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Technical Memorandum 33-446

Energy Levels and Transition Matrix Elements of Paramagnetic Crystals for Maser Applications

Robert W. Berwin



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Technical Memorandum 33-446

Energy Levels and Transition Matrix Elements of Paramagnetic Crystals for Maser Applications

Robert W. Berwin

JET PROPULSION LABORATORY CALIFORNIA INSTITUTE OF TECHNOLOGY PASADENA, CALIFORNIA

March 1, 1970

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Preface

The work described in this report was performed by the Telecommunications Division of the Jet Propulsion Laboratory. The subroutine which diagonalizes the Hermitian matrix was kindly furnished by R. J. Hanson of the Computation and Analysis Section.

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A-1. Plot of energy levels of Cr(+3) in beryl (emerald) vs external dc magnetic field for $\theta = 90 \text{ deg}$.

Abstract

Computer programs on the Univac 1108 have been developed at the Jet Propulsion Laboratory to give the energy levels and transition probabilities for ruby, emerald, iron-doped rutile, iron-doped zinc tungstate, and chromium-doped rutile. These programs also generate SC-4020 plots of energy levels vs an external dc magnetic field which is at any orientation with respect to the crystal magnetic axes.

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Energy Levels and Transition Matrix Elements of Paramagnetic Crystals for Maser Applications

I. Introduction

Investigation of maser performance of paramagnetic crystals is a continuing program in the Microwave Electronics Group at the Jet Propulsion Laboratory (JPL). As the need arises for higher signal frequencies, it is necessary to evaluate the maser qualities of many crystals. Efficient study of maser crystal performance can be achieved by the use of a set of fine structure energy levels and transition probabilities. Such information allows the investigator to determine the optimum orientation of the crystal magnetic axes with respect to the external dc magnetic field and the polarization of the signal and pump frequencies.

To meet this goal, Fortran V language programs for the Univac 1108 computer at JPL have been implemented to diagonalize the spin Hamiltonians of ruby, emerald, irondoped rutile, iron-doped zinc tungstate, and chromiumdoped rutile. For each of these crystals, eigenvalues in GHz, normalized eigenvectors, and transition probabilities are computed, and a plot by the Stromberg-Carlson SC-4020 Plotter is made of eigenvalues vs the external dc magnetic field.

II. Discussion

A. Spin Hamiltonian

The spin Hamiltonian for the case of ruby was derived in detail in Ref. 1. If H_s is the spin Hamiltonian which, because of the physical nature of the problem, is Hermitian then the equation to be solved is

$$H_s|\psi_i\rangle = E_i|\psi_i\rangle \qquad i = 1, \cdots, n = 2S+1 \qquad (1)$$

where eigenvalues E_i are real, and S is the effective total spin of the ion in the crystal, H_s can be diagonalized by a unitary matrix with the result that the eigenvalues occur along the diagonal of the transformed matrix. $|\psi_i\rangle$ is an

n-fold vector representing a linear combination of the *n*-pure spin states:

$$|\psi_i\rangle = a_i |S\rangle + b_i |S-1\rangle + c_i |S-2\rangle + \cdots + x_i |-S\rangle$$

The $|S\rangle$, etc., are the base states corresponding to the 2S + 1 positions of the spin dipole in a magnetic field.

The diagonalization of H_s by computer methods can be conveniently handled by expanding the $n \times n$ Hermitian matrix into a $2n \times 2n$ real matrix.

Thus, if H_s and $|\psi_i\rangle$ are expressed as $H_s = H_{s1} + iH_{s2}$ and $|\psi_i\rangle = |\psi_i\rangle_1 + i|\psi_i\rangle_2$ then Eq. (1) takes the form

$$\begin{bmatrix} H_{s_1} - H_{s_2} \\ H_{s_2} & H_{s_1} \end{bmatrix} \begin{bmatrix} |\psi_i\rangle_1 \\ |\psi_i\rangle_2 \end{bmatrix} = E_i \begin{bmatrix} |\psi_i\rangle_1 \\ |\psi_i\rangle_2 \end{bmatrix}$$
(2)

Eq. (3), for S = 3/2 becomes

B. Transition Probability Matrix Elements

From first order perturbation, the transition probability per unit time of a transition from state ψ_i to state ψ_j is

$$W_{ij} = \frac{1}{4} \gamma^2 G(f) |\langle \psi_i | H' | \psi_j \rangle|^2$$
 (3)

where $\gamma = g\beta\mu_0/h$, H' is the applied perturbation, and G(f) is the density of states as a function of energy. When an RF magnetic field $\mathbf{H}_1 = H_1^0(\phi_1 \mathbf{i} + \phi_2 \mathbf{j} + \phi_3 \mathbf{k})$ is applied to the crystal, the dipole interaction energy is $H' = \boldsymbol{\mu} \cdot \mathbf{H}_1 = g\beta \mathbf{S} \cdot \mathbf{H}_1$, where ϕ_1 , ϕ_2 , and ϕ_3 are the direction cosines of \mathbf{H}_1 with respect to the magnetic axes x, y, z of the crystal.

