NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

Technical Memorandum 33-440

Paramagnetic Energy Levels of the Ground State of Cr^{+3} in Al_2O_3 (Ruby)

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Preface

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Abstract

The orbital splitting of the chromium (+3) ion in a host lattice of Al_2O_3 (ruby) is calculated on the basis of crystalline field theory. Spin-orbit coupling and the Zeeman energy are treated as a perturbation on the orbital singlet ground state in order to derive the spin Hamiltonian. A program has been written for the Univac 1108 computer to diagonalize the spin Hamiltonian matrix. Plots of fine-structure energy levels vs magnetic field are given for $\theta = 54°44'$ and 90°, where θ is the angle between the C axis of ruby and the external dc magnetic field.

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I. Introduction

Chromium-doped Al_2O_3 (ruby) has represented a vitally important component in maser development at JPL. It is essential to investigate the basic maser properties of ruby, among which are fine-structure energy levels and theoretical transition probabilities, in order to know to first order the performance of ruby as a maser material. Therefore, this study was undertaken in an attempt to develop an insight into the problem of what makes a good candidate for a maser material, while providing useful information concerning ruby. Treatises on the various subjects in this report are cited, and an attempt is made to compile these subjects into a detailed treatment.

One of the results of this study is a computer program which plots the fine-structure energy levels as a function of magnetic field and gives the transition probability matrix elements for chromium (+3) in Al_2O_3 (ruby).

The motivation for this paper has been to provide an introduction of the subject.

II. Crystalline Electric Field

It is appropriate to begin with the Hamiltonian of the free Cr^{+++} ion, the electron configuration of which is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$. A typical characteristic of a transition group element is illustrated by this configuration in that the outer s shell ($4s$) begins to fill before the inner shell ($3d$). The result is that for the case of Cr^{+++}, the $4s^1$ electron and two of the $3d^5$ electrons are used for chemical bonding in the Al_2O_3 crystal, leaving an inner shell $3d^3$ configuration, which gives the magnetic properties of this ion. In the central field approximation for N electrons and a nuclear charge Ze, the Hamiltonian is given by a sum of Coulomb and spin-orbit interaction terms[1]

$$\mathcal{H} = \mathcal{H}_{coul} + \mathcal{H}_{LS} \tag{1}$$

where

$$\mathcal{H}_{coul} = \sum_{k=1}^{N} \left(\frac{P_k^2}{2m} - \frac{Ze^2}{r_k} \right) + \sum_{j<k}^{N} \frac{e^2}{r_{jk}}$$

and

$$\mathcal{H}_{LS} = \sum_{k=1}^{N} \lambda \mathbf{L}_k \cdot \mathbf{S}_k$$

The form of $\mathcal{H}_{LS}$ is the result of assuming Russel–Saunders (L-S) coupling in which L and S are total angular momentum and spin of the N electrons. Consequently, each eigenstate can be labeled by L, S, M_L, M_S (or J,M_J),

[1]The chromium ion ($Z = 54$) has no nuclear spin; for this discussion, nuclear interaction terms are not listed.

where M_L, M_S, and M_J are the z components of L, S, and $J = L + S$, respectively, in a magnetic field. The interaction energies of $\mathcal{H}_{coul}$ and $\mathcal{H}_{LS}$ are approximately 10^5 cm^{-1} and 10^2 cm^{-1}, respectively.

The $\mathcal{H}_{coul}$ for $3d$ electrons gives rise to energy levels separated by optical transition frequencies. The ground state of the Cr^{+++} ion is labeled by the term $^4F_{3/2}$, where $S = 3/2$, $L = 3$, and $J = 3/2$. The orbital degeneracy is 7 and each orbital level has a spin degeneracy of 4.

When the Cr^{+++} ion is placed in the crystal of Al_2O_3, the electrostatic fields exert an influence on the unfilled $3d$ shell, and the orbital degeneracy of the ion is lifted by means of an internal Stark effect. The crystalline field theory assumes that the charges surrounding the ion are point charges and the potential at the ion site is determined from Laplace's equation. The symmetry of the electrostatic fields simplifies the form of the potential considerably and determines the orbital splitting. The interaction energy of the crystal potential V_c for the Cr^{+++} ion in Al_2O_3 is of the order of 10^4 cm^{-1}, and thus falls between the Coulomb and spin-orbit coupling terms. The potential energy due to the crystalline field is treated as a perturbation on the ground state $^4F_{3/2}$ term. Later, in deriving the spin Hamiltonian, the spin-orbit and Zeeman terms are taken together and treated as a perturbation on one of the nondegenerate orbital energy levels.

The Hamiltonian of the crystalline field is expressed as

$$\mathcal{H}_c = -|e|\sum_i V_c(r_i, \theta_i, \phi_i)$$

where the sum is over each of the surrounding charges making up the symmetry of the electrostatic field in the crystal, and V_c is the potential of each charge satisfying $\nabla^2 V_c = 0$. The potential at $\mathbf{r}$ due to point charges q at R_i (see Fig. 1) is

$$V_c(r, \theta, \phi) = q\sum_i \frac{1}{|\mathbf{R}_i - \mathbf{r}|}$$

$$= q\sum_i \frac{1}{R_i}\left[1 + \frac{r^2}{R_i^2} - \frac{r\cos\omega_i}{R_i}\right]^{-1/2}$$

The square root can be expressed in terms of spherical harmonics

$$V_c(r, \theta, \phi) = \sum_n \sum_i q\frac{r^n}{R_i^{n+1}} P_n(\cos\omega_i)$$

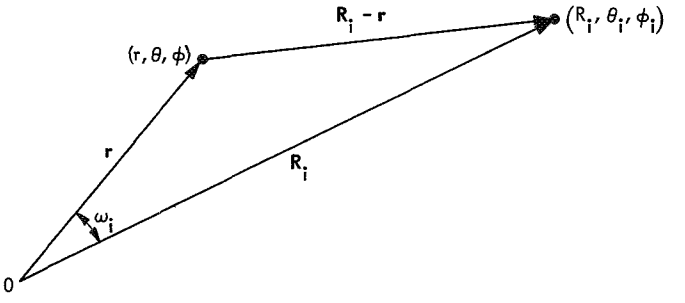


Fig. 1. Coordinate system depicting potential at r due to point charges at R_i

From the addition theorem for spherical harmonics (Ref. 1),

$$P_n(\cos\omega_i) = \frac{4\pi}{2n+1}\sum_{m=-n}^{n}(-1)^m Y_n^m(\theta, \phi)\, Y_n^{-m}(\theta_i, \phi_i)$$

Therefore,

$$V_c(r, \theta, \phi) =$$

$$\sum_i \sum_{m=-n}^{n} q\frac{r^n}{R_i^{n+1}}\frac{4\pi}{2n+1}(-1)^m Y_n^m(\theta, \phi)\, Y_n^{-m}(\theta_i, \phi_i)$$

Since the spherical harmonics are complex for $m > 0$, it is convenient to express the potential in terms of tesseral harmonics, defined as

$$Z_{n0}(\theta, \phi) = Y_n^0(\theta, \phi)$$

$$Z_{nm}^c(\theta, \phi) = \frac{1}{(2)^{1/2}}[Y_n^{-m} + (-1)^m Y_n^m]$$

$$Z_{nm}^s(\theta, \phi) = \frac{i}{(2)^{1/2}}[Y_n^{-m} - (-1)^m Y_n^m]$$

Therefore,

$$V_c(r, \theta, \phi) = \sum_{n=0}^{\infty}\sum_{\alpha}\gamma_{n\alpha} r^n Z_{n\alpha}(\theta, \phi) \qquad (2)$$

where

$$\gamma_{n\alpha} = \sum_i \frac{4\pi}{2n+1} q\frac{Z_{n\alpha}(\theta_i, \phi_i)}{R_i^{n+1}} \qquad (2a)$$

The objective in determining the splitting of the degenerate orbital levels in the crystalline field is to find the matrix elements $\langle L, M_L|V_c|L, M_L'\rangle$ of the 7×7 perturbation matrix. The elements $|L, M_L\rangle$ are the ground state orbital eigenfunctions

$$\psi_{L,M_L} = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

and each matrix element can be found from

$$\int \psi^*_{L,M_L} V_c \psi_{L,M'_L} d\tau$$

For the $3d$ electron, ψ_{L,M_L} has the form

$$\psi_{L,M_L} = R(r)\,\Theta(\theta)\,e^{iM_L\phi}$$

Thus,

$$\int \psi^*_{L,M_L} V_c \psi_{L,M'_L} d\tau \sim \int_{r,\theta} \int_{\phi=0}^{2\pi} e^{-iM_L\phi}\, e^{im\phi}\, e^{iM'_L\phi}\, dr\, d\theta\, d\phi = 0$$

unless $M_L = m + M'_L$, where we have used the spherical harmonic representation for $V_c \sim e^{im\phi}$. Since L is constant in these calculations, the matrix elements will be denoted by $\langle M_L | V_c | M'_L \rangle$, where $L = 3$ is implicit. Symmetry considerations of the crystalline field, in this case three-fold symmetry about an axis, will retain only certain terms in the expansion, Eq. (2). If $R(\phi, z)$ represents a rotation transformation of the spherical harmonics about the z axis by an angle ϕ, then for a three-fold symmetry axis, $\phi = 2\pi/3$ and

$$R\left(\frac{2\pi}{3}, z\right) Y^m_n = e^{im2\pi/3} Y^m_n = Y^m_n$$

since the spherical harmonics must be invariant under the rotation of ϕ degrees. Therefore, $e^{im2\pi/3} = 1$ and $m = 0, \pm 3, \pm 6, \cdots$. Since the matrix elements must be invariant under inversion, and

$$Y^m_n(-x, -y, -z) = (-1)^n\, Y^m_n(x, y, z),$$

n must be an even integer since the ground state wave function product $\psi^*_{M_L}\psi_{M'_L}$ is invariant under inversion.

