Thesis - geology

Elastic constants and computer programs
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ELASTIC CONSTANTS AND COMPUTER PROGRAMS FOR CALCULATING THE ELASTIC PARAMETERS OF MATERIALS SUBJECTED TO MODEST PRESSURES OR TEMPERATURES

A THESIS SUBMITTED TO THE GRADUATE DIVISION OF THE
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By

Thomas Joseph Sokolowski

Thesis Committee:

Kost A. Pankiwskyj, Chairman
Richard P. Shaw
Pow-Foong Fan

We certify that we have read this thesis and that in our opinion it is satisfactory in scope and quality as a thesis for the degree of Master of Science in Geosciences - Geology.

THESIS COMMITTEE

Kost A. Pawlowsky

Richard Paul Shaw

Pow Foong Tan

ABSTRACT

The purpose of this work is to relate laboratory data, obtained at standard and above-standard atmospheric conditions of temperature and pressure, to the elastic stiffness constants $[C_{ij}]$ which are used to obtain the bulk modulus and other elastic parameters. Each crystalline or non-crystalline system is characterized by a particular group of stiffness constants which are determined by the system's crystallographic symmetry together with Hooke's law. Stiffness constant assemblages have been derived for all crystalline systems and for the isotropic system.

The "pulse superposition" method was used in the laboratory to obtain the longitudinal (V_p) and shear (V_s) velocities for a specimen. These velocities together with the density of the specimen are used to obtain values for the stiffness constants. Formulas, relating the stiffness constants to the other elastic parameters, have been consolidated from the current literature and are given here.

Four computer programs with input-output explanations were included for performing the elastic parameter calculations. Two programs are for pressure or temperature computations concerning an isotropic material. The remaining programs are for pressure or temperature computations for a tetragonal crystalline specimen.

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INTRODUCTION

In the past few decades much interest has been generated concerning rock specimens that are subjected to modest pressures or temperatures. It would be desirable to be able to duplicate, experimentally, the higher pressure-temperature conditions (< shock wave experimental conditions) of the earth, but this is not as yet possible. However, it is possible to study specimens at lower pressures than those that exist in the earth to gain an initial understanding of the elastic behavior of materials under moderate pressures or temperatures; the upper limit of the pressure in this case is approximately 10 kilobars and that of the temperature is about 500 degrees centigrade.

One approach to the study of the elastic behavior of isotropic or crystalline materials is through their stiffness constants (also called rigidity constants). Therefore, the first part of this paper presents some of the basic theory pertaining to the derivation of the stiffness constants for all systems of crystalline and non-crystalline material. Partial derivations of the elastic constants can be found in Voigt (1928), Wooster (1938), Love (1944), Sokolnikoff (1946), Kittel (1960), Federov (1968), and others. The stiffness constants were derived for a homogeneous, isotropic material and for all crystal classes. For all crystal classes, point group stereograms and corresponding class symbols are given with their appropriate stiffness constants derivations. Hooke's law and the symmetry of the material structure form the basis of the derivations. Symmetry is a

basic property of all crystals and can be considered here as of two basic types: symmetry with respect to a plane (mirror reflection) and symmetry with respect to an axis of revolution. Grouping of crystals into 32 classes is predicted on symmetry and those classes which have similar axial sets can be grouped into a crystal system. With this type of grouping, the 32 crystal classes comprise seven crystal systems: monoclinic, orthorhombic, tetragonal, cubic, hexagonal, trigonal, and triclinic.

The elastic parameters of a material are computed from the stiffness constants of the material. These computations are tedious and lengthy but can easily be done by a computer. Therefore, the second part of this paper presents the basic formulas extracted from the current literature, and computer programs for elastic parameter calculations. The computer programs show how these basic computations are performed for a few specific cases. These programs can be modified for computations based on other systems.

DERIVATION OF ELASTIC STIFFNESS CONSTANTS FOR THE ISOTROPIC SYSTEM

The basis of the mathematical theory of elasticity concerning small deformations of elastic bodies is Hooke's law. This law states that there is a proportionality between forces and displacements on a body. The generalized Hooke's law relating stress as a linear function of strain is given by Frederick and Chang (1965) and has the form

$$t_{ij} = C_{ijk\ell} e_{k\ell} \tag{1.1}$$

where the $C_{ijk\ell}$ are the elastic constants, t_{ij} is the stress and $C_{k\ell}$ is the strain. The stress-strain subscripts indicate orientation of the stress-strain vectors. Frederick and Chang have shown that the maximum number of independent constants of (1.1) is 36 and by making the substitution

$$t_{11} = t_1,\ t_{22} = t_2,\ t_{33} = t_3,\ t_{23} = t_4,\ t_{31} = t_5,\ t_{12} = t_6$$
$$e_{11} = e_1,\ e_{22} = e_2,\ e_{33} = e_3,\ 2e_{23} = e_4,\ 2e_{31} = e_5,\ 2e_{12} = e_6 \tag{1.2}$$

then (1.1) can be expressed in more compact indexing as

$$t_i = C_{ij}e_j \qquad (i,j = 1,\ldots,6) \tag{1.3}$$

Equation (1.3) expanded becomes

$$\begin{aligned}
t_1 &= C_{11}e_1 + C_{12}e_2 + C_{13}e_3 + C_{14}e_4 + C_{15}e_5 + C_{16}e_6 \\
t_2 &= C_{21}e_1 + C_{22}e_2 + C_{23}e_3 + C_{24}e_4 + C_{25}e_5 + C_{26}e_6 \\
t_3 &= C_{31}e_1 + C_{32}e_2 + C_{33}e_3 + C_{34}e_4 + C_{35}e_5 + C_{36}e_6 \\
t_4 &= C_{41}e_1 + C_{42}e_2 + C_{43}e_3 + C_{44}e_4 + C_{45}e_5 + C_{46}e_6 \\
t_5 &= C_{51}e_1 + C_{52}e_2 + C_{53}e_3 + C_{54}e_4 + C_{55}e_5 + C_{56}e_6 \\
t_6 &= C_{61}e_1 + C_{62}e_2 + C_{63}e_3 + C_{64}e_4 + C_{65}e_5 + C_{66}e_6
\end{aligned} \tag{1.4}$$

The 6 x 6 matrix of elastic constants $[C_{ij}]$ of (1.3) has been shown by Love (1944) to be symmetric. The symmetry of $[C_{ij}]$ is not assumed for the isotropic case.

An isotropic body is defined as one that has the same elastic properties in any direction about a point of the body. Therefore, an isotropic body can have symmetry planes in any direction. Then (1.3) must not alter under any transformation of the coordinates with respect to these symmetry planes. The equations for the stress and strain transformations are given as

$$t'_{ij} = \ell_{ir}\ell_{js}t_{rs} \tag{1.5}$$

$$e'_{ij} = \ell_{ir}\ell_{js}e_{rs} \tag{1.6}$$

where ℓ_{ir} and ℓ_{js} are direction cosines. After transformation of the coordinates, (1.3) has the form

$$t'_i = C_{ij}e'_j \qquad (i,j = 1,\ldots,6) \tag{1.7}$$

The coordinate axes of a body will in general be chosen such that these axes will coincide with the symmetry of structure. A right-handed cartesian coordinate system (X_1,X_2,X_3) is chosen at the center of the body. Arbitrarily, the (X_1X_2) plane is chosen to be a mirror plane. Since this is a symmetry plane the elastic constants $[C_{ij}]$ must then be invariant with respect to this plane. The coordinate transformations with respect to this mirror plane are given by $X_1 = X'_1$, $X_2 = X'_2$, $X_3 = -X'_3$ and the corresponding direction cosine

scheme is

	X_1	X_2	X_3
X_1'	1	0	0
X_2'	0	1	0
X_3'	0	0	-1

where $\ell_{11} = 1$, $\ell_{22} = 1$, $\ell_{33} = -1$, and the remaining $\ell_{ij} = 0$. (1.8)

Equation (1.5) can then be expanded as

$$\begin{aligned} t'_{11} = {} & \ell_{11}(\ell_{11}t_{11} + \ell_{12}t_{12} + \ell_{13}t_{13}) \\ & + \ell_{12}(\ell_{11}t_{21} + \ell_{12}t_{22} + \ell_{13}t_{23}) \\ & + \ell_{13}(\ell_{11}t_{31} + \ell_{12}t_{32} + \ell_{13}t_{33}) \end{aligned}$$

$$\begin{aligned} t'_{22} = {} & \ell_{21}(\ell_{21}t_{11} + \ell_{22}t_{12} + \ell_{23}t_{13}) \\ & + \ell_{22}(\ell_{21}t_{21} + \ell_{22}t_{22} + \ell_{23}t_{23}) \\ & + \ell_{23}(\ell_{21}t_{31} + \ell_{22}t_{32} + \ell_{23}t_{33}) \end{aligned}$$

$$\begin{aligned} t'_{33} = {} & \ell_{31}(\ell_{31}t_{11} + \ell_{32}t_{12} + \ell_{33}t_{13}) \\ & + \ell_{32}(\ell_{31}t_{21} + \ell_{32}t_{22} + \ell_{33}t_{23}) \\ & + \ell_{33}(\ell_{31}t_{31} + \ell_{32}t_{32} + \ell_{33}t_{33}) \end{aligned}$$

$$\begin{aligned} t'_{23} = {} & \ell_{21}(\ell_{31}t_{11} + \ell_{32}t_{12} + \ell_{33}t_{13}) \\ & + \ell_{22}(\ell_{31}t_{21} + \ell_{32}t_{22} + \ell_{33}t_{23}) \\ & + \ell_{23}(\ell_{31}t_{31} + \ell_{32}t_{32} + \ell_{33}t_{33}) \end{aligned}$$

$$t'_{31} = \ell_{31}(\ell_{11}t_{11} + \ell_{12}t_{12} + \ell_{13}t_{13}) + \ell_{32}(\ell_{11}t_{21} + \ell_{12}t_{22} + \ell_{13}t_{23}) + \ell_{33}(\ell_{11}t_{31} + \ell_{12}t_{32} + \ell_{13}t_{33})$$

$$t'_{12} = \ell_{11}(\ell_{21}t_{11} + \ell_{22}t_{12} + \ell_{23}t_{13}) + \ell_{12}(\ell_{21}t_{21} + \ell_{22}t_{22} + \ell_{23}t_{23}) + \ell_{13}(\ell_{21}t_{31} + \ell_{22}t_{32} + \ell_{23}t_{33})$$