 $\frac{\langle \psi_i | g\mathbf{H}_1 \cdot \mathbf{S} | \psi_i \rangle}{H_1^0} = \left[a_i^* b_i^* c_i^* d_i^* \right] \begin{bmatrix} 3\phi_3 & (3)^{\frac{1}{2}} (\phi_1 - i\phi_2) & 0 & 0\\ (3)^{\frac{1}{2}} (\phi_1 + i\phi_2) & \phi_3 & 2(\phi_1 - i\phi_2) \\ 0 & 2(\phi_1 + i\phi_2) & -\phi_3 & (3)^{\frac{1}{2}} (\phi_1 - i\phi_2) \\ 0 & 0 & (3)^{\frac{1}{2}} (\phi_1 + i\phi_2) & -3\phi_3 \end{bmatrix} \begin{bmatrix} a_i \\ b_i \\ c_i \\ d_i \end{bmatrix}$

 $\equiv \alpha_{ij} \phi_1 + i\beta_{ij} \phi_2 + \gamma_{ij} \phi_3$

where

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

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

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

Similar equations can be derived for the case of S = 5/2.

C. Main Programs

1. RUBYCR

- a. Purpose
- (1) Calculate the eigenvalues of the spin Hamiltonian of chromium (+3) in Al₂O₃ (ruby).
- (2) Calculate the transition probability matrix elements.

(3) Plot eigenvalues vs external de magnetic field, $H_{de^{\mu}}$

b. Input data

- THETA ($0 \deg \le \theta \le 90 \deg$) is the angle between c axis and external dc magnetic field (see Fig. 1).
- HMIN, HMAX, DH defines respectively minimum, maximum, and incremental external dc magnetic field for calculations and plots.

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c. Spin Hamiltonian (Ref. 2)

$$H_s = g\beta H_{dc} \cdot S + D \left[S_z^2 - \frac{1}{3} S (S+1) \right]$$
$$g = 1.99$$
$$D = -5.73 \text{ GHz}$$
$$H_{dc} = H_0 (\sin \theta \mathbf{i} + \cos \theta \mathbf{j})$$
$$S = \frac{3}{2}$$

Fig. 1. Orientation of H_{dc} and c axis

d. Spin Hamiltonian matrix

$\frac{3}{2}geta H_0\cos heta+D$	$\frac{3}{2}geta H_0\sin heta$	0	0
$rac{3}{2} geta H_0 \sin heta$	$\frac{1}{2}g\beta H_0\cos\theta-D$	$geta H_0$ sin $ heta$	0
0	$geta H_{\mathfrak{o}}\sin heta$	$-rac{1}{2}geta H_u\cos heta-D$	$rac{3}{2}geta H_0\sin heta$
0	0	$rac{3}{2} geta H_0 \sin heta$	$-\frac{3}{2}g\beta H_0\cos\theta+D$

2. TIO2FE

a. Purpose

- (1) Calculate the eigenvalues of the spin Hamiltonian of Fe(+3) in rutile (TiO_2) .
- (2) Calculate the transition probability matrix elements.
- (3) Plot eigenvalues vs external dc magnetic field, H_{dc} .

b. Input data

- THETA, PHI $[0 \deg \le (\theta, \phi) \le 90 \deg]$ are the spherical coordinates of external dc magnetic field with respect to crystal magnetic axes x, y, z (see Fig. 2).
- c. Spin Hamiltonian (Ref. 3)

$$H_{s} = g\beta H_{dc} \cdot S + D \left[S_{z}^{2} - \frac{1}{3} s (s+1) \right] + E \left(S_{x}^{2} - S_{y}^{2} \right)$$
$$+ \frac{a}{6} \left(S_{x}^{4} + S_{y}^{4} + S_{z}^{4} - \frac{707}{16} \right)$$
$$+ \frac{7}{36} F \left(S_{z}^{4} - \frac{75}{14} S_{z}^{2} + \frac{81}{16} \right)$$

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D = 20.35 GHz	a =	1.1 GHz
$E = 2.21 \mathrm{GHz}$	//	2.0
$F = -0.5 \mathrm{GHz}$	 S =	5/2



Fig. 2. Orientation of H_{dc} and crystal magnetic axes x, y, z; crystalline axes a, b, c shown with c axis along y direction; a and b axes in x-z plane

d. Spin Hamiltonian matrix

	0	(5) ¹⁻ a	0	(10);F	$\frac{(5)^{i_2}}{2} \frac{g_B H}{l_5} \sin \theta e^{i \Phi}$	$-\frac{5}{2}\frac{g\beta i i}{h}\cos\theta + \left(\frac{i0}{3}D \pm \frac{a}{2} \pm \frac{F}{3}\right)$
	رة)، 1-2-4	0	3 (2) ¹⁵ E	$(2)^{i_2} \frac{g\beta H}{h} \sin \theta e^{i\phi}$	$-\frac{3}{2}\frac{g\rho H}{h}\cos\theta$ $-\left(\frac{2}{3}D+\frac{3}{2}a+F\right)$	$\frac{(5)^{i\pm}}{2}\frac{g\beta H}{h}\sin\theta e^{-i\phi}$
	0	3 (2) ¹⁴ E	$\frac{3}{2}\frac{\mathrm{g}\mathrm{\beta}H}{\hbar}\sin heta\mathrm{e}^{\mathrm{i}\phi}$	$-\frac{1}{2}\frac{g\beta H}{h}\cos\theta + \left(-\frac{8}{3}D \pm a + \frac{2}{3}F\right)$	$(2)^{\frac{2}{2}}\frac{g\beta H}{h}\sin\theta e^{-i\phi}$	(10) ¹⁵ E
	$(10)^{14}E$	$(2)^{i\pm}rac{geta H}{h}\sin hetae^{i\phi}$	$\frac{1}{2} \frac{\frac{g\beta H}{h}}{2} \cos \theta + \left(-\frac{8}{3}D + a + \frac{2}{3}F\right)$	$rac{3}{2}rac{geta H}{h}\sin hetae^{-i\phi}$	3 (2) ¹⁵ E	0
-	$\frac{(5)^{i_2}}{2}\frac{g_\beta H}{h}\sin\thetae^{i_{\frac{1}{T}}}$	$\frac{3}{2} \frac{g\beta H}{h} \cos \theta \\ -\left(\frac{2}{3}D + \frac{3}{2}a + F\right)$	$(2)^{rac{14}{h}}rac{geta H}{h}\sin hetae^{-i\phi}$	3 (2) ¹⁴ E	0	$\frac{(5)^{i_2}}{2}a$
	$\frac{5}{2} \frac{g\beta H}{h} \cos \theta + \left(\frac{10}{3}D + \frac{a}{2} + \frac{F}{3}\right)$	$\left(\frac{5}{2}\right)^{14}\frac{g\beta H}{h}\sin\thetae^{-i\phi}$	(10) ¹⁴ <i>E</i>	0	$\frac{(5)!^4}{2}a$	0

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3. EMERCR

- a. Purpose
- (1) Calculate the eigenvalues of the spin Hamiltonian of chromium (+3) in beryl (emerald: $Be_3Al_2Si_6O_{18}$).
- (2) Calculate the transition probability matrix elements.
- (3) Plot eigenvalues vs external de magnetic field, H_{dc} .

b. Input data

- THETA (0 deg $\leq \theta \leq 90$ deg) is the angle between c axis and external dc magnetic field (see Fig. 1).
- HMIN, HMAX, DH defines respectively minimum, maximum, and incremental external dc magnetic field for calculations and plots.
- c. Spin Hamiltonian (Ref. 4)

$$H_{s} = g\beta \mathbf{H}_{dc} \cdot \mathbf{S} + D \left[S_{z}^{2} - \frac{1}{3} \mathbf{S} (\mathbf{S} + 1) \right]$$
$$D = -26 \text{ GHz}$$
$$g = 1.97$$
$$\mathbf{S} = 3/2$$

The Hamiltonian matrix is the same as that for ruby (see Case 1 in Section C1d).

An example of the computer printout and plot for $\theta = 90 \text{ deg}$ is given in the appendix.

4. ZNWOFE

a. Purpose

(1) Calculate the eigenvalues of the spin Hamiltonian of Fe(+3) in ZnWO₄ (zinc tungstate).

Fig. 3. Orientation of H_{dc} and crystal magnetic axes x, y, z; a, b, c crystalline axes with a and c axes in x-z plane

- (2) Calculate the transition probability matrix elements.
- (3) Plot eigenvalues vs external de magnetic field, H_{de} .

b. Input data

- THETA, PHI $[0 \deg \leq (\theta, \phi) \leq 90 \deg]$ are the spherical coordinates of external de magnetic field with respect to crystal magnetic axes x, y, z (see Fig. 3).
- HMIN, HMAX, DH defines respectively minimum, maximum, and incremental dc external magnetic field for calculations and plots.

c. Spin Hamiltonian (Ref. 5)

$$H_{s} = \frac{g\beta H}{2} \left(2S_{z} \cos \theta + S_{+} e^{-i\phi} \sin \theta + S_{-} e^{i\phi} \sin \theta \right)$$

$$+ B_{02} \left[3S_{z}^{2} - S \left(S + 1 \right) \right] + \frac{1}{2} B_{22} \left(S_{+}^{2} + S_{-}^{2} \right)$$

$$+ B_{04} \left[35S_{z}^{4} - 30S \left(S + 1 \right) S_{z}^{2} + 25S_{z}^{2} - 6S \left(S + 1 \right) \right]$$

$$+ 3S^{2} \left(S + 1 \right)^{2} \right]$$

$$+ \frac{1}{2} B_{24} \left\{ S_{+}^{2} \left[7S_{z}^{2} + 4S_{z} - S \left(S + 1 \right) + 9 \right] \right\}$$

$$+ S_{-}^{2} \left[7S_{z}^{2} - 14S_{z} - S \left(S + 1 \right) + 9 \right] \right\}$$

$$+ \frac{1}{2} B_{44} \left(S_{+}^{4} + S_{-}^{4} \right)$$

$$B_{02} = -6.987 \text{ GHz}$$

$$S_{z} = S_{x} \pm iS_{y}$$

$$B_{04} = 0.00326 \text{ GHz}$$
 $g = 2.0019$
 $B_{24} = -0.00178 \text{ GHz}$
 $B_{44} = -0.0173 \text{ GHz}$ $S = 5/2$



-					
$\frac{10B_{02}+60B_{04}}{+\frac{5}{2}}g\beta H_0\cos\theta$	$\frac{(5)^{j_{h}}}{2}g_{\beta}H_{\mathfrak{n}}\sin\thetae^{\mathrm{i}\phi}$	$(10)^{!!_2}(B_{22} \div 9B_{24})$	0	12 (5) ¹⁵ B++	0
$\frac{(5)^{ik}}{2}g_{\beta}H_{0}\sin\theta^{-i\phi}$	$-2B_{02} - 180B_{04} + rac{3}{2} geta H_0 \cos heta$	$(2)^{rac{3}{2}} geta H_{n} \sin heta e^{rac{1}{2}\phi}$	$3(2)^{16}(B_{22}-5B_{24})$	0	12 (5) ^{1<u>5</u>} B ₄₄
$(10)^{rac{1}{2}}(B_{zz}+9B_{z4})$	$(2)^{j_2} \mathrm{g} eta H_{\mathrm{o}} \sin heta e^{-\mathrm{i} \phi}$	$- 8B_{ m oz} + 120B_{ m out} + rac{1}{2} geta H_{ m o}\cos heta$	$rac{3}{2}$ g $eta H_0 \sin heta e^{i\phi}$	$3(2)^{i\underline{i}}(B_{zz}-5B_{zi})$	0
0	$3(2)^{rac{1}{2}}(B_{zz}-5B_{z4})$	$rac{3}{2}$ g $eta H_0$ sin $ heta e^{-i\phi}$	$egin{array}{l} -8B_{\mathrm{oz}}+120B_{\mathrm{o}4}\ -rac{1}{2}\mathrm{g}eta H_{\mathrm{o}}\cos heta \end{array}$	$(2)^{i4} g eta H_n \sin heta e^{i\phi}$	(10) ¹ ¹ (B ₂₂ + 9B ₂₄)
12 (5) ^{1/2} B ₄₄	0	$3(2)^{!!}(B_{zz}-5B_{zz})$	$(2)^{j_{k}}$ g $eta H_{a}\sin heta$ $e^{-i\phi}$	$-\frac{2B_{02}-180B_{01}}{-\frac{3}{2}}g\beta H_0\cos\theta$	$\frac{(5)^{i\underline{s}}}{2}g\beta H_{\mathfrak{a}}\sin\theta e^{i\phi}$
0	$12(5)^{l_{4}}B_{44}$	0	$(10)^{\frac{1}{2}}(B_{22}+9B_{24})$	$\frac{(5)^{1\frac{\alpha}{2}}}{2}g\beta H_0\sin\theta e^{-i\phi}$	$10B_{02} + 60B_{04}$ $- \frac{5}{2} g_{\beta} H_0 \cos \vartheta$

d. Spin Hamiltonian matrix

5. TIO2CR

- a. Purpose
- (1) Calculate the eigenvalues of the spin Hamiltonian of Cr(+3) in rutile (TiO_2) .
- (2) Calculate the transition probability matrix elements.
- (3) Plot eigenvalues vs external de magnetic field, H_{dc} .

b. Input data

THETA, PHI $[0 \deg \leq (\theta, \phi) \leq 90 \deg]$ are the spherical coordinates of external dc magnetic field with respect to crystal magnetic axes x, y, z (see Fig. 2).

- HMIN, HMAX, DH defines minimum, maximum, and incremental dc external magnetic field for calculations and plots.
- c. Spin Hamiltonian

$$H_{s} = g\beta H_{dv} \cdot S + D \left[S_{z}^{2} - \frac{1}{3} S \left(S + 1 \right) \right] + E \left(S_{x}^{2} - S_{y}^{2} \right)$$
$$D = -20.4 \text{ GHz}$$
$$E = -4.2 \text{ GHz}$$
$$\mathcal{G} = 1.97$$
$$S = 3/2$$

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d. Spin Hamiltonian matrix

$\frac{3}{2}g\beta H_0\cos\theta+D$	$-\frac{(3)^{1/2}}{2}geta H_{\scriptscriptstyle 0}\sin hetae^{-i\phi}$	(3)½ E	0
${(3)^{\frac{1}{2}}\over 2}geta H_{v}\sin hetae^{i\phi}$	$rac{1}{2} geta H_0 \cos heta - D$	$geta H_0\sin heta \ e^{-i\phi}$	(3) ^½ E
(3)½ <i>E</i>	$geta H_{\scriptscriptstyle 0}\sin heta \ e^{i\phi}$	$-rac{1}{2}geta H_{0}\cos heta-D$	$\frac{(3)^{\frac{1}{2}}}{2}g\beta H_0\sin\theta e^{-i\phi}$
0	(3)½ <i>E</i>	${(3)^{\frac{1}{2}}\over 2}geta H_0\sin hetae^{i\phi}$	$-rac{3}{2}geta H_{0}\cos heta+D$

Appendix

Energy Levels and Computer Output for the Case of Cr(+3) in Beryl (Emerald) for θ = 90 deg With External dc Magnetic Field as a Parameter



Fig. A-1. Plot of energy levels of Cr(+3) in beryl (emerald) vs external dc magnetic field for $\theta = 90 \text{ deg}$

ENERGY LEVELS AND FCR (r(+j) în bert	TRANSITION PR	OBABILITY MATRIX	ELEMENTS			
THETAN PORDDO DEC	REES H.	.O GAUSS	் நடித்துதல் பிருந்துகளுக்கு அனை அனை அன்று கேட்டிய	فر شیه ۲	÷	a à
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JPL TECHNICAL MEMORANDUM 33-446

FOR TORISTIN REPLICENT HATRIX ELEMENTS THETA= 70.000 DEGREES H= 2000.0 GAUSS FIRST ROW OF EIGENVECTOR IS REAL PART, SECONG ROW IS IMAG. PART EIGENVECTOR FOR EIGI- 31.91875 GH2 .404018-05 .2497050-04 .2497051-04 .044 .404018-05 .2497050-04 .2497051-04 .044 .404018-05 .2497050-04 .2497051-04 .044 .4033 .6034 .031 .0034 .4034018-05 .2497050-05 573489-06 .1034+47-07 .4131 .8131 .6134 6044+47-07 .4132 .8133 613 6034+47-07 .4132 .8132 1034447-00 .1034447-07 .4132 .8123 1034447-00 .10414-000 .703498700 2198758-06 1047144000 1047144000 .703498700 .121922-07 1652224-07 194795-06 047144000 .104915-06 1972457900 1972457900 1973457900 1972457900 EIGENVECTOR FOR E(1)= -22.48735 GH2 197475-06 9722 TRAMSITION PROBASILITY HATRIX ELEMENTS 19855 </th <th>ENERGY I</th> <th>NELÉ AND</th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th>	ENERGY I	NELÉ AND								
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<pre>(1,2)00000000 .00000 .0000 .0000 .0000 .0000 .0000 .0000 .0000 .000</pre>		REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
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(1)4) **0000 0000 0000 *0001 *1*5278 **1447 0000 *1487 (2:3) *0000 *0000 *0000 *0000 *0000 *2211 **0000 *2211 (2:4) 1*5445 *0001 1*5445 *0000 <td< td=""><td>(1.3)</td><td>1.8981</td><td>.0000</td><td>1.8981</td><td>0000 00000</td><td>•0000</td><td>0000</td><td>₩407₩28 10004</td><td>•0000</td><td>.0000</td></td<>	(1.3)	1.8981	.0000	1.8981	0000 00000	•0000	0000	₩407₩28 10004	•0000	.0000
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(3,4) *.0000 *0000 *.0001 *.0001 *1.0165 *0000 1.0165 TR(K,L) *25*(ALPHA**2*GAMMA**2) *25*(BETA**2) *25*(BETA**2) *1.0006 (1,2) 2.2242 *0006 *0006 *1.0165 *0006 (1,3) *9007 *0000 *0000 *1.0161 *1.0161 (1,4) *0052 *5850 *2.23) *0000 *1.0161	{2,4}	1+5445	••0001	1+5445		-+0000	•0000	• 0000	0000	.0000
TR(K,L) •25+(ALPHA++2+GAMMA++2) •25+(BETA++2) (1,2) 2.2242 •0006 (1,3) •9007 •0000 (1,4) •0052 •5850 (2,3) •0122 •8982 (2,4) •5964 •0000 (3,4) •2583 1+0161	13471			•0000	=+0n01	• <u>3</u> •01•0	2+0100	*1:0105	•000	1+0102
	TR(K,L)	•25+(AL	PHA + + 2+ GAMH	14=02)	+ 25+ (BETA	++ ? }	₩.j. °P		· · · }	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$.					_				
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(2,3) .0122 .8982 (2,4) .5964 .0000 (3,4) .2583 1.0161			. 7007 . 705 2		•00	50 50				
(2,4) ,5964 ,0000 (3,4) ,2583 1+0161	(2.3)		0122		· · · · · · · · · · · · · · · · · · ·	82				
(3,4) ,2583 1+0161	(2,4)		.5964		• 0 0	00	e e a	1 # 7	i in the	···· V
	(3,4)		.2583	.÷.	1+01	6]		-		

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS FOR CRI+3) IN BERYL(EMERALD)

THETA = 90.000 DEGREES H# 4000+0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAGE PART

EIGENVECTOR FAR A(4) • 6479976=06 • 1038015+00	E(4)= 38,46715 B(4) ,4366408=05 ,6994464=00	GHZ C(4) •4366408=05 •6994464=00	D(4) • 6479977=06 • 1038015+00		
EIGENVECTOR FOR A(3) • 3783482=07 • • 1533087=00	E(3)= 17.07751 B(3) .1703549=06 =.6992872=00	GHZ C(3) F,1703549706 2後年02872700	0(3) ••3783482=07 \$1533087#00	6 V	1 - 22 - Y - 1 - 1
EIGENVECTOR FOR A(2) +7070543=08 +6994441=00	E(2)= -27,41983 B(2) =.1049304=08 =.1038010+00	GHZ C(2) =,1049314=08 #,1038020+00	0(2) •7070590=08 •6994487=00		
EIGENVECTOR FOR A(1) • 1751704+07 =• 6902895+00	E(1)= -28.12483 B(1) =.3890428-08 .1533091-00	GHZ C(1) •3890411=08 •,1533084+00	D(1) #+1751693=07 +6902849=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)

E(4)+E(1)

46,5920

1

TRANSITION PROBABILITY MATRIX ELEMENTS

E(4)=E(2)

45+8870

E(4) = E(3)

21,3896

TR(K.L)		AI PHATK .LI			POBETALK.	L)	a i ta di b i a	GAHMACK	L.) ¹
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1.2)	* •0000	.0000	•0000	. .0000	-+1869	.1869	=2,9287	.0000	2.92#7
(1,3)	1.9925	.0000	1.9925		0000	•0000	.0000	.0000	.0000
(1,4)	0000	•0000	.0000		-1-27-7	1 2787	**X155	1000	.2155
(2.3)	+0000	.0000	.0000	•0000	+2+0143	2.0143			.5001
(2.4)	1.3470		1.3470			0000	0000	•0000	.0000
(3,4)		.0000	.0000	-,0000	-2.0545	2.0545	•1.0411	•0000	1.0411

E(3)-E(2)

44.4973

45.2023

+25+(BETA++2) TRIKALE +25+ (ALPHA++2+GAMMA++2)

(1.2)	2.1444	• 0 0 \$ 7
(1.3)	.9925	•0000
(1,4)	.0116	• 4 2 1 7
(2,3)	.0625	1•01**3
(2+4)	.4672	• 0 0 0 0
(3,4)	. 2815	1+0553

11

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS' For cr(+3) in Beryl(Emerald)

THETA- TO.DOD DEGREES H. ADDD+D GAUSS

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

EIGENVECTOR FOR A(4) • 5418089*07 • 1372370=00	E(4)= 45.45326 B(4) •2697673=06 •6932626=00	GHZ C(4) •2697874=D6 •6932627=D0	D(4) •5418070=07 •1372370+00		
EIGENVECTOR FOR A(3) •7813764=D8 =,2361047=D0	E(3)= 14+51258 B(3) +2205826+07 ++6665242-00	6HZ C(3) *•2205826#07 •6665242+00	D(3) +7813765-08 -7813765-08		
EIGENVECTOR FOR A(2) • 1985 48=06 • 6932616=00	E(2)= +28,88228 8(2) +,3987028-07 -,1392366-00	GHZ C(2) % - 3987049=07 = .1392374=00	D(2) 11785154406 06932636400	• • •	 .
EIGENVECTOR FOR A(1) • 3057854-07 = • 6645252=00	E(1)= -31.08356 B(1) 1083192-07 .2361051=00	GHZ C(1) +1083190=07 -,2361047=00	D(1) = \$ 3057#44=07 }\$\$\$5232=00		-
E(4)-E(3)	E(4)=E(2)	E(4)=E(1)	E(3)+E(2)	° E(3)-E(1)	E(2)-E())
30 • 9407	74•3355	74+5368	43.3949	45.5961	2+2013

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K.L)			1 BETAIK, L)			GAHMA(K.L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	INAG	ABS
(1,2) (1,3) (2,3) (2,4) (2,4) (3,4)	- 0000 1 • 9753 - 0000 0000 1 • 2116 - 0000	.0000 .0000 .0000 .0000 .0000 .0000	0000 0000 0000 0000 0000 0000	- 0000 0000 0000 - 0000 - 0000 - 0000	-+3770 +0000 +1+0578 -2+0858 -+0000 +2+0938	.3770 .0000 1.0598 2.0858 .0000 2.0938	+2.8382 .0000 +2245 7945 0000 71.1214	0000 0000 0000 0000 0000 0000 0000	2.8392 .0000 .2295 .7965 .0000 1.1214
TR(K,L)	+25+(ALP	HA++2+GAM	44+2)	+25+18ETA+	• 2)				-
(1.2)				E			п		

N & N & I	£ 4 W I J 7	
(1+3)	• 9755	• 0 0 0 0
(1,4)	.0132	+2808
(2,3)	.1586	1+0676
(2+4)	.3670	+0800
(3,4)	.3144	1+0960
		· · ·

Pun Chiv	37 IN BERT	LICENERALD	1	andro an in try in administration in antitic stationaries and set of	ann an Annailte	an san ang ang ang ang ang ang ang ang ang a			the second by the second second
THETTH	0.000 DE0	REES		GAUSS		and a state of the second s		anna a tha an	
FIRST	ROW OF EIG	ENVECTOR	IS REAL P	ARTI SECOND	ROW 15 1H	AG. PART		···	
EIGENVEC	TOR FOR ES	4)= 52.7 8(4)	4425 GH	[Z C (4)	D(4)	. مند در . مدم	- <u></u> 180 <u>2012</u> 010 - 201520	n an a	na na atraac
• 1 6 6	7653=00	+6871110	-D	047540-00 871118-00	+1+69+53	+07 +00	*****	n land afgegesennen of Agened 2 geboor	if the , press science of the second second
EIGENVEC	TOR FOR EL	3) 8 13.2	 3448 gH			n - Constant and Same in any	ne na ta Kasakanina na Sakakananina di Jawa	n an	
A	(3)	8(3)		C (3)		unite de la serie de la se	in and the second s	R 	
.137	4947-07	.2823567	-072	823567=07	++1376967	-07			
	++27-00	***3555921	-00	355592=00		*JU	****		
EIGENVEC	TOR FOR ET	2)=-30.6	496 j - GH	2 - 11,22 - 11,22 - 12,122 - 12	a a <u>alaa a sababa ahaan ka ka ka</u>		Andreastic and Mary	an a san ar san	an ar what is an statement
	(2)	8(2)		C(2)	D(2)				
	0417=07	2987863	•00 •••2	787874=08	.1230421	•07	an an an an ann an an an an an an an an	an a definition and a second	
• 6 6 •	1112-00	1667650	•00 ••1	447456-00	+6871124	=00			
EIGENVEC	TOR FOR EL	1)= -35.3:	3132 GH	2					
· A			and and a second se	C(1))	0117		n na hain an la taga na hiring na hirin na hainn an hainn	ى <u>مەرىپە بەر</u> ئەھلەردىكە «مەر <u>اپەتەر بەرە</u> تە».	Second and the second secon
	3912-00		+04 +1	701051-06		-04			
	570-00	•3077427	• <u>0</u> 0 · · · · • • • 3	099425-00		*00		a la si kanyi tire si sekan yanga sing	n digina kajar kaja di kaja di kaja kaja kaja kaja kaja kaja kaja kaj
E (4	1+213)	EINTHET	2) E	(4)=E(1)	E131-E1	2) E(37-2117	E(2)+E(1)
3.9	.5076	83+3934	tean chian		43.886	3 4		4.681	7
TRANSITI	ON PROBABI	LITY MATRI	X ELEMEN	TS	ه نورهمی و امیشند اور میکند در ا	1	ali interación da construction da construction de construction de construction de construction de construction	 المنابعة <u>فيتركونو</u> والمتحدث ومحدث ال	an a
- TRIK		T WHET T							
	REAL	1 MÁG	ABS	REAL	INAG	1. 188	in É a i	GAMMATK	L)
		a se in the se		an a	• • • • • • • • • • • • • • • • • • •		an a a P	1044	402
(1,2)	0000-	.0000	.0000	0000	++5771	.5771	•2.7237	.0000	2.723
(1+3)	1.8544	0000	1+8544	.0000	+0000	.0000	.0000	+.0000	.000
	-0000-	.0000	.0000	++0000	**8402	18402	*+2108	+0000	-210
(2)3)	•0000	.0000	+0000	•0000	-2+1165	2+1145	#1+Q454	0000	1.045
······································	1.0800-		1.0,00	-0000		•0000	•0000-	.0000	
13947		•0000	0000 • • • • • • • • • • • • • • • • • •	0400	-2+1149	2.1169	-1.1839	.0000	1.105.
TR(K,L)	+25+(ALP	HA++2+6AM	14++2)	+25+(BETA	•2)				
(1+2)		1.8546	and high and a set of the set of	•043]]	۵.۵۰۵ و دوندوکرد در دور در مهاره در معارف در معارف در میکند. مربع رو دور میکنو در معارف در	a da la companya da serie da s	ang sa si pang pangan na sa si na si n	andi i buransan <u>ai katakan</u> ina
***37	_ · · · · ·	.8397		• 600	10	and the state of the			
(2.2)		28.30		•170	5	an ann an bhill da ann an Bhline ann an A		and a second	alanaan ta sadiin ah ta saalaa ah ta sada
	·····			1.1.1.1					
(3.4)		.3504		1.1.1.90)4				
				1.444					

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS

10800 1+1243

(2+3) (2+4) (3+4)	•0000 •9697 •0000	0000 0000 0000	•0000 •9497 •0000	+ 0000 + 0000 + 0000	-2+1207 -+0000 -2+1207	2 • 1 2 0 7 • 0 0 0 0 2 • 1 2 0 7	+1,2825 +,0000 +1,2405	•0000 •0000 •0000	1.2025
TR(K.L)	+25+(ALP)	HA••2*GAMP	1A+ 62)	•25•1BETA•)ežý	1991 - 1992 - 1992 - 1992 - 1992 - 1992 - 1992 - 1993 - 1994 - 1995 -		an a	an a
(1:2) (1:3)	n n i san an analasis tatal ayyo'	1+6760 •7035	u nomina na ser sera	•143	1	a anti-arrange data patri da ana ana kana a		ka maalaan ka	antina (international de s
(1+4) -	18 .	,0081	a an and an an an	+105		an a	ander and the state of the stat		
12 + 3) {-2		+4112		1+124	3				

101010	ALTHANKILI				I TOLTAIKIL	• !	GAMMA(K.L)		
	KEAL	IMAG	ADS	REAL	IMAG	ABS	REAL	IMAG	ABS
								and have a first of the second se	, na singerenden die stationen
(1,2)	0000	*,0000	.0000	,0000	* • 7566	.7566	02,6046	0000	2.0096
(1+3)	1+4775	••0000	1.6775	•0000	+0000	.0000	.0000	-,U000	.0000
(2.5)		- 0000	0000	10000			-1901	-+0000	

EIGENVECTOR FOR E	(1)= =40+65491	GHZ			
=,3223433=07 =,6029322=p0	•1975032-07 •3694230+00	1975031-07 3699228-00	0111 63223429+07 66029314=00	n mananan mananan mananan kananan kanan Mananan mananan mananan kananan kananan kananan kanana kanana kananan kanana kanana kanana kanana kanana kanana 	nennenn geberen unterstellen einer unterstellte socher des socher unterstellten.
E(+)=E(3)	EINIEIZI	E(4)+E(1)	E(3)=E(2)	£13)=E(1)	E(2)+E(1)
47.2144	72+8637	100.9059	45.6473	63.4916	

+6813728-00

A(4)	8(4)	C(4)	D(4)	
+ 100775-07 + 1007560-00	•6813924=00	.6813724-00	+1887560+00	nen men etter en men het per un sen per und het men het men men men men men men men men etter het het bemen ver
EIGENVECTOR FOR A [3] # • 9280882=04	E(3)= 13.0366; B(3) =.1514725=05	GHZ C13)		and and an and an an an analysis and an a The second sec
	***027318*00		+3+++229=00	
EIGENVECTOR FOR A(2)	E(Z)= +32,63271 B(2)	GH2 C(2)	D(2)	
~,30/9/10007~	.10.0414=07	.1020417407	**3*77714*07	

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX EVEMENTS FOR CR(+3) IN BERYL(EMERALD)

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

GHZ

-,1887563+00

THETAS PORDO DEGREES HE TODOURD GAUSS

-+1087557+00

. 3847

TRANSITION PROBABILITY MATRIX ELEMENTS

EIGENVECTOR FAR EINI# 40.25101

+4813920-00

(3,4)

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