At this point we resort to the fundamental matrix element theorem (Ref. 2). If, in the matrix element

$$\langle \psi_{M_L} | Y^m_n | \psi_{M'_L} \rangle$$

the functions ψ_{M_L}, Y^m_n and $\psi_{M'_L}$ transform according to the irreducible representations $D^{(L)}$, $D^{(n)}$, and $D^{(L')}$ of the full rotation group, the matrix element is nonzero only if the reduction of the product representation $D^{(n)} \times D^{(L')}$ contains the representation $D^{(L)}$. Thus, since ψ_{M_L} are eigenfunctions for the d electrons, they transform according to $D^{(2)}$ of the full rotation group. The matrix elements are nonzero only if

$$D^{(n)} \times D^{(2)} = D^{n+2} + D^{n+1} + \cdots + D^{|n-2|}$$

contains $D^{(2)}$. The allowed values of n are then $n \leq 4$. From all this, the only spherical harmonics representing the axially symmetric, three-fold potential are those for which n is even and ≤ 4 and $l = 0, \pm 3$. Thus,

$$V_c(r, \theta, \phi) = \gamma_{00} Z_{00}(\theta, \phi) + \gamma_{20} r^2 Z_{20}(\theta, \phi) + \gamma_{40} r^4 Z_{40}(\theta, \phi) + \gamma_{43} r^4 Z_{43}(\theta, \phi)$$

The Z_{00} term can be neglected since it adds a constant term to the potential and we are left to determine the matrix elements of

$$V_c(r, \theta, \phi) = r^2 \gamma_{20} Y^0_2(\theta, \phi) + r^4 \{\gamma_{40} Y^0_4(\theta, \phi) + \gamma_{43} [Y^{-3}_4(\theta, \phi) - Y^3_4(\theta, \phi)]\} \quad (3)$$

The coefficients in this potential are determined from the symmetrical nature of the crystal field.

To illustrate the method of determining the coefficients, we choose an eight-fold cubic coordination (Fig. 2) where the point charges are at the corners of the cube. The coordinates of each atom are shown on the figure, with the assumption that the origin of the xyz axes is at the physical center of the cube. If the xyz axes are rotated into $x'y'z'$ such that the positive z' axis is in the $0 \rightarrow (a,a,a)$ direction and the positive x' axis is in the $z,0,(a,a,a)$ plane

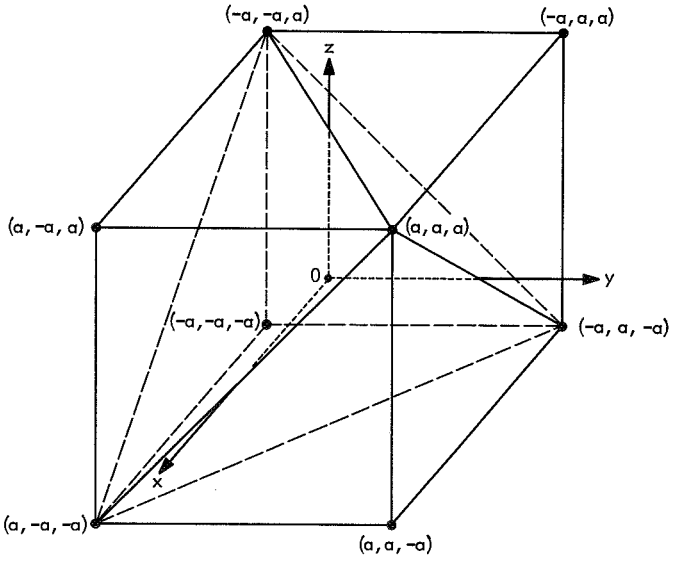


Fig. 2. Arrangement of atoms in an eight-fold cubic coordination showing tetrahedron and three-fold symmetry about diagonal $(a, a, a) \rightarrow (-a, -a, -a)$

(with $\angle z0x'$ acute), then the atomic arrangement of the tetrahedron, as shown in Fig. 2, has three-fold symmetry about the z' axis. This transformation from xyz to $x'y'z'$ can be accomplished easily by three successive rotations about Eulerian angles ϕ, θ, ψ. The definition of the Eulerian angles used here follows that in Ref. 3. The successive rotations are $\phi = 135°$, $\theta = \tan^{-1}(2)^{1/2}$, and $\psi = 90°$. The resultant transformation is given by

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\phi \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

with the result

$$x' = \left(\frac{2}{3}\right)^{1/2}\left(-\frac{1}{2}x - \frac{1}{2}y + z\right)$$

$$y' = \frac{(2)^{1/2}}{2}(x - y)$$

$$z' = \frac{1}{(3)^{1/2}}(x + y + z)$$

Table 1 gives the coordinates of the four point charges in terms of the $x'y'z'$ axes in Cartesian and spherical coordinates, where

$$x' = r'\sin\theta\cos\phi$$

$$y' = r'\sin\theta\sin\phi$$

$$z' = r'\cos\theta$$

$$r' = (x'^2 + y'^2 + z'^2)^{1/2} = (3)^{1/2}a$$

For our purposes, a rather complete list of spherical and tesseral harmonics is given in Refs. 4 and 5. From these references we obtain

$$Z_{20} = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1)$$

$$Z_{40} = Y_4^0 = \frac{3}{16\sqrt{\pi}}(35\cos^4\theta - 30\cos^2\theta + 3)$$

$$Y_4^{\pm 3} = \mp\frac{3}{8}\sqrt{\frac{35}{\pi}}\sin^3\theta\cos\theta\, e^{\pm 3i\phi}$$

$$Z_{43}^c = \frac{3}{8}\sqrt{\frac{70}{\pi}}\sin^3\theta\cos\theta\cos 3\phi$$

$$Z_{43}^s = \frac{3}{8}\sqrt{\frac{70}{\pi}}\sin^3\theta\cos\theta\sin 3\phi$$

Table 2 gives the values of Z_{40} and Z_{43} for each of the four point charges of the tetrahedron.

Substituting the values from Table 2 into Eq. (2a) gives

$$\gamma_{20} = 0$$

$$\gamma_{40} = \frac{2}{3}(\pi)^{1/2}\frac{q}{d^5}\frac{28}{27}$$

and

$$\gamma_{43} = -\frac{2}{3}(\pi)^{1/2}\frac{q}{d^5}\left(\frac{10}{7}\right)^{1/2}\frac{28}{27}(2)^{1/2}$$

where $d = (3)^{1/2}a$. Equation (2) becomes

$$V_c = \frac{q}{d^5}\frac{2}{3}(\pi)^{1/2}\frac{28}{27}\left[Y_4^0 - \left(\frac{10}{7}\right)^{1/2}(Y_4^{-3} - Y_4^{3})\right] \qquad (4)$$

III. Matrix Elements of the Crystalline Potential V_c

The equation $\int\psi^*_{M_L}V_c\psi_{M'_L}\,d\tau$ is the most direct way to evaluate matrix elements but requires the knowledge of the ground state eigenfunctions for the $3d$ electrons. Although it is possible to perform the integrations in the usual way (see Ref. 6 for a discussion of this method), we shall consider a more convenient method, introduced by Stevens (Ref. 7), called the "operator equivalent method." In this method, the potential, Eq. (4), is expressed as a function of Cartesian coordinates, and x,y,z are replaced by the angular momentum operators L_x, L_y, L_z, respectively.

Although x, y, and z commute, the commutation rules for the angular momentum operators must be observed. (It is not the purpose of this report to expound on the reasoning behind the equivalence of the resulting matrix elements, as it involves a discourse on group theory.) The reader can resort to the references dealing with the Wigner-Eckart theorem (Refs. 8, 9, and 10), which is the basis for the operator equivalent method of Stevens.