Equations (1.8), (1.5), and (1.2) yield

$$t'_1 = t_1,\ t'_2 = t_2,\ t'_3 = t_3,\ t'_4 = -t_4,\ t'_5 = -t_5,\ t'_6 = t_6 \qquad (1.9)$$

and (1.8), (1.6), and (1.2) give

$$e'_1 = e_1,\ e'_2 = e_2,\ e'_3 = e_3,\ e'_4 = -e_4,\ e'_5 = -e_5,\ e'_6 = e_6 \qquad (1.10)$$

The invariance of the $[C_{ij}]$ must be considered with respect to the symmetry plane. This is done by comparing the coefficients in Hooke's law (1.3) before transformation of coordinates to the coeeficients in Hooke's law (1.7) after transformation of the coordinates.

Substituting (1.9) and (1.10) into the first equation of (1.7) yields equation

$$t_1 = C_{11}e_1 + C_{12}e_2 + C_{13}e_3 - C_{14}e_4 - C_{15}e_5 + C_{16}e_6 \qquad (1.11)$$

Equating (1.11) with the first equation in (1.4) gives

$$C_{14} = C_{15} = 0 \tag{1.12}$$

Substituting (1.9) and (1.10) into the remaining five equations of (1.7) gives five equations that can then be equated to the corresponding five equations of (1.4). These equalities yield

$$\begin{aligned} C_{24} = C_{25} = C_{34} = C_{35} = C_{41} = C_{42} = C_{43} = 0 \\ C_{51} = C_{52} = C_{53} = C_{56} = C_{64} = C_{65} = C_{46} = 0 \end{aligned} \tag{1.13}$$

From (1.12) and (1.13), the stiffness constant matrix of (1.3) can be written as

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{21} & C_{22} & C_{23} & 0 & 0 & C_{26} \\ C_{31} & C_{32} & C_{33} & 0 & 0 & C_{36} \\ 0 & 0 & 0 & C_{44} & C_{55} & 0 \\ 0 & 0 & 0 & C_{54} & C_{55} & 0 \\ C_{61} & C_{62} & C_{63} & 0 & 0 & C_{66} \end{bmatrix} \tag{1.14}$$

The matrix (1.14) substituted into (1.3) represents the stress-strain relationships for a body that has one plane of symmetry and the stiffness constants have been reduced from 36 to 20. The first equation of

(1.3) can now be written as

$$t_1 = C_{11}e_1 + C_{12}e_2 + C_{13}e_3 + C_{16}e_6 \tag{1.15}$$

Similarly, the first equation of (1.7) is

$$t_1' = C_{11}e_1' + C_{12}e_2' + C_{13}e_3' + C_{16}e_6' \tag{1.16}$$

Since our body is isotropic, another mirror plane (X_2X_3) can be introduced normal to the (X_1X_2) plane. The coordinate transformation for this symmetry operation is given by $X_1 = -X_1'$, $X_2 = X_2'$, $X_3 = X_3'$ and the direction cosine scheme is given by

	X_1	X_2	X_3
X_1'	-1	0	0
X_2'	0	1	0
X_3'	0	0	1

where $\ell_{11} = -1$, $\ell_{22} = 1$, $\ell_{33} = 1$, and the remaining $\ell_{ij} = 0$. (1.17)

As before, equations (1.5), (1.6), (1.2), and (1.17) give

$$\begin{aligned} &t_1' = t_1,\ t_2' = t_2,\ t_3' = t_3,\ t_4' = t_4,\ t_5' = -t_5,\ t_6' = -t_6 \\ &e_1' = e_1,\ e_2' = e_2,\ e_3' = e_3,\ e_4' = e_4,\ e_5' = -e_5,\ e_6' = -e_6 \end{aligned} \tag{1.18}$$

From (1.18), (1.14), and (1.7), six equations are obtained that can then be compared to those equations obtained from (1.14) and (1.3). The results of these equalities are

$$C_{16} = C_{26} = C_{36} = C_{45} = C_{54} = C_{61} = C_{62} = C_{63} = 0 \qquad (1.19)$$

Incorporating (1.19) into (1.14) yields

$$\begin{matrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{21} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{31} & C_{32} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{matrix} \qquad (1.20)$$

Equation (1.3) with the matrix $[C_{ij}]$ defined as that of (1.20) represents the stress-strain relationship for a body with two planes of symmetry normal to each other. These two planes of symmetry have reduced the stiffness constants to 12.

Tne (X_1X_3) plane can now be considered as a mirror plane but no new information will be obtained concerning the $[C_{ij}]$. This lack of information is because two orthogonal mirror planes imply the existence of a third mutually orthogonal mirror plane. Since the body is isotropic, the elastic properties must be the same irrespective of orientation of the coordinate axes. Therefore,

90-degree rotations can be considered about the X_1 and X_3 axes and a 45-degree rotation about the X_3 axis. The coordinate transformation for a 90-degree rotation about the X_1 axis gives $X_1 = X_1'$, $X_2 = -X_3'$, $X_3 = X_2'$ and the direction cosine table is given as

	X_1	X_2	X_3
X_1'	1	0	0
X_2'	0	0	-1
X_3'	0	1	0

Using $\ell_{11} = 1$, $\ell_{23} = -1$, and $\ell_{32} = 1$ with equations (1.5), (1.6), and (1.2) gives

$$\begin{aligned} t_1' &= t_1,\ t_2' = t_3,\ t_3' = t_2,\ t_4' = -t_4,\ t_5' = t_6,\ t_6' = -t_5 \\ e_1' &= e_1,\ e_2' = e_3,\ e_3' = e_2,\ e_4' = -e_4,\ e_5' = e_6,\ e_6' = -e_5 \end{aligned} \tag{1.21}$$

The resulting equations obtained from the substitutions of (1.21) into (1.7), where the $[C_{ij}]$ is defined as (1.20), are equated to those equations obtained from (1.3) and (1.20). These equalities yield

$$C_{12} = C_{13},\ C_{21} = C_{31},\ C_{22} = C_{33},\ C_{32} = C_{23},\ C_{66} = C_{55} \tag{1.22}$$

Matrix (1.20) now has form

$$\begin{matrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{21} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{21} & C_{23} & C_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{matrix} \qquad (1.23)$$

Tne 90-degree rotation about the X_3 axis has direction cosines

	X_1	X_2	X_3
X_1'	0	1	0
X_2'	-1	0	0
X_3'	0	0	1

Computations for this rotation are performed in similar manner to the previous one but give

$$C_{12} = C_{21},\ C_{11} = C_{22},\ C_{12} = C_{23},\ C_{21} = C_{23},\ C_{44} = C_{55} \qquad (1.24)$$

Tne array of coefficients of (1.23) can now be written as

$$\begin{matrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{matrix} \tag{1.25}$$

A 45-degree rotation about the X_3 axis yields a relationship among the remaining three stiffness constants. This rotation of coordinates has direction cosines given by

	X_1	X_2	X_3
X_1'	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	0
X_2'	$-\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	0
X_3'	0	0	1

Using the direction cosines, (1.5), (1.6), and (1.2) yield

$$t_6' = -\frac{1}{2}t_1 + \frac{1}{2}t_2 \tag{1.26}$$

$$e_6' = -e_1 + e_2 \tag{1.27}$$

Relationships (1.25) and (1.7) give

$$t_6' = C_{44}e_6' \tag{1.28}$$

Combining equations (1.26), (1.27), and (1.28) gives

$$-\frac{1}{2}t_1 + \frac{1}{2}t_2 = C_{44}(e_2-e_1) \tag{1.29}$$

Equation (1.29) represents the stress-strain relationship of the transformed coordinates. Since the same stress-strain relationship must exist prior to transformation, an expression equivalent to (1.29) can be obtained prior to transformation. Using the first two equations of the set of (1.3) and (1.2) and (1.25) give

$$t_1 = C_{11}e_1 + C_{12}e_2 + C_{12}e_3 \tag{1.30}$$

and

$$t_2 = C_{12}e_1 + C_{11}e_2 + C_{12}e_3 \tag{1.31}$$

Equations (1.30) and (1.31) are combined to give

$$-\frac{1}{2}t_1 + \frac{1}{2}t_2 = \frac{1}{2}(C_{11}-C_{12})(e_2-e_1) \tag{1.32}$$

The equality of (1.29) and (1.32) gives

$$C_{44} = \frac{1}{2}(C_{11}-C_{12})$$

Two of these constants are independent. Letting $C_{44} = \mu$ and $C_{12} = \lambda$, and using (1.3) and (1.25), the generalized Hooke's law for an isotropic body can be written as

$$t_{ij} = \lambda\delta_{ij}e_{ii} + 2\mu e_{ij}(i,j, = 1,2,3) \tag{1.33}$$

where λ and μ are the constants of Lame.

