ELECTRON SPIN RESONANCE STUDY OF THE E_2' CENTER IN QUARTZ

By

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CHAPTER I

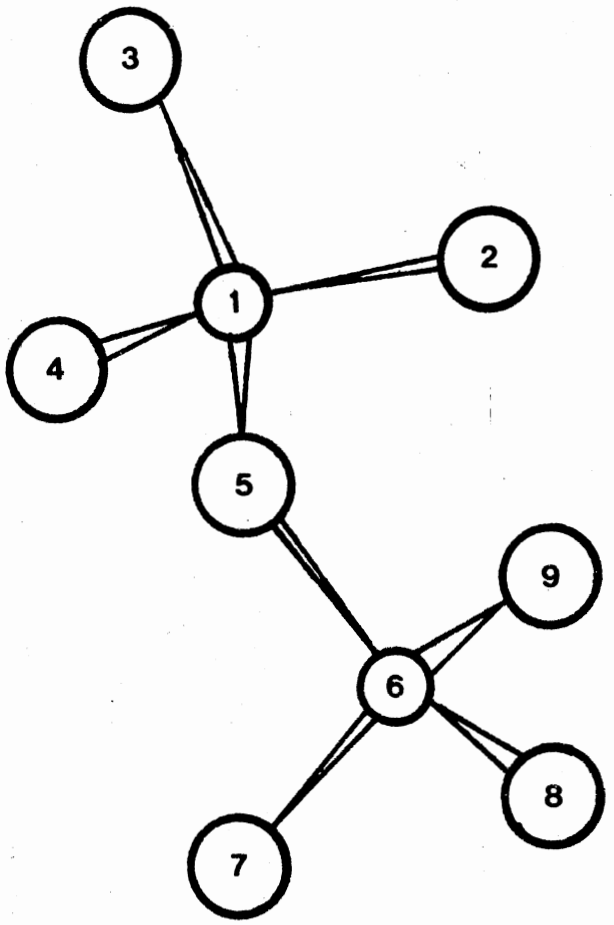
INTRODUCTION

Radiation-induced defects in solids have been studied extensively for the last sixty years. It is well known that high energy irradiation produces defects in crystals. Study of these defects is important since many materials are being used in various industrial areas involving high energy irradiation.

Electron spin resonance has been used as one of the important tools to visualize the crystalline environment in the vicinity of well-localized defects (called point defects) in crystalline solids.

Quartz (SiO_2) is different from other oxides, in that it is neither completely ionic nor completely covalent. This makes its study much more difficult. It does not have a high symmetry crystal structure (1). The crystal structure for SiO_2 is shown in Figure 1. For quite some time now quartz has been used for oscillators in space satellites and hence has been exposed to various kinds of irradiation in outer space. It has been observed that properties of the oscillators do not remain the same as a consequence of its exposure to high energy irradiation (2).

The E' center in quartz is similar to the F center in ionic materials in which an electron is trapped at a negative ion vacancy. The notation was first introduced by R. A. Weeks and C. M. Nelson (3) for this paramagnetic defect in quartz. There are three different




Oxygen


Silicon

Si(1) - Ox(5)	Long Bond = 1.6120 A^{o}
Si(6) - Ox(5)	Short Bond =1.6072 A^{o}
Si(1) - Ox(5)-Si(6)	Angle =143.5^{o}

Figure 1. Structure of Right Quartz. (Projection on z-plane with +z axis coming out of plane of paper)

types of E' centers reported in the literature. They are the E_1' center, the E_2' center and the E_4' center. Some E' type centers are shown in Figure 2. The E_2' and E_4' centers are different from the E_1' center in that proton hyperfine effects are associated with them.

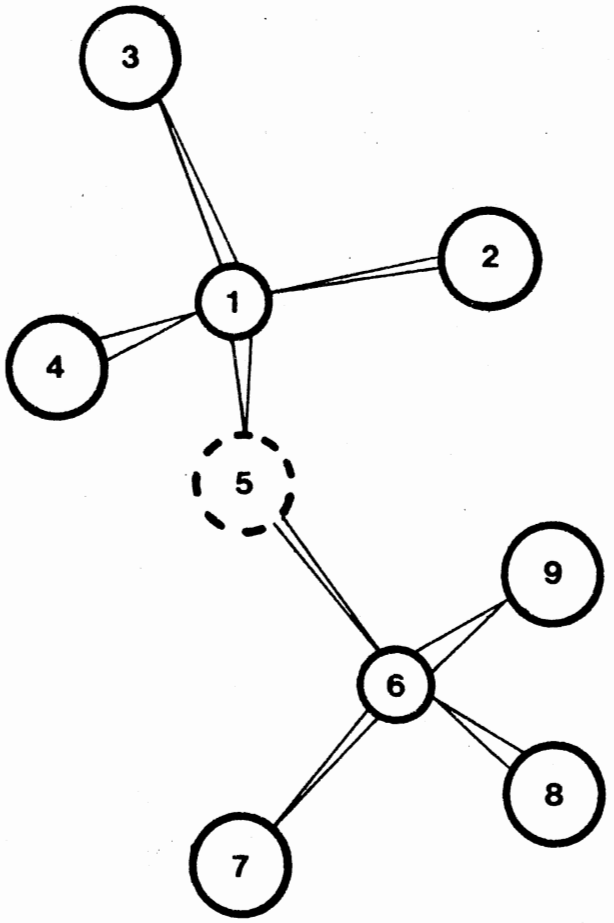
The E_1' center was originally reported by R. A. Weeks (4). This study inspired many other people to carry out theoretical and experimental investigations of the E' centers in SiO_2. Some of these studies are discussed briefly in the following few paragraphs.

R. A. Weeks and C. M. Nelson (3)

The correlation of optical bands with ESR spectra was established by a series of optical bleaching and thermal annealing experiments. They used ^{60}Co γ-irradiated synthetic crystalline quartz in this study. It was concluded from this study that an optical band at 210 nm is associated with the E_1' center and an absorption band at 230 nm is associated with the E_2' center. Defect models were proposed for the E_1', the E_1'' and the E_2' centers.

R. H. Silsbee (5)

A detailed electron spin resonance study of E_1' centers produced by fast neutron-irradiation of crystalline quartz was done. The parameters for the g tensor and hyperfine tensor were reported for the E_1' center. It was concluded that the E_1' center, produced by low neutron doses, consisted of an unpaired electron in a non-bonding orbital on a silicon. The complete breakdown of the crystalline structure was observed at high doses of neutron irradiation. A pair of weak lines 400



E_1 - Contains no electrons

E_1' - Trapped a single electron

E_1'' - Trapped two electrons

Figure 2. Different E'-Type Center Models

gauss apart were attributed to a single ^{29}Si strong hyperfine interaction.

Kwok Leung Yip and W. Beall Fowler (6)

Theoretical analysis of the E_1' center in the α-quartz structure of SiO_2 was done using a linear combination of localized orbital-molecular orbital (LCLO-MO) cluster method. Similar analysis was also done for the E_1'(Ge) center which is an electron trapped by a germanium ion substituted for a silicon ion neighboring an oxygen vacancy in SiO_2. It was also concluded from this theoretical study that the E_1' center is an electron trapped at an oxygen vacancy. The trapped electron at the defect site is strongly localized in a non-bonding sp^3 hybrid orbital centered on silicon (or Ge substituted for Si) and oriented almost along a Si-O short bond direction toward the oxygen vacancy.

R. A. Weeks (7)

The E_2' center was studied in detail using the electron spin resonance technique. A spectrum consisting of two lines about 0.4 ± 0.1 gauss apart was observed for the magnetic field oriented along the c axis. An angular dependence study was done for this spectrum and the g tensor parameters were calculated. It was concluded from this study that the E_2' center is an electron trapped at an oxygen vacancy with a proton nearby. In addition to the primary doublet spectrum, an additional pair of similar doublets about 412 gauss apart was observed for the magnetic field along the c axis. The widely split pair of doublets was attributed to the strong hyperfine interaction with ^{29}Si.

F. J. Feigl and J. H. Anderson (8)

Paramagnetic defects produced by low energy ionizing radiation in crystalline quartz doped with Ge were studied through electron spin resonance. Their analysis indicated that these defects are similar to the E_1' and the E_2' centers in pure crystalline quartz, with a Ge ion substituted for the central Si ion in the E'-defect structures. The parameters for these Ge-related defects were calculated and compared with the parameters reported by R. H. Silsbee (5) and R. A. Weeks (7). It was concluded from this investigation that the unpaired electron occupies a non-bonding orbital strongly localized on the Ge impurity. A single oxygen vacancy model for the entire E' class of center was adequate to explain their data.

L. E. Halliburton and J. A. Weil (9)

The E_4' center first reported by R. A. Weeks and C. M. Nelson (3), was studied in detail using electron spin resonance. Nelson and Weeks suggested that the four equally spaced and equally intense line spectrum was a result of an unpaired electron interacting with an alkali ion ($I = 3/2$). The complete angular dependence study of the four line spectrum was done and the parameters for the g tensor and A tensors were calculated. It was concluded from this study that the E_4' center has $S = 1/2$ and the hyperfine structure arises from interactions with a proton ($I = 1/2$) in a situation permitting observation of all $2S(2I+1)^2$ possible ESR transitions.

Present Study

In the present study, the angular dependence study of the two

pairs of lines due to strong hyperfine interaction with ^{29}Si for the E_2' center is reported. This study provides additional information from which the precise model for the E_2' center in quartz may be determined.

CHAPTER II

EXPERIMENTAL PROCEDURE

In this chapter, the experimental procedure and equipment used to study the E_2' center in SiO_2 is described. In Section I, sample preparation and defect production in SiO_2 is discussed. The ESR spectrometer and operating procedure is outlined in Section II.

I. Sample Preparation and Defect Production

The sample used in this study was obtained from R. A. Weeks, Oak Ridge National Laboratory. The main difficulty in this study was that the history of treatments received by this sample was not available. It was known that the crystal had been irradiated in a ^{60}Co γ-cell, receiving a dosage of 4.5×10^9 R at some time in the past.

The next important question was how one explains defect production in the crystal. One of the possible explanations is that oxygen vacancies were already present in the crystal as a result of the hydrothermal growth process. This seems reasonable, since it was observed that Sawyer Electronic Grade samples, on being irradiated by electrons from a Van de Graaff accelerator, give similar ESR signals as from our γ-irradiated samples. Dimensions of the Sawyer Electronic Grade sample were nearly one-half of our γ-irradiated samples. The irradiation dose received by our Sawyer samples is not sufficient to create oxygen vacancies. Hence we conclude that oxygen vacancies are initially pres-

ent in the sample. Electron irradiation or γ-irradiation just moves around the charges to form paramagnetic defects.

II. ESR Spectrometer

The x-band homodyne spectrometer used to obtain the ESR spectra in this study is shown in the block diagram in Figure 3. The microwave power was supplied by a Varian VA-153C klystron. The klystron was locked to the resonant frequency of the sample cavity with the help of a reflector-modulated stabilizer. The sample was placed inside a rectangular microwave cavity operating in the TE_{102} mode. The precision attenuator in the sample arm regulated the microwave power incident on the sample. The microwave frequency was measured using a Hewlett-Packard frequency counter.

A Varian 9-inch V-7200 electro-magnet was used to produce the magnetic field. Any variations in the field intensity were detected by a Hall probe mounted on one of the pole caps. This probe supplies an error signal which adjusts the magnet current to maintain stability of the field. Magnetic field values could be directly read in gauss from the field set controls. But this method was not precise enough to yield correct field values, thus a different method was used.

