6	3.60	.000	.000	.000	.000	.000	.000	.002	.002	.000

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 75.00 PHI = .00 B = 2000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.8443	.043	.000	−.201	.000	.623	.000	−.705	.000	.268	.000	−.026	.000
−.4304	−.057	.000	.391	.000	−.601	.000	−.445	.000	.514	.000	−.143	.000
−.0714	−.103	.000	.460	.000	−.033	.000	−.446	.000	−.708	.000	.277	.000
.0934	.265	.000	−.719	.000	−.494	.000	−.314	.000	−.247	.000	.095	.000
.5091	.005	.000	.009	.000	.015	.000	−.076	.000	−.317	.000	−.945	.000
.7436	.956	.000	.281	.000	.070	.000	.044	.000	.013	.000	.001	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	12.42	.001	2.534	.467	.002	.008	.016	.056	1.888	3.812
1–3	23.19	.516	.008	.000	2.345	4.684	.400	1.957	.057	.072
1–4	28.13	.038	.137	.007	.397	.703	.044	.173	.773	1.961
1–5	40.60	.005	.000	.002	.467	.430	.001	.053	.069	.441
1–6	47.63	.000	.002	.002	.244	.399	.019	.047	.032	.312
2–3	10.77	.112	2.508	.706	.126	.047	.326	.210	1.499	.377
2–4	15.72	1.287	.361	.024	.237	.252	.977	2.067	.297	.005
2–5	28.18	.083	.061	.012	.611	1.614	.239	.890	.712	.971
2–6	35.22	.018	.036	.000	1.094	1.304	.009	.312	.335	1.257
3–4	4.94	.354	.776	.911	1.328	.700	.100	.093	.000	2.392
3–5	17.41	.866	.981	.093	1.223	.000	1.245	3.291	2.447	.456
3–6	24.45	.156	.152	.001	.038	.296	.122	1.035	.992	.185
4–5	12.47	.179	.221	.007	1.188	.491	.151	.491	.417	.907
4–6	19.50	1.077	.971	.105	2.465	.213	1.229	3.319	2.621	.832
5–6	7.03	.001	.001	.001	.021	.015	.000	.004	.006	.019

THETA = 75.00 PHI = .00 B = 3000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.0540	.051	.000	−.227	.000	.600	.000	−.690	.000	.325	.000	−.054	.000
−.5181	−.096	.000	.436	.000	−.546	.000	−.331	.000	.588	.000	−.219	.000
−.0665	−.184	.000	.546	.000	.010	.000	−.473	.000	−.551	.000	.375	.000
.2260	.353	.000	−.558	.000	−.567	.000	−.389	.000	−.185	.000	.238	.000
.5382	.046	.000	−.010	.000	−.050	.000	−.184	.000	−.458	.000	−.867	.000
.8744	.910	.000	.386	.000	.133	.000	.069	.000	.027	.000	.007	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	16.08	.000	2.320	.570	.008	.019	.051	.100	2.562	4.752
1–3	29.63	.350	.002	.002	2.006	4.846	.616	2.128	.002	.002
1–4	38.40	.006	.045	.003	.129	.273	.027	.068	.537	1.323
1–5	47.77	.002	.000	.001	.236	.240	.000	.040	.038	.166
1–6	57.85	.000	.001	.001	.108	.201	.014	.034	.019	.144
2–3	13.55	.004	2.605	1.022	.056	.105	.313	.147	1.791	.003
2–4	22.32	.772	.112	.004	.003	1.635	1.489	2.680	.143	.090
2–5	31.69	.049	.062	.011	.258	1.153	.320	.838	.771	.727
2–6	41.77	.011	.023	.000	.678	.975	.027	.294	.299	.851
3–4	8.78	.234	1.408	1.190	.436	.161	.067	.097	.056	2.150
3–5	18.14	.667	.619	.130	1.331	.124	2.270	2.910	1.240	.230
3–6	28.23	.181	.178	.005	.023	.563	.357	1.383	1.248	.274
4–5	9.37	.312	.474	.174	2.797	.506	.924	.528	.187	1.840
4–6	19.45	.987	.881	.210	3.809	.208	2.235	2.753	1.500	1.247
5–6	10.09	.020	.022	.018	.284	.124	.033	.000	.010	.202

