THE EFFECT OF UNIAXIAL STRESS ON
THE ELECTRON PARAMAGNETIC RESONANCE OF RUBY

by

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ABSTRACT

The effect of uniaxial stress on the EPR lines in 0.05% ruby may be described by the addition of a term to the spin Hamiltonian of the form: $H_{\text{SL}} = \mathbf{S} \cdot \mathbf{D} \cdot \mathbf{S}$. $D_{ij}$ is a linear function of the strain, $e_{k\ell}$ in the crystal: $D_{ij} = G_{ij\kappa\ell} e_{k\ell}$, where $G_{ij\kappa\ell} = n_1 G_{ij\kappa\ell}^1 + n_2 G_{ij\kappa\ell}^2$. $G'$ and $G''$ are the magneto-elastic coupling tensors for each of the two inequivalent $\text{Cr}^{3+}$ sites in the lattice. $n_1$ and $n_2$ are descriptive of the relative population of paramagnetic ions in the two sites. The $G$-tensors are fourth-rank tensors whose components are related by the symmetry of the lattice sites with which they are associated.

The components of the $G$-tensor may be ascertained from the shift of the resonance field with strain at various directions in the crystal as a function of the angle between the applied magnetic field and the c-axis of the crystal. The strain in the sample is measured using four strain gages; one bonded to each side of the sample.

Linear shifts of the lines have been measured for all observable transitions at 9.9 Gc on samples with four different stress-axes. The results were fitted to the theory by a least-squares analysis, yielding the following values for the independent components of $G'$ and $G''$ (in Voigt-reduced notation and units of Gc/unit strain):

- $G_{11} = 137.2 \pm 10\%$
- $G_{12} = -58.13 \pm 10\%$
- $G_{22} = 192.3 \pm 10\%$
- $G_{33} = 59.19 \pm 15\%$
- $G_{44} = -12.80 \pm 30\%$
- $G_{41} = -18.88 \pm 50\%$

$G_{15} + 2 \left( \frac{S_{44}}{S_{44}} \right) G_{14} = -45.0$

$G_{51} - \left( \frac{S_{14}}{S_{14}} \right) G_{45} = -45.0$
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I. INTRODUCTION

The purpose of this experiment is to determine the spin-lattice coupling of Cr$^{3+}$ in 0.05% ruby. This is an extension of an investigation begun by R. B. Hemphill in 1963 for his Ph.D. thesis at Rice. He shows that the effect can be accounted for by the addition of a term of the form: $H_{SL} = \hat{S} \cdot \hat{D} \cdot \hat{S}$ to the spin Hamiltonian. He shows that $\hat{D}$ can be taken as a symmetric, traceless tensor of second-rank. $\hat{D}$ is related to the strain as follows: $D_{ij} = G_{ijkl} e_{kl}$ where $G$ is a fourth-rank tensor called the magneto-elastic coupling tensor.

Hemphill assumed a form for the $G$-tensor which has since been found to be inadequate. The symmetry of the $Al_2O_3$ lattice dictates that certain components must be zero and relations must hold between others of the components. Hemphill attributed too much symmetry to the Cr$^{3+}$ (i.e. Al$^{3+}$) sites and thus obtained too many zero terms.

The non-zero components are found by measuring the shift of resonance field with strain at various directions in the crystal as a function of the angle between the applied magnetic field and the c-axis of the crystal. The strain is measured with four constantan strain gages, one on each side of the rod. The stress is adjusted so that all four gages register the same strain, thus eliminating all bending in the rod. Measurements were made for four separate directions of applied stress with a simple, absorption-type spectrometer at 9.9 Gc employing phase-sensitive detection. The results indicated a good linear relation between the field shift and the measured strain.
II. THEORY

The effective-spin Hamiltonian which describes the spin-resonance experiment with uniaxial applied stress has been shown by Hemphill\(^1\) to be given by:

\[
\mathbf{H} = \frac{g\beta}{\hbar} \mathbf{B} \cdot \mathbf{S} + D \left( S_z^2 - \frac{5}{4} \right) + \mathbf{S} \cdot \mathbf{D} \cdot \mathbf{S}.
\]

\(\mathbf{B}\) is a second-rank tensor which must be symmetric and real, since \(\mathbf{H}\) must be a Hermitian operator. Moreover, no generality is lost by taking \(\mathbf{D}\) traceless, as Hemphill shows the trace corresponds to a shift in the zero level of the energy.

\(D_{ij}\) is assumed to be linear in the strain, \(e_{kl}\):

\[
D_{ij} = \sum_{k,l=1}^{3} G_{ijk\ell} e_{k\ell}
\]

for \(i, j = 1, 2, 3\)

where \(G\) will, in general, be a fourth-rank tensor having eighty-one independent components. Now \(\mathbf{e}\) and \(\mathbf{D}\) are both real, symmetric tensors, so that equation (II-2) must be invariant to an interchange of the indices \(i\) and \(j\), or of the indices \(k\) and \(l\). Hence we must have,

\[
G_{ijk\ell} = G_{jik\ell} = G_{ij\ell k} = G_{ij k\ell}.
\]

This relation shows that the number of independent components of \(G\) is at most thirty-six. Therefore, we may use the Voigt notation\(^2\) to rewrite equation (II-2):

\[
D_k = \sum_{m=1}^{6} G_{km} e_m
\]

for \(k = 1, 2, \ldots, 6\).

The strain, \(\varepsilon\), is related to the stress, \(\underline{T}\), by a fourth-rank tensor called the elastic-compliance tensor:

\[
\varepsilon_{ij} = \sum_{k, l=1}^{3} S_{ij k\ell} T_{k\ell}
\]
Rewriting in Voigt notation:

\[(\Pi-4') \quad \epsilon_m = \sum_{\eta=1}^{b} S_{mn} T_n \quad \text{m = 1, 2, ..., 6.} \]
III. THE FORM OF THE G-TENSOR IN RUBY

In section II we showed that the G-tensor has at most thirty-six independent components, we will now show that the symmetry of the crystal further reduces the number of independent components to ten.

Figure 1 shows a portion of the $\alpha$-Al $O$ lattice, which is the host lattice in ruby. The Cr$^{3+}$ atoms substitute into the lattice at the Al$^{3+}$ sites which are the small black spheres. It will be seen that the point symmetry at these sites is only $C_3$. The sites marked b and c are completely equivalent; but sites a and b are found to be magnetically inequivalent$^1$. a and b are physically equivalent and one can be carried into the other by a rotation of $180^\circ$ about an a-axis through the oxygen plane between them. Hence we may relate the physical properties of these two sites by performing the necessary rotations.

There will be a G-tensor related to each of the inequivalent sites. Both of these G-tensors will have the same form, since the point symmetry is $C_3$ at each site. In general, a rotation of the G-tensor is given by the following expression:

\[
G'_{ij\kappa\lambda} = \sum_{\rho\sigma\rho'} \chi_{i\rho} \chi_{j\sigma} \chi_{k\rho'} \chi_{\lambda\sigma'} G_{\rho\sigma\rho'\sigma'}
\]

If the $\chi_{i\rho}$ are components of the $120^\circ$ rotation about z-axis:

\[
C_3 = \begin{pmatrix}
-\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\
-\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

the tensor must have been left invariant, $G'_{ij\kappa\lambda} = G_{ij\kappa\lambda}$
FIGURE 1  $\text{Al}_2\text{O}_3$ LATTICE  
(from Hemphill$^1$)
This condition, together with the requirement that $\tilde{\mathbf{D}}$ be traceless, allows us to write, for either $G$-tensor, in the Voigt notation:

$$\mathbf{G} = \begin{pmatrix}
G_{11} & G_{12} & -\frac{1}{2}G_{33} & G_{14} & G_{15} & G_{16} \\
G_{12} & G_{11} & -\frac{1}{2}G_{33} & -G_{14} & -G_{15} & -G_{16} \\
-G_{33} & G_{33} & G_{33} & G_{34} & G_{35} & G_{36} \\
-G_{14} & -G_{14} & G_{14} & G_{15} & G_{16} & G_{17} \\
-G_{15} & -G_{15} & -G_{15} & -G_{16} & -G_{17} & -G_{18} \\
-G_{16} & -G_{16} & -G_{16} & -G_{17} & -G_{18} & -G_{19}
\end{pmatrix}$$

(III-3)

If we call the $G$-tensor for site $b$, $\mathbf{G}$ and that for site $a$, $\mathbf{G}'$, then we may apply equation (III-1), with the $\gamma_{ij}$ being components of the $180^\circ$ rotation about the $x$-axis, to obtain the relations:

$$\begin{align*}
(III-4) & \quad G'_{ij} = -G_{ij} \quad \text{for } i, j = 1, 5; 1, 6; 5, 1; \text{ or } 4, 5 \\
& \quad G'_{ij} = G_{ij} \quad \text{otherwise.}
\end{align*}$$

Thus we have reduced the total number of independent components for the two $G$-tensors from 162, possible, to 10 at most.

If we let

$$\begin{align*}
(III-5) & \quad G''_{ij} = \gamma G_{ij} + \gamma' G'_{ij}
\end{align*}$$

where $\gamma + \gamma' = 1$

$n = \text{relative number of Cr}^{3+} \text{ ions in sites equivalent to } b$

$n' = \text{relative number of Cr}^{3+} \text{ ions in sites equivalent to } a$

the forms of section II will be valid descriptions of the experiment. We will assume that there is no preferential filling of the two sites,
so that \( n = n' \); i.e. the two sites will be assumed to be equally populated.
IV. DIAGONALIZATION OF THE EFFECTIVE-SPIN HAMILTONIAN

In the Voigt notation, equation (II-1) for the Hamiltonian is just

\[ H = \sum \beta \left( B_x S_x + B_y S_y + B_z S_z \right) + D \left( S_z^2 - \frac{5}{4} \right) + \\
D_1 S_x^2 + D_2 S_y^2 + D_3 S_z^2 + D_4 (S_y S_z + S_z S_y) + D_5 (S_x S_z + S_z S_x) + D_6 (S_x S_y + S_y S_x) \]

We would like now to solve an energy-eigenvalue problem of the following sort:

\[ (IV-1) \quad H |k\rangle = E_k |k\rangle \]

We will assume that we may take the state \(|k\rangle\) as a linear combination of the spin-eigenstates for \(S_z\) which have the following relations:

\[ S_z |m_s\rangle = m_s |m_s\rangle \]

\[ S_x |m_s\rangle = \frac{1}{2} \left[ \sqrt{(\frac{3}{2} + m_s)(\frac{5}{2} - m_s)} |m_s - 1\rangle + \sqrt{(\frac{3}{2} - m_s)(\frac{5}{2} + m_s)} |m_s + 1\rangle \right] \]

\[ S_y |m_s\rangle = \frac{1}{2} \left[ \sqrt{(\frac{3}{2} + m_s)(\frac{5}{2} - m_s)} |m_s - 1\rangle - \sqrt{(\frac{3}{2} - m_s)(\frac{5}{2} + m_s)} |m_s + 1\rangle \right] \]

For the case of ruby where \(S = \frac{3}{2}\), \(m_s\) may take on the values: \(3/2, 1/2, -1/2, -3/2\). Therefore, we take

\[ (IV-3) \]

Now, the spin-states, \(|m_s\rangle\), form a complete, orthogonal basis for a system of spin \(3/2\), so we have

\[ (IV-4) \quad \langle m_s' | m_s \rangle = \delta_{m_s, m_s'} \]

If we write, for convenience sake, \(|i\rangle = |m_s\rangle\) where \(i = 1\) for \(m_s = 3/2\), 2 for \(m_s = 1/2\), 3 for \(m_s = -1/2\), and 4 for \(m_s = -3/2\), then multiplying equation (IV-1) by \(\langle i |\), \(i = 1, 2, 3, 4\), we obtain,
using relations (IV-3) and (IV-4):

\[ (IV-5) \sum_{j=1}^{4} \left( H_{ij} - E \delta_{ij} \right) a_{kj} = 0 \quad i = 1, 2, 3, 4 \]

where

\[ (IV-6) H_{ij} = \langle i | H | j \rangle \]

Upon substituting equation (II-1') in (IV-6) and employing relations (IV-2), we are able to evaluate the matrix elements \( H_{ij} \).

In order that the solutions of (IV-5) be non-trivial, it is necessary that the secular determinant of the set of equations be zero. If we choose a coordinate system so that the magnetic field \( B \) lies in the x-z plane, we will have \( B_y = 0 \) in equation (II-1'). In this case the secular determinant is the following:

\[ (IV-7) \begin{vmatrix} 
\left( \frac{\delta}{2} GB \cos \theta + \delta - E \right) \left( \frac{G}{4} GB \sin \theta + E \right) & \nu & 0 \\
\left( \frac{\delta}{2} GB \sin \theta + E \right) \left( \frac{G}{4} GB \cos \theta - \delta - E \right) & \left( GB \sin \theta \right) & \nu^* \\
0 & \left( GB \sin \theta \right) & \left( \frac{\delta}{2} GB \cos \theta - E \right) \left( \frac{G}{4} GB \sin \theta + \delta - E \right) 
\end{vmatrix} \]

where

\[ G = \frac{a B^2}{\mu} \]
\[ \delta = D + \frac{3}{2} D_3 \]
\[ \varepsilon = \sqrt{3} \left( D_5 - i D_4 \right) \]
\[ \nu = \sqrt{3} / 2 \left( D_{12} - i 2 D_6 \right) \]

and

\[ D_{12} = D_1 - D_2 \]

Now, since the stress applied to the crystal is very small, we will assume that the components of \( \hat{D} \) are much smaller than the terms \( D \) and \( G \). That this is valid can be seen from the fact that we are treating the stress effects as a perturbation. If the \( \hat{D} \) terms are not much smaller than \( D \) and \( G \), then this perturbation treatment is not
valid. Using this fact, we will neglect all terms in the expansion of (IV-7) which are of second-order or higher in the terms of \( \mathbf{D} \). When this is done, the following secular equation is obtained upon expanding (IV-7).

\[
(IV-8) \quad 0 = E^4 - \alpha E^2 + \beta E + \gamma + D_{12} F_{D_{12}} + D_{3} F_{D_{3}} + D_{5} F_{D_{5}}
\]

where:

\[
\begin{align*}
\alpha &= \frac{5}{2} G^2 B^4 + 2D^2 \\
\beta &= 2G^2B^2D(1-3\cos^2\Theta) \\
\gamma &= D^4 + \frac{3}{2} G^4 B^4 + \frac{1}{2} G^2 B^4 D^3 (1-6 \cos^2 \Theta) \\
F_{D_{12}} &= 3G^2 B^2 (D - E) \sin^2 \Theta \\
F_{D_{3}} &= 6D (D^2 - E^2) + \frac{3}{2} G^2 B^2 D (1-6 \cos^2 \Theta) + 3G^2 B^2 (1-3 \cos^2 \Theta) \\
F_{D_{5}} &= -6G^2 B^2 (D + 2E) \cos \Theta \sin \Theta \\
G &= 2.7789 \quad Gc/kG \\
D &= -5.733 \quad Gc
\end{align*}
\]

It is of interest to note that for \( \mathbf{B} \) lying in the x-z plane the secular equation is dependent on only four of the six components of \( \mathbf{D} \).
V. STRAIN DEPENDENCE IN SECULAR FORM

The secular equation (IV-8) may be written:

\[(V-1) \quad F(E, B, D_{12}, D_3, D_5, \Theta) = 0\]

The total differential of this function is just:

\[(V-2) \quad dF = F_E dE + F_B dB + F_{D_{12}} dD_{12} + F_{D_3} dD_3 + F_{D_5} dD_5 + F_\Theta d\Theta = 0\]

where \( F_\alpha = \partial F/\partial \alpha \)

The secular equation will have four roots which we will denote as \( E_i \), \( i = 1, 2, 3, 4 \), where for convenience we will denote these so that for fixed \( B, 0, D_{12}, D_3, \) and \( D_5, E_1 \geq E_2 \geq E_3 \geq E_4 \). When \( E \) is replaced by \( E_i \) in the secular equation, we will write it as:

\[(V-1') \quad F^i (E_i, B, D_{12}, D_3, D_5, \Theta) = 0 \quad ; \quad i = 1, 2, 3, 4\]

In this notation (V-2) becomes:

\[(V-2') \quad dF^i = F_{E_i}^i dE_i + F_B^i dB + F_{D_{12}}^i dD_{12} + F_{D_3}^i dD_3 + F_{D_5}^i dD_5 + F_\Theta^i d\Theta = 0\]

If we consider an experiment in which \( \Theta \) is held constant, so \( d\Theta = 0 \) and where the energy difference \( E_i - E_j = E_0 \) is constant, \( i > j \), so \( d(E_i - E_j) = 0 \), (as a microwave experiment at a constant microwave frequency \( \nu \), where \( h\nu = E_0 \) would be), then we would write:

\[(V-3) \quad F_{E_j}^i dE_i - F_{E_i}^i dE_j = 0 = F_{E_j}^i \left[ F_{E_j}^i dE_i + F_B^i dB + F_{D_{12}}^i dD_{12} + F_{D_3}^i dD_3 + F_{D_5}^i dD_5 \right] - F_{E_i}^i \left[ F_{E_i}^i dE_j + F_B^i dB + F_{D_{12}}^i dD_{12} + F_{D_3}^i dD_3 + F_{D_5}^i dD_5 \right]

\[= F_{E_j}^i - F_{E_i}^i \left( dE_i - dE_j \right) + \left( F_{E_j}^i F_B^i - F_{E_i}^i F_B^i \right) dB + \sum_{k=2,3,5} \left( F_{E_j}^i F_{D_k}^i - F_{E_i}^i F_{D_k}^i \right) dD_k\]
If we solve for dB in equation (V-3) we obtain:

(V-4) \[
\frac{dB}{d\nu} = \left[ \sum_{k=1,3,5} (F_{E_i}^i F_{B}^i - F_{E_i}^j F_{B}^j) dD_k \right]^{-1} \left[ \sum_{k=1,3,5} (F_{E_i}^i F_{D_k}^j - F_{E_i}^j F_{D_k}^j) dD_k \right]
\]

But if we consider

(V-5) \[B = B(D_{12}, D_3, D_5)\]

then

(V-4') \[\frac{dB}{d\nu} = \frac{\partial B}{\partial D_{12}} dD_{12} + \frac{\partial B}{\partial D_3} dD_3 + \frac{\partial B}{\partial D_5} dD_5\]

so (V-4) and (V-4') show that

(V-6) \[\frac{\partial B}{\partial D_k} = \frac{F_{E_i}^i F_{D_k}^j - F_{E_i}^j F_{D_k}^i}{F_{E_i}^i F_{B}^j - F_{E_i}^j F_{B}^i}\]

Now we see from section IV that we are able to calculate all of the derivations of F which appear in (V-4) and (V-6) to first order in the small quantities:

(V-7) \[F_{E_i}^i = 4 E_i^3 - (5G^2B^2 + 4D^2)E_i + 2G^2B^2 D (1 - 3\cos^2 \Theta)\]
\[F_{E_i}^j = G^2B^2 \left[ (4G^2B^2 - 5E_i^2 + 4DE_i)(1 - 3\cos^2 \Theta) + D^2(1 - 6\cos^2 \Theta) \right]\]

In this experiment we held \(\Theta\) fixed and operated at a constant frequency \(E_0/\hbar\) so that equation (V-4') was valid. When stress is applied the crystal is strained and (V-4') tells us:

(V-8) \[\frac{dB}{d\epsilon} = \frac{\partial B}{\partial D_{12}} \frac{dD_{12}}{d\epsilon} + \frac{\partial B}{\partial D_3} \frac{dD_3}{d\epsilon} + \frac{\partial B}{\partial D_5} \frac{dD_5}{d\epsilon}\]

so we measure the shift, \(dB/d\epsilon\), calculate the components \(\partial B/\partial D_k\)

from the relations in (V-7) and (V-6), and calculate \(dD_k/d\epsilon\).
For the two types of sites we obtain from (II-2') and (III-4):

\[
D_{i2} = \left( G_{i1} - G_{i2} \right) (e_1 - e_2) + \frac{2}{G_{i3}} \left( G_{i4} e_4 + G_{i5} e_5 + G_{i6} e_6 \right)
\]
\[
D_{i3}' = \left( G_{i1} - G_{i3} \right) (e_1 - e_3) + \frac{2}{G_{i4}} \left( G_{i4} e_4 - G_{i5} e_5 - G_{i6} e_6 \right)
\]
\[
D_4 = -\left( G_{i1} + G_{i2} \right) (e_1 + e_2) + G_{i3} e_3
\]
\[
D_4' = D_3
\]
\[
D_5 = \frac{G_{i5}}{G_{i1}} (e_1 - e_5) - \frac{G_{i5}}{G_{i4}} e_4 + G_{i4} e_5 + G_{i6} e_6
\]
\[
D_5' = -\frac{G_{i5}}{G_{i1}} (e_1 - e_5) + G_{i4} e_4 + G_{i4} e_5 + G_{i4} e_6
\]

Consider the coordinate system below, where X, Y, Z is the crystalline system corresponding to that in Figure 1, and \( \bar{B} \) and \( \bar{T} \) lie in the x-z plane. \( \Theta \) is the angle from the c-axis to \( \bar{T} \) going toward the x-axis. \( \Phi \) is the angle from the +a-axis to the little x-axis.
The stress is applied uniaxially along the axis of the sample rod, and in coordinate system, $\xi$, $\eta$, $\zeta$, which has $T$ applied along the $\zeta$-axis and where $\eta = y$-axis we have

$$\mathbf{T}_{\xi\eta\zeta} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \mathbf{T}_{\text{lab}}$$

In this coordinate system the measured strain, $e$, is just

$$\text{(V-9)} \quad e = s''_{\parallel} \mathbf{T}_{\text{lab}}$$

where $s''_{\parallel}$ is the elastic compliance component in the $\xi$, $\eta$, $\zeta$ system.

Applying a rotation $\pi/2 - \Theta$ about the $\eta$-axis brings us into the laboratory system:

$$\mathbf{T}_{x'y'z'} = \begin{pmatrix} \sin^2 \Theta \\ 0 \\ -\sin \Theta \cos \Theta \end{pmatrix} \mathbf{T}_{\text{lab}}$$

A further rotation by $-\Phi$ about the $z$-axis brings us to the crystalline system:

$$\mathbf{T}_{x'y'z'} = \begin{pmatrix} \sin^2 \Phi & \cos \Phi & 0 \\ \sin \Phi \cos \Phi & \cos^2 \Phi & 0 \\ -\sin \Phi & -\cos \Phi \sin \Phi & \cos \Phi \end{pmatrix} \mathbf{T}_{\text{lab}}$$

So that

$$\text{(V-10)} \quad \mathbf{e}_{\text{crys.}} = \begin{pmatrix} S_{11} \sin^2 \Phi + S_{12} \sin^2 \Phi + S_{13} \sin^2 \Phi + S_{14} \sin \Phi \cos \Phi + S_{15} \cos^2 \Phi + S_{16} \sin \Phi \cos \Phi \\ S_{22} \sin^2 \Phi + S_{23} \sin^2 \Phi + S_{24} \sin \Phi \cos \Phi + S_{25} \cos^2 \Phi + S_{26} \sin \Phi \cos \Phi + S_{27} \cos^2 \Phi \\ S_{33} \sin^2 \Phi + S_{34} \sin \Phi \cos \Phi + S_{35} \cos^2 \Phi + S_{36} \sin \Phi \cos \Phi + S_{37} \cos^2 \Phi \\ S_{44} \sin^2 \Phi + S_{45} \sin \Phi \cos \Phi + S_{46} \cos^2 \Phi + S_{47} \sin \Phi \cos \Phi + S_{48} \cos^2 \Phi \\ S_{55} \sin^2 \Phi + S_{56} \sin \Phi \cos \Phi + S_{57} \cos^2 \Phi + S_{58} \sin \Phi \cos \Phi + S_{59} \cos^2 \Phi \\ S_{66} \sin^2 \Phi + S_{67} \sin \Phi \cos \Phi + S_{68} \cos^2 \Phi + S_{69} \sin \Phi \cos \Phi + S_{610} \cos^2 \Phi \end{pmatrix}$$
Likewise a similarity transformation of rotation $\pm \Phi$ about the $z$-axis will bring $\mathbf{D}$ from the crystalline system into the laboratory system.

$$
\mathbf{D}_{lb} = \begin{pmatrix}
D_1 \cos^2 \Phi + D_2 \sin^2 \Phi + 2D_6 \cos \Phi \sin \Phi \\
D_1 \sin^2 \Phi + D_2 \cos^2 \Phi - 2D_6 \cos \Phi \sin \Phi \\
D_3 \\
-D_5 \sin \Phi + D_4 \cos \Phi \\
D_5 \cos \Phi + D_4 \sin \Phi \\
-D_{12} \cos \Phi \sin \Phi - D_6 (\sin^2 \Phi - \cos^2 \Phi)
\end{pmatrix}
$$

So that we have in the laboratory system

\begin{align*}
(D-11) \quad D_{12 \ lb} &= D_{12} \cos 2\Phi + 2D_6 \sin 2\Phi \\
D_3 \ lb &= D_3 \\
D_5 \ lb &= D_5 \cos \Phi + D_4 \sin \Phi
\end{align*}

Using, then, equations (V-11), (V-10), and (V-9) and differentiating with respect to the measured strain we obtain

\begin{align*}
(D-12) \quad \frac{dD_{12}}{de} &= (G_{11} - G_{12}) \left[ (\frac{s_{11} - s_{13}}{s_{11}''}) \sin^2 \Theta - \frac{s_{14}}{s_{11}''} \sin 2\Theta \sin 3\Phi \right] \\
&\quad + G_{14} \left[ \frac{s_{14}}{s_{11}''} 2 \sin^2 \Theta - \frac{s_{14}}{s_{11}''} \sin 2\Theta \sin 3\Phi \right] \\
&\quad + G_{15} \left[ -\frac{s_{14}}{s_{11}''} \sin 2\Theta \cos 3\Phi \right] \\
&\quad + G_{16} \left[ -\frac{s_{14}}{s_{11}''} 2 \sin 2\Theta \cos 3\Phi \right] \\
\frac{dD_3}{de} &= -(G_{11} + G_{12}) \left[ (\frac{s_{11} + s_{13}}{s_{11}''}) \sin^2 \Theta + \frac{s_{14}}{s_{11}''} 2 \cos^2 \Theta \right] \\
&\quad + G_{23} \left[ \frac{s_{14}}{s_{11}''} \sin^2 \Theta + \frac{s_{14}}{s_{11}''} \cos^2 \Theta \right] \\
\frac{dD_5}{de} &= G_{41} \left[ (\frac{s_{11} + s_{13}}{s_{11}''}) \sin^2 \Theta \sin 3\Phi - \frac{s_{14}}{s_{11}''} \sin 2\Theta \right] \\
&\quad + G_{44} \left[ \frac{s_{14}}{s_{11}''} \sin^2 \Theta \sin 3\Phi - \frac{s_{14}}{s_{11}''} \sin 2\Theta \right] \\
&\quad + G_{45} \left[ -\frac{s_{14}}{s_{11}''} \sin^2 \Theta \cos 3\Phi \right] \\
&\quad + G_{51} \left[ (\frac{s_{11} + s_{13}}{s_{11}''}) \sin^2 \Theta \cos 3\Phi \right]
\end{align*}

and the forms for $D_{12}'$, $D_3'$, and $D_5'$, will be those of (V-12) with the appropriate sign changes.
With the information contained in equations (V-12) and the corresponding equations for the other site, we see that in order to have the shift $\frac{dB}{de}$ the same for both sites we must choose stress axes such that the factors multiplying $G_{15}$, $G_{16}$, $G_{45}$, and $G_{51}$ are zero. These factors are:

$$\sin 2\Theta \cos 3\Phi$$ for $G_{15}$ and $G_{14}$

$$\sin^2\Theta \cos 3\Phi$$ for $G_{45}$ and $G_{51}$

So we see that it suffices to choose $\Theta = 0$ or $\Phi = \frac{\pi}{6}$ or $\frac{\pi}{2}$.

We choose thusly, three rods in order to evaluate the six components of $G$ which are invariant to the difference between the two sites.

<table>
<thead>
<tr>
<th>Rod Number</th>
<th>$\Theta$</th>
<th>$\Phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0°</td>
<td>90°</td>
</tr>
<tr>
<td>2</td>
<td>45°</td>
<td>90°</td>
</tr>
<tr>
<td>3</td>
<td>90°</td>
<td>90°</td>
</tr>
</tbody>
</table>

In order to evaluate the derivatives in (V-12) we must obtain $s''_{11}$ in terms of the components of the compliance tensor in the crystalline system, $s_{ij}$. To do this, we must perform a similarity rotation on $s_{ij}$ of $\Phi$ about the z-axis and then one of $\Theta - \frac{\pi}{2}$ about the y-axis, yielding:

\begin{align*}
(V-13) \quad s''_{11} &= \sin^4\Theta \left( \cos^4\Phi + \sin^4\Phi \right) s_{11} + 6 \sin^4\Theta \\
& \quad \cos^2\Phi \sin^2\Phi s_{12} + 12 \sin^3\Theta \cos\Theta \\
& \quad \cos\Theta \sin\Phi s_{14} + 6 \sin^2\Theta \cos^2\Theta s_{13} + \\
& \quad \cos^4\Theta s_{33}
\end{align*}

For $\Phi = 90^\circ$ we may rewrite (V-13):
Thus we have the following result, employing the values for $S_{ij}$ given by Wachtman, et al.\textsuperscript{3}:

<table>
<thead>
<tr>
<th>ROD</th>
<th>$S_{ii}$</th>
<th>$dD_{1}/de$</th>
<th>$dD_{3}/de$</th>
<th>$dD_{5}/de$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$S_{33}$</td>
<td>0</td>
<td>$-(G_{ii}+G_{ii}) 2^{3/4}S_{iii}$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>$(G_{ii}+G_{ii})$</td>
<td>$\frac{S_{ii}-S_{ii}^{2}+2S_{ii}^{2}}{2S_{ii}}$</td>
<td>$-(G_{ii}+G_{ii}) \frac{S_{ii}^{3}+S_{ii}^{3}+S_{ii}^{3}}{2S_{ii}}$</td>
<td>$G_{44} (\frac{S_{ii}^{3}+S_{ii}^{3}}{2S_{ii}})$</td>
</tr>
<tr>
<td>3</td>
<td>$S_{ii}$</td>
<td>$G_{ii} \frac{S_{ii}^{3}+S_{ii}^{3}}{2S_{ii}}$</td>
<td>$-(G_{ii}+G_{ii}) \frac{S_{ii}^{3}+S_{ii}^{3}}{2S_{ii}}$</td>
<td>$G_{44} (\frac{S_{ii}^{3}+S_{ii}^{3}}{2S_{ii}})$</td>
</tr>
</tbody>
</table>

Thus we are in a position to calculate the value of the components $G_{11}$, $G_{12}$, $G_{13}$, $G_{33}$, $G_{14}$, and $G_{44}$.

In order to find the other four components, we wish to use a stress direction such that $\sin^{2} \Theta \cos 3 \phi \times \sin 2 \Theta \cos 3 \phi \neq 0$. It suffices thus to choose $\Theta = \pi/4$, $\phi = 0$ and then to measure, rather than $d\theta /de$, $\Delta (d\theta /de)$, i.e., to ignore the individual shifts of the two different sites, but measure only the splitting of the lines. In this case we have from (v-8) and (v-12):

\[(v-13) \quad \Delta (d\theta /de) = -2 \partial^{2}B / \partial d_{12} (G_{i5} S_{ii}^{4} S_{ii}^{4} + 2 G_{i6} S_{ii}^{4} S_{ii}^{4}) - \partial^{2}B / \partial d_{5} (G_{i5} S_{ii}^{4} S_{ii}^{4} - G_{i5} (S_{ii}^{3} S_{ii}^{3} S_{ii}^{3})) \]

which for $\Theta = 45^\circ$, $\phi = 0^\circ$ is just

\[\Delta (d\theta /de) = -2 \partial^{2}B / \partial d_{12} (G_{i5} S_{ii}^{4} S_{ii}^{4} + 2 G_{i6} S_{ii}^{4} S_{ii}^{4}) - \partial^{2}B / \partial d_{5} (G_{i5} S_{ii}^{4} S_{ii}^{4} - G_{i5} (S_{ii}^{3} S_{ii}^{3} S_{ii}^{3})) \]

where $S_{ii} = \frac{1}{4} (S_{ii} + 6 S_{12} + S_{33})$.
We see that no matter what values of $\Theta$ and $\Phi$ we choose; it is impossible to evaluate more than the combinations of the splitting terms of $G$ in (V-13). So the variables for splitting are
\[
(G_{15} + 2^{S_W/S_{44}} G_{16})
\]
and \[
(G_{51} - S_{45}/(s_n-s_s) G_{45}).
\]
VI. EXPERIMENTAL PROCEDURE AND RESULTS FOR NON-SPLITTING CASE

In section V we considered an experiment in which $\Theta$ was held constant and where $E_i - E_j = E_\phi$ was constant. This is exactly the manner in which the experiment was performed. The experimental procedure was essentially that described by Hemphill in his thesis. Figure 2 is a block diagram of the EPR spectrometer which was used in this experiment. This design was developed by T. D. Black in the course of his investigation of stress effects on rare-earths in $^{4}$CaF$_2$. The equipment is described in detail in Black's and Hemphill's theses.

Figure 3 is a photograph of the sample cavity and stress-mechanism which we developed to try to eliminate the bending we encountered in attempting to employ Hemphill's cavity. The cavity proper is shown separately in Figure 4 together with a diagram indicating the magnetic-field lines and sample orientation. The cavity is a rectangular cavity which is excited in the TE$_{201}$ mode. The sample is placed in a region of high magnetic field which is perpendicular to the axis of the rod.

The stress mechanism is shown in Figure 5 with the cavity removed. Stress is applied to the rod along its axis by means of the large, hand wheel.

All rotational motion is removed by means of a push rod which is restricted to linear motion. The stress is adjusted to lie along the axis of the rod by means of an adjustable ball socket on the static end of the rod.
FIGURE 2  EPR SPECTROMETER
FIGURE 3  CAVITY & STRESS SYSTEM
FIGURE 4  $\text{TE}_{201}$ CAVITY
FIGURE 5  STRESS MECHANISM
The strain was measured by means of four constantan foil, paper base SR-4 strain gages, type FAP-12-12 which were attached to the four sides of the rod using Eastman 910 adhesive.

For each rod, all gages were taken from the same lot and all had the same gage factors. In addition a comparison, or dummy, gage of the same lot as the gages on the rod, was employed to eliminate any temperature dependent drift.

The samples were prepared in exactly the same manner as described by Hemphill, but were slightly longer than his samples.

The experimental procedure was very simple: The magnet base readings were calibrated to the angle \( \theta \) with respect to the c-axis by employing the angular dependence of the unstressed spectrum in the vicinity of 0° and 90°. The frequency of the microwaves was held constant by locking the klystron frequency to the resonant frequency of the sample cavity. The magnet base was set for the angle necessary to have \( B \) at an angle \( \theta \) to the c-axis, and the magnetic field was adjusted to a value where a resonance was observed. The magnetic field was measured with the NMR Gaussmeter. Strain readings were recorded for the four gages. Stress was applied and the new strain readings recorded. The ball seat was adjusted until the strain differences were approximately equal on the four sides. The magnetic field was readjusted for resonance and this field measured. This was repeated for higher stresses and then the stress was removed and the field was found to return to its initial value. The measurements were repeated for various values of \( \theta \) and for several
C LEAST-SQUARES ANALYSIS OF RUBY STRAIN DATA E.D. MC DONALD, P.L. DONOH

DIMENSION GA(6,1000), W(1000), F(1000), AL(6), A(6,6), VARG1(6), VARG2(6)

1, ALP(6), G(6), GP(6)

COMMON NLOOP1, NLOOP2, TH, B, DUMMY, FD12, FD3, FD5, ET

NW=4

K=0

21 READ INPUT TAPE 2,1, NR, I, J, TH, B, Q, Y, NC, ET

1 FORMAT(11, 2X2I11, 4F10.5, 4X11, 4XF10.3)

K=K+1

CALL MESS (I, J)

IF (NLOOP1-2) 700, 200, 200

700 IF (NLOOP2-2) 701, 200, 200

200 WRITE OUTPUT TAPE 6,2, NLOOP1, NLOOP2, I, J, TH, B, DUMMY, FD12, FD3, FD5,

1 ET, NW, K

2 FORMAT(2I2, 2X2I1, F5.1, 6(3XE10.3), 2X2I2)

701 GO TO (11, 12, 13), NR

11 GA(1,K)=.335*FD3

GA(2,K)=0.0

GA(3,K)=1.0*FD3

GA(4,K)=0.0

GA(5,K)=0.0

GA(6,K)=0.0

GO TO 20

12 GA(1,K)=-0.186*FD3

GA(2,K)=0.429*FD12

GA(3,K)=0.370*FD3

GA(4,K)=1.322*FD5

GA(5,K)=-2.645*FD12

GA(6,K)=-0.429*FD5

GO TO 20

13 GA(1,K)=-0.696*FD3

GA(2,K)=1.304*FD12

GA(3,K)=-0.155*FD3

GA(4,K)=-0.208*FD5

GA(5,K)=0.416*FD12

GA(6,K)=-1.304*FD5

GO TO 20

20 W(K)=Y

F(K)=-Q

GO TO (21, 22), NC

22 DO 23 M=1, 6

AL(M)=0.0

DO 23 L=1, 6

23 A(M, L)=0.0

DO 25 KT=1, K

DO 24 M=1, 6

AL(M)=AL(M)+W(KT)*F(KT)*GA(M, KT)

DO 24 L=1, 6

24 A(M, L)=A(M, L)+W(KT)*GA(M, KT)*GA(L, KT)

25 CONTINUE

CALL SOLVE(A, AL, G)

VARF=0.0

DO 26 KT=1, K

300 F0=0.0

DO 27 M=1, 6
FO = FO + G(M) * GA(M, KT)

VARF = VARF + (fi(KT) - FO) * 2
VARF = VARF / FLOATF(K)

DO 28 L = 1, 6
   VARG1(L) = 0.0
28
VARG2(L) = 0.0

DO 29 KT = 1, K
   DO 30 M = 1, 6
      ALP(M) = W(KT) * GA(M, KT)
      CALL SOLVE (A, ALP, GP)
      DO 31 M = 1, 6
         VARG1(M) = VARG1(M) + GP(M) * 2 / W(KT)
      31
      VARG2(M) = VARG2(M) + GP(M) * 2
   30
   CONTINUE
   DO 32 M = 1, 6
      VARG2(M) = VARG2(M) * VARF
   32
   CONTINUE
2000 CONTINUE

WRITE OUTPUT TAPE 3, 2010
2010 FORMAT(23H1 WEIGHTED AS PER CARDS)
GO TO 2009

WRITE OUTPUT TAPE 3, 2011
2011 FORMAT(28H1 WEIGHTED DBDE**2 OF CARDS)
GO TO 2009

WRITE OUTPUT TAPE 3, 2012
2012 FORMAT(16H1 EQUAL WEIGHTS)

WRITE OUTPUT TAPE 3, 33, G, VARG1, VARG2, VARF
33 FORMAT (1H0, 14X5H11+12, 10X5H11-12, 12X2H33, 13X2H44, 13X2H14, 13X2H41/110H0
       6F15.5/10H0 VAR.1  6F15.5/10H0 VAR.2  6F15.5/10HOVA
       2R. DBDE F15.5)
      CALL DBDE(G, VARG2)
      NW = NW - 1
      GO TO (35, 36, 760), NW
760 DO 761 KT = 1, K
761 W(KT) = F(KT) * 2 * W(KT)
GO TO 22
35 CALL EXIT
36 DO 37 KT = 1, K
37 W(KT) = 1.0
GO TO 22
END

SUBROUTINESOLVE(G, GL, X)
DIMENSION(A(6, 6), AL(6), BL(6), CL(5), D(4, 3), DL(4), E(3, 21), EL(3), F(2, 2), FL(2), X(6), T(7, 6), TL(7), V(6, 5), VL(6), G(6, 6), GL(6))

DO 401 I = 1, 6
   AL(I) = GL(I)
   DO 401 J = 1, 6
   A(I, J) = G(I, J)
N = 6
DO 401 I = 1, 6
   TL(I) = AL(I)
   DO 401 J = 1, 6
   T(I, J) = A(I, J)
M=1
GOTO100
200 DO201I=1,6
   AL(I)=TL(I)
   DO201J=1,6
201 A(I,J)=T(I,J)
   DO2I=1,5
   BL(I)=VL(I)
   TL(I)=VL(I)
   DO2J=1,5
   B(I,J)=V(I,J)
   2 T(I,J)=V(I,J)
   N=5
   M=2
   GOTO100
300 DO301I=1,5
   BL(I)=TL(I)
   DO301J=1,5
301 B(I,J)=T(I,J)
   DO31=1,4
   CL(I)=VL(I)
   TL(I)=VL(I)
   DO3J=1,4
   C(I,J)=V(I,J)
   3 T(I,J)=V(I,J)
   N=4
   M=3
   GOTO100
400 DO801I=1,4
   CL(I)=TL(I)
   DO801J=1,4
401 C(I,J)=T(I,J)
   DO41=1,3
   DL(I)=VL(I)
   TL(I)=VL(I)
   DO4J=1,3
   D(I,J)=V(I,J)
   4 T(I,J)=V(I,J)
   N=3
   M=4
   GOTO100
500 DO501I=1,3
   DL(I)=TL(I)
   DO501J=1,3
501 D(I,J)=T(I,J)
   DO51=1,2
   EL(I)=VL(I)
   TL(I)=VL(I)
   DO5J=1,2
   E(I,J)=V(I,J)
   5 T(I,J)=V(I,J)
   N=2
   M=5
   GOTO100
F(1,1)=V(1,1)
DO601I=1,2
EL(1)=TL(1)
DO601J=1,2
601 E(I,J)=T(I,J)
FL(1)=VL(1)
X(1)=FL(1)/F(1,1)
X(2)=EL(2)-E(2,1)*X(1)/E(2,2)
X(3)=(DL(3)-D(3,1)*X(1)-D(3,2)*X(2))/D(3,3)
X(4)=(CL(4)-C(4,1)*X(1)-C(4,2)*X(2)-C(4,3)*X(3))/C(4,4)
X(5)=(BL(5)-B(5,1)*X(1)-B(5,2)*X(2)-B(5,3)*X(3)-B(5,4)*X(4))/B(5,5)
X(6)=(AL(6)-A(6,1)*X(1)-A(6,2)*X(2)-A(6,3)*X(3)-A(6,4)*X(4)-A(6,5))
1*X(5))/A(6,6)
RETURN
100 BIG=ABS(T(1,N))
DO101J=1,N
IF (ABS(T(J,N))<BIG) 101,102,102
102 BIG=ABS(T(J,N))
L=J
101 CONTINUE
J=L
TL(N+1)=TL(J)
DO103K=1,N
103 T(N+1,K)=T(J,K)
JP=J+1
KP=N+1
DO104K=JP,KP
TL(K-1)=T(K)
DO104L=1,N
104 T(K-1,L)=T(K,L)
NP=N-1
DO501I=1,NP
Z=T(I,N)/T(N,N)
VL(I)=TL(I)-TL(N)*Z
DO50J=1,NP
50 V(I,J)=T(I,J)-Z*T(N,J)
GOTO(200,300,400,500,600),M
END
SUBROUTINE DBDE(G,VARG)
COMMON NL00P1,NL00P2,TH,B0,B,FD12,FD3,FD5,ET
DIMENSION G(6),VARG(6),GA(6,2),NRM(5),IM(6),JM(6),BOM(6)
IF (SENSE SWITCH 1) 1,2
1 RETURN
2 CONTINUE
NRM(1)=1
NRM(2)=2
NRM(3)=3
IM(1)=1
IM(2)=2
IM(3)=2
IM(4)=3
IM(5)=1
IM(6)=1
JM(1)=2
JM(2)=3
JM(3)=3
JM(4)=4
JM(5)=3
JM(6)=3
BOM(1)=7.69
BOM(2)=0.27
BOM(3)=3.83
BOM(4)=1.19
BOM(5)=0.56
BOM(6)=3.57
K=1
DO69M1=1,3
DO69M2=1,6
I=IM(M2)
J=JM(M2)
TH=0.0
BO=BOM(M2)
NR=NRM(M1)
ET=9.93
WRITE OUTPUT TAPE 3,3,NR,I,J
3 FORMAT(1H1,6X,2HNR,4X,1HI,4X,1HJ,6X,2HTH,14X,1HB,12X,4HDBDE,7X,15H
1STD. DEV. DBDE /1H0I8,215)
DTH=2.
DO40N=1.45
TH=TH+DTH
CALLMESS(I,J)
GO TO (32,69),NLOOP1
32 GO TO (33,69),NLOOP2
33 IF(B)69,34,34
34 CONTINUE
GO TO (11,12,13),NR
11 GA(1,K)=.335*FD3
GA(2,K)=0.0
GA(3,K)=1.0*FD3
GA(4,K)=0.0
GA(5,K)=0.0
GA(6,K)=0.0
GO TO 20
12 GA(1,K)=-0.186*FD3
GA(2,K)=0.429*FD12
GA(3,K)=0.370*FD3
GA(4,K)=1.322*FD5
GA(5,K)=-2.645*FD12
GA(6,K)=-0.429*FD5
GO TO 20
13 GA(1,K)=-0.696*FD3
GA(2,K)=1.304*FD12
GA(3,K)=-0.155*FD3
GA(4,K)=0.208*FD5
GA(5,K)=0.416*FD12
GA(6,K)=1.304*FD5
20 CONTINUE
F = 0.
VARF = 0.
DO 4 M = 1, 6
   F = F + G(M) * GA(M, K)
4    VARF = VARF + VARG(M) * GA(M, K) * 2
   STD = SQRTF(VARF)
WRITE OUTPUT TAPE 3, 5, TH, B, F, STD
FORMAT(1H, 19X, 4F15.5)
CONTINUE
RETURN
END
SUBROUTINE MESS(I, J)
FNTF(E) = 3. * G2 * B2 * SF**2 * (D - E)
DIMENSION E(4)
COMMON NLOOP1, NLOOP2, TH, B0, B, DBDD12, DBDD3, DBDD5, ET
D = (-5.733)
G = 2.7789
G2 = G * G
T = TH / 57.29578
CF = COSF(T)
SF = SINF(T)
C3 = 1. - 3. * CF * CF
C6 = 1. - 6. * CF * CF
B = B0
L = 0
500   L = L + 1
   IF(L - 25) 400, 301, 301
301   NLOOP1 = 2
      GO TO 300
400   B2 = B * B
      AL = 2.5 * G2 * B2 + 2. * D2
      GA = D2 * D2 + 5625 * (G2 * B2) * 2.5 * G2 * B2 * D2 * C6
      DEL = D - 1.5 * G * B
      EIP = DEL
      K = 0
1     K = K + 1
      IF(K - 25) 10, 200, 200
200   NLOOP2 = 2
      GO TO 5
10    EI = EIP
      EIP = EI - (EI**4 - AL * EI**2 + BE * EI + GA) / (4. * EI**3 - 2. * AL * EI + BE)
      IF(ABS(EI - EIP) - 0.00001) 2, 2, 1
      2   E(1) = EIP
      EIP = DEL
      K = 0
3     K = K + 1
      IF(K - 25) 30, 200, 200
EI=EIP
EIP=EI-(EI**4-AL*EI**2+8*EI+GA)/(4.*EI**3-2.*AL*EI+BE)
IF(ABS(EI-EIP)-0.00001)4,4,3
4
E(4)=EIP
E(2)=0.5*(-(E(1)+E(4)))+SQR((E(1)+E(4))^2-4.*GA/(E(1)*E(4)))
E(3)=(-(E(1)+E(2)+E(4)))
NLOOP2=1
5 CONTINUE
GOTO(20,300),NLOOP2
20
FT=E(I)-E(J)-ET
FTP=FNNF(E(J))/FNMF(E(J))-FNNF(E(I))/FNMF(E(I))
B=B-FT/FTP
IF(ABS(FT/FTP)-.0001)50,50,500
50
B2=B*B
DEN=FNMF(E(J))*FNNF(E(I))-FNMF(E(I))*FNNF(E(J))
TOP=FNNF(E(I))*FNPF(E(J))-FNMF(E(J))*FNPFE(I))
TOPS=FNMF(E(I))*FNSF(E(J))-FNMF(E(J))*FNSFE(I))
TOPT=FNMF(E(I))*FNTF(E(J))-FNMF(E(J))*FNTFE(I))
DBD03=TOPR/DEN
DBDD5=TOPS/DEN
DBD12=TOPT/DEN
DTH=1./57.29578
B0=B+DTH*TOPP/DEN
NLOOP1=1
300 RETURN
END
C

LEAST SQUARES FIT OF STRAIN DATA R. B. HEMPHILL RICE UNIV.

DIMENSION SUM(9), DB(20), DE(20), WT(20)

3 FORMAT (11,2X,2I1,4F5.0,2F10.1,F5.3,F5.0,4X,I1)

4 FORMAT(11,2X2I1,4F10.5,4XI1,4XF10.3)

5 FORMAT (106H1, ROD TRANS THETA DB/DE)

1 BINT VAR DB/DE SIG DB/DE WT DB/DE N)

6 FORMAT (12XI1,7X2I1,7XF5.1,4XF10.2,4XF8.2,F14.6,F12.6,F14.6,4XI2)

7 PRINT 5

10 DO 20 I = 1,9

20 SUM (I) = 0.0

N = 0

30 N = N+1

READ 3,NROD,I,J,TH,BI,B,F0,DE(N),NCTRL

BA=BI/4257.76

WT(N)=-DE(N)

IF (SENSE SWITCH 2) 31,32

31 WT(N) = 1.0

32 CONTINUE

DB(N) = (B-BI)/4257.76

DE(N) = DE(N)*1.0E-6

SUM(1) = SUM(1)+WT(N)*DB(N)

SUM(2) = SUM(2)+WT(N)*DE(N)*DE(N)

SUM(3) = SUM(3)+WT(N)*DE(N)*DB(N)

SUM(4) = SUM(4)+WT(N)*DE(N)

SUM(5) = SUM(5)+WT(N)

SUM(6) = SUM(6)+(WT(N)*DE(N))*2

SUM(7) = SUM(7)+WT(N)*WT(N)

SUM(8) = SUM(8)+WT(N)*WT(N)*DE(N)

IF (NCTRL) 30,30,40

40 DELTA = SUM(5)*SUM(2)-SUM(4)*2

BINT = (SUM(1)*SUM(2)-SUM(3)*SUM(4))/DELTA

DBDE = (SUM(5)*SUM(3)-SUM(4)*SUM(1))/DELTA

DO 50 K = 1,N

50 SUM(9) = SUM(9)+WT(K)*DBDE*DE(K)+BINT-DB(K)*2

VARA=SUM(9)/SUM(5)

VARB=5.53E-8

IF (ABS (VARA) = ABSF (VARB)) 51,51,52.

51 VAR=VARB

GO TO 53

52 VAR=VARA

53 VARM = VAR*(SUM(5)*SUM(5)-SUM(6)-2.0*SUM(5)*SUM(8)*SUM(4)+SUM(4)*S

1UM(4)*SUM(7))/DELTA**2

SIGM = SQRTF (VARM)

IF (VARM-1.0E-6) 54,55,55

54 WT = 0.0

GO TO 56

55 WT = 1.0/VARM

56 IF (SENSE SWITCH 3) 57,58

57 WT = 1.0

58 NCT = 1

IF (NCTRL-2) 80,60,70

60 NCT = 1

GO TO 80

70 NCT = 2
80 IF (SENSE SWITCH 1) 81,82
81 PUNCH 4,NROD,I,J,TH,BA,DBDE,WTT,NCT,FO
82 BINT = BINT*1.0E+3
   PRINT 6,NROD,I,J,TH,DBDE,BINT,VARM,SIGM,WTT,N
   IF (NCTRL-2) 10,7,90
90 PAUSE
   GO TO 7
END
BIBLIOGRAPHY