The static magnetic field was amplitude modulated at 100 kHz. The modulation coils were mounted on the outside of a glass Dewar. The microwave signal was detected using a properly biased low-noise Schottky barrier diode. This signal was then amplified by a broad-band amplifier (Micro-Now Instruments Co., Model 521). The amplified signal was fed to a phase sensitive detector (PAR Model 128) which greatly enhanced the signal-to-noise ratio. The reference signal for the phase sensitive

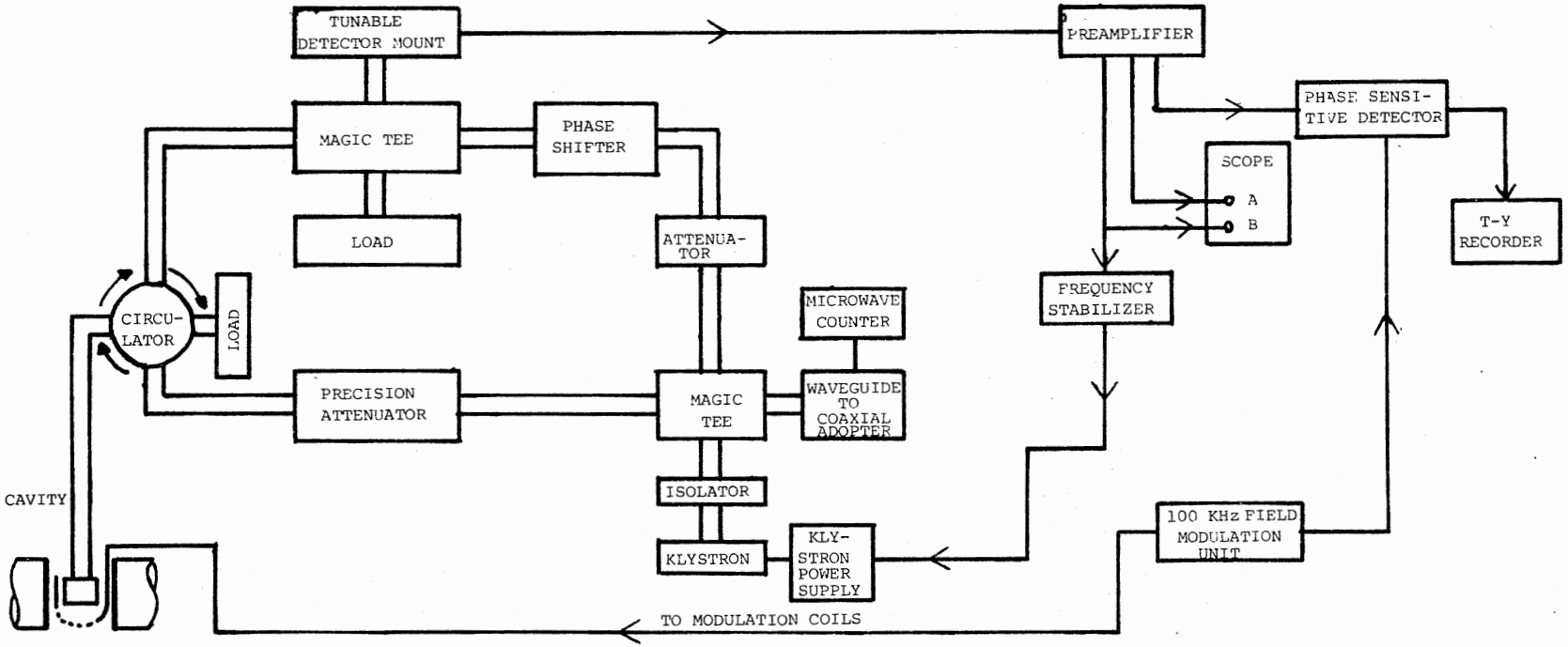


Figure 3. ESR Spectrometer

detector was obtained from the oscillator which amplitude-modulated the magnetic field. The output from the phase sensitive detector was fed into a strip chart recorder (Leeds and Northrup) which yielded a first derivative ESR spectrum.

Magnetic field measurements were made using an NMR marginal oscillator and proton probe. The probe essentially consisted of coaxial cable surrounded by a brass tube. At one end of the probe a rigid BNC connector was provided for connecting to the marginal oscillator. At the other end of the coaxial cable an inductor which consisted of 18-20 turns of copper wire was wound on a glass capsule containing the NMR sample. Since the probe could not be placed at the same position as the ESR sample in the cavity, a correction was made to the measured field values using a standard Cr^{3+}-doped MgO sample whose g-value is 1.9799.

CHAPTER III

THEORETICAL ANALYSIS AND EXPERIMENTAL RESULTS

This chapter is divided into two sections. The theoretical format for analysis of the E_2' center spectra is presented in Section I. Experimental results and computer programs for data reduction are discussed in Section II. Some of the results obtained using these computer programs are also presented in Section II. Conclusions reached in this study will be presented in the next chapter.

I. Theoretical Analysis

The spin Hamiltonian describing the E_2' center is given by

$$H = \beta \vec{H} \cdot \overleftrightarrow{g} \cdot \vec{S} + \vec{I}_1 \cdot \overleftrightarrow{A}_1 \cdot \vec{S} + \vec{I}_2 \cdot \overleftrightarrow{A}_2 \cdot \vec{S} - (g_N \beta_N)_1 \vec{H} \cdot \vec{I}_1 - (g_N \beta_N)_2 \vec{H} \cdot \vec{I}_2$$

where the first term represents the electron Zeeman interaction, the second and the third terms represent hyperfine interactions due to a proton (H^+) nucleus and a ^{29}Si (I = 1/2, 4.7% abundant) nucleus, respectively, with the unpaired electron. The last two terms represent nuclear Zeeman interactions for the two nuclei, respectively.

The following coordinate systems are used in converting the Hamiltonian to a suitable form for computer programming.

x,y,z: Magnetic field coordinate system chosen such that the magnetic field is along the z direction.

x_c, y_c, z_c: Crystal coordinate system.

x_g, y_g, z_g: Principal axes of the g tensor.

x_1, y_1, z_1: Principal axes system for the proton hyperfine tensor, $\overleftrightarrow{A}_1$.

x_2, y_2, z_2: Principal axes system for the ^{29}Si hyperfine tensor, $\overleftrightarrow{A}_2$.

Rewriting the Hamiltonian in terms of different coordinate systems, we have

$$H = \beta[S_{x_g} g_x H_{x_g} + S_{y_g} g_y H_{y_g} + S_{z_g} g_z H_{z_g}]$$

$$+ I_{x_1} A_{x_1} S_{x_1} + I_{y_1} A_{y_1} S_{y_1} + I_{z_1} A_{z_1} S_{z_1}$$

$$+ I_{x_2} A_{x_2} S_{x_2} + I_{y_2} A_{y_2} S_{y_2} + I_{z_2} A_{z_2} S_{z_2}$$

$$- (g_N\beta_N)_1 H I_{z_1} - (g_N\beta_N)_2 H I_{z_2}$$

The relationships between the different coordinate systems are

$$\begin{pmatrix} x_g \\ y_g \\ z_g \end{pmatrix} = [TG] \begin{pmatrix} x \\ y \\ z \end{pmatrix},$$

$$\begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} = [TH] \begin{pmatrix} x \\ y \\ z \end{pmatrix},$$

and

$$\begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix} = [TM] \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

where the transformation matrices are defined as follows:

[G]: Transforms principal axes of the g tensor to crystal coordinate system.

[H]: Transforms principal axes of the hyperfine tensor A_1 to crystal coordinate system.

[M]: Transforms principal axes of the hyperfine tensor A_2 to crystal coordinate system.

[R]: Transforms the crystal coordinate system to the magnetic field coordinate system.

[TG] = [G] [R]: Transforms principal axes of the g tensor to the magnetic field coordinate system.

[TH] = [H] [R]: Transforms principal axes system of hyperfine tensor A_1 to the magnetic field coordinate system.

[TM] = [M] [R]: Transforms principal axes system of hyperfine tensor A_2 to the magnetic field coordinate system.

Now using the above transformations, the Hamiltonian is written in terms of the magnetic field coordinate system only, as follows:

$$H = W1\,S_x + W2\,S_y + W3\,S_z + W4\,I_{1x}S_x + W5\,I_{1x}S_y + W6\,I_{1x}S_z + W5\,I_{1y}S_x + W7\,I_{1y}S_y + W8\,I_{1y}S_z + W6\,I_{1z}S_x + W8\,I_{1z}S_y + W9\,I_{1z}S_z + W10\,I_{2x}S_x + W11\,I_{2x}S_y + W12\,I_{2x}S_z + W11\,I_{2y}S_x + W13\,I_{2y}S_y + W14\,I_{2y}S_z + W12\,I_{2z}S_x + W14\,I_{2z}S_y + W15\,I_{2z}S_z - (g_N\beta_N)_1\,HI_{1z} - (g_N\beta_N)_2\,HI_{2z}$$

where

$$W1 = \beta H[g_x\,TG(1,1)TG(1,3) + g_y\,TG(2,1)TG(2,3) + g_x\,TG(3,1)TG(3,3)]$$

$$W2 = \beta H[g_x\,TG(1,2)TG(1,3) + g_y\,TG(2,2)TG(2,3) + g_z\,TG(3,2)TG(3,3)]$$

$$W3 = \beta H[g_x\,TG(1,3)TG(1,3) + g_y\,TG(2,3)TG(2,3) + g_z\,TG(3,3)TG(3,3)]$$

$$W4 = A_{1x}\,TH(1,1)TH(1,1) + A_{1y}\,TH(2,1)TH(2,1) + A_{1z}\,TH(3,1)TH(3,1)$$

$$W5 = A_{1x}\,TH(1,1)TH(1,2) + A_{1y}\,TH(2,1)TH(2,2) + A_{1z}\,TH(3,1)TH(3,2)$$

$$W6 = A_{1x}\,TH(1,1)TH(1,3) + A_{1y}\,TH(2,1)TH(2,3) + A_{1z}\,TH(3,1)TH(3,3)$$

$$W7 = A_{1x}\,TH(1,2)TH(1,2) + A_{1y}\,TH(2,2)TH(2,2) + A_{1z}\,TH(3,2)TH(3,2)$$

$$W8 = A_{1x}\,TH(1,2)TH(1,3) + A_{1y}\,TH(2,2)TH(2,3) + A_{1z}\,TH(3,2)TH(3,3)$$

$$W9 = A_{1x}\,TH(1,3)TH(1,3) + A_{1y}\,TH(2,3)TH(2,3) + A_{1z}\,TH(3,3)TH(3,3)$$

$$W10 = A_{2x}\,TM(1,1)TM(1,1) + A_{2y}\,TM(2,1)TM(2,1) + A_{2z}\,TM(3,1)TM(3,1)$$

$$W11 = A_{2x}\,TM(1,1)TM(1,2) + A_{2y}\,TM(2,1)TM(2,2) + A_{2z}\,TM(3,1)TM(3,2)$$

$$W12 = A_{2x}\,TM(1,1)TM(1,3) + A_{2y}\,TM(2,1)TM(2,3) + A_{2z}\,TM(3,1)TM(3,3)$$

$$W13 = A_{2x}\,TM(1,2)TM(1,2) + A_{2y}\,TM(2,2)TM(2,2) + A_{2z}\,TM(3,2)TM(3,2)$$

$$W14 = A_{2x}\,TM(1,2)TM(1,3) + A_{2y}\,TM(2,2)TM(2,3) + A_{2z}\,TM(3,2)TM(3,3)$$

$$W15 = A_{2x}\,TM(1,3)TM(1,3) + A_{2y}\,TM(2,3)TM(2,3) + A_{2z}\,TM(3,3)TM(3,3)\ .$$

Using the raising and the lowering operators

$$S_+ = S_x + iS_y \ , \ S_- = S_x - iS_y \ ,$$

$$I_+ = I_x + iI_y \ , \ I_- = I_x - iI_y \ ,$$

we can write the Hamiltonian in the following form,

$$\begin{aligned} H = {} & W3\, S_z + W9\, I_{1z} S_z + W15\, I_{2z} S_z - (g_N \beta_N)_1 HI_{1z} \\ & - (g_N \beta_N)_2 HI_{2z} + Q1^* S_+ + Q1 S_- + Q2^* I_{1+} S_+ \\ & + Q3 I_{1+} S_- + Q3 I_{1-} S_+ + Q2 I_{1-} S_- + Q4^* I_{1+} S_z \\ & + Q4 I_{1-} S_z + Q4^* I_{1z} S_+ + Q4 I_{1z} S_- + Q5^* I_{2+} S_+ \\ & + Q6 I_{2+} S_- + Q6 I_{2-} S_+ + Q5 I_{2-} S_- + Q7^* I_{2+} S_z \\ & + Q7 I_{2-} S_z + Q7^* I_{2z} S_+ + Q7 I_{2z} S_- \end{aligned}$$

where

$$\begin{aligned} Q1 &= 1/2(W1 + iW2) \\ Q2 &= 1/4(W4 - W7) + 1/2\ W5 \\ Q3 &= 1/4(W4 + W7) \\ Q4 &= 1/2(W6 + iW8) \\ Q5 &= 1/4(W10 - W13) + 1/2\ W11 \\ Q6 &= 1/4(W10 + W13) \\ Q7 &= 1/2(W12 + iW14) \ . \end{aligned}$$

Since the ^{29}Si nucleus has I = 1/2 and the proton (H^+) nucleus has I = 1/2, the basis set chosen is $|M_s = \pm 1/2, M_{I_1} = \pm 1/2, M_{I_2} = \pm 1/2\rangle$. This basis set consists of eight vectors, which allows one to write the Hamiltonian in an 8 x 8 matrix form. The Hamiltonian being hermitian, the lower half of the matrix elements are sufficient to calculate the

energy eigenvalues.

The notation for the lower half of the matrix elements is presented in Table I. The non-zero elements are given as follows:

$$A(1,1) = 1/2\ W3 + 1/4(W9+W15) - 1/2(g_N\beta_N)_1\ H - 1/2(g_N\beta_N)_2\ H$$

$$A(2,1) = 1/2\ Q4$$

$$A(3,1) = Q1 + 1/2(Q4+Q7)$$

$$A(4,1) = Q2$$

$$A(5,1) = 1/2\ Q7$$

$$A(7,1) = Q5$$

$$A(2,2) = 1/2\ W3 - 1/4(W9-W15) + 1/2(g_N\beta_N)_1\ H - 1/2(g_N\beta_N)_2\ H$$

$$A(3,2) = Q3$$

$$A(4,2) = Q1 - 1/2(Q4-Q7)$$

$$A(6,2) = 1/2\ Q7$$

$$A(8,2) = Q5$$

$$A(3,3) = -\ 1/2\ W3 - 1/4(W9+W15) - 1/2(g_N\beta_N)_1\ H - 1/2(g_N\beta_N)_2\ H$$

$$A(4,3) = -\ 1/2\ Q4$$

$$A(5,3) = Q6$$

$$A(7,3) = -\ 1/2\ Q7$$

$$A(4,4) = -\ 1/2\ W3 + 1/4(W9-W15) + 1/2(g_N\beta_N)_1\ H - 1/2(g_N\beta_N)_2\ H$$

$$A(6,4) = Q6$$

$$A(8,4) = -\ 1/2\ Q7$$

$$A(5,5) = 1/2\ W3 + 1/4(W9-W15) - 1/2(g_N\beta_N)_1\ H + 1/2(g_N\beta_N)_2\ H$$

$$A(6,5) = 1/2\ Q4$$

$$A(7,5) = Q1 + 1/2(Q4-Q7)$$

$$A(8,5) = Q2$$

TABLE I

THE LOWER HALF OF THE HAMILTONIAN MATRIX

	$\left\vert\frac{1}{2},\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\vert\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\vert-\frac{1}{2},\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\vert-\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\vert\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle$	$\left\vert\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right\rangle$	$\left\vert-\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle$	$\left\vert-\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right\rangle$
$\left\vert\frac{1}{2},\frac{1}{2},\frac{1}{2}\right\rangle$	A(1,1)							
$\left\vert\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right\rangle$	A(2,1)	A(2,2)						
$\left\vert-\frac{1}{2},\frac{1}{2},\frac{1}{2}\right\rangle$	A(3,1)	A(3,2)	A(3,3)					
$\left\vert-\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right\rangle$	A(4,1)	A(4,2)	A(4,3)	A(4,4)				
$\left\vert\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle$	A(5,1)	0	A(5,3)	0	A(5,5)			
$\left\vert\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right\rangle$	0	A(6,2)	0	A(6,4)	A(6,5)	A(6,6)		
$\left\vert-\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle$	A(7,1)	0	A(7,3)	0	A(7,5)	A(7,6)	A(7,7)	
$\left\vert-\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right\rangle$	0	A(8,2)	0	A(8,4)	A(8,5)	A(8,6)	A(8,7)	A(8,8)

$$A(6,6) = 1/2\ W3 - 1/4(W9+W15) + 1/2(g_N\beta_N)_1\ H + 1/2(g_N\beta_N)_2\ H$$

$$A(7,6) = Q3$$

$$A(8,6) = Q1 - 1/2(Q4 + Q7)$$

$$A(7,7) = -\ 1/2\ W3 - 1/4(W9-W15) - 1/2(g_N\beta_N)_1\ H + 1/2(g_N\beta_N)_2\ H$$

$$A(8,7) = -\ 1/2\ Q4$$

$$A(8,8) = -\ 1/2\ W3 + 1/4(W9+W15) + 1/2(g_N\beta_N)_1\ H + 1/2(g_N\beta_N)_2\ H$$

II. Experimental Results

The principal E_2' center ESR spectrum for the magnetic field along the [001] direction consists of two equally intense lines 0.37 ± 0.02 gauss apart as shown in Figure 4. The other four lines in the figure represent the E_4' center. This data was obtained at 300K. The lowest field E_4' center line was used to check the alignment. The two lines associated with the E_2' center arise as a result of the interaction of an electron trapped at an oxygen vacancy with a proton near the defect site (3).

In addition to this primary doublet for the E_2' center, two additional weak pairs of lines were observed with the magnetic field along the [001] direction as shown in Figure 5. The separation of each of these pairs of lines is nearly 0.37 ± 0.02 gauss, the same as the primary doublet. One pair of lines was approximately 198.6 gauss above the primary doublet and the other pair was nearly 226.8 gauss below the primary doublet. The separation between these two pairs of doublets is 425.4 gauss which is greater than the value 412 gauss reported in the literature by R. A. Weeks [7]. These low and high field pairs of doublets are attributed to a strong hyperfine interaction with a ^{29}Si

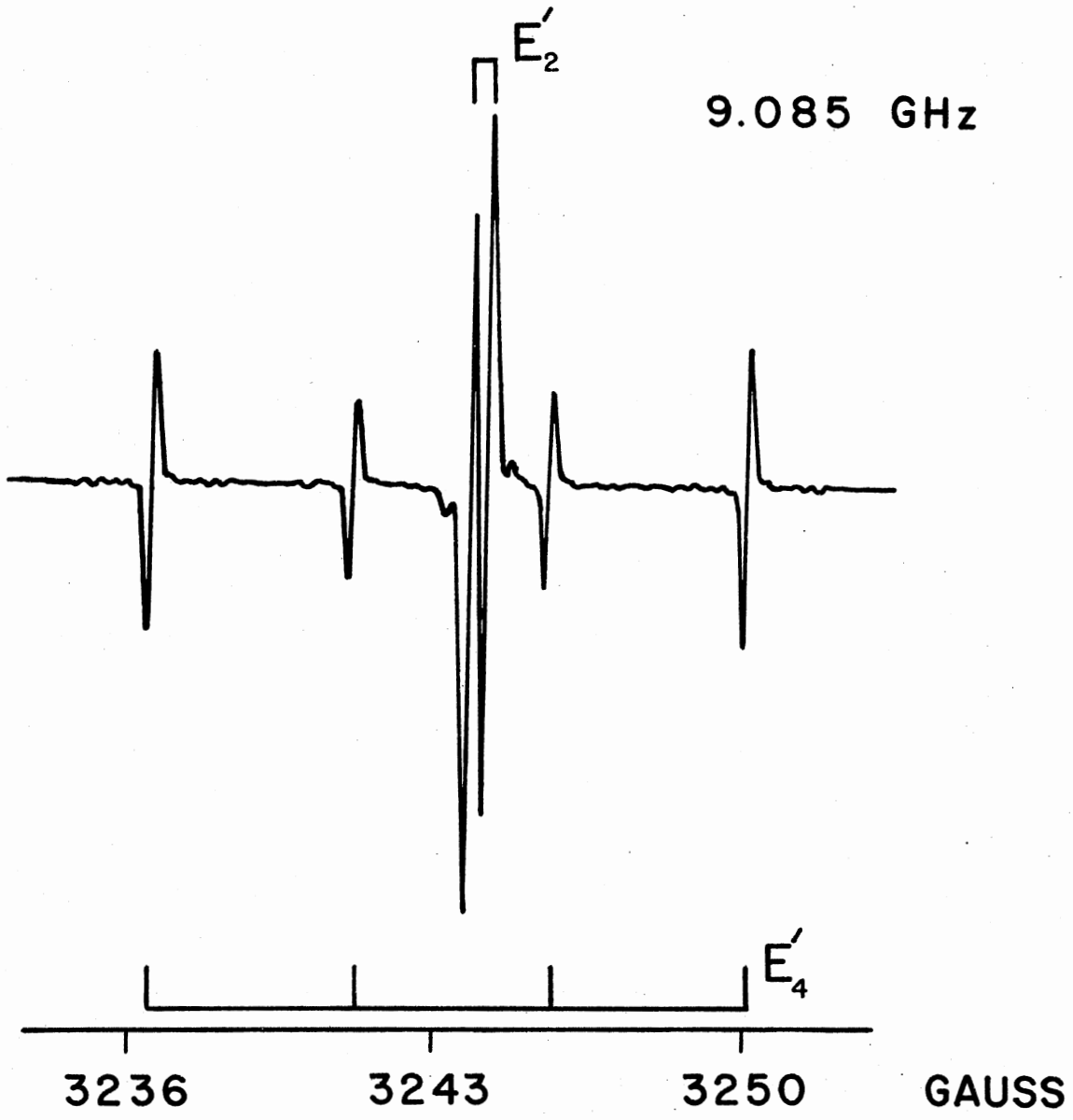


Figure 4. ESR Spectrum for the E_2' and the E_4' Center With Magnetic Field Along the [001] Direction at 300K

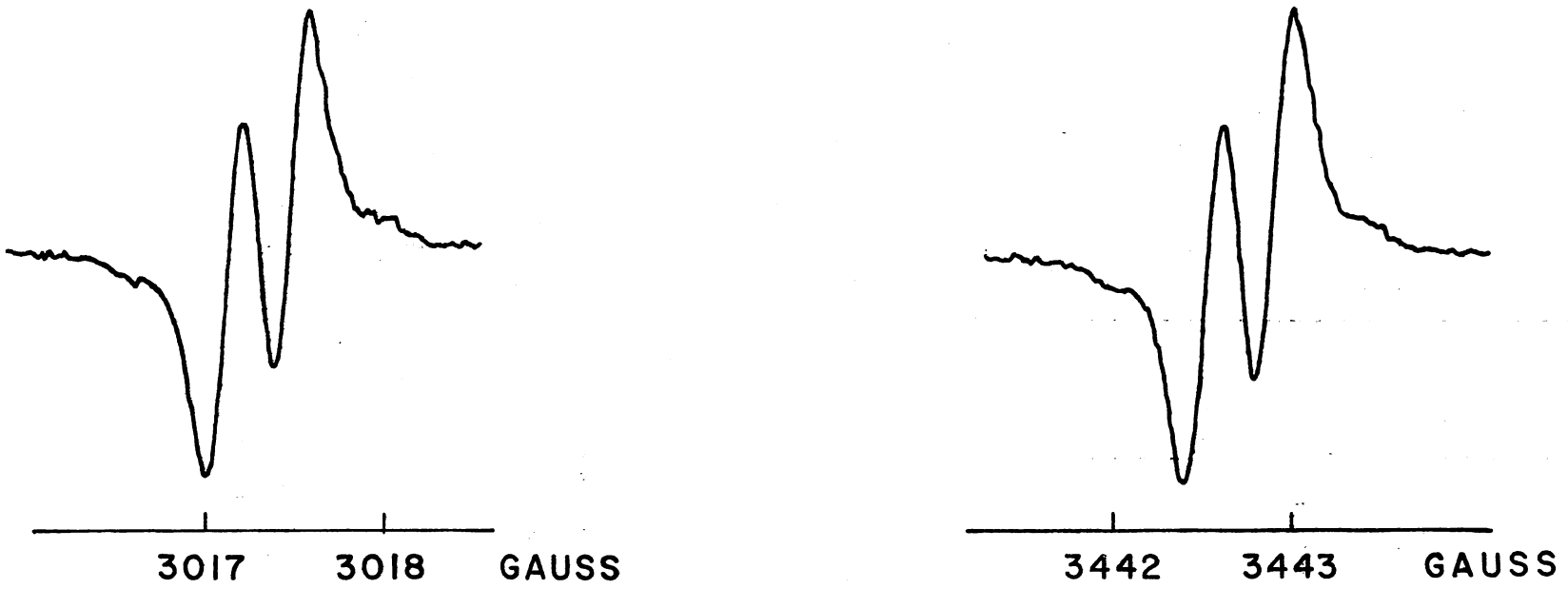


Figure 5. ESR Spectrum for ^{29}Si Hyperfine Interaction With Magnetic Field Along the [001] Direction at 300 K

nucleus ($I = \frac{1}{2}$, 4.7% natural abundance).

An angular dependence study of the low and high field pairs of doublets was carried out at 300K. The magnetic field was rotated about the two-fold crystal axis and spectra were obtained at 15° intervals. Data were taken up to 70° of rotation on each side from the [001] direction. The intensity of the signal dropped rapidly beyond 70°, because the microwave magnetic field component perpendicular to the static magnetic field is proportional to $\cos^2\theta$. The results of this study are presented in Figure 6, for both the low and high field pairs of lines. In this figure, proton hyperfine effects are not illustrated. Each line in this figure represents the average of the doublet. The proton hyperfine effects are illustrated in Figure 7 for the high field doublet.

An isochronal temperature anneal study was done by holding the sample at a desired temperature for 3 minutes and then taking an ESR spectrum at room temperature. Results of this study are shown in Figure 8. At 450K, half of the E_2' centers have decayed. The initial growth of the E_2' center is questionable and additional experimental verification will be required.

Two separate programs were written to analyze the experimental data presented in Figure 7. These are listed in Appendices A and B, respectively. The first program, listed in Appendix A, calculates the transition frequencies for a given set of spin Hamiltonian parameters and an assumed magnetic field value. This is equivalent to obtaining data at a fixed value of magnetic field by scanning the microwave frequency. The second program, listed in Appendix B, calculates the final set of parameters (g and A tensors) using the experimental data as in-

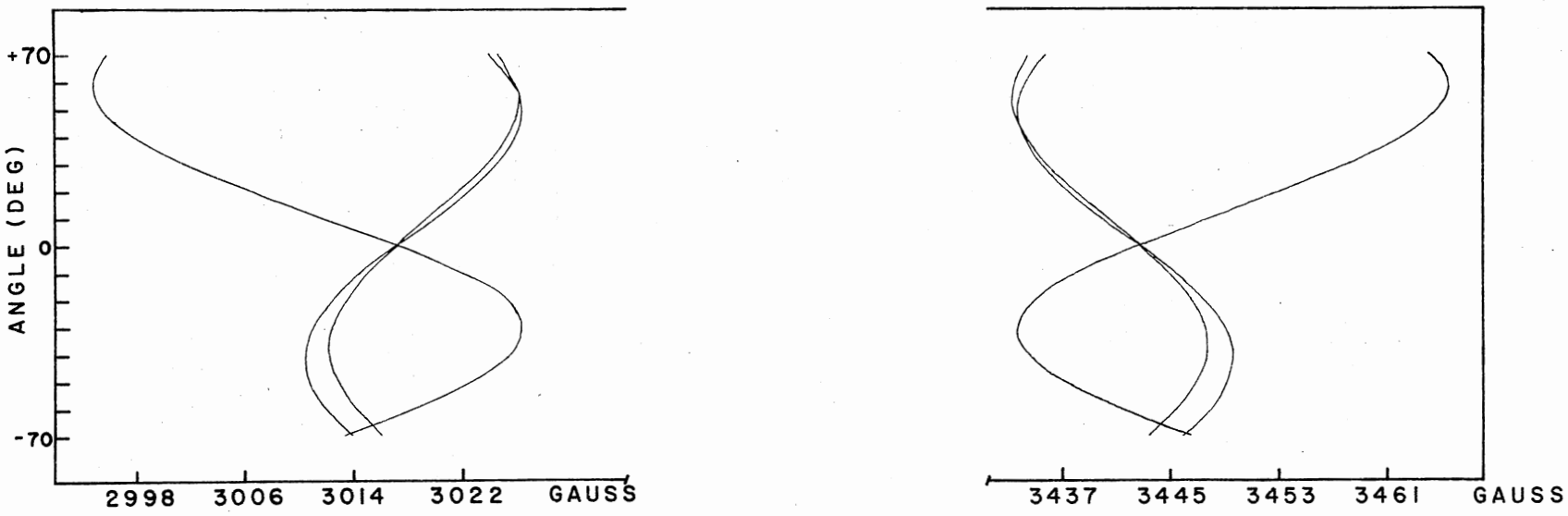


Figure 6. Angular Dependence for ^{29}Si Hyperfine Interaction

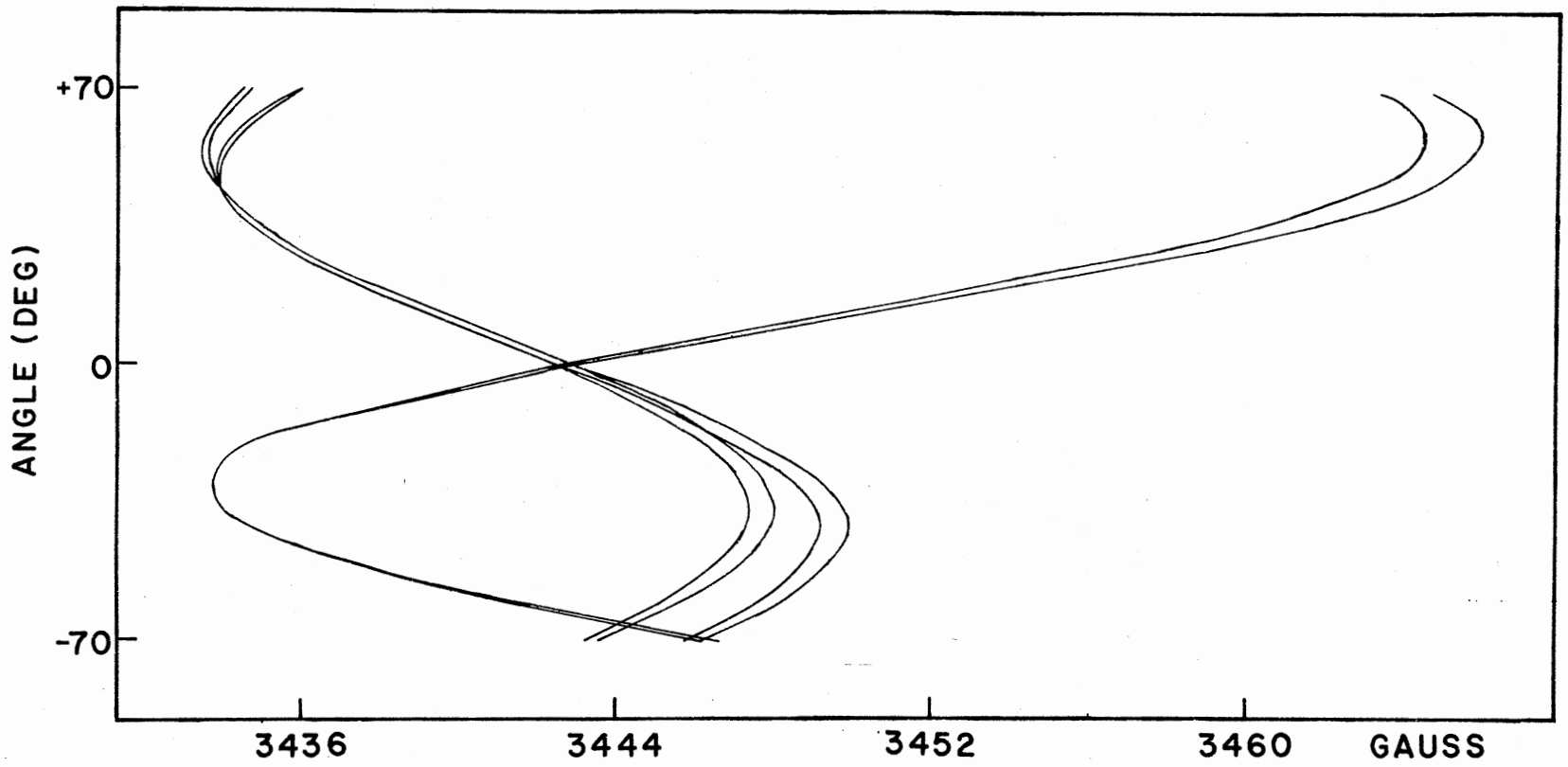


Figure 7. Angular Dependence for the High Field Doublet Illustrating the Proton Effects

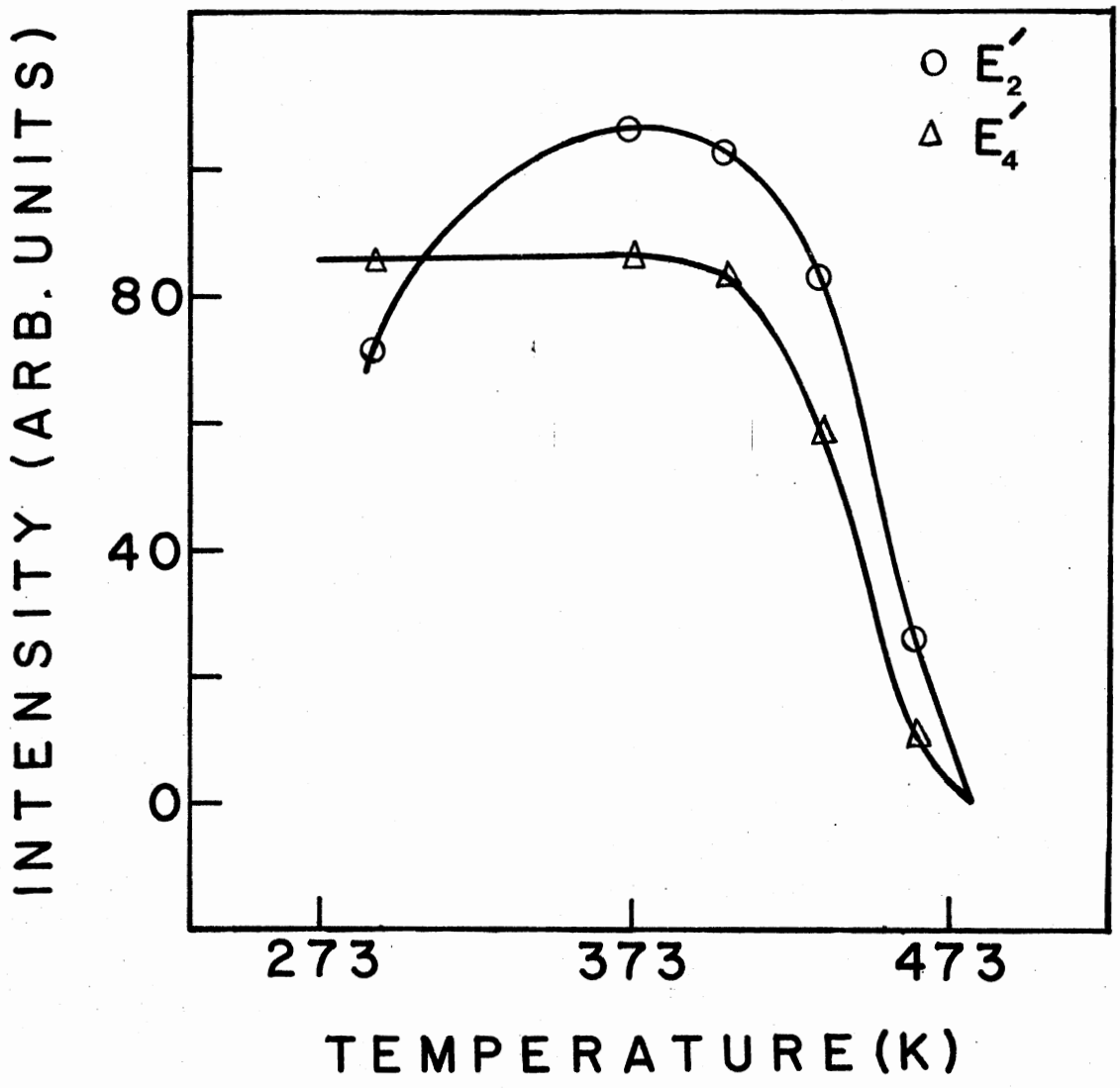


Figure 8. Pulse Anneal Study of the E_2' and the E_4' Center in SiO_2

put.

In the first program, it was assumed that the parameters for the g and A tensors are known. The magnetic field values associated with different ESR resonance lines are predicted by an iteration scheme. An initial value of magnetic field, H, is assigned. The direction of the magnetic field relative to the defect site is specified by the parameters alpha (α) and beta (β). For each set of these angles there are four transitions according to the spin selection rules $\Delta M_s = \pm 1$, $\Delta M_{I_1} = 0$ and $\Delta M_{I_2} = 0$. These possible four transitions are shown in Figure 9. The 8 x 8 matrix shown in Table I is diagonalized and eight energy eigenvalues D(I) given in order of ascending value are obtained. The four transitions are given by

$$h\nu_1 = D(8) - D(2) ,$$

$$h\nu_2 = D(7) - D(1) ,$$

$$h\nu_3 = D(6) - D(4) ,$$

$$h\nu_4 = D(5) - D(3) .$$

The assigned field value is then varied and the microwave frequency corresponding to a particular transition is recalculated and compared with the experimental microwave frequency 9.085 GHz. If the calculated microwave frequency lies within 0.1 MHz of the experimental frequency, then the microwave frequency for the other, 3 transitions are calculated by iteration.

In the second program, the values of different parameters are systematically varied until a good agreement between the calculated and experimental magnetic field positions is obtained. An initial set of

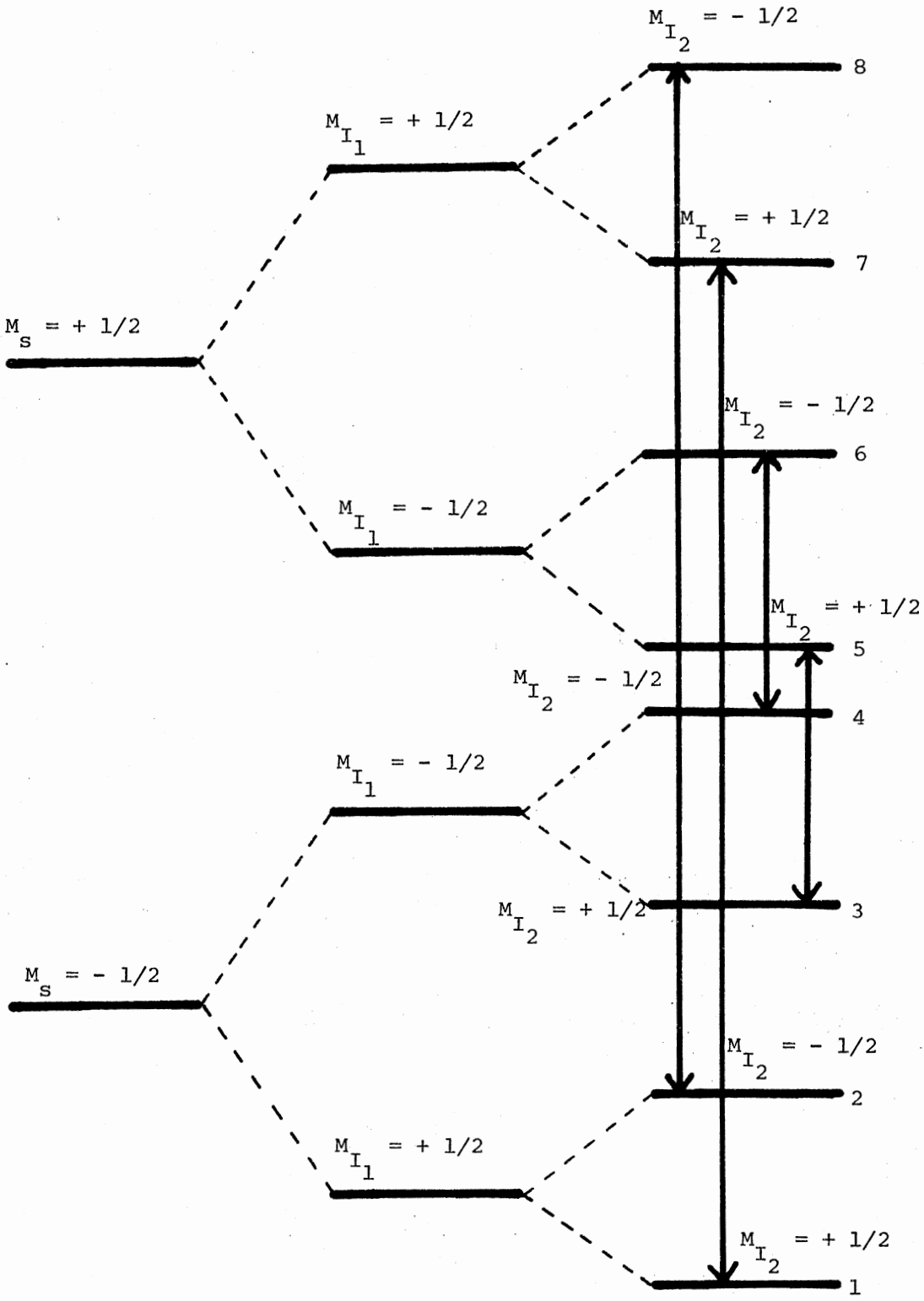


Figure 9. Energy Levels and Possible Transitions in an S = 1/2, I_1 = 1/2 and I_2 = 1/2 System

parameters is assumed and the magnetic field positions for different orientations of the magnetic field are provided as experimental data. Using this information the energy eigenvalues are obtained as in the first program and the microwave frequency associated with each resonance is calculated.

Since the assumed parameters are not the correct ones, the calculated microwave frequency is not the same as the experimental value. Therefore a quantity called SUM

$$\text{SUM} = \sum_{i=1}^{28} [\nu_i^{exp} - \nu_i^{cal}]^2$$

is calculated. Now the value of SUM is minimized by an iteration technique. Using the assumed set of parameters, the value of SUM is calculated. One of the parameters then is increased by a pre-determined amount and a new set of calculated microwave frequencies are obtained by diagonalization of the matrix. Thus, a new value of SUM is obtained and compared with the previous value of SUM. If the new value of SUM is greater than the previous value, then the value of the parameter (which was increased) is decreased by twice the specified increment. All the microwave frequencies are obtained again and SUM is recalculated. This SUM is compared with the initial value of SUM and the value of the parameter which gives the smallest SUM is retained. This procedure is repeated for all the other parameters.

The final set of parameters was reached when any variation in the parameters failed to lower the value of SUM. The parameters obtained from the computer programs are listed in Table II. The final parameters obtained in this study for the g tensor and proton hyperfine tensor are in good agreement with the parameters listed in Table III

TABLE II

SPIN HAMILTONIAN PARAMETERS FOR THE E_2' CENTER FROM PRESENT STUDY

		z-component	x-component	y-component
Zeeman	g-tensor	2.0020 (120°, 149°)	2.0006 (67°, 73°)	2.0004 (140°, 14°)
H^+	hfs.	4.21 MHz (237°, 26°)	-0.23 MHz (134°, 24°)	-0.56 MHz (117°, -83°)
Si^{29}	hfs.	1312.95 MHz (59°, 27°)	1135.54 MHz (67°, -48°)	1135.51 MHz (140°, -72°)

TABLE III

SPIN HAMILTONIAN PARAMETERS REPORTED BY FEIGEL AND ANDERSON

		z-component	x-component	y-component
Zeeman	g-tensor	2.0020 (120°, 208°)	2.0007 (67°, 133°)	2.0005 (39°, 253°)
H^{+}	hfs.	4.5 MHz (126°, 215°)	-0.3 MHz (44°, 257°)	-0.59 MHz (70°, 140°)
Si^{29}	Strong hfs.	Not Measured Directly		

which were reported by Feigl and Anderson (8). Discrepancies exists in the angles describing the principal axes directions because of the failure of Feigl and Anderson to choose an appropriate coordinate system. The estimated errors in computing the principal values and directions from this present study are

$$\Delta g = \pm 0.000006$$

$$\Delta A = \pm 0.1 \text{ MHz}$$

$$\Delta\theta = \pm 1^{\circ}$$

$$\Delta\phi = \pm 1^{\circ}$$

CHAPTER IV

DISCUSSION

The E_4' center has been studied in detail recently by L. E. Halliburton and J. A. Weil (10). They have suggested that the E_4' center is a hydride ion (H^-) sitting in the oxygen vacancy bonding with one silicon with the unpaired electron localized in an sp^3 hybrid orbital on the opposite silicon.

In general, a hyperfine interaction tensor can be separated into two parts--an isotropic part and an anisotropic part with zero trace.

$$\overleftrightarrow{A} = A_o \overleftrightarrow{1} + \overleftrightarrow{B}$$

The isotropic interaction term (also called the Fermi contact term) is proportional to the probability density of the unpaired electron at the interacting nucleus and is given by

$$A_o = (8/3)\ \pi\ g\beta\ g_N\beta_N\ |\psi(\gamma_i)|^2$$

The anisotropic term describes the dipole-dipole interaction of the nuclear magnetic moment with the distributed electronic magnetic moment. The elements of the B tensor are given by

$$B_{ij} = g\beta\ g_N\beta_N \int \left[\frac{3x_i x_j}{\gamma^5} - \left(\frac{\delta_{ij}}{\gamma^3}\right)\right] |\psi(\gamma)|^2\ d\tau$$

where x_1, x_2 and x_3 are the Cartesian coordinates of the distributed electronic dipole with respect to the point nuclear dipole.

Now for the E_2' and the E_4' center let's assume momentarily that the distributed electronic dipole moment is a point dipole with separation γ from the nuclear magnetic moment along the z axis of the principal coordinate system of the A tensor. From the anisotropic part of the hyperfine tensor A we get

$$\gamma = 1.4\ A^{o} \qquad \text{for the } E_4' \text{ center}$$

and

$$\gamma = 3.2\ A^{o} \qquad \text{for the } E_2' \text{ center.}$$

Different γ values for the E_4' and the E_2' centers from the simple calculations suggests that these two centers are different in nature. But at the same time we have evidence from our thermal anneal study which suggests that these two centers must be similar in nature. A recent thermal anneal study at low temperatures after various low and high temperature electron irradiation by Mark E. Markes and L. E. Halliburton (11) supports the idea that these two defect centers must be similar in nature. The main question is to find where the proton is sitting in the E_2' center configuration.

A complete set of experimental data for the ground state of the E_2' center has now been obtained. But this accumulation of information is insufficient to suggest any concrete model for the E_2' center. Further theoretical investigations probably will allow one to propose a definite defect model for the E_2' center in agreement with the experimental data available.

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APPENDIX A

```
CARD
0001          IMPLICIT  REAL * 8 (A-H,O-Z)
0002          REAL * 8 AR(8,8),AI(8,8),E(8),E2(8),TAU(2,8),D(8),HF(8),P(18),
0003         CG(3,3),H(3,3),Z(3,3),RM(3,3),R2(3,3),R3(3,3),RT(3,3),TG(3,3),
0004         CTH(3,3),TZ(3,3),R(3,3),PQ(18)
0005          P(1)=2.0005840+00
0006          P(2)=2.0003780+00
0007          P(3)=2.001710+00
0008          P(4)=120.3D+00
0009          P(5)=238.8D+00
0010          P(6)=153.2D+00
0011          P(7)=1135.540+00
0012          P(8)=1135.510+00
0013          P(9)=1312.95D+00
0014          P(10)=58.70+00
0015          P(11)=62.60+00
0016          P(12)=153.2D+00
0017          P(13)=-0.232D+00
0018          P(14)=-0.559D+00
0019          P(15)=4.2140+00
0020          P(16)=237.00+00
0021          P(17)=63.5D+00
0022          P(18)=56.5D+00
0023    C     THE PARAMETERS FOR THE G TENSOR ARE 1-GX, 2-GY, 3-GZ, 4-THETA,
0024    C     5-PHI, 6-PSI.  THE PARAMETERS FOR THE HYPERFINE TENSOR ARE 7-AX,
0025    C     8-AY, 9-AZ, 10-THETA, 11-PHI, 12-PSI.
0026    C     THE PARAMETERS FOR  PROTON TENSOR ARE 13-A,14-AY,15-AZ,16-THETA,
0027    C     17-PHI,18-PSI.
0028          WRITE(6,10) (P(I),I=1,18)
0029       10 FORMAT(9F10.5)
0030          B=9.2741D+00/6.6262D+00
0031          GBN1=8.458D-04
0032          GBN2=4.257708D-03
0033          FREQQ=9.085D+03
0034          N=8
0035          NM=8
0036          ALPHA= 0.0D+00
0037          BETA= -9.0D+01
0038          DO  91  L=1,3
0039          P(L+3)=P(L+3)*(3.14159D+00/1.8D+02)
0040          P(L+9)=P(L+9)*(3.14159D+00/1.8D+02)
0041       91 P(L+15)=P(L+15)*(3.14159D+00/1.8D+02)
0042          AG=DSIN(P(4))
0043          AAG=DCOS(P(4))
0044          CG=DSIN(P(5))
0045          CCG=DCOS(P(5))
0046          FG=DSIN(P(6))
0047          FFG=DCOS(P(6))
0048          AH=DSIN(P(10))
0049          AAH=DCOS(P(10))
0050          CH=DSIN(P(11))
0051          CCH=DCOS(P(11))
0052          FH=DSIN(P(12))
0053          FFH=DCOS(P(12))
0054          AZ=DSIN(P(16))
0055          AAZ=DCOS(P(16))
0056          CZ=DSIN(P(17))
0057          CCZ=DCOS(P(17))
0058          FZ=DSIN(P(18))
0059          FFZ=DCOS(P(18))
0060          CO=DCOS(2.094395D+00)
0061          SI=DSIN(2.094395D+00)
0062          G(1,1)=FFG*CCG-AAG*CG*FG
0063          G(1,2)=FFG*CG+AAG*CCG*FG
0064          G(1,3)=FG*AG
0065          G(2,1)=-FG*CCG-AAG*CG*FFG
0066          G(2,2)=-FG*CG+AAG*CCG*FFG
0067          G(2,3)=FFG*AG
0068          G(3,1)=AG*CG
```

```
0069          G(3,2)=-AG*CCG
0070          G(3,3)=AAG
0071          H(1,1)=FFH*CCH-AAH*CH*FH
0072          H(1,2)=FFH*CH+AAH*CCH*FH
0073          H(1,3)=FH*AH
0074          H(2,1)=-FH*CCH-AAH*CH*FFH
0075          H(2,2)=-FH*CH+AAH*CCH*FFH
0076          H(2,3)=FFH*AH
0077          H(3,1)=AH*CH
0078          H(3,2)=-AH*CCH
0079          H(3,3)=AAH
0080          Z(1,1)=FFZ*CCZ-AAZ*CZ*FZ
0081          Z(1,2)=FFZ*CZ+AAZ*CCZ*FZ
0082          Z(1,3)=FZ*AZ
0083          Z(2,1)=-FZ*CCZ-AAZ*CZ*FFZ
0084          Z(2,2)=-FZ*CZ+AAZ*CCZ*FFZ
0085          Z(2,3)=FFZ*AZ
0086          Z(3,1)=AZ*CZ
0087          Z(3,2)=-AZ*CCZ
0088          Z(3,3)=AAZ
0089       20 ALPHAR=ALPHA*(3.14159D+00/1.8D+02)
0090          BETAR=BETA*(3.14159D+00/1.8D+02)
0091          WRITE(6,30) ALPHA, BETA
0092       30 FORMAT('0',2F15.3)
0093          RM(1,1)=DCOS(ALPHAR)
0094          RM(1,2)=-DSIN(ALPHAR)*DSIN(BETAR)
0095          RM(1,3)=DSIN(ALPHAR)*DCOS(BETAR)
0096          RM(2,1)=0.0D+00
0097          RM(2,2)=DCOS(BETAR)
0098          RM(2,3)=DSIN(BETAR)
0099          RM(3,1)=-DSIN(ALPHAR)
0100          RM(3,2)=-DCOS(ALPHAR)*DSIN(BETAR)
0101          RM(3,3)=DCOS(ALPHAR)*DCOS(BETAR)
0102          K = 1
0103       40 GO  TO  (50,50,50,60,60,60),K
0104       50 R2(1,1)=1.0D+00
0105          R2(1,2)=0.0D+00
0106          R2(1,3)=0.0D+00
0107          R2(2,1)=0.0D+00
0108          R2(2,2)=1.0D+00
0109          R2(2,3)=0.0D+00
0110          R2(3,1)=0.0D+00
0111          R2(3,2)=0.0D+00
0112          R2(3,3)=1.0D+00
0113          GO TO (70,80,90),K
0114       60 R2(1,1)=1.0D+00
0115          R2(1,2)=0.0D+00
0116          R2(1,3)=0.0D+00
0117          R2(2,1)=0.0D+00
0118          R2(2,2)=-1.0D+00
0119          R2(2,3)=0.0D+00
0120          R2(3,1)=0.0D+00
0121          R2(3,2)=0.0D+00
0122          R2(3,3)=-1.0D+00
0123          KK = K-3
0124          GO TO (70,80,90),KK
0125       70 R3(1,1)=1.0D+00
0126          R3(1,2)=0.0D+00
0127          R3(1,3)=0.0D+00
0128          R3(2,1)=0.0D+00
0129          R3(2,2)=1.0D+00
0130          R3(2,3)=0.0D+00
0131          R3(3,1)=0.0D+00
0132          R3(3,2)=0.0D+00
0133          R3(3,3)=1.0D+00
0134          GO TO 100
0135       80 R3(1,1)=CO
0136          R3(1,2)=SI
0137          R3(1,3)=0.0D+00
0138          R3(2,1)=-SI
```

```
0139          R3(2,2)=CO
0140          R3(2,3)=0.0D+00
0141          R3(3,1)=0.0D+00
0142          R3(3,2)=0.0D+00
0143          R3(3,3)=1.0D+00
0144          GO TO 100
0145       90 R3(1,1)=CO
0146          R3(1,2)=-SI
0147          R3(1,3)=0.0D+00
0148          R3(2,1)=SI
0149          R3(2,2)=CO
0150          R3(2,3)=0.0D+00
0151          R3(3,1)=0.0D+00
0152          R3(3,2)=0.0D+00
0153          R3(3,3)=1.0D+00
0154      100 DO 110 L=1,3
0155          DO 110 M=1,3
0156      110 RT(L,M)=R2(L,1)*R3(1,M)+R2(L,2)*R3(2,M)+R2(L,3)*R3(3,M)
0157          DO 120 L=1,3
0158          DO 120 M=1,3
0159      120 R(L,M)=RT(L,1)*RM(1,M)+RT(L,2)*RM(2,M)+RT(L,3)*RM(3,M)
0160          DO 130 L=1,3
0161          DO 130 M=1,3
0162          TG(L,M)=G(L,1)*R(1,M)+G(L,2)*R(2,M)+G(L,3)*R(3,M)
0163          TH(L,M)=H(L,1)*R(1,M)+H(L,2)*R(2,M)+H(L,3)*R(3,M)
0164      130 TZ(L,M)=Z(L,1)*R(1,M)+Z(L,2)*R(2,M)+Z(L,3)*R(3,M)
0165          I=1
0166      140 HH=6.00D+03
0167      150 W1=8*HH*(P(1)*TG(1,1)*TG(1,3)+P(2)*TG(2,1)*TG(2,3)+P(3)*TG(3,1)*
0168         CTG(3,3))
0169          W2=8*HH*(P(1)*TG(1,2)*TG(1,3)+P(2)*TG(2,2)*TG(2,3)+P(3)*TG(3,2)*
0170         CTG(3,3))
0171          W3=8*HH*(P(1)*TG(1,3)*TG(1,3)+P(2)*TG(2,3)*TG(2,3)+P(3)*TG(3,3)*
0172         CTG(3,3))
0173          W4=P(7)*TH(1,1)*TH(1,1)+P(8)*TH(2,1)*TH(2,1)+P(9)*TH(3,1)*TH(3,1)
0174          W5=P(7)*TH(1,1)*TH(1,2)+P(8)*TH(2,1)*TH(2,2)+P(9)*TH(3,1)*TH(3,2)
0175          W6=P(7)*TH(1,1)*TH(1,3)+P(8)*TH(2,1)*TH(2,3)+P(9)*TH(3,1)*TH(3,3)
0176          W7=P(7)*TH(1,2)*TH(1,2)+P(8)*TH(2,2)*TH(2,2)+P(9)*TH(3,2)*TH(3,2)
0177          W8=P(7)*TH(1,2)*TH(1,3)+P(8)*TH(2,2)*TH(2,3)+P(9)*TH(3,2)*TH(3,3)
0178          W9=P(7)*TH(1,3)*TH(1,3)+P(8)*TH(2,3)*TH(2,3)+P(9)*TH(3,3)*TH(3,3)
0179          W10=P(13)*TZ(1,1)*TZ(1,1)+P(14)*TZ(2,1)*TZ(2,1)+P(15)*TZ(3,1)
0180         C*TZ(3,1)
0181          W11=P(13)*TZ(1,1)*TZ(1,2)+P(14)*TZ(2,1)*TZ(2,2)+P(15)*TZ(3,1)
0182         C*TZ(3,2)
0183          W12=P(13)*TZ(1,1)*TZ(1,3)+P(14)*TZ(2,1)*TZ(2,3)+P(15)*TZ(3,1)
0184         C*TZ(3,3)
0185          W13=P(13)*TZ(1,2)*TZ(1,2)+P(14)*TZ(2,2)*TZ(2,2)+P(15)*TZ(3,2)
0186         C*TZ(3,2)
0187          W14=P(13)*TZ(1,2)*TZ(1,3)+P(14)*TZ(2,2)*TZ(2,3)+P(15)*TZ(3,2)
0188         C*TZ(3,3)
0189          W15=P(13)*TZ(1,3)*TZ(1,3)+P(14)*TZ(2,3)*TZ(2,3)+P(15)*TZ(3,3)
0190         C*TZ(3,3)
0191          Q1R=W1/2.00+00
0192          Q1I= W2/2.00+00
0193          Q2R= (W4-W7)/4.00+00
0194          Q2I= W5/2.00+00
0195          Q3= (W4+W7)/4.00+00
0196          Q4R= W6/2.00+00
0197          Q4I= W8/2.00+00
0198          Q5R=(W10-W13)/4.00+00
0199          Q5I=W11/2.00+00
0200          Q6=(W10+W13)/4.00+00
0201          Q7R=W12/2.00+00
0202          Q7I=W14/2.00+00
0203          DO 160 L=1,8
0204          DO 160 M=1,8
0205          AR(L,M)= 0.00+00
0206      160 AI(L,M)= 0.00+00
0207          AR(1,1)=W3/2.00+00+W9/4.00+00+W15/4.00+00-(GBN1*HH)/2.00+00
0208         C-(GBN2*HH)/2.00+00
```

```
0209        AR(2,2)=W3/2.0D+00-W9/4.0D+00+W15/4.0D+00+(GBN1*HH)/2.0D+00
0210       C-(GBN2*HH)/2.0D+00
0211        AR(3,3)=-W3/2.0D+00-W9/4.0D+00-W15/4.0D+00-(GBN1*HH)/2.0D+00
0212       C-(GBN2*HH)/2.0D+00
0213        AR(4,4)=-W3/2.0D+00+W9/4.0D+00-W15/4.0D+00+(GBN1*HH)/2.0D+00
0214       C-(GBN2*HH)/2.0D+00
0215        AR(5,5)=W3/2.0D+00+W9/4.0D+00-W15/4.0D+00-(GBN1*HH)/2.0D+00
0216       C+(GBN2*HH)/2.0D+00
0217        AR(6,6)=W3/2.0D+00-W9/4.0D+00-W15/4.0D+00+(GBN1*HH)/2.0D+00
0218       C+(GBN2*HH)/2.0D+00
0219        AR(7,7)=-W3/2.0D+00-W9/4.0D+00+W15/4.0D+00-(GBN1*HH)/2.0D+00
0220       C+(GBN2*HH)/2.0D+00
0221        AR(8,8)=-W3/2.0D+00+W9/4.0D+00+W15/4.0D+00+(GBN1*HH)/2.0D+00
0222       C+(GBN2*HH)/2.0D+00
0223        AR(2,1)=Q4R/2.0D+00
0224        AI(2,1)=Q4I/2.0D+00
0225        AR(3,1)=Q1R+Q4R/2.0D+00+Q7R/2.0D+00
0226        AI(3,1)=Q1I+Q4I/2.0D+00+Q7I/2.0D+00
0227        AR(4,1)=Q2R
0228        AI(4,1)=Q2I
0229        AR(5,1)=Q7R/2.0D+00
0230        AI(5,1)=Q7I/2.0D+00
0231        AR(7,1)=Q5R
0232        AI(7,1)=Q5I
0233        AR(3,2)=Q3
0234        AR(4,2)=Q1R-Q4R/2.0D+00+Q7R/2.0D+00
0235        AI(4,2)=Q1I-Q4I/2.0D+00+Q7I/2.0D+00
0236        AR(6,2)=AR(5,1)
0237        AI(6,2)=AI(5,1)
0238        AR(8,2)=AR(7,1)
0239        AI(8,2)=AI(7,1)
0240        AR(4,3)=-AR(2,1)
0241        AI(4,3)=-AI(2,1)
0242        AR(5,3)=Q6
0243        AR(7,3)=-AR(5,1)
0244        AI(7,3)=-AI(5,1)
0245        AR(6,4)=AR(5,3)
0246        AR(8,4)=AR(7,3)
0247        AI(8,4)=AI(7,3)
0248        AR(6,5)=-AR(4,3)
0249        AI(6,5)=-AI(4,3)
0250        AR(7,5)=Q1R+Q4R/2.0D+00-Q7R/2.0D+00
0251        AI(7,5)=Q1I+Q4I/2.0D+00-Q7I/2.0D+00
0252        AR(8,5)=AR(4,1)
0253        AI(8,5)=AI(4,1)
0254        AR(7,6)=AR(3,2)
0255        AR(8,6)=Q1R-Q4R/2.0D+00-Q7R/2.0D+00
0256        AI(8,6)=Q1I-Q4I/2.0D+00-Q7I/2.0D+00
0257        AR(8,7)=-Q4R/2.0D+00
0258        AI(8,7)=-Q4I/2.0D+00
0259        CALL  HTRIDI (NM,N,AR,AI,D,E,E2,TAU)
0260        CALL  IMTQL1  (N,D,E,IERR)
0261        GO TO (170,180,190,200),I
0262    170 FREQ=D(8)-D(2)
0263        GO TO 210
0264    180 FREQ=D(7)-D(1)
0265        GO TO 210
0266    190 FREQ=D(6)-D(4)
0267        GO TO 210
0268    200 FREQ=D(5)-D(3)
0269    210 IF(DABS(FREQQ-FREQ)-1.0D-01)220,220,230
0270    220 HF(I)=HH
0271        GO TO 240
0272    230 HH=HH*(FREQQ/FREQ)
0273        GO TO 150
0274    240 IF(I-4)250,260,260
0275    250 I=I+1
0276        GO TO 140
0277    260 WRITE(6,270) (HF(I),I=1,4)
0278    270 FORMAT(4F20.2)
```

```
0279          IF(K-6)280,290,290
0280      280 K=K+1
0281          GO TO 40
0282      290 BETA=BETA+5.0D+00
0283          IF(BETA-9.1D+01)20,300,300
0284      300 WRITE(6,310) (P(I),I=1,18)
0285      310 FORMAT('0',9F10.5)
0286          PQ(1)=DARCOS(G(1,3))
0287          PQ(2)=DATAN(G(1,2)/G(1,1))
0288          PQ(3)=DARCOS(G(2,3))
0289          PQ(4)=DATAN(G(2,2)/G(2,1))
0290          PQ(5)=P(4)
0291          PQ(6)=DARCOS(CG)
0292          PQ(7)=DARCOS(H(1,3))
0293          PQ(8)=DATAN(H(1,2)/H(1,1))
0294          PQ(9)=DARCOS(H(2,3))
0295          PQ(10)=DATAN(H(2,2)/H(2,1))
0296          PQ(11)=P(10)
0297          PQ(12)=DARCOS(CH)
0298          PQ(13)=DARCOS(Z(1,3))
0299          PQ(14)=DATAN(Z(1,2)/Z(1,1))
0300          PQ(15)=DARCOS(Z(2,3))
0301          PQ(16)=DATAN(Z(2,2)/Z(2,1))
0302          PQ(17)=P(16)
0303          PQ(18)=DARCOS(CZ)
0304          DO 320 L=1,18
0305      320 PQ(L)=PQ(L)*(1.8D+02/3.14159D+00)
0306          WRITE(6,330) (PQ(I),I=1,18)
0307      330 FORMAT('0',6F15.5)
0308          STOP
0309          END
```