The elastic constants, λ and μ, are used to obtain the various elastic parameters for an isotropic material. Relationships between the various elastic parameters and these stiffness constants are given by Birch (1961).

DERIVATION OF THE ELASTIC STIFFNESS CONSTANTS FOR THE CRYSTALLINE SYSTEMS

The generalized Hermann-Mauguin symbols for crystal classes are given by Mason and Berry (1968) as n, $\bar{n}$, n/m, nm, $\bar{n}$m, n2, and n/mm . The letter n represents a rotation axis of symmetry and m represents a plane of symmetry. A two-, three-, four-, or sixfold rotation axis of symmetry is denoted by n being 2, 3, 4, or 6. A bar over the n indicates an inversion axis and a plane of symmetry parallel to the principal symmetry axis is denoted as n/m. The crystal class symbols and corresponding stereograms are given for all classes for which elastic stiffness constants have been derived.

Some of the symmetry operations imply the existence of others, and only those symmetry operations that produce all other symmetries in a given system have been considered. Furthermore, some coordinate transformations yield the same elastic constants. This implies that, mathematically, the symmetry operations producing the transformations are equivalent. Two such equivalent operations are, the symmetry plane and a diad axis perpendicular to it. A mathematical verification of this equivalence of symmetry operations is by showing that the elastic constants are the same for the two symmetry operations.

The transformation of the elastic constants is given by Frederick and Chang (1965) as

$$C'_{rs} = \ell_{ri}\ell_{sj}C_{ij} \tag{1.34}$$

Consider a symmetry plane perpendicular to the X_3 axis in a right-hand coordinate system. This symmetry operation results in $X_1 = X'_1$, $X_2 = X'_2$, and $X_3 = -X'_3$. The direction cosines are $\ell_{11} = 1$, $\ell_{22} = 1$, and $\ell_{33} = -1$. The direction cosines and (1.34) give

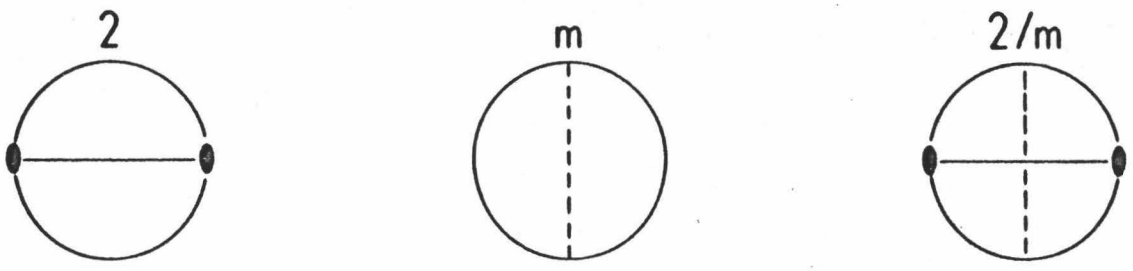
$$\begin{aligned} C'_{11} = C_{11},\ C'_{22} = C_{22},\ C'_{33} = C_{33} \\ C'_{13} = -C_{13},\ C'_{23} = -C_{23},\ C'_{12} = -C_{12} \end{aligned} \tag{1.35}$$

For X_3 as a diad axis, the coordinate transformations are $X_1 = -X'_1$, $X_2 = -X'_2$, and $X_3 = X'_3$. The direction cosines, $\ell_{11} = -1$, $\ell_{22} = -1$, and $\ell_{33} = 1$, substituted into (1.34) gives

$$\begin{aligned} C'_{11} = C_{11},\ C'_{22} = C_{22},\ C'_{33} = C_{33} \\ C'_{13} = -C_{13},\ C'_{23} = -C_{23},\ C'_{12} = -C_{12} \end{aligned} \tag{1.36}$$

The elastic constants of (1.35) are the same as those of (1.36). Therefore, with regard to the stiffness constants, a twofold axis is equivalent to a mirror plane that is perpendicular to the twofold axis. Similarly it can be shown that an inversion axis symmetry operation does not alter the stiffness constants.

A. MONOCLINIC SYSTEM. The symmetry operations of the monoclinic system are a twofold (diad) axis, a mirror plane or both. The symmetry symbols and stereograms are given as



Since a diad is mathematically equivalent to a mirror plane perpendicular to it, then all classes in this system are equivalent to a diad axis. Therefore, the derivation of stiffness constants for the monoclinic case will be with regard to a diad axis arbitrarily oriented parallel to the X_3 axis. The direction cosines table for the coordinate transformation is given as

	X_1	X_2	X_3
X_1'	-1	0	0
X_2'	0	-1	0
X_3'	0	0	1

The direction cosines, (1.5), (1.6), and (1.2) give

$$t_1' = t_1,\ t_2' = t_2,\ t_3' = t_3,\ t_4' = -t_4,\ t_5' = -t_5,\ t_6' = t_6$$
$$e_1' = e_1,\ e_2' = e_2,\ e_3' = e_3,\ e_4' = -e_4,\ e_5' = -e_5,\ e_6' = e_6 \qquad (1.37)$$

Equations (1.37), (1.7), and (1.3) give

$$\begin{aligned} C_{14} = C_{15} = C_{24} = C_{25} = C_{34} = C_{35} = C_{41} = C_{42} = 0 \\ C_{51} = C_{52} = C_{53} = C_{56} = C_{64} = C_{65} = C_{46} = C_{43} = 0 \end{aligned} \tag{1.38}$$

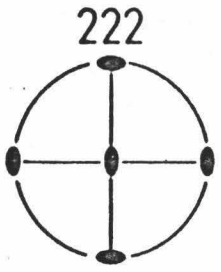
Using (1.38) and the symmetrical properties of the stiffness constants, the $[C_{ij}]$ of (1.3) has the form

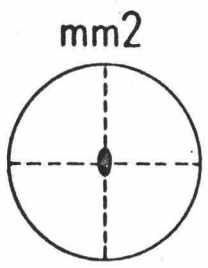
$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{22} & C_{23} & 0 & 0 & C_{26} \\ C_{13} & C_{23} & C_{33} & 0 & 0 & C_{36} \\ 0 & 0 & 0 & C_{44} & C_{45} & 0 \\ 0 & 0 & 0 & C_{45} & C_{55} & 0 \\ C_{16} & C_{26} & C_{36} & 0 & 0 & C_{66} \end{bmatrix} \tag{1.39}$$

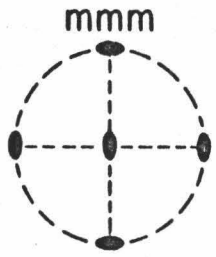
The monoclinic system (2, m, 2/m) is characterized by 13 different stiffness constants:

$$\begin{aligned} C_{11}, C_{12}, C_{13}, C_{16}, C_{22}, C_{23}, C_{26} \\ C_{33}, C_{36}, C_{44}, C_{45}, C_{55}, C_{66} \end{aligned} \tag{1.40}$$

B. ORTHORHOMBIC SYSTEM. All classes in this system have three mutually orthogonal symmetry operations. The classes and stereograms are given as







The 222 and the mmm classes have as minimum symmetry operations, three mutually orthogonal diad axes. The mm2 class, has two mirror planes normal to each other which can be considered as diads perpendicular to each mirror plane. Thus all three classes can be made to have common mathematical symmetry operations. The stiffness constants may be obtained by considering three mutually orthogonal diad axes. Let the first diad axis be parallel to the X_3 axis. The stiffness constant matrix would be the same as (1.39).