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 75.00 PHI = .00 B = 4000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.2706	.058	.000	−.241	.000	.583	.000	−.679	.000	.363	.000	−.080	.000
−.6278	−.122	.000	.453	.000	−.518	.000	−.258	.000	.607	.000	−.277	.000
−.0791	−.238	.000	.561	.000	.030	.000	−.481	.000	−.441	.000	.449	.000
.3369	−.417	.000	.451	.000	.570	.000	.358	.000	.031	.000	−.410	.000
.6128	−.147	.000	.042	.000	.162	.000	.318	.000	.550	.000	.739	.000
1.0278	.854	.000	.465	.000	.201	.000	.105	.000	.048	.000	.018	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	19.29	.001	2.139	.648	.024	.025	.098	.132	2.966	5.121
1–3	35.75	.249	.006	.004	1.636	4.692	.787	2.202	.001	.028
1–4	48.23	.001	.017	.001	.049	.133	.021	.036	.416	.978
1–5	56.50	.000	.001	.001	.130	.149	.001	.029	.005	.022
1–6	68.95	.000	.000	.001	.046	.099	.010	.021	.009	.064
2–3	16.46	.001	2.567	1.202	.073	.109	.359	.153	2.005	.093
2–4	28.94	.531	.040	.000	.104	3.083	2.055	3.428	.053	.091
2–5	37.22	.007	.047	.007	.066	.455	.174	.359	.676	.635
2–6	49.67	.005	.012	.000	.427	.683	.030	.220	.212	.551
3–4	12.48	.110	1.936	1.449	.048	.061	.001	.020	.233	1.652
3–5	20.76	.542	.228	.070	1.137	.486	3.111	3.044	.452	.055
3–6	33.21	.136	.138	.006	.026	.732	.481	1.314	1.148	.343
4–5	8.28	.219	.724	.817	2.810	.088	1.906	.413	.012	2.491
4–6	20.73	.851	.757	.271	3.936	.051	3.091	2.585	.895	1.065
5–6	12.45	.128	.137	.128	1.363	.345	.337	.044	.025	.811

THETA = 75.00 PHI = .00 B = 5000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.4914	.063	.000	−.248	.000	.569	.000	−.670	.000	.390	.000	−.101	.000
−.7481	−.140	.000	.461	.000	−.502	.000	−.208	.000	.607	.000	−.322	.000
−.1038	−.274	.000	.559	.000	.038	.000	−.484	.000	−.357	.000	.500	.000
.4150	−.446	.000	.377	.000	.538	.000	.281	.000	−.125	.000	−.524	.000
.7281	−.265	.000	.043	.000	.252	.000	.416	.000	.575	.000	.601	.000
1.2002	.795	.000	.519	.000	.265	.000	.146	.000	.074	.000	.030	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	22.30	.002	2.004	.710	.050	.027	.150	.157	3.231	5.272
1–3	41.63	.186	.008	.004	1.329	4.475	.927	2.237	.006	.053
1–4	57.19	.001	.008	.001	.026	.088	.018	.027	.324	.717
1–5	66.59	.000	.001	.001	.076	.099	.001	.021	.000	.000
1–6	80.75	.000	.000	.000	.019	.049	.007	.012	.004	.027
2–3	19.33	.008	2.506	1.322	.107	.107	.427	.171	2.117	.282
2–4	34.90	.382	.020	.000	.167	3.961	2.500	3.868	.023	.076
2–5	44.29	.000	.031	.004	.003	.065	.039	.062	.553	.581
2–6	58.45	.001	.006	.000	.270	.458	.025	.150	.137	.346
3–4	15.57	.058	2.193	1.658	.003	.074	.107	.003	.319	1.187
3–5	24.96	.433	.036	.014	.790	.974	3.518	3.262	.081	.012
3–6	39.12	.087	.092	.005	.034	.767	.477	1.094	.955	.374
4–5	9.39	.044	.953	1.497	1.241	.032	1.668	.277	.345	2.857
4–6	23.56	.638	.559	.239	3.053	.010	3.417	2.485	.610	.589
5–6	14.16	.289	.333	.358	2.927	.471	1.050	.174	.109	1.626