Using the transformations $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$,

$$Z_{40} = \frac{3}{16(\pi)^{1/2}}\frac{35z^4 - 30z^2r^2 + 3r^4}{r^4}$$

and

$$Z_{43}^c = \frac{3}{8}\left(\frac{70}{\pi}\right)^{1/2}\frac{z(x^3 - 3xy^2)}{r^4}$$

Table 1. Spherical and Cartesian coordinates of point charges of tetrahedron (Fig. 2) expressed in transformed coordinates (along diagonal of cube)

xyz coordinate	x′y′z′ coordinate (Cartesian)	Spherical coordinates					
		cos θ	sin θ	θ	cos φ	sin φ	φ, deg
(a,a,a)	$(0,0,\sqrt{3}\,a)$	1	0	0	—	—	—
(a,−a,−a)	$\left(-\sqrt{\frac{2}{3}}a,\ \sqrt{2}\,a,\ -\frac{1}{\sqrt{3}}a\right)$	$-\frac{1}{3}$	$2\frac{\sqrt{2}}{3}$	$\tan^{-1}2\sqrt{2}$	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	120
(−a,a,−a)	$\left(-\sqrt{\frac{2}{3}}a,\ -\sqrt{2}\,a,\ -\frac{1}{\sqrt{3}}a\right)$	$-\frac{1}{3}$	$2\frac{\sqrt{2}}{3}$	$\tan^{-1}2\sqrt{2}$	$-\frac{1}{2}$	$-\frac{\sqrt{3}}{2}$	240
(−a,−a,a)	$\left(2\sqrt{\frac{2}{3}}a,\ 0,\ -\frac{1}{\sqrt{3}}a\right)$	$-\frac{1}{3}$	$2\frac{\sqrt{2}}{3}$	$\tan^{-1}2\sqrt{2}$	1	0	0

Table 2. Values of Z_{40} and Z_{43} for point charges of the tetrahedron

Coordinate	Z_{20}	Z_{40}	Z^c_{43}	Z^s_{43}
(a,a,a)	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\,2$	$8\,\frac{3}{16\sqrt{\pi}}$	0	0
(a,−a,−a)	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(-\frac{2}{3}\right)$	$\frac{8}{81}\,\frac{3}{16\sqrt{\pi}}$	$-\frac{16\sqrt{2}}{81}\,\frac{3}{8}\sqrt{\frac{70}{\pi}}$	0
(−a,a,−a)	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(-\frac{2}{3}\right)$	$\frac{8}{81}\,\frac{3}{16\sqrt{\pi}}$	$-\frac{16\sqrt{2}}{81}\,\frac{3}{8}\sqrt{\frac{70}{\pi}}$	0
(−a,−a,a)	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(-\frac{2}{3}\right)$	$\frac{8}{81}\,\frac{3}{16\sqrt{\pi}}$	$-\frac{16\sqrt{2}}{81}\,\frac{3}{8}\sqrt{\frac{70}{\pi}}$	0

The operator equivalents for these tesseral harmonics are

$$\sum_i (35z_i^4 - 30z_i r_i^2 + 3r_i^4) = \langle r^4\rangle \beta_L [35L_z^4 - 30L(L+1)L_z^2 + 25L_z^2 - 6L(L+1) + 3L^2(L+1)^2] \equiv \langle r^4\rangle \beta_L O_4^0$$

and

$$\sum_i z_i (x_i^3 - 3x_i y_i^2) = \langle r^4\rangle \beta_L \frac{1}{4}[L_z(L_+^3 + L_-^3) + (L_+^3 + L_-^3)L_z] \equiv \langle r^4\rangle \beta_L O_4^3$$

where $\langle r^4\rangle = \int [f(r)]^2 r^6\,dr$, $f(r)$ is the radial part of the wave function, β_L is a multiplying factor which is equal to 2/315 for the ground state ${}^4F_{3/2}$ of Cr^{+++}, and $L_\pm = L_x \pm iL_y$.

With these definitions, the potential, Eq. (4), becomes

$$V_c = -\frac{2}{3}\frac{|e|}{d^5}\frac{7}{36}\beta_L \langle r^4\rangle [O_4^0 - 20(2)^{1/2} O_4^3] \qquad (5)$$

The matrix elements $\langle M_L|O_n^m|M'_L\rangle$ have been tabulated in Refs. 4 and 11. The only nonzero matrix elements are those where $M_L = m + M'_L$. Thus, for O_4^0, $M_L = M'_L$, and the diagonal elements are

$$\langle 3|O_4^0|3\rangle = 180 \qquad \langle 1|O_4^0|1\rangle = 60$$
$$\langle 2|O_4^0|2\rangle = -420 \qquad \langle 0|O_4^0|0\rangle = 360$$

For O_4^3, the off-diagonal elements $\langle M_L|O_4^3|M'_L\rangle$ are

$$\langle 2|O_4^3|-1\rangle = -120(5)^{1/2}$$
$$\langle 3|O_4^3|0\rangle = -180(10)^{1/2}$$

The matrix, then, with

$$\langle -M_L|O_4^3|-M'_L\rangle = -\langle M_L|O_4^3|M'_L\rangle,$$

is

L	3	2	1	0	−1	−2	−3
3	180	0	0	$-180(10)^{1/2}$	0	0	0
2	0	−420	0	0	$-120(5)^{1/2}$	0	0
1	0	0	60	0	0	$120(5)^{1/2}$	0
0	$-180(10)^{1/2}$	0	0	360	0	0	$180(10)^{1/2}$
−1	0	$-120(5)^{1/2}$	0	0	60	0	0
−2	0	0	$120(5)^{1/2}$	0	0	−420	0
−3	0	0	0	$180(10)^{1/2}$	0	0	180

Diagonalization of this 7×7 matrix yields the following eigenvalues:

$$E = 1080 \text{ (singlet)}$$
$$E = 180 \text{ (triplet)}$$
$$E = 540 \text{ (triplet)}$$

and the Hamiltonian H_c has the following eigenvalues:

$$E_1 = 18\text{K (triplet)}$$
$$E_2 = -6\text{K (triplet)}$$
$$E_3 = -36\text{K (singlet)}$$

where

$$K = \frac{2}{3}\frac{q|e|}{d^5}\frac{7}{36}30\beta_L\langle r^4\rangle$$

Thus, the ground state of the Cr^{+++} ion in an eight-fold cubic coordination taken along the diagonal axis which has three-fold symmetry, is split up into two orbital triplets and a singlet. The singlet is actually four-fold spin-degenerate, and our next task is to apply spin-orbit coupling and Zeeman perturbations on this singlet level in the form of a spin Hamiltonian.

IV. Spin Hamiltonian

The experimental values of the g factor of Cr^{+++} in Al_2O_3 show a slight anisotropy; i.e., $g_{\parallel} = 1.984$ and $g_{\perp} = 1.9867$, where $g_{\parallel}$ refers to the z' direction ($\theta = 0°$) and $g_{\perp} =$ refers to the plane perpendicular to the z' axis ($\theta = 90°$). However, it is noteworthy that the average g is close to the spin-only value of 2.0, compared to $g = 0.4$ if angular momentum is included. Thus, the atom acts as if $L \approx 0$; i.e., the magnetic moment is quenched. In fact, disregarding spin-orbit coupling, the angular momentum of the orbital singlet is totally quenched and has no angular momentum. The slight anisotropy of the g value is a result of spin-orbit coupling which admixes the singlet ground state with the upper states and thus restores some of the angular momentum. The spin-orbit coupling then accounts for the difference between the spin-only g value and the actual value. In the derivation of the spin Hamiltonian, the nondegenerate ground state is treated as an unperturbed, isolated level (which is four-fold spin-degenerate), and all other orbital levels are ignored. This isolated level is considered to be a dipole with $2S + 1$ orientations and a g factor (usually anisotropic) which is close to the free spin value. The success of using this method depends on the spin-orbit coupling and Zeeman energies being small compared with the separation between the orbital levels; also, the spin-orbit coupling must be smaller than the Zeeman separation energies.

The perturbing Hamiltonian has the form

$$\mathcal{H}' = \lambda\mathbf{L}\cdot\mathbf{S} + \beta\mathbf{H}\cdot(\mathbf{L} + 2\mathbf{S})$$

where the first term is spin-orbit coupling and the second term is the Zeeman energy.

Up to second order, the perturbed energy is

$$\mathcal{H}_s = W_1 + W_2 = \langle 0|\mathcal{H}'|0\rangle - \sum_{n\neq 0}\frac{\langle 0|\mathcal{H}'|n\rangle\langle n|\mathcal{H}'|0\rangle}{E_n - E_0}$$

where $|0\rangle$ is the ground state eigenfunction (the orbital singlet) and $|n\rangle$ are eigenfunctions of the higher-lying orbitals. Since the ground state possesses no angular momentum, then $\langle 0|L_i|0\rangle = 0$ for $i = x, y, z$. Therefore,

$$W_1 = \langle 0|\lambda\mathbf{L}\cdot\mathbf{S} + \beta\mathbf{H}\cdot(\mathbf{L} + 2\mathbf{S})|0\rangle = 2\beta\mathbf{H}\cdot\mathbf{S}\langle 0|0\rangle$$
$$= 2\beta\mathbf{H}\cdot\mathbf{S}$$

The second-order term is

$$W_2 = -\sum_{n\neq 0}\frac{\langle 0|\lambda\mathbf{L}\cdot\mathbf{S} + \beta\mathbf{H}\cdot(\mathbf{L} + 2\mathbf{S})|n\rangle\langle n|\lambda\mathbf{L}\cdot\mathbf{S} + \beta\mathbf{H}\cdot(\mathbf{L} + 2\mathbf{S})|0\rangle}{E_n - E_0}$$

The orbital angular momentum operates on the eigenfunctions, and terms not including L can be factored out of the matrix element. Thus, for example,

$$\langle 0|\lambda\mathbf{L}\cdot\mathbf{S}|n\rangle\langle n|\lambda\mathbf{L}\cdot\mathbf{S}|0\rangle = \frac{\lambda^2[\langle 0|L_xS_x|n\rangle\langle n|L_xS_x|0\rangle + \langle 0|L_yS_y|n\rangle\langle n|L_yS_y|0\rangle + \cdots + \langle 0|L_xS_x|n\rangle\langle n|L_yS_y|0\rangle + \cdots]}{(E_n - E_0)}$$
$$= \lambda^2\sum_{ij}S_iS_j\frac{\langle 0|L_i|n\rangle\langle n|L_j|0\rangle}{E_n - E_0}$$