Now consider the diad axis oriented parallel to the X_2 axis. The direction cosine scheme is given as

	X_1	X_2	X_3
X_1'	-1	0	0
X_2'	0	1	0
X_3'	0	0	-1

The direction cosines, (1.5), (1.6), and (1.2) give

$$\begin{aligned} t_1' &= t_1,\ t_2' = t_2,\ t_3' = t_3,\ t_4' = -t_4,\ t_5' = -t_5,\ t_6' = -t_6 \\ e_1' &= e_1,\ e_2' = e_2,\ e_3' = e_3,\ e_4' = -e_4,\ e_5' = -e_5,\ e_6' = -e_6 \end{aligned} \tag{1.41}$$

and equations (1.41), (1.39), (1.7), and (1.3) give

$$C_{16} = C_{26} = C_{36} = 0 \tag{1.42}$$

Matrix (1.39) can now be written as

$$\begin{matrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & C_{45} & 0 \\ 0 & 0 & 0 & C_{45} & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{matrix} \tag{1.43}$$

The third diad axis, mutually orthogonal to the previous two, will be parallel to X_1 axis with direction cosine scheme as

	X_1	X_2	X_3
X_1'	1	0	0
X_2'	0	-1	0
X_3'	0	0	-1

The transformed stresses and strains become

$$t_1' = t_1,\ t_2' = t_2,\ t_3' = t_3,\ t_4' = t_4,\ t_5' = -t_5,\ t_6' = -t_6$$
$$e_1' = e_1,\ e_2' = e_2,\ e_3' = e_3,\ e_4' = e_4,\ e_5' = -e_5,\ e_6' = -e_6 \qquad (1.44)$$

And applying previous procedures gives

$$C_{45} = 0$$

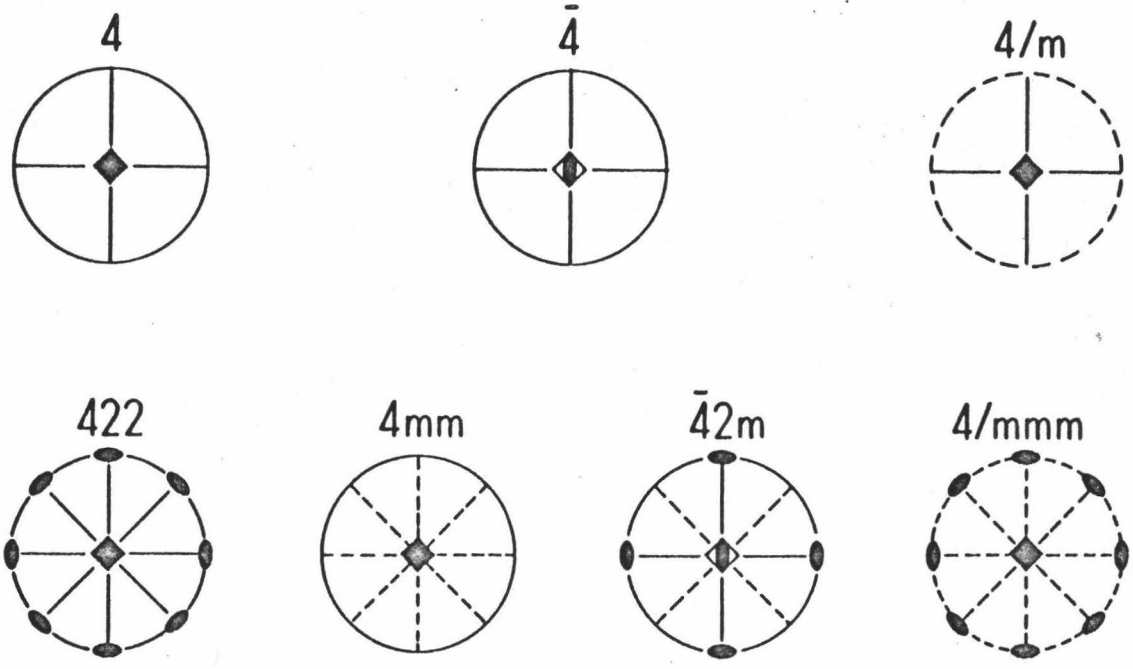
Matrix (1.43) can be written as

$$\begin{matrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{matrix} \qquad (1.45)$$

Therefore, the orthorhombic system (222, mm2, mmm) is characterized by nine stiffness constants:

$$C_{11},\ C_{12},\ C_{13},\ C_{22},\ C_{23},\ C_{33},\ C_{44},\ C_{55},\ C_{66} \qquad (1.46)$$

C. TETRAGONAL SYSTEM. This system contains the classes whose symbols and stereograms are given as



Two sets of stiffness constants are obtained. One set, for classes 4, $\bar{4}$, 4/m, and the second set for the remaining classes. The former has a twofold and a fourfold axis of rotation parallel to the X_3 coordinate. Since the twofold axis of rotation is included in the fourfold axis of rotation, only the fourfold axis of rotation is considered. The fourfold operation yields a coordinate transformation whose tabular form of the direction cosine is

	X_1	X_2	X_3
X_1'	0	-1	0
X_2'	1	0	0
X_3'	0	0	1

The direction cosines, (1.5), (1.6), and (1.2) give

$$\begin{aligned} t_1' &= t_2,\ t_2' = t_1,\ t_3' = t_3,\ t_4' = t_5,\ t_5' = -t_4,\ t_6' = -t_6 \\ e_1' &= e_2,\ e_2' = e_1,\ e_3' = e_3,\ e_4' = e_5,\ e_5' = -e_4,\ e_6' = -e_6 \end{aligned} \tag{1.47}$$

Relationships (1.48), (1.7), and (1.3) result in seven non-zero stiffness constants. The diad symmetry element does not affect the stiffness constants and the matrix $[C_{ij}]$ for classes 4, $\bar{4}$, and $4/m$ can be written as

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{11} & C_{13} & 0 & 0 & -C_{16} \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ C_{16} & -C_{16} & 0 & 0 & 0 & C_{66} \end{bmatrix} \tag{1.48}$$

The seven stiffness constants for tetragonal classes 4, $\bar{4}$, and $4/m$ are

$$C_{11},\ C_{12},\ C_{13},\ C_{33},\ C_{44},\ C_{66},\ C_{16} \tag{1.49}$$

Classes 422, $4mm$, $\bar{4}2m$, and $4/mmm$ have a symmetry operation in addition to the symmetry operations of the previous set of classes. Since a mirror plane can be considered equivalent to a diad axis

perpendicular to it, then these remaining four classes have, as an additional symmetry operation, a diad axis normal to the X_3 coordinate. Using the results from the previous classes, the diad axis is placed arbitrarily parallel to the X_1 axis. The direction cosine scheme for this transformation is the same as that used to obtain equations (1.44).

Equations (1.44), (1.7), and (1.3) give

$$c_{16} = 0$$

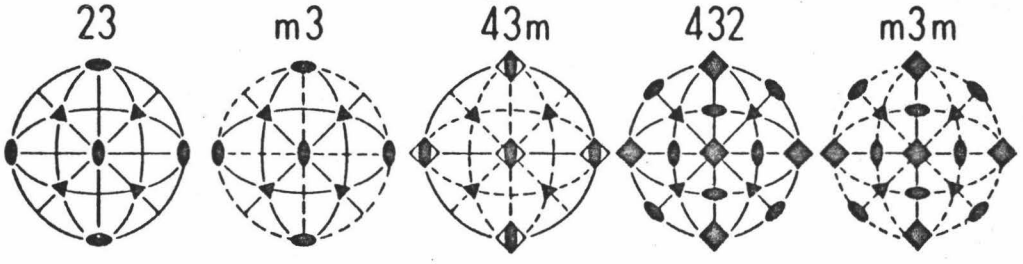
and the stiffness constant matrix (1.49) can be written as

$$\begin{matrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{matrix}$$

The tetragonal classes 422, 4mm, $\bar{4}$2m, and 4/mmm are characterized by six stiffness constants:

$$c_{11}, c_{12}, c_{13}, c_{33}, c_{44}, c_{66} \qquad (1.50)$$

D. CUBIC SYSTEM. The symbols and stereograms for this system are given by



The minimum symmetry operations, to obtain the stiffness constants for this system, are three mutually orthogonal diad axes and a triad axis. Considering the diad axes, the results are the same as those of the orthorhombic system and the stiffness constants are those of (1.45). The triad axis is perpendicular to the diagonal axes of the cube. Successive symmetry operations of a triad axis yields coordinate transformations given by

$$X_1 = X_1', \; X_2 = X_3', \; X_3 = X_2'$$

and (1.51)

$$X_1 = X_3', \; X_2 = X_2', \; X_3 = X_1'$$

Their respective direction cosine schemes are

	X_1	X_2	X_3
X_1'	1	0	0
X_2'	0	0	1
X_3'	0	1	0

(1.52)

and

$$\begin{array}{cccc} & X_1 & X_2 & X_3 \\ X_1' & 0 & 0 & 1 \\ X_2' & 0 & 1 & 0 \\ X_3' & 1 & 0 & 0 \end{array} \tag{1.53}$$

Using (1.52), (1.53), (1.5), (1.6), (1.2), (1.45), (1.7), and (1.3) gives

$$C_{12} = C_{13} = C_{23},\ C_{11} = C_{22} = C_{33},\ C_{44} = C_{55} = C_{66} \tag{1.54}$$

The matrix of stiffness constants (1.45) can now be written as

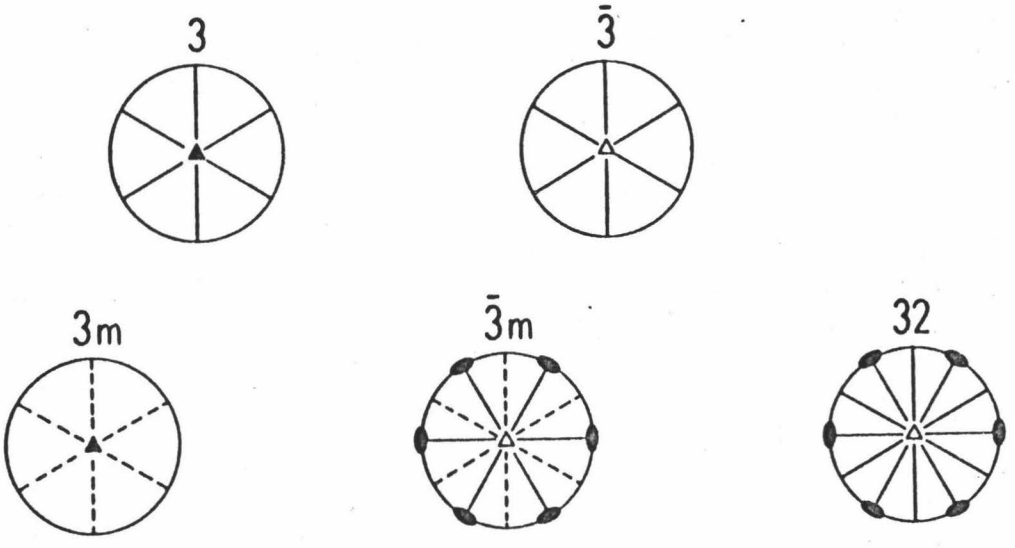
$$\begin{array}{cccccc} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{array} \tag{1.55}$$

The cubic classes 23, m3, 432, $\bar{4}3m$, and m3m, have three stiffness constants:

$$C_{11},\ C_{12},\ C_{44} \tag{1.56}$$

E. HEXAGONAL AND TRIGONAL SYSTEMS. The hexagonal and trigonal systems will be considered together. These systems are characterized by three stiffness constant matrices. The first and second sets of matrix constants are obtained for the trigonal classes (3, $\bar{3}$) and (32, $\bar{3}$m, 3m). The third set represents all classes of the hexagonal system.

The symbols and stereograms for the trigonal system are



Classes 3 and $\bar{3}$ have a triad axis parallel to the X_3 axis. This symmetry operation corresponds to a 120-degree rotation. The direction cosine table for this transformation of coordinates is given by

	X_1	X_2	X_3
X_1'	Cos θ	Sin θ	0
X_2'	-Sin θ	Cos θ	0
X_3'	0	0	1

(1.57)

where $\theta = 120$ degrees.

Relationships (1.57), (1.5), (1.6), and (1.2) give

$$
\begin{aligned}
t_1' &= t_1\mathrm{Cos}^2\theta + t_2\mathrm{Sin}^2\theta + t_6\mathrm{Sin}\ 2\theta \\
t_2' &= t_1\mathrm{Sin}^2\theta + t_2\mathrm{Cos}^2\theta - t_6\mathrm{Sin}\ 2\theta \\
t_3' &= t_3 \\
t_4' &= t_4\mathrm{Cos}\ \theta - t_5\mathrm{Sin}\ \theta \\
t_5' &= t_4\mathrm{Sin}\ \theta + t_5\mathrm{Cos}\ \theta \\
t_6' &= \tfrac{1}{2}(t_2 - t_1)\mathrm{Sin}\ 2\theta + t_6\mathrm{Cos}\ 2\theta
\end{aligned}
\tag{1.58}
$$

$$
\begin{aligned}
e_1' &= e_1\mathrm{Cos}^2\theta + e_2\mathrm{Sin}^2\theta + \tfrac{1}{2}e_6\mathrm{Sin}\ 2\theta \\
e_2' &= e_1\mathrm{Sin}^2\theta + e_2\mathrm{Cos}^2\theta - \tfrac{1}{2}e_6\mathrm{Sin}\ 2\theta \\
e_3' &= e_3 \\
e_4' &= e_4\mathrm{Cos}\ \theta - e_5\mathrm{Sin}\ \theta \\
e_5' &= e_4\mathrm{Sin}\ \theta + e_5\mathrm{Cos}\ \theta \\
e_6' &= (e_2 - e_1)\mathrm{Sin}\ 2\theta + e_6\mathrm{Cos}\ 2\theta
\end{aligned}
\tag{1.59}
$$

The substitution of (1.58) and (1.59) into the first equation of (1.7) results in an equation relating t_1, t_2, and t_6 as a function of the various strains. This represents the stress-strain relationship after transformation of coordinates and has the form

$$t_1\cos^2\theta + t_2\sin^2\theta + t_6\sin 2\theta = [C_{11}\cos^2\theta + C_{12}\sin^2\theta - C_{16}\sin 2\theta]\, e_1$$
$$+ [C_{11}\sin^2\theta + C_{12}\cos^2\theta + C_{16}\sin 2\theta]\, e_2$$
$$+ C_{13}e_3$$
$$+ [C_{14}\cos\theta + C_{15}\sin\theta]\, e_4$$
$$+ [C_{15}\cos\theta - C_{14}\sin\theta]\, e_5$$
$$+ [\tfrac{1}{2}C_{11}\sin 2\theta - \tfrac{1}{2}C_{12}\sin 2\theta + C_{16}\cos 2\theta]\, e_6 \qquad (1.60)$$

From the first equation of (1.3) and using (1.58) and (1.59) yields

$$t_1\cos^2\theta + t_2\sin^2\theta + t_6\sin 2\theta = [C_{11}\cos^2\theta + C_{21}\sin^2\theta + C_{61}\sin 2\theta]\, e_1$$
$$+ [C_{12}\cos^2\theta + C_{22}\sin^2\theta + C_{62}\sin 2\theta]\, e_2$$
$$+ [C_{13}\cos^2\theta + C_{23}\sin^2\theta + C_{63}\sin 2\theta]\, e_3$$
$$+ [C_{14}\cos^2\theta + C_{24}\sin^2\theta + C_{64}\sin 2\theta]\, e_4$$
$$+ [C_{15}\cos^2\theta + C_{25}\sin^2\theta + C_{65}\sin 2\theta]\, e_5$$
$$+ [C_{16}\cos^2\theta + C_{26}\sin^2\theta + C_{66}\sin 2\theta]\, e_6 \qquad (1.61)$$

Since the $[C_{ij}]$ must be invariant with regard to the transformation, then an equality must exist between (1.60) and (1.61). This equality

yields six equations of the type

$$C_{11}\text{Cos}^2\theta + C_{12}\text{Sin}^2\theta - C_{16}\text{Sin } 2\theta = C_{11}\text{Cos}^2\theta + C_{21}\text{Sin}^2\theta + C_{61}\text{Sin } 2\theta \tag{1.62}$$

which implies that

$$C_{12} = C_{21} \quad \text{and} \quad C_{16} = C_{61} = 0 \tag{1.63}$$

A repetition of the previous procedure is applied to the remaining equations of (1.7). An equality is obtained for each of these equations with corresponding equations obtained from (1.3). The final results, of these six equalities of the type (1.60) and (1.61), give 36 soluble equations. Solving various combinations from these 36 equations gives

$$\begin{aligned} C_{16} = C_{26} = C_{34} = C_{35} = C_{36} = C_{43} = C_{45} = C_{53} = C_{54} \\ = C_{61} = C_{62} = C_{63} = 0 \end{aligned} \tag{1.64}$$

and

$$\begin{aligned} &C_{15} = -C_{25},\ C_{21} = C_{12},\ C_{22} = C_{11},\ C_{23} = C_{13}, \\ &C_{24} = -C_{14},\ C_{31} = C_{13},\ C_{32} = C_{13},\ C_{41} = C_{14}, \\ &C_{42} = -C_{14},\ C_{46} = C_{25},\ C_{51} = -C_{25},\ C_{52} = C_{25}, \\ &C_{55} = C_{44},\ C_{56} = C_{14},\ C_{64} = C_{25},\ C_{65} = C_{14}, \\ &C_{66} = \tfrac{1}{2}(C_{11}-C_{12}) \end{aligned} \tag{1.65}$$

Using (1.64) and (1.65), the $[C_{ij}]$ can be written as

$$\begin{matrix} C_{11} & C_{12} & C_{13} & C_{14} & -C_{25} & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & C_{25} & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & C_{25} \\ -C_{25} & C_{25} & 0 & 0 & C_{44} & C_{14} \\ 0 & 0 & 0 & C_{25} & C_{14} & \frac{C_{11}-C_{12}}{2} \end{matrix} \tag{1.66}$$