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 90.00 PHI = .00 B = 1000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.6535	.034	.000	−.165	.000	.688	.000	−.688	.000	.158	.000	.006	.000
−.3991	−.006	.000	.271	.000	−.648	.000	−.649	.000	.287	.000	−.054	.000
−.0664	.109	.000	−.708	.000	−.161	.000	.161	.000	.649	.000	−.117	.000
−.0406	−.122	.000	.610	.000	.280	.000	.280	.000	.668	.000	−.100	.000
.5796	.230	.000	.032	.000	−.024	.000	.024	.000	.157	.000	.959	.000
.5800	−.959	.000	−.158	.000	−.031	.000	−.031	.000	.030	.000	.231	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	7.63	.000	2.522	.337	.002	.002	.000	.004	.769	1.680
1–3	17.61	.954	.001	.001	3.536	5.460	.208	2.047	.013	.008
1–4	18.39	.001	.664	.016	.007	.004	.000	.010	1.520	3.714
1–5	36.99	.005	.001	.002	.473	.323	.014	.014	.057	1.043
1–6	37.01	.001	.005	.005	.919	1.171	.015	.069	.022	.391
2–3	9.98	.000	2.931	.231	.004	.007	.001	.012	1.815	2.041
2–4	10.75	2.591	.000	.003	2.565	.722	.565	2.078	.012	.008
2–5	29.36	.038	.005	.008	1.890	2.524	.046	.362	.131	.789
2–6	29.37	.004	.038	.001	.886	.697	.011	.084	.303	2.190
3–4	.77	.000	.151	1.976	.002	.003	.000	.012	.028	1.441
3–5	19.38	.314	.899	.024	.061	.013	.132	1.090	3.062	.056
3–6	19.39	.899	.314	.003	.256	.000	.276	3.758	1.539	.004
4–5	18.61	.861	.358	.001	.783	.151	.246	3.471	1.401	.221
4–6	18.62	.357	.862	.031	.458	.071	.168	.989	2.805	.414
5–6	.01	.000	.000	1.253	.001	.001	.000	.002	.082	.001

THETA = 90.00 PHI = .00 B = 2000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−.8565	.051	.000	−.241	.000	.665	.000	−.665	.000	.232	.000	−.018	.000
−.4306	−.076	.000	.445	.000	−.530	.000	−.530	.000	.470	.000	−.117	.000
−.0530	−.211	.000	.658	.000	.235	.000	−.235	.000	−.603	.000	.218	.000
.0784	.233	.000	−.463	.000	−.462	.000	−.462	.000	−.518	.000	.191	.000
.6289	.346	.000	.118	.000	.044	.000	−.044	.000	−.278	.000	−.886	.000
.6328	.879	.000	.286	.000	.077	.000	.077	.000	.129	.000	.341	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	12.78	.000	2.498	.478	.004	.003	.000	.007	1.924	3.872
1–3	24.11	.524	.001	.002	2.650	5.350	.470	2.163	.010	.008
1–4	28.05	.001	.147	.006	.004	.001	.001	.003	.833	2.010
1–5	44.56	.003	.000	.003	.605	.632	.000	.072	.016	.120
1–6	44.68	.000	.003	.001	.072	.180	.024	.031	.074	.588
2–3	11.33	.000	2.918	.713	.000	.004	.001	.004	1.821	.280
2–4	15.27	1.426	.000	.005	.313	.336	1.298	2.408	.003	.008
2–5	31.79	.022	.068	.005	.231	.628	.097	.270	.891	1.897
2–6	31.90	.059	.023	.001	1.515	2.232	.069	.821	.145	.396
3–4	3.94	.000	.791	1.591	.003	.007	.001	.030	.006	2.465
3–5	20.46	.876	.193	.028	.443	.195	1.225	3.795	.430	.014
3–6	20.57	.193	.852	.054	.125	.008	.197	.909	3.357	.009
4–5	16.52	.170	1.083	.094	.528	.137	.127	.681	2.321	1.989
4–6	16.63	1.071	.171	.062	4.072	.633	1.494	2.801	.268	.316
5–6	.11	.000	.002	2.638	.005	.004	.000	.007	.980	.028

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 90.00 PHI = .00 B = 3000.00

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.0718	.068	.000	−.281	.000	.649	.000	−.649	.000	.272	.000	−.039	.000
−.5172	−.133	.000	.508	.000	−.453	.000	−.453	.000	.534	.000	−.170	.000
−.0545	−.294	.000	.607	.000	.272	.000	−.272	.000	−.556	.000	.298	.000
.2121	.347	.000	−.330	.000	−.517	.000	−.517	.000	−.385	.000	.295	.000
.7055	.490	.000	.233	.000	.074	.000	−.074	.000	−.341	.000	−.761	.000
.7259	.729	.000	.364	.000	.163	.000	.163	.000	.261	.000	.464	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	16.64	.000	2.294	.584	.004	.003	.000	.006	2.620	4.832
1–3	30.52	.333	.001	.002	2.034	5.094	.690	2.264	.008	.007
1–4	38.52	.001	.044	.002	.004	.000	.002	.000	.535	1.259
1–5	53.32	.001	.001	.003	.317	.387	.003	.063	.004	.018
1–6	53.93	.000	.001	.000	.005	.039	.016	.012	.047	.279
2–3	13.88	.000	2.771	1.015	.000	.002	.002	.001	2.031	.001
2–4	21.88	.802	.000	.004	.000	1.766	1.751	2.964	.001	.008
2–5	36.68	.006	.065	.005	.032	.187	.065	.115	1.012	1.564
2–6	37.30	.042	.007	.000	.941	1.895	.165	.897	.037	.083
3–4	8.00	.000	1.391	1.529	.002	.009	.003	.041	.034	2.192
3–5	22.80	.804	.050	.018	.545	.681	2.442	4.367	.059	.002
3–6	23.41	.050	.685	.083	.050	.006	.092	.254	2.760	.009
4–5	14.80	.044	1.370	.404	.199	.052	.047	.169	1.223	3.383
4–6	15.41	1.249	.045	.067	7.245	.633	3.596	2.834	.008	.131
5–6	.61	.001	.025	4.195	.010	.007	.000	.011	3.144	.231

THETA = 90.00 PHI = .00 B = 4000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.2932	.081	.000	−.305	.000	.636	.000	−.636	.000	.296	.000	−.055	.000
−.6254	−.176	.000	.531	.000	−.409	.000	−.409	.000	.556	.000	−.208	.000
−.0697	.355	.000	−.560	.000	−.292	.000	.292	.000	.514	.000	−.356	.000
.3238	−.446	.000	.212	.000	.515	.000	.515	.000	.266	.000	−.394	.000
.8019	.520	.000	.307	.000	.101	.000	−.100	.000	−.385	.000	−.684	.000
.8627	.606	.000	.415	.000	.261	.000	.261	.000	.347	.000	.452	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	20.03	.000	2.124	.664	.004	.003	.000	.005	3.057	5.231
1–3	36.70	.232	.001	.002	1.588	4.823	.876	2.333	.007	.006
1–4	48.51	.001	.018	.001	.003	.000	.003	.000	.396	.891
1–5	62.85	.000	.001	.002	.157	.211	.004	.041	.001	.004
1–6	64.68	.000	.000	.000	.000	.014	.009	.007	.017	.098
2–3	16.67	.000	2.658	1.201	.000	.001	.002	.000	2.233	.144
2–4	28.47	.532	.000	.004	.069	3.046	2.198	3.540	.000	.007
2–5	42.82	.002	.042	.003	.007	.082	.041	.059	.854	1.177
2–6	44.64	.014	.002	.900	.509	1.185	.141	.585	.012	.025
3–4	11.80	.000	1.823	1.637	.001	.010	.005	.042	.170	1.631
3–5	26.15	.629	.019	.012	.490	1.274	3.345	4.487	.010	.000
3–6	27.97	.019	.399	.062	.027	.003	.047	.092	1.911	.081
4–5	14.34	.017	1.537	.903	.084	.020	.022	.059	.336	3.881
4–6	16.17	1.106	.018	.057	7.708	.199	5.433	2.736	.004	.063
5–6	1.83	.001	.108	3.910	.013	.008	.001	.013	4.753	.761