Expanding W_2 similarly for the other terms gives

$$W_2 = -\sum_{ij} [\lambda^2 \Lambda_{ij} S_i S_j + \beta^2 \Lambda_{ij} H_i H_j + 2\beta\lambda\Lambda_{ij} S_i H_j]$$

where

$$\Lambda_{ij} \equiv \sum_{n \neq 0} \frac{\langle 0|L_i|n\rangle \langle n|L_j|0\rangle}{E_n - E_0}$$

Therefore,

$$\mathcal{H}_s = \sum_{ij} [-\lambda^2 \Lambda_{ij} S_i S_j - \beta^2 \Lambda_{ij} H_i H_j + 2\beta(\delta_{ij} - \lambda\Lambda_{ij}) S_i H_j]$$

If we define

$$g_{ij} = 2(\delta_{ij} - \lambda\Lambda_{ij})$$

and

$$D_{ij} = -\lambda^2 \Lambda_{ij}$$

then

$$\mathcal{H}_s = \sum_{ij} [g_{ij}\beta S_i H_j + D_{ij} S_i S_j], \qquad (i, j = x, y, z) \tag{6}$$

where we have omitted the quadratic term of the magnetic field $-\beta^2 \Lambda_{ij} H_i H_j$ since it is a constant independent of spin. The g_{ij} is the g factor tensor, and D_{ij} determines the zero field splitting of the orbital singlet.

In ruby, the only directions we are concerned with in the g and D tensors are the z axis and the x–y plane.[2] Therefore, we define

$$\Lambda_{xx} = \Lambda_{yy} \equiv \Lambda_\perp, \qquad \Lambda_{zz} \equiv \Lambda_\parallel$$

and

$$g_{xx} = g_{yy} \equiv g_\perp = 2(1 - \lambda\Lambda_{xx}), \qquad g_{zz} \equiv g_\parallel = 2(1 - \lambda\Lambda_{zz})$$

Then,

$$\begin{aligned} \sum_{ij} D_{ij} S_i S_j &= -\lambda^2 [\Lambda_\perp (S_x^2 + S_y^2) + \Lambda_\parallel S_z^2] \\ &= \lambda^2 [(\Lambda_\perp - \Lambda_\parallel) S_z^2 - \Lambda_\perp S(S+1)] \\ &= D\left[S_z^2 - \frac{1}{3} S(S+1)\right] - \frac{\lambda^2}{3} S(S+1)(\Lambda_\parallel + 2\Lambda_\perp) \end{aligned} \tag{7}$$

where we have substituted $S_x^2 + S_y^2 = S(S+1) - S_z^2$ and defined $D = \lambda^2(\Lambda_\perp - \Lambda_\parallel)$. The second term in Eq. (7) can be neglected since it represents a constant term in the Hamiltonian.

For our purposes we can neglect the slight anisotropy of the g factor and use an average value, g. The first term in Eq. (6) becomes $g\beta\mathbf{H} \cdot \mathbf{S}$, and the final spin Hamiltonian becomes

$$\mathcal{H}_s = g\beta\mathbf{H} \cdot \mathbf{S} + D\left[S_z^2 - \frac{1}{3} S(S+1)\right] \tag{8}$$

where $S = 3/2$.

To compute the energy levels of the spin Hamiltonian, we must find the eigenvalues of $\hat{\mathcal{H}}_s|\psi_i\rangle = E_i|\psi_i\rangle$. This equation is easily solved by forming the matrix $[\mathcal{H}_s]$ and solving the secular equation $|\hat{\mathcal{H}}_s - E_i I| = 0$ for the eigenvalues $E_i, i = 1, \cdots, 4$. The method of finding $[\mathcal{H}_s]$ can be found in the literature (Refs. 12 and 13), and one of several but equivalent methods can be used. As mentioned before, the orbital ground state of the Cr^{+++} ion is four-fold degenerate. The eigenvector $|\psi_i\rangle$ can be expressed as a linear combination of the four pure spin states:

$$|\psi_i\rangle = a_i \left|\frac{3}{2}\right\rangle + b_i \left|\frac{1}{2}\right\rangle + c_i \left|-\frac{1}{2}\right\rangle + d_i \left|-\frac{3}{2}\right\rangle$$

where $|3/2\rangle$, etc., are the base states referring to the $2S + 1$ positions of the dipole in the magnetic field.

In the Hamiltonian, Eq. (8), we substitute

$$\begin{aligned} H_x &= H_0 \sin\theta \cos\phi \\ H_y &= H_0 \sin\theta \sin\phi \\ H_z &= H_0 \cos\theta \end{aligned}$$

where H_0 is the maximum value of the dc field which makes an angle θ with the z axis (Fig. 3). Since $\mathcal{H}_s$ has axial symmetry about the z axis, we can let $\phi = 0$. Therefore,

$$\mathcal{H}_s = g\beta H_0 (S_x \sin\theta + S_z \cos\theta) + D\left(S_z^2 - \frac{5}{4}\right) \tag{9}$$

[2] In the following, primes are omitted from $x'y'z'$ and the z axis is taken to be along the diagonal of the cube in Fig. 2. The z axis is then the C axis of the crystal.

It is convenient to express S_x and S_z as matrix operators of the following form (Ref. 14):

$$S_x = \frac{1}{2}\begin{bmatrix} 0 & (3)^{1/2} & 0 & 0 \\ (3)^{1/2} & 0 & 2 & 0 \\ 0 & 2 & 0 & (3)^{1/2} \\ 0 & 0 & (3)^{1/2} & 0 \end{bmatrix}, \quad S_y = \frac{1}{2}\begin{bmatrix} 0 & -(3)^{1/2}i & 0 & 0 \\ (3)^{1/2}i & 0 & -2i & 0 \\ 0 & 2i & 0 & -(3)^{1/2}i \\ 0 & 0 & (3)^{1/2}i & 0 \end{bmatrix}, \quad S_z = \frac{1}{2}\begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix} \tag{10}$$

Substitution of these matrices into Eq. (9) gives

$$[\mathcal{H}_s] = \begin{bmatrix} \frac{3}{2}g\beta H_0\cos\theta + D & \frac{(3)^{1/2}}{2}g\beta H_0\sin\theta & 0 & 0 \\ \frac{(3)^{1/2}}{2}g\beta H_0\sin\theta & \frac{1}{2}g\beta H_0\cos\theta - D & g\beta H_0\sin\theta & 0 \\ 0 & g\beta H_0\sin\theta & -\frac{1}{2}g\beta H_0\cos\theta - D & \frac{(3)^{1/2}}{2}g\beta H_0\sin\theta \\ 0 & 0 & \frac{(3)^{1/2}}{2}g\beta H_0\sin\theta & -\frac{3}{2}g\beta H_0\cos\theta + D \end{bmatrix} \tag{11}$$

The stimulated transition probability per unit time of a transition from state ψ_i to state ψ_j is given by (Ref. 14, p. 199)

$$W_{ij} = \frac{1}{4}\gamma^2 G(f)\,|\langle\psi_i|\mathcal{H}'|\psi_j\rangle|^2 \tag{12}$$

where H' is the applied perturbation, $G(f)$ is the density of states, and $\gamma = g\beta\mu_0/\hbar$. For an rf magnetic field H_1 applied to the spin system in the crystal, the dipole interaction energy is $\boldsymbol{\mu}\cdot\mathbf{H}_1 = g\beta\mathbf{S}\cdot\mathbf{H}_1$. Therefore,

$$W_{ij} = \frac{1}{4}\gamma^2 G(f)\, g\beta\,|\langle\psi_i|\mathbf{H}_1\cdot\mathbf{S}|\psi_j\rangle|^2$$

If ϕ_1, ϕ_2, and ϕ_3 are direction cosines of $\mathbf{H}_1$ with respect to the x, y, z axes in Fig. 3, then $\mathbf{H}_1 = H_1^0(\phi_1\hat{i} + \phi_2\hat{j} + \phi_3\hat{k})$, and matrix elements of Eq. (12) become, using Eqs. (10) for the representation of S,