The trigonal classes 3 and $\bar{3}$ are characterized by seven stiffness constants:

$$C_{11}, C_{12}, C_{13}, C_{14}, C_{25}, C_{33}, C_{44} \tag{1.67}$$

The trigonal classes 3m, $\bar{3}$m, and 32 have the same symmetry operation as the previous classes and in addition, a diad axis normal to the triad axis. If we let the diad be parallel to the X_1 axis, the transformation scheme is the same as that used to obtain (1.44). Equations (1.44), (1.7), and (1.3) give

$$C_{25} = 0 \tag{1.68}$$

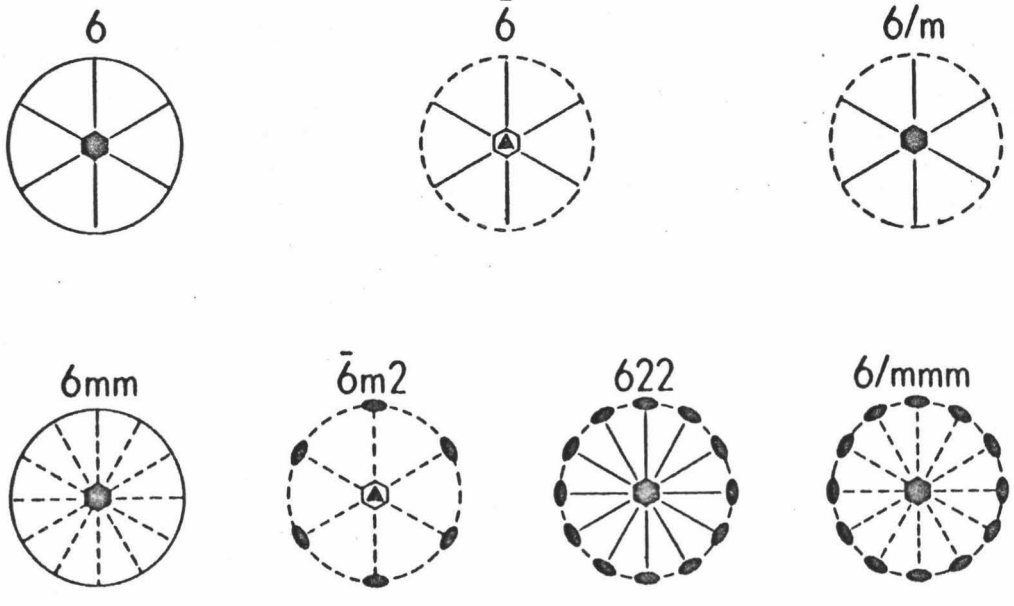
The matrix of (1.66) can be written as

$$\begin{matrix} C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & C_{14} \\ 0 & 0 & 0 & 0 & C_{14} & \frac{C_{11}-C_{12}}{2} \end{matrix} \qquad (1.69)$$

The trigonal classes 3m, $\bar{3}$, and 32 are characterized by six stiffness constants:

$$C_{11}, C_{12}, C_{13}, C_{14}, C_{33}, C_{44} \qquad (1.70)$$

The symbols and stereograms for the hexagonal system are



The stiffness constants for the six hexagonal crystal classes are obtained by simultaneously applying a twofold and threefold rotation axes. Elastically, these two simultaneous operations are equivalent to either a reflection-rotation sixfold axis or a single axis [Federov, (1968)]. Considering the threefold axis first we obtain (1.66). Introducing a diad axis parallel to the X_3 axis yields the direction cosine table

	X_1	X_2	X_3
X_1'	-1	0	0
X_2'	0	-1	0
X_3'	0	0	-1

The direction cosines, (1.5), (1.6), and (1.2) give

$$\begin{aligned} t_1' = t_1,\ t_2' = t_2,\ t_3' = t_3,\ t_4' = -t_4,\ t_5' = -t_5,\ t_6' = t_6 \\ e_1' = e_1,\ e_2' = e_2,\ e_3' = e_3,\ e_4' = -e_4,\ e_5' = -e_5,\ e_6' = e_6 \end{aligned} \tag{1.71}$$

Equations (1.71), (1.7), and (1.3) give

$$C_{14} = C_{25} = 0 \tag{1.72}$$

and the matrix of (1.66) can be written as

$$\begin{matrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} \end{matrix} \tag{1.73}$$

All hexagonal classes are characterized by five stiffness constants:

$$C_{11}, C_{12}, C_{13}, C_{33}, C_{44} \tag{1.74}$$

F. TRICLINIC SYSTEM. The triclinic system has two classes. One class has a full rotation axis and the other has a center of inversion. Neither of these symmetry operations reduce the number of independent stiffness constants from the original 21.

G. RELATIONSHIPS BETWEEN ELASTIC STIFFNESS AND COMPLIANCE CONSTANTS.

In some instances, it may be desired to have the strain as a linear function of the stress and this relationship [Frederick and Chang, 1965] may be expressed as

$$e_i = S_{ij} t_j \qquad (i,j = 1,\ldots,6) \tag{1.75}$$

where e_i is the strain, t_j is the stress, and $[S_{ij}]$ are the elastic compliance constants. From equations (1.3) and (1.75), a relationship between the stiffness and compliance constants is

$$[C]\,[S] = I \tag{1.76}$$

where [C] and [S] are the matrices of stiffness and compliance constants, respectively, and I is the identity matrix. Matrix equation (1.76) can be solved for each system, resulting in a relationship between the $[C_{ij}]$ and $[S_{ij}]$. These equations for the most common classes are given by Nye (1967) as

Cubic System

$$\begin{aligned} C_{11} &= (S_{11}+ S_{12}) \,/\, (S_{11}- S_{12})(S_{11}+ 2\, S_{12}) \\ C_{12} &= -S_{12} \,/\, (S_{11}- S_{12})(S_{11}+ 2\, S_{12}) \\ C_{44} &= 1/S_{44} \end{aligned} \tag{1.77}$$

Hexagonal System

$$\text{let } S = S_{33}(S_{11}+ S_{12}) - 2\, S_{13}^2$$

$$\begin{aligned} C_{11}+ C_{12} &= S_{33}/S \\ C_{11}- C_{12} &= 1/(S_{11}- S_{12}) \\ C_{13} &= -S_{13}/S \\ C_{33} &= (S_{11}+ S_{12})/S \\ C_{44} &= 1/S_{44} \end{aligned} \tag{1.78}$$

Tetragonal System (classes 4mm, $\bar{4}$2m, 422, 4/mmm)

$$\text{let } S = S_{33}(S_{11} + S_{12}) - 2\,S_{13}^2$$

$$\begin{aligned} C_{11} + C_{12} &= S_{33}/S \\ C_{11} - C_{12} &= 1/(S_{11} - S_{12}) \\ C_{13} &= -S_{13}/S \\ C_{33} &= (S_{11} + S_{12})/S \\ C_{44} &= 1/S_{44} \\ C_{66} &= 1/S_{66} \end{aligned} \tag{1.79}$$

Trigonal System (classes 3m, 32, $\bar{3}$m)

$$\text{let } S = S_{33}(S_{11} + S_{12}) - 2\,S_{13}^2$$

$$S' = S_{44}(S_{11} - S_{12}) - 2\,S_{14}^2$$

$$\begin{aligned} C_{11} + C_{12} &= S_{33}/S \\ C_{11} - C_{12} &= S_{44}/S' \\ C_{13} &= -S_{13}/S \\ C_{14} &= -S_{14}/S' \\ C_{33} &= (S_{11} + S_{12})/S \\ C_{44} &= (S_{11} - S_{12})/S' \end{aligned} \tag{1.80}$$

BASIC EXPERIMENTAL DATA

The "pulse superposition" ultrasonic interferometry method is used to obtain the basic experimental data for isotropic and non-isotropic materials subjected to a pressure-temperature environment. This method has been described in detail by McSkimin (1950, 1961) and Schrieber and Anderson (1966). A block diagram of the electronic equipment is shown in Figure 1. The carrier wave oscillator is designated as CW and the pulse repetition frequency as prf .

A quartz transducer to generate elastic wave pulses is attached to one of the two parallel faces of the specimen. The frequency of the CW pulse is equalized to the natural frequency of the transducer. A radio frequency pulse (rf) from the tone burst generator is applied to the transducer. The waves travel through the specimen and are reflected and received by the transducer. When the interval (i.e., the period) between the applied rf pulses is equal to an integral multiple (p) of the round-trip transit time of the wave pulses in the specimen, the echoes are superimposed. By properly gating the incident pulses, the echo pulses travel through transformers and amplifiers and are then displayed on an oscilloscope. The prf of the applied pulse is measured with a frequency counter, and the elastic wave velocity in the specimen is calculated from the basic experimental prf data and the specimen length. The basic data is obtained at equal intervals of increasing or decreasing pressure and temperature. Fifteen to thirty minutes are allowed at each

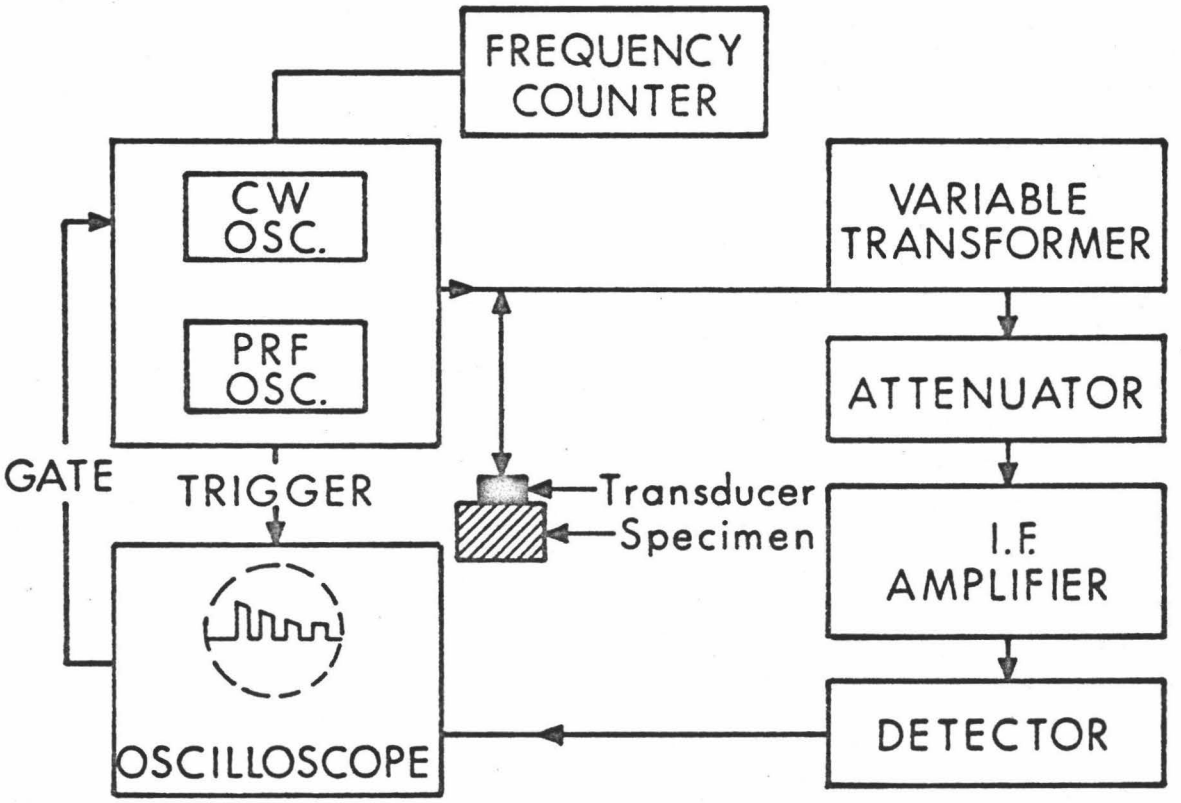


FIGURE 1. ELECTRONIC EQUIPMENT

interval for the specimen to reach equilibrium with the environment. Twenty to forty MHz x-cut and y-cut quartz transducers are commonly used for measuring the longitudinal- and shear-wave velocities in the specimens. The transducers are bonded to the specimen by a thin film of Dow Corning resin 276-V9. The effect of the phase shift due to reflection at the specimen-seal interface is less than 1° for a properly prepared seal [McSkimin and Andreatch (1962), Schrieber and Anderson (1966)] and is therefore negligible.

A block diagram of the pressure system is shown in Figure 2. The main components are a two-stage nitrogen gas pumping system, a pressure vessel, a Harwood manganin pressure cell [Johnson and Newhall (1953), Johnson et al. (1957), Newhall (1962)] and a Carey-Foster resistance bridge. The latter is used for measuring and monitoring the pressure in the vessel containing the specimen. The temperature of the specimen can be maintained at 25±0.1°C by a constant-temperature water jacket around the vessel and monitored with a chromel-alumel thermo-couple and a potentiometer.

Figure 3 shows a block diagram of the temperature system. This equipment is designed for elevated temperatures and 1 bar pressure. The main components are the furnace, the heating unit, and a potentiometer. The latter is used to measure and monitor the temperature within an accuracy of ±0.1°C. The upper limit of the temperature is approximately 500°C.

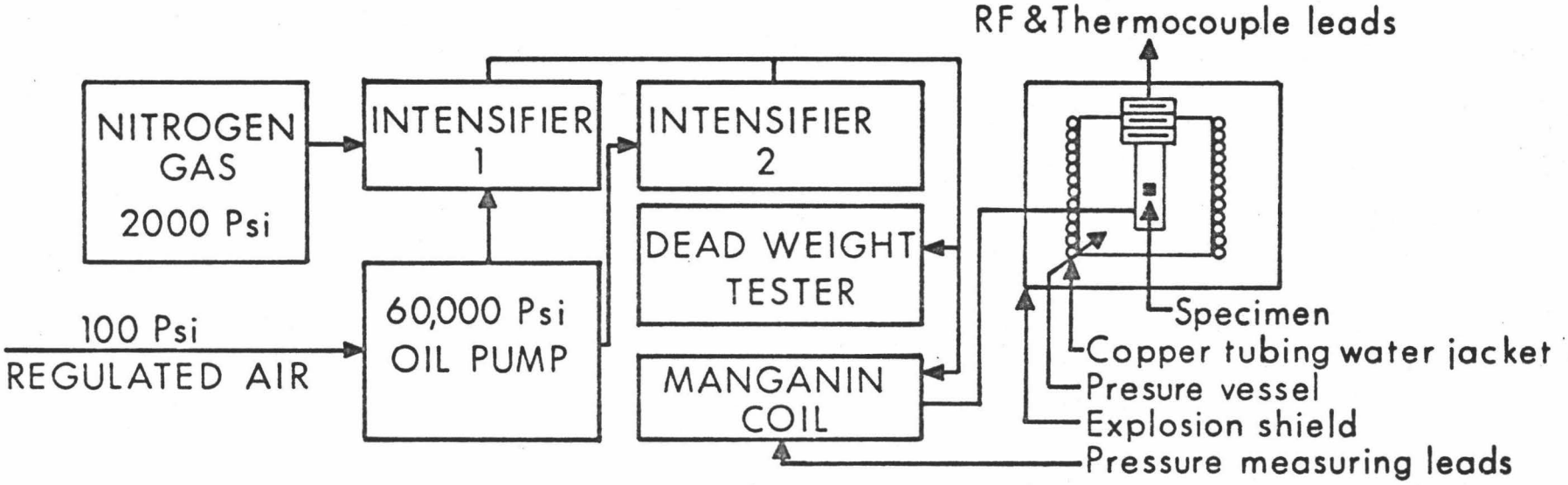


FIGURE 2. PRESSURE SYSTEM

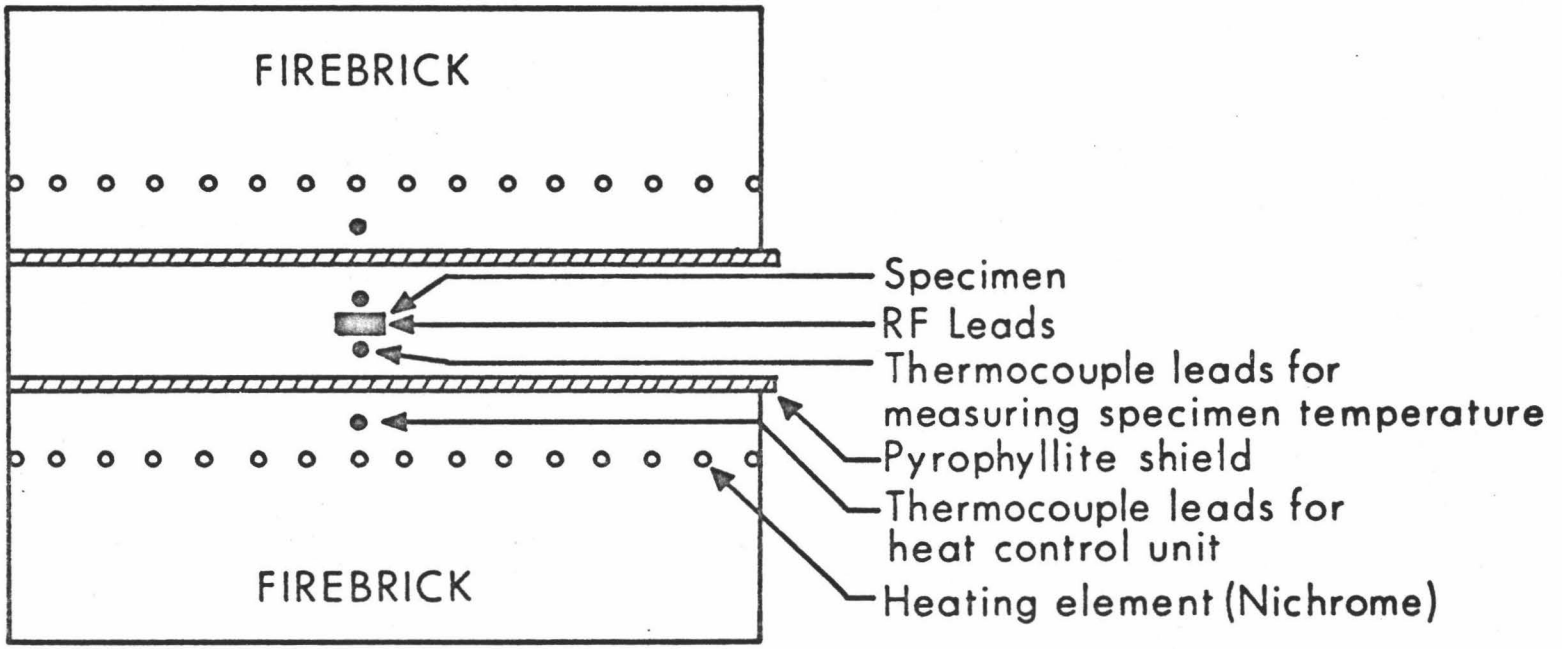


FIGURE 3. TEMPERATURE SYSTEM

Each specimen is prepared for wave velocity measurements, at 1 bar at 25°C, by grinding and polishing the two parallel faces to within 1 part in 4. The specimen is measured with a micrometer. The longitudinal-wave velocity (V_p) and the shear-wave velocity (V_s) is obtained from the relationship

$$V = 2\ell f \tag{2.1}$$

where V is the velocity in the specimen, ℓ is the specimen length, and f is the pulse repetition frequency (prf) of the applied pulse.

ISOTROPIC ELASTIC PARAMETER MEASUREMENTS AT MODERATE PRESSURES OR TEMPERATURES

The hydrostatic pressure changes the dimension and density of the specimen. The length change is given by Cook (1957) as

$$(\ell_o/\ell) = 1 + \frac{1+\Delta}{\rho_o} \int_o^P \frac{dP}{3A-4B}$$

where $(1+\Delta)$ is the ratio of the adiabatic bulk modulus to the isothermal bulk modulus, ρ_o is the initial density, $A = (V_{p_o} f/f_o)^2$ for longitudinal waves, and $B = (V_{s_o} f/f_o)^2$ for shear waves. The zero subscripts denote initial 1 bar conditions. The quantity Δ is equal to $\alpha\gamma T$, where α is the coefficient of volumetric expansion, γ is the Gruneisen parameter, and T is the temperature (°K). For those materials where $\alpha \leq 10^{-6}/°C$, Δ will be negligible. With an increase in hydrostatic pressure, the density and velocity are assumed

to vary linearly over small intervals. The density can then be written as a ratio

$$(\rho/\rho_o) = (m/v)/(m/v_o) \tag{2.3}$$

where ρ is the density at an increase in pressure, ρ_o is the initial density at 1 bar, m is the mass, v is the volume at an increased pressure, and v_o is the initial volume.

For an isotropic material, the length change is the same in all directions, and (2.3) can be written as

$$\rho = \rho_o(\ell_o/\ell)^3 \tag{2.4}$$

where (ℓ_o/ℓ) is given in equation (2.2).

Similarly, for an increase in pressure the velocity ratio over small intervals can be written as

$$(V/V_o) = (\ell/\ell_o)(f/f_o) \tag{2.5}$$

or rewritten

$$V = V_o(\ell/\ell_o)(f/f_o) \tag{2.6}$$

The density and velocity after an increase in hydrostatic pressure are given by equations (2.4) and (2.6), respectively.

The dimensions and density of a specimen also change when the specimen is subjected to an increase in temperature. The length after an increase in temperature is given by

$$\ell = \ell_o (1.0 + \alpha \Delta t) \tag{2.7}$$

where α is the coefficient of linear thermal expansion per centigrade degree, and Δt is the temperature difference in °C. By substituting (2.7) into (2.4) and (2.6), the density and velocity of the specimen are obtained for the increased temperature.

From the velocity, density, and the isotropic stiffness constants, the bulk-, shear-, and Young's moduli, Poisson's ratio and compressibility are obtained. Formulas relating all of these parameters [Birch (1961)] are given in Table I.

CRYSTALLINE (TETRAGONAL) EIASTIC PARAMETER MEASUREMENTS AT MODERATE PRESSURES OR TEMPERATURES

In contrast to the isotropic case, a crystal is characterized by more stiffness constants and consequently, prf data must be obtained to compute the different stiffness constants. The six constants for the tetragonal case are given by (1.46). Pressure or temperature f_{ij} (experimental prf data) values are needed for each different $[C_{ij}]$. The stiffness constants are related to the velocity of a wave propagated through the crystal in a particular direction. These velocity relationships [Verma (1960), Birch (1960)] for waves propagated with a given particle motion direction, in various directions through the

crystal, are given in Table II. This table also includes the experimental prf data which corresponds to the appropriate stiffness constant in the velocity relation column.

The experimental data (f_{ij}), equation (2.1), and the velocity relationships of Table II, are used to obtain the 1 bar values for C_{11}, C_{33}, C_{44}, C_{66}, C_{PQ}, C_{TU}, and C_{RS}. C_{12} is obtained indirectly from velocity relation involving C_{PQ} or C_{TU} given in Table II. Similarly, C_{13} is obtained from velocity relation involving C_{RS}.

TABLE I. IDENTITIES FOR STIFFNESS CONSTANTS OF ISOTROPIC BODIES

K = bulk modulus	σ = Poisson's ratio
E = Young's modulus	ρ = density
μ = shear modulus	$R_1 = V_p/V_s$
β = compressibility	$R_2^2 = K/(\rho V_s^2)$
λ = Lame's constant	$R_3^2 = K/(\rho V_p^2)$

K	E	λ	σ	ρV_p^2	$\rho V_s^2 = \mu$
$\lambda + 2\mu/3$	$\mu\,\frac{3\lambda + 2\mu}{\lambda + \mu}$		$\frac{\lambda}{2(\lambda + \mu)}$	$\lambda + 2\mu$	
	$9K\,\frac{9K\mu}{3K + \mu}$		$\frac{\lambda}{3K - \lambda}$	$3K - 2\lambda$	$3(K-\lambda)/2$
	$\frac{9K\mu}{3K + \mu}$	$K - 2\mu/3$	$\frac{3K - 2\mu}{2(3K + \mu)}$	$K + 4\mu/3$	
$\frac{E\mu}{3(3\mu - E)}$		$\mu\,\frac{E - 2\mu}{3\mu - E}$	$E/(2\mu) - 1$	$\mu\,\frac{4\mu - E}{3\mu - E}$	
		$3K\,\frac{3K - E}{9K - E}$	$\frac{3K - E}{6K}$	$3K\,\frac{3K + E}{9K - E}$	$\frac{3KE}{9K - E}$
$\lambda\,\frac{1 + \sigma}{3\sigma}$	$\lambda\,\frac{(1+\sigma)(1-2\sigma)}{\sigma}$			$\lambda\,\frac{1 - \sigma}{\sigma}$	$\lambda\,\frac{1 - 2\sigma}{2\sigma}$
$\mu\,\frac{2(1 + \sigma)}{3(1 - 2\sigma)}$	$2\mu(1 + \sigma)$	$\mu\,\frac{2\sigma}{1 - 2\sigma}$		$\mu\,\frac{2 - 2\sigma}{1 - 2\sigma}$	
	$3K(1 - 2\sigma)$	$3K\,\frac{\sigma}{1 + \sigma}$		$3K\,\frac{1 - \sigma}{1 + \sigma}$	$3K\,\frac{1 - 2\sigma}{2 + 2\sigma}$
$\frac{E}{3(1 - 2\sigma)}$		$\frac{E\sigma}{(1+\sigma)(1-2\sigma)}$		$\frac{E(1-\sigma)}{(1+\sigma)(1-2\sigma)}$	$\frac{E}{2 + 2\sigma}$
$\rho(V_p^2 - V_s^2)$	$\frac{9\rho V_s^2 R_2^2}{3R_2^2 + 1}$	$\rho(V_p^2 - 2V_s^2)$	See Below		

$$2\sigma = (R_1^2 - 2)/(R_1^2 - 1) = (3R_2^2 - 2)/(3R_2^2 + 1) = 2(3R_3^2 - 1)/(3R_3^2 + 1)$$

TABLE II. EXPERIMENTAL DATA AND VELOCITY RELATIONSHIPS USED IN THE TETRAGONAL COMPUTER PROGRAMS

Wave Propagation Direction	Particle Motion Direction	Mode	prf	Velocity Relation
[001]	[001]	C	f_{33}	$\rho V^2 = C_{33}$
[100]	[100]	C	f_{11}	$\rho V^2 = C_{11}$
[001]	Any direction in [001]	S	$+f_{44}$	$\rho V^2 = C_{44}$
[100]	[001]	S	$+f_{44A}$	$\rho V^2 = C_{44}$
[110]	[001]	S	$+f_{44A}$	$\rho V^2 = C_{44}$
[100]	[010]	S	f_{66}	$\rho V^2 = C_{66}$
[110]	[110]	S	$*f_{PQ}$	$\rho V^2 = (C_{11} - C_{12})/2 = *C_{PQ}$
[110]	[110]	C	$*f_{TU}$	$\rho V^2 = (C_{11} + C_{12} + 2C_{66})/2 = *C_{TU}$
Inclined at 45° to [100] and [001]	[110]	C	$*f_{RS}$	$*C_{RS} = **$

C Compressional

S Shear

* Defined by author

** $\rho V^2 = \left\{C_{11} + C_{33} + 2C_{44} + [(C_{11} - C_{33})^2 + 4(C_{13} + C_{44})^2]^{\frac{1}{2}}\right\}/4$

\+ Indicates experimental data used to obtain the same elastic constant C_{44}.

A. COMPRESSIBILITY. The adiabatic linear and volumetric compressibilities [Fisher (1964)] were computed using the formulas

$$\begin{aligned} \beta_1 &= S_{11} + S_{12} + S_{13} \\ \beta_2 &= S_{33} + 2S_{13} \\ \beta_v &= 2S_{11} + S_{33} + 2S_{12} + 4S_{13} \end{aligned} \tag{2.8}$$

where β_1 and β_2 are the compressibilities perpendicular and parallel to the c axis and β_v is the volumetric compressibility.

The pressure measurements in the laboratory are made under adiabatic conditions. Therefore, the compressibilities of (2.8) are converted to isