COMPUTATION OF ANGULAR VARIATION OF EPR SPECTRA

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ABSTRACT

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The determination of angular variation of the EPR spectra for different spin values and symmetries is presented. This has been done by exact computer diagonalization of the spin-Hamiltonian matrix instead of using perturbation theory, or series expansions, as done by previous researchers.

First, the initial resonant magnetic field values $H = H(\Theta)$ for an angle Θ between the applied magnetic field and the Z-axis are obtained graphically using exact computer diagonalization of the spin-Hamiltonian matrix. Secondly, a Taylor series expansion of the resonant field values with respect to the angle Θ is made to give the new resonant field values H' at $\Theta + \delta\Theta$: $H'(\Theta+\delta\Theta) = H(\Theta) + \delta\Theta \frac{\partial H}{\partial \Theta} + \ldots\ldots$ This expansion, combined with the fact that a resonant field value is a solution of an equation describing the transition between two different energy eigenvalues of the spin-Hamiltonian matrix, leads, through a least-squares fitting procedure, to the formula: $H' = H - \frac{\partial S'/\partial H}{\partial^2 S'/\partial H^2}$ where

$\partial S'/\partial H$, $\partial^2 S'/\partial H^2$ are functions of $\delta\Theta$ and directly related to the first and second derivatives of the energy eigenvalues of the spin-Hamiltonian matrix. These derivatives are evaluated using Feynman's theorem. The results are cast into a form suitable for computer calculation.

The angular variation of the EPR spectra is computed for external magnetic field orientation in the ZX-plane. Hyperfine interaction terms have also been considered.

The theoretical results obtained by the method mentioned above are in excellent agreement with theoretical results for spin values 1,3/2 published by Hutton[7] and experimental results published by Misra[13] for spin values 5/2,7/2.

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CHAPTER I

INTRODUCTION

A substance may be defined as paramagnetic when it possesses no resultant magnetic moment in the absence of an external magnetic field but acquires a magnetic moment in the direction of an applied magnetic field.[1] When a magnetic field is applied to a paramagnetic substance Zeeman splitting of the energy levels occurs, and photons having energies equal to the gaps between Zeeman levels can induce transitions. The energy absorbed as a function of the magnetic field is referred to as the paramagnetic resonance spectrum of the substance.[2]

The angular variation of the spectrum consists of the angular variation at constant frequency and variable magnetic field of the allowed and forbidden transitions.

The importance of the angular dependence of the resonance spectrum is that it reflects the local symmetry of the paramagnetic complex. It enables one to evaluate the different constants appearing in the Hamiltonian and thus to check any supposedly accurate Hamiltonian. If the symmetry is cubic then the g factor is isotropic. If it is axial there are two g factors $g_{||}$ and $g_{\perp}$ and the spectrum is axially symmetric in the XY-plane (see Fig. 1); if it is orthorombic then there are three g factors g_x, g_y, g_z. Distortions from a given symmetry can also be detected.

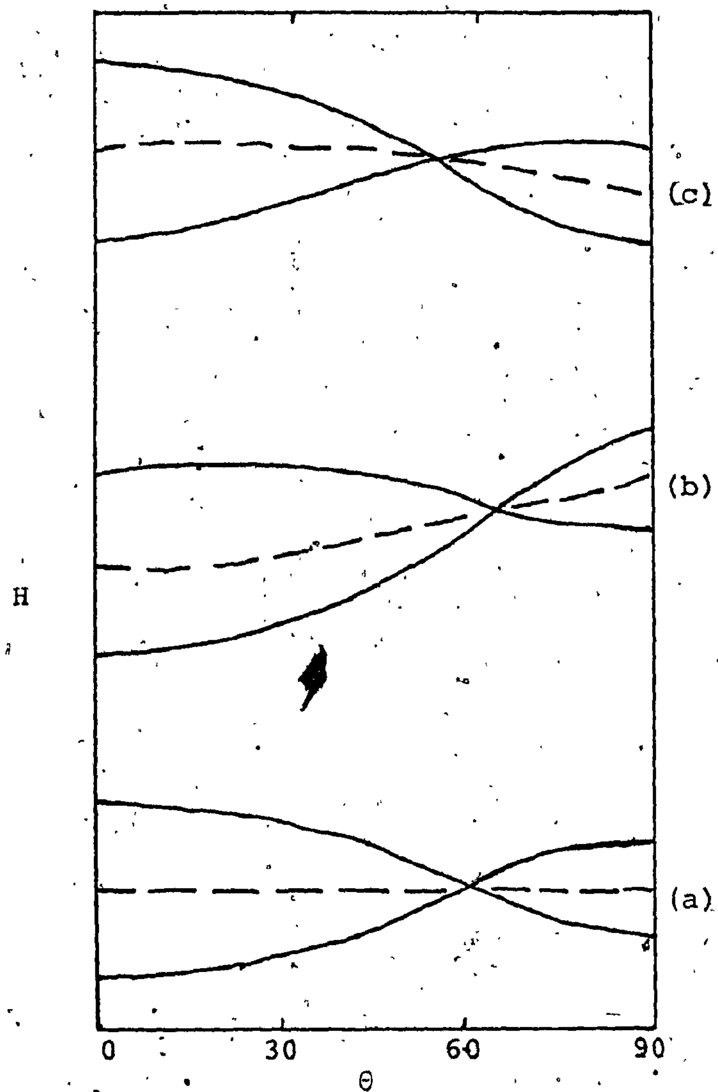

FIG. 1: Angular variation of constant frequency with variable H of the two strongly allowed transitions for s=1 when H makes an angle Θ with the Z-axis and the spin-Hamiltonian is $\mathcal{H} = \beta(H.g.\tilde{S}) + D\{\tilde{S}_z^2 - \frac{1}{3}\tilde{S}(\tilde{S}+1)$. $\tilde{S}$ is the effective spin

(a) g isotropic (approximation: $D \ll g\beta H$)

(b) g axially anisotropic ($|g_{||}| > g_{\perp}$)

(c) g axially anisotropic ($|g_{||}| < g_{\perp}$)

The broken lines show the coincident transitions if D were zero[1].

CHAPTER II

THE STATE OF ART

Electron paramagnetic resonance was discovered in 1944 by E. Zavoisky in U.S.S.R. who observed strong resonance absorption in several paramagnetic salts.

Since then EPR has developed into a major scientific technique. The main contributions to the experimental techniques and theoretical apparatus for interpretation of the results have come from the Oxford group (Pryce, Abragoun, Stevens, Elliot, Judd).

As far as the determination of the angular variation of the EPR spectrum is concerned the methods used by previous researchers are perturbation theory,[1,2,16] series expansions[4,5] and diagnonalization of the spin-Hamiltonian matrix[6,15].

In the first case the axis of quantization for the electronic spin is chosen such that the Zeeman term is diagonalized. Bleaney[1] and Low[2] showed that this term is diagonalized in a coordinate system with spherical coordinates (Θ',ϕ') with respect to the symmetry axis of the crystalline potential when the orientation of the magnetic field is (Θ, ϕ) if the g-factor is anisotropic. These coordinates describe the direction of the principal axis of the g-tensor. It can be shown, following Low[2], that

$$\sin\Theta' = \frac{g_{\perp}}{g}\sin\Theta \qquad \cos\phi' = \frac{g_x}{g_{\perp}}\cos\phi$$

$$\cos\Theta' = \frac{g_{||}}{g}\cos\Theta \qquad \sin\phi' = \frac{g_y}{g_{\perp}}\sin\phi$$

where $$g^2 = g_{||}^2 \cos^2\Theta + g_{\perp}^2 \sin^2\Theta$$

$$g_{\perp}^2 = g_x^2 \cos^2\phi + g_y^2 \sin^2\phi$$

$$g_{||} = g_z$$

Vinokurov et al.[16] extended the calculations by Baker and Williams[17] of the matrix elements for the crystalline electric potential when the Z-axis is parallel to the direction of the magnetic field by tabulating the transformation of the angular momentum operator equivalents into a new coordinate system which is diagonal in the Zeeman energy; however, they attempted to use the Stevens[18] definition of the operator equivalents which do not transform properly as it has been pointed out by Buckmaster.[19]

In the second case, the secular equation is solved for cubic symmetry only and certain directions of the applied magnetic field. Kronig and Bouwkamp[5], for example, give first the roots of the secular equation, i.e. the energy eigenvalues, for external magnetic field parallel to one of the fourfold cubic axes.

These roots for spin 5/2 are:

$$\left.\begin{matrix} W_1 \\ W_2 \end{matrix}\right\} = a \pm b$$

$$\left.\begin{matrix} W_3 \\ W_4 \end{matrix}\right\} = -\frac{1}{2}a \mp b \pm \sqrt{(4b \mp a)^2 + \frac{5}{4}a^2}$$

$$\left.\begin{matrix} W_5 \\ W_6 \end{matrix}\right\} = -\frac{1}{2}a \pm b \pm \sqrt{(4b \pm a)^2 + \frac{5}{4}a^2}$$

where $b = \beta H$, β is the Bohr magneton, H the applied magnetic field and 3a is the total separation of the energy levels in the absence of the magnetic field. Then, for arbitrary directions of H, the roots are approximated by power series in b. Thus, for example, for $b >> a$, i.e. for strong magnetic fields;

$$\left.\begin{matrix} W_1 \\ W_2 \end{matrix}\right\} = \pm b + pa \pm q_1 a^2 b^{-1} + r_1 a^3 b^{-2} \pm \ldots$$

$$\left.\begin{matrix} W_3 \\ W_4 \end{matrix}\right\} = \pm 3b - \frac{3}{2}pa \pm q_2 a^2 b^{-1} + r_2 a^2 b^{-2} \pm \ldots$$

$$\left.\begin{matrix} W_5 \\ W_6 \end{matrix}\right\} = \pm 5b + \frac{1}{2}pa \pm q_3 a^2 b^{-1} + r_3 a^3 b^{-2} \pm \ldots$$

where $p, q_1, q_2, q_3, r_1, r_2, r_3$ are known functions of φ and $\varphi = a_2^2 a_3^2 + a_3^2 a_1^2 + a_1^2 a_2^2$ with a_1, a_2, a_3 being the direction cosines of the magnetic field H with respect to the cubic axes. They also give analogous expressions for weak magnetic fields and for the case in which the magnetic field is oriented along the body diagonal.

Lacroix[4] gives a solution for the case of cubic symmetry and spin value 7/2 when the magnetic field, initially oriented along the (001) direction, is rotated into the plane normal to the (011) direction. The energy eigenvalues obtained by a series expansion in $u = \frac{g\beta\mu H}{\delta}$ for the case $u \gg 1$ are:

$$M = \pm \tfrac{1}{2}\} \quad \pm \frac{u}{2} + a_1 \pm \frac{b_1}{u} + \frac{c_1}{u^2}$$

$$M = \pm \tfrac{3}{2}\} \quad \pm \frac{3u}{2} + a_2 \pm \frac{b_2}{u} + \frac{c_2}{u^2}$$

$$M = \pm \tfrac{5}{2}\} \quad \pm \frac{5u}{2} + a_3 \pm \frac{b_3}{u} + \frac{c_3}{u^2}$$

$$M = \pm \tfrac{7}{2}\} \quad \pm \frac{7u}{2} + a_4 \pm \frac{b_4}{u} + \frac{c_4}{u^2}$$

where H is the magnetic field, g is the g-factor, β is the Bohr magneton, μ_0 is the permeability of empty space, 8δ is the separation of the energy levels in the absence of the magnetic field, M is the magnetic quantum number and a_i, b_i, c_i (i=1,2,3,4) are known functions of φ and Ψ where $\varphi = \ell^2 m^2 + m^2 n^2 + n^2 \ell^2 = \frac{1}{4}$, $\Psi = \ell^2 m^2 n^2 = 0$ with ℓ,m,n being the direction cosines of H with respect to the cubic axes.

Hutton[7] gives results for cubic symmetry and spin value 5/2 in the same plane as Lacroix, but he does not incidate the way he obtained them.

In the third case, the spin-Hamiltonian is diagonalized either directly in the high field region, where the Zeeman term is the largest one and some of the off-diagonal elements are taken to be zero[6], or after a transformation of the spin-Hamiltonian is made into a system of magnetic coordinates.[15] The advantage arises when the magnitude of the Zeeman term is large compared to the crystalline field terms and the anisotropy of the g-factor is small. The orientation of the external magnetic field with respect to the crystal coordinate system can be specified in spherical coordinates by an azimuthal angle ϕ and a polar angle Θ. The Euler angles describing this transformation are $a = \phi$, $\beta = \Theta$, $\gamma = 0$. Then the tensor operators transform in a way which facilitates the diagonalization of the spin-Hamiltonian matrix. Yet this diagonalization is not exact. It is based on the fact that the Zeeman term is the largest one and the g-factor is small.

Another method of solving the problem of the angular variation of EPR spectra is the graphical method. It is based on an exact computer diagonalization of the spin-Hamiltonian matrix which gives the energy eigenvalues. Once these eigenvalues are found, the computer is programmed to solve the transition equations, where the only variable is the applied magnetic field. But this is extremely time consuming, a brute-force method and for this reason less interesting from a physics point of view. It can only serve as a test of the LSF procedure discussed later.

In all cases mentioned above, except the graphical method, the results are applicable only when the perturbation approximation, or series expansion method is valid, i.e. the spin-Hamiltonian can be broken into two parts, $\mathcal{H}_o + \mathcal{H}_1$, where $\mathcal{H}_1 << \mathcal{H}_0$ and exact results for $\mathcal{H}_0$ can be computed. The diagonalization technique of the third case is not exact. There are no calculations for intermediate values of the magnetic field. Also there are symmetry limitations on the applicability of these methods.

A few angular variation spectra have been reported by Poole[6], mainly for the hyperfine interaction, and by Hutton[7] who does not indicate the way he obtained them. In general no systematic treatment for different symmetries and spin values has been given.

The advantage of the LSF procedure is that it is based on an exact diagonalization of the spin-Hamiltonian matrix, it is not limited to certain symmetries, spin values, or the size of the magnetic field. It can be readily subjected to computer techniques. The only approximation used is a Taylor series expansion of the resonant magnetic field values with respect to the angle Θ between the magnetic field and a certain axis. This expansion combined with the LSF method and Feynman's theorem for the derivatives of the energy eigenvalues gives the resonant field values at $\Theta + \delta\Theta$ as a function of those at Θ with $\delta\Theta$ taken sufficiently small $(\delta\Theta = \frac{1}{4} \times \frac{\pi}{180})$.

In Chapter III the spin-Hamiltonian is discussed. In Chapter IV we discuss the least-squares fitting procedure as applied by Misra to the analysis of EPR spectra. Chapters V, VI, VII, deal with the application of the least-squares fitting procedure to different symmetries and spin values, and comparison with experimental results. In Chapter VIII hyperfine terms are discussed and comparison with experiment is made again. Finally an overall discussion of the least-squares fitting method is the content of Chapter IX. The conclusion constitutes the last chapter.

CHAPTER III

SPIN HAMILTONIAN

1. GENERAL HAMILTONIAN

The energy of an atom or radical containing unpaired electrons and nuclei with nonzero spins is expressed in terms of the Hamiltonian operator[6]:

$$\mathcal{H} = \mathcal{H}_{e\ell} + \mathcal{H}_{CF} + \mathcal{H}_{LS} + \mathcal{H}_{ze} + \mathcal{H}_{HF} + \mathcal{H}_{zn} + \mathcal{H}_{II} + \mathcal{H}_{q} + \mathcal{H}_{ss}$$

The electronic operator $\mathcal{H}_{e\ell}$ is the sum of the kinetic energy of each electron, $mv_i^2/2 = p_i^2/2m$, the potential energy of each electron relative to the nuclei, $-Z_n e^2/r_{ni}$, and the interelectronic repulsion energies, e^2/r_{ij}:

$$\mathcal{H}_{e\ell} = \sum_i \frac{p_i^2}{2m} - \sum_{i,n} \frac{Z_m e^2}{r_{ni}} + \sum_{i>j} \frac{e^2}{r_{ij}}$$

where n denotes the sum over the nuclei and i,j denote the sum over the electrons.

The crystal field term $\mathcal{H}_{CF}$ arises from the electrostatic action of the crystalline environment. In the crystal field or point charge approximation ordinarily only nearest-neighbor ligands are taken into account. It is essentially a Stark effect resulting from an electric potential of the type $V = \sum_{i,j} \frac{Q_j}{r_{ij}}$ where the summation is over the Q_j charges and the i electrons.

The spin-orbit interaction for an atom may be writen as $\mathcal{H}_{LS} = \lambda\vec{L}.\vec{S}$ where λ is the spin-orbit coupling constant and L,S the orbital angular and the spin angular momenta.

The spin-spin interaction has the form:

$$\mathcal{H}_{SS} = D(S_z^2 - \frac{1}{3} S(S+1)) + E(S_x^2 - S_y^2)$$

where D,E are constants. The electronic Zeeman term

$$\mathcal{H}_{ze} = \beta\vec{H}.(\vec{L}+2\vec{S}) = \beta\vec{S}.\vec{\vec{g}}.\vec{H}$$

stands for the interaction of the electrons with the applied magnetic field, β is the Bohr magnetron, $\vec{\vec{g}}$ is the spectroscopic splitting tensor. The nuclear Zeeman term

$$\mathcal{H}_{zn} = - \sum_i g_{ni}\beta_n\vec{H}.\vec{I}_i$$

represents the interaction of the magnetic field $\vec{H}$ with the nuclear spin $\vec{I}$.

The hyperfine interaction between the electronic and the nuclear spins

$$\mathcal{H}_{HF} = \vec{S}\sum_i.\vec{\vec{A}}_i.\vec{I}_i$$

and the nuclear spin-spin interaction

$$\mathcal{H}_{II} = \sum_{i>j} \vec{I}_i.\vec{\vec{J}}_{ij}.\vec{I}_j$$

are of the same form ($\vec{\vec{A}}$ is the hyperfine splitting tensor).

The main quadrupolar energy term is

$$\mathcal{H}_q = \frac{e^2Q}{4I(2I-1)} \left(\frac{\partial^2 V}{\partial z^2}\right)[3I_z^2 - I(I+1) + n(I_x^2 - I_y^2)]$$

where Q is the quadrupole moment, $\frac{\partial^2 V}{\partial z^2}$ is the field gradient and n is the asymmetry parameter:

$$n = \frac{\partial^2 V/\partial x^2 - \partial^2 V/\partial y^2}{\partial^2 V/\partial z^2}$$

The order of magnitude of these interactions, excluding $\mathcal{H}_{CF}$, can be estimated from observed atomic spectra for the rare earths:

$$\mathcal{H}_{e\ell} \sim 10^5 cm^{-1},\ \mathcal{H}_{LS} \sim 10^3 cm^{-1},\ \mathcal{H}_{ss} \sim cm^{-1},$$

$$\mathcal{H}_{ze} = 10^{-1} cm^{-1},\ \mathcal{H}_{zn} \sim 10^{-3} cm^{-1},\ \mathcal{H}_{HF} \sim 10^{-3} cm^{-1},$$

$$\mathcal{H}_{II} \sim 10^{-3} cm^{-1},\ \mathcal{H}_{q} \sim 10^{-3} cm^{-1}$$

2. SPIN HAMILTONIAN

In the previous Hamiltonian the spin-dependent part or spin-Hamiltonian is:

$$\mathcal{H}_{spin} = \mathcal{H}_{LS} + \mathcal{H}_{ss} + \mathcal{H}_{ze} + \mathcal{H}_{HF} + \mathcal{H}_{zn} + \mathcal{H}_{II} + \mathcal{H}_{q}$$

we can drop the spin-independent terms from $\mathcal{H}$ since they shift the energy levels equally and thus do not enter into the energy differences. Ordinarily only the first three or four terms will be present at a time, given the order of magnitude of the different terms.

3. EQUIVALENT OPERATORS

The spin-Hamiltonian for an unpaired spin $\vec{S}$ interacting with a nuclear spin $\vec{I}$ can also be writen as

$$\mathcal{H} = \vec{S}.\vec{g}.\vec{H} - \beta_n \vec{H}.\vec{g}_n.\vec{I} + \vec{S}.\vec{A}.\vec{I} + \sum_{k,q} B_k^q O_k^q$$

where O_k^q are spin operators and the coefficients B_k^q assume definite values for specific interactions. Some of those spin operators are given by the following expressions.

$$D[S_z^2 - \frac{1}{3}S(S+1)] = B_2^0 O_2^0$$

$$E(S_x^2 - S_x^2) = B_2^2 O_2^2$$

where D,E are the zero field splitting interactions. Most of the operators O_k^q are listed by Abragam and Bleaney[1].

CHAPTER IV

PROCEDURE FOR COMPUTATION OF ANGULAR VARIATION OF EPR SPECTRA

1. ANALYSIS OF EPR DATA BY THE LSF METHOD

The spin-Hamiltonian for a single ion is described using the notation of Abragam and Bleaney[1], as

$$\mathcal{H} = \beta\vec{H}.\vec{\vec{g}}.\vec{S} + \sum_{\ell,m} B_\ell^m O_\ell^m \qquad (1)$$

$$(\ell \text{ even}, |m| \leq \ell)$$

where $\vec{S}$ is the ionic spin, $\vec{H}$ the external magnetic field $\vec{\vec{g}}$ is the g-tensor, O_ℓ^m are spin operators and β is the Bohr magneton. Suppose that the external magnetic field makes an angle Θ with the Z-axis and the resonance occurs at values of the magnetic field H_r. As the angle Θ varies by $\delta\Theta$ the resonant field values H_r vary by ΔH_r so that the new ones become $H_r' = H_r + \Delta H_r$. Making a Taylor series expansion of the resonant field values with respect to the angle Θ:

$$H(\Theta + \delta\Theta) = H(\Theta) + \delta\Theta \frac{\partial H}{\partial \Theta} + \ldots \quad \text{with } H_r' = H(\Theta+\delta\Theta)$$

and $H_r = H(\Theta)$ leads[8], through the application of a least-squares fitting procedure (LSF), to the formula

$$H_r' = H_r - \frac{(\partial S'/\partial H)_{H_r}}{(\partial^2 S'/\partial H^2)_{H_r}} \qquad (2)$$

where S' (chi-squared) for EPR data is

$$S' = \sum_i [(|\Delta E_i| - h\nu)^2/\sigma_i^2] \quad (3)$$

and $\Delta E_i \equiv E_{i'} - E_{i''}$ ($E_{i'}$ and $E_{i''}$ are the energy levels between which transitions occur), h is Planck's constant, ν is the Klystron frequency and σ_i is a weight factor (related to standard deviation).

Following Misra[3], with $a_\ell = a_j = H_{i',i''}$, where a_ℓ, a_j stand for the various parameters of equation (1), and $\sigma_i=1$, we get from equation (3):

$$\frac{\partial S'}{\partial H_{i',i''}} = 2\frac{\Delta E_i}{|\Delta E_i|}(|\Delta E_i| - h\nu)\left(\frac{\partial E_{i'}}{\partial H_{i',i''}} - \frac{\partial E_{i''}}{\partial H_{i',ii''}}\right) \quad (4)$$

and from equation (4) we get:

$$\frac{\partial^2 S'}{\partial H^2_{i',i''}} = 2\left(\frac{\partial E_{i'}}{\partial H_{i',i''}} - \frac{\partial E_{i''}}{\partial H_{i',i''}}\right)^2 + 2\frac{\Delta E_i}{|\Delta E_i|}(|\Delta E_i| - h\nu)\times$$

$$\left(\frac{\partial^2 E_{i'}}{\partial H^2_{i',i''}} - \frac{\partial^2 E_{i''}}{\partial H^2_{i',i''}}\right) \quad (5)$$

where $H_{i',i''}$ in equations (4) is the resonant magnetic field value for the transition $E_{i'} \leftrightarrow E_{i''}$. Thus, the problem reduces to the evaluation of first and second derivatives of the energy eigenvalues.

2. NUMERICAL EVALUATION OF THE FIRST AND SECOND DERIVATIVES OF THE ENERGY EIGENVALUES.

Suppose that the spin-Hamiltonian $\mathcal{H}$ is represented by a $(2S+1) \times (2S+1)$ matrix with eigenvectors $|\varphi_{i'}\rangle$ and corresponding eigenvalues E_i. Then the j'i' element of the matrix which diagonalizes $\mathcal{H}$ is given by

$$V_{j'i'} = |\varphi_{i'}\rangle_{j'} \qquad (6)$$

where $|\varphi_{i'}\rangle_{j'}$ is the j'th element of the column vector $|\varphi_{i'}\rangle$.

From Feynman's theorem[9] we have:

$$\frac{\partial E_{i'}}{\partial H_{i',i''}} = \langle\varphi_{i'}|\frac{\partial \mathcal{H}}{\partial H_{i',i''}}|\varphi_{i'}\rangle \qquad (7)$$

which, rewritten for numerical computation, is

$$\frac{\partial E_{i'}}{\partial H_{i',i''}} = Tr[\frac{\partial \mathcal{H}}{\partial H_{i',i''}}(|\varphi_{i'}\rangle \times \langle\varphi_{i'}|)] \qquad (8)$$

In equation (8), Tr stands for Trace and $|\varphi_{i'}\rangle \times \langle\varphi_{i'}|$ represents the (2S+1) x (2S+1) matrix obtained by taking the outer product of $|\varphi_{i'}\rangle$ with itself, i.e. $(|\varphi_{i'}\rangle \times \langle\varphi_{i'}|)_{pq} = |\varphi_{i'}\rangle_p |\varphi_{i'}\rangle_q^*$.

For the numerical evaluation of equation (8) the $|\varphi_{i'}\rangle$ are obtained by computer diagonalization of $\mathcal{H}$ and $\frac{\partial \mathcal{H}}{\partial H_{i',i''}}$ from the known matrix representation of S_x, S_y, S_z and O_ℓ^m (see equation (1))

When the spin-Hamiltonian is given by equation (1), equation (5) can be simplified. Suppose that in equation (1) g is isotropic and that the magnetic field lies in the ZX-plane (the treatment is the same when g is a tensor).

Then $$\frac{\partial \mathcal{H}}{\partial H_{i',i''}} = \frac{\partial}{\partial H_{i',i''}} (\beta \vec{H}.\vec{g}.\vec{S} + \sum_{\ell,m} B_\ell^m O_\ell^m)$$

$$(\ell \text{ even}, |m| \leq \ell)$$

or, in the ZX-plane,

$$\frac{\partial \mathcal{H}}{\partial H_{i',i''}} = \frac{\partial}{\partial H_{i',i''}} (g\beta S_z \cos\Theta\ H_{i',i''} + g\beta S_x \sin\Theta\ H_{i',i''})$$

$$= g\beta \cos\Theta S_z + g\beta \sin\Theta S_x \qquad (9)$$

where Θ is the angle between the magnetic field and the Z-axis. From equations (8) and (9) we get:

$$\frac{\partial E_{i'}}{\partial H_{i',i''}} = \mathrm{Tr}\,[(g\beta\cos\Theta S_z + g\beta\cos\Theta S_x)(|\varphi_{i'}\rangle \times \langle\varphi_{i'}|)]$$

$$= g\beta\cos\Theta\ \mathrm{Tr}\,(S_z|\varphi_{i'}\rangle \times \langle\varphi_{i'}|) +$$

$$g\beta\sin\Theta\ \mathrm{Tr}\,(S_x|\varphi_{i'}\rangle \times \langle\varphi_{i'}|) \qquad (10)$$

From equation (10) we have $\frac{\partial^2 E_{i'}}{\partial H^2_{i',i''}} = 0$. Equation (5) then reduces to:

$$\frac{\partial^2 S'}{\partial H^2_{i',i''}} = 2\left(\frac{\partial E_{i'}}{\partial H_{i',i''}} - \frac{\partial E_{i''}}{\partial H_{i',i''}}\right)^2 \qquad (11)$$

From equations (2), (4), (11) and $H_r = H_{i',i''}$ we get the final form for the new resonant magnetic field values which is suitable for computer procedures:

$$H'_{i',i''} = H_{i',i''} - \frac{\Delta E_i}{|\Delta E_i|}(|\Delta E_i| - h\nu)\left(\frac{\partial E_{i'}}{\partial H_{i',i''}} - \frac{\partial E_{i''}}{\partial H_{i',i''}}\right) x$$

$$\left(\frac{\partial E_{i'}}{\partial H_{i',i''}} - \frac{\partial E_{i''}}{\partial H_{i',i''}}\right)^{-2} \qquad (12)$$

where $\frac{\partial E_{i'}}{\partial H_{i',i''}}$ is given by equation (10) and so is $\frac{\partial E_{i''}}{\partial H_{i',i''}}$ on replacing $E_{i'}$ by $E_{i''}$.

To assure the applicability of equation (2) which is based on a Taylor series expansion of the resonant magnetic field values with respect to the angle Θ

$H(0+\delta\theta) = H(0) + \delta\Theta\left(\frac{\partial H}{\partial \Theta}\right)_{\Theta=0} + \ldots.$ we take $\delta\Theta = \frac{1}{4}\,\frac{\pi}{180}$ which turned out to be sufficiently small (even if we take $\delta\Theta = \frac{\pi}{180}$ the results are almost the same).

The resonant magnetic field values for $\Theta = 0^{\circ}$ and for the different transitions are obtained by exact computer diagonalization of the spin-Hamiltonian matrix.

CHAPTER V

SPIN S = 1

As mentioned earlier in detail, in Chapter II, previous researchers have used perturbation theory, series expansions and not exact diagonalization techniques to determine the angular variation of EPR spectra. In this chapter, as well as in the next one, we give first the graphical solution and then the LSF one for comparison purposes.

1. GRAPHICAL SOLUTION

The spin-Hamiltonian matrix is:

$$\mathcal{H} = g\beta\vec{H}.\vec{S} + D(S_z^2 - \frac{1}{3}S(S+1)) + E(S_x^2 - S_y^2)$$

in the ZX-plane it becomes:

$$\mathcal{H} = g\beta H\cos\Theta\, S_z + g\beta H\sin\Theta\, S_x + D(S_z^2 - \frac{1}{3}S(S+1) + E(S_x^2 - S_y^2)$$

Its matrix form is:

M \ M	1	0	-1
1	$\frac{D}{3} + a_1$	a_2	E
0	a_2	$-\frac{2}{3}D$	a_2
-1	E	a_2	$\frac{D}{3} - a_1$

where $a_1 = g\beta H\cos\Theta$, $a_2 = \frac{\sqrt{2}}{2} g\beta H \sin\Theta$. H is the applied magnetic field making an angle Θ with the Z-axis, g is the g-factor, β is the Bohr magneton and D,E the zero field splittings.

The equation $\det||\mathcal{H} - \lambda\mathbb{1}|| = 0$ becomes

$(\frac{\lambda}{D})^3 - q(\frac{\lambda}{D}) + r = 0$ where λ stands for the energy

eigenvalues, $q = \frac{1}{3} + (\frac{E}{D})^2 + (\frac{g\beta H}{D})^2$ and

$$r = \frac{2}{3}(\frac{1}{9} - (\frac{E}{D})^2) + (\frac{g\beta H}{D})^2(\sin^2\Theta(1 - \frac{E}{D}) - \frac{2}{3})$$

The three real solutions of the cubic equation in λ/D are[10]:

$$\frac{\lambda_1}{D} = 2R^{1/3}\cos\frac{\varphi}{3}, \quad \frac{\lambda_2}{D} = 2R^{1/3}\cos\frac{\varphi+2\pi}{3}, \quad \frac{\lambda_3}{D} = 2R^{1/3}\cos\frac{\varphi+4\pi}{3}$$

where $R = \sqrt{\frac{r^2}{4} + |\frac{r^2}{4} + \frac{q^3}{27}|}$ and $\tan\varphi = \frac{\sqrt{|\frac{r^2}{4} + \frac{q^3}{27}|}}{-\frac{r}{2}}$

Thus the equations for the transitions become:

$$||\frac{\lambda_1}{D} - \frac{\lambda_2}{D}| - \frac{W}{D}| = |2|R^{1/3}||\cos\frac{\phi}{3} - \cos\frac{\phi+2\pi}{3}| - \frac{W}{D}| = 0$$

$$||\frac{\lambda_2}{D} - \frac{\lambda_3}{D}| - \frac{W}{D}| = |2|R^{1/3}||\cos\frac{\phi+2\pi}{3} - \cos\frac{\phi+4\pi}{3}| - \frac{W}{D}| = 0$$

$$||\frac{\lambda_3}{D} - \frac{\lambda_1}{D}| - \frac{W}{D}| = |2|R^{1/3}||\cos\frac{\phi+4\pi}{3} - \cos\frac{\phi}{3}| - \frac{W}{D}| = 0$$

where $W = h\nu$ is the energy absorbed in those transitions. These equations in $g\beta H/D$ are solved graphically using the computer. The resonant G values, where $G = g\beta H/D$, as a function of the angle Θ, for different values of the parameters E/D and W/D, where W is the energy absorbed at resonance, are plotted on the next two pages. The results are the same as those given by Hutton[7], except that he doesn't show the so-called forbidden transition for $\frac{W}{D} = 1.6$ and $\frac{W}{D} = 6.4$

2. THE LSF SOLUTION

As mentioned earlier, the initial resonant field values are obtained by diagonalizing the hamiltonian matrix for $\Theta = 0^{o}$ and programming appropriately a computer to give the field values for the different transitions. This being done, the computer is programmed to give the new resonant field values according to equation (12) of the preceding chapter in which we replace H by G, where $G = g\beta H/D$. Accordingly, equation (10) of the preceding chapter becomes:

$$\frac{\partial E_{i'}}{\partial G_{i',i''}} = \cos\Theta \, \mathrm{Tr}(S_z|\varphi_{i'}\rangle\langle\varphi_{i'}|) + \mathrm{Sin}\Theta \, \mathrm{Tr}(S_x|\varphi_{i'}\rangle\langle\varphi_{i'}|).$$

Results, i.e. G values, are neglected once they become negative, since physically, we have only one direction of the applied magnetic field.

The results are exactly the same as those given in part 1 so that no further graphs are necessary.