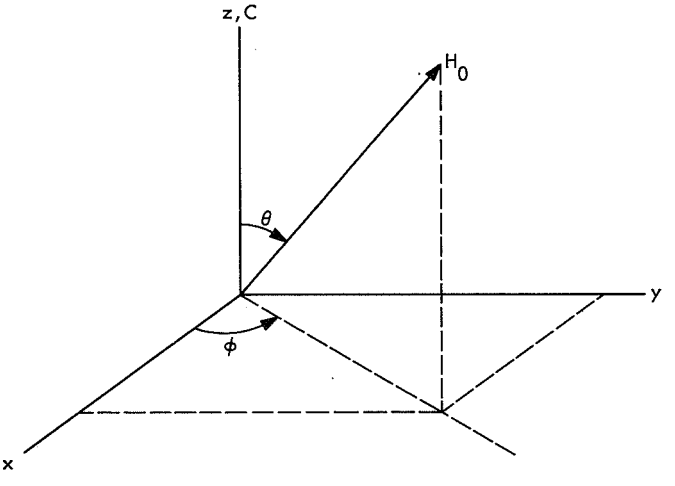


Fig. 3. Coordinate system of the external dc magnetic field $\mathbf{H}_0$

$$\frac{\langle\psi_i|\mathbf{H}_1\cdot\mathbf{S}|\psi_j\rangle}{H_1^0} =$$

$$[a_i^* b_i^* c_i^* d_i^*]\begin{bmatrix} 3\phi_3 & (3)^{1/2}(\phi_1 - i\phi_2) & 0 & 0 \\ (3)^{1/2}(\phi_1 + i\phi_2) & \phi_3 & 2(\phi_1 - i\phi_2) & 0 \\ 0 & 2(\phi_1 + i\phi_2) & -\phi_3 & (3)^{1/2}(\phi_1 - i\phi_2) \\ 0 & 0 & (3)^{1/2}(\phi_1 + i\phi_2) & -3\phi_3 \end{bmatrix}\begin{bmatrix} a_j \\ b_j \\ c_j \\ d_j \end{bmatrix} \equiv \alpha_{ij}\phi_1 + i\beta_{ij}\phi_2 + \gamma_{ij}\phi_3 \tag{13}$$

where

$$\alpha_{ij} = (3)^{1/2}(a_i^* b_j + b_i^* a_j + c_i^* d_j + d_i^* c_j) + 2(b_i^* c_j + c_i^* b_j)$$

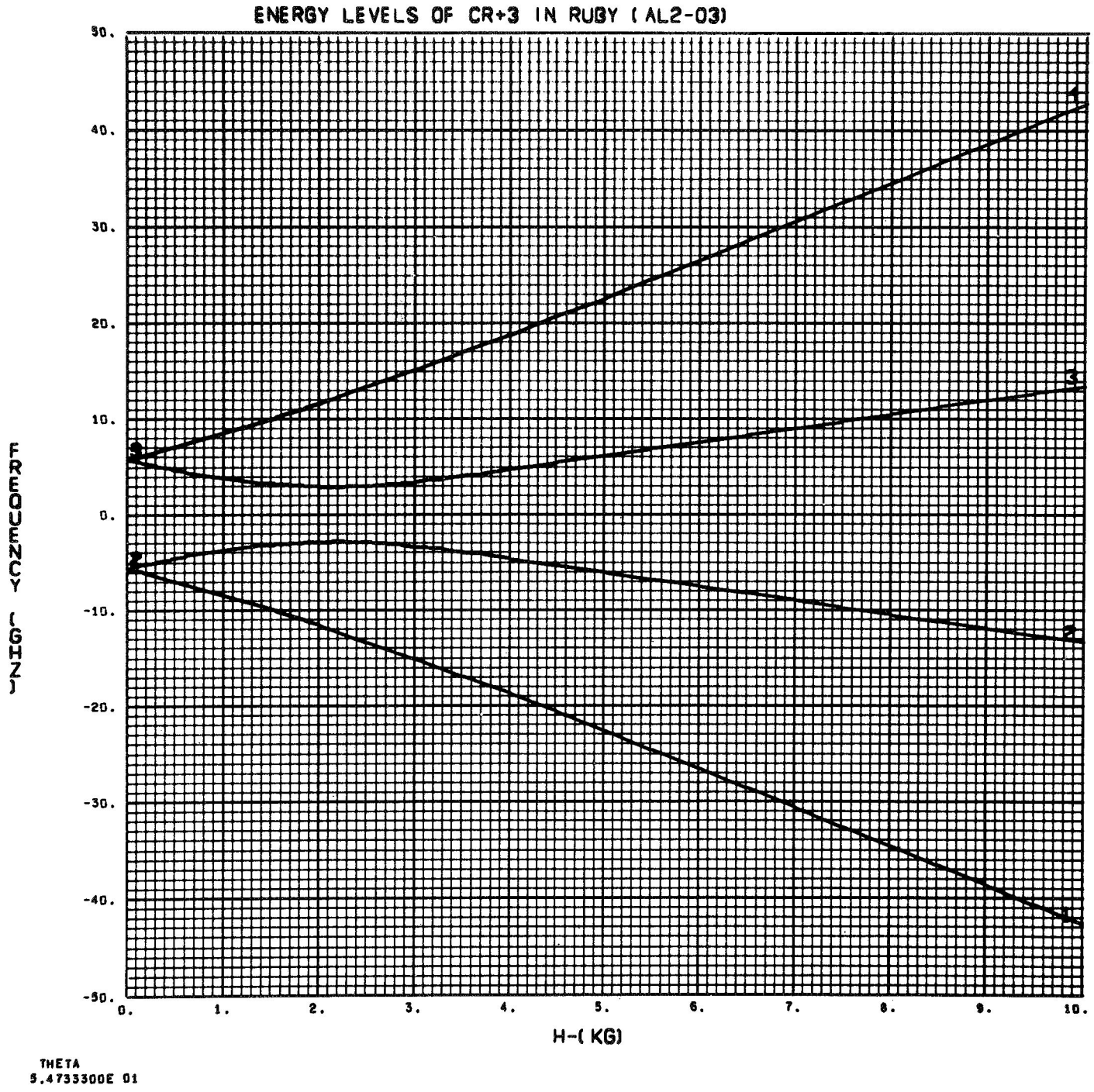
$$\beta_{ij} = (3)^{1/2}(-a_i^* b_j + b_i^* a_j - c_i^* d_j + d_i^* c_j) + 2(-b_i^* c_j + c_i^* b_j)$$

$$\gamma_{ij} = 3(a_i^* a_j - d_i^* d_j) + b_i^* b_j - c_i^* c_j$$

Diagonalization of the spin Hamiltonian, Eq. (11), and computation of the transition probability matrix elements (i.e., α_{ij}, β_{ij}, and γ_{ij}, have been programmed in Fortran V language for the Univac 1108. The program computes eigenvalues and orthonormal eigenvector coefficients a_i, b_i, c_i, d_i. A plot is also made of the eigenvalues vs magnetic field from 0 to 10 kG for a given value of θ. The results of these computations are listed in the Appendix for $\theta = 54°44'$ and 90°.

Appendix

Computer Output of Energy Levels and Transition Probability Matrix Elements for Ruby at $\theta = 54°44'$ and 90°



THETA
5.4733300E 01

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 54.733 DEGREES H= 0.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 5.73000 GHZ

A(4)	B(4)	C(4)	D(4)
0.8931108E-34	0.6962002E 00	0.5071397E 00	0.8763578E-34
0.4006738E-33	0.4936993E 00	0.1198984E 00	0.5235862E-33

EIGENVECTOR FOR E(3)= 5.73000 GHZ

A(3)	B(3)	C(3)	D(3)
0.2357551E-34	-0.2962759E-01	-0.5675999E 00	0.1545277E-33
0.1079737E-32	0.7210653E 00	-0.3962541E 00	0.1234076E-32

EIGENVECTOR FOR E(2)= -5.73000 GHZ

A(2)	B(2)	C(2)	D(2)
0.1401714E 00	0.1275324E-33	0.4942286E-33	0.6229365E-01
0.4789766E 00	0.1230159E-34	0.3250896E-33	0.8643222E 00

EIGENVECTOR FOR E(1)= -5.73000 GHZ

A(1)	B(1)	C(1)	D(1)
-0.1685672E 00	0.1479543E-33	0.7008233E-33	0.9754711E 00
0.1011655E 00	0.7160902E-33	0.1480275E-33	-0.9902935E-01

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
0.0000	11.4600	11.4600	11.4600	11.4600	-0.0000

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.1490	-2.8326	2.8365
(1,3)	-0.7560	-0.9722	1.2316	-0.5615	1.0260	1.1696	0.0000	-0.0000	0.0000
(1,4)	0.7195	0.0234	0.7199	0.5557	-0.9530	1.1032	0.0000	-0.0000	0.0000
(2,3)	-0.0634	1.0066	1.0086	0.6073	1.2455	1.3857	-0.0000	0.0000	0.0000
(2,4)	0.8128	-1.2040	1.4527	-0.2886	0.3444	0.4493	-0.0000	0.0000	0.0000
(3,4)	-1.0387	-0.7472	1.2795	0.7298	1.3244	1.5122	0.6707	-0.6495	0.9337

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	2.0115	0.0000
(1,3)	0.3792	0.3420
(1,4)	0.1296	0.3043
(2,3)	0.2543	0.4800
(2,4)	0.5276	0.0505
(3,4)	0.6272	0.5717

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 54.733 DEGREES H= 2000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 11.63081 GHZ

A(4)	B(4)	C(4)	D(4)
0.2209415E 00	0.7015915E 00	0.4693284E 00	0.8343376E-01
0.1213400E 00	0.3853107E 00	0.2577529E 00	0.4582142E-01

EIGENVECTOR FOR E(3)= 2.86723 GHZ

A(3)	B(3)	C(3)	D(3)
-0.4033737E 00	-0.3849092E 00	0.7273033E 00	0.2136661E 00
0.1450575E 00	0.1384175E 00	-0.2615461E 00	-0.7683665E-01

EIGENVECTOR FOR E(2)= -2.86691 GHZ

A(2)	B(2)	C(2)	D(2)
0.5254458E 00	-0.2622836E 00	0.1326357E 00	0.6799965E-01
0.6899240E 00	-0.3443852E 00	0.1741541E 00	0.8928531E-01

EIGENVECTOR FOR E(1)= -11.63113 GHZ

A(1)	B(1)	C(1)	D(1)
-0.2463838E-01	0.6703029E-01	-0.2578059E 00	0.9517895E 00
0.3740838E-02	-0.1017719E-01	0.3914259E-01	-0.1445099E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
8.7636	14.4977	23.2619	5.7341	14.4984	8.7642

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	0.3311	0.6057	0.6903	0.6098	-0.3333	0.6949	-0.1733	-0.3170	0.3612
(1,3)	1.4439	-0.2845	1.4717	-0.2768	-1.4048	1.4318	-0.4414	0.0870	0.4499
(1,4)	0.3972	0.3038	0.5001	0.3098	-0.4050	0.5099	-0.0793	-0.0607	0.0999
(2,3)	-0.2723	0.8630	0.9049	-1.4210	-0.4484	1.4900	-0.3563	1.1289	1.1838
(2,4)	0.9509	-0.4220	1.0404	0.2066	0.4655	0.5093	0.1463	-0.0649	0.1600
(3,4)	0.2412	0.2732	0.3644	1.6298	-1.4391	2.1742	-0.7481	-0.8472	1.1303

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	0.1518	0.1207
(1,3)	0.5921	0.5125
(1,4)	0.0650	0.0650
(2,3)	0.5551	0.5551
(2,4)	0.2770	0.0648
(3,4)	0.3526	1.1818

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 54.733 DEGREES H= 4000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 18.84546 GHZ

A(4)	B(4)	C(4)	D(4)
0.2736778E 00	0.5171491E 00	0.3245446E 00	0.7479146E-01
0.3005740E 00	0.5679728E 00	0.3564397E 00	0.8214172E-01

EIGENVECTOR FOR E(3)= 4.67359 GHZ

A(3)	B(3)	C(3)	D(3)
-0.7128297E 00	-0.6672811E-01	0.6486593E 00	0.2550454E 00
0.2866153E-01	0.2683011E-02	-0.2608136E-01	-0.1025489E-01

EIGENVECTOR FOR E(2)= -4.67310 GHZ

A(2)	B(2)	C(2)	D(2)
0.4839336E 00	-0.5279271E 00	0.3703368E 00	0.2725487E 00
0.2985461E 00	-0.3256863E 00	0.2284665E 00	0.1681395E 00

EIGENVECTOR FOR E(1)= -18.84594 GHZ

A(1)	B(1)	C(1)	D(1)
-0.4145993E-01	0.1196968E 00	-0.3292722E 00	0.7528807E 00
0.2770562E-01	-0.7998748E-01	0.2200363E 00	-0.5031129E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
14.1719	23.5186	37.6914	9.3467	23.5195	14.1728

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	0.5302	1.1593	1.2748	1.2335	-0.5641	1.3564	-0.3627	-0.7930	0.8720
(1,3)	0.7770	0.4752	0.9108	0.4568	-0.7470	0.8756	-0.2894	-0.1770	0.3392
(1,4)	0.0365	0.2425	0.2453	0.2499	-0.0376	0.2528	-0.0091	-0.0604	0.0611
(2,3)	0.3232	-0.2178	0.3897	-0.9764	-1.4490	1.7472	-1.4125	0.9518	1.7032
(2,4)	0.7126	0.2045	0.7413	0.0709	-0.2470	0.2569	-0.0957	-0.0275	0.0995
(3,4)	0.1767	0.2105	0.2748	1.5716	-1.3195	2.0521	-0.8483	-1.0104	1.3193

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	0.5963	0.4599
(1,3)	0.2361	0.1917
(1,4)	0.0160	0.0160
(2,3)	0.7632	0.7632
(2,4)	0.1399	0.0165
(3,4)	0.4540	1.0527

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 54.733 DEGREES H= 6000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 26.62367 GHZ

A(4)	B(4)	C(4)	D(4)
0.3260342E 00	0.4918651E 00	0.2956715E 00	0.7469604E-01
0.3668990E 00	0.5535150E 00	0.3327307E 00	0.8405837E-01

EIGENVECTOR FOR E(3)= 7.57222 GHZ

A(3)	B(3)	C(3)	D(3)
-0.6926710E 00	0.6994532E-01	0.5845673E 00	0.2488876E 00
-0.2455645E 00	0.2479689E-01	0.2072398E 00	0.8823518E-01

EIGENVECTOR FOR E(2)= -7.57165 GHZ

A(2)	B(2)	C(2)	D(2)
0.2399894E 00	-0.3312925E 00	0.2317362E 00	0.2167272E 00
-0.3966029E 00	0.5474891E 00	-0.3829638E 00	-0.3581601E 00

EIGENVECTOR FOR E(1)= -26.62424 GHZ

A(1)	B(1)	C(1)	D(1)
-0.2936079E-01	0.8779319E-01	-0.2134482E 00	0.3949444E 00
-0.5692808E-01	0.1702235E 00	-0.4138580E 00	0.7657636E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
19.0515	34.1953	53.2479	15.1439	34.1965	19.0526

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	-0.6918	-1.1272	1.3226	-1.2895	0.7914	1.5129	0.5677	0.9250	1.0853
(1,3)	0.4586	-0.4306	0.6290	-0.4082	-0.4347	0.5963	-0.1737	0.1631	0.2383
(1,4)	0.1309	-0.0335	0.1351	-0.0346	-0.1355	0.1398	-0.0348	0.0089	0.0359
(2,3)	0.1619	0.7847	0.8012	1.8218	-0.3759	1.8602	-0.3392	-1.6441	1.6788
(2,4)	-0.1637	0.5289	0.5537	0.3149	0.0974	0.3296	0.0389	-0.1258	0.1317
(3,4)	0.3762	0.2073	0.4295	0.9367	-1.6999	1.9409	-1.2195	-0.6719	1.3923

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	0.7318	0.5722
(1,3)	0.1131	0.0889
(1,4)	0.0049	0.0049
(2,3)	0.8651	0.8651
(2,4)	0.0810	0.0272
(3,4)	0.5308	0.9418

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 54.733 DEGREES H= 8000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 34.65038 GHZ

A(4)	B(4)	C(4)	D(4)
0.5331336E 00	0.7111348E 00	0.4154470E 00	0.1098027E 00
0.8607282E-01	0.1148106E 00	0.6707267E-01	0.1772732E-01

EIGENVECTOR FOR E(3)= 10.50438 GHZ

A(3)	B(3)	C(3)	D(3)
-0.6827994E 00	0.1339299E 00	0.5790559E 00	0.2569526E 00
-0.2455493E 00	0.4816405E-01	0.2082409E 00	0.9240567E-01

EIGENVECTOR FOR E(2)= -10.50379 GHZ

A(2)	B(2)	C(2)	D(2)
0.4011253E 00	-0.6126562E 00	0.4150245E 00	0.4499614E 00
-0.1254076E 00	0.1915405E 00	-0.1297530E 00	-0.1406757E 00

EIGENVECTOR FOR E(1)= -34.65097 GHZ

A(1)	B(1)	C(1)	D(1)
0.1283144E-01	-0.3923142E-01	0.8969429E-01	-0.1475854E 00
-0.7111393E-01	0.2174269E 00	-0.4971004E 00	0.8179421E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
24.1460	45.1542	69.3013	21.0082	45.1554	24.1472

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	-0.5999	-1.1480	1.2953	-1.3962	0.7296	1.5753	0.5506	1.0536	1.1888
(1,3)	0.0796	-0.4730	0.4796	-0.4430	-0.0745	0.4492	-0.0301	0.1788	0.1813
(1,4)	-0.0015	-0.0832	0.0832	-0.0863	0.0016	0.0863	0.0004	0.0227	0.0227
(2,3)	0.7591	0.5749	0.9523	1.1555	-1.5255	1.9137	-1.3233	-1.0023	1.6600
(2,4)	0.3915	0.1955	0.4375	0.1348	-0.2700	0.3018	-0.1090	-0.0544	0.1218
(3,4)	0.5423	-0.1016	0.5517	-0.3472	-1.8535	1.8857	-1.3988	0.2620	1.4231

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	0.7728	0.6204
(1,3)	0.0657	0.0504
(1,4)	0.0019	0.0019
(2,3)	0.9156	0.9156
(2,4)	0.0516	0.0228
(3,4)	0.5824	0.8890

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 54.733 DEGREES H= 10000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 42.80011 GHZ

A(4)	B(4)	C(4)	D(4)
0.4583615E 00	0.5661965E 00	0.3242855E 00	0.8800243E-01
0.3411054E 00	0.4213545E 00	0.2413282E 00	0.6549002E-01

EIGENVECTOR FOR E(3)= 13.40302 GHZ

A(3)	B(3)	C(3)	D(3)
0.2464149E 00	-0.6282331E-01	-0.2123505E 00	-0.9675386E-01
-0.6700862E 00	0.1708380E 00	0.5774535E 00	0.2631067E 00

EIGENVECTOR FOR E(2)= -13.40241 GHZ

A(2)	B(2)	C(2)	D(2)
0.3465850E 00	-0.5593129E 00	0.3673969E 00	0.4395140E 00
-0.1941739E 00	0.3133545E 00	-0.2058337E 00	-0.2462372E 00

EIGENVECTOR FOR E(1)= -42.80072 GHZ

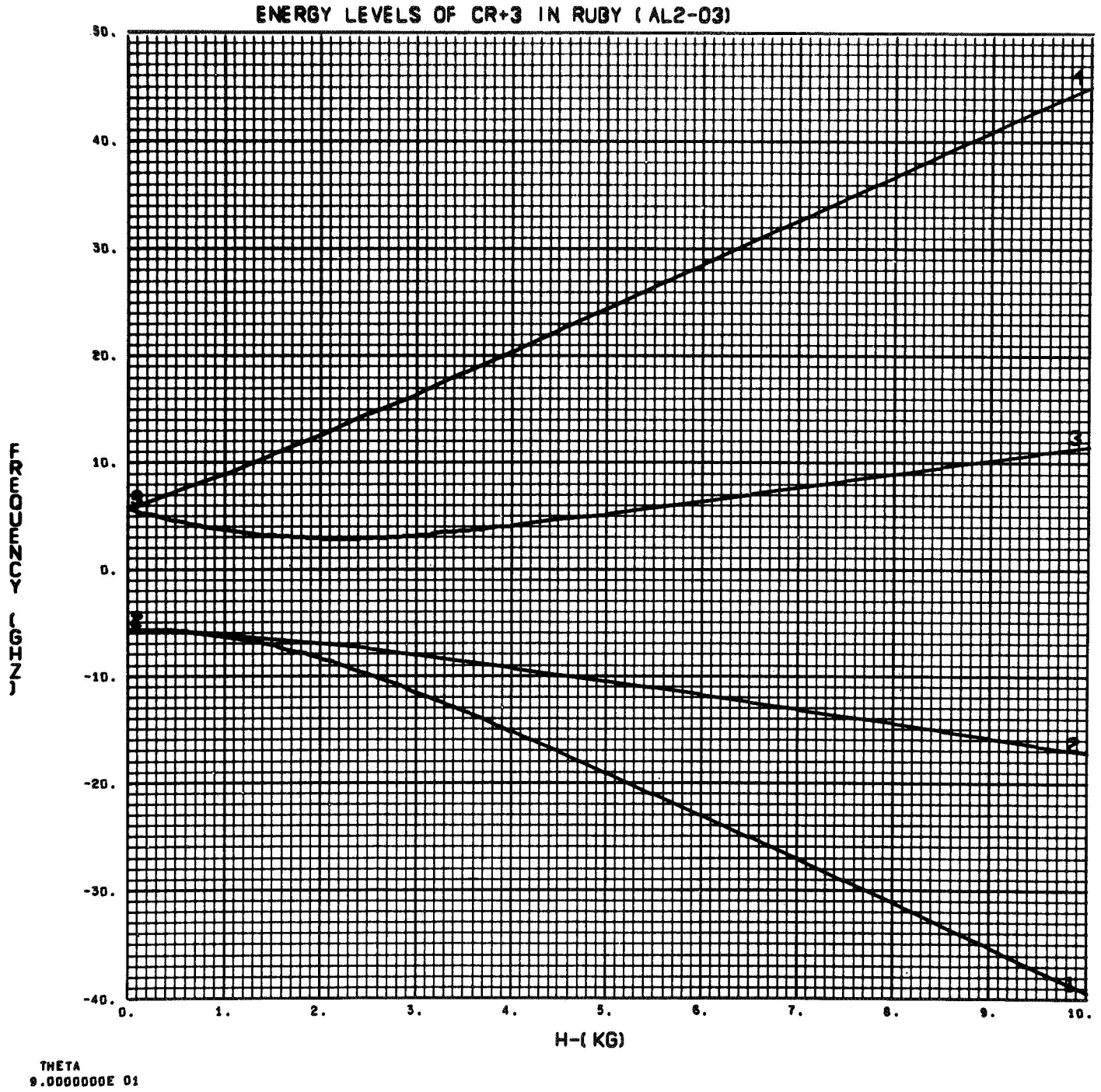
A(1)	B(1)	C(1)	D(1)
-0.6762784E-01	0.2099206E 00	-0.4629027E 00	0.7074158E 00
-0.3765385E-01	0.1168797E 00	-0.2577351E 00	0.3938752E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
29.3971	56.2025	85.6008	26.8054	56.2037	29.3983

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	0.6615	-1.0739	1.2613	-1.3702	-0.8440	1.6093	-0.6539	1.0616	1.2469
(1,3)	0.0600	0.3822	0.3868	0.3545	-0.0556	0.3589	-0.0225	-0.1437	0.1454
(1,4)	0.0553	0.0073	0.0558	0.0076	-0.0573	0.0578	-0.0153	-0.0020	0.0154
(2,3)	-0.7779	0.6656	1.0238	1.2626	1.4757	1.9422	1.2540	-1.0729	1.6504
(2,4)	0.1469	0.3287	0.3601	0.2423	-0.1083	0.2654	-0.0439	-0.0982	0.1076
(3,4)	0.1803	-0.6101	0.6362	-1.7776	-0.5254	1.8536	-0.4071	1.3774	1.4363

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	0.7864	0.6474
(1,3)	0.0427	0.0322
(1,4)	0.0008	0.0008
(2,3)	0.9430	0.9430
(2,4)	0.0353	0.0176
(3,4)	0.6169	0.8589


ENERGY LEVELS OF CR+3 IN RUBY (AL2-03)
50.
40.
30.
20.
10.
0.
-10.
-20.
-30.
-40.
FREQUENCY (GHZ)
0.
1.
2.
3.
4.
5.
6.
7.
8.
9.
10.
H-(KG)
1
2
3
4
THETA
9.0000000E 01

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 90.000 DEGREES H= 0.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 5.73000 GHZ

A(4)	B(4)	C(4)	D(4)
0.2818598E-33	0.4361551E 00	0.3148621E 00	0.5128783E-34
0.1787986E-33	0.3161147E 00	0.7814742E 00	0.3324911E-33

EIGENVECTOR FOR E(3)= 5.73000 GHZ

A(3)	B(3)	C(3)	D(3)
0.1011291E-32	0.2958702E 00	0.6753012E 00	0.8325003E-33
0.5755642E-33	0.3490809E 00	-0.5784217E 00	0.5933537E-33

EIGENVECTOR FOR E(2)= -5.73000 GHZ

A(2)	B(2)	C(2)	D(2)
0.3977284E 00	0.2184034E-33	0.7837963E-33	0.8849286E 00
0.2032546E 00	0.3136773E-33	0.5751073E-33	0.1319133E 00

EIGENVECTOR FOR E(1)= -5.73000 GHZ

A(1)	B(1)	C(1)	D(1)
0.3737572E-01	0.2018054E-33	0.1259577E-32	-0.2580811E 00
0.9538448E 00	0.8100750E-33	0.8453049E-33	0.1489204E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
0.0000	11.4600	11.4600	11.4600	11.4600	-0.0000

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	1.2524	-0.6178	1.3965
(1,3)	0.1448	-0.3818	0.4084	0.5506	1.0469	1.1829	0.0000	-0.0000	0.0000
(1,4)	0.6113	-1.1307	1.2853	0.2696	0.4897	0.5590	-0.0000	-0.0000	0.0000
(2,3)	1.2296	-0.9045	1.5265	-1.1772	-0.5762	1.3106	-0.0000	-0.0000	0.0000
(2,4)	1.0729	1.1901	1.6023	1.0616	-0.2494	1.0905	-0.0000	-0.0000	0.0000
(3,4)	0.9553	1.1741	1.5136	0.6889	0.5085	0.8563	0.4788	-0.7686	0.9055

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	0.4876	0.0000
(1,3)	0.0417	0.3498
(1,4)	0.4130	0.0781
(2,3)	0.5825	0.4294
(2,4)	0.6419	0.2973
(3,4)	0.7778	0.1833

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 90.000 DEGREES H= 2000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 12.58468 GHZ

A(4)	B(4)	C(4)	D(4)
0.1042252E 00	0.3950279E 00	0.3950279E 00	0.1042252E 00
0.1472356E 00	0.5580428E 00	0.5580428E 00	0.1472356E 00

EIGENVECTOR FOR E(3)= 2.86650 GHZ

A(3)	B(3)	C(3)	D(3)
0.2971850E 00	0.5286935E 00	-0.5286935E 00	-0.2971850E 00
0.1781381E 00	0.3169086E 00	-0.3169086E 00	-0.1781382E 00

EIGENVECTOR FOR E(2)= -7.00494 GHZ

A(2)	B(2)	C(2)	D(2)
0.6253559E 00	-0.1649957E 00	-0.1649955E 00	0.6253557E 00
0.2763855E 00	-0.7292234E-01	-0.7292228E-01	0.2763854E 00

EIGENVECTOR FOR E(1)= -8.44624 GHZ

A(1)	B(1)	C(1)	D(1)
0.2072887E 00	-0.1165195E 00	0.1165195E 00	-0.2072888E 00
-0.5804990E 00	0.3263056E 00	-0.3263056E 00	0.5804992E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
9.7182	19.5896	21.0309	9.8714	11.3127	1.4413

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	0.0000	-0.0000	0.0000	-0.6836	-0.0501	0.6855	-0.1940	2.6465	2.6536
(1,3)	-0.3435	1.7207	1.7546	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
(1,4)	0.0000	-0.0000	0.0000	-0.5966	-0.4186	0.7288	-0.1111	0.1583	0.1934
(2,3)	0.0000	0.0000	0.0000	-0.2620	2.1049	2.1212	1.1898	0.1481	1.1990
(2,4)	0.8698	0.5198	1.0133	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
(3,4)	-0.0000	-0.0000	0.0000	-0.8549	1.9413	2.1212	1.1146	0.4908	1.2179

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	1.7604	0.1175
(1,3)	0.7697	0.0000
(1,4)	0.0093	0.1328
(2,3)	0.3594	1.1249
(2,4)	0.2567	0.0000
(3,4)	0.3708	1.1249

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 90.000 DEGREES H= 4000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 20.45625 GHZ

A(4)	B(4)	C(4)	D(4)
0.1575809E 00	0.4269750E 00	0.4269750E 00	0.1575809E 00
0.1873711E 00	0.5076935E 00	0.5076935E 00	0.1873711E 00

EIGENVECTOR FOR E(3)= 4.08582 GHZ

A(3)	B(3)	C(3)	D(3)
-0.8614643E-03	-0.8749624E-03	0.8749624E-03	0.8614643E-03
0.4960975E 00	0.5038707E 00	-0.5038708E 00	-0.4960975E 00

EIGENVECTOR FOR E(2)= -9.29677 GHZ

A(2)	B(2)	C(2)	D(2)
0.1809009E 00	-0.6676394E-01	-0.6676392E-01	0.1809009E 00
0.6382282E 00	-0.2355468E 00	-0.2355467E 00	0.6382281E 00

EIGENVECTOR FOR E(1)= -15.24530 GHZ

A(1)	B(1)	C(1)	D(1)
-0.7350251E-01	0.7236858E-01	-0.7236859E-01	0.7350252E-01
0.4984815E 00	-0.4907915E 00	0.4907915E 00	-0.4984817E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
16.3704	29.7530	35.7015	13.3826	19.3311	5.9485

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	-0.0000	0.0000	0.0000	0.4915	1.0931	1.1985	2.0506	-0.9221	2.2484
(1,3)	1.0161	-0.1480	1.0268	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000
(1,4)	-0.0000	0.0000	0.0000	0.1963	0.1739	0.2622	0.0544	-0.0613	0.0820
(2,3)	0.0000	0.0000	0.0000	-0.5685	1.9926	2.0721	1.6616	0.4741	1.7279
(2,4)	0.6083	-0.2739	0.6671	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000
(3,4)	-0.0000	0.0000	0.0000	1.3220	1.5664	2.0497	1.0678	-0.9012	1.3973

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	1.2639	0.3591
(1,3)	0.2636	0.0000
(1,4)	0.0017	0.0172
(2,3)	0.7464	1.0734
(2,4)	0.1113	0.0000
(3,4)	0.4881	1.0503

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 90.000 DEGREES H= 6000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 28.59212 GHZ

A(4)	B(4)	C(4)	D(4)
0.1444047E 00	0.3418925E 00	0.3418925E 00	0.1444047E 00
0.2341825E 00	0.5544505E 00	0.5544505E 00	0.2341825E 00

EIGENVECTOR FOR E(3)= 6.36533 GHZ

A(3)	B(3)	C(3)	D(3)
-0.3342972E 00	-0.2789234E 00	0.2789234E 00	0.3342972E 00
0.4278203E 00	0.3569550E 00	-0.3569551E 00	-0.4278203E 00

EIGENVECTOR FOR E(2)= -11.85290 GHZ

A(2)	B(2)	C(2)	D(2)
0.5510435E 00	-0.2327435E 00	-0.2327434E 00	0.5510435E 00
0.3473571E 00	-0.1467127E 00	-0.1467127E 00	0.3473571E 00

EIGENVECTOR FOR E(1)= -23.10455 GHZ

A(1)	B(1)	C(1)	D(1)
0.4525955E 00	-0.5424479E 00	0.5424480E 00	-0.4525956E 00
0.1929945E-01	-0.2313092E-01	0.2313092E-01	-0.1929946E-01

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
22.2268	40.4450	51.6967	18.2182	29.4699	11.2516

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	-0.0000	-0.0000	0.0000	-0.6909	1.2072	1.3909	1.7959	1.0279	2.0693
(1,3)	-0.3917	0.5479	0.6735	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
(1,4)	-0.0000	-0.0000	0.0000	-0.1035	0.0701	0.1250	0.0227	0.0335	0.0405
(2,3)	-0.0000	-0.0000	0.0000	-2.0278	-0.2052	2.0382	-0.1885	1.8632	1.8727
(2,4)	0.4407	0.2160	0.4908	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000
(3,4)	-0.0000	0.0000	0.0000	1.8507	0.6859	1.9737	0.5166	-1.3938	1.4864

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	1.0705	0.4836
(1,3)	0.1134	0.0000
(1,4)	0.0004	0.0039
(2,3)	0.8768	1.0386
(2,4)	0.0602	0.0000
(3,4)	0.5524	0.9739

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 90.000 DEGREES H= 8000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 36.82767 GHZ

A(4)	B(4)	C(4)	D(4)
0.2545461E 00	0.5604538E 00	0.5604538E 00	0.2545461E 00
0.1439034E 00	0.3168433E 00	0.3168433E 00	0.1439034E 00

EIGENVECTOR FOR E(3)= 8.91740 GHZ

A(3)	B(3)	C(3)	D(3)
-0.1793656E 00	-0.1359237E 00	0.1359237E 00	0.1793656E 00
0.5342626E 00	0.4048656E 00	-0.4048656E 00	-0.5342626E 00

EIGENVECTOR FOR E(2)= -14.50872 GHZ

A(2)	B(2)	C(2)	D(2)
0.4830033E 00	-0.2193698E 00	-0.2193697E 00	0.4830033E 00
0.4256828E 00	-0.1933360E 00	-0.1933360E 00	0.4256828E 00

EIGENVECTOR FOR E(1)= -31.23635 GHZ

A(1)	B(1)	C(1)	D(1)
0.4083025E 00	-0.5387980E 00	0.5387980E 00	-0.4083025E 00
0.1252217E 00	-0.1652432E 00	0.1652432E 00	-0.1252218E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
27.9103	51.3364	68.0640	23.4261	40.1538	16.7276

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	-0.0000	-0.0000	0.0000	-0.6114	1.3516	1.4835	1.8034	0.8158	1.9793
(1,3)	-0.0130	0.4942	0.4943	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000
(1,4)	-0.0000	0.0000	0.0000	-0.0155	0.0703	0.0720	0.0231	0.0051	0.0236
(2,3)	-0.0000	-0.0000	0.0000	-1.8643	0.7849	2.0228	0.7478	1.7762	1.9272
(2,4)	0.3783	-0.0798	0.3867	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000
(3,4)	-0.0000	0.0000	0.0000	1.8893	0.3646	1.9241	0.2916	-1.5108	1.5387

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	0.9794	0.5502
(1,3)	0.0611	0.0000
(1,4)	0.0001	0.0013
(2,3)	0.9286	1.0230
(2,4)	0.0374	0.0000
(3,4)	0.5919	0.9256

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN RUBY (AL2-03)

THETA= 90.000 DEGREES H= 10000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 45.11069 GHZ

A(4)	B(4)	C(4)	D(4)
0.1754916E 00	0.3692779E 00	0.3692779E 00	0.1754916E 00
0.2476288E 00	0.5210725E 00	0.5210725E 00	0.2476288E 00

EIGENVECTOR FOR E(3)= 11.57144 GHZ

A(3)	B(3)	C(3)	D(3)
0.5328108E-01	0.3815406E-01	-0.3815406E-01	-0.5328108E-01
-0.5724311E 00	-0.4099122E 00	0.4099123E 00	0.5724311E 00

EIGENVECTOR FOR E(2)= -17.21200 GHZ

A(2)	B(2)	C(2)	D(2)
0.4489009E 00	-0.2133308E 00	-0.2133308E 00	0.4489009E 00
0.4542803E 00	-0.2158873E 00	-0.2158872E 00	0.4542803E 00

EIGENVECTOR FOR E(1)= -39.47013 GHZ

A(1)	B(1)	C(1)	D(1)
-0.9144489E-02	0.1277003E-01	-0.1277003E-01	0.9144491E-02
0.4115825E 00	-0.5747635E 00	0.5747636E 00	-0.4115826E 00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
33.5393	62.3227	84.5808	28.7834	51.0416	22.2581

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	-0.0000	0.0000	0.0000	1.1044	1.0690	1.5370	1.3399	-1.3842	1.9265
(1,3)	-0.3879	-0.0274	0.3889	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
(1,4)	-0.0000	0.0000	0.0000	0.0278	0.0374	0.0466	0.0123	-0.0092	0.0154
(2,3)	0.0000	0.0000	0.0000	1.5431	-1.2959	2.0150	-1.2560	-1.4956	1.9531
(2,4)	0.3143	0.0517	0.3185	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000
(3,4)	0.0000	-0.0000	0.0000	-1.2315	-1.4347	1.8908	-1.1934	1.0244	1.5728

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	0.9279	0.5906
(1,3)	0.0378	0.0000
(1,4)	0.0001	0.0005
(2,3)	0.9537	1.0151
(2,4)	0.0254	0.0000
(3,4)	0.6184	0.8937

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