APPENDIX B

```
CARD
0001          IMPLICIT  REAL * 8 (A-H,O-Z)
0002          REAL * 8 AR(8,8),AI(8,8),E(8),E2(8),TAU(2,8),D(8),HF(8),P(18),
0003         CG(3,3),H(3,3),Z(3,3),RM(3,3),R2(3,3),R3(3,3),RT(3,3),TG(3,3),
0004         CTH(3,3),TZ(3,3),R(3,3),FREQ1(28)
0005          P(1)=2.000584D+00
0006          P(2)=2.000378D+00
0007          P(3)=2.00171D+00
0008          P(4)=120.3D+00
0009          P(5)=238.8D+00
0010          P(6)=153.2D+00
0011          P(7)=1135.54D+00
0012          P(8)=1135.51D+00
0013          P(9)=1312.95D+00
0014          P(10)=58.7D+00
0015          P(11)=62.6D+00
0016          P(12)=153.2D+00
0017          P(13)=-0.232D+00
0018          P(14)=-0.559D+00
0019          P(15)=4.214D+00
0020          P(16)=237.0D+00
0021          P(17)=63.5D+00
0022          P(18)=56.5D+00
0023    C     THE PARAMETERS FOR THE G TENSOR ARE 1-GX, 2-GY, 3-GZ, 4-THETA,
0024    C     5-PHI, 6-PSI.  THE PARAMETERS FOR THE HYPERFINE TENSOR ARE 7-AX,
0025    C     8-AY, 9-AZ, 10-THETA, 11-PHI, 12-PSI.
0026    C     THE PARAMETERS FOR  PROTON TENSOR ARE 13-A,14-AY,15-AZ,16-THETA,
0027    C     17-PHI,18-PSI.
0028          WRITE(6,10) (P(I),I=1,18)
0029       10 FORMAT('0',6F10.5)
0030          B=9.2741D+00/6.6262D+00
0031          GBN1=8.458D-04
0032          GBN2=4.257708D-03
0033          FREQQ=9.085D+03
0034          N=8
0035          NM=8
0036          ALPHA= 0.0D+00
0037          DO  91  L=1,3
0038          P(L+3)=P(L+3)*(3.14159D+00/1.8D+02)
0039          P(L+9)=P(L+9)*(3.14159D+00/1.8D+02)
0040       91 P(L+15)=P(L+15)*(3.14159D+00/1.8D+02)
0041       92 DO 93 LL=13,18
0042       94 K1=1
0043       95 MM=1
0044       96 GO TO (358,359,360,361,362,363,364,365,366,367,368,369,370,
0045         C371,372,373,374,375,376,377,378,379,380,381,382,383,384,385),MM
0046      358 HH=2996.655D+00
0047          BETA=70.0D+00
0048          K=2
0049          I=1
0050          GO TO 97
0051      359 HH=3434.567D+00
0052          K=1
0053          I=3
0054          GO TO 97
0055      360 HH=3435.957D+00
0056          K=3
0057          I=4
0058          GO TO 97
0059      361 HH=2995.592D+00
0060          BETA=60.0D+00
0061          K=2
0062          I=1
0063          GO TO 97
0064      362 HH=3433.756D+00
0065          K=1
0066          I=4
0067          GO TO 97
0068      363 HH=2997.236D+00
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```
0069          BETA=45.0D+00
0070          K=2
0071          I=1
0072          GO TO 97
0073      364 HH=2995.776D+00
0074          I=2
0075      365 HH=3025.92D+00
0076          K=1
0077          I=2
0078          GO TO 97
0079      366 HH=3026.275D+00
0080          K=3
0081          GO TO 97
0082      367 HH=3002.303D+00
0083          BETA=30.0D+00
0084          K=2
0085          I=1
0086          GO TO 97
0087      368 HH=3024.028D+00
0088          K=1
0089          I=1
0090          GO TO 97
0091      369 HH=3024.7035D+00
0092          K=3
0093          GO TO 97
0094      370 HH=3009.712D+00
0095          BETA=15.0D+00
0096          K=2
0097          I=1
0098          GO TO 97
0099      371 HH=3020.9D+00
0100          K=1
0101          I=1
0102          GO TO 97
0103      372 HH=3021.411D+00
0104          K=3
0105          GO TO 97
0106      373 HH=3017.523D+00
0107          BETA=0.0D+00
0108          K=2
0109          I=1
0110          GO TO 97
0111      374 HH=3023.642D+00
0112          BETA=-15.0D+00
0113          K=2
0114          I=1
0115          GO TO 97
0116      375 HH=3026.277D+00
0117          BETA=-30.0D+00
0118          K=2
0119          I=1
0120          GO TO 97
0121      376 HH=3011.467D+00
0122          K=3
0123          I=1
0124          GO TO 97
0125      377 HH=3012.85D+00
0126          K=1
0127          I=1
0128          GO TO 97
0129      378 HH=3024.387D+00
0130          BETA=-45.0D+00
0131          K=2
0132          I=1
0133          GO TO 97
0134      379 HH=3012.81D+00
0135          K=1
0136          I=1
0137          GO TO 97
0138      380 HH=3010.903D+00
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```
0139          K=3
0140          I=1
0141          GO TO 97
0142      381 HH=3018.668D+00
0143          BETA=-60.0D+00
0144          K=2
0145          I=1
0146          GO TO 97
0147      382 HH=3014.451D+00
0148          K=1
0149          I=1
0150          GO TO 97
0151      383 HH=3012.308D+00
0152          K=3
0153          I=1
0154          GO TO 97
0155      384 HH=3014.211D+00
0156          BETA=-70.0D+00
0157          K=3
0158          I=1
0159          GO TO 97
0160      385 HH=3445.787D+00
0161          K=3
0162          I=4
0163       97 AG=DSIN(P(4))
0164          AAG=DCOS(P(4))
0165          CG=DSIN(P(5))
0166          CCG=DCOS(P(5))
0167          FG=DSIN(P(6))
0168          FFG=DCOS(P(6))
0169          AH=DSIN(P(10))
0170          AAH=DCOS(P(10))
0171          CH=DSIN(P(11))
0172          CCH=DCOS(P(11))
0173          FH=DSIN(P(12))
0174          FFH=DCOS(P(12))
0175          AZ=DSIN(P(16))
0176          AAZ=DCOS(P(16))
0177          CZ=DSIN(P(17))
0178          CCZ=DCOS(P(17))
0179          FZ=DSIN(P(18))
0180          FFZ=DCOS(P(18))
0181          CO=DCOS(2.094395D+00)
0182          SI=DSIN(2.094395D+00)
0183          G(1,1)=FFG*CCG-AAG*CG*FG
0184          G(1,2)=FFG*CG+AAG*CCG*FG
0185          G(1,3)=FG*AG
0186          G(2,1)=-FG*CCG-AAG*CG*FFG
0187          G(2,2)=-FG*CG+AAG*CCG*FFG
0188          G(2,3)=FFG*AG
0189          G(3,1)=AG*CG
0190          G(3,2)=-AG*CCG
0191          G(3,3)=AAG
0192          H(1,1)=FFH*CCH-AAH*CH*FH
0193          H(1,2)=FFH*CH+AAH*CCH*FH
0194          H(1,3)=FH*AH
0195          H(2,1)=-FH*CCH-AAH*CH*FFH
0196          H(2,2)=-FH*CH+AAH*CCH*FFH
0197          H(2,3)=FFH*AH
0198          H(3,1)=AH*CH
0199          H(3,2)=-AH*CCH
0200          H(3,3)=AAH
0201          Z(1,1)=FFZ*CCZ-AAZ*CZ*FZ
0202          Z(1,2)=FFZ*CZ+AAZ*CCZ*FZ
0203          Z(1,3)=FZ*AZ
0204          Z(2,1)=-FZ*CCZ-AAZ*CZ*FFZ
0205          Z(2,2)=-FZ*CZ+AAZ*CCZ*FFZ
0206          Z(2,3)=FFZ*AZ
0207          Z(3,1)=AZ*CZ
0208          Z(3,2)=-AZ*CCZ
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0209          Z(3,3)=AAZ
0210       20 ALPHAR=ALPHA*(3.141590+00/1.80+02)
0211          BETAR=BETA*(3.14159D+00/1.8D+02)
0212          RM(1,1)=DCOS(ALPHAR)
0213          RM(1,2)=-DSIN(ALPHAR)*DSIN(BETAR)
0214          RM(1,3)=DSIN(ALPHAR)*DCOS(BETAR)
0215          RM(2,1)=0.0D+00
0216          RM(2,2)=DCOS(BETAR)
0217          RM(2,3)=DSIN(BETAR)
0218          RM(3,1)=-DSIN(ALPHAR)
0219          RM(3,2)=-DCOS(ALPHAR)*DSIN(BETAR)
0220          RM(3,3)=DCOS(ALPHAR)*DCOS(BETAR)
0221       40 GO  TO  (50,50,50,60,60,60),K
0222       50 R2(1,1)=1.0D+00
0223          R2(1,2)=0.0D+00
0224          R2(1,3)=0.0D+00
0225          R2(2,1)=0.0D+00
0226          R2(2,2)=1.0D+00
0227          R2(2,3)=0.0D+00
0228          R2(3,1)=0.0D+00
0229          R2(3,2)=0.0D+00
0230          R2(3,3)=1.0D+00
0231          GO TO (70,80,90),K
0232       60 R2(1,1)=1.0D+00
0233          R2(1,2)=0.0D+00
0234          R2(1,3)=0.0D+00
0235          R2(2,1)=0.0D+00
0236          R2(2,2)=-1.0D+00
0237          R2(2,3)=0.0D+00
0238          R2(3,1)=0.0D+00
0239          R2(3,2)=0.0D+00
0240          R2(3,3)=-1.0D+00
0241          KK = K-3
0242          GO TO (70,80,90),KK
0243       70 R3(1,1)=1.0D+00
0244          R3(1,2)=0.0D+00
0245          R3(1,3)=0.0D+00
0246          R3(2,1)=0.0D+00
0247          R3(2,2)=1.0D+00
0248          R3(2,3)=0.0D+00
0249          R3(3,1)=0.0D+00
0250          R3(3,2)=0.0D+00
0251          R3(3,3)=1.0D+00
0252          GO TO 100
0253       80 R3(1,1)=CO
0254          R3(1,2)=SI
0255          R3(1,3)=0.0D+00
0256          R3(2,1)=-SI
0257          R3(2,2)=CO
0258          R3(2,3)=0.0D+00
0259          R3(3,1)=0.0D+00
0260          R3(3,2)=0.0D+00
0261          R3(3,3)=1.0D+00
0262          GO TO 100
0263       90 R3(1,1)=CO
0264          R3(1,2)=-SI
0265          R3(1,3)=0.0D+00
0266          R3(2,1)=SI
0267          R3(2,2)=CO
0268          R3(2,3)=0.0D+00
0269          R3(3,1)=0.0D+00
0270          R3(3,2)=0.0D+00
0271          R3(3,3)=1.0D+00
0272      100 DO 110 L=1,3
0273          DO 110 M=1,3
0274      110 RT(L,M)=R2(L,1)*R3(1,M)+R2(L,2)*R3(2,M)+R2(L,3)*R3(3,M)
0275          DO 120 L=1,3
0276          DO 120 M=1,3
0277      120 R(L,M)=RT(L,1)*RM(1,M)+RT(L,2)*RM(2,M)+RT(L,3)*RM(3,M)
0278          DO 130 L=1,3
```

```
0279          DO 130 M=1,3
0280          TG(L,M)=G(L,1)*R(1,M)+G(L,2)*R(2,M)+G(L,3)*R(3,M)
0281          TH(L,M)=H(L,1)*R(1,M)+H(L,2)*R(2,M)+H(L,3)*R(3,M)
0282      130 TZ(L,M)=Z(L,1)*R(1,M)+Z(L,2)*R(2,M)+Z(L,3)*R(3,M)
0283      150 W1=8*HH*(P(1)*TG(1,1)*TG(1,3)+P(2)*TG(2,1)*TG(2,3)+P(3)*TG(3,1)*
0284         CTG(3,3))
0285          W2=8*HH*(P(1)*TG(1,2)*TG(1,3)+P(2)*TG(2,2)*TG(2,3)+P(3)*TG(3,2)*
0286         CTG(3,3))
0287          W3=8*HH*(P(1)*TG(1,3)*TG(1,3)+P(2)*TG(2,3)*TG(2,3)+P(3)*TG(3,3)*
0288         CTG(3,3))
0289          W4=P(7)*TH(1,1)*TH(1,1)+P(8)*TH(2,1)*TH(2,1)+P(9)*TH(3,1)*TH(3,1)
0290          W5=P(7)*TH(1,1)*TH(1,2)+P(8)*TH(2,1)*TH(2,2)+P(9)*TH(3,1)*TH(3,2)
0291          W6=P(7)*TH(1,1)*TH(1,3)+P(8)*TH(2,1)*TH(2,3)+P(9)*TH(3,1)*TH(3,3)
0292          W7=P(7)*TH(1,2)*TH(1,2)+P(8)*TH(2,2)*TH(2,2)+P(9)*TH(3,2)*TH(3,2)
0293          W8=P(7)*TH(1,2)*TH(1,3)+P(8)*TH(2,2)*TH(2,3)+P(9)*TH(3,2)*TH(3,3)
0294          W9=P(7)*TH(1,3)*TH(1,3)+P(8)*TH(2,3)*TH(2,3)+P(9)*TH(3,3)*TH(3,3)
0295          W10=P(13)*TZ(1,1)*TZ(1,1)+P(14)*TZ(2,1)*TZ(2,1)+P(15)*TZ(3,1)
0296         C*TZ(3,1)
0297          W11=P(13)*TZ(1,1)*TZ(1,2)+P(14)*TZ(2,1)*TZ(2,2)+P(15)*TZ(3,1)
0298         C*TZ(3,2)
0299          W12=P(13)*TZ(1,1)*TZ(1,3)+P(14)*TZ(2,1)*TZ(2,3)+P(15)*TZ(3,1)
0300         C*TZ(3,3)
0301          W13=P(13)*TZ(1,2)*TZ(1,2)+P(14)*TZ(2,2)*TZ(2,2)+P(15)*TZ(3,2)
0302         C*TZ(3,2)
0303          W14=P(13)*TZ(1,2)*TZ(1,3)+P(14)*TZ(2,2)*TZ(2,3)+P(15)*TZ(3,2)
0304         C*TZ(3,3)
0305          W15=P(13)*TZ(1,3)*TZ(1,3)+P(14)*TZ(2,3)*TZ(2,3)+P(15)*TZ(3,3)
0306         C*TZ(3,3)
0307          Q1R=W1/2.0D+00
0308          Q1I= W2/2.0D+00
0309          Q2R= (W4-W7)/4.0D+00
0310          Q2I= W5/2.0D+00
0311          Q3= (W4+W7)/4.0D+00
0312          Q4R= W6/2.0D+00
0313          Q4I= W8/2.0D+00
0314          Q5R=(W10-W13)/4.0D+00
0315          Q5I=W11/2.0D+00
0316          Q6=(W10+W13)/4.0D+00
0317          Q7R=W12/2.0D+00
0318          Q7I=W14/2.0D+00
0319          DO 160 L=1,8
0320          DO 160 M=1,8
0321          AR(L,M)= 0.0D+00
0322      160 AI(L,M)= 0.0D+00
0323          AR(1,1)=W3/2.0D+00+W9/4.0D+00+W15/4.0D+00-(GBN1*HH)/2.0D+00
0324         C-(GBN2*HH)/2.0D+00
0325          AR(2,2)=W3/2.0D+00-W9/4.0D+00+W15/4.0D+00+(GBN1*HH)/2.0D+00
0326         C-(GBN2*HH)/2.0D+00
0327          AR(3,3)=-W3/2.0D+00-W9/4.0D+00-W15/4.0D+00-(GBN1*HH)/2.0D+00
0328         C-(GBN2*HH)/2.0D+00
0329          AR(4,4)=-W3/2.0D+00+W9/4.0D+00-W15/4.0D+00+(GBN1*HH)/2.0D+00
0330         C-(GBN2*HH)/2.0D+00
0331          AR(5,5)=W3/2.0D+00+W9/4.0D+00-W15/4.0D+00-(GBN1*HH)/2.0D+00
0332         C+(GBN2*HH)/2.0D+00
0333          AR(6,6)=W3/2.0D+00-W9/4.0D+00-W15/4.0D+00+(GBN1*HH)/2.0D+00
0334         C+(GBN2*HH)/2.0D+00
0335          AR(7,7)=-W3/2.0D+00-W9/4.0D+00+W15/4.0D+00-(GBN1*HH)/2.0D+00
0336         C+(GBN2*HH)/2.0D+00
0337          AR(8,8)=-W3/2.0D+00+W9/4.0D+00+W15/4.0D+00+(GBN1*HH)/2.0D+00
0338         C+(GBN2*HH)/2.0D+00
0339          AR(2,1)=Q4R/2.0D+00
0340          AI(2,1)=Q4I/2.0D+00
0341          AR(3,1)=Q1R+Q4R/2.0D+00+Q7R/2.0D+00
0342          AI(3,1)=Q1I+Q4I/2.0D+00+Q7I/2.0D+00
0343          AR(4,1)=Q2R
0344          AI(4,1)=Q2I
0345          AR(5,1)=Q7R/2.0D+00
0346          AI(5,1)=Q7I/2.0D+00
0347          AR(7,1)=Q5R
0348          AI(7,1)=Q5I
```

```
0349          AR(3,2)=Q3
0350          AR(4,2)=Q1R-Q4R/2.0D+00+Q7R/2.0D+00
0351          AI(4,2)=Q1I-Q4I/2.0D+00+Q7I/2.0D+00
0352          AR(6,2)=AR(5,1)
0353          AI(6,2)=AI(5,1)
0354          AR(8,2)=AR(7,1)
0355          AI(8,2)=AI(7,1)
0356          AR(4,3)=-AR(2,1)
0357          AI(4,3)=-AI(2,1)
0358          AR(5,3)=Q6
0359          AR(7,3)=-AR(5,1)
0360          AI(7,3)=-AI(5,1)
0361          AR(6,4)=AR(5,3)
0362          AR(8,4)=AR(7,3)
0363          AI(8,4)=AI(7,3)
0364          AR(6,5)=-AR(4,3)
0365          AI(6,5)=-AI(4,3)
0366          AR(7,5)=Q1R+Q4R/2.0D+00-Q7R/2.0D+00
0367          AI(7,5)=Q1I+Q4I/2.0D+00-Q7I/2.0D+00
0368          AR(8,5)=AR(4,1)
0369          AI(8,5)=AI(4,1)
0370          AR(7,6)=AR(3,2)
0371          AR(8,6)=Q1R-Q4R/2.0D+00-Q7R/2.0D+00
0372          AI(8,6)=Q1I-Q4I/2.0D+00-Q7I/2.0D+00
0373          AR(8,7)=-Q4R/2.0D+00
0374          AI(8,7)=-Q4I/2.0D+00
0375          CALL  HTRIDI (NM,N,AR,AI,D,E,E2,TAU)
0376          CALL  IMTQL1  (N,D,E,IERR)
0377          GO TO (170,180,190,200),I
0378      170 FREQ=D(8)-D(2)
0379          GO TO 210
0380      180 FREQ=D(7)-D(1)
0381          GO TO 210
0382      190 FREQ=D(6)-D(4)
0383          GO TO 210
0384      200 FREQ=D(5)-D(3)
0385      210 FREQ1(MM)=FREQ
0386          MM=MM+1
0387          IF(MM-28)96,96,399
0388      399 SUM=0.0D+00
0389          DO 400 MM=1,28
0390      400 SUM=SUM+(FREQ1(MM)-FREQQ)**2
0391          GO TO (401,407,409),K1
0392      401 SUM2=SUM
0393          IF(LL-13)402,402,403
0394      402 SUM1=SUM
0395      403 LLL=LL-12
0396          GO TO (404,404,404,405,405,405),LLL
0397      404 PP=1.0D-03
0398          GO TO 406
0399      405 PP=0.5D+00*(3.14159D+00/180.0D+00)
0400      406 P(LL)=P(LL)+PP
0401          K1=K1+1
0402          GO TO 95
0403      407 IF(SUM-SUM2)93,408,408
0404      408 P(LL)=P(LL)-2.0D+00*PP
0405          K1=K1+1
0406          GO TO 95
0407      409 IF(SUM-SUM2)93,410,410
0408      410 P(LL)=P(LL)+PP
0409       93 CONTINUE
0410          IF(SUM-SUM2)411,412,412
0411      411 SUM2=SUM
0412      412 CONTINUE
0413          WRITE(6,420)SUM2
0414      420 FORMAT(' SUM2 EQUALS',F12.5)
0415          WRITE(6,430) (P(I),I=1,18)
0416      430 FORMAT('0',6F15.6)
0417          IF(SUM1-SUM2)450,450,92
0418      450 CONTINUE
0419          STOP
0420          END
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VITA [2]

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Master of Science

Thesis: ELECTRON SPIN RESONANCE STUDY OF THE E_2' CENTER IN QUARTZ

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