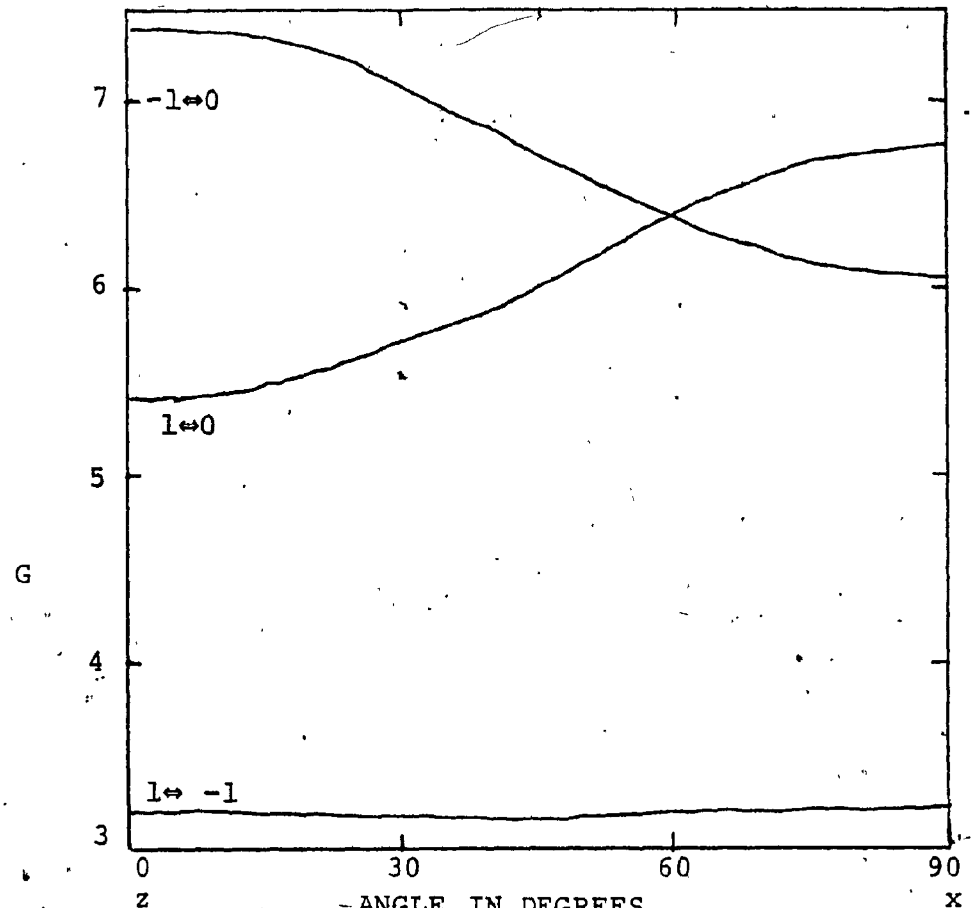

FIG. 2: Angular variation of EPR spectrum in the ZX-plane for spin S = 1(W/D = 6.4, E/D = .1)

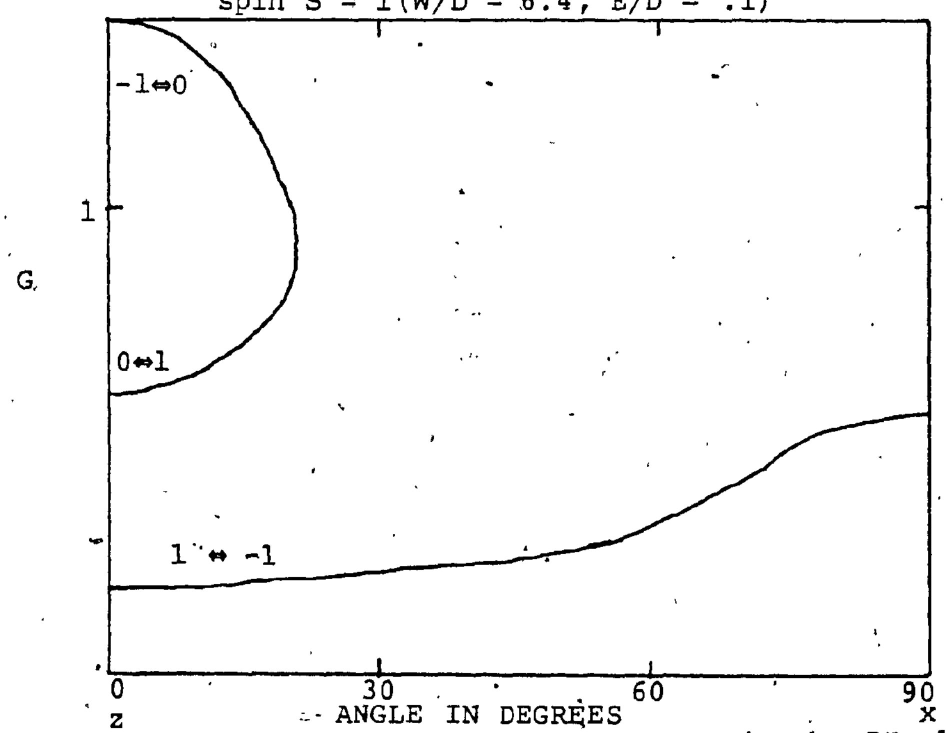

FIG. 3: Angular variation of EPR spectrum in the ZX-plane for spin S = 1(W/D = .4, E/D = .1)

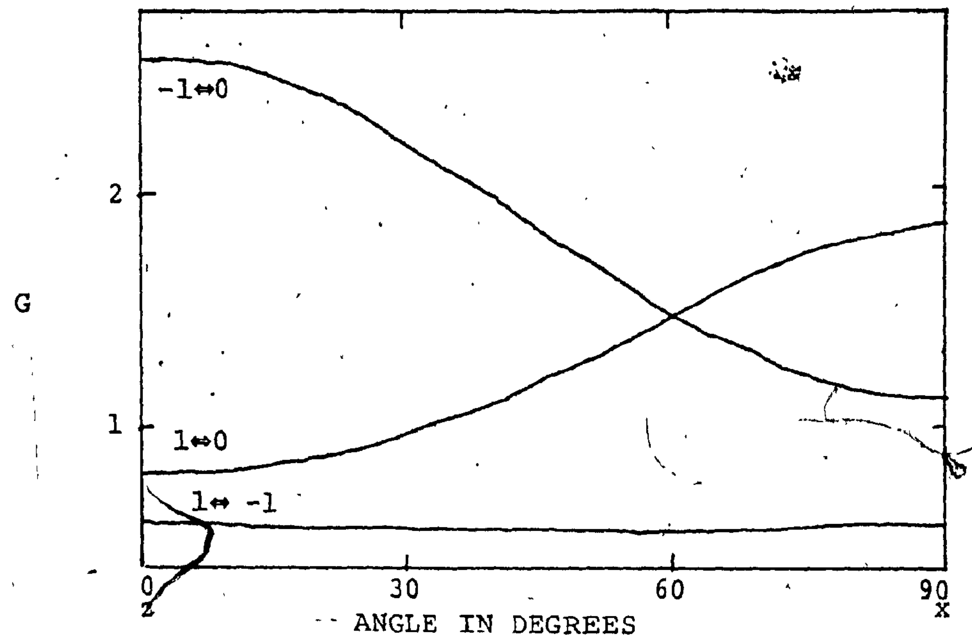

FIG. 4: Angular variation of EPR spectrum in the ZX-plane for spin S = 1(W/D = 1.6, E/D = .1)

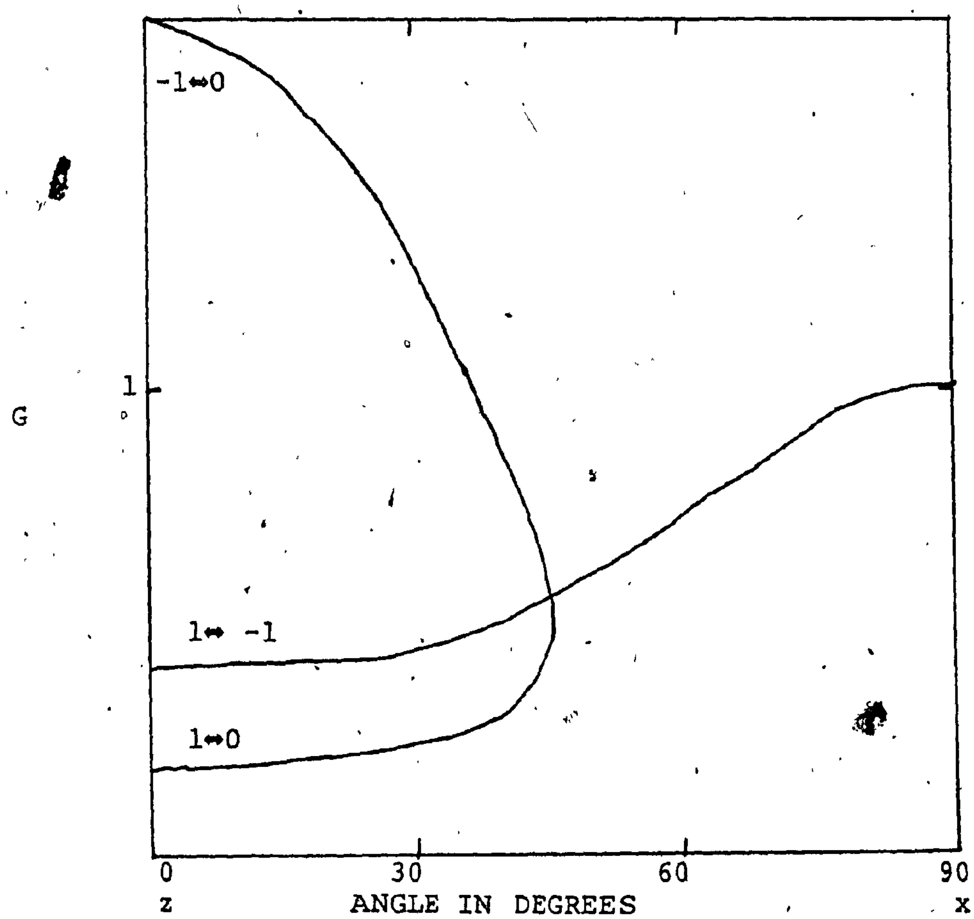

FIG. 5: Angular variation of EPR spectrum in the ZX-plane for spin S = 1(W/D = .8, E/D = .1)

CHAPTER VI

SPIN S = 3/2

1. GRAPHICAL SOLUTION

The spin-Hamiltonian is the same as that of the preceding chapter. In the ZX-plane the spin-Hamiltonian matrix is:

M \ M	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$
$\frac{3}{2}$	$\frac{3}{2}G_1+D$	$\frac{\sqrt{3}}{2}G_2$	$\sqrt{3}\,E$	0
$\frac{1}{2}$	$\frac{\sqrt{3}}{2}G_2$	$\frac{1}{2}G_1-D$	G_2	$\sqrt{3}\,E$
$-\frac{1}{2}$	$\sqrt{3}\,E$	G_2	$-\frac{1}{2}G_1-D$	$\frac{\sqrt{3}}{2}G_2$
$-\frac{3}{2}$	0	$\sqrt{3}\,E$	$\frac{\sqrt{3}}{2}G_2$	$-\frac{3}{2}G_1+D$

where $G_1 = g\beta H\cos\Theta$ and $G_2 = g\beta H\sin\Theta$. H is the applied magnetic field making an angle Θ with the Z-axis, g is the g-factor, β is the Bohr magneton and D,E are the zero field splittings.

The equation $\det\|\mathcal{H}-\lambda\mathbb{1}\| = 0$ becomes

$$A_4\left(\frac{\lambda}{D}\right)^4 + 2A_3\left(\frac{\lambda}{D}\right)^3 + A_2\left(\frac{\lambda}{D}\right)^2 + A_1\left(\frac{\lambda}{D}\right) + A_0 = 0 \quad \text{where:}$$

$A_4 = 1$, $A_3 = 0$, $A_2 = -2-6\left(\frac{E}{D}\right)^2-\frac{5}{2}\left(\frac{G}{D}\right)^2$

$$A_1 = 2(\frac{G}{D})^2(1-3\frac{E}{D}) - 6(\frac{G}{D})^2 \cos^2\Theta(1-\frac{E}{D}),$$

$$A_0 = (1+3(\frac{E}{D})^2)^2 + \frac{1}{2}(\frac{G}{D})^2[1-9(\frac{E}{D})^2+\frac{9}{8}(\frac{G}{D})^2+12\frac{E}{D}]-3(\frac{G}{D})^2\cos^2\Theta(1-3(\frac{E}{D})^2+2\frac{E}{D})$$

and $G = g\beta H/D$

Comparing the equation above with the equation

$$x^4 + 2px^3 + qx^2 + 2rx + s = 0$$

which is solved in reference (10), we identify:

$$p = A_3 = 0, \quad q = A_2, \quad r = \frac{A_1}{2}, \quad s = A_0.$$

The roots of our equation finally are the roots of the following two quadratic equations:

$$x^2 - ax + (y-b) = 0$$

$$x^2 + ax + (y+b) = 0$$

where $a = \sqrt{2(y+\frac{A_2}{6}) - A_2}$, $b = -\frac{A_1}{2a}$ and y is the real root of the cubic equation:

$$y^3 + [-A_0 - \frac{A_2^2}{12}]y + [-2\frac{A_2^3}{6^3} - 2\frac{A_2A_0}{6} + \frac{A_2A_0-A_4^2}{2}] = 0,$$

which was found by substituting $y+\frac{q}{6}$ for k in

$$2k^3 - qk^2 + 2(pr-s)k - p^2s+qs-r^2 = 0 \text{ (Reference 10)}.$$

Writing $S_1 = \sqrt{(p-a)^2-4(y-b)}$ and $S_2 = \sqrt{(p+a)^2-4(y+b)}$, with p,a,b given above in terms of A_1, A_2, A_3, A_0, the roots of the two quadratic equations are:

$$\frac{\lambda_1}{D} = \frac{a-p+S_1}{2} \qquad \frac{\lambda_3}{D} = \frac{-(a+p)+S_2}{2}$$

and

$$\frac{\lambda_1}{D} = \frac{a-p-S_1}{2} \qquad \frac{\lambda_4}{D} = \frac{-(a+p)-S_2}{2}$$

respectively. Thus the transition equations become:

1) $\left| |S_1| - \frac{W}{D} \right| = 0$

2) $\left| |2a+S_1-S_2|/2 - \frac{W}{D} \right| = 0$

3) $\left| |2a+S_1+S_2|/2 - \frac{W}{D} \right| = 0$

4) $\left| |2a-S_1-S_2|/2 - \frac{W}{D} \right| = 0$

5) $\left| |2a-S_1+S_2|/2 - \frac{W}{D} \right| = 0$

6) $\left| |S_2| - \frac{W}{D} \right| = 0$

Those equations in G are solved graphically using the computer. The results are the same as those given by Hutton[7]. The resonant G values, where $G = g\beta H/D$, as a function of the angle Θ, for the different values of the parameters E/D and W/D, where W is the energy absorbed at resonance, are plotted on the next two pages.

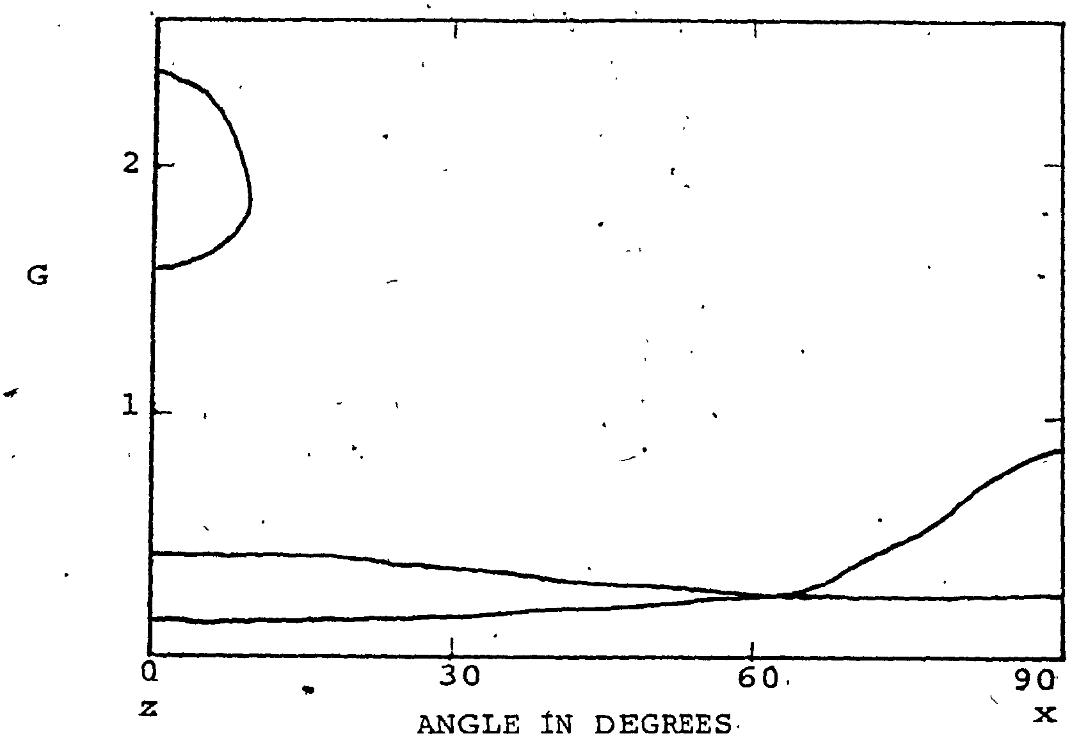

FIG. 6: Angular variation of EPR spectrum in the ZX-plane for spin S = 3/2 (W/D = .4, E/D = .1)

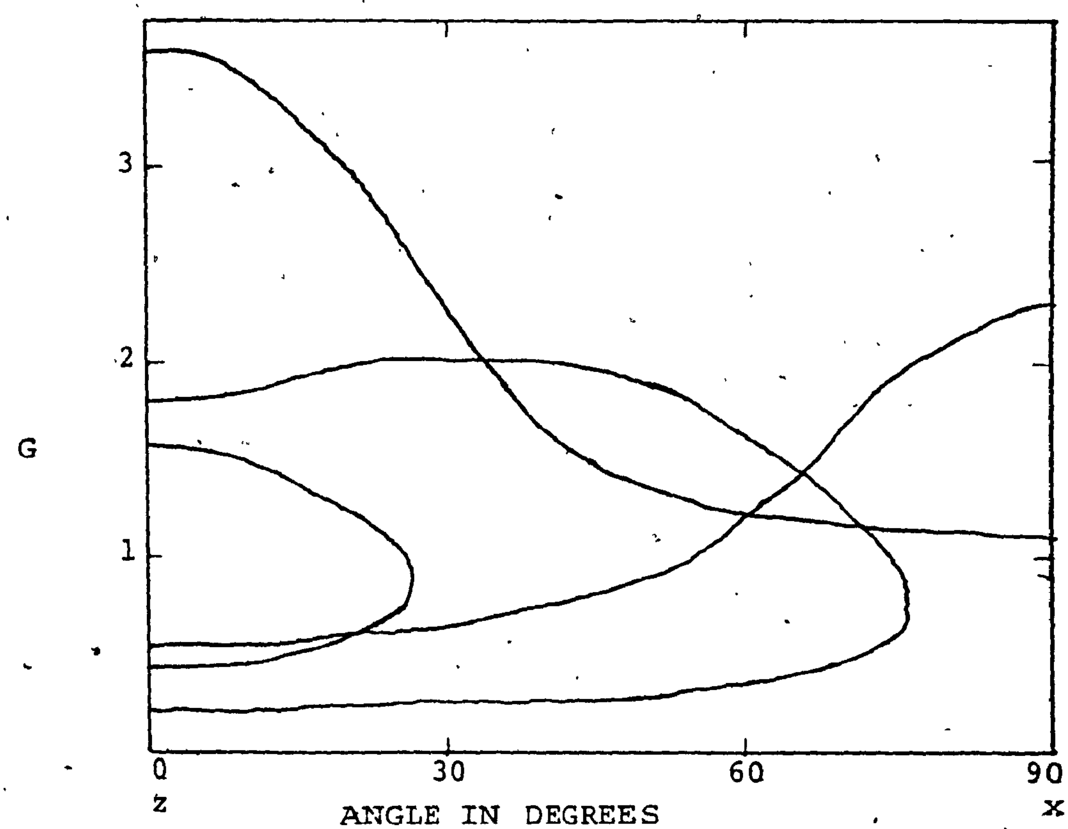

FIG. 7: Angular variation of EPR spectrum in the ZX-plane for spin S = 3/2 (W/D = 1.6, E/D = .1)

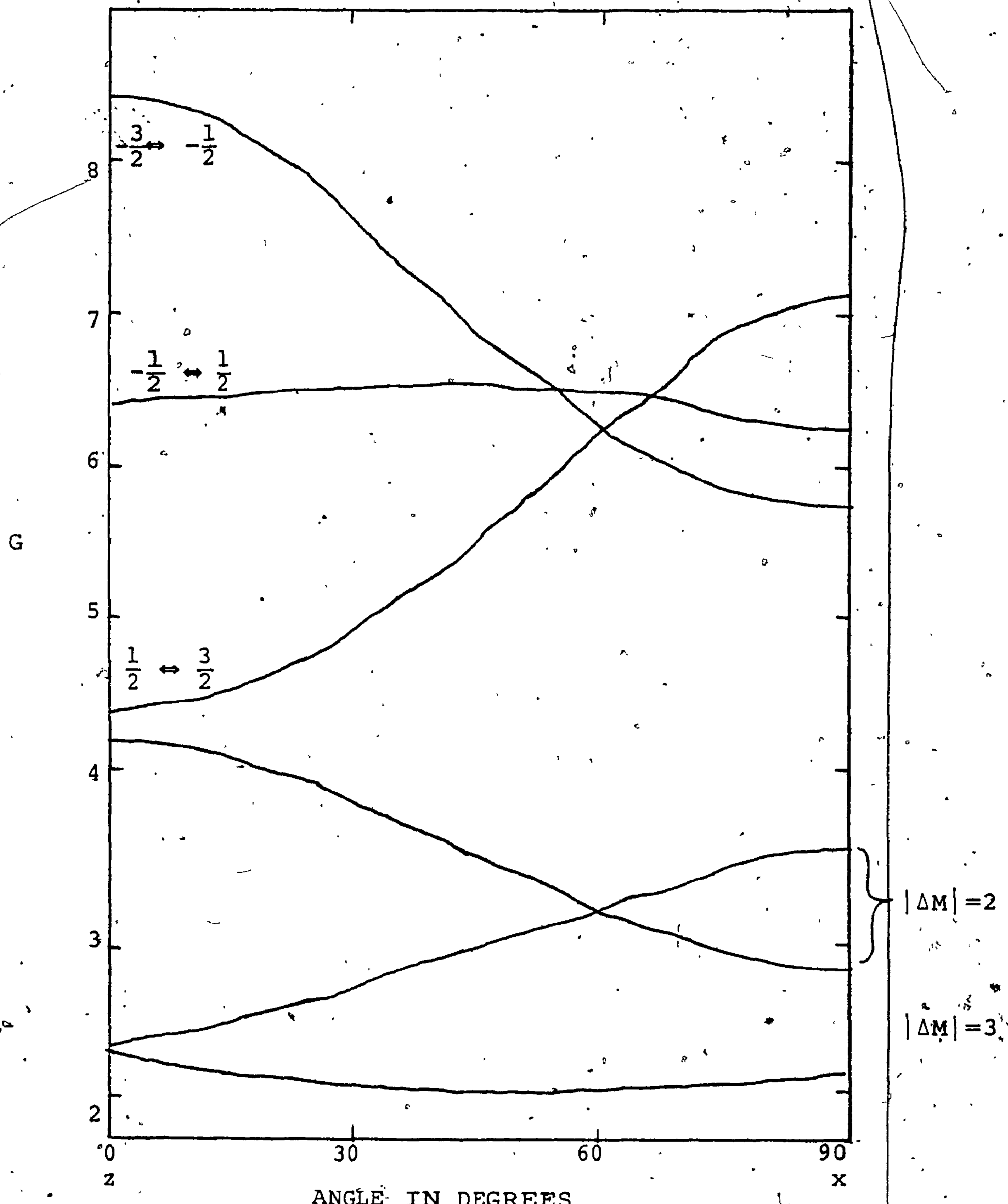

FIG. 8: Angular variation of EPR spectrum in the ZX-plane for spin S = 3/2(W/D = 6.4, E/D = .1)

2. THE LSF SOLUTION

We proceed in exactly the same manner as in Part 2 of the preceding chapter. The results are exactly the same as those of Part 1, so that no further graphs are necessary.

CHAPTER VII

HIGHER SPIN VALUES

The spin-Hamiltonian which is used throughout this chapter is the same as that of Chapter V. H is the external magnetic field making an angle Θ with the Z-axis, g is the g-factor, β is the Bohr magneton and D,E are the zero field splittings. We follow the same precedure as that of Part 2 of Chapter V.

1. SPIN S = 2

The spin-Hamiltonian matrix in the ZX-plane becomes:

M \ M	2	1	0	-1	-2
2	2C+2	S	$\sqrt{6}\,\frac{E}{D}$	0	0
1	S	C-1	$\sqrt{\frac{3}{2}}\,S$	$3\,\frac{E}{D}$	0
0	$\sqrt{6}$ E/D	$\sqrt{\frac{3}{2}}\,S$	-2	$\sqrt{\frac{3}{2}}\,S$	$\sqrt{6}\,\frac{E}{D}$
-1	0	$3\,\frac{E}{D}$	$\sqrt{\frac{3}{2}}\,S$	-C-1	S
-2	0	0	$\sqrt{6}\,\frac{E}{D}$	S	-2C+2

where $C = \frac{g\beta H \cos\Theta}{D}$ and $S = \frac{g\beta H \sin\Theta}{D}$. The resonant G values, where G = gβH/D, as a function of the angle Θ for different values of the parameters E/D and W/D, where W is the energy absorbed at resonance, are plotted on the next two pages.

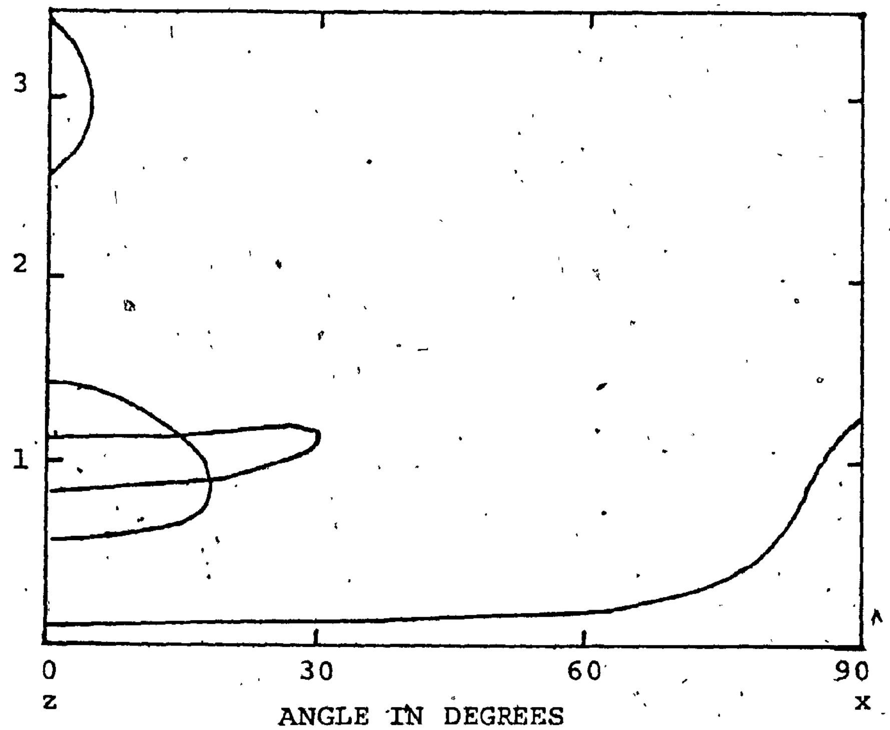

FIG. 9: Angular variation of EPR spectrum in the ZX-plane for spin S = 2(W/D = .4, E/D = .1)

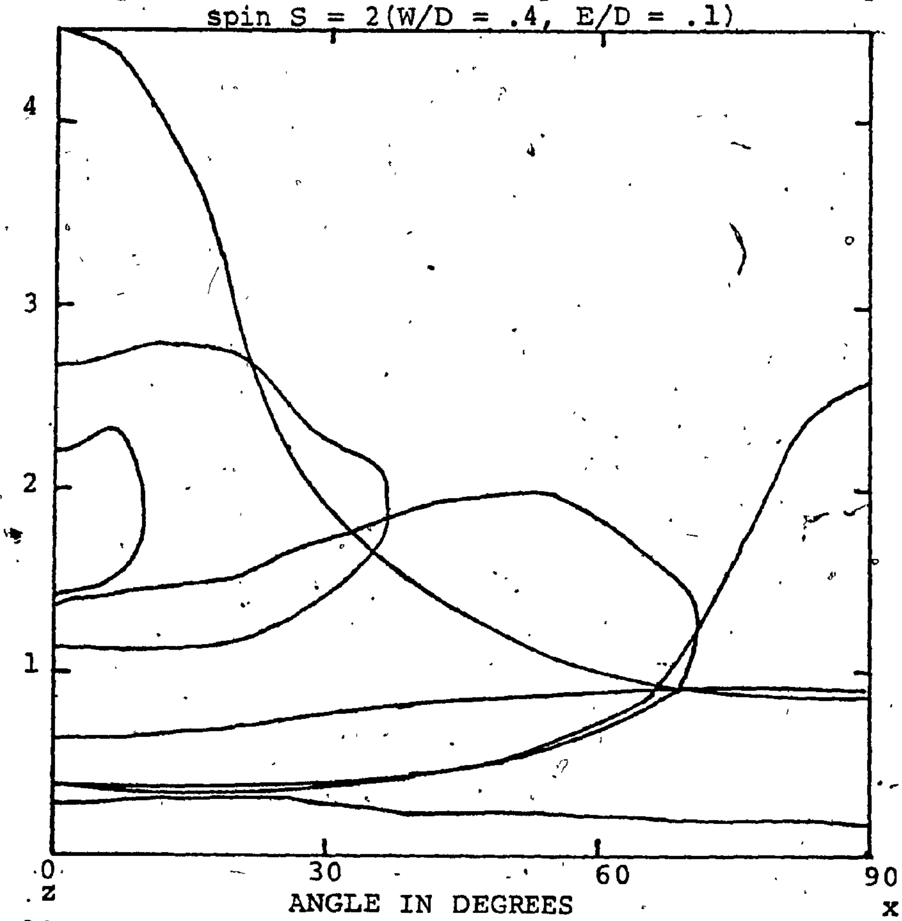

FIG. 10: Angular variation of EPR spectrum in the ZX-plane for spin S = 2(W/D = 1.6, E/D = .1)

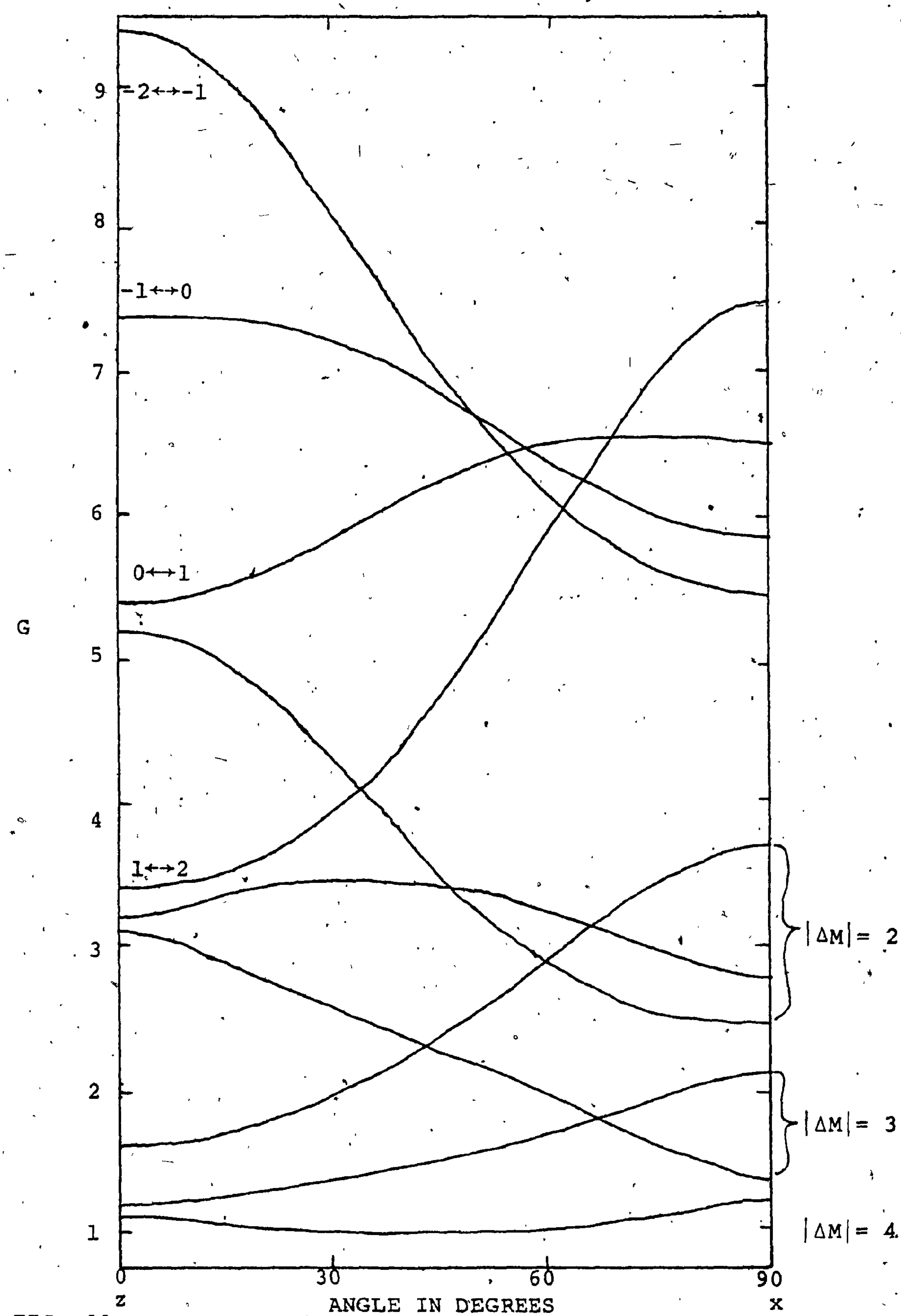

FIG. 11: Angular variation of EPR spectrum in the ZX-plane for spin S = 2(W/D = 6.4, E/D = 1)

2. SPIN S = 5/2

The spin-Hamiltonian matrix in the ZX-plane is:

M \ M	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
$\frac{5}{2}$	$\frac{5}{2}C+\frac{10}{3}$	$\frac{\sqrt{5}}{2}S$	$\sqrt{10}\frac{E}{D}$	0	0	0
$\frac{3}{2}$	$\frac{\sqrt{5}}{2}S$	$\frac{3}{2}C-\frac{2}{3}$	$\sqrt{2}\ S$	$3\sqrt{2}\ \frac{E}{D}$	0	0
$\frac{1}{2}$	$\sqrt{10}\frac{E}{D}$	$\sqrt{2}\ S$	$\frac{1}{2}C-\frac{8}{3}$	$\frac{3}{2}\ S$	$3\sqrt{2}\ \frac{E}{D}$	0
$-\frac{1}{2}$	0	$3\sqrt{2}\frac{E}{D}$	$\frac{3}{2}\ S$	$-\frac{1}{2}C-\frac{8}{3}$	$\sqrt{2}\ S$	$\sqrt{10}\frac{E}{D}$
$-\frac{3}{2}$	0	0	$3\sqrt{2}\ \frac{E}{D}$	$\sqrt{2}\ S$	$-\frac{3}{2}C-\frac{2}{3}$	$\frac{\sqrt{5}}{2}\ S$
$-\frac{5}{2}$	0	0	0	$\sqrt{10}\frac{E}{D}$	$\frac{\sqrt{5}}{2}\ S$	$-\frac{5}{2}\ C$

where $C = \frac{g\beta H}{D}\cos\Theta$ and $S = \frac{g\beta H}{D}\sin\Theta$. The resonant G values, where $G = g\beta H/D$, as a function of the angle Θ for different values of the parameters E/D and W/D, where W is the energy absorbed at resonance, are plotted on the next three pages.

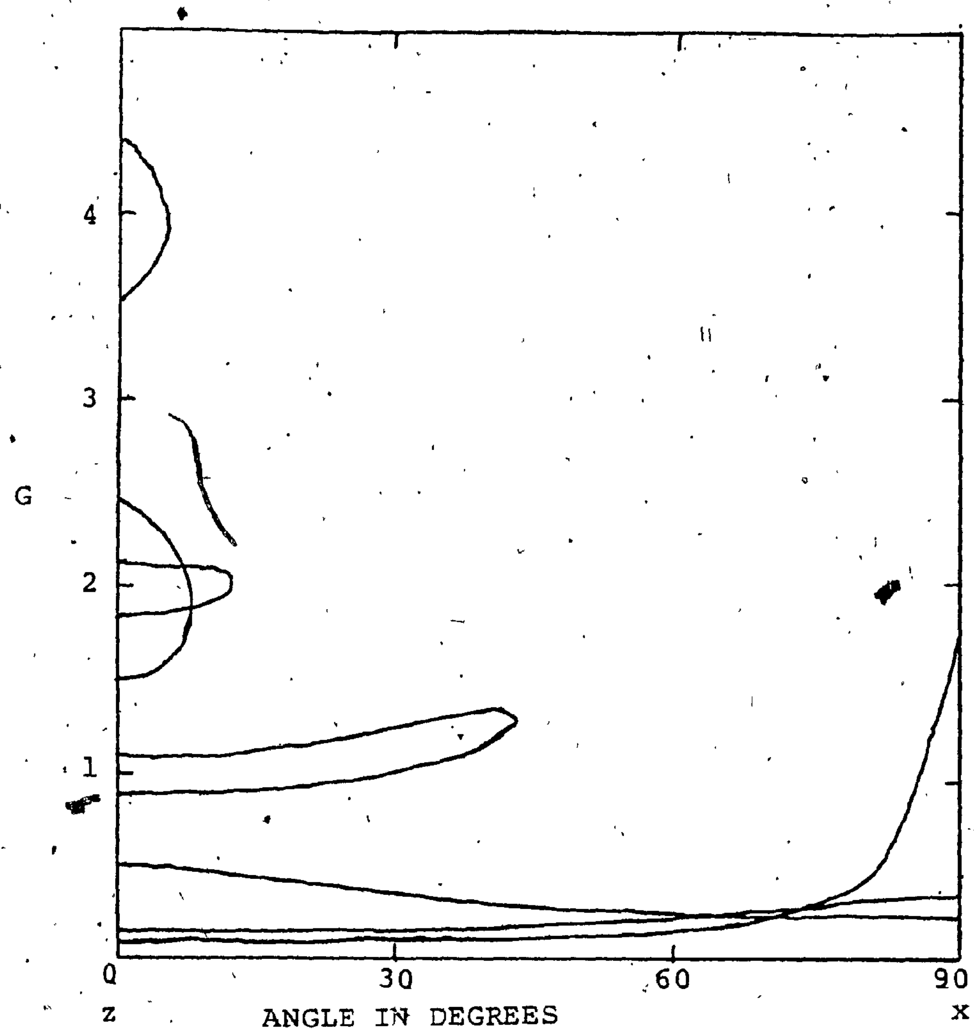

FIG. 12: Angular variation of EPR spectrum in the ZX-plane for spin S = 5/2 (W/D = .4, E/D = .1)

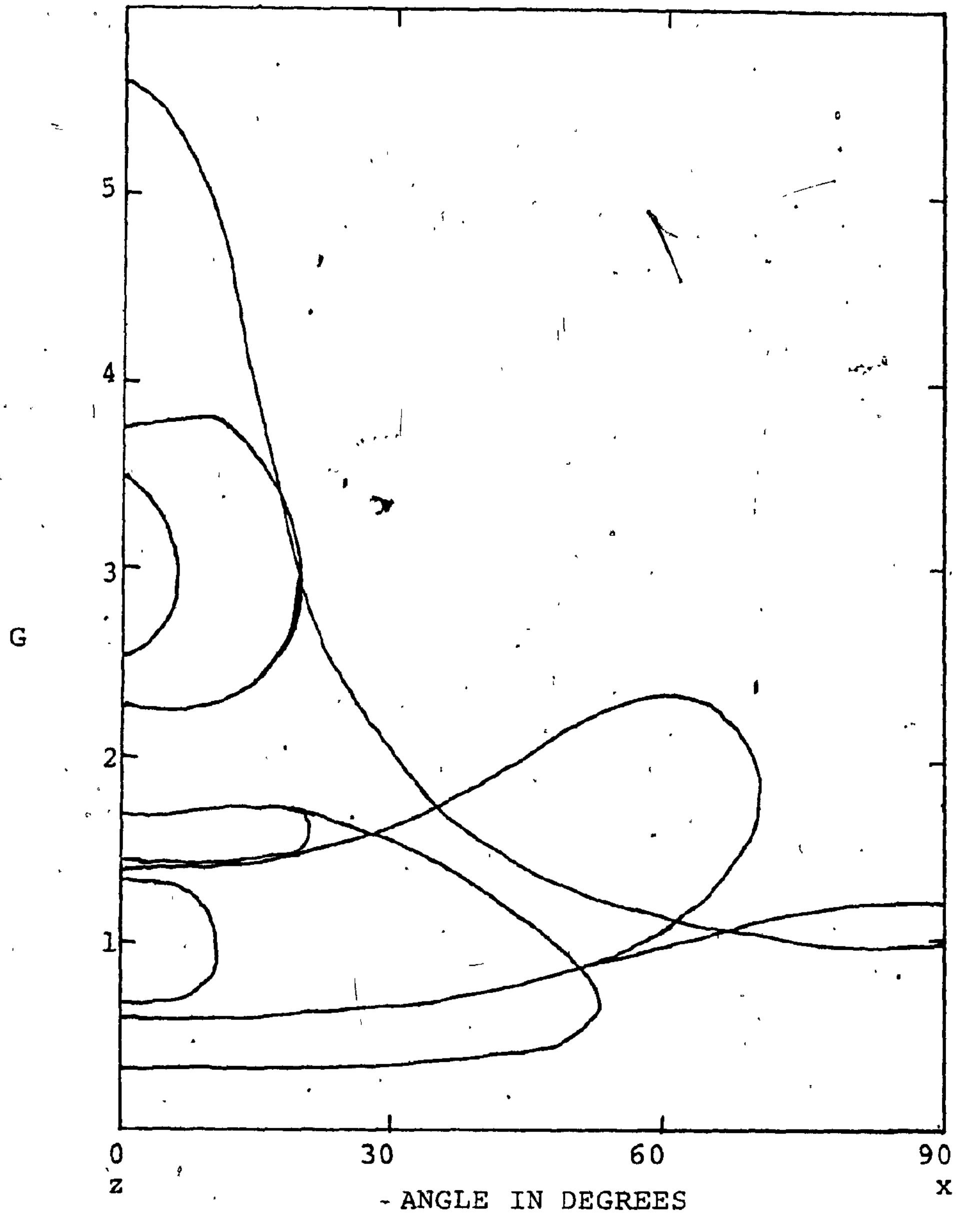

FIG. 13: Angular variation for EPR spectrum in the ZX-plane for spin S = 5/2(W/D = 1.6, E/D = .1)

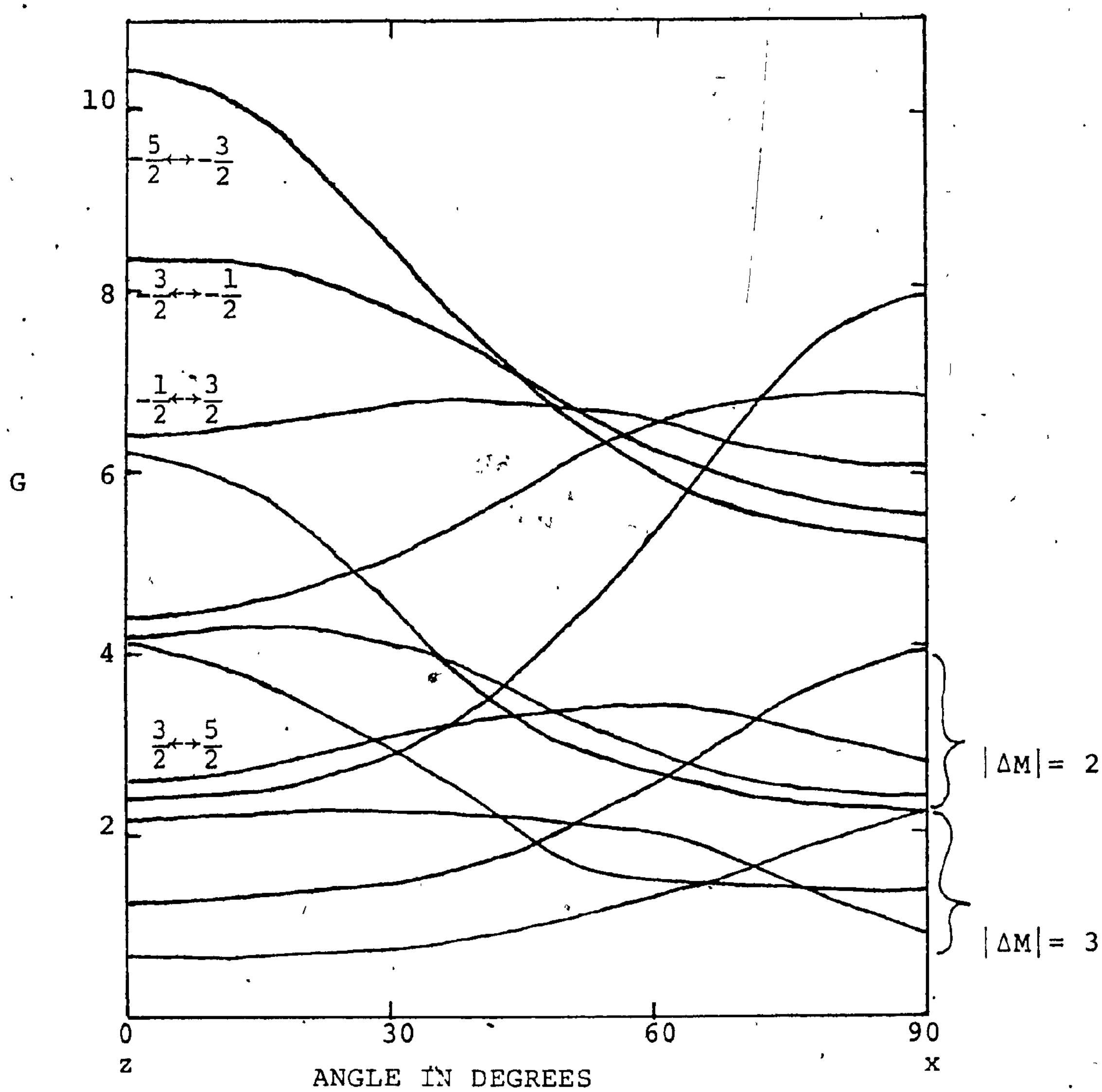

FIG. 14: Angular variation of EPR spectrum in the ZX-plane for spin $S = 5/2$ ($W/D = 6.4$, $E/D = .1$)

3. SPIN S = 7/2

The spin-Hamiltonian Matrix in the ZX-plane is:

M \ M	$\frac{7}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$	$-\frac{7}{2}$
$\frac{7}{2}$	$\frac{7}{2}C+7$	$\frac{\sqrt{7}}{2}S$	$\sqrt{21}\frac{E}{D}$	0	0	0	0	0
$\frac{5}{2}$	$\frac{\sqrt{7}}{2}S$	$\frac{5}{2}C+1$	$\sqrt{3}S$	$\sqrt{45}\frac{E}{D}$	0	0	0	0
$\frac{3}{2}$	$\sqrt{21}\frac{E}{D}$	$\sqrt{3}S$	$\frac{3}{2}C-3$	$\frac{\sqrt{15}}{2}S$	$2\sqrt{15}\frac{E}{D}$	0	0	0
$\frac{1}{2}$	0	$\sqrt{45}\frac{E}{D}$	$\frac{\sqrt{15}}{2}S$	$\frac{1}{2}C-S$	$2S$	$2\sqrt{15}\frac{E}{D}$	0	0
$-\frac{1}{2}$	0	0	$2\sqrt{15}\frac{E}{D}$	$2S$	$-\frac{1}{2}C-S$	$\frac{\sqrt{15}}{2}S$	$\sqrt{45}\frac{E}{D}$	0
$-\frac{3}{2}$	0	0	0	$2\sqrt{15}\frac{E}{D}$	$\frac{\sqrt{15}}{5}S$	$-\frac{3}{2}C-3$	$\sqrt{3}S$	$\sqrt{21}\frac{E}{D}$
$-\frac{5}{2}$	0	0	0	0	$\sqrt{45}\frac{E}{D}$	$\sqrt{3}S$	$-\frac{5}{2}C+1$	$\frac{\sqrt{7}}{2}S$
$-\frac{7}{2}$	0	0	0	0	0	$\sqrt{21}\frac{E}{D}$	$\frac{\sqrt{7}}{2}S$	$-\frac{7}{2}C+7$

where $C = \frac{g\beta H}{D}\cos\Theta$, $S = \frac{g\beta H}{D}\sin\Theta$. The resonant G values, where $G = g\beta H/D$, as a function of the angle Θ for different values of the parameters E/D and W/D, where W is the energy absorbed at resonance, are plotted on the next three pages.