TABLE 1. *Energy levels, wave functions, and transition probabilities for angles and field strengths indicated*—Continued

THETA = 90.00 PHI = .00 B = 5000.0

Energy levels and wave functions

E(CM−1)	(5/2)		(3/2)		(1/2)		(−1/2)		(−3/2)		(−5/2)	
−1.5180	.091	.000	−.322	.000	.627	.000	−.627	.000	.313	.000	−.069	.000
−.7439	−.207	.000	.542	.000	−.380	.000	−.380	.000	.565	.000	−.236	.000
−.0948	−.398	.000	.520	.000	.303	.000	−.304	.000	−.479	.000	.397	.000
.4096	.511	.000	−.117	.000	−.491	.000	−.491	.000	−.167	.000	.464	.000
.9114	.520	.000	.356	.000	.123	.000	−.123	.000	−.415	.000	−.633	.000
1.0357	.508	.000	.439	.000	.339	.000	.339	.000	.391	.000	.407	.000

Transition probabilities

I, J	D(GC)	PSX	PSY	PSZ	PSXSX	PSYSY	PSZSZ	PSYSZ	PSXSZ	PSXSY
1–2	23.22	.000	1.997	.726	.003	.002	.000	.004	3.359	5.411
1–3	42.70	.171	.001	.002	1.262	4.571	1.030	2.380	.005	.005
1–4	57.83	.001	.008	.001	.003	.000	.003	.000	.306	.651
1–5	72.88	.000	.000	.001	.082	.116	.003	.025	.001	.002
1–6	76.61	.000	.000	.000	.000	.006	.005	.004	.005	.030
2–3	19.47	.000	2.570	1.330	.000	.001	.002	.000	2.368	.357
2–4	34.61	.382	.000	.003	.131	3.878	2.584	3.936	.000	.005
2–5	49.66	.001	.026	.002	.002	.045	.028	.035	.677	.885
2–6	53.39	.003	.001	.000	.267	.652	.085	.318	.005	.009
3–4	15.13	.000	2.068	1.767	.000	.008	.006	.037	.279	1.153
3–5	30.19	.478	.009	.008	.402	1.816	3.927	4.517	.002	.000
3–6	33.91	.009	.205	.034	.016	.001	.027	.039	1.264	.150
4–5	15.05	.008	1.616	1.375	.041	.008	.012	.025	.014	3.841
4–6	18.78	.809	.009	.039	6.186	.001	6.058	2.668	.011	.036
5–6	3.73	.001	.241	3.332	.012	.007	.001	.011	5.572	1.464

6. Appendix 1. Some Remarks on the Program

The matrix to be diagonalized is a 6 by 6 hermitian matrix. This matrix is equivalent to a 12 by 12 real symmetric matrix replacing each element:

$$a_{ij}+ib_{ij} \quad \text{by} \quad \begin{pmatrix} a_{ij} & -b_{ij} \\ b_{ij} & a_{ij} \end{pmatrix}.$$

The wave functions are treated similarly. The functions in the 12 column vector represent the real part of the wave functions at the odd positions, the imaginary part at the even positions. The diagonalization is performed using the Jacobi's method [29]. This method consists of the following steps:

The first subroutine will select the largest off-diagonal element a_{ij}; it will diagonalize the 2 by 2 matrix consisting of a_{ii}, a_{jj}, and a_{ji}. A second subroutine will rotate the wave functions $|i\rangle$ and $|j\rangle$ to accomplish this diagonalization. As a result of this transformation all elements will be modified. The procedure is then repeated by looking again for the largest matrix element (which may be larger than the first matrix element). Beyond a certain iteration, the largest element will decrease.

The convergence of the method is based on the relation:

$$\sum_{ij} (a_{ij}^2+b_{ij}^2)=\sum_i \lambda_i^2,$$

where λ_i are the eigenvalues of the matrix. One can estimate the number of steps necessary to obtain elements of a certain magnitude; it is proportional to (n^2-n) where n is the dimensionality of the matrix [29]. The matrix is considered diagonalized if the off diagonal elements are less than a predetermined value. Actually, a weighted criterion was used based on the second order correction of the perturbation theory:

$$\sum_j \left| \frac{a_{ij}^2}{a_{ii}-a_{jj}} \right| < \epsilon \quad \text{for all } i$$

and ϵ was chosen to be 10^{-5}. Smaller values led to "accidental" divergences. The machine was prevented from using this criterion if a_{ii} was equal to a_{jj}. The number of iterations range from 4 (the minimum) to about 150.

Finally two more subroutines were used, one to order the levels, and one to calculate the dipolar and quadrupolar transition probabilities as indicated in eqs (2) and (3).

7. References

[1] Kagan, M. R., Lally, J. F., Meister, R., and Meijer, P. H. E., Phys. Rev. **166,** 234 (1968).
[2] Mattuck, R. D., and Strandberg, M. W. P., Phys. Rev. Letters **3,** 369, (1959).
[3] Mattuck, R. D., and Strandberg, M. W. P., Phys. Rev. **119,** 1204 (1960).
[4] Dobrov, W. I., Phys. Rev. **134,** 734 (1964).
[5] Howarth, D. J., Royal Radar Establishment (1960).
[6] Cross, C. S., and Kikuchi, R., Technical Report, University of Michigan Z 1238. (24 June 1959).
[7] Unpublished figures obtained from the Bell Tel. Lab.
[8] Lessin, I., U.S.A.F. Cambridge Report AFCRL 66–692 (1966).
[9] Moore, C. E., NBS (US) Circ. No. 467.
[10] Moorjani, K., and Mc Avoy, N., Phys. Rev. **132,** 504 (1963).
[11] Geschwind, S., and Remeika, J. P., Phys. Rev. **122,** 751 (1961).
[12] Borgnis, F. E., Phys. Rev. **98,** 1000 (1955).
[13] Desilets, E. H., and Meister, R., J. Appl. Phys. **36,** 261 (1965).
[14] Kornienko, L. S., and Prokhorov, A. M., JETP **33,** 805, 1955 (Trans. JETP **6,** 620, 1958).
[15] Bogle, G. S., and Symmons, J. F., Proc. Phys. Soc. (London) **73,** 531, (1959).
[16] Symmons, H. F., and Bogle, G. S., Proc. Phys. Soc. (London) **79,** 468, (1962).
[17] Abragam, A., and Pryce, M. H. L., Proc. Roy, Soc. **A205,** 135, (1951).
[18] Bleaney, B., and Trenam, R. S., Proc. Roy. Soc. (London) **223,** 1 (1954).
[19] Bleaney, B., and Ingram, D. J. E., Proc. Roy. Soc. **A205,** 336, (1951).
[20] de L. Kronig, R., and Bouwkamp, C. J., Physica **6,** 290, (1939).
[21] Stevens, K. W. H., Proc. Phys. Soc. (London) **A65,** 209 (1952).
[22] Hutchings, M. T., Solid State Physics **16,** 227 (1964).
[23] Shiren, N. S., and Tucker, E. B., Phys. Rev. Letters **6,** 105, (1961).
[24] Shiren, N. S., Bull. Am. Phys. Soc. **7,** 29 (1962).
[25] Tucker, E. B., Phys. Rev. Letters **6,** 183 (1962).
126] Dobrov, W. I., Phys. Rev. **134,** 734 (1964).
[27] Guermeur, R., Joffrin, J., Levelut, A., and Penne, J., Compt. Rend. Acad. Sc. (Paris) **260,** 108 (1965).
[28] Nye, J. F., Physical Properties of Crystals (Oxford University Press, 1957) and Birss, R. R., Symmetry and Magnetism (North Holland Publishing Company, Amsterdam, 1964).
[29] Wilkinson, J. H., Algebraic Eigenvalue Problems (Oxford, Oxford University Press 1965).

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