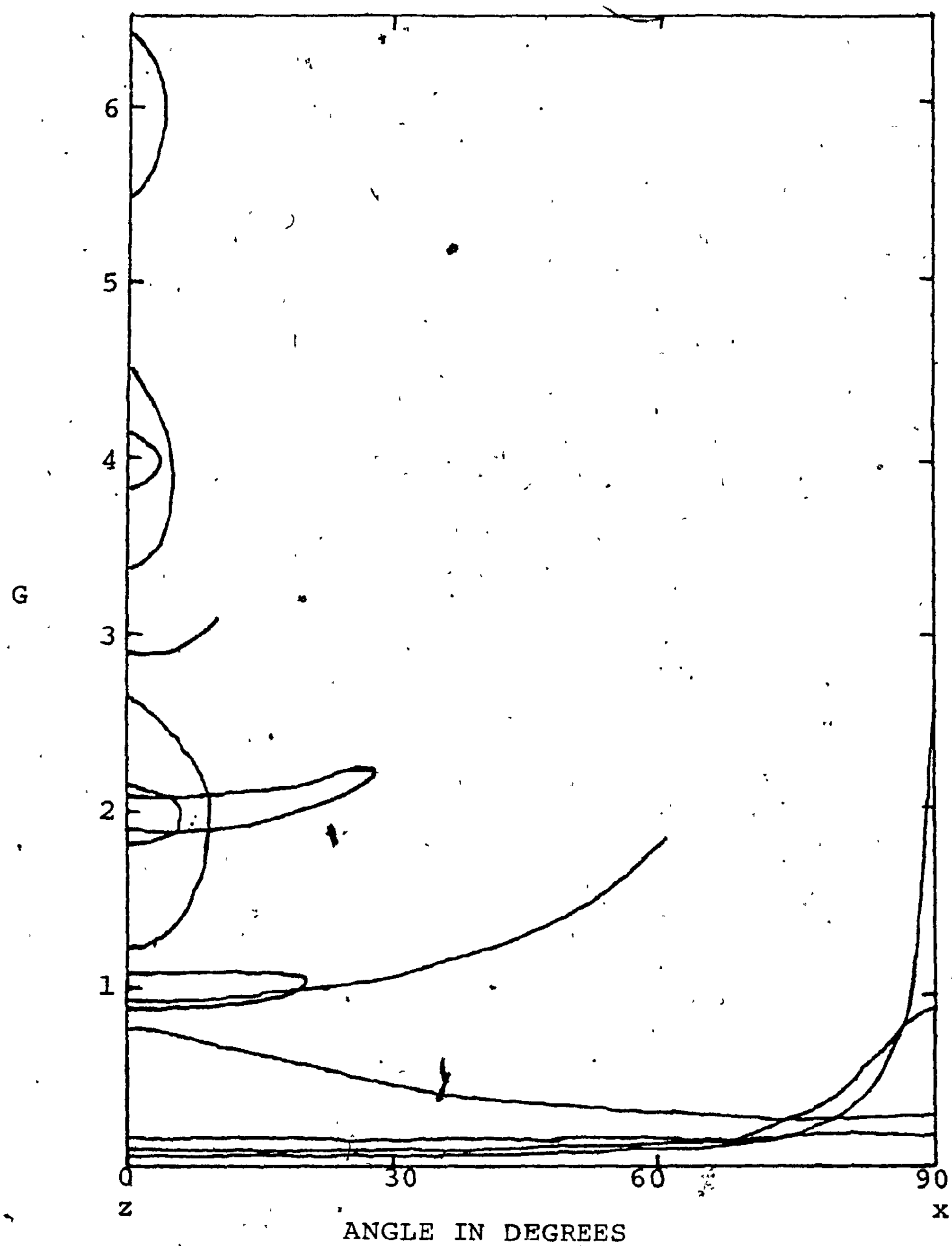

FIG. 15: Angular variation of EPR spectrum in the ZX-plane for spin S = 7/2 (W/D = .4, E/D = .1)

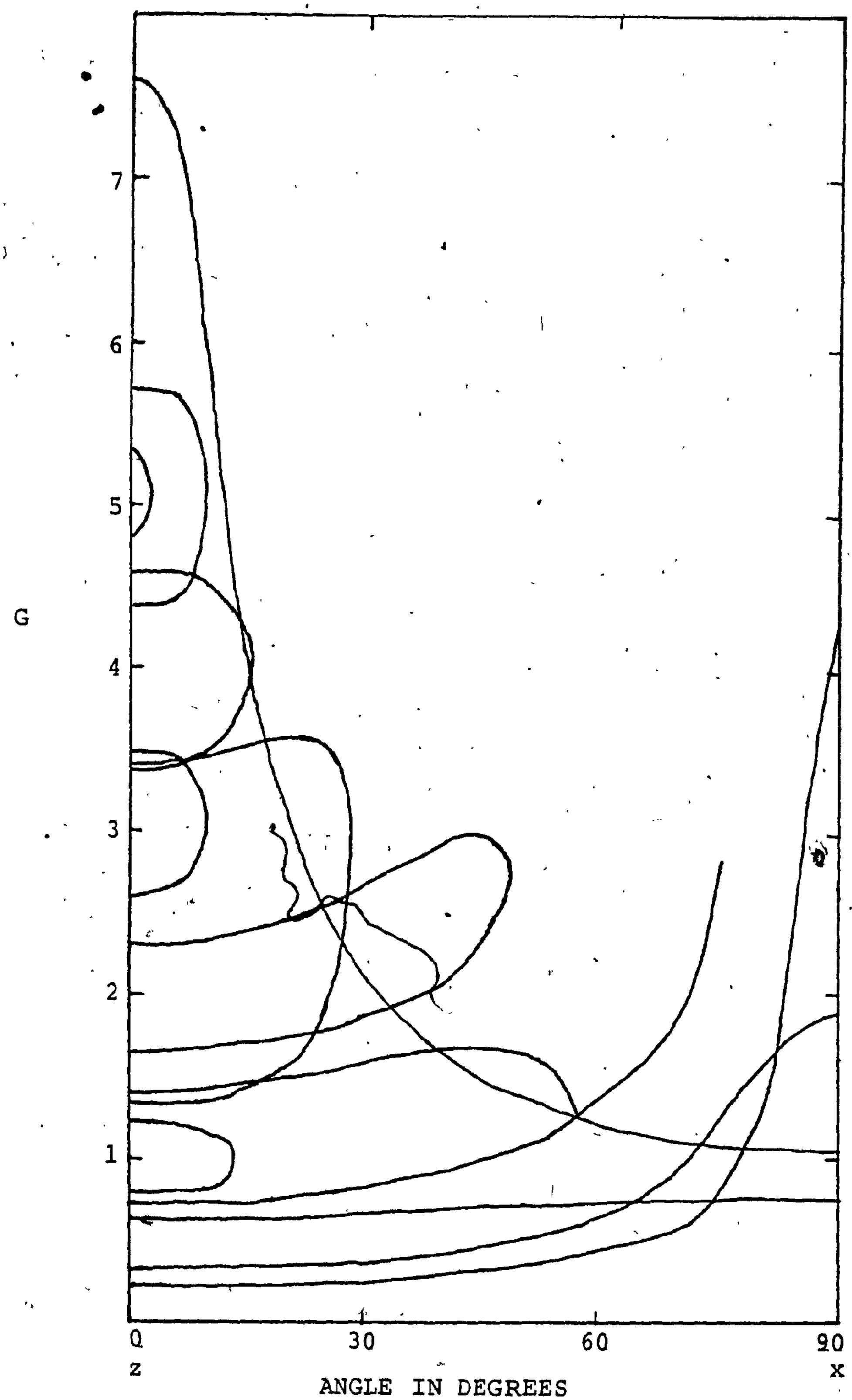

FIG. 16: Angular variation of EPR spectrum in the ZX-plane for spin S = 7/2 (W/D = 1.6, E/D = .1).

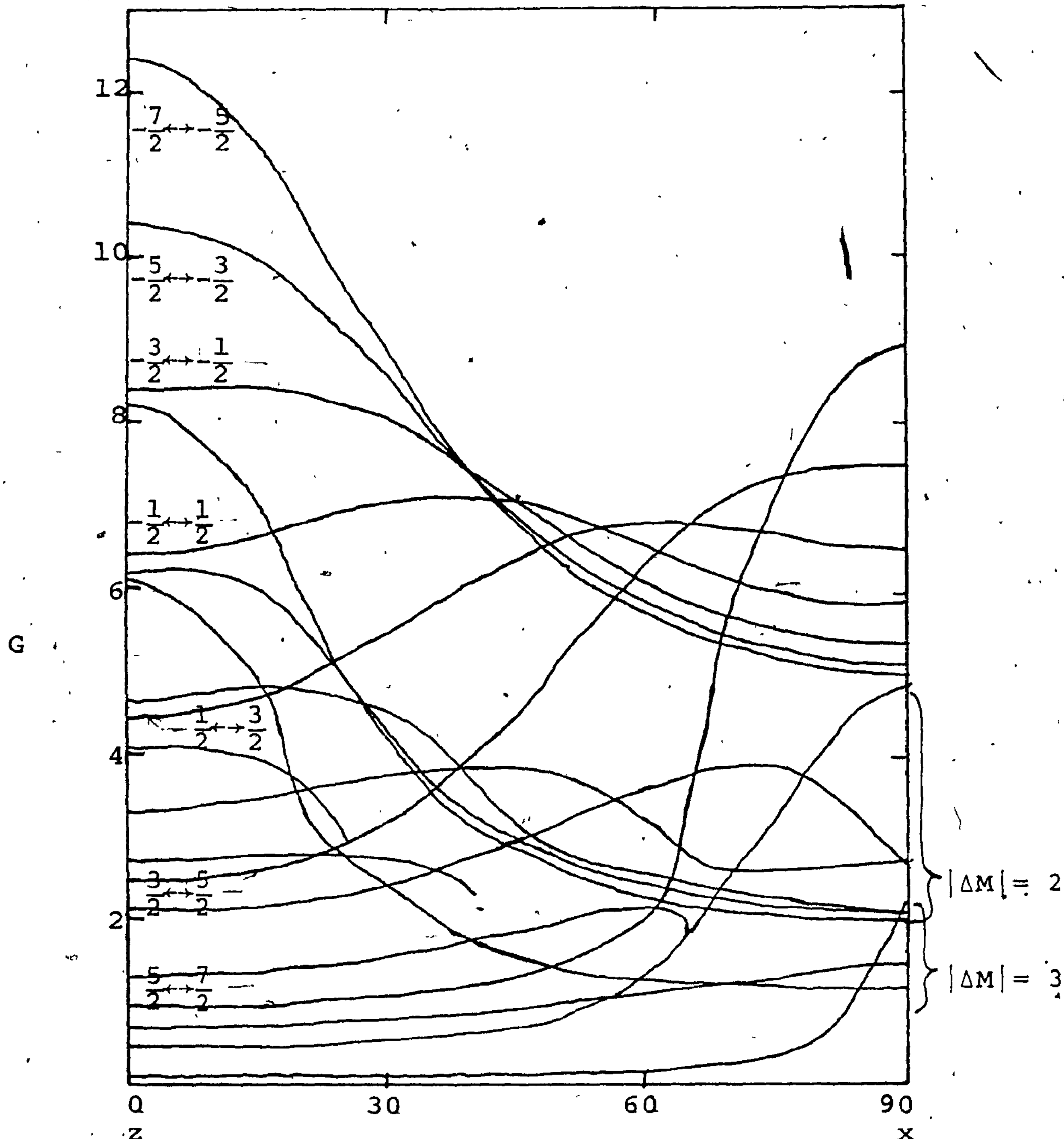

FIG. 17: Angular variation of EPR spectrum in the ZX-plane for spin S = 7/2 (W/D = 6.4, E/D = .1)

4. AGREEMENT WITH EXPERIMENT

A. MONOCLINIC SYMMETRY, SPIN S = 7/2

EPR SPECTRUM OF Gd^{3+} IN $NdCl_3 \cdot 6H_2O$

The spin-Hamiltonian for this case is[11]:

$$\mathcal{H} = \beta \vec{H} \cdot \vec{\vec{g}} \cdot \vec{S} + B_2^0 O_2^0 + B_2^2 O_2^2 + B_4^0 O_4^0 + B_4^2 O_4^2 + B_4^4 O_4^4 + B_6^0 O_6^0 + B_6^2 O_6^2 + B_6^4 O_6^4 + B_6^6 O_6^6$$

where $\vec{H}$ is the applied static magnetic field, $\vec{S}$ is the ionic spin, B_ℓ^m are constants and the $O_{2r}^{2s} (s \leq r)$ are spin operators the same as those given by Abragam and Bleany: β is the Bohr magneton, $\vec{\vec{g}}$ is the g tensor. The spin-Hamiltonian in the ZX-plane takes on the following matrix form: (See Page 42)

M \ M	$\frac{7}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$	$-\frac{7}{2}$
$\frac{7}{2}$	$7A_1+7A_2+7A_3+7/2C$	$\frac{\sqrt{7}}{2}S$	$\sqrt{21}(\frac{B_1}{3}+\frac{B_2}{2}+\frac{2}{21}B_3)$	0	$\sqrt{35}(\frac{C_1}{5}+\frac{C_2}{7})$	0	$\frac{2\sqrt{7}}{7}C_3$	0
$\frac{3}{2}$	$\frac{\sqrt{7}}{2}S$	$A_1-13A_2-5A_3+\frac{5}{2}C$	$\sqrt{3}S$	$\sqrt{5}(B_1+\frac{B_2}{10}-\frac{2}{5}B_3)$	0	$\sqrt{3}(C_1-\frac{C_2}{3})$	0	$\frac{2\sqrt{7}}{7}C_3$
$\frac{3}{2}$	$\sqrt{21}(\frac{B_1}{3}+\frac{B_2}{21}+B_3)$	$\sqrt{3}S$	$-3A_1-3A_2+9A_3+\frac{3}{2}C$	$\frac{\sqrt{15}}{2}S$	$\sqrt{15}(\frac{2}{3}B_1-\frac{2}{5}B_2+\frac{14}{105}B_3)$	0	$\sqrt{3}(C_1-\frac{C_2}{3})$	0
$\frac{1}{2}$	0	$\sqrt{5}(B_1+\frac{B_2}{10}-\frac{2}{3}B_3)$	$\frac{\sqrt{15}}{2}S$	$-5A_1+9A_2-5A_3+\frac{1}{2}C$	$2S$	$\sqrt{15}(\frac{2}{3}B_1-\frac{2}{5}B_2+\frac{14}{105}B_3)$	0	$\sqrt{35}(\frac{C_1}{5}+\frac{C_2}{7})$
$-\frac{1}{2}$	$\sqrt{35}(\frac{C_1}{5}+\frac{C_2}{7})$	0	$\sqrt{15}(\frac{2}{3}B_1-\frac{2}{5}B_2+\frac{14}{105}B_3)$	$2S$	$-5A_1+9A_2-5A_3-\frac{1}{2}C$	$\frac{\sqrt{15}}{2}S$	$\sqrt{5}(B_1+\frac{B_2}{10}-\frac{2}{5}B_3)$	0
$-\frac{3}{2}$	0	$\sqrt{3}(C_1-\frac{C_2}{5})$	0	$\sqrt{15}(\frac{2}{3}B_1-\frac{2}{5}B_2+\frac{14}{105}B_3)$	$\frac{\sqrt{15}}{2}S$	$-3A_1-3A_2+9A_3-\frac{3}{2}C$	$\sqrt{3}S$	$\sqrt{21}(\frac{B_1}{3}+\frac{B_2}{2}+\frac{2}{21}B_3)$
$-\frac{5}{2}$	$\frac{2\sqrt{7}}{7}C_3$	0	$\sqrt{3}(C_1-\frac{C_2}{3})$	0	$\sqrt{5}(B_1+\frac{B_2}{10}-\frac{2}{5}B_3)$	$\sqrt{3}S$	$A_1-13A_2-5A_3-\frac{5}{2}C$	$\frac{\sqrt{7}}{2}S$
$-\frac{7}{2}$	0	$\frac{2\sqrt{7}}{7}C_3$	0	$\sqrt{35}(\frac{C_1}{5}+\frac{C_2}{7})$	0	$\sqrt{21}(\frac{B_1}{3}+\frac{B_2}{2}+\frac{2}{21}B_3)$	$\frac{\sqrt{7}}{2}S$	$7A_1+7A_2+A_3-7/2C$

where $C = g_{zz}\beta H\cos\Theta$, $S = g_{xx}\beta H\sin\Theta$, $g_{zz} = 1.992$, $g_x = 1.993$, $A_1 = 3B_2^0 = 1.857$, $A_2 = 60B_4^0 = -.032$, $A_3 = 1260B_6^0 = .000$, $B_1 = 3B_2^0 = -1.058$, $B_2 = 60B_4^2 = .006$, $B_3 = 1260B_6^2 = .001$, $C_1 = 60B_4^4 = -.024$, $C_2 = 1260B_6^4 = -.029$, $C_3 = 1260B_0^0 = -.023$. These values of the constants have been taken from Reference 11 at room temperature. The units are GHz. The results for the $\Delta M = \pm 1$ transitions, i.e. the resonant magnetic field values as a function of Θ, in the ZX-plane and in the ZY-plane are plotted on pages 45-47.

The Hamiltonian matrix in the ZY-plane has been obtained by transforming the $O_{2r}^{2s}(s\leq r)$ operators on rotation of the Z-axis into the perpendicular plane xy so that the ZX-plane becomes the same with the Z'Y'. Y' is parallel to Z[12]. The operators O_{2r}^{2s} transform[12] as follows:

$$O_2^0 \rightarrow -\frac{1}{2}O_2^0 - \frac{3}{2}O_2^2$$

$$O_2^2 \rightarrow \frac{1}{2}O_2^0 - \frac{1}{2}O_2^2$$

$$O_4^0 \rightarrow \frac{3}{8}O_4^0 + \frac{5}{2}O_4^2 + \frac{35}{8}O_4^4$$

$$O_4^2 \rightarrow -\frac{1}{8}O_4^0 - \frac{1}{2}O_4^2 + \frac{7}{8}O_4^4$$

$$O_4^4 \rightarrow \frac{1}{8}O_4^0 - \frac{1}{2}O_4^2 + \frac{1}{8}O_4^4$$

$$O_6^0 \rightarrow -\frac{5}{16}O_6^0 - \frac{105}{32}O_6^2 - \frac{63}{16}O_6^4 - \frac{231}{32}O_6^6$$

$$O_6^2 \rightarrow \frac{1}{16}O_6^0 + \frac{17}{32}O_6^2 + \frac{3}{16}O_6^4 - \frac{33}{32}O_6^6$$

$$O_6^4 \rightarrow -\frac{1}{16} O_6^0 - \frac{5}{32} O_6^2 + \frac{13}{16} O_6^4 - \frac{11}{32} O_6^6$$

$$O_6^6 \rightarrow \frac{1}{16} O_6^0 - \frac{15}{32} O_3^2 + \frac{3}{16} O_6^4 - \frac{1}{32} O_6^6$$

Comparison with the results reported by Misra[11] shows excellent agreement.

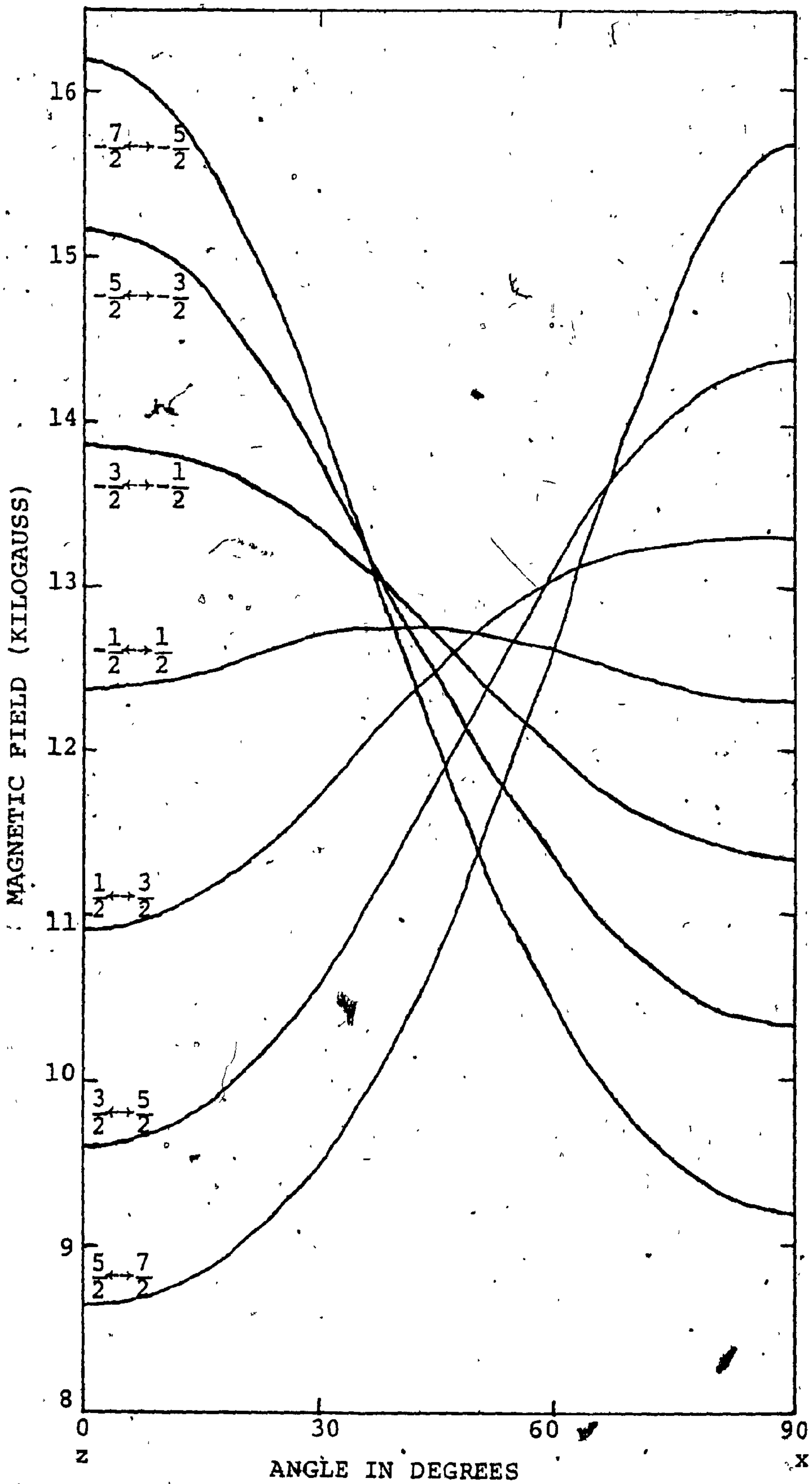

FIG. 18: Angular variation of EPR spectrum in the ZX-plane for Gd^{3+} in $NdCl_3.6H_2O$ at room temperature (ν=34.55GHz)

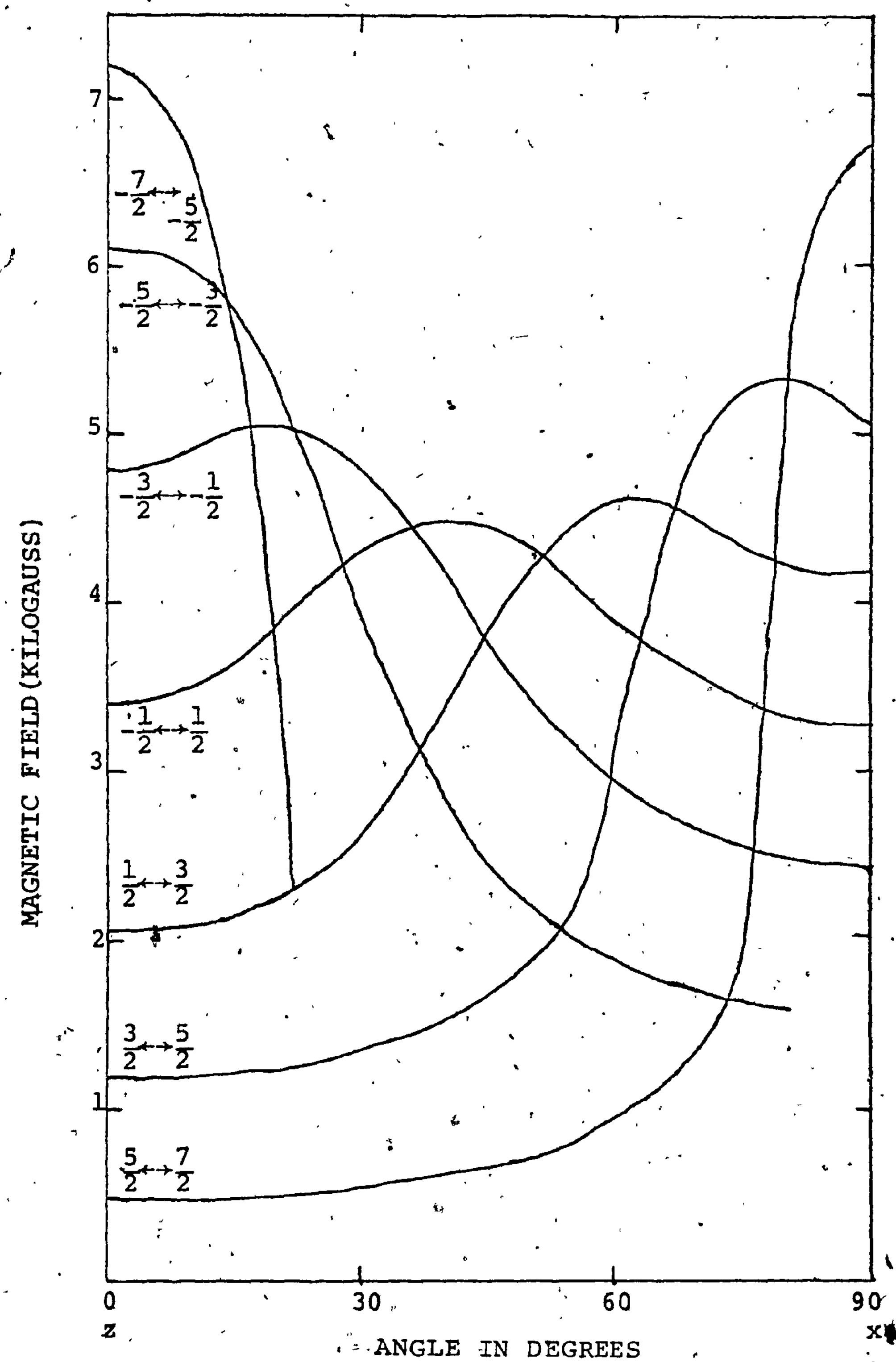

FIG. 19: Angular variation of EPR spectrum in the ZX-plane for Gd^{3+} in $NdCl_3.6H_2O$ at room temperature (ν = 9.43GHz)

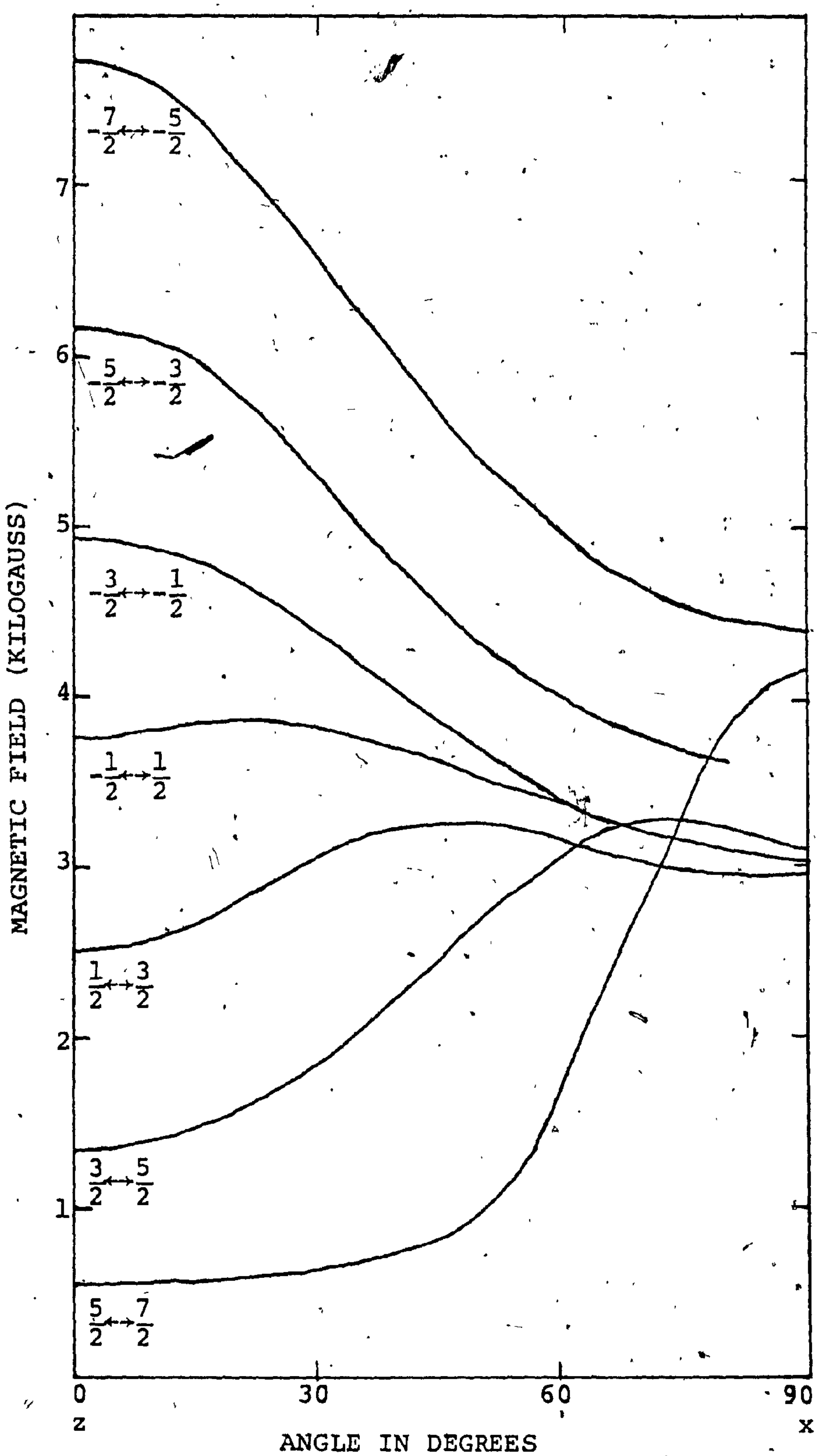

FIG. 20: Angular variation of EPR spectrum in the ZY-plane at room temperature ($\nu = 10.37$ GHz) for Gd^{3+} in $NdC\ell_3 . 6H_2O$.

B. C_{3u} SYMMETRY, SPIN S = 5/2

EPR SPECTRUM OF Fe^{3+} SUBSTITUTED FOR Al^{3+} IN $C(NH_2)_3Al(SO_4)_2 \cdot 6H_2O$.

The spin-Hamiltonian is[13]:

$$\mathcal{H} = \beta\vec{H}.\vec{\vec{g}}.\vec{S} + B_2^0O_2^0 + B_4^0O_4^0 + B_4^3O_4^3 + B_4^{-3}O_4^{-3}$$

where β is the Bohr magneton, $\vec{\vec{g}}$ is the g-factor, $\vec{H}$ is the applied magnetic field, $\vec{S}$ is the ionic spin and the O_ℓ^m are operator equivalents as described by Abragam and Bleany[1]. In the ZX-plane the spin-Hamiltonian takes on the following matrix form:

M \ M	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
$\frac{5}{2}$	$\frac{10}{3}A_1+A_2+\frac{5}{2}C$	$\frac{\sqrt{5}}{2}S$	0	$\frac{\sqrt{10}}{20}(A_3-iAy)$	0	0
$\frac{3}{2}$	$\frac{\sqrt{5}}{2}S$	$-\frac{2}{3}A_1-3A_2+\frac{3}{2}C$	$\sqrt{2}\ S$	0	0	0
$\frac{1}{2}$	0	$\sqrt{2}\ S$	$-\frac{8}{3}A_1+2A_2+\frac{1}{C}$	$\frac{3}{2}S$	0	$-\frac{\sqrt{10}}{20}(A_3-iAy)$
$-\frac{1}{2}$	$\frac{\sqrt{10}}{20}(A_3+iAy)$	0	$\frac{3}{2}S$	$-8A_1+2A_2-\frac{1}{2}C$	$\sqrt{2}\ S$	0
$-\frac{3}{2}$	0	0	0	$\sqrt{2}\ S$	$-2A_1-3A_3-\frac{3}{2}C$	$\frac{\sqrt{5}}{2}S$
$-\frac{5}{2}$	0	0	$-\frac{\sqrt{10}}{20}(A_3+iAy)$	0	$\frac{\sqrt{5}}{2}S$	$\frac{10}{3}A_1+A_2-\frac{5}{2}C$

where $C = g_{zz}\beta H\cos\Theta$, $S = g_{xx}\beta H\sin\Theta$, $g_{zz} = 2.001$, $g_{xx} = 2.004$, $A_1 = -8.622$, $A_2 = .181$, $A_3 = .531$, $A_y = 2.712$. The units of the constants A_i are GHz and they are taken from reference 13. The results are exactly the same as those reported by Misra[13]. They are plotted as a function of Θ on the next page.

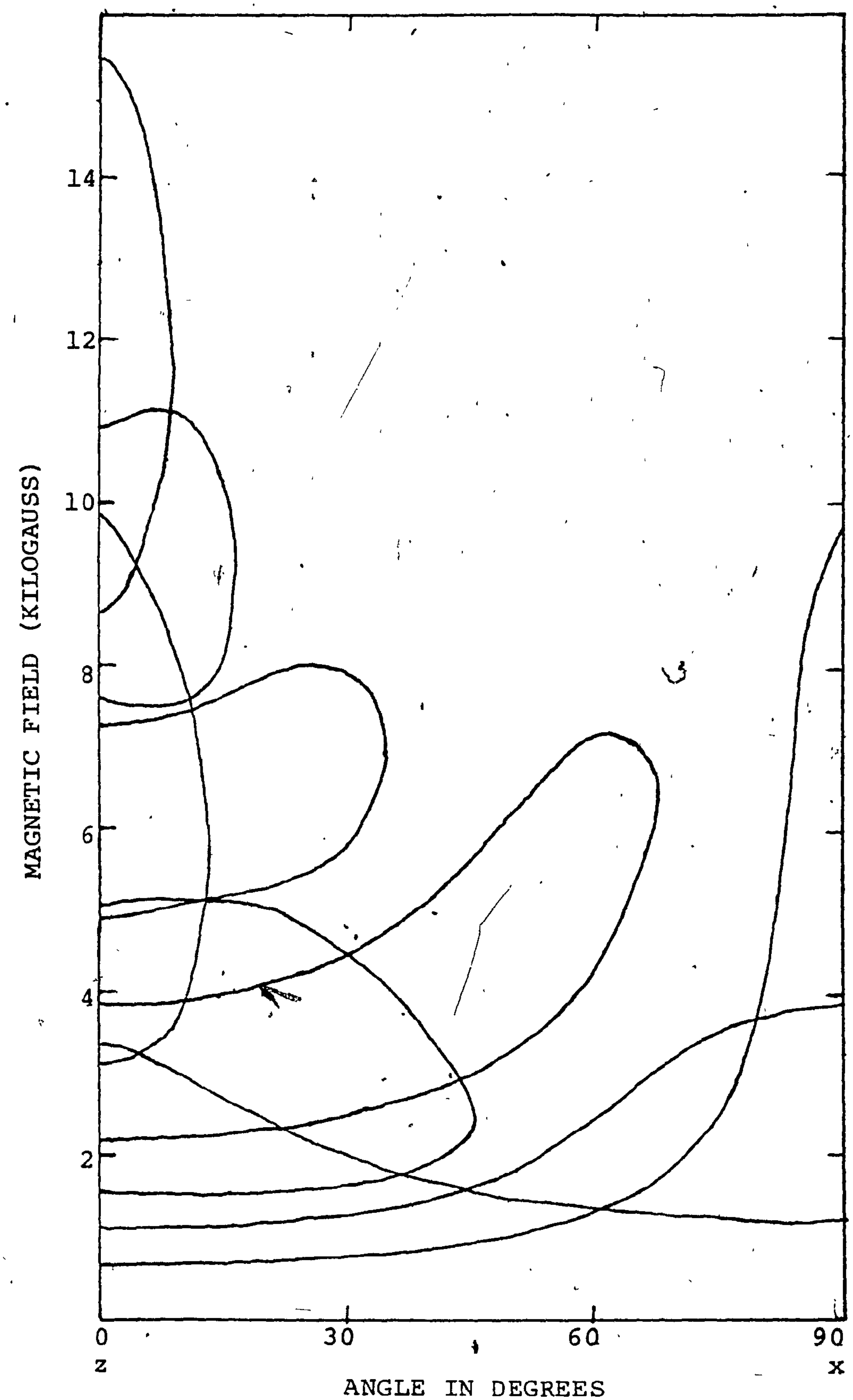

FIG. 21: Angular variation of EPR spectrum for Fe^{3+} in GASH in the ZX-plane at room temperature (ν = 9.40GHz)

CHAPTER VIII

EPR SPECTRUM INCLUDING HYPERFINE INTERACTION

In this chapter we consider the interaction of two spins, the electronic spin S and the nuclear spin I, with an external magnetic field and with each other. We apply the LSF method to obtain the angular variation of the spectrum.

1. S = I = 1/2.

The spin-Hamiltonian, neglecting the nuclear Zeeman interaction, is given by:

$$\mathcal{H} = \beta\vec{H}.\vec{\vec{g}}.\vec{S} + \vec{S}.\vec{\vec{A}}.\vec{I}$$

where β is the Bohr magneton, $\vec{H}$ is the static magnetic field, $\vec{\vec{g}}$ is the g tensor and $\vec{\vec{A}}$ the hyperfine splitting tensor. To obtain the matrix form of $\mathcal{H}$ we use the direct product expansion of matrices. In the ZX-plane, with Θ being the angle between the Z-axis and the magnetic field, $\mathcal{H}$ takes on the following matrix form:

M,m \ M,m	$\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$	$-\frac{1}{2}, \frac{1}{2}$	$-\frac{1}{2}, -\frac{1}{2}$
$\frac{1}{2}, \frac{1}{2}$	$\frac{K_1}{2} + \frac{A_z}{4}$	0	$\frac{K_2}{2}$	$A_x - A_y$
$\frac{1}{2}, -\frac{1}{2}$	0	$\frac{K_1}{2} - \frac{A_z}{4}$	$A_x + A_y$	$\frac{K_2}{2}$
$-\frac{1}{2}, \frac{1}{2}$	$\frac{K_2}{2}$	$A_x + A_y$	$-\frac{K_1}{2} - \frac{A_z}{4}$	0
$-\frac{1}{2}, -\frac{1}{2}$	$A_x - A_y$	$\frac{K_2}{2}$	0	$-\frac{K_1}{2} + \frac{A_z}{4}$

where $K_1 = g_z\beta H \cos\Theta$, $K_2 = g_x\beta H \sin\Theta$ and g_z, g_x, A_x, A_y, A_z are the principal values of the g and A tensors respectively. We consider the following four cases:

1) $g_z=g_x=2$ $A_x=A_y=A_z=1.42GH_z$ (isotropic g, isotropic A)

2) $g_z=2, g_x=1.95$ $A_x=A_y=A_2=1.42GH_z$ (anisotropic g, isotropic A)

3) $g_z=2, g_x=1.95$ $A_x=A_y=.71GH_z, A_2=1.42GH_z$ (anisotropic g; anisotropic A)

4) $g_z=g_x=2$ $A_x=A_y=.71GH_z, A_2=1.42GH_z$ (isotropic g, anisotropic A).

The results, i.e. the resonant magnetic field values as a function of Θ, for the strong transitions $\Delta M = \pm 1$, $\Delta m = 0$, are plotted on the next two pages. M and m are the electronic and nuclear magnetic quantum numbers respectively.

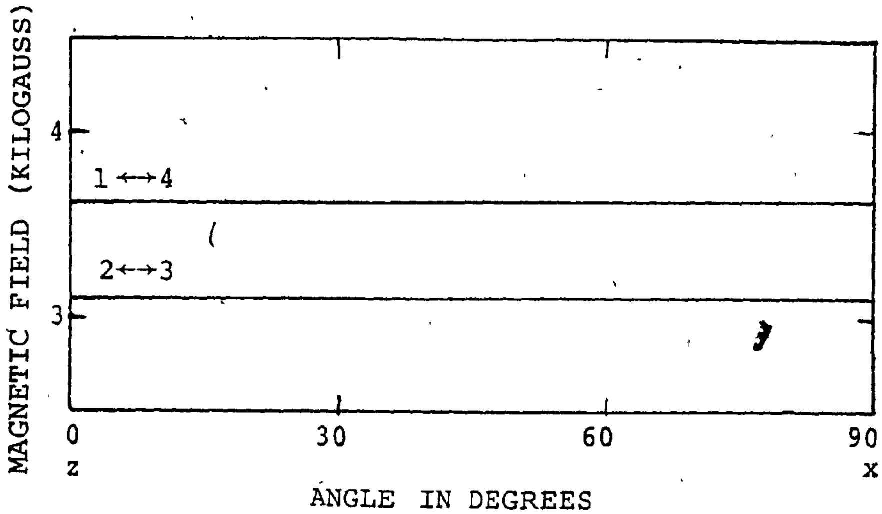

FIG. 22: Angular variation of EPR spectrum in the ZX-plane for spin S = 1/2, I = 1/2. g and A are isotropic.

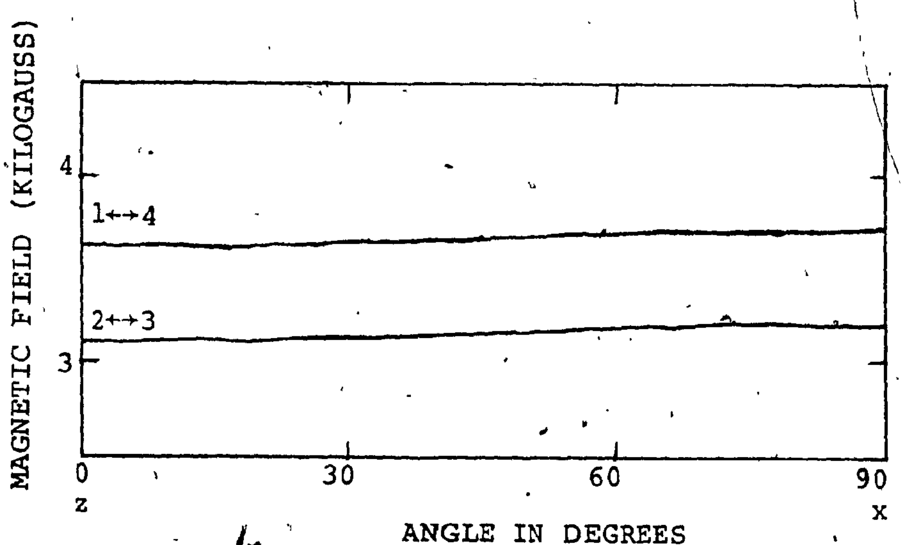

FIG. 23: Angular variation of EPR spectrum in the ZX-plane for spin S = 1/2, I = 1/2. g is anisotropic, A is isotropic.

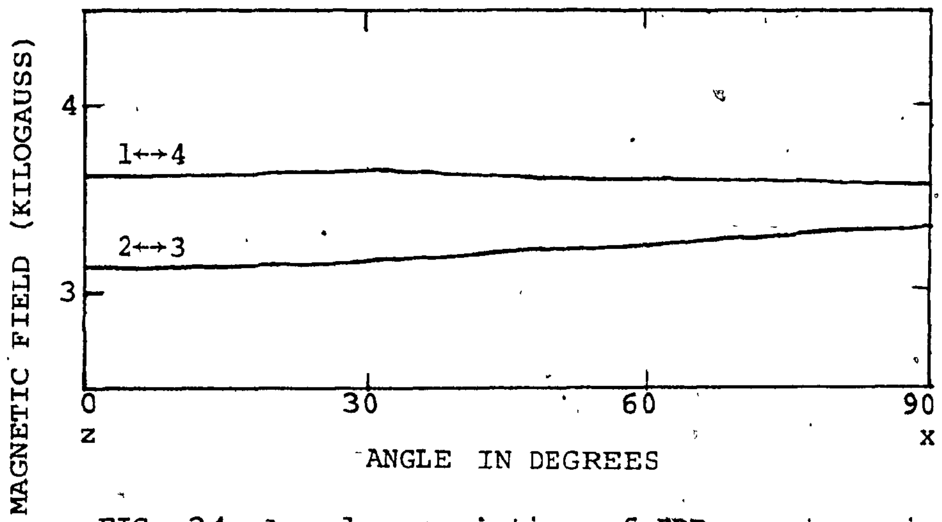

FIG. 24: Angular variation of EPR spectrum in the ZX-plane for spins S = 1/2, I = 1/2. g and A are anisotropic.

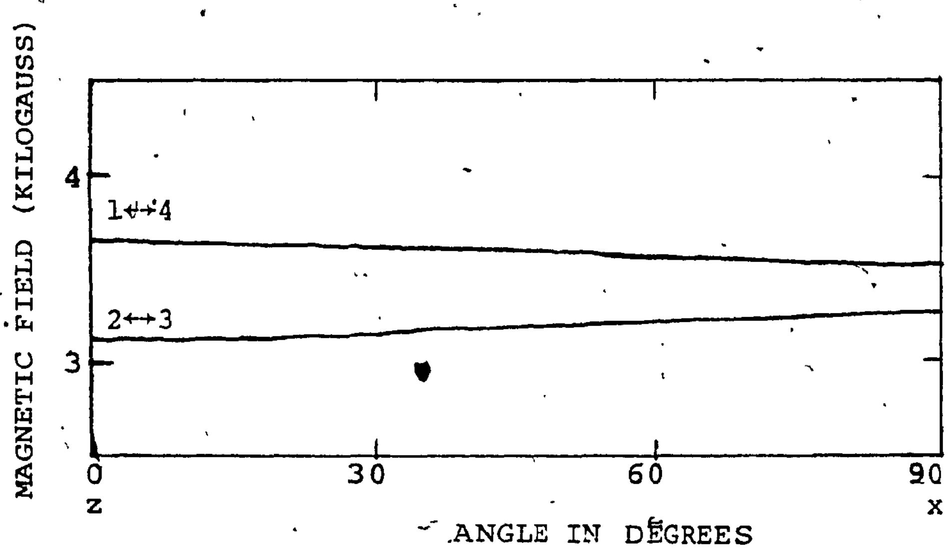

FIG. 25: Angular variation of EPR spectrum in the ZX-plane for spins S = 1/2, I = 1/2. g is isotropic, A is anisotropic.

2. $S = I = 1$

The spin-Hamiltonian is:

$$\mathcal{H} = \beta\vec{H}.\vec{\vec{g}}.\vec{S} + D(S_z^2 - \tfrac{1}{3}S(S+1)) + E(S_x^2 - S_y^2) + \vec{S}.\vec{\vec{A}}.\vec{I}$$

where $\vec{H}, \vec{\vec{g}}, \vec{\vec{A}}$ are the static magnetic field, the g tensor and the hyperfine tensor respectively. D and E are the zero field splitting constants. We neglect again the nuclear Zeeman interaction.

Using the direct product expansion of matrices we find that in the ZX-plane $\mathcal{H}$ takes on the following matrix form:

M,m \ M,m	1,1	1,0	1,-1	0,1	0,0	0,-1	-1,-1	-1,0	-1;-1
1,1	$K_1+\frac{D}{3}+A$	0	0	K_2	0	0	E	0	0
1,0	0	$K_1+\frac{D}{3}$	0	A	K_2	0	0	E	0
1,-1	0	0	$K_1+\frac{D}{3}-A$		A	K_2	0	0	E
0,1	K_2	A	0	$-\frac{2}{3}D$	0	0	K_2	0	0
0,0	0	K_2	A	0	$-\frac{2}{3}D$	0	A	K_2	0
0,-1	0	0	K_2	0	0	$-\frac{2}{3}D$	0	A	K_2
-1,1	E	0	0	K_2	A		$-K_1+\frac{D}{3}-A$	0	0
-1,0	0	E	0	0	K_2	A	0	$-K_2+\frac{D}{3}$	0
-1,-1	0	0	E	0	0	K_2	0	0	$-K_1+\frac{D}{3}+A$

where $K_1 = g_z \beta H \cos\theta$, $K_2 = \frac{\sqrt{2}}{2} g_x \beta H \sin\theta$, $g_z = 2$, $g_x = 1.993$,

$A = A_x = A_y = A_z = -.27$GHz, $D = -.78$GHz, $E = .093$GHz.

The results, i.e. the resonant magnetic field values as a function of θ, for the strong transitions $\Delta M = \pm 1$, $\Delta m = 0$, are plotted on the next page.

3. $S = I = 5/2$

EPR SPECTRUM OF Mn^{2+} IN $Ni(CH_3COO)_2 \cdot 4H_2O$

The spin-Hamiltonian in the ZX-plane is[14]:

$$\mathcal{H} = \beta g_z H_z S_z + \beta g_x H_x S_x + D[S_z^2 - \frac{1}{3} S(S+1)] + E(S_x^2 - S_y^2)$$

$$+ AS_z I_z + B(S_x I_x + S_y I_y)$$

where the values of the constants are [14]:

$g_z = 1.996$, $D = 1.29067$ GHz, $E = .25$GHz and $A = -B = -.25142$GHz.

The value of the energy absorbed at resonance is 9.5GHz. For g_x we used the value 1.996.

The spin-Hamiltonian matrix is again obtained using the direct product expansion of the known matrices $S_x, S_y, S_z, I_x, I_y, I_z$ (see Appendix II). The results, i.e. the resonant magnetic field values as a function of θ, for the strong transitions $\Delta M = \pm 1$, $\Delta m = 0$, where M and m are the electronic and nuclear magnetic quantum numbers respectively, are plotted on page 58. (To obtain agreement with the experimental results as obtained by Misra et al[20], it was necessary to use a negative sign for E, rather than a positive sign as given by Janakiraman et al[14].).

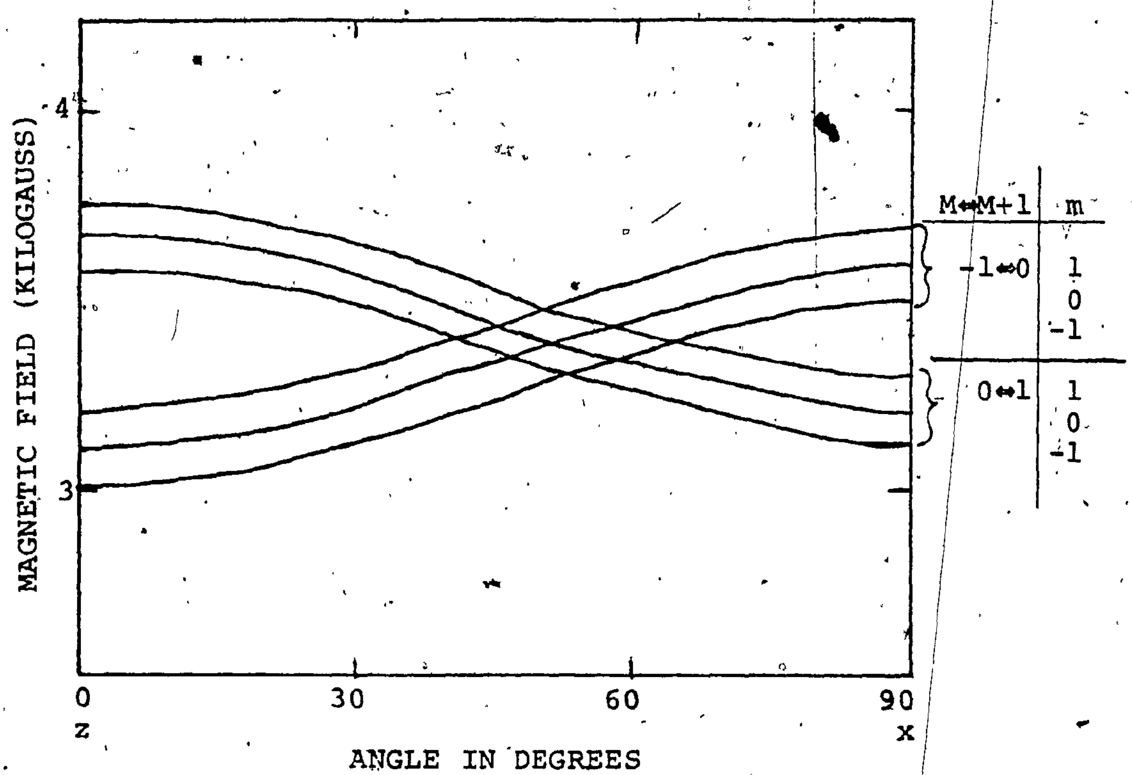

FIG. 26: Angular variation of EPR spectrum in the ZX-plane for spins S = I = 1 (ν = 9.5GHz)

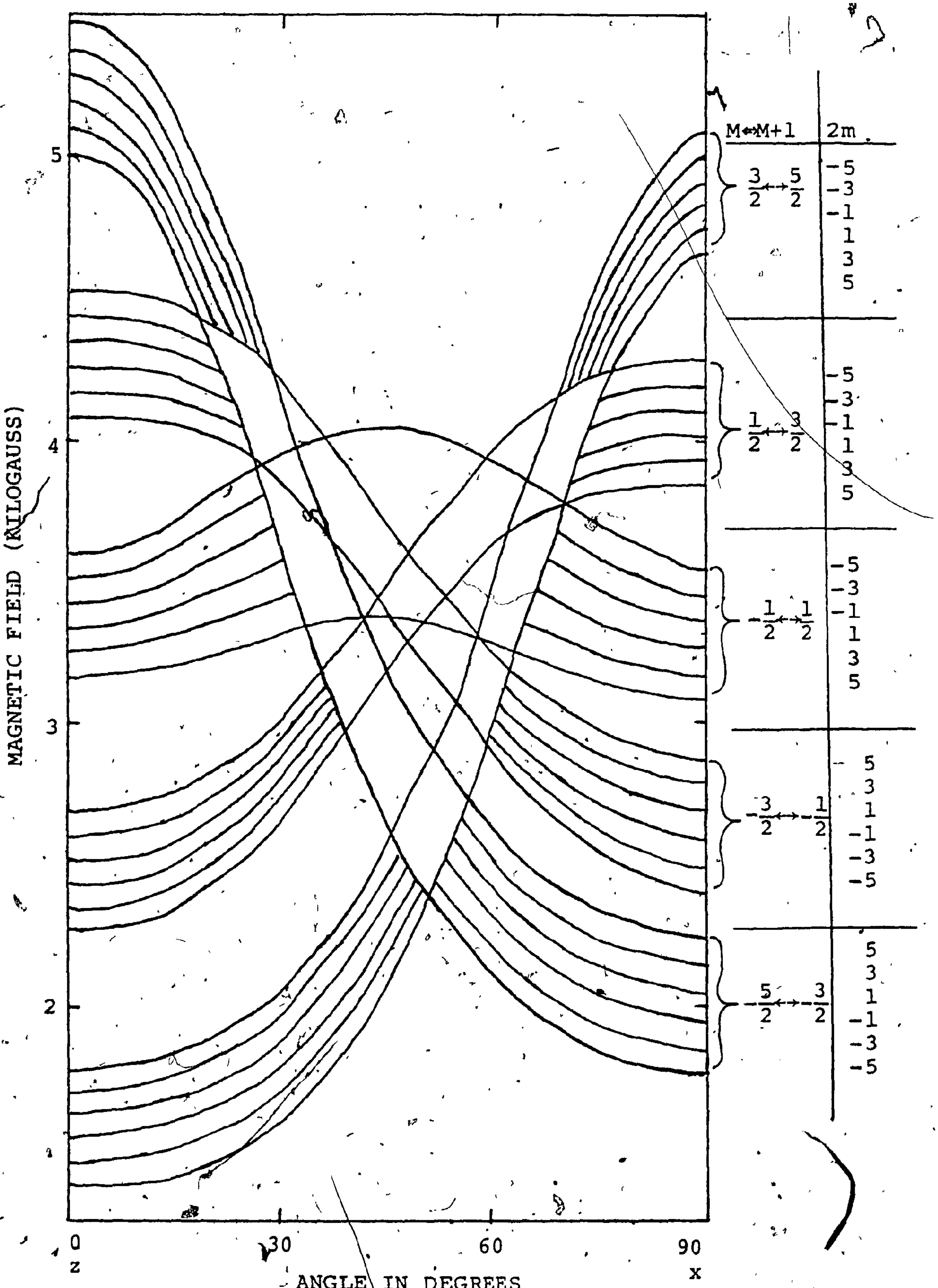

FIG. 27: Angular variation of EPR spectrum of Mn^{2+} in $Ni(CH_3COO)_2 \cdot 4H_2O$ at room temperature (ν = 9.5GHz) in the ZX-plane.

CHAPTER IX

DISCUSSION

In this chapter the problems encountered in applying the LSF procedure are discussed.

The problem of finding the initial resonant field values, when the applied magnetic field is parallel to the Z-axis, can be easily solved by using computer techniques in case they are not available from experiment. An exact computer diagonalization of the spin-Hamiltonian matrix is used. The computer program, i.e. the appropriate SUBROUTINE, which was available to us from the Computer Center of Concordia University, gives the energy eigenvalues of the spin-Hamiltonian matrix. This being done, the computer is programmed to solve the equations describing the transitions between different energy eigenvalues. The only variable in these equations is the applied magnetic field. This is exactly the graphical method of Chapter II.

The second problem, not encountered by us, was the appearance of transitions for intermediate angles Θ, between the Z-axis and the applied magnetic field not present at $\Theta = 0^0$. The situation has not been discussed previously. An examination of the results as given by the LSF procedure presented here in conjunction with those given by the graphical method, at selected intermediate angles, helps to solve the problem.

The third problem, which we faced in the case of C_{3u} symmetry and $S = 5/2$, was the following: for $\Theta = 0^{\circ}$ a transition takes place between, say, the E_1 and E_2 energy levels and between the E_1 and E_3 energy levels for an intermediate angle. This means that the transition equation is altered. This can be overcome by programming the computer appropriately since the transition energy is kept constant (see computer programs).

CHAPTER X

CONCLUSION

From the work reported in this thesis, it can be said with certainty that the problem of determining the angular variation of EPR spectra can be solved if one uses the LSF method, for all symmetries and spin values no matter what the size of the applied magnetic field or the off-diagonal elements are. No approximation methods, like perturbation theory, or series expansion, or transformations of the spin-Hamiltonian are required.

Furthermore, the method presented here is capable of taking into account the anisotropic g-factor and parameters of any size (corresponding to diagonal or off-diagonal spin-Hamiltonian matrix elements).

APPENDIX D

SPIN MATRICES FOR DIFFERENT SPIN VALUES

$S = 1$

$$S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad S_x = \frac{1}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

$$S_y = \frac{i}{2}\begin{pmatrix} 0 & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

$S = 3/2$

$$S_z = \frac{1}{2}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix} \quad S_x = \frac{1}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

$$S_y = \frac{i}{2}\begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

$S = 2$

$$S_z = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix} \qquad S_x = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \sqrt{3/2} & 0 & 0 \\ 0 & \sqrt{3/2} & 0 & \sqrt{3/2} & 0 \\ 0 & 0 & \sqrt{3/2} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$S_y = i \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & -\sqrt{3/2} & 0 & 0 \\ 0 & \sqrt{3/2} & 0 & -\sqrt{3/2} & 0 \\ 0 & 0 & \sqrt{3/2} & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$S = 5/2$

$$S_z = \begin{pmatrix} 5/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -3/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -5/2 \end{pmatrix}$$

$$S = 5/2$$

$$S_x = \begin{pmatrix} 0 & \sqrt{5/2} & 0 & 0 & 0 & 0 \\ \sqrt{5/2} & 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 3/2 & 0 & 0 \\ 0 & 0 & 3/2 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & \sqrt{5/2} \\ 0 & 0 & 0 & 0 & \sqrt{5/2} & 0 \end{pmatrix}$$

$$S_y = i \begin{pmatrix} 0 & -\sqrt{5/2} & 0 & 0 & 0 & 0 \\ \sqrt{5/2} & 0 & -\sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & -3/2 & 0 & 0 \\ 0 & 0 & 3/2 & 0 & -\sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & -\sqrt{5/2} \\ 0 & 0 & 0 & 0 & \sqrt{5/2} & 0 \end{pmatrix}$$

$$S = 7/2$$

$$S_z = \begin{pmatrix} 7/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -3/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -5/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -7/2 \end{pmatrix}$$

$S = 7/2$

$$S_x = \begin{pmatrix} 0 & \sqrt{7}/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{7}/2 & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & \sqrt{15}/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{15}/2 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & \sqrt{15}/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{15}/2 & 0 & \sqrt{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{3} & 0 & \sqrt{7}/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{7}/2 & 0 \end{pmatrix}$$

$$S_y = i \begin{pmatrix} 0 & -\sqrt{7}/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{7}/2 & 0 & -\sqrt{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & -\sqrt{15}/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{15}/2 & 0 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & -\sqrt{15}/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{15}/2 & 0 & -\sqrt{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{3} & 0 & -\sqrt{7}/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{7}/2 & 0 \end{pmatrix}$$

APPENDIX II

DIRECT PRODUCT EXPANSION OF MATRICES

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \times \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} Aa & Ab & Ba & Bb \\ Ac & Ad & Bc & Bd \\ Ca & Cb & Da & Db \\ Cc & Cd & Dc & Dd \end{pmatrix}$$

APPENDIX III

COMPUTER PROGRAMS USED FOR THE CALCULATIONS

```
      PROGRAM TAKIS1(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION R1(201,20),R2(201,20),R3(201,20),K4(300)
      WD=6.4
      ED=.1
      DO 15 I=1,19
      AI=5.*FLOAT(I-1)

      THETA=AI*3.14159264/180.
      SN=SIN(THETA)
      CN=COS(THETA)
      DO 5 K1=1,270
      K=0+2*K1
      K4(K1)=K
      GD=FLOAT(K-1)/100.
      Q=-(1./3.+(ED**2)+(GD**2))
      R=2./27.-(2./3.)*(ED**2)+(GD**2)*((SN**2)*(1.-ED)-2./3.)
      A=-R/2.
      QR=(R**2)/4.+(Q**3)/27.
      B=SQRT(ABS(QR))
      BA=B/A
      P=ATAN(BA)
      PIE=3.14159264
      P1=P/3.
      P2=(P+2.*PIE)/3.
      P3=(P+4.*PIE)/3.
      C1=COS(P1)
      C2=COS(P2)
      C3=COS(P3)
      AA=1./3.
      RT=ABS(SQRT(A**2+ABS(QR)))
      RS=RT**AA
      R1(K1,I)=ABS(2.*RS*(ABS(C1-C2))-WD)
      R2(K1,I)=ABS(2.*RS*(ABS(C2-C3))-WD)
      R3(K1,I)=ABS(2.*RS*(ABS(C3-C1))-WD)
    5 CONTINUE
   15 CONTINUE
      DO 105 I1=1,19
      WRITE(6,106)I1
  106 FORMAT(5X,*I=*,I2,/)
      WRITE(6,107)((K4(K),R1(K,I1)),K=1,270)
  107 FORMAT(5(5X,*R1(*,I3,*,I)=*,E10.4))
      WRITE(6,108)((K4(K),R2(K,I1)),K=1,270)
  108 FORMAT(5(5X,*R2(*,I3,*,I)=*,E10.4))
      WRITE(6,109)((K4(K),R3(K,I1)),K=1,270)
  109 FORMAT(5(5X,*R3(*,I3,*,I)=*,E10.4))
  105 CONTINUE
      STOP
      END
```

```
      ROGRAM TAKIS3(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SPH(3,3),A(6),W(3),ZR(3,3),SI(3,3),SZ(3,3),SX(3,3),
     7SZX(3,3),EV1(3,3),EV2(3,3),EV3(3,3),GDD(180,3),GD(3),
     8D1(3),D2(3),D3(3),TR(3,3),I6(3),I7(3)
      ED=.1
      WD=.8
   10 CONTINUE
      WRITE(6,15)WD,ED
   15 FORMAT(5X,*WD=*,E10.4,*ED=*,E10.4)
      R2=1./SQRT(2.)
      PI=3.14159264
C     GD(1),GD(2),GD(3) REPRESENT RES. VALUES FOR THETA=0
      GD(1)=SQRT((WD-1.)**2-ED**2)
      GD(2)=SQRT((WD+1.)**2-ED**2)
      GD(3)=SQRT((1./4.)*(WD**2)-ED**2)
      GDD(1,1)=GD(1)
      GDD(1,2)=GD(2)
      GDD(1,3)=GD(3)
      SZ(1,1)=1.
      SZ(1,2)=0.
      SZ(1,3)=0.
      SZ(2,1)=0.
      SZ(2,2)=0.
      SZ(2,3)=0.
      SZ(3,1)=0.
      SZ(3,2)=0.
      SZ(3,3)=-1.
      SX(1,1)=0.
      SX(1,2)=R2
      SX(1,3)=0.
      SX(2,1)=R2
      SX(2,2)=0.
      SX(2,3)=R2
      SX(3,1)=0.
      SX(3,2)=R2
      SX(3,3)=0.
      DO 40 IK=1,179
      DELTA=PI/360.
      THETA=DELTA*FLOAT(IK-1)
      CN=COS(THETA)
      SN=SIN(THETA)
      DO 1 I=1,3
C     SPH REPRESENTS THE SPIN-HAMILTONIAN
      SPH(1,1)=1./3.+GDD(IK,I)*CN
      SPH(1,2)=GDD(IK,I)*R2*SN
      SPH(1,3)=ED
      SPH(2,1)=GDD(IK,I)*R2*SN
      SPH(2,2)=-2./3.
      SPH(2,3)=GDD(IK,I)*R2*SN
      SPH(3,1)=ED
      SPH(3,2)=GDD(IK,I)*R2*SN
      SPH(3,3)=1./3.-GDD(IK,I)*CN
      DO 995 I1=1,3
      W(I1)=0.
```

```
      DO 995 I2=1,3
      SI(I1,I2)=0.
  995 ZR(I1,I2)=0.
      DO 999 II=1,3
      DO 999 JJ=1,II
      KK=II*(II-1)/2+JJ
  999 A(KK)=SPH(II,JJ)
      CALL EIGRS(A,3,1,W,ZR,3,SI,IER)
      IF (IER) 997,996,997
  997 CONTINUE
      WRITE(6,998)IER
  996 CONTINUE
  998 FORMAT(5X,*IER=*,I3)
      I6(I)=1
      I7(I)=2
      AMIN=ABS(ABS(W(1)-W(2))-WD)
      DO 100 L=1,2
      L1=L+1
      DO 100 M=L1,3
      TEMP=ABS(ABS(W(L)-W(M))-WD)
      IF (TEMP-AMIN) 105,110,110
  105 AMIN=TEMP
      I6(I)=L
      I7(I)=M
  110 CONTINUE
  100 CONTINUE
      DO 25 I2=1,3
      WRITE(6,20)W(I2),I2,I
      WRITE(6,30)(ZR(I1,I2),I1=1,3)
   20 FORMAT(5X,*W(I2)=*,E10.4,5X,*I2=*,I2,*I=*,I2)
   30 FORMAT(5X,*ZR(I1,I2)=*,E10.4)
   25 CONTINUE
      DO 11 K=1,3
      DO 11 J=1,3
      SZX(K,J)=SZ(K,J)*CN+SX(K,J)*SN
      EV1(K,J)=ZR(K,1)*ZR(J,1)
      EV2(K,J)=ZR(K,2)*ZR(J,2)
      EV3(K,J)=ZR(K,3)*ZR(J,3)
   11 CONTINUE
      TR(1,I)=0.
      TR(2,I)=0.
      TR(3,I)=0.
      DO 12 K=1,3
      DO 12 J=1,3
      TR(1,I)=TR(1,I)+SZX(K,J)*EV1(J,K)
      TR(2,I)=TR(2,I)+SZX(K,J)*EV2(J,K)
      TR(3,I)=TR(3,I)+SZX(K,J)*EV3(J,K)
   12 CONTINUE
      D1(I)=W(I6(1))-W(I7(1))
      D2(I)=W(I6(2))-W(I7(2))
      D3(I)=W(I6(3))-W(I7(3))
    1 CONTINUE
      S1=2.*(D1(1)/ABS(D1(1)))*(ABS(D1(1))-WD)*(TR(I6(1),1)-TR(I7(1),1))
```

```
      S2=2.*((TR(I6(1),1)-TR(I7(1),1))**2)
      S3=2.*(D2(2)/ABS(D2(2)))*(ABS(D2(2))-WD)*(TR(I6(2),2)-TR(I7(2),2))
      S4=2.*((TR(I6(2),2)-TR(I7(2),2))**2)
      S5=2.*(D3(3)/ABS(D3(3)))*(ABS(D3(3))-WD)*(TR(I6(3),3)-TR(I7(3),3))
      S6=2.*((TR(I6(3),3)-TR(I7(3),3))**2)
      IK1=IK+1
      GDD(IK1,1)=GDD(IK,1)-S1/S2
      GDD(IK1,2)=GDD(IK,2)-S3/S4
      GDD(IK1,3)=GDD(IK,3)-S5/S6
      WRITE(6,50)IK1,GDD(IK1,1),GDD(IK1,2),GDD(IK1,3)
   50 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,1)=*,E10.4,2X,
     9*GDD(IK1,2)=*,E10.4,2X,*GDD(IK1,3)=*,E10.4)
   40 CONTINUE
      STOP
      END
```

```
      PROGRAM TAKIS2(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      ED=.1
      WD=1.6
    1 CONTINUE
      WRITE(6,2)WD
    2 FORMAT(5X,*WD=*,E10.4)
      DO 15 I=1,19
      AI=5.*FLOAT(I-1)
      THETA=AI*3.14159264/180.
      SN=SIN(THETA)
      CN=COS(THETA)
      DO 5 K=1,360,3
      GD=FLOAT(K-1)/100.
      AO=(1.+3.*(ED**2))**2-3.*((GD*CN)**2)*(1.+2.*ED-3.*(ED**2))
     3+(1./2.)*(GD**2)*(1.+12.*ED-9.*(ED**2)+(9./8.)*(GD**2))
      A1=2.*(GD**2)*(1.-3.*ED)-6.*((GD*CN)**2)*(1.-ED)
      A2=-2.-6.*(ED**2)-(5./2.)*(GD**2)
      A3=0.
      AA=1./3.
      Q=A3*(A1/2.)-AO-(A2**2)/12.
      R=-2.*((A2/6.)**3)+(A2/6.)*(A3*(A1/2.)-AO)
     7-((A3**2)*AO-A2*AO+(A1/2.)**2)/2.
      QR=(R**2)/4.+(Q**3)/27.
      IF (QR) 50,60,70
   50 P=ATAN(SQRT(ABS(QR))/(-R/2.))
      PIE=3.14159264
      PSI=2.*((SQRT((R**2)/4.+ABS(QR)))**AA)*COS(P/3.)
      GO TO 200
   60 PSI=2.*((ABS(-R/2.))**AA)
      GO TO 200
   70 SGN=-1.
      Q1=-R/2.+SQRT(QR)
      Q2=-R/2.-SQRT(QR)
      IF (Q1.GT.0.) QA1=Q1**AA
      IF (Q2.GT.0.) QA2=Q2**AA
      IF (Q1.LT.0.) QA1=SGN*((ABS(Q1))**AA)
      IF (Q2.LT.0.) QA2=SGN*((ABS(Q2))**AA)
      PSI=QA1+QA2
  200 CONTINUE
      ETA1=A3**2+2.*(PSI+A2/6.)-A2
      IF (ETA1.LT.0.) GO TO 5
      T1=SQRT(ETA1)
      IF (T1.EQ.0.) GO TO 5
      T2=(A3*(PSI+A2/6.)-A1/2.)/T1
      ETA2=(A3-T1)**2-4.*(PSI+A2/6.-T2)
      IF (ETA2.LT.0.) GO TO 5
      ETA3=(A3+T1)**2-4.*(PSI+A2/6.+T2)
      IF (ETA3.LT.0.) GO TO 5
      S1=SQRT(ETA2)
      S2=SQRT(ETA3)
      R1=ABS(ABS(S1)-WD)
      R2=ABS(ABS(2.*T1+S1-S2)/2.-WD)
      R3=ABS(ABS(2.*T1+S1+S2)/2.-WD)
      R4=ABS(ABS(S2)-WD)
```

```
      R5=ABS(ABS(2.*T1-S1-S2)/2.-WD)
      R6=ABS(ABS(2.*T1-S1+S2)/2.-WD)
      WRITE(6,998)K,I,R1,R2,R3
  998 FORMAT(5X,*K=*,I3,*I=*,I2,*R1=*,E10.4,*R2=*,E10.4,2X,*R3=*,E10.4)
      WRITE(6,999)K,I,R4,R5,R6
  999 FORMAT(5X,*K=*,I3,*I=*,I2,*R4=*,E10.4,*R5=*,E10.4,2X,*R6=*,E10.4)
    5 CONTINUE
   15 CONTINUE
      STOP
      END
```

```
      PROGRAM TAKIS4(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SPH(4,4),A(10),W(4),ZR(4,4),SI(4,4),SZ(4,4),SX(4,4),
     7SZX(4,4),EV1(4,4),EV2(4,4),EV3(4,4),EV4(4,4),
     8D1(6),D2(6),D3(6),TR(4,6),I6(6),I7(6),D4(6),D5(6),D6(6),GDD(180,6)
      ED=.1
      WD=.4
      R2=1./SQRT(2.)
      R3=SQRT(3.)
      PI=3.14159264
      GDD(1,1)=.12
      GDD(1,2)=.42
      GDD(1,3)=1.59
      GDD(1,4)=2.4
      SZ(1,1)=(R2*R3)**2
      SZ(1,2)=0.
      SZ(1,3)=0.
      SZ(1,4)=0.
      SZ(2,1)=0.
      SZ(2,2)=R2**2
      SZ(2,3)=0.
      SZ(2,4)=0.
      SZ(3,1)=0.
      SZ(3,2)=0.
      SZ(3,3)=-R2**2
      SZ(3,4)=0.
      SZ(4,1)=0.
      SZ(4,2)=0.
      SZ(4,3)=0.
      SZ(4,4)=-(R2*R3)**2
      SX(1,1)=0.
      SX(1,2)=R3*(R2**2)
      SX(1,3)=0.
      SX(1,4)=0.
      SX(2,1)=R3*(R2**2)
      SX(2,2)=0.
      SX(2,3)=1.
      SX(2,4)=0.
      SX(3,1)=0.
      SX(3,2)=1.
      SX(3,3)=0.
      SX(3,4)=R3*(R2**2)
      SX(4,1)=0.
      SX(4,2)=0.
      SX(4,3)=R3*(R2**2)
      SX(4,4)=0.
      DO 40 IK=1,179
      DELTA=PI/360.
      THETA=DELTA*FLOAT(IK-1)
      CN=COS(THETA)
      SN=SIN(THETA)
      DO 1 I=1,4
C     SPH REPRESENTS THE SPIN HAMILTONIAN
      SPH(1,1)=1.+((R3*R2)**2)*GDD(IK,I)*CN
      SPH(1,2)=GDD(IK,I)*R3*(R2**2)*SN
```

```
      SPH(1,3)=R3*ED
      SPH(1,4)=0.
      SPH(2,1)=GDD(IK,I)*R3*(R2**2)*SN
      SPH(2,2)=(R2**2)*GDD(IK,I)*CN-1.
      SPH(2,3)=GDD(IK,I)*SN
      SPH(2,4)=R3*ED
      SPH(3,1)=R3*ED
      SPH(3,2)=GDD(IK,I)*SN
      SPH(3,3)=-(R2**2)*GDD(IK,I)*CN-1.
      SPH(3,4)=R3*(R2**2)*GDD(IK,I)*SN
      SPH(4,1)=0.
      SPH(4,2)=R3*ED
      SPH(4,3)=R3*(R2**2)*GDD(IK,I)*SN
      SPH(4,4)=-((R3*R2)**2)*GDD(IK,I)*CN+1.
      DO 995 I1=1,4
      W(I1)=0.
      DO 995 I2=1,4
      SI(I1,I2)=0.
  995 ZR(I1,I2)=0.
      DO 999 II=1,4
      DO 999 JJ=1,II
      KK=II*(II-1)/2+JJ
  999 A(KK)=SPH(II,JJ)
      CALL EIGRS(A,4,1,W,ZR,4,SI,IER)
      IF (IER) 997,996,997
  997 CONTINUE
      WRITE(6,998)IER
  996 CONTINUE
  998 FORMAT(5X,*IER=*,I3)
      GO TO 111
      I6(I)=1
      I7(I)=2
      IEQ=0.
      AMIN=ABS(ABS(W(1)-W(2))-WD)
      DO 100 L=1,3
      L1=L+1
      DO 100 M=L1,4
      TEMP=ABS(ABS(W(L)-W(M))-WD)
      IF (TEMP-AMIN) 105,106,110
  105 AMIN=TEMP
      I6(I)=L
      I7(I)=M
      GO TO 110
  106 IEQ=IEQ+1.
  110 CONTINUE
  100 CONTINUE
  111 CONTINUE
      I6(4)=1
      I7(4)=2
      I6(3)=1
      I7(3)=2
      I6(2)=1
      I7(2)=2
```

```
      I6(1)=3
      I7(1)=4
      DO 25 I2=1,4
      WRITE(6,20)W(I2),I2,I,ZR(1,I2),ZR(2,I2),ZR(3,I2),ZR(4,I2)
   20 FORMAT(5X,*W(I2)=*,E10.4,2X,*I2=*,I1,2X,*I=*,I1,2X,*ZR(1,I2)=*,
     2E10.4,2X,*ZR(2,I2)=*,E10.4,2X,*ZR(3,I2)=* E10.4,2X,*ZR(4,I2)=*,
     3E10.4)
   25 CONTINUE
      DO 11 K=1,4
      DO 11 J=1,4
      SZX(K,J)=SZ(K,J)*CN+SX(K,J)*SN
      EV1(K,J)=ZR(K,1)*ZR(J,1)
      EV2(K,J)=ZR(K,2)*ZR(J,2)
      EV3(K,J)=ZR(K,3)*ZR(J,3)
      EV4(K,J)=ZR(K,4)*ZR(J,4)
   11 CONTINUE
      TR(1,I)=0.
      TR(2,I)=0.
      TR(3,I)=0.
      TR(4,I)=0.
      DO 12 K=1,4
      DO 12 J=1,4
      TR(1,I)=TR(1,I)+SZX(K,J)*EV1(J,K)
      TR(2,I)=TR(2,I)+SZX(K,J)*EV2(J,K)
      TR(3,I)=TR(3,I)+SZX(K,J)*EV3(J,K)
      TR(4,I)=TR(4,I)+SZX(K,J)*EV4(J,K)
   12 CONTINUE
      D1(I)=W(I6(1))-W(I7(1))
      D2(I)=W(I6(2))-W(I7(2))
      D3(I)=W(I6(3))-W(I7(3))
      D4(I)=W(I6(4))-W(I7(4))
      GO TO 1
      D5(I)=W(I6(5))-W(I7(5))
      D6(I)=W(I6(6))-W(I7(6))
    1 CONTINUE
      S1=(D1(1)/ABS(D1(1)))*(ABS(D1(1))-WD)*(TR(I6(1),1)-TR(I7(1),1))
      S2=(TR(I6(1),1)-TR(I7(1),1))**2
      S3=(D2(2)/ABS(D2(2)))*(ABS(D2(2))-WD)*(TR(I6(2),2)-TR(I7(2),2))
      S4=(TR(I6(2),2)-TR(I7(2),2))**2
      S5=(D3(3)/ABS(D3(3)))*(ABS(D3(3))-WD)*(TR(I6(3),3)-TR(I7(3),3))
      S6=(TR(I6(3),3)-TR(I7(3),3))**2
      S7=(D4(4)/ABS(D4(4)))*(ABS(D4(4))-WD)*(TR(I6(4),4)-TR(I7(4),4))
      S8=(TR(I6(4),4)-TR(I7(4),4))**2
      GO TO 13
      S9=(D5(5)/ABS(D5(5)))*(ABS(D5(5))-WD)*(TR(I6(5),5)-TR(I7(5),5))
      S10=(TR(I6(5),5)-TR(I7(5),5))**2
      S11=(D6(6)/ABS(D6(6)))*(ABS(D6(6))-WD)*(TR(I6(6),6)-TR(I7(6),6))
      S12=(TR(I6(6),6)-TR(I7(6),6))**2
   13 CONTINUE
      IK1=IK+1
      GDD(IK1,1)=GDD(IK,1)-S1/S2
      GDD(IK1,2)=GDD(IK,2)-S3/S4
      GDD(IK1,3)=GDD(IK,3)-S5/S6
```

```
      GDD(IK1,4)=GDD(IK,4)-S7/S8
      GO TO 14
      GDD(IK1,5)=GDD(IK,5)-S9/S10
      GDD(IK1,6)=GDD(IK,6)-S11/S12
   14 CONTINUE
      WRITE(6,50)IK1,GDD(IK1,1),GDD(IK1,2),GDD(IK1,3)
      WRITE(6,55)IK1,GDD(IK1,4),GDD(IK1,5),GDD(IK1,6)
   50 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,1)=*,E10.4,2X,
     9*GDD(IK1,2)=*,E10.4,2X,*GDD(IK1,3)=*,E10.4)
   55 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,4)=*,E10.4,2X,
     1*GDD(IK1,5)=*,E10.4,2X,*GDD(IK1,6)=*,E10.4)
   40 CONTINUE
      STOP
      END
```

```
      PROGRAM TAKIS6(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SPH(5,5),A(15),W(5),ZR(5,5),SI(5,5),SZ(5,5),SX(5,5),
     7SZX(5,5),EV1(5,5),EV2(5,5),EV3(5,5),EV4(5,5),EV5(5,5),
     8D1(10),D2(10),D3(10),TR(5,10),I6(10),I7(10),D4(10),D5(10),D6(10),
     9D7(10),D8(10),D9(10),D10(10),GDD(450,10)
      ED=.1
      WD=6.4
      R2=1./SQRT(2.)
      R3=SQRT(3.)
      PI=3.14159264
      GDD(1,1)=1.11
      GDD(1,2)=1.17
      GDD(1,3)=1.61
      GDD(1,4)=3.11
      GDD(1,5)=3.19
      GDD(1,6)=3.41
      GDD(1,7)=5.19
      GDD(1,8)=5.39
      GDD(1,9)=7.39
      GDD(1,10)=9.41
    2 CONTINUE
      SZ(1,1)=2.
      SZ(1,2)=0.
      SZ(1,3)=0.
      SZ(1,4)=0.
      SZ(1,5)=0.
      SZ(2,1)=0.
      SZ(2,2)=1.
      SZ(2,3)=0.
      SZ(2,4)=0.
      SZ(2,5)=0.
      SZ(3,1)=0.
      SZ(3,2)=0.
      SZ(3,3)=0.
      SZ(3,4)=0.
      SZ(3,5)=0.
      SZ(4,1)=0.
      SZ(4,2)=0.
      SZ(4,3)=0.
      SZ(4,4)=-1.
      SZ(4,5)=0.
      SZ(5,1)=0.
      SZ(5,2)=0.
      SZ(5,3)=0.
      SZ(5,4)=0.
      SZ(5,5)=-2.
      SX(1,1)=0.
      SX(1,2)=1.
      SX(1,3)=0.
      SX(1,4)=0.
      SX(1,5)=0.
      SX(2,1)=1.
      SX(2,2)=0.
      SX(2,3)=R3*R2
```

```
      SX(2,4)=0.
      SX(2,5)=0.
      SX(3,1)=0.
      SX(3,2)=R3*R2
      SX(3,3)=0.
      SX(3,4)=R3*R2
      SX(3,5)=0.
      SX(4,1)=0.
      SX(4,2)=0.
      SX(4,3)=R3*R2
      SX(4,4)=0.
      SX(4,5)=1.
      SX(5,1)=0.
      SX(5,2)=0.
      SX(5,3)=0.
      SX(5,4)=1.
      SX(5,5)=0.
      DO 40 IK=1,359
      DELTA=PI/720.
      THETA=DELTA*FLOAT(IK-1)
      CN=COS(THETA)
      SN=SIN(THETA)
      DO 1 I=1,10
C     SPH REPRESENTS THE SPIN HAMILTONIAN
      SPH(1,1)=2.+2.*GDD(IK,I)*CN
      SPH(1,2)=GDD(IK,I)*SN
      SPH(1,3)=SQRT(6.)*ED
      SPH(1,4)=0.
      SPH(1,5)=0.
      SPH(2,1)=GDD(IK,I)*SN
      SPH(2,2)=GDD(IK,I)*CN-1.
      SPH(2,3)=R3*R2*GDD(IK,I)*SN
      SPH(2,4)=3.*ED
      SPH(2,5)=0.
      SPH(3,1)=SQRT(6.)*ED
      SPH(3,2)=R3*R2*GDD(IK,I)*SN
      SPH(3,3)=-2.
      SPH(3,4)=R3*R2*GDD(IK,I)*SN
      SPH(3,5)=SQRT(6.)*ED
      SPH(4,1)=0.
      SPH(4,2)=3.*ED
      SPH(4,3)=R3*R2*GDD(IK,I)*SN
      SPH(4,4)=-GDD(IK,I)*CN-1.
      SPH(4,5)=GDD(IK,I)*SN
      SPH(5,1)=0.
      SPH(5,2)=0.
      SPH(5,3)=SQRT(6.)*ED
      SPH(5,4)=GDD(IK,I)*SN
      SPH(5,5)=2.-2.*GDD(IK,I)*CN
      DO 995 I1=1,5
      W(I1)=0.
      DO 995 I2=1,5
      SI(I1,I2)=0.
```

```
995 ZR(I1,L2)=0.
    DO 999 II=1,5
    DO 999 JJ=1,II
    KK=II*(II-1)/2+JJ
999 A(KK)=SPH(II,JJ)
    CALL EIGRS(A,5,1,W,ZR,5,SI,IER)
    IF (IER) 997,996,997
997 CONTINUE
    WRITE(6,998)IER
996 CONTINUE
998 FORMAT(5X,*IER=*,I3)
    GO TO 111
    I6(I)=1
    I7(I)=2
    IEQ=0.
    AMIN=ABS(ABS(W(1)-W(2))-WD)
    DO 100 L=1,4
    L1=L+1
    DO 100 M=L1,5
    TEMP=ABS(ABS(W(L)-W(M))-WD)
    IF (TEMP-AMIN) 105,106,110
105 AMIN=TEMP
    I6(I)=L
    I7(I)=M
    GO TO 110
106 IEQ=IEQ+1.
110 CONTINUE
100 CONTINUE
111 CONTINUE
    I6(4)=4
    I7(4)=1
    I6(3)=5
    I7(3)=3
    I6(2)=5
    I7(2)=2
    I6(1)=5
    I7(1)=1
    I6(5)=4
    I7(5)=2
    I6(6)=5
    I7(6)=4
    I6(7)=3
    I7(7)=1
    I6(8)=4
    I7(8)=3
    I6(9)=3
    I7(9)=2
    I6(10)=2
    I7(10)=1
    GO TO 25
    WRITE(6,20)I,W(1),W(2),W(3),W(4),W(5)
 20 FORMAT(5X,*I=*,I2,2X,*W(1)=*,E10.4,2X,*W(2)=*,E10.4,
   62X,*W(3)=*,E10.4,2X,*W(4)=*,E10.4,2X,*W(5)=*,E10.4,/)
```

```
25 CONTINUE
   DO 11 K=1,5
   DO 11 J=1,5
   SZX(K,J)=SZ(K,J)*CN+SX(K,J)*SN
   EV1(K,J)=ZR(K,1)*ZR(J,1)
   EV2(K,J)=ZR(K,2)*ZR(J,2)
   EV3(K,J)=ZR(K,3)*ZR(J,3)
   EV4(K,J)=ZR(K,4)*ZR(J,4)
   EV5(K,J)=ZR(K,5)*ZR(J,5)
11 CONTINUE
   TR(1,I)=0.
   TR(2,I)=0.
   TR(3,I)=0.
   TR(4,I)=0.
   TR(5,I)=0.
   DO 12 K=1,5
   DO 12 J=1,5
   TR(1,I)=TR(1,I)+SZX(K,J)*EV1(J,K)
   TR(2,I)=TR(2,I)+SZX(K,J)*EV2(J,K)
   TR(3,I)=TR(3,I)+SZX(K,J)*EV3(J,K)
   TR(4,I)=TR(4,I)+SZX(K,J)*EV4(J,K)
   TR(5,I)=TR(5,I)+SZX(K,J)*EV5(J,K)
12 CONTINUE
   D1(I)=W(I6(1))-W(I7(1))
   D2(I)=W(I6(2))-W(I7(2))
   D3(I)=W(I6(3))-W(I7(3))
   D4(I)=W(I6(4))-W(I7(4))
   D5(I)=W(I6(5))-W(I7(5))
   D6(I)=W(I6(6))-W(I7(6))
   D7(I)=W(I6(7))-W(I7(7))
   D8(I)=W(I6(8))-W(I7(8))
   D9(I)=W(I6(9))-W(I7(9))
   D10(I)=W(I6(10))-W(I7(10))
 1 CONTINUE
   S1=(D1(1)/ABS(D1(1)))*(ABS(D1(1))-WD)*(TR(I6(1),1)-TR(I7(1),1))
   S2=(TR(I6(1),1)-TR(I7(1),1))**2
   S3=(D2(2)/ABS(D2(2)))*(ABS(D2(2))-WD)*(TR(I6(2),2)-TR(I7(2),2))
   S4=(TR(I6(2),2)-TR(I7(2),2))**2
   S5=(D3(3)/ABS(D3(3)))*(ABS(D3(3))-WD)*(TR(I6(3),3)-TR(I7(3),3))
   S6=(TR(I6(3),3)-TR(I7(3),3))**2
   S7=(D4(4)/ABS(D4(4)))*(ABS(D4(4))-WD)*(TR(I6(4),4)-TR(I7(4),4))
   S8=(TR(I6(4),4)-TR(I7(4),4))**2
   S9=(D5(5)/ABS(D5(5)))*(ABS(D5(5))-WD)*(TR(I6(5),5)-TR(I7(5),5))
   S10=(TR(I6(5),5)-TR(I7(5),5))**2
   S11=(D6(6)/ABS(D6(6)))*(ABS(D6(6))-WD)*(TR(I6(6),6)-TR(I7(6),6))
   S12=(TR(I6(6),6)-TR(I7(6),6))**2
   S13=(D7(7)/ABS(D7(7)))*(ABS(D7(7))-WD)*(TR(I6(7),7)-TR(I7(7),7))
   S14=(TR(I6(7),7)-TR(I7(7),7))**2
   S15=(D8(8)/ABS(D8(8)))*(ABS(D8(8))-WD)*(TR(I6(8),8)-TR(I7(8),8))
   S16=(TR(I6(8),8)-TR(I7(8),8))**2
   S17=(D9(9)/ABS(D9(9)))*(ABS(D9(9))-WD)*(TR(I6(9),9)-TR(I7(9),9))
   S18=(TR(I6(9),9)-TR(I7(9),9))**2
   S19=(D10(10)/ABS(D10(10)))*(ABS(D10(10))-WD)*(TR(I6(10),10)
```

```
  5-TR(I7(10),10))
   S20=(TR(I6(10),10)-TR(I7(10),10))**2
13 CONTINUE
   IK1=IK+1
   GDD(IK1,1)=GDD(IK,1)-S1/S2
   GDD(IK1,2)=GDD(IK,2)-S3/S4
   GDD(IK1,3)=GDD(IK,3)-S5/S6
   GDD(IK1,4)=GDD(IK,4)-S7/S8
   GDD(IK1,5)=GDD(IK,5)-S9/S10
   GDD(IK1,6)=GDD(IK,6)-S11/S12
 7 CONTINUE
   GDD(IK1,7)=GDD(IK,7)-S13/S14
   GDD(IK1,8)=GDD(IK,8)-S15/S16
   GDD(IK1,9)=GDD(IK,9)-S17/S18
   GDD(IK1,10)=GDD(IK,10)-S19/S20
 3 CONTINUE
   WRITE(6,50)IK1,GDD(IK1,1),GDD(IK1,2),GDD(IK1,3)
   WRITE(6,55)IK1,GDD(IK1,4),GDD(IK1,5),GDD(IK1,6)
   WRITE(6,66)IK1,GDD(IK1,7),GDD(IK1,8),GDD(IK1,9),GDD(IK1,10)
50 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,1)=*,E10.4,2X,
  9*GDD(IK1,2)=*,E10.4,2X,*GDD(IK1,3)=*,E10.4,/)
55 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,4)=*,E10.4,2X,
  1*GDD(IK1,5)=*,E10.4,2X,*GDD(IK1,6)=*,E10.4,/)
66 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,7)=*,E10.4,2X,*GDD(IK1,8)=*,
  2E10.4,2X,*GDD(IK1,9)=*,E10.4,2X,*GDD(IK1,10)=*,E10.4,//)
40 CONTINUE
   STOP
   END
```

```
      PROGRAM TAKIS7(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SPH(6,6),A(21),W(6),ZR(6,6),SI(6,6),SZ(6,6),SX(6,6),
     7SZX(6,6),EV1(6,6),EV2(6,6),EV3(6,6),EV4(6,6),EV5(6,6),EV6(6,6),
     8D1(15),D2(15),D3(15),TR(6,15),I6(15),I7(15),D4(15),D5(15),D6(15),
     9D7(15),D8(15),D9(15),D10(15),GDD(450,15),D11(15),D12(15),
     4D13(15),D14(15),D15(15)
      ED=.1
      WD=6.4
      R1=1./2.
      R2=SQRT(2.)
      R3=SQRT(5.)
      R4=1./3.
      PI=3.14159264
      GDD(1,1)=.09
      GDD(1,2)=.12
      GDD(1,3)=.65
      GDD(1,4)=1.29
      GDD(1,5)=2.09
      GDD(1,6)=2.15
      GDD(1,7)=2.41
      GDD(1,8)=2.63
      GDD(1,9)=4.11
      GDD(1,10)=4.17
      GDD(1,11)=4.41
      GDD(1,12)=6.19
      GDD(1,13)=6.39
      GDD(1,14)=8.39
      GDD(1,15)=10.41
    2 CONTINUE
      SZ(1,1)=5.*R1
      SZ(1,2)=0.
      SZ(1,3)=0.
      SZ(1,4)=0.
      SZ(1,5)=0.
      SZ(1,6)=0.
      SZ(2,1)=0.
      SZ(2,2)=3.*R1
      SZ(2,3)=0.
      SZ(2,4)=0.
      SZ(2,5)=0.
      SZ(2,6)=0.
      SZ(3,1)=0.
      SZ(3,2)=0.
      SZ(3,3)=R1
      SZ(3,4)=0.
      SZ(3,5)=0.
      SZ(3,6)=0.
      SZ(4,1)=0.
      SZ(4,2)=0.
      SZ(4,3)=0.
      SZ(4,4)=-R1
      SZ(4,5)=0.
      SZ(4,6)=0.
      SZ(5,1)=0.
```

```
SZ(5,2)=0.
SZ(5,3)=0.
SZ(5,4)=0.
SZ(5,5)=-3.*R1
SZ(5,6)=0.
SZ(6,1)=0.
SZ(6,2)=0.
SZ(6,3)=0.
SZ(6,4)=0.
SZ(6,5)=0.
SZ(6,6)=-5.*R1
SX(1,1)=0.
SX(1,2)=R1*R3
SX(1,3)=0.
SX(1,4)=0.
SX(1,5)=0.
SX(1,6)=0.
SX(2,1)=R1*R3
SX(2,2)=0.
SX(2,3)=R2
SX(2,4)=0.
SX(2,5)=0.
SX(2,6)=0.
SX(3,1)=0.
SX(3,2)=R2
SX(3,3)=0
SX(3,4)=3.*R1
SX(3,5)=0.
SX(3,6)=0.
SX(4,1)=0.
SX(4,2)=0.
SX(4,3)=3.*R1
SX(4,4)=0.
SX(4,5)=R2
SX(4,6)=0.
SX(5,1)=0.
SX(5,2)=0.
SX(5,3)=0.
SX(5,4)=R2
SX(5,5)=0.
SX(5,6)=R1*R3
SX(6,1)=0.
SX(6,2)=0.
SX(6,3)=0.
SX(6,4)=0.
SX(6,5)=R1*R3
SX(6,6)=0.
DO 40 IK=1,359
DELTA=PI/720.
THETA=DELTA*FLOAT(IK-1)
CN=COS(THETA)
SN=SIN(THETA)
DO 1 I=1,15
```

```
C      SPH REPRESENTS THE SPIN HAMILTONIAN
       SPH(1,1)=10.*R4+5.*R1*GDD(IK,I)*CN
       SPH(1,2)=R1*R3*GDD(IK,I)*SN
       SPH(1,3)=R2*R3*ED
       SPH(1,4)=0.
       SPH(1,5)=0.
       SPH(1,6)=0.
       SPH(2,1)=R1*R3*GDD(IK,I)*SN
       SPH(2,2)=3.*R1*GDD(IK,I)*CN-2.*R4
       SPH(2,3)=R2*GDD(IK,I)*SN
       SPH(2,4)=3.*R2*ED
       SPH(2,5)=0.
       SPH(2,6)=0.
       SPH(3,1)=R2*R3*ED
       SPH(3,2)=R2*GDD(IK,I)*SN
       SPH(3,3)=-8.*R4+R1*GDD(IK,I)*CN
       SPH(3,4)=3.*R1*GDD(IK,I)*SN
       SPH(3,5)=3.*R2*ED
       SPH(3,6)=0.
       SPH(4,1)=0.
       SPH(4,2)=3.*R2*ED
       SPH(4,3)=3.*R1*GDD(IK,I)*SN
       SPH(4,4)=-R1*GDD(IK,I)*CN-8.*R4
       SPH(4,5)=R2*GDD(IK,I)*SN
       SPH(4,6)=R2*R3*ED
       SPH(5,1)=0.
       SPH(5,2)=0.
       SPH(5,3)=3.*R2*ED
       SPH(5,4)=R2*GDD(IK,I)*SN
       SPH(5,5)=-2.*R4-3.*R1*GDD(IK,I)*CN
       SPH(5,6)=R1*R3*GDD(IK,I)*SN
       SPH(6,1)=0.
       SPH(6,2)=0.
       SPH(6,3)=0.
       SPH(6,4)=R2*R3*ED
       SPH(6,5)=R1*R3*GDD(IK,I)*SN
       SPH(6,6)=10.*R4-5.*R1*GDD(IK,I)*CN
       DO 995 I1=1,6
       W(I1)=0.
       DO 995 I2=1,6
       SI(I1,I2)=0.
   995 ZR(I1,I2)=0.
       DO 999 II=1,6
       DO 999 JJ=1,II
       KK=II*(II-1)/2+JJ
   999 A(KK)=SPH(II,JJ)
       CALL EIGRS(A,6,1,W,ZR,6,SI,IER)
       IF (IER) 997,996,997
   997 CONTINUE
       WRITE(6,998)IER
   996 CONTINUE
   998 FORMAT(5X,*IER=*,I3)
       GO TO 111
```

```
      I6(I)=1
      I7(I)=2
      IEQ=0.
      AMIN=ABS(ABS(W(1)-W(2))-WD)
      DO 100 L=1,5
      L1=L+1
      DO 100 M=L1,6
      TEMP=ABS(ABS(W(L)-W(M))-WD)
      IF (TEMP-AMIN) 105,106,110
  105 AMIN=TEMP
      I6(I)=L
      I7(I)=M
      GO TO 110
  106 IEQ=IEQ+1.
  110 CONTINUE
  100 CONTINUE
  111 CONTINUE
      I6(1)=6
      I7(1)=1
      I6(2)=6
      I7(2)=2
      I6(3)=6
      I7(3)=3
      I6(4)=6
      I7(4)=4
      I6(5)=5
      I7(5)=1
      I6(6)=5
      I7(6)=2
      I6(7)=6
      I7(7)=5
      I6(8)=5
      I7(8)=3
      I6(9)=4
      I7(9)=1
      I6(10)=4
      I7(10)=2
      I6(11)=5
      I7(11)=4
      I6(12)=3
      I7(12)=1
      I6(13)=4
      I7(13)=3
      I6(14)=3
      I7(14)=2
      I6(15)=2
      I7(15)=1
      GO TO 25
      WRITE(6,20)I,W(1),W(2),W(3),W(4),W(5),W(6)
   20 FORMAT(5X,*I=*,I2,2X,*W(1)=*,E10.4,2X,*W(2)=*,E10.4,
     32X,*W(3)=*,E10.4,
     62X,*W(4)=*,E10.4,2X,*W(5)=*,E10.4,2X,*W(6)=*,E10.4,/)
   25 CONTINUE
```

```
      DO 11 K=1,6
      DO 11 J=1,6
      SZX(K,J)=SZ(K,J)*CN+SX(K,J)*SN
      EV1(K,J)=ZR(K,1)*ZR(J,1)
      EV2(K,J)=ZR(K,2)*ZR(J,2)
      EV3(K,J)=ZR(K,3)*ZR(J,3)
      EV4(K,J)=ZR(K,4)*ZR(J,4)
      EV5(K,J)=ZR(K,5)*ZR(J,5)
      EV6(K,J)=ZR(K,6)*ZR(J,6)
   11 CONTINUE
      TR(1,I)=0.
      TR(2,I)=0.
      TR(3,I)=0.
      TR(4,I)=0.
      TR(5,I)=0.
      TR(6,I)=0.
      DO 12 K=1,6
      DO 12 J=1,6
      TR(1,I)=TR(1,I)+SZX(K,J)*EV1(J,K)
      TR(2,I)=TR(2,I)+SZX(K,J)*EV2(J,K)
      TR(3,I)=TR(3,I)+SZX(K,J)*EV3(J,K)
      TR(4,I)=TR(4,I)+SZX(K,J)*EV4(J,K)
      TR(5,I)=TR(5,I)+SZX(K,J)*EV5(J,K)
      TR(6,I)=TR(6,I)+SZX(K,J)*EV6(J,K)
   12 CONTINUE
      D1(I)=W(I6(1))-W(I7(1))
      D2(I)=W(I6(2))-W(I7(2))
      D3(I)=W(I6(3))-W(I7(3))
      D4(I)=W(I6(4))-W(I7(4))
      D5(I)=W(I6(5))-W(I7(5))
      D6(I)=W(I6(6))-W(I7(6))
      D7(I)=W(I6(7))-W(I7(7))
      D8(I)=W(I6(8))-W(I7(8))
      D9(I)=W(I6(9))-W(I7(9))
      D10(I)=W(I6(10))-W(I7(10))
      D11(I)=W(I6(11))-W(I7(11))
      D12(I)=W(I6(12))-W(I7(12))
      D13(I)=W(I6(13))-W(I7(13))
      D14(I)=W(I6(14))-W(I7(14))
      D15(I)=W(I6(15))-W(I7(15))
    1 CONTINUE
      S1=(D1(1)/ABS(D1(1)))*(ABS(D1(1))-WD)*(TR(I6(1),1)-TR(I7(1),1))
      S2=(TR(I6(1),1)-TR(I7(1),1))**2
      S3=(D2(2)/ABS(D2(2)))*(ABS(D2(2))-WD)*(TR(I6(2),2)-TR(I7(2),2))
      S4=(TR(I6(2),2)-TR(I7(2),2))**2
      S5=(D3(3)/ABS(D3(3)))*(ABS(D3(3))-WD)*(TR(I6(3),3)-TR(I7(3),3))
      S6=(TR(I6(3),3)-TR(I7(3),3))**2
      S7=(D4(4)/ABS(D4(4)))*(ABS(D4(4))-WD)*(TR(I6(4),4)-TR(I7(4),4))
      S8=(TR(I6(4),4)-TR(I7(4),4))**2
      S9=(D5(5)/ABS(D5(5)))*(ABS(D5(5))-WD)*(TR(I6(5),5)-TR(I7(5),5))
      S10=(TR(I6(5),5)-TR(I7(5),5))**2
      S11=(D6(6)/ABS(D6(6)))*(ABS(D6(6))-WD)*(TR(I6(6),6)-TR(I7(6),6))
      S12=(TR(I6(6),6)-TR(I7(6),6))**2
```

```
      S13=(D7(7)/ABS(D7(7)))*(ABS(D7(7))-WD)*(TR(I6(7),7)-TR(I7(7),7))
      S14=(TR(I6(7),7)-TR(I7(7),7))**2
      S15=(D8(8)/ABS(D8(8)))*(ABS(D8(8))-WD)*(TR(I6(8),8)-TR(I7(8),8))
      S16=(TR(I6(8),8)-TR(I7(8),8))**2
      S17=(D9(9)/ABS(D9(9)))*(ABS(D9(9))-WD)*(TR(I6(9),9)-TR(I7(9),9))
      S18=(TR(I6(9),9)-TR(I7(9),9))**2
      S19=(D10(10)/ABS(D10(10)))*(ABS(D10(10))-WD)*(TR(I6(10),10)
     5-TR(I7(10),10))
      S20=(TR(I6(10),10)-TR(I7(10),10))**2
      S21=(D11(11)/ABS(D11(11)))*(ABS(D11(11))-WD)*(TR(I6(11),11)
     1-TR(I7(11),11))
      S22=(TR(I6(11),11)-TR(I7(11),11))**2
      S23=(D12(12)/ABS(D12(12)))*(ABS(D12(12))-WD)*(TR(I6(12),12)
     2-TR(I7(12),12))
      S24=(TR(I6(12),12)-TR(I7(12),12))**2
      S25=(D13(13)/ABS(D13(13)))*(ABS(D13(13))-WD)*(TR(I6(13),13)
     3-TR(I7(13),13))
      S26=(TR(I6(13),13)-TR(I7(13),13))**2
      S27=(D14(14)/ABS(D14(14)))*(ABS(D14(14))-WD)*(TR(I6(14),14)
     4-TR(I7(14),14))
      S28=(TR(I6(14),14)-TR(I7(14),14))**2
      S29=(D15(15)/ABS(D15(15)))*(ABS(D15(15))-WD)*(TR(I6(15),15)
     5-TR(I7(15),15))
      S30=(TR(I6(15),15)-TR(I7(15),15))**2
   13 CONTINUE
      IK1=IK+1
      GDD(IK1,1)=GDD(IK,1)-S1/S2
      GDD(IK1,2)=GDD(IK,2)-S3/S4
      GDD(IK1,3)=GDD(IK,3)-S5/S6
      GDD(IK1,4)=GDD(IK,4)-S7/S8
      GDD(IK1,5)=GDD(IK,5)-S9/S10
      GDD(IK1,6)=GDD(IK,6)-S11/S12
      GDD(IK1,7)=GDD(IK,7)-S13/S14
      GDD(IK1,8)=GDD(IK,8)-S15/S16
      GDD(IK1,9)=GDD(IK,9)-S17/S18
      GDD(IK1,10)=GDD(IK,10)-S19/S20
      GDD(IK1,11)=GDD(IK,11)-S21/S22
      GDD(IK1,12)=GDD(IK,12)-S23/S24
      GDD(IK1,13)=GDD(IK,13)-S25/S26
      GDD(IK1,14)=GDD(IK,14)-S27/S28
      GDD(IK1,15)=GDD(IK,15)-S29/S30
    3 CONTINUE
      WRITE(6,50)IK1,GDD(IK1,1),GDD(IK1,2),GDD(IK1,3)
      WRITE(6,55)IK1,GDD(IK1,4),GDD(IK1,5),GDD(IK1,6)
      WRITE(6,66)IK1,GDD(IK1,7),GDD(IK1,8),GDD(IK1,9),GDD(IK1,10)
      WRITE(6,77)IK1,GDD(IK1,11),GDD(IK1,12),
     6GDD(IK1,13),GDD(IK1,14),GDD(IK1,15)
   50 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,1)=*,E10.4,2X,
     9*GDD(IK1,2)=*,E10.4,2X,*GDD(IK1,3)=*,E10.4,/)
   55 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,4)=*,E10.4,2X,
     1*GDD(IK1,5)=*,E10.4,2X,*GDD(IK1,6)=*,E10.4,/)
   66 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,7)=*,E10.4,2X,*GDD(IK1,8)=*,
     2E10.4,2X,*GDD(IK1,9)=*,E10.4,2X,*GDD(IK1,10)=*,E10.4,/)
```

```
77 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,11)=*,E10.4,2X,
  7*GDD(IK1,12)=*,E10.4,2X,*GDD(IK1,13)=*,E10.4,2X,
  8*GDD(IK1,14)=*,E10.4,2X,*GDD(IK1,15)=*,E10.4,//)
40 CONTINUE
   STOP
   END
```

```
      PROGRAM TAKIS9(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION T1(800),T2(800),T3(800),T4(800),T5(800),T6(800),
     1T7(800),T8(800),T9(800),T10(800),K4(800),T11(800),T12(800),
     3SPH(8,8),A(36),W(8),ZR(8,8),SI(8,8),T13(800),T14(800),T15(800),
     1T16(800),T17(800),T18(800),T19(800),T20(800),T21(800),T22(800),
     2T23(800),T24(800),T25(800),T26(800),T27(800),T28(800)
      ED=.1
      R1=1./2.
      R2=SQRT(3.)
      R3=SQRT(7.)
      R4=SQRT(15.)
      WD=1.6
    2 CONTINUE
      WRITE(6,10)WD
   10 FORMAT(5X,*WD=*,E10.4)
      PI=3.14159264
      DO 5 K1=1,451
      K=0+2*K1
      K4(K1)=K
      GD=FLOAT(K-1)/100.
      SPH(1,1)=7.*R1*GD+7.
      SPH(1,2)=0.
      SPH(1,3)=R2*R3*ED
      SPH(1,4)=0.
      SPH(1,5)=0.
      SPH(1,6)=0.
      SPH(1,7)=0.
      SPH(1,8)=0.
      SPH(2,1)=0.
      SPH(2,2)=5.*R1*GD+1.
      SPH(2,3)=0.
      SPH(2,4)=R4*R2*ED
      SPH(2,5)=0.
      SPH(2,6)=0.
      SPH(2,7)=0.
      SPH(2,8)=0.
      SPH(3,1)=R2*R3*ED
      SPH(3,2)=0.
      SPH(3,3)=3.*R1*GD-3.
      SPH(3,4)=0.
      SPH(3,5)=2.*R4*ED
      SPH(3,6)=0.
      SPH(3,7)=0.
      SPH(3,8)=0.
      SPH(4,1)=0.
      SPH(4,2)=R4*R2*ED
      SPH(4,3)=0.
      SPH(4,4)=R1*GD-5.
      SPH(4,5)=0.
      SPH(4,6)=2.*R4*ED
      SPH(4,7)=0.
      SPH(4,8)=0.
      SPH(5,1)=0.
      SPH(5,2)=0.
```

```
      SPH(5,3)=2.*R4*ED
      SPH(5,4)=0.
      SPH(5,5)=-R1*GD-5.
      SPH(5,6)=0.
      SPH(5,7)=R2*R4*ED
      SPH(5,8)=0.
      SPH(6,1)=0.
      SPH(6,2)=0.
      SPH(6,3)=0.
      SPH(6,4)=2.*R4*ED
      SPH(6,5)=0.
      SPH(6,6)=-3.*R1*GD-3.
      SPH(6,7)=0.
      SPH(6,8)=R2*R3*ED
      SPH(7,1)=0.
      SPH(7,2)=0.
      SPH(7,3)=0.
      SPH(7,4)=0.
      SPH(7,5)=R2*R4*ED
      SPH(7,6)=0.
      SPH(7,7)=-5.*R1*GD+1.
      SPH(7,8)=0.
      SPH(8,1)=0.
      SPH(8,2)=0.
      SPH(8,3)=0.
      SPH(8,4)=0.
      SPH(8,5)=0.
      SPH(8,6)=R2*R3*ED
      SPH(8,7)=0.
      SPH(8,8)=-7.*R1*GD+7.
      DO 995 I1=1,8
      W(I1)=0.
      DO 995 I2=1,8
      SI(I1,I2)=0.
  995 ZR(I1,I2)=0.
      DO 999 II=1,8
      DO 999 JJ=1,II
      KK=II*(II-1)/2+JJ
  999 A(KK)=SPH(II,JJ)
      CALL EIGRS(A,8,1,W,ZR,8,SI,IER)
      IF (IER) 997,996,997
  997 CONTINUE
      WRITE(6,998)IER
  996 CONTINUE
  998 FORMAT(5X,*IER=*,I3)
      T1(K1)=ABS(ABS(W(1)-W(2))-WD)
      T2(K1)=ABS(ABS(W(1)-W(3))-WD)
      T3(K1)=ABS(ABS(W(1)-W(4))-WD)
      T4(K1)=ABS(ABS(W(1)-W(5))-WD)
      T11(K1)=ABS(ABS(W(1)-W(6))-WD)
      T16(K1)=ABS(ABS(W(1)-W(7))-WD)
      T22(K1)=ABS(ABS(W(1)-W(8))-WD)
      T5(K1)=ABS(ABS(W(2)-W(3))-WD)
```

```
      T6(K1)=ABS(ABS(W(2)-W(4))-WD)
      T7(K1)=ABS(ABS(W(2)-W(5))-WD)
      T12(K1)=ABS(ABS(W(2)-W(6))-WD)
      T17(K1)=ABS(ABS(W(2)-W(7))-WD)
      T23(K1)=ABS(ABS(W(2)-W(8))-WD)
      T8(K1)=ABS(ABS(W(3)-W(4))-WD)
      T9(K1)=ABS(ABS(W(3)-W(5))-WD)
      T13(K1)=ABS(ABS(W(3)-W(6))-WD)
      T18(K1)=ABS(ABS(W(3)-W(7))-WD)
      T24(K1)=ABS(ABS(W(3)-W(8))-WD)
      T10(K1)=ABS(ABS(W(4)-W(5))-WD)
      T14(K1)=ABS(ABS(W(4)-W(6))-WD)
      T19(K1)=ABS(ABS(W(4)-W(7))-WD)
      T25(K1)=ABS(ABS(W(4)-W(8))-WD)
      T15(K1)=ABS(ABS(W(5)-W(6))-WD)
      T20(K1)=ABS(ABS(W(5)-W(7))-WD)
      T26(K1)=ABS(ABS(W(5)-W(8))-WD)
      T21(K1)=ABS(ABS(W(6)-W(7))-WD)
      T27(K1)=ABS(ABS(W(6)-W(8))-WD)
      T28(K1)=ABS(ABS(W(7)-W(8))-WD)
    5 CONTINUE
      WRITE(6,11)((K4(K),T1(K)),K=1,451)
      WRITE(6,12)((K4(K),T2(K)),K=1,451)
      WRITE(6,13)((K4(K),T3(K)),K=1,451)
      WRITE(6,14)((K4(K),T4(K)),K=1,451)
      WRITE(6,15)((K4(K),T5(K)),K=1,451)
      WRITE(6,16)((K4(K),T6(K)),K=1,451)
      WRITE(6,17)((K4(K),T7(K)),K=1,451)
      WRITE(6,18)((K4(K),T8(K)),K=1,451)
      WRITE(6,19)((K4(K),T9(K)),K=1,451)
      WRITE(6,20)((K4(K),T10(K)),K=1,451)
      WRITE(6,21)((K4(K),T11(K)),K=1,451)
      WRITE(6,22)((K4(K),T12(K)),K=1,451)
      WRITE(6,23)((K4(K),T13(K)),K=1,451)
      WRITE(6,24)((K4(K),T14(K)),K=1,451)
      WRITE(6,25)((K4(K),T15(K)),K=1,451)
      WRITE(6,26)((K4(K),T16(K)),K=1,451)
      WRITE(6,27)((K4(K),T17(K)),K=1,451)
      WRITE(6,28)((K4(K),T18(K)),K=1,451)
      WRITE(6,29)((K4(K),T19(K)),K=1,451)
      WRITE(6,30)((K4(K),T20(K)),K=1,451)
      WRITE(6,31)((K4(K),T21(K)),K=1,451)
      WRITE(6,32)((K4(K),T22(K)),K=1,451)
      WRITE(6,33)((K4(K),T23(K)),K=1,451)
      WRITE(6,34)((K4(K),T24(K)),K=1,451)
      WRITE(6,35)((K4(K),T25(K)),K=1,451)
      WRITE(6,36)((K4(K),T26(K)),K=1,451)
      WRITE(6,37)((K4(K),T27(K)),K=1,451)
      WRITE(6,38)((K4(K),T28(K)),K=1,451)
   11 FORMAT(5(5X,*T1(*,I4,*)=*,E10.4))
   12 FORMAT(5(5X,*T2(*,I4,*)=*,E10.4))
   13 FORMAT(5(5X,*T3(*,I4,*)=*,E10.4))
   14 FORMAT(5(5X,*T4(*,I4,*)=*,E10.4))
```

```
15 FORMAT(5(5X,*T5(*,I4,*)=*,E10.4))
16 FORMAT(5(5X,*T6(*,I4,*)=*,E10.4))
17 FORMAT(5(5X,*T7(*,I4,*)=*,E10.4))
18 FORMAT(5(5X,*T8(*,I4,*)=*,E10.4))
19 FORMAT(5(5X,*T9(*,I4,*)=*,E10.4))
20 FORMAT(5(5X,*T10(*,I4,*)=*,E10.4))
21 FORMAT(5(5X,*T11(*,I4,*)=*,E10.4))
22 FORMAT(5(5X,*T12(*,I4,*)=*,E10.4))
23 FORMAT(5(5X,*T13(*,I4,*)=*,E10.4))
24 FORMAT(5(5X,*T14(*,I4,*)=*,E10.4))
25 FORMAT(5(5X,*T15(*,I4,*)=*,E10.4))
26 FORMAT(5(5X,*T16(*,I4,*)=*,E10.4))
27 FORMAT(5(5X,*T17(*,I4,*)=*,E10.4))
28 FORMAT(5(5X,*T18(*,I4,*)=*,E10.4))
29 FORMAT(5(5X,*T19(*,I4,*)=*,E10.4))
30 FORMAT(5(5X,*T20(*,I4,*)=*,E10.4))
31 FORMAT(5(5X,*T21(*,I4,*)=*,E10.4))
32 FORMAT(5(5X,*T22(*,I4,*)=*,E10.4))
33 FORMAT(5(5X,*T23(*,I4,*)=*,E10.4))
34 FORMAT(5(5X,*T24(*,I4,*)=*,E10.4))
35 FORMAT(5(5X,*T25(*,I4,*)=*,E10.4))
36 FORMAT(5(5X,*T26(*,I4,*)=*,E10.4))
37 FORMAT(5(5X,*T27(*,I4,*)=*,E10.4))
38 FORMAT(5(5X,*T28(*,I4,*)=*,E10.4))
   STOP
   END
```

```
PROGRAM TAKIS8(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
DIMENSION SPH(8,8),A(36),W(8),ZR(8,8),SI(8,8),SZ(8,8),SX(8,8),
7SZX(8,8),EV1(8,8),EV2(8,8),EV3(8,8),EV4(8,8),EV5(8,8),EV6(8,8),
8D1(28),D2(28),D3(28),TR(8,28),I6(28),I7(28),D4(28),D5(28),D6(28),
9D7(28),D8(28),D9(28),D10(28),GDD(450,28),D11(28),D12(28),
4D13(28),D14(28),D15(28),D16(28),D17(28),D18(28),D19(28),D20(28),
1D21(28),D22(28),D23(28),D24(28),D25(28),D26(28),D27(28),
2D28(28),EV7(8,8),EV8(8,8)
ED=.1
WD=.4
R1=1./2.
R2=SQRT(3.)
R3=SQRT(7.)
R4=SQRT(15.)
PI=3.14159264
GO TO 7
GDD(1,1)=.05
GDD(1,2)=.09
GDD(1,3)=.15
GDD(1,4)=.77
GDD(1,5)=.91
GDD(1,6)=.93
GDD(1,7)=1.07
GDD(1,8)=1.25
GDD(1,9)=1.83
GDD(1,10)=1.91
GDD(1,11)=2.07
GDD(1,12)=2.15
GDD(1,13)=2.65
GDD(1,14)=2.89
7 CONTINUE
GDD(1,15)=3.37
GO TO 8
GDD(1,16)=3.83
GDD(1,17)=4.13
GDD(1,18)=4.51
8 CONTINUE
GDD(1,19)=5.51
GDD(1,20)=6.39
GO TO 2
GDD(1,21)=8.19
GDD(1,22)=8.39
GDD(1,23)=10.39
GDD(1,24)=12.41
GDD(1,25)=5.69
GDD(1,26)=7.61
2 CONTINUE
SZ(1,1)=7.*R1
SZ(1,2)=0.
SZ(1,3)=0.
SZ(1,4)=0.
SZ(1,5)=0.
SZ(1,6)=0.
SZ(1,7)=0.
```

```
SZ(1,8)=0.
SZ(2,1)=0.
SZ(2,2)=5.*R1
SZ(2,3)=0.
SZ(2,4)=0.
SZ(2,5)=0.
SZ(2,6)=0.
SZ(2,7)=0.
SZ(2,8)=0.
SZ(3,1)=0.
SZ(3,2)=0.
SZ(3,3)=3.*R1
SZ(3,4)=0.
SZ(3,5)=0.
SZ(3,6)=0.
SZ(3,7)=0.
SZ(3,8)=0.
SZ(4,1)=0.
SZ(4,2)=0.
SZ(4,3)=0.
SZ(4,4)=R1
SZ(4,5)=0.
SZ(4,6)=0.
SZ(4,7)=0.
SZ(4,8)=0.
SZ(5,1)=0.
SZ(5,2)=0.
SZ(5,3)=0.
SZ(5,4)=0.
SZ(5,5)=-R1
SZ(5,6)=0.
SZ(5,7)=0.
SZ(5,8)=0.
SZ(6,1)=0.
SZ(6,2)=0.
SZ(6,3)=0.
SZ(6,4)=0.
SZ(6,5)=0.
SZ(6,6)=-3.*R1
SZ(6,7)=0.
SZ(6,8)=0.
SZ(7,1)=0.
SZ(7,2)=0.
SZ(7,3)=0.
SZ(7,4)=0.
SZ(7,5)=0.
SZ(7,6)=0.
SZ(7,7)=-5.*R1
SZ(7,8)=0.
SZ(8,1)=0.
SZ(8,2)=0.
SZ(8,3)=0.
SZ(8,4)=0.
```

```
SZ(8,5)=0.
SZ(8,6)=0.
SZ(8,7)=0.
SZ(8,8)=-7.*R1
SX(1,1)=0.
SX(1,2)=R1*R3
SX(1,3)=0.
SX(1,4)=0.
SX(1,5)=0.
SX(1,6)=0.
SX(1,7)=0.
SX(1,8)=0.
SX(2,1)=R1*R3
SX(2,2)=0.
SX(2,3)=R2
SX(2,4)=0.
SX(2,5)=0.
SX(2,6)=0.
SX(2,7)=0.
SX(2,8)=0.
SX(3,1)=0.
SX(3,2)=R2
SX(3,3)=0.
SX(3,4)=R1*R4
SX(3,5)=0.
SX(3,6)=0.
SX(3,7)=0.
SX(3,8)=0.
SX(4,1)=0.
SX(4,2)=0.
SX(4,3)=R4*R1
SX(4,4)=0.
SX(4,5)=2.
SX(4,6)=0.
SX(4,7)=0.
SX(4,8)=0.
SX(5,1)=0.
SX(5,2)=0.
SX(5,3)=0.
SX(5,4)=2.
SX(5,5)=0.
SX(5,6)=R1*R4
SX(5,7)=0.
SX(5,8)=0.
SX(6,1)=0.
SX(6,2)=0.
SX(6,3)=0.
SX(6,4)=0.
SX(6,5)=R1*R4
SX(6,6)=0.
SX(6,7)=R2
SX(6,8)=0.
SX(7,1)=0.
```

```
      SX(7,2)=0.
      SX(7,3)=0.
      SX(7,4)=0.
      SX(7,5)=0.
      SX(7,6)=R2
      SX(7,7)=0.
      SX(7,8)=R1*R3
      SX(8,1)=0.
      SX(8,2)=0.
      SX(8,3)=0.
      SX(8,4)=0.
      SX(8,5)=0.
      SX(8,6)=0.
      SX(8,7)=R1*R3
      SX(8,8)=0.
      DO 40 IK=1,359
      DELTA=PI/720.
      THETA=DELTA*FLOAT(IK-1)
      CN=COS(THETA)
      SN=SIN(THETA)
      DO 1 I=1,26
C     SPH REPRESENTS THE SPIN HAMILTONIAN
      SPH(1,1)=7.*R1*GDD(IK,I)*CN+7.
      SPH(1,2)=R1*R3*GDD(IK,I)*SN
      SPH(1,3)=R2*R3*ED
      SPH(1,4)=0.
      SPH(1,5)=0.
      SPH(1,6)=0.
      SPH(1,7)=0.
      SPH(1,8)=0.
      SPH(2,1)=R1*R3*GDD(IK,I)*SN
      SPH(2,2)=5.*R1*GDD(IK,I)*CN+1.
      SPH(2,3)=R2*GDD(IK,I)*SN
      SPH(2,4)=R4*R2*ED
      SPH(2,5)=0.
      SPH(2,6)=0.
      SPH(2,7)=0.
      SPH(2,8)=0.
      SPH(3,1)=R2*R3*ED
      SPH(3,2)=R2*GDD(IK,I)*SN
      SPH(3,3)=-3.+3.*R1*GDD(IK,I)*CN
      SPH(3,4)=R4*R1*GDD(IK,I)*SN
      SPH(3,5)=2.*R4*ED
      SPH(3,6)=0.
      SPH(3,7)=0.
      SPH(3,8)=0.
      SPH(4,1)=0.
      SPH(4,2)=R4*R2*ED
      SPH(4,3)=R4*R1*GDD(IK,I)*SN
      SPH(4,4)=R1*GDD(IK,I)*CN-5.
      SPH(4,5)=2.*GDD(IK,I)*SN
      SPH(4,6)=2.*R4*ED
      SPH(4,7)=0.
```

```
      SPH(4,8)=0.
      SPH(5,1)=0.
      SPH(5,2)=0.
      SPH(5,3)=2.*R4*ED
      SPH(5,4)=2.*GDD(IK,I)*SN
      SPH(5,5)=-5.-R1*GDD(IK,I)*CN
      SPH(5,6)=R1*R4*GDD(IK,I)*SN
      SPH(5,7)=R2*R4*ED
      SPH(5,8)=0.
      SPH(6,1)=0.
      SPH(6,2)=0.
      SPH(6,3)=0.
      SPH(6,4)=2.*R4*ED
      SPH(6,5)=R1*R4*GDD(IK,I)*SN
      SPH(6,6)=-3.-3.*R1*GDD(IK,I)*CN
      SPH(6,7)=R2*GDD(IK,I)*SN
      SPH(6,8)=R2*R3*ED
      SPH(7,1)=0.
      SPH(7,2)=0.
      SPH(7,3)=0.
      SPH(7,4)=0.
      SPH(7,5)=R2*R4*ED
      SPH(7,6)=R2*GDD(IK,I)*SN
      SPH(7,7)=-5.*R1*GDD(IK,I)*CN+1.
      SPH(7,8)=R1*R3*GDD(IK,I)*SN
      SPH(8,1)=0.
      SPH(8,2)=0.
      SPH(8,3)=0.
      SPH(8,4)=0.
      SPH(8,5)=0.
      SPH(8,6)=R2*R3*ED
      SPH(8,7)=R1*R3*GDD(IK,I)*SN
      SPH(8,8)=-7.*R1*GDD(IK,I)*CN+7.
      DO 995 I1=1,8
      W(I1)=0.
      DO 995 I2=1,8
      SI(I1,I2)=0.
  995 ZR(I1,I2)=0.
      DO 999 II=1,8
      DO 999 JJ=1,II
      KK=II*(II-1)/2+JJ
  999 A(KK)=SPH(II,JJ)
      CALL EIGRS(A,8,1,W,ZR,8,SI,IER)
      IF (IER) 997,996,997
  997 CONTINUE
      WRITE(6,998)IER
  996 CONTINUE
  998 FORMAT(5X,*IER=*,I3)
      GO TO 111
      I6(I)=1
      I7(I)=2
      IEQ=0.
      AMIN=ABS(ABS(W(1)-W(2))-WD)
```

```
      DO 100 L=1,7
      L1=L+1
      DO 100 M=L1,8
      TEMP=ABS(ABS(W(L)-W(M))-WD)
      IF (TEMP-AMIN) 105,106,110
  105 AMIN=TEMP
      I6(I)=L
      I7(I)=M
      GO TO 110
  106 IEQ=IEQ+1.
  110 CONTINUE
  100 CONTINUE
  111 CONTINUE
      I6(1)=8
      I7(1)=7
      I6(2)=6
      I7(2)=5
      I6(3)=4
      I7(3)=3
      I6(4)=2
      I7(4)=1
      I6(5)=5
      I7(5)=4
      I6(6)=7
      I7(6)=6
      I6(7)=5
      I7(7)=4
      I6(8)=2
      I7(8)=1
      I6(9)=4
      I7(9)=3
      I6(10)=6
      I7(10)=5
      I6(11)=6
      I7(11)=5
      I6(12)=4
      I7(12)=3
      I6(13)=2
      I7(13)=1
      I6(14)=5
      I7(14)=4
      I6(15)=2
      I7(15)=1
      I6(16)=4
      I7(16)=3
      I6(17)=4
      I7(17)=3
      I6(18)=2
      I7(18)=1
      I6(19)=2
      I7(19)=1
      I6(20)=2
      I7(20)=1
```

```
      I6(21)=3
      I7(21)=1
      I6(22)=4
      I7(22)=3
      I6(23)=3
      I7(23)=2
      I6(24)=2
      I7(24)=1
      I6(25)=3
      I7(25)=2
      I6(26)=2
      I7(26)=1
      GO TO 25
      WRITE(6,20)I,W(1),W(2),W(3),W(4),W(5),W(6),W(7),W(8)
   20 FORMAT(2X,*I=*,I2,1X,*W(1)=*,E10.4,1X,*W(2)=*,E10.4,
     31X,*W(3)=*,E10.4,1X,*W(4)=*,E10.4,1X,*W(5)=*,E10.4,
     61X,*W(6)=*,E10.4,1X,*W(7)=*,E10.4,1X,*W(8)=*,E10.4,/)
   25 CONTINUE
      DO 11 K=1,8
      DO 11 J=1,8
      SZX(K,J)=SZ(K,J)*CN+SX(K,J)*SN
      EV1(K,J)=ZR(K,1)*ZR(J,1)
      EV2(K,J)=ZR(K,2)*ZR(J,2)
      EV3(K,J)=ZR(K,3)*ZR(J,3)
      EV4(K,J)=ZR(K,4)*ZR(J,4)
      EV5(K,J)=ZR(K,5)*ZR(J,5)
      EV6(K,J)=ZR(K,6)*ZR(J,6)
      EV7(K,J)=ZR(K,7)*ZR(J,7)
      EV8(K,J)=ZR(K,8)*ZR(J,8)
   11 CONTINUE
      TR(1,I)=0.
      TR(2,I)=0.
      TR(3,I)=0.
      TR(4,I)=0.
      TR(5,I)=0.
      TR(6,I)=0.
      TR(7,I)=0.
      TR(8,I)=0.
      DO 12 K=1,8
      DO 12 J=1,8
      TR(1,I)=TR(1,I)+SZX(K,J)*EV1(J,K)
      TR(2,I)=TR(2,I)+SZX(K,J)*EV2(J,K)
      TR(3,I)=TR(3,I)+SZX(K,J)*EV3(J,K)
      TR(4,I)=TR(4,I)+SZX(K,J)*EV4(J,K)
      TR(5,I)=TR(5,I)+SZX(K,J)*EV5(J,K)
      TR(6,I)=TR(6,I)+SZX(K,J)*EV6(J,K)
      TR(7,I)=TR(7,I)+SZX(K,J)*EV7(J,K)
      TR(8,I)=TR(8,I)+SZX(K,J)*EV8(J,K)
   12 CONTINUE
      D1(I)=W(I6(1))-W(I7(1))
      D2(I)=W(I6(2))-W(I7(2))
      D3(I)=W(I6(3))-W(I7(3))
      D4(I)=W(I6(4))-W(I7(4))
```

```
      D5(I)=W(I6(5))-W(I7(5))
      D6(I)=W(I6(6))-W(I7(6))
      D7(I)=W(I6(7))-W(I7(7))
      D8(I)=W(I6(8))-W(I7(8))
      D9(I)=W(I6(9))-W(I7(9))
      D10(I)=W(I6(10))-W(I7(10))
      D11(I)=W(I6(11))-W(I7(11))
      D12(I)=W(I6(12))-W(I7(12))
      D13(I)=W(I6(13))-W(I7(13))
      D14(I)=W(I6(14))-W(I7(14))
      D15(I)=W(I6(15))-W(I7(15))
      D16(I)=W(I6(16))-W(I7(16))
      D17(I)=W(I6(17))-W(I7(17))
      D18(I)=W(I6(18))-W(I7(18))
      D19(I)=W(I6(19))-W(I7(19))
      D20(I)=W(I6(20))-W(I7(20))
      D21(I)=W(I6(21))-W(I7(21))
      D22(I)=W(I6(22))-W(I7(22))
      D23(I)=W(I6(23))-W(I7(23))
      D24(I)=W(I6(24))-W(I7(24))
      D25(I)=W(I6(25))-W(I7(25))
      D26(I)=W(I6(26))-W(I7(26))
    1 CONTINUE
      S1=(D1(1)/ABS(D1(1)))*(ABS(D1(1))-WD)*(TR(I6(1),1)-TR(I7(1),1))
      S2=(TR(I6(1),1)-TR(I7(1),1))**2
      S3=(D2(2)/ABS(D2(2)))*(ABS(D2(2))-WD)*(TR(I6(2),2)-TR(I7(2),2))
      S4=(TR(I6(2),2)-TR(I7(2),2))**2
      S5=(D3(3)/ABS(D3(3)))*(ABS(D3(3))-WD)*(TR(I6(3),3)-TR(I7(3),3))
      S6=(TR(I6(3),3)-TR(I7(3),3))**2
      S7=(D4(4)/ABS(D4(4)))*(ABS(D4(4))-WD)*(TR(I6(4),4)-TR(I7(4),4))
      S8=(TR(I6(4),4)-TR(I7(4),4))**2
      S9=(D5(5)/ABS(D5(5)))*(ABS(D5(5))-WD)*(TR(I6(5),5)-TR(I7(5),5))
      S10=(TR(I6(5),5)-TR(I7(5),5))**2
      S11=(D6(6)/ABS(D6(6)))*(ABS(D6(6))-WD)*(TR(I6(6),6)-TR(I7(6),6))
      S12=(TR(I6(6),6)-TR(I7(6),6))**2
      S13=(D7(7)/ABS(D7(7)))*(ABS(D7(7))-WD)*(TR(I6(7),7)-TR(I7(7),7))
      S14=(TR(I6(7),7)-TR(I7(7),7))**2
      S15=(D8(8)/ABS(D8(8)))*(ABS(D8(8))-WD)*(TR(I6(8),8)-TR(I7(8),8))
      S16=(TR(I6(8),8)-TR(I7(8),8))**2
      S17=(D9(9)/ABS(D9(9)))*(ABS(D9(9))-WD)*(TR(I6(9),9)-TR(I7(9),9))
      S18=(TR(I6(9),9)-TR(I7(9),9))**2
      S19=(D10(10)/ABS(D10(10)))*(ABS(D10(10))-WD)*(TR(I6(10),10)
     5-TR(I7(10),10))
      S20=(TR(I6(10),10)-TR(I7(10),10))**2
      S21=(D11(11)/ABS(D11(11)))*(ABS(D11(11))-WD)*(TR(I6(11),11)
     1-TR(I7(11),11))
      S22=(TR(I6(11),11)-TR(I7(11),11))**2
      S23=(D12(12)/ABS(D12(12)))*(ABS(D12(12))-WD)*(TR(I6(12),12)
     2-TR(I7(12),12))
      S24=(TR(I6(12),12)-TR(I7(12),12))**2
      S25=(D13(13)/ABS(D13(13)))*(ABS(D13(13))-WD)*(TR(I6(13),13)
     3-TR(I7(13),13))
      S26=(TR(I6(13),13)-TR(I7(13),13))**2
```

```
      S27=(D14(14)/ABS(D14(14)))*(ABS(D14(14))-WD)*(TR(I6(14),14)
     4-TR(I7(14),14))
      S28=(TR(I6(14),14)-TR(I7(14),14))**2
      S29=(D15(15)/ABS(D15(15)))*(ABS(D15(15))-WD)*(TR(I6(15),15)
     5-TR(I7(15),15))
      S30=(TR(I6(15),15)-TR(I7(15),15))**2
      S31=(D16(16)/ABS(D16(16)))*(ABS(D16(16))-WD)*(TR(I6(16),16)
     1-TR(I7(16),16))
      S32=(TR(I6(16),16)-TR(I7(16),16))**2
      S33=(D17(17)/ABS(D17(17)))*(ABS(D17(17))-WD)*(TR(I6(17),17)
     1-TR(I7(17),17))
      S34=(TR(I6(17),17)-TR(I7(17),17))**2
      S35=(D18(18)/ABS(D18(18)))*(ABS(D18(18))-WD)*(TR(I6(18),18)
     1-TR(I7(18),18))
      S36=(TR(I6(18),18)-TR(I7(18),18))**2
      S37=(D19(19)/ABS(D19(19)))*(ABS(D19(19))-WD)*(TR(I6(19),19)
     1-TR(I7(19),19))
      S38=(TR(I6(19),19)-TR(I7(19),19))**2
      S39=(D20(20)/ABS(D20(20)))*(ABS(D20(20))-WD)*(TR(I6(20),20)
     1-TR(I7(20),20))
      S40=(TR(I6(20),20)-TR(I7(20),20))**2
      S41=(D21(21)/ABS(D21(21)))*(ABS(D21(21))-WD)*(TR(I6(21),21)
     1-TR(I7(21),21))
      S42=(TR(I6(21),21)-TR(I7(21),21))**2
      S43=(D22(22)/ABS(D22(22)))*(ABS(D22(22))-WD)*(TR(I6(22),22)
     1-TR(I7(22),22))
      S44=(TR(I6(22),22)-TR(I7(22),22))**2
      S45=(D23(23)/ABS(D23(23)))*(ABS(D23(23))-WD)*(TR(I6(23),23)
     1-TR(I7(23),23))
      S46=(TR(I6(23),23)-TR(I7(23),23))**2
      S47=(D24(24)/ABS(D24(24)))*(ABS(D24(24))-WD)*(TR(I6(24),24)
     1-TR(I7(24),24))
      S48=(TR(I6(24),24)-TR(I7(24),24))**2
      S49=(D25(25)/ABS(D25(25)))*(ABS(D25(25))-WD)*(TR(I6(25),25)
     1-TR(I7(25),25))
      S50=(TR(I6(25),25)-TR(I7(25),25))**2
      S51=(D26(26)/ABS(D26(26)))*(ABS(D26(26))-WD)*(TR(I6(26),26)
     1-TR(I7(26),26))
      S52=(TR(I6(26),26)-TR(I7(26),26))**2
   13 CONTINUE
      IK1=IK+1
      GDD(IK1,1)=GDD(IK,1)-S1/S2
      GDD(IK1,2)=GDD(IK,2)-S3/S4
      GDD(IK1,3)=GDD(IK,3)-S5/S6
      GDD(IK1,4)=GDD(IK,4)-S7/S8
      GDD(IK1,5)=GDD(IK,5)-S9/S10
      GDD(IK1,6)=GDD(IK,6)-S11/S12
      GDD(IK1,7)=GDD(IK,7)-S13/S14
      GDD(IK1,8)=GDD(IK,8)-S15/S16
      GDD(IK1,9)=GDD(IK,9)-S17/S18
    9 CONTINUE
      GDD(IK1,10)=GDD(IK,10)-S19/S20
      GDD(IK1,11)=GDD(IK,11)-S21/S22
```

```
      GDD(IK1,12)=GDD(IK,12)-S23/S24
      GDD(IK1,13)=GDD(IK,13)-S25/S26
      GDD(IK1,14)=GDD(IK,14)-S27/S28
    6 CONTINUE
      GDD(IK1,15)=GDD(IK,15)-S29/S30
      GDD(IK1,16)=GDD(IK,16)-S31/S32
      GDD(IK1,17)=GDD(IK,17)-S33/S34
      GDD(IK1,18)=GDD(IK,18)-S35/S36
      GDD(IK1,19)=GDD(IK,19)-S37/S38
      GDD(IK1,20)=GDD(IK,20)-S39/S40
      GO TO 3
      GDD(IK1,21)=GDD(IK,21)-S41/S42
      GDD(IK1,22)=GDD(IK,22)-S43/S44
      GDD(IK1,23)=GDD(IK,23)-S45/S46
      GDD(IK1,24)=GDD(IK,24)-S47/S48
      GDD(IK1,25)=GDD(IK,25)-S49/S50
      GDD(IK1,26)=GDD(IK,26)-S51/S52
      WRITE(6,50)IK1,GDD(IK1,1),GDD(IK1,2),GDD(IK1,3),
     1GDD(IK1,4),GDD(IK1,5)
      WRITE(6,55)IK1,GDD(IK1,6),GDD(IK1,7),GDD(IK1,8),
     1GDD(IK1,9),GDD(IK1,10)
    3 CONTINUE
      WRITE(6,66)IK1,GDD(IK1,11),GDD(IK1,12),GDD(IK1,13),
     1GDD(IK1,14),GDD(IK1,15)
      WRITE(6,77)IK1,GDD(IK1,16),GDD(IK1,17),GDD(IK1,18),
     1GDD(IK1,19),GDD(IK1,20)
      GO TO 41
      WRITE(6,88)IK1,GDD(IK1,21),GDD(IK1,22),GDD(IK1,23),
     1GDD(IK1,24)
   41 CONTINUE
   50 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,1)=*,E10.4,2X,*GDD(IK1,2)=*,E10.4,
     12X,*GDD(IK1,3)=*,E10.4,*GDD(IK1,4)=*,E10.4,*GDD(IK1,5)=*,E10.4,/)
   55 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,6)=*,E10.4,2X,*GDD(IK1,7)=*,E10.4,
     12X,*GDD(IK1,8)=*,E10.4,*GDD(IK1,9)=*,E10.4,*GDD(IK1,10)=*,E10.4,/)
   66 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,11)=*,E10.4,*GDD(IK1,12)=*,E10.4,
     1*GDD(IK1,13)=*,E10.4,*GDD(IK1,14)=*,E10.4,*GDD(IK1,15)=*,E10.4,/)
   77 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,16)=*,E10.4,*GDD(IK1,17)=*,E10.4,
     1*GDD(IK1,18)=*,E10.4,*GDD(IK1,19)=*,E10.4,*GDD(IK1,20)=*,E10.4,//)
   88 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,21)=*,E10.4,2X,*GDD(IK1,22)=*,
     1E10.4,2X,*GDD(IK1,23)=*,E10.4,2X,*GDD(IK1,24)=*,E10.4,//)
   40 CONTINUE
      STOP
      END
```

```
      PROGRAM TAKI1(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SPH(8,8),A(36),W(8),ZR(8,8),SI(8,8),SZ(8,8),SX(8,8),
     7SZX(8,8),EV1(8,8),EV2(8,8),EV3(8,8),EV4(8,8),EV5(8,8),EV6(8,8),
     8D1(28),D2(28),D3(28),TR(8,28),I6(28),I7(28),D4(28),D5(28),D6(28),
     9D7(28),D8(28),D9(28),D10(28),GDD(540,28),D11(28),D12(28),
     4D13(28),D14(28),D15(28),D16(28),D17(28),D18(28),D19(28),D20(28),
     1D21(28),D22(28),D23(28),D24(28),D25(28),D26(28),D27(28),
     2D28(28),EV7(8,8),EV8(8,8)
      PI=3.14159264
      R1=1./2.
      R2=SQRT(3.)
      R3=SQRT(7.)
      R4=SQRT(5.)
      GDD(1,1)=.55
      GDD(1,2)=1.125
      GDD(1,3)=2.33
      GDD(1,4)=3.73
      GDD(1,5)=5.12
      GDD(1,6)=6.45
      GDD(1,7)=7.55
      GO TO 2
      GDD(1,8)=1.19
      GDD(1,9)=1.61
      GDD(1,10)=1.85
      GDD(1,11)=1.91
      GDD(1,12)=2.07
      GDD(1,13)=2.17
    7 CONTINUE
      GDD(1,14)=2.87
      GDD(1,15)=3.41
      GDD(1,16)=3.65
      GDD(1,17)=4.79
      GDD(1,18)=4.93
      GDD(1,19)=6.11
      GDD(1,20)=7.19
      GDD(1,21)=5.33
      GDD(1,22)=5.69
      GDD(1,23)=7.61
      GDD(1,24)=5.27
      GDD(1,25)=5.69
      GDD(1,26)=7.61
    2 CONTINUE
      SZ(1,1)=7.*R1
      SZ(1,2)=0.
      SZ(1,3)=0.
      SZ(1,4)=0.
      SZ(1,5)=0.
      SZ(1,6)=0.
      SZ(1,7)=0.
      SZ(1,8)=0.
      SZ(2,1)=0.
      SZ(2,2)=5.*R1
      SZ(2,3)=0.
      SZ(2,4)=0.
```

```
SZ(2,5)=0.
SZ(2,6)=0.
SZ(2,7)=0.
SZ(2,8)=0.
SZ(3,1)=0.
SZ(3,2)=0.
SZ(3,3)=3.*R1
SZ(3,4)=0.
SZ(3,5)=0.
SZ(3,6)=0.
SZ(3,7)=0.
SZ(3,8)=0.
SZ(4,1)=0.
SZ(4,2)=0.
SZ(4,3)=0.
SZ(4,4)=R1
SZ(4,5)=0.
SZ(4,6)=0.
SZ(4,7)=0.
SZ(4,8)=0.
SZ(5,1)=0.
SZ(5,2)=0.
SZ(5,3)=0.
SZ(5,4)=0.
SZ(5,5)=-R1
SZ(5,6)=0.
SZ(5,7)=0.
SZ(5,8)=0.
SZ(6,1)=0.
SZ(6,2)=0.
SZ(6,3)=0.
SZ(6,4)=0.
SZ(6,5)=0.
SZ(6,6)=-3.*R1
SZ(6,7)=0.
SZ(6,8)=0.
SZ(7,1)=0.
SZ(7,2)=0.
SZ(7,3)=0.
SZ(7,4)=0.
SZ(7,5)=0.
SZ(7,6)=0.
SZ(7,7)=-5.*R1
SZ(7,8)=0.
SZ(8,1)=0.
SZ(8,2)=0.
SZ(8,3)=0.
SZ(8,4)=0.
SZ(8,5)=0.
SZ(8,6)=0.
SZ(8,7)=0.
SZ(8,8)=-7.*R1
SX(1,1)=0.
```

```
SX(1,2)=R1*R3
SX(1,3)=0.
SX(1,4)=0.
SX(1,5)=0.
SX(1,6)=0.
SX(1,7)=0.
SX(1,8)=0.
SX(2,1)=R1*R3
SX(2,2)=0.
SX(2,3)=R2
SX(2,4)=0.
SX(2,5)=0.
SX(2,6)=0.
SX(2,7)=0.
SX(2,8)=0.
SX(3,1)=0.
SX(3,2)=R2
SX(3,3)=0.
SX(3,4)=R1*R4
SX(3,5)=0.
SX(3,6)=0.
SX(3,7)=0.
SX(3,8)=0.
SX(4,1)=0.
SX(4,2)=0.
SX(4,3)=R4*R1
SX(4,4)=0.
SX(4,5)=2.
SX(4,6)=0.
SX(4,7)=0.
SX(4,8)=0.
SX(5,1)=0.
SX(5,2)=0.
SX(5,3)=0.
SX(5,4)=2.
SX(5,5)=0.
SX(5,6)=R1*R4
SX(5,7)=0.
SX(5,8)=0.
SX(6,1)=0.
SX(6,2)=0.
SX(6,3)=0.
SX(6,4)=0.
SX(6,5)=R1*R4
SX(6,6)=0.
SX(6,7)=R2
SX(6,8)=0.
SX(7,1)=0.
SX(7,2)=0.
SX(7,3)=0.
SX(7,4)=0.
SX(7,5)=0.
SX(7,6)=R2
```

```
SPH(2,3)=R2*GX*B*GDD(IK,I)*SN
SPH(2,4)=R4*(3.*B11+B22*6.-21.*24.*B33)
SPH(2,5)=0.
SPH(2,6)=R2*(60.*C11-420.*C22)
SPH(2,7)=0.
SPH(2,8)=360.*R3*C33
SPH(3,1)=R2*R3*(B11+B22*30.+B33*120.)
SPH(3,2)=R2*GX*B*GDD(IK,I)*SN
SPH(3,3)=-3.*A11-3.*A22+9.*A33+3.*R1*GDD(IK,I)*B*GZ*CN
SPH(3,4)=R1*R2*R4*GX*B*GDD(IK,I)*SN
SPH(3,5)=R2*R4*(2.*B11-24.*B22+168.*B33)
SPH(3,6)=0.
SPH(3,7)=R2*(60.*C11-420.*C22)
SPH(3,8)=0.
SPH(4,1)=0.
SPH(4,2)=R4*(3.*B11+B22*6.-21.*24.*B33)
SPH(4,3)=R1*R2*R4*GX*B*GDD(IK,I)*SN
SPH(4,4)=-5.*A11+9.*A22-5.*A33+R1*GDD(IK,I)*B*GZ*CN
SPH(4,5)=2.*GX*B*GDD(IK,I)*SN
SPH(4,6)=R2*R4*(2.*B11-24.*B22+168.*B33)
SPH(4,7)=0.
SPH(4,8)=R3*R4*(12.*C11+180.*C22)
SPH(5,1)=R3*R4*(12.*C11+180.*C22)
SPH(5,2)=0.
SPH(5,3)=R2*R4*(2.*B11-24.*B22+168.*B33)
SPH(5,4)=2.*GX*B*GDD(IK,I)*SN
SPH(5,5)=-5.*A11+9.*A22-5.*A33-R1*GDD(IK,I)*B*GZ*CN
SPH(5,6)=R1*R2*R4*GX*B*GDD(IK,I)*SN
SPH(5,7)=R4*(3.*B11+6.*B22-21.*24.*B33)
SPH(5,8)=0.
SPH(6,1)=0.
SPH(6,2)=R2*(60.*C11-420.*C22)
SPH(6,3)=0.
SPH(6,4)=R2*R4*(2.*B11-24.*B22+168.*B33)
SPH(6,5)=R1*R2*R4*GX*B*GDD(IK,I)*SN
SPH(6,6)=-3.*A11-3.*A22+9.*A33-3.*R1*GDD(IK,I)*B*GZ*CN
SPH(6,7)=R2*GX*B*GDD(IK,I)*SN
SPH(6,8)=R2*R3*(B11+30.*B22+120.*B33)
SPH(7,1)=360.*R3*C33
SPH(7,2)=0.
SPH(7,3)=R2*(60.*C11-420.*C22)
SPH(7,4)=0.
SPH(7,5)=R4*(3.*B11+6.*B22-21.*24.*B33)
SPH(7,6)=R2*GX*B*GDD(IK,I)*SN
SPH(7,7)=A11-13.*A22-5.*A33-5.*R1*GDD(IK,I)*B*GZ*CN
SPH(7,8)=R1*R3*GX*B*GDD(IK,I)*SN
SPH(8,1)=0.
SPH(8,2)=360.*R3*C33
SPH(8,3)=0.
SPH(8,4)=R3*R4*(12.*C11+180.*C22)
SPH(8,5)=0.
SPH(8,6)=R2*R3*(B11+30.*B22+120.*B33)
SPH(8,7)=R1*R3*GX*B*GDD(IK,I)*SN
```

```
SX(7,7)=0.
SX(7,8)=R1*R3
SX(8,1)=0.
SX(8,2)=0.
SX(8,3)=0.
SX(8,4)=0.
SX(8,5)=0.
SX(8,6)=0.
SX(8,7)=R1*R3
SX(8,8)=0.
R5=SQRT(35.)
R6=1./3.
R7=1./7.
R8=1./105.
R9=1./5.
A1=1.864
A2=-.033
A3=.001
B1=-1.053
B2=.028
B3=.034
C1=-.002
C2=.047
C3=.038
GZ=1.993
GX=1.992
B=9.274/6.626
WD=10.3702
A11=(1./2.)*(B1-A1)
A22=(1./8.)*(3.*A2-B2+C1)
A33=(1./16.)*(-5.*A3+B3-C2+C3)
B11=-(1./6.)*(3.*A1+B1)
B22=(1./120.)*(5.*A2-B2-C1)
B33=(1./32.)*(1./1260.)*(-105.*A3+17.*B3-5.*C2-15.*C3)
C11=(1./480.)*(35.*A2+7.*B2+C1)
C22=(1./16.)*(1./1260.)*(-63.*A3+3.*B3+13.*C2+3.*C3)
C33=-(1./32.)*(1./1260.)*(231.*A3+33.*B3+11.*C2+C3)
DO 40 IK=1,179
DELTA=PI/360.
THETA=DELTA*FLOAT(IK-1)
CN=COS(THETA)
SN=SIN(THETA)
DO 1 I=1,7
SPH(1,1)=7.*R1*GDD(IK,I)*B*GZ*CN+7.*A11+7.*A22+A33
SPH(1,2)=R1*R3*GX*B*GDD(IK,I)*SN
SPH(1,3)=R2*R3*(B11+B22*30.+B33*120.)
SPH(1,4)=0.
SPH(1,5)=R5*(12.*C11+180.*C22)
SPH(1,6)=0.
SPH(1,7)=360.*R3*C33
SPH(1,8)=0.
SPH(2,1)=R1*R3*GX*B*GDD(IK,I)*SN
SPH(2,2)=A11-13.*A22-5.*A33+5.*R1*GDD(IK,I)*B*GZ*CN
```

```
      SPH(8,8)=7.*A11+7.*A22+A33-7.*R1*GDD(IK,I)*B*GZ*CN
      DO 995 I1=1,8
      W(I1)=0.
      DO 995 I2=1,8
      SI(I1,I2)=0.
  995 ZR(I1,I2)=0.
      DO 999 II=1,8
      DO 999 JJ=1,II
      KK=II*(II-1)/2+JJ
  999 A(KK)=SPH(II,JJ)
      CALL EIGRS(A,8,1,W,ZR,8,SI,IER)
      IF (IER) 997,996,997
  997 CONTINUE
      WRITE(6,998)IER
  996 CONTINUE
  998 FORMAT(5X,*IER=*,I3)
      GO TO 111
      I6(I)=1
      I7(I)=2
      IEQ=0.
      AMIN=ABS(ABS(W(1)-W(2))-WD)
      DO 100 L=1,7
      L1=L+1
      DO 100 M=L1,8
      TEMP=ABS(ABS(W(L)-W(M))-WD)
      IF (TEMP-AMIN) 105,106,110
  105 AMIN=TEMP
      I6(I)=L
      I7(I)=M
      GO TO 110
  106 IEQ=IEQ+1.
  110 CONTINUE
  100 CONTINUE
  111 CONTINUE
      I6(1)=8
      I7(1)=7
      I6(2)=7
      I7(2)=6
      I6(3)=6
      I7(3)=5
      I6(4)=5
      I7(4)=4
      I6(5)=4
      I7(5)=3
      I6(6)=3
      I7(6)=2
      I6(7)=2
      I7(7)=1
      I6(8)=6
      I7(8)=5
      I6(9)=6
      I7(9)=5
      I6(10)=6
```

```
      I7(10)=4
      I6(11)=6
      I7(11)=5
      I6(12)=6
      I7(12)=5
      I6(13)=3
      I7(13)=2
      I6(14)=7
      I7(14)=5
      I6(15)=6
      I7(15)=4
      I6(16)=7
      I7(16)=5
      I6(17)=7
      I7(17)=5
      I6(18)=3
      I7(18)=2
      I6(19)=4
      I7(19)=3
      I6(20)=3
      I7(20)=1
      I6(21)=3
      I7(21)=1
      I6(22)=3
      I7(22)=2
      I6(23)=2
      I7(23)=1
      I6(24)=4
      I7(24)=3
      I6(25)=3
      I7(25)=2
      I6(26)=2
      I7(26)=1
      GO TO 25
      WRITE(6,20)I,W(1),W(2),W(3),W(4),W(5),W(6),W(7),W(8)
   20 FORMAT(2X,*I=*,I2,1X,*W(1)=*,E10.4,1X,*W(2)=*,E10.4/
     31X,*W(3)=*,E10.4,1X,*W(4)=*,E10.4,1X,*W(5)=*,E10.4,
     61X,*W(6)=*,E10.4,1X,*W(7)=*,E10.4,1X,*W(8)=*,E10.4,/)
   25 CONTINUE
      DO 11 K=1,8
      DO 11 J=1,8
      SZX(K,J)=SZ(K,J)*CN*GZ*B+SX(K,J)*SN*GX*B
      EV1(K,J)=ZR(K,1)*ZR(J,1)
      EV2(K,J)=ZR(K,2)*ZR(J,2)
      EV3(K,J)=ZR(K,3)*ZR(J,3)
      EV4(K,J)=ZR(K,4)*ZR(J,4)
      EV5(K,J)=ZR(K,5)*ZR(J,5)
      EV6(K,J)=ZR(K,6)*ZR(J,6)
      EV7(K,J)=ZR(K,7)*ZR(J,7)
      EV8(K,J)=ZR(K,8)*ZR(J,8)
   11 CONTINUE
      TR(1,I)=0.
      TR(2,I)=0.
```

```
      TR(3,I)=0.
      TR(4,I)=0.
      TR(5,I)=0.
      TR(6,I)=0.
      TR(7,I)=0.
      TR(8,I)=0.
      DO 12 K=1,8
      DO 12 J=1,8
      TR(1,I)=TR(1,I)+SZX(K,J)*EV1(J,K)
      TR(2,I)=TR(2,I)+SZX(K,J)*EV2(J,K)
      TR(3,I)=TR(3,I)+SZX(K,J)*EV3(J,K)
      TR(4,I)=TR(4,I)+SZX(K,J)*EV4(J,K)
      TR(5,I)=TR(5,I)+SZX(K,J)*EV5(J,K)
      TR(6,I)=TR(6,I)+SZX(K,J)*EV6(J,K)
      TR(7,I)=TR(7,I)+SZX(K,J)*EV7(J,K)
      TR(8,I)=TR(8,I)+SZX(K,J)*EV8(J,K)
   12 CONTINUE
      D1(I)=W(I6(1))-W(I7(1))
      D2(I)=W(I6(2))-W(I7(2))
      D3(I)=W(I6(3))-W(I7(3))
      D4(I)=W(I6(4))-W(I7(4))
      D5(I)=W(I6(5))-W(I7(5))
      D6(I)=W(I6(6))-W(I7(6))
      D7(I)=W(I6(7))-W(I7(7))
      D8(I)=W(I6(8))-W(I7(8))
      D9(I)=W(I6(9))-W(I7(9))
      D10(I)=W(I6(10))-W(I7(10))
      D11(I)=W(I6(11))-W(I7(11))
      D12(I)=W(I6(12))-W(I7(12))
      D13(I)=W(I6(13))-W(I7(13))
      D14(I)=W(I6(14))-W(I7(14))
      D15(I)=W(I6(15))-W(I7(15))
      D16(I)=W(I6(16))-W(I7(16))
      D17(I)=W(I6(17))-W(I7(17))
      D18(I)=W(I6(18))-W(I7(18))
      D19(I)=W(I6(19))-W(I7(19))
      D20(I)=W(I6(20))-W(I7(20))
      D21(I)=W(I6(21))-W(I7(21))
      D22(I)=W(I6(22))-W(I7(22))
      D23(I)=W(I6(23))-W(I7(23))
      D24(I)=W(I6(24))-W(I7(24))
      D25(I)=W(I6(25))-W(I7(25))
      D26(I)=W(I6(26))-W(I7(26))
    1 CONTINUE
      S1=(D1(1)/ABS(D1(1)))*(ABS(D1(1))-WD)*(TR(I6(1),1)-TR(I7(1),1))
      S2=(TR(I6(1),1)-TR(I7(1),1))**2
      S3=(D2(2)/ABS(D2(2)))*(ABS(D2(2))-WD)*(TR(I6(2),2)-TR(I7(2),2))
      S4=(TR(I6(2),2)-TR(I7(2),2))**2
      S5=(D3(3)/ABS(D3(3)))*(ABS(D3(3))-WD)*(TR(I6(3),3)-TR(I7(3),3))
      S6=(TR(I6(3),3)-TR(I7(3),3))**2
      S7=(D4(4)/ABS(D4(4)))*(ABS(D4(4))-WD)*(TR(I6(4),4)-TR(I7(4),4))
      S8=(TR(I6(4),4)-TR(I7(4),4))**2
      S9=(D5(5)/ABS(D5(5)))*(ABS(D5(5))-WD)*(TR(I6(5),5)-TR(I7(5),5))
```

```
      S10=(TR(I6(5),5)-TR(I7(5),5))**2
      S11=(D6(6)/ABS(D6(6)))*(ABS(D6(6))-WD)*(TR(I6(6),6)-TR(I7(6),6))
      S12=(TR(I6(6),6)-TR(I7(6),6))**2
      S13=(D7(7)/ABS(D7(7)))*(ABS(D7(7))-WD)*(TR(I6(7),7)-TR(I7(7),7))
      S14=(TR(I6(7),7)-TR(I7(7),7))**2
      GO TO 13
      S15=(D8(8)/ABS(D8(8)))*(ABS(D8(8))-WD)*(TR(I6(8),8)-TR(I7(8),8))
      S16=(TR(I6(8),8)-TR(I7(8),8))**2
      S17=(D9(9)/ABS(D9(9)))*(ABS(D9(9))-WD)*(TR(I6(9),9)-TR(I7(9),9))
      S18=(TR(I6(9),9)-TR(I7(9),9))**2
      S19=(D10(10)/ABS(D10(10)))*(ABS(D10(10))-WD)*(TR(I6(10),10)
     5-TR(I7(10),10))
      S20=(TR(I6(10),10)-TR(I7(10),10))**2
      S21=(D11(11)/ABS(D11(11)))*(ABS(D11(11))-WD)*(TR(I6(11),11)
     1-TR(I7(11),11))
      S22=(TR(I6(11),11)-TR(I7(11),11))**2
      S23=(D12(12)/ABS(D12(12)))*(ABS(D12(12))-WD)*(TR(I6(12),12)
     2-TR(I7(12),12))
      S24=(TR(I6(12),12)-TR(I7(12),12))**2
      S25=(D13(13)/ABS(D13(13)))*(ABS(D13(13))-WD)*(TR(I6(13),13)
     3-TR(I7(13),13))
      S26=(TR(I6(13),13)-TR(I7(13),13))**2
    8 CONTINUE
      S27=(D14(14)/ABS(D14(14)))*(ABS(D14(14))-WD)*(TR(I6(14),14)
     4-TR(I7(14),14))
      S28=(TR(I6(14),14)-TR(I7(14),14))**2
      S29=(D15(15)/ABS(D15(15)))*(ABS(D15(15))-WD)*(TR(I6(15),15)
     5-TR(I7(15),15))
      S30=(TR(I6(15),15)-TR(I7(15),15))**2
      S31=(D16(16)/ABS(D16(16)))*(ABS(D16(16))-WD)*(TR(I6(16),16)
     1-TR(I7(16),16))
      S32=(TR(I6(16),16)-TR(I7(16),16))**2
      S33=(D17(17)/ABS(D17(17)))*(ABS(D17(17))-WD)*(TR(I6(17),17)
     1-TR(I7(17),17))
      S34=(TR(I6(17),17)-TR(I7(17),17))**2
      S35=(D18(18)/ABS(D18(18)))*(ABS(D18(18))-WD)*(TR(I6(18),18)
     1-TR(I7(18),18))
      S36=(TR(I6(18),18)-TR(I7(18),18))**2
      S37=(D19(19)/ABS(D19(19)))*(ABS(D19(19))-WD)*(TR(I6(19),19)
     1-TR(I7(19),19))
      S38=(TR(I6(19),19)-TR(I7(19),19))**2
      S39=(D20(20)/ABS(D20(20)))*(ABS(D20(20))-WD)*(TR(I6(20),20)
     1-TR(I7(20),20))
      S40=(TR(I6(20),20)-TR(I7(20),20))**2
      S41=(D21(21)/ABS(D21(21)))*(ABS(D21(21))-WD)*(TR(I6(21),21)
     1-TR(I7(21),21))
      S42=(TR(I6(21),21)-TR(I7(21),21))**2
      S43=(D22(22)/ABS(D22(22)))*(ABS(D22(22))-WD)*(TR(I6(22),22)
     1-TR(I7(22),22))
      S44=(TR(I6(22),22)-TR(I7(22),22))**2
      S45=(D23(23)/ABS(D23(23)))*(ABS(D23(23))-WD)*(TR(I6(23),23)
     1-TR(I7(23),23))
      S46=(TR(I6(23),23)-TR(I7(23),23))**2
```

```
      S47=(D24(24)/ABS(D24(24)))*(ABS(D24(24))-WD)*(TR(I6(24),24)
     1-TR(I7(24),24))
      S48=(TR(I6(24),24)-TR(I7(24),24))**2
      S49=(D25(25)/ABS(D25(25)))*(ABS(D25(25))-WD)*(TR(I6(25),25)
     1-TR(I7(25),25))
      S50=(TR(I6(25),25)-TR(I7(25),25))**2
      S51=(D26(26)/ABS(D26(26)))*(ABS(D26(26))-WD)*(TR(I6(26),26)
     1-TR(I7(26),26))
      S52=(TR(I6(26),26)-TR(I7(26),26))**2
   13 CONTINUE
      IK1=IK+1
      GDD(IK1,1)=GDD(IK,1)-S1/S2
      GDD(IK1,2)=GDD(IK,2)-S3/S4
      GDD(IK1,3)=GDD(IK,3)-S5/S6
      GDD(IK1,4)=GDD(IK,4)-S7/S8
      GDD(IK1,5)=GDD(IK,5)-S9/S10
      GDD(IK1,6)=GDD(IK,6)-S11/S12
      GDD(IK1,7)=GDD(IK,7)-S13/S14
      GO TO 3
      GDD(IK1,8)=GDD(IK,8)-S15/S16
      GDD(IK1,9)=GDD(IK,9)-S17/S18
      GDD(IK1,10)=GDD(IK,10)-S19/S20
      GDD(IK1,11)=GDD(IK,11)-S21/S22
      GDD(IK1,12)=GDD(IK,12)-S23/S24
      GDD(IK1,13)=GDD(IK,13)-S25/S26
    9 CONTINUE
      GDD(IK1,14)=GDD(IK,14)-S27/S28
      GDD(IK1,15)=GDD(IK,15)-S29/S30
      GDD(IK1,16)=GDD(IK,16)-S31/S32
      GDD(IK1,17)=GDD(IK,17)-S33/S34
      GDD(IK1,18)=GDD(IK,18)-S35/S36
      GDD(IK1,19)=GDD(IK,19)-S37/S38
      GDD(IK1,20)=GDD(IK,20)-S39/S40
      GDD(IK1,21)=GDD(IK,21)-S41/S42
      GDD(IK1,22)=GDD(IK,22)-S43/S44
      GDD(IK1,23)=GDD(IK,23)-S45/S46
      GDD(IK1,24)=GDD(IK,24)-S47/S48
      GDD(IK1,25)=GDD(IK,25)-S49/S50
      GDD(IK1,26)=GDD(IK,26)-S51/S52
    3 CONTINUE
      WRITE(6,50)IK1,GDD(IK1,1),GDD(IK1,2),GDD(IK1,3),
     1GDD(IK1,4),GDD(IK1,5)
      WRITE(6,55)IK1,GDD(IK1,6),GDD(IK1,7),GDD(IK1,8),
     1GDD(IK1,9),GDD(IK1,10)
      GO TO 41
      WRITE(6,66)IK1,GDD(IK1,11),GDD(IK1,12),GDD(IK1,13),
     1GDD(IK1,14),GDD(IK1,15)
      WRITE(6,77)IK1,GDD(IK1,16),GDD(IK1,17),GDD(IK1,18),
     1GDD(IK1,19),GDD(IK1,20)
      WRITE(6,88)IK1,GDD(IK1,21),GDD(IK1,22),GDD(IK1,23)
   41 CONTINUE
   50 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,1)=*,E10.4,2X,*GDD(IK1,2)=*,E10.4,
     12X,*GDD(IK1,3)=*,E10.4,*GDD(IK1,4)=*,E10.4,*GDD(IK1,5)=*,E10.4,/)
```

```
55 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,6)=*,E10.4,2X,*GDD(IK1,7)=*,E10.4,
  12X,*GDD(IK1,8)=*,E10.4,*GDD(IK1,9)=*,E10.4,
  1*GDD(IK1,10)=*,E10.4,//)
   GO TO 40
66 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,11)=*,E10.4,*GDD(IK1,12)=*,E10.4,
  1*GDD(IK1,13)=*,E10.4,*GDD(IK1,14)=*,E10.4,*GDD(IK1,15)=*,E10.4,/)
77 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,16)=*,E10.4,*GDD(IK1,17)=*,E10.4,
  1*GDD(IK1,18)=*,E10.4,*GDD(IK1,19)=*,E10.4,*GDD(IK1,20)=*,E10.4,//)
88 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,21)=*,E10.4,2X,*GDD(IK1,22)=*,
  1E10.4,2X,*GDD(IK1,23)=*,E10.4,//)
40 CONTINUE
   STOP
   END
```

```
      PROGRAM TAKI2(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION T1(800),T2(800),T3(800),T4(800),T5(800),T6(800),
     1T7(800),T8(800),T9(800),T10(800),K4(800),T11(800),T12(800),
     3T13(800),T14(800),T15(800),AR(6,6),AI(6,6),ZR(6,6),ZI(6,6),
     1W(6),FV1(6),FM1(2,6)
      R1=1./2.
      R2=1./3.
      R3=SQRT(10.)
      R4=1./20.
      R5=SQRT(5.)
      R6=SQRT(2.)
      GX=2.004
      WD=9.4038
      B=9.274/6.626
      GZ=2.001
      A1=-8.622
      A2=.181
      A3=.531
      A4=-2.712
      WRITE(6,10)WD
   10 FORMAT(5X,*WD=*,E10.4)
      PI=3.14159264
      THETA=43.*PI/180.
      CN=COS(THETA)
      SN=SIN(THETA)
      DO 5 K1=1,201
      K=0+2*K1
      K4(K1)=K
      GD=FLOAT(K-1)/100.
      AR(1,1)=5.*R1*GZ*CN*B*GD+A2+10.*R2*A1
      AR(1,2)=R1*R5*GX*SN*B*GD
      AR(1,3)=0.
      AR(1,4)=R3*R4*A3
      AR(1,5)=0.
      AR(1,6)=0.
      AR(2,1)=R1*R5*GX*SN*B*GD
      AR(2,2)=3.*R1*GZ*CN*B*GD-3.*A2-2.*R2*A1
      AR(2,3)=R6*GX*SN*B*GD
      AR(2,4)=0.
      AR(2,5)=0.
      AR(2,6)=0.
      AR(3,1)=0.
      AR(3,2)=R6*GX*SN*B*GD
      AR(3,3)=R1*GZ*CN*B*GD+2.*A2-8.*R2*A1
      AR(3,4)=3.*R1*GX*SN*B*GD
      AR(3,5)=0.
      AR(3,6)=-R3*R4*A3
      AR(4,1)=R3*R4*A3
      AR(4,2)=0.
      AR(4,3)=3.*R1*GX*SN*B*GD
      AR(4,4)=-R1*GZ*CN*B*GD+2.*A2-8.*R2*A1
      AR(4,5)=R6*GX*SN*B*GD
      AR(4,6)=0.
      AR(5,1)=0.
```

```
      AR(5,2)=0.
      AR(5,3)=0.
      AR(5,4)=R6*GX*SN*B*GD
      AR(5,5)=-3.*R1*GZ*CN*B*GD-3.*A2-2.*R2*A1
      AR(5,6)=R1*R5*GX*SN*B*GD
      AR(6,1)=0.
      AR(6,2)=0.
      AR(6,3)=-R3*R4*A3
      AR(6,4)=0.
      AR(6,5)=R1*R5*GX*SN*B*GD
      AR(6,6)=-5.*R1*GZ*CN*B*GD+A2+10.*R2*A1
      DO 33 I=1,6
      DO 33 J=1,6
      AI(I,J)=0.
   33 CONTINUE
      AI(1,4)=R3*R4*A4
      AI(3,6)=-R3*R4*A4
      AI(4,1)=-R3*R4*A4
      AI(6,3)=R3*R4*A4
      CALL HTRIDI(6,6,AR,AI,W,FV1,FV1,FM1)
      DO 100 I=1,6
      DO 50 J=1,6
      ZR(I,J)=0.
   50 CONTINUE
      ZR(I,I)=1.
  100 CONTINUE
      CALL TQL2(6,6,W,FV1,ZR,IERR)
      IF(IERR.NE.0) WRITE(6,44)IERR
      CALL HTRIBK(6,6,AR,AI,FM1,6,ZR,ZI)
   44 FORMAT(5X,*IERR=*,I3)
      T1(K1)=ABS(ABS(W(1)-W(2))-WD)
      T2(K1)=ABS(ABS(W(1)-W(3))-WD)
      T3(K1)=ABS(ABS(W(1)-W(4))-WD)
      T4(K1)=ABS(ABS(W(1)-W(5))-WD)
      T11(K1)=ABS(ABS(W(1)-W(6))-WD)
      T5(K1)=ABS(ABS(W(2)-W(3))-WD)
      T6(K1)=ABS(ABS(W(2)-W(4))-WD)
      T7(K1)=ABS(ABS(W(2)-W(5))-WD)
      T12(K1)=ABS(ABS(W(2)-W(6))-WD)
      T8(K1)=ABS(ABS(W(3)-W(4))-WD)
      T9(K1)=ABS(ABS(W(3)-W(5))-WD)
      T13(K1)=ABS(ABS(W(3)-W(6))-WD)
      T10(K1)=ABS(ABS(W(4)-W(5))-WD)
      T14(K1)=ABS(ABS(W(4)-W(6))-WD)
      T15(K1)=ABS(ABS(W(5)-W(6))-WD)
    5 CONTINUE
      WRITE(6,11)((K4(K),T1(K)),K=1,201)
      WRITE(6,12)((K4(K),T2(K)),K=1,201)
      WRITE(6,13)((K4(K),T3(K)),K=1,201)
      WRITE(6,14)((K4(K),T4(K)),K=1,201)
      WRITE(6,15)((K4(K),T5(K)),K=1,201)
      WRITE(6,16)((K4(K),T6(K)),K=1,201)
      WRITE(6,17)((K4(K),T7(K)),K=1,201)
```

```
      WRITE(6,18)((K4(K),T8(K)),K=1,201)
      WRITE(6,19)((K4(K),T9(K)),K=1,201)
      WRITE(6,20)((K4(K),T10(K)),K=1,201)
      WRITE(6,21)((K4(K),T11(K)),K=1,201)
      WRITE(6,22)((K4(K),T12(K)),K=1,201)
      WRITE(6,23)((K4(K),T13(K)),K=1,201)
      WRITE(6,24)((K4(K),T14(K)),K=1,201)
      WRITE(6,25)((K4(K),T15(K)),K=1,201)
   11 FORMAT(5(5X,*T1(*,I4,*)=*,E10.4))
   12 FORMAT(5(5X,*T2(*,I4,*)=*,E10.4))
   13 FORMAT(5(5X,*T3(*,I4,*)=*,E10.4))
   14 FORMAT(5(5X,*T4(*,I4,*)=*,E10.4))
   15 FORMAT(5(5X,*T5(*,I4,*)=*,E10.4))
   16 FORMAT(5(5X,*T6(*,I4,*)=*,E10.4))
   17 FORMAT(5(5X,*T7(*,I4,*)=*,E10.4))
   18 FORMAT(5(5X,*T8(*,I4,*)=*,E10.4))
   19 FORMAT(5(5X,*T9(*,I4,*)=*,E10.4))
   20 FORMAT(5(5X,*T10(*,I4,*)=*,E10.4))
   21 FORMAT(5(5X,*T11(*,I4,*)=*,E10.4))
   22 FORMAT(5(5X,*T12(*,I4,*)=*,E10.4))
   23 FORMAT(5(5X,*T13(*,I4,*)=*,E10.4))
   24 FORMAT(5(5X,*T14(*,I4,*)=*,E10.4))
   25 FORMAT(5(5X,*T15(*,I4,*)=*,E10.4))
      STOP
      END
```

```
 PROGRAM TAKI3(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
 DIMENSION AR(6,6),AI(6,6),W(6),ZR(6,6),ZI(6,6),SZ(6,6),SX(6,6),
7SZX(6,6),EV1(6,6),EV2(6,6),EV3(6,6),EV4(6,6),EV5(6,6),EV6(6,6),
8D1(15),D2(15),D3(15),TR(6,15),I6(15),I7(15),D4(15),D5(15),D6(15),
9D7(15),D8(15),D9(15),D10(15),GDD(450,15),D11(15),D12(15),
4D13(15),D14(15),D15(15),FV1(6),FM1(2,6)
 WD=9.4038
 R1=1./2.
 R2=1./3.
 R3=SQRT(10.)
 R4=1./20.
 R5=SQRT(5.)
 R6=SQRT(2.)
 B=9.274/6.626
 GZ=2.001
 GX=2.004
 A1=-8.622
 A2=.181
 A3=.531
 A4=-2.712
 PI=3.14159264
 GO TO 2
 GDD(1,1)=.67
 GDD(1,2)=1.11
 GDD(1,3)=1.57
 GDD(1,4)=2.17
 GDD(1,5)=3.13
 GDD(1,6)=3.39
 GDD(1,7)=15.41
 GDD(1,8)=3.85
 GDD(1,9)=4.93
 GDD(1,10)=5.07
 GDD(1,11)=7.29
 GDD(1,12)=7.59
 GDD(1,13)=8.71
2 CONTINUE
 GDD(200,14)=3.39
 GDD(200,15)=1.91
 SZ(1,1)=5.*R1
 SZ(1,2)=0.
 SZ(1,3)=0.
 SZ(1,4)=0.
 SZ(1,5)=0.
 SZ(1,6)=0.
 SZ(2,1)=0.
 SZ(2,2)=3.*R1
 SZ(2,3)=0.
 SZ(2,4)=0.
 SZ(2,5)=0.
 SZ(2,6)=0.
 SZ(3,1)=0.
 SZ(3,2)=0.
 SZ(3,3)=R1
 SZ(3,4)=0.
```

```
SZ(3,5)=0.
SZ(3,6)=0.
SZ(4,1)=0.
SZ(4,2)=0.
SZ(4,3)=0.
SZ(4,4)=-R1
SZ(4,5)=0.
SZ(4,6)=0.
SZ(5,1)=0.
SZ(5,2)=0.
SZ(5,3)=0.
SZ(5,4)=0.
SZ(5,5)=-3.*R1
SZ(5,6)=0.
SZ(6,1)=0.
SZ(6,2)=0.
SZ(6,3)=0.
SZ(6,4)=0.
SZ(6,5)=0.
SZ(6,6)=-5.*R1
SX(1,1)=0.
SX(1,2)=R1*R3
SX(1,3)=0.
SX(1,4)=0.
SX(1,5)=0.
SX(1,6)=0.
SX(2,1)=R1*R3
SX(2,2)=0.
SX(2,3)=R2
SX(2,4)=0.
SX(2,5)=0.
SX(2,6)=0.
SX(3,1)=0.
SX(3,2)=R2
SX(3,3)=0.
SX(3,4)=3.*R1
SX(3,5)=0.
SX(3,6)=0.
SX(4,1)=0.
SX(4,2)=0.
SX(4,3)=3.*R1
SX(4,4)=0.
SX(4,5)=R2
SX(4,6)=0.
SX(5,1)=0.
SX(5,2)=0.
SX(5,3)=0.
SX(5,4)=R2
SX(5,5)=0.
SX(5,6)=R1*R3
SX(6,1)=0.
SX(6,2)=0.
SX(6,3)=0.
```

```
      SX(6,4)=0.
      SX(6,5)=R1*R3
      SX(6,6)=0.
      DO 40 IK=200,299
      DELTA=PI/900.
      THETA=DELTA*FLOAT(IK-1)
      CN=COS(THETA)
      SN=SIN(THETA)
      DO 1 I=14,15
      AR(1,1)=10.*R2*A1+A2+5.*R1*GDD(IK,I)*GZ*B*CN
      AR(1,2)=R1*R5*GDD(IK,I)*GX*B*SN
      AR(1,3)=0.
      AR(1,4)=R3*R4*A3
      AR(1,5)=0.
      AR(1,6)=0.
      AR(2,1)=R1*R5*GDD(IK,I)*GX*B*SN
      AR(2,2)=3.*R1*GDD(IK,I)*GZ*B*CN-2.*R2*A1-3.*A2
      AR(2,3)=R6*GDD(IK,I)*GX*B*SN
      AR(2,4)=0.
      AR(2,5)=0.
      AR(2,6)=0.
      AR(3,1)=0.
      AR(3,2)=R6*GDD(IK,I)*GX*B*SN
      AR(3,3)=-8.*R2*A1+2.*A2+R1*GDD(IK,I)*GZ*B*CN
      AR(3,4)=3.*R1*GDD(IK,I)*GX*B*SN
      AR(3,5)=0.
      AR(3,6)=-R3*R4*A3
      AR(4,1)=R3*R4*A3
      AR(4,2)=0.
      AR(4,3)=3.*R1*GDD(IK,I)*GX*B*SN
      AR(4,4)=-R1*GDD(IK,I)*GZ*B*CN-8.*R2*A1+2.*A2
      AR(4,5)=R6*GDD(IK,I)*GX*B*SN
      AR(4,6)=0.
      AR(5,1)=0.
      AR(5,2)=0.
      AR(5,3)=0.
      AR(5,4)=R6*GDD(IK,I)*GX*B*SN
      AR(5,5)=-2.*R2*A1-3.*A2-3.*R1*GDD(IK,I)*GZ*B*CN
      AR(5,6)=R1*R5*GDD(IK,I)*GX*B*SN
      AR(6,1)=0.
      AR(6,2)=0.
      AR(6,3)=-R3*R4*A3
      AR(6,4)=0.
      AR(6,5)=R1*R5*GDD(IK,I)*GX*B*SN
      AR(6,6)=10.*R2*A1+A2-5.*R1*GDD(IK,I)*GZ*B*CN
      DO 33 K=1,6
      DO 33 J=1,6
      AI(K,J)=0.
   33 CONTINUE
      AI(1,4)=R3*R4*A4
      AI(3,6)=-R3*R4*A4
      AI(4,1)=-R3*R4*A4
      AI(6,3)=R3*R4*A4
```

```
      CALL HTRIDI(6,6,AR,AI,W,FV1,FV1,FM1)
      DO 200 K=1,6
      DO 90 J=1,6
      ZR(K,J)=0.
   90 CONTINUE
      ZR(K,K)=1.
  200 CONTINUE
      CALL TQL2(6,6,W,FV1,ZR,IERR)
      IF(IERR.NE.0) WRITE(6,44)IERR
      CALL HTRIBK(6,6,AR,AI,FM1,6,ZR,ZI)
   44 FORMAT(5X,*IERR=*,I3)
      GO TO 111
      I6(I)=1
      I7(I)=2
      IEQ=0.
      AMIN=ABS(ABS(W(1)-W(2))-WD)
      DO 100 L=1,5
      L1=L+1
      DO 100 M=L1,6
      TEMP=ABS(ABS(W(L)-W(M))-WD)
      IF (TEMP-AMIN) 105,106,110
  105 AMIN=TEMP
      I6(I)=L
      I7(I)=M
      GO TO 110
  106 IEQ=IEQ+1.
  110 CONTINUE
  100 CONTINUE
  111 CONTINUE
      I6(1)=2
      I7(1)=1
      I6(2)=4
      I7(2)=3
      I6(3)=5
      I7(3)=4
      I6(4)=3
      I7(4)=2
      I6(5)=6
      I7(5)=4
      I6(6)=6
      I7(6)=4
      I6(7)=6
      I7(7)=5
      I6(8)=3
      I7(8)=2
      I6(9)=5
      I7(9)=4
      I6(10)=4
      I7(10)=3
      I6(11)=4
      I7(11)=3
      I6(12)=5
      I7(12)=4
```

```
      I6(13)=6
      I7(13)=4
      I6(14)=5
      I7(14)=4
      I6(15)=5
      I7(15)=4
      GO TO 25
      WRITE(6,20)I,W(1),W(2),W(3),W(4),W(5),W(6)
   20 FORMAT(5X,*I=*,I2,2X,*W(1)=*,E10.4,2X,*W(2)=*,E10.4,
     32X,*W(3)=*,E10.4,
     62X,*W(4)=*,E10.4,2X,*W(5)=*,E10.4,2X,*W(6)=*,E10.4,/)
   25 CONTINUE
      DO 11 K=1,6
      DO 11 J=1,6
      SZX(K,J)=SZ(K,J)*GZ*B*CN+SX(K,J)*GX*B*SN
      EV1(K,J)=ZR(K,1)*ZR(J,1)+ZI(K,1)*ZI(J,1)
      EV2(K,J)=ZR(K,2)*ZR(J,2)+ZI(K,2)*ZI(J,2)
      EV3(K,J)=ZR(K,3)*ZR(J,3)+ZI(K,3)*ZI(J,3)
      EV4(K,J)=ZR(K,4)*ZR(J,4)+ZI(K,4)*ZI(J,4)
      EV5(K,J)=ZR(K,5)*ZR(J,5)+ZI(K,5)*ZI(J,5)
      EV6(K,J)=ZR(K,6)*ZR(J,6)+ZI(K,6)*ZI(J,6)
   11 CONTINUE
      TR(1,I)=0.
      TR(2,I)=0.
      TR(3,I)=0.
      TR(4,I)=0.
      TR(5,I)=0.
      TR(6,I)=0.
      DO 12 K=1,6
      DO 12 J=1,6
      TR(1,I)=TR(1,I)+SZX(K,J)*EV1(J,K)
      TR(2,I)=TR(2,I)+SZX(K,J)*EV2(J,K)
      TR(3,I)=TR(3,I)+SZX(K,J)*EV3(J,K)
      TR(4,I)=TR(4,I)+SZX(K,J)*EV4(J,K)
      TR(5,I)=TR(5,I)+SZX(K,J)*EV5(J,K)
      TR(6,I)=TR(6,I)+SZX(K,J)*EV6(J,K)
   12 CONTINUE
      D1(I)=W(I6(1))-W(I7(1))
      D2(I)=W(I6(2))-W(I7(2))
      D3(I)=W(I6(3))-W(I7(3))
      D4(I)=W(I6(4))-W(I7(4))
      D5(I)=W(I6(5))-W(I7(5))
      D6(I)=W(I6(6))-W(I7(6))
      D7(I)=W(I6(7))-W(I7(7))
      D8(I)=W(I6(8))-W(I7(8))
      D9(I)=W(I6(9))-W(I7(9))
      D10(I)=W(I6(10))-W(I7(10))
      D11(I)=W(I6(11))-W(I7(11))
      D12(I)=W(I6(12))-W(I7(12))
      D13(I)=W(I6(13))-W(I7(13))
      D14(I)=W(I6(14))-W(I7(14))
      D15(I)=W(I6(15))-W(I7(15))
    1 CONTINUE
```

```
      GO TO 7
      S1=(D1(1)/ABS(D1(1)))*(ABS(D1(1))-WD)*(TR(I6(1),1)-TR(I7(1),1))
      S2=(TR(I6(1),1)-TR(I7(1),1))**2
      S3=(D2(2)/ABS(D2(2)))*(ABS(D2(2))-WD)*(TR(I6(2),2)-TR(I7(2),2))
      S4=(TR(I6(2),2)-TR(I7(2),2))**2
      S5=(D3(3)/ABS(D3(3)))*(ABS(D3(3))-WD)*(TR(I6(3),3)-TR(I7(3),3))
      S6=(TR(I6(3),3)-TR(I7(3),3))**2
      S7=(D4(4)/ABS(D4(4)))*(ABS(D4(4))-WD)*(TR(I6(4),4)-TR(I7(4),4))
      S8=(TR(I6(4),4)-TR(I7(4),4))**2
      S9=(D5(5)/ABS(D5(5)))*(ABS(D5(5))-WD)*(TR(I6(5),5)-TR(I7(5),5))
      S10=(TR(I6(5),5)-TR(I7(5),5))**2
      S11=(D6(6)/ABS(D6(6)))*(ABS(D6(6))-WD)*(TR(I6(6),6)-TR(I7(6),6))
      S12=(TR(I6(6),6)-TR(I7(6),6))**2
      S13=(D7(7)/ABS(D7(7)))*(ABS(D7(7))-WD)*(TR(I6(7),7)-TR(I7(7),7))
      S14=(TR(I6(7),7)-TR(I7(7),7))**2
      S15=(D8(8)/ABS(D8(8)))*(ABS(D8(8))-WD)*(TR(I6(8),8)-TR(I7(8),8))
      S16=(TR(I6(8),8)-TR(I7(8),8))**2
      S17=(D9(9)/ABS(D9(9)))*(ABS(D9(9))-WD)*(TR(I6(9),9)-TR(I7(9),9))
      S18=(TR(I6(9),9)-TR(I7(9),9))**2
      S19=(D10(10)/ABS(D10(10)))*(ABS(D10(10))-WD)*(TR(I6(10),10)
     5-TR(I7(10),10))
      S20=(TR(I6(10),10)-TR(I7(10),10))**2
      S21=(D11(11)/ABS(D11(11)))*(ABS(D11(11))-WD)*(TR(I6(11),11)
     1-TR(I7(11),11))
      S22=(TR(I6(11),11)-TR(I7(11),11))**2
      S23=(D12(12)/ABS(D12(12)))*(ABS(D12(12))-WD)*(TR(I6(12),12)
     2-TR(I7(12),12))
      S24=(TR(I6(12),12)-TR(I7(12),12))**2
      S25=(D13(13)/ABS(D13(13)))*(ABS(D13(13))-WD)*(TR(I6(13),13)
     3-TR(I7(13),13))
      S26=(TR(I6(13),13)-TR(I7(13),13))**2
    7 CONTINUE
      S27=(D14(14)/ABS(D14(14)))*(ABS(D14(14))-WD)*(TR(I6(14),14)
     4-TR(I7(14),14))
      S28=(TR(I6(14),14)-TR(I7(14),14))**2
      S29=(D15(15)/ABS(D15(15)))*(ABS(D15(15))-WD)*(TR(I6(15),15)
     5-TR(I7(15),15))
      S30=(TR(I6(15),15)-TR(I7(15),15))**2
   13 CONTINUE
      IK1=IK+1
      GO TO 8
      GDD(IK1,1)=GDD(IK,1)-S1/S2
      GDD(IK1,2)=GDD(IK,2)-S3/S4
      GDD(IK1,3)=GDD(IK,3)-S5/S6
      GDD(IK1,4)=GDD(IK,4)-S7/S8
      GDD(IK1,5)=GDD(IK,5)-S9/S10
      GDD(IK1,6)=GDD(IK,6)-S11/S12
      GDD(IK1,7)=GDD(IK,7)-S13/S14
      GDD(IK1,8)=GDD(IK,8)-S15/S16
      GDD(IK1,9)=GDD(IK,9)-S17/S18
      GDD(IK1,10)=GDD(IK,10)-S19/S20
      GDD(IK1,11)=GDD(IK,11)-S21/S22
      GDD(IK1,12)=GDD(IK,12)-S23/S24
```

```
      GDD(IK1,13)=GDD(IK,13)-S25/S26
    8 CONTINUE
      GDD(IK1,14)=GDD(IK,14)-S27/S28
      GDD(IK1,15)=GDD(IK,15)-S29/S30
      GO TO 9
      WRITE(6,50)IK1,GDD(IK1,1),GDD(IK1,2),GDD(IK1,3)
      WRITE(6,55)IK1,GDD(IK1,4),GDD(IK1,5),GDD(IK1,6)
      WRITE(6,66)IK1,GDD(IK1,7),GDD(IK1,8),GDD(IK1,9),GDD(IK1,10)
    9 CONTINUE
      WRITE(6,77)IK1,GDD(IK1,11),GDD(IK1,12),
     6GDD(IK1,13),GDD(IK1,14),GDD(IK1,15)
      GO TO 41
   50 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,1)=*,E10.4,2X,
     9*GDD(IK1,2)=*,E10.4,2X,*GDD(IK1,3)=*,E10.4,/)
   55 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,4)=*,E10.4,2X,
     1*GDD(IK1,5)=*,E10.4,2X,*GDD(IK1,6)=*,E10.4,/)
   66 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,7)=*,E10.4,2X,*GDD(IK1,8)=*,
     2E10.4,2X,*GDD(IK1,9)=*,E10.4,2X,*GDD(IK1,10)=*,E10.4,/)
   41 CONTINUE
   77 FORMAT(5X,*IK1=*,I3,2X,*GDD(IK1,11)=*,E10.4,2X,
     7*GDD(IK1,12)=*,E10.4,2X,*GDD(IK1,13)=*,E10.4,2X,
     8*GDD(IK1,14)=*,E10.4,2X,*GDD(IK1,15)=*,E10.4,//)
   40 CONTINUE
      STOP
      END
```

```
      PROGRAM TAKI11(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SPH(4,4),A(10),W(4),ZR(4,4),SI(4,4),
     1T1(800),T2(800),K4(800)
      WD=9.5
      GZ=2.
      GX=1.95
      B=9.274/6.626
      BB=1.42
      AA=1.42
      R1=1./4.
      PI=3.14159264
      THETA=0.
      CN=COS(THETA)
      SN=SIN(THETA)
      AK1=GZ*B*CN
      AK2=GX*B*SN
      DO 5 K3=1,301
      K=0+2*K3
      K4(K3)=K
      GD=FLOAT(K-1)/100.
C     SPH REPRESENTS THE SPIN HAMILTONIAN
      SPH(1,1)=R1*(GD*AK1*2.+AA)
      SPH(1,2)=0.
      SPH(1,3)=R1*AK2*GD*2.
      SPH(1,4)=0.
      SPH(2,1)=0.
      SPH(2,2)=R1*(GD*AK1*2.-AA)
      SPH(2,3)=2.*BB*R1
      SPH(2,4)=R1*AK2*GD*2.
      SPH(3,1)=R1*AK2*GD*2.
      SPH(3,2)=2.*BB*R1
      SPH(3,3)=-R1*(GD*AK1*2.+AA)
      SPH(3,4)=0.
      SPH(4,1)=0.
      SPH(4,2)=R1*AK2*GD*2.
      SPH(4,3)=0.
      SPH(4,4)=-R1*(GD*AK1*2.-AA)
      DO 995 I1=1,4
      W(I1)=0.
      DO 995 I2=1,4
      SI(I1,I2)=0.
  995 ZR(I1,I2)=0.
      DO 999 II=1,4
      DO 999 JJ=1,II
      KK=II*(II-1)/2+JJ
  999 A(KK)=SPH(II,JJ)
      CALL EIGRS(A,4,1,W,ZR,4,SI,IER)
      IF (IER) 997,996,997
  997 CONTINUE
      WRITE(6,998)IER
  996 CONTINUE
  998 FORMAT(5X,*IER=*,I3)
      T1(K3)=ABS(ABS(W(1)-W(3))-WD)
      T2(K3)=ABS(ABS(W(2)-W(4))-WD)
```

```
    5 CONTINUE
      WRITE(6,11)((K4(K),T1(K)),K=1,301)
      WRITE(6,12)((K4(K),T2(K)),K=1,301)
   11 FORMAT(5(5X,*T1(*,I4,*)=*,E10.4))
   12 FORMAT(5(5X,*T2(*,I4,*)=*,E10.4))
      STOP
      END
```

```
      PROGRAM TAKI52(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION T1(800),T2(800),T3(800),T4(800),T5(800),T6(800),
     1T7(800),T8(800),T9(800),T10(800),T11(800),T12(800),
     1T13(800),T14(800),T15(800),T16(800),T17(800),T18(800),
     1T19(800),T20(800),T21(800),T22(800),T23(800),T24(800),
     1T25(800),T26(800),T27(800),T28(800),T29(800),T30(800),
     1SH(36,36),A(666),W(36),ZR(36,36),SI(36,36),K4(800)
      R1=1./4.
      R2=1./3.
      R3=SQRT(2.)
      R4=SQRT(5.)
      WD=9.5
      GG=1.996
      B=9.274/6.626
      D=GG*B*.462
      E=-GG*B*.09
      AA=-GG*B*.09
      BB=GG*B*.09
      PI=3.14159264
      THETA=PI/2.
      CN=COS(THETA)
      SN=SIN(THETA)
      DO 5 K1=1,301
      K=0+2*K1
      K4(K1)=K
      GD=GG*B*FLOAT(K-1)/100.
      DO 45 I=1,36
      DO 45 J=1,36
      SH(I,J)=0.
   45 CONTINUE
      SH(1,1)=R1*(2.*5.*GD*CN+5.*5.*AA+40.*R2*D)
      SH(2,2)=R1*(2.*5.*GD*CN+3.*5.*AA+40.*R2*D)
      SH(3,3)=R1*(2.*5.*GD*CN+1.*5.*AA+40.*R2*D)
      SH(4,4)=R1*(2.*5.*GD*CN-1.*5.*AA+40.*R2*D)
      SH(5,5)=R1*(2.*5.*GD*CN-3.*5.*AA+40.*R2*D)
      SH(6,6)=R1*(2.*5.*GD*CN-5.*5.*AA+40.*R2*D)
      SH(7,7)=R1*(2.*3.*GD*CN+5.*3.*AA-8.*R2*D)
      SH(8,8)=R1*(2.*3.*GD*CN+3.*3.*AA-8.*R2*D)
      SH(9,9)=R1*(2.*3.*GD*CN+1.*3.*AA-8.*R2*D)
      SH(10,10)=R1*(2.*3.*GD*CN-1.*3.*AA-8.*R2*D)
      SH(11,11)=R1*(2.*3.*GD*CN-3.*3.*AA-8.*R2*D)
      SH(12,12)=R1*(2.*3.*GD*CN-5.*3.*AA-8.*R2*D)
      SH(13,13)=R1*(2.*GD*CN+5.*AA-32.*R2*D)
      SH(14,14)=R1*(2.*GD*CN+3.*AA-32.*R2*D)
      SH(15,15)=R1*(2.*GD*CN+1.*AA-32.*R2*D)
      SH(16,16)=R1*(2.*GD*CN-1.*AA-32.*R2*D)
      SH(17,17)=R1*(2.*GD*CN-3.*AA-32.*R2*D)
      SH(18,18)=R1*(2.*GD*CN-5.*AA-32.*R2*D)
      SH(19,19)=R1*(-2.*GD*CN-5.*AA-32.*R2*D)
      SH(20,20)=R1*(-2.*GD*CN-3.*AA-32.*R2*D)
      SH(21,21)=R1*(-2.*GD*CN-1.*AA-32.*R2*D)
      SH(22,22)=R1*(-2.*GD*CN+1.*AA-32.*R2*D)
      SH(23,23)=R1*(-2.*GD*CN+3.*AA-32.*R2*D)
      SH(24,24)=R1*(-2.*GD*CN+5.*AA-32.*R2*D)
```

```
SH(25,25)=R1*(-2.*3.*GD*CN-5.*3.*AA-8.*R2*D)
SH(31,31)=R1*(-2.*5.*GD*CN-5.*5.*AA+40.*R2*D)
SH(32,32)=R1*(-2.*5.*GD*CN-3.*5.*AA+40.*R2*D)
SH(33,33)=R1*(-2.*5.*GD*CN-1.*5.*AA+40.*R2*D)
SH(34,34)=R1*(-2.*5.*GD*CN+1.*5.*AA+40.*R2*D)
SH(35,35)=R1*(-2.*5.*GD*CN+3.*5.*AA+40.*R2*D)
SH(36,36)=R1*(-2.*5.*GD*CN+5.*5.*AA+40.*R2*D)
SH(26,26)=R1*(-2.*3.*GD*CN-3.*3.*AA-8.*R2*D)
SH(27,27)=R1*(-2.*3.*GD*CN-1.*3.*AA-8.*R2*D)
SH(28,28)=R1*(-2.*3.*GD*CN+1.*3.*AA-8.*R2*D)
SH(29,29)=R1*(-2.*3.*GD*CN+3.*3.*AA-8.*R2*D)
SH(30,30)=R1*(-2.*3.*GD*CN+5.*3.*AA-8.*R2*D)
SH(1,7)=2.*R1*R4*GD*SN
SH(2,8)=2.*R1*R4*GD*SN
SH(3,9)=2.*R1*R4*GD*SN
SH(4,10)=2.*R1*R4*GD*SN
SH(5,11)=2.*R1*R4*GD*SN
SH(6,12)=2.*R1*R4*GD*SN
SH(7,13)=R3*GD*SN
SH(8,14)=R3*GD*SN
SH(9,15)=R3*GD*SN
SH(10,16)=R3*GD*SN
SH(11,17)=R3*GD*SN
SH(12,18)=R3*GD*SN
SH(13,19)=6.*R1*GD*SN
SH(14,20)=6.*R1*GD*SN
SH(15,21)=6.*R1*GD*SN
SH(16,22)=6.*R1*GD*SN
SH(17,23)=6.*R1*GD*SN
SH(18,24)=6.*R1*GD*SN
SH(19,25)=R3*GD*SN
SH(20,26)=R3*GD*SN
SH(21,27)=R3*GD*SN
SH(22,28)=R3*GD*SN
SH(23,29)=R3*GD*SN
SH(24,30)=R3*GD*SN
SH(25,31)=2.*R1*R4*GD*SN
SH(26,32)=2.*R1*R4*GD*SN
SH(27,33)=2.*R1*R4*GD*SN
SH(28,34)=2.*R1*R4*GD*SN
SH(29,35)=2.*R1*R4*GD*SN
SH(30,36)=2.*R1*R4*GD*SN
SH(2,7)=2.*R1*R4*BB*R4
SH(3,8)=2.*R1*R4*BB*2.*R3
SH(4,9)=2.*R1*R4*BB*3.
SH(5,10)=2.*R1*R4*BB*2.*R3
SH(6,11)=2.*R1*R4*BB*R4
SH(8,13)=R2*BB*R4
SH(9,14)=R2*BB*2.*R3
SH(10,15)=R2*BB*3.
SH(11,16)=R2*BB*2.*R3
SH(12,17)=R2*BB*R4
SH(14,19)=2.*R1*3.*BB*R4
```

```
      SH(15,20)=2.*R1*3.*BB*2.*R3
      SH(16,21)=2.*R1*3.*BB*3.
      SH(17,22)=2.*R1*3.*BB*2.*R3
      SH(18,23)=2.*R1*3.*BB*R4
      SH(20,25)=R2*BB*R4
      SH(21,26)=R2*BB*2.*R3
      SH(22,27)=R2*BB*3.
      SH(23,28)=R2*BB*2.*R3
      SH(24,29)=R2*BB*R4
      SH(26,31)=2.*R1*R4*BB*R4
      SH(27,32)=2.*R1*R4*BB*2.*R3
      SH(28,33)=2.*R1*R4*BB*3.
      SH(29,34)=2.*R1*R4*BB*2.*R3
      SH(30,35)=2.*R1*R4*BB*R4
      SH(1,13)=R3*R4*E
      SH(2,14)=R3*R4*E
      SH(3,15)=R3*R4*E
      SH(4,16)=R3*R4*E
      SH(5,17)=R3*R4*E
      SH(6,18)=R3*R4*E
      SH(7,19)=3.*R3*E
      SH(8,20)=3.*R3*E
      SH(9,21)=3.*R3*E
      SH(10,22)=3.*R3*E
      SH(11,23)=3.*R3*E
      SH(12,24)=3.*R3*E
      SH(13,25)=3.*R3*E
      SH(14,26)=3.*R3*E
      SH(15,27)=3.*R3*E
      SH(16,28)=3.*R3*E
      SH(17,29)=3.*R3*E
      SH(18,30)=3.*R3*E
      SH(19,31)=R3*R4*E
      SH(20,32)=R3*R4*E
      SH(21,33)=R3*R4*E
      SH(22,34)=R3*R4*E
      SH(23,35)=R3*R4*E
      SH(24,36)=R3*R4*E
      DO 55 I=1,36
      DO 55 J=1,36
      IF(I.GT.J) SH(I,J)=SH(J,I)
   55 CONTINUE
      DO 995 I1=1,36
      W(I1)=0.
      DO 995 I2=1,36
      SI(I1,I2)=0.
  995 ZR(I1,I2)=0.
      DO 999 II=1,36
      DO 999 JJ=1,II
      KK=II*(II-1)/2+JJ
  999 A(KK)=SH(II,JJ)
      CALL EIGRS(A,36,1,W,ZR,36,SI,IER)
      IF(IER) 997,996,997
```

```
997 CONTINUE
    WRITE(6,998)IER
996 CONTINUE
998 FORMAT(5X,*IER=*,I3)
    T1(K1)=ABS(ABS(W(1)-W(7))-WD)
    T2(K1)=ABS(ABS(W(2)-W(8))-WD)
    T3(K1)=ABS(ABS(W(3)-W(9))-WD)
    T4(K1)=ABS(ABS(W(4)-W(10))-WD)
    T5(K1)=ABS(ABS(W(5)-W(11))-WD)
    T6(K1)=ABS(ABS(W(6)-W(12))-WD)
    T7(K1)=ABS(ABS(W(7)-W(13))-WD)
    T8(K1)=ABS(ABS(W(8)-W(14))-WD)
    T9(K1)=ABS(ABS(W(9)-W(15))-WD)
    T10(K1)=ABS(ABS(W(10)-W(16))-WD)
    T11(K1)=ABS(ABS(W(11)-W(17))-WD)
    T12(K1)=ABS(ABS(W(12)-W(18))-WD)
    T13(K1)=ABS(ABS(W(18)-W(19))-WD)
    T14(K1)=ABS(ABS(W(17)-W(20))-WD)
    T15(K1)=ABS(ABS(W(16)-W(21))-WD)
    T16(K1)=ABS(ABS(W(15)-W(22))-WD)
    T17(K1)=ABS(ABS(W(14)-W(23))-WD)
    T18(K1)=ABS(ABS(W(13)-W(24))-WD)
    T19(K1)=ABS(ABS(W(19)-W(25))-WD)
    T20(K1)=ABS(ABS(W(20)-W(26))-WD)
    T21(K1)=ABS(ABS(W(21)-W(27))-WD)
    T22(K1)=ABS(ABS(W(22)-W(28))-WD)
    T23(K1)=ABS(ABS(W(23)-W(29))-WD)
    T24(K1)=ABS(ABS(W(24)-W(30))-WD)
    T25(K1)=ABS(ABS(W(25)-W(31))-WD)
    T26(K1)=ABS(ABS(W(26)-W(32))-WD)
    T27(K1)=ABS(ABS(W(27)-W(33))-WD)
    T28(K1)=ABS(ABS(W(28)-W(34))-WD)
    T29(K1)=ABS(ABS(W(29)-W(35))-WD)
    T30(K1)=ABS(ABS(W(30)-W(36))-WD)
  5 CONTINUE
    WRITE(6,11)((K4(K),T1(K)),K=1,301)
    WRITE(6,12)((K4(K),T2(K)),K=1,301)
    WRITE(6,13)((K4(K),T3(K)),K=1,301)
    WRITE(6,14)((K4(K),T4(K)),K=1,301)
    WRITE(6,15)((K4(K),T5(K)),K=1,301)
    WRITE(6,16)((K4(K),T6(K)),K=1,301)
    WRITE(6,17)((K4(K),T7(K)),K=1,301)
    WRITE(6,18)((K4(K),T8(K)),K=1,301)
    WRITE(6,19)((K4(K),T9(K)),K=1,301)
    WRITE(6,20)((K4(K),T10(K)),K=1,301)
    WRITE(6,21)((K4(K),T11(K)),K=1,301)
    WRITE(6,22)((K4(K),T12(K)),K=1,301)
    WRITE(6,23)((K4(K),T13(K)),K=1,301)
    WRITE(6,24)((K4(K),T14(K)),K=1,301)
    WRITE(6,25)((K4(K),T15(K)),K=1,301)
    WRITE(6,26)((K4(K),T16(K)),K=1,301)
    WRITE(6,27)((K4(K),T17(K)),K=1,301)
    WRITE(6,28)((K4(K),T18(K)),K=1,301)
```

```
      WRITE(6,29)((K4(K),T19(K)),K=1,301)
      WRITE(6,30)((K4(K),T20(K)),K=1,301)
      WRITE(6,31)((K4(K),T21(K)),K=1,301)
      WRITE(6,32)((K4(K),T22(K)),K=1,301)
      WRITE(6,33)((K4(K),T23(K)),K=1,301)
      WRITE(6,34)((K4(K),T24(K)),K=1,301)
      WRITE(6,35)((K4(K),T25(K)),K=1,301)
      WRITE(6,36)((K4(K),T26(K)),K=1,301)
      WRITE(6,37)((K4(K),T27(K)),K=1,301)
      WRITE(6,38)((K4(K),T28(K)),K=1,301)
      WRITE(6,39)((K4(K),T29(K)),K=1,301)
      WRITE(6,40)((K4(K),T30(K)),K=1,301)
   11 FORMAT(5(5X,*T1(*,I4,*)=*,E10.4))
   12 FORMAT(5(5X,*T2(*,I4,*)=*,E10.4))
   13 FORMAT(5(5X,*T3(*,I4,*)=*,E10.4))
   14 FORMAT(5(5X,*T4(*,I4,*)=*,E10.4))
   15 FORMAT(5(5X,*T5(*,I4,*)=*,E10.4))
   16 FORMAT(5(5X,*T6(*,I4,*)=*,E10.4))
   17 FORMAT(5(5X,*T7(*,I4,*)=*,E10.4))
   18 FORMAT(5(5X,*T8(*,I4,*)=*,E10.4))
   19 FORMAT(5(5X,*T9(*,I4,*)=*,E10.4))
   20 FORMAT(5(5X,*T10(*,I4,*)=*,E10.4))
   21 FORMAT(5(5X,*T11(*,I4,*)=*,E10.4))
   22 FORMAT(5(5X,*T12(*,I4,*)=*,E10.4))
   23 FORMAT(5(5X,*T13(*,I4,*)=*,E10.4))
   24 FORMAT(5(5X,*T14(*,I4,*)=*,E10.4))
   25 FORMAT(5(5X,*T15(*,I4,*)=*,E10.4))
   26 FORMAT(5(5X,*T16(*,I4,*)=*,E10.4))
   27 FORMAT(5(5X,*T17(*,I4,*)=*,E10.4))
   28 FORMAT(5(5X,*T18(*,I4,*)=*,E10.4))
   29 FORMAT(5(5X,*T19(*,I4,*)=*,E10.4))
   30 FORMAT(5(5X,*T20(*,I4,*)=*,E10.4))
   31 FORMAT(5(5X,*T21(*,I4,*)=*,E10.4))
   32 FORMAT(5(5X,*T22(*,I4,*)=*,E10.4))
   33 FORMAT(5(5X,*T23(*,I4,*)=*,E10.4))
   34 FORMAT(5(5X,*T24(*,I4,*)=*,E10.4))
   35 FORMAT(5(5X,*T25(*,I4,*)=*,E10.4))
   36 FORMAT(5(5X,*T26(*,I4,*)=*,E10.4))
   37 FORMAT(5(5X,*T27(*,I4,*)=*,E10.4))
   38 FORMAT(5(5X,*T28(*,I4,*)=*,E10.4))
   39 FORMAT(5(5X,*T29(*,I4,*)=*,E10.4))
   40 FORMAT(5(5X,*T30(*,I4,*)=*,E10.4))
      STOP
      END
```

```
      PROGRAM TAKI53(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SH(36,36),A(666),W(36),ZR(36,36),SI(36,36),SZ(36,36),
     1SX(36,36),EV3(36,36),EV9(36,36),EV15(36,36),EV22(36,36),
     1EV28(36,36),EV34(36,36),TR(36,5),I6(5),I7(5),GD(360,5),
     1D1(5),D2(5),D3(5),D4(5),D5(5),SZX(36,36)
      R1=1./4.
      R2=1./3.
      R3=SQRT(2.)
      R4=SQRT(5.)
      WD=9.5
      B=9.274/6.626
      GG=1.996
      D=GG*B*.462
      E=-GG*B*.09
      AA=-GG*B*.09
      BB=GG*B*.09
      PI=3.14159264
      GD(1,1)=5.15
      GD(1,2)=4.33
      GD(1,3)=3.25
      GD(1,4)=2.51
      GD(1,5)=1.49
      DO 5 I=1,36
      DO 5 J=1,36
      SZ(I,J)=0.
    5 CONTINUE
      SZ(1,1)=2.*R1*5.
      SZ(2,2)=2.*R1*5.
      SZ(3,3)=2.*R1*5.
      SZ(4,4)=2.*R1*5.
      SZ(5,5)=2.*R1*5.
      SZ(6,6)=2.*R1*5.
      SZ(7,7)=2.*R1*3.
      SZ(8,8)=2.*R1*3.
      SZ(9,9)=2.*R1*3.
      SZ(10,10)=2.*R1*3.
      SZ(11,11)=2.*R1*3.
      SZ(12,12)=2.*R1*3.
      SZ(13,13)=2.*R1
      SZ(14,14)=2.*R1
      SZ(15,15)=2.*R1
      SZ(16,16)=2.*R1
      SZ(17,17)=2.*R1
      SZ(18,18)=2.*R1
      SZ(19,19)=-2.*R1
      SZ(20,20)=-2.*R1
      SZ(21,21)=-2.*R1
      SZ(22,22)=-2.*R1
      SZ(23,23)=-2.*R1
      SZ(24,24)=-2.*R1
      SZ(25,25)=-2.*R1*3.
      SZ(26,26)=-2.*R1*3.
      SZ(27,27)=-2.*R1*3.
      SZ(28,28)=-2.*R1*3.
```

```
      SZ(29,29)=-2.*R1*3.
      SZ(30,30)=-2.*R1*3.
      SZ(31,31)=-2.*R1*5.
      SZ(32,32)=-2.*R1*5.
      SZ(33,33)=-2.*R1*5.
      SZ(34,34)=-2.*R1*5.
      SZ(35,35)=-2.*R1*5.
      SZ(36,36)=-2.*R1*5.
      DO 15 I=1,36
      DO 15 J=1,36
      SX(I,J)=0.
   15 CONTINUE
      SX(1,7)=2.*R1*R4,
      SX(2,8)=2.*R1*R4
      SX(3,9)=2.*R1*R4
      SX(4,10)=2.*R1*R4
      SX(5,11)=2.*R1*R4
      SX(6,12)=2.*R1*R4
      SX(7,13)=R3
      SX(8,14)=R3
      SX(9,15)=R3
      SX(10,16)=R3
      SX(11,17)=R3
      SX(12,18)=R3
      SX(13,19)=6.*R1
      SX(14,20)=6.*R1
      SX(15,21)=6.*R1
      SX(16,22)=6.*R1
      SX(17,23)=6.*R1
      SX(18,24)=6.*R1
      SX(19,25)=R3
      SX(20,26)=R3
      SX(21,27)=R3
      SX(22,28)=R3
      SX(23,29)=R3
      SX(24,30)=R3
      SX(25,31)=2.*R1*R4
      SX(26,32)=2.*R1*R4
      SX(27,33)=2.*R1*R4
      SX(28,34)=2.*R1*R4
      SX(29,35)=2.*R1*R4
      SX(30,36)=2.*R1*R4
      DO 25 I=1,36
      DO 25 J=1,36
      IF(I.GT.J) SX(I,J)=SX(J,I)
   25 CONTINUE
      DO 40 IK=1,179
      DELTA=PI/360.
      THETA=DELTA*FLOAT(IK-1)
      CN=COS(THETA)
      SN=SIN(THETA)
      DO 1 I=1,5
      DO 35 K=1,36
```

```
      DO 35 J=1,36
      SH(K,J)=0.
   35 CONTINUE
      SH(1,1)=R1*(2.*5.*GG*B*GD(IK,I)*CN+5.*5.*AA+40.*R2*D)
      SH(2,2)=R1*(2.*5.*GG*B*GD(IK,I)*CN+3.*5.*AA+40.*R2*D)
      SH(3,3)=R1*(2.*5.*GG*B*GD(IK,I)*CN+1.*5.*AA+40.*R2*D)
      SH(4,4)=R1*(2.*5.*GG*B*GD(IK,I)*CN-1.*5.*AA+40.*R2*D)
      SH(5,5)=R1*(2.*5.*GG*B*GD(IK,I)*CN-3.*5.*AA+40.*R2*D)
      SH(6,6)=R1*(2.*5.*GG*B*GD(IK,I)*CN-5.*5.*AA+40.*R2*D)
      SH(7,7)=R1*(2.*3.*GG*B*GD(IK,I)*CN+5.*3.*AA-8.*R2*D)
      SH(8,8)=R1*(2.*3.*GG*B*GD(IK,I)*CN+3.*3.*AA-8.*R2*D)
      SH(9,9)=R1*(2.*3.*GG*B*GD(IK,I)*CN+1.*3.*AA-8.*R2*D)
      SH(10,10)=R1*(2.*3.*GG*B*GD(IK,I)*CN-1.*3.*AA-8.*R2*D)
      SH(11,11)=R1*(2.*3.*GG*B*GD(IK,I)*CN-3.*3.*AA-8.*R2*D)
      SH(12,12)=R1*(2.*3.*GG*B*GD(IK,I)*CN-5.*3.*AA-8.*R2*D)
      SH(13,13)=R1*(2.*GG*B*GD(IK,I)*CN+5.*AA-32.*R2*D)
      SH(14,14)=R1*(2.*GG*B*GD(IK,I)*CN+3.*AA-32.*R2*D)
      SH(15,15)=R1*(2.*GG*B*GD(IK,I)*CN+1.*AA-32.*R2*D)
      SH(16,16)=R1*(2.*GG*B*GD(IK,I)*CN-1.*AA-32.*R2*D)
      SH(17,17)=R1*(2.*GG*B*GD(IK,I)*CN-3.*AA-32.*R2*D)
      SH(18,18)=R1*(2.*GG*B*GD(IK,I)*CN-5.*AA-32.*R2*D)
      SH(19,19)=R1*(-2.*GG*B*GD(IK,I)*CN-5.*AA-32.*R2*D)
      SH(20,20)=R1*(-2.*GG*B*GD(IK,I)*CN-3.*AA-32.*R2*D)
      SH(21,21)=R1*(-2.*GG*B*GD(IK,I)*CN-1.*AA-32.*R2*D)
      SH(22,22)=R1*(-2.*GG*B*GD(IK,I)*CN+1.*AA-32.*R2*D)
      SH(23,23)=R1*(-2.*GG*B*GD(IK,I)*CN+3.*AA-32.*R2*D)
      SH(24,24)=R1*(-2.*GG*B*GD(IK,I)*CN+5.*AA-32.*R2*D)
      SH(25,25)=R1*(-2.*3.*GG*B*GD(IK,I)*CN-5.*3.*AA-8.*R2*D)
      SH(31,31)=R1*(-2.*5.*GG*B*GD(IK,I)*CN-5.*5.*AA+40.*R2*D)
      SH(32,32)=R1*(-2.*5.*GG*B*GD(IK,I)*CN-3.*5.*AA+40.*R2*D)
      SH(33,33)=R1*(-2.*5.*GG*B*GD(IK,I)*CN-1.*5.*AA+40.*R2*D)
      SH(34,34)=R1*(-2.*5.*GG*B*GD(IK,I)*CN+1.*5.*AA+40.*R2*D)
      SH(35,35)=R1*(-2.*5.*GG*B*GD(IK,I)*CN+3.*5.*AA+40.*R2*D)
      SH(36,36)=R1*(-2.*5.*GG*B*GD(IK,I)*CN+5.*5.*AA+40.*R2*D)
      SH(26,26)=R1*(-2.*3.*GG*B*GD(IK,I)*CN-3.*3.*AA-8.*R2*D)
      SH(27,27)=R1*(-2.*3.*GG*B*GD(IK,I)*CN-1.*3.*AA-8.*R2*D)
      SH(28,28)=R1*(-2.*3.*GG*B*GD(IK,I)*CN+1.*3.*AA-8.*R2*D)
      SH(29,29)=R1*(-2.*3.*GG*B*GD(IK,I)*CN+3.*3.*AA-8.*R2*D)
      SH(30,30)=R1*(-2.*3.*GG*B*GD(IK,I)*CN+5.*3.*AA-8.*R2*D)
      SH(1,7)=2.*R1*R4*GG*B*GD(IK,I)*SN
      SH(2,8)=2.*R1*R4*GG*B*GD(IK,I)*SN
      SH(3,9)=2.*R1*R4*GG*B*GD(IK,I)*SN
      SH(4,10)=2.*R1*R4*GG*B*GD(IK,I)*SN
      SH(5,11)=2.*R1*R4*GG*B*GD(IK,I)*SN
      SH(6,12)=2.*R1*R4*GG*B*GD(IK,I)*SN
      SH(7,13)=R3*GG*B*GD(IK,I)*SN
      SH(8,14)=R3*GG*B*GD(IK,I)*SN
      SH(9,15)=R3*GG*B*GD(IK,I)*SN
      SH(10,16)=R3*GG*B*GD(IK,I)*SN
      SH(11,17)=R3*GG*B*GD(IK,I)*SN
      SH(12,18)=R3*GG*B*GD(IK,I)*SN
      SH(13,19)=6.*R1*GG*B*GD(IK,I)*SN
      SH(14,20)=6.*R1*GG*B*GD(IK,I)*SN
```

```
SH(15,21)=6.*R1*GG*B*GD(IK,I)*SN
SH(16,22)=6.*R1*GG*B*GD(IK,I)*SN
SH(17,23)=6.*R1*GG*B*GD(IK,I)*SN
SH(18,24)=6.*R1*GG*B*GD(IK,I)*SN
SH(19,25)=R3*GG*B*GD(IK,I)*SN
SH(20,26)=R3*GG*B*GD(IK,I)*SN
SH(21,27)=R3*GG*B*GD(IK,I)*SN
SH(22,28)=R3*GG*B*GD(IK,I)*SN
SH(23,29)=R3*GG*B*GD(IK,I)*SN
SH(24,30)=R3*GG*B*GD(IK,I)*SN
SH(25,31)=2.*R1*R4*GG*B*GD(IK,I)*SN
SH(26,32)=2.*R1*R4*GG*B*GD(IK,I)*SN
SH(27,33)=2.*R1*R4*GG*B*GD(IK,I)*SN
SH(28,34)=2.*R1*R4*GG*B*GD(IK,I)*SN
SH(29,35)=2.*R1*R4*GG*B*GD(IK,I)*SN
SH(30,36)=2.*R1*R4*GG*B*GD(IK,I)*SN
SH(2,7)=2.*R1*R4*BB*R4
SH(3,8)=2.*R1*R4*BB*2.*R3
SH(4,9)=2.*R1*R4*BB*3.
SH(5,10)=2.*R1*R4*BB*2.*R3
SH(6,11)=2.*R1*R4*BB*R4
SH(8,13)=R3*BB*R4
SH(9,14)=R3*BB*2.*R3
SH(10,15)=R3*BB*3.
SH(11,16)=R3*BB*2.*R3
SH(12,17)=R3*BB*R4
SH(14,19)=2.*R1*3.*BB*R4
SH(15,20)=2.*R1*3.*BB*2.*R3
SH(16,21)=2.*R1*3.*BB*3.
SH(17,22)=2.*R1*3.*BB*2.*R3
SH(18,23)=2.*R1*3.*BB*R4
SH(20,25)=R3*BB*R4
SH(21,26)=R3*BB*2.*R3
SH(22,27)=R3*BB*3.
SH(23,28)=R3*BB*2.*R3
SH(24,29)=R3*BB*R4
SH(26,31)=2.*R1*R4*BB*R4
SH(27,32)=2.*R1*R4*BB*2.*R3
SH(28,33)=2.*R1*R4*BB*3.
SH(29,34)=2.*R1*R4*BB*2.*R3
SH(30,35)=2.*R1*R4*BB*R4
SH(1,13)=R3*R4*E
SH(2,14)=R3*R4*E
SH(3,15)=R3*R4*E
SH(4,16)=R3*R4*E
SH(5,17)=R3*R4*E
SH(6,18)=R3*R4*E
SH(7,19)=3.*R3*E
SH(8,20)=3.*R3*E
SH(9,21)=3.*R3*E
SH(10,22)=3.*R3*E
SH(11,23)=3.*R3*E
SH(12,24)=3.*R3*E
```

```
      SH(13,25)=3.*R3*E
      SH(14,26)=3.*R3*E
      SH(15,27)=3.*R3*E
      SH(16,28)=3.*R3*E
      SH(17,29)=3.*R3*E
      SH(18,30)=3.*R3*E
      SH(19,31)=R3*R4*E
      SH(20,32)=R3*R4*E
      SH(21,33)=R3*R4*E
      SH(22,34)=R3*R4*E
      SH(23,35)=R3*R4*E
      SH(24,36)=R3*R4*E
      DO 45 K=1,36
      DO 45 J=1,36
      IF(K.GT.J) SH(K,J)=SH(J,K)
   45 CONTINUE
      DO 995 I1=1,36
      W(I1)=0.
      DO 995 I2=1,36
      SI(I1,I2)=0.
  995 ZR(I1,I2)=0.
      DO 999 II=1,36
      DO 999 JJ=1,II
      KK=II*(II-1)/2+JJ
  999 A(KK)=SH(II,JJ)
      CALL EIGRS(A,36,1,W,ZR,36,SI,IER)
      IF(IER) 997,996,997
  997 CONTINUE
      WRITE(6,998)IER
  996 CONTINUE
  998 FORMAT(5X,*IER=*,I3)
      GO TO 111
      I6(I)=1
      I7(I)=7
      IEQ=0.
      AMIN=ABS(ABS(W(1)-W(7))-WD)
      DO 100 L=1,35
      L1=L+1
      DO 100 M=L1,36
      TEMP=ABS(ABS(W(L)-W(M))-WD)
      IF (TEMP-AMIN) 105,106,110
  105 AMIN=TEMP
      I6(I)=L
      I7(I)=M
      GO TO 110
  106 IEQ=IEQ+1.
  110 CONTINUE
  100 CONTINUE
  111 CONTINUE
      I6(1)=3
      I7(1)=9
      I6(2)=9
      I7(2)=15
```

```
      I6(3)=15
      I7(3)=22
      I6(4)=22
      I7(4)=28
      I6(5)=28
      I7(5)=34
      GO TO 26
      WRITE(6,20)I,W(1),W(2),W(3),W(4),W(5),W(6)
   20 FORMAT(5X,*I=*,I2,2X,*W(1)=*,E10.4,2X,*W(2)=*,E10.4,
     32X,*W(3)=*,E10.4,
     62X,*W(4)=*,E10.4,2X,*W(5)=*,E10.4,2X,*W(6)=*,E10.4,/)
   26 CONTINUE
      DO 11 K=1,36
      DO 11 J=1,36
      SZX(K,J)=SZ(K,J)*GG*B*CN+SX(K,J)*GG*B*SN
      EV3(K,J)=ZR(K,3)*ZR(J,3)
      EV9(K,J)=ZR(K,9)*ZR(J,9)
      EV15(K,J)=ZR(K,15)*ZR(J,15)
      EV22(K,J)=ZR(K,22)*ZR(J,22)
      EV28(K,J)=ZR(K,28)*ZR(J,28)
      EV34(K,J)=ZR(K,34)*ZR(J,34)
   11 CONTINUE
      DO 14 K=1,36
      TR(K,I)=0.
   14 CONTINUE
      DO 12 K=1,36
      DO 12 J=1,36
      TR(3,I)=TR(3,I)+SZX(K,J)*EV3(J,K)
      TR(9,I)=TR(9,I)+SZX(K,J)*EV9(J,K)
      TR(15,I)=TR(15,I)+SZX(K,J)*EV15(J,K)
      TR(22,I)=TR(22,I)+SZX(K,J)*EV22(J,K)
      TR(28,I)=TR(28,I)+SZX(K,J)*EV28(J,K)
      TR(34,I)=TR(34,I)+SZX(K,J)*EV34(J,K)
   12 CONTINUE
      D1(I)=W(I6(1))-W(I7(1))
      D2(I)=W(I6(2))-W(I7(2))
      D3(I)=W(I6(3))-W(I7(3))
      D4(I)=W(I6(4))-W(I7(4))
      D5(I)=W(I6(5))-W(I7(5))
    1 CONTINUE
      S1=(D1(1)/ABS(D1(1)))*(ABS(D1(1))-WD)*(TR(I6(1),1)-TR(I7(1),1))
      S2=(TR(I6(1),1)-TR(I7(1),1))**2
      S3=(D2(2)/ABS(D2(2)))*(ABS(D2(2))-WD)*(TR(I6(2),2)-TR(I7(2),2))
      S4=(TR(I6(2),2)-TR(I7(2),2))**2
      S5=(D3(3)/ABS(D3(3)))*(ABS(D3(3))-WD)*(TR(I6(3),3)-TR(I7(3),3))
      S6=(TR(I6(3),3)-TR(I7(3),3))**2
      S7=(D4(4)/ABS(D4(4)))*(ABS(D4(4))-WD)*(TR(I6(4),4)-TR(I7(4),4))
      S8=(TR(I6(4),4)-TR(I7(4),4))**2
      S9=(D5(5)/ABS(D5(5)))*(ABS(D5(5))-WD)*(TR(I6(5),5)-TR(I7(5),5))
      S10=(TR(I6(5),5)-TR(I7(5),5))**2
      IK1=IK+1
      GD(IK1,1)=GD(IK,1)-S1/S2
      GD(IK1,2)=GD(IK,2)-S3/S4
```

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      GD(IK1,3)=GD(IK,3)-S5/S6
      GD(IK1,4)=GD(IK,4)-S7/S8
      GD(IK1,5)=GD(IK,5)-S9/S10
      WRITE(6,50)IK1,GD(IK1,1),GD(IK1,2),GD(IK1,3),
     1GD(IK1,4),GD(IK1,5)
   50 FORMAT(5X,*IK1=*,I3,2X,*GD(IK1,1)=*,E10.4,2X,
     1*GD(IK1,2)=*,E10.4,2X,*GD(IK1,3)=*,E10.4,2X,
     1*GD(IK1,4)=*,E10.4,2X,*GD(IK1,5)=*,E10.4,//)
   40 CONTINUE
      STOP
      END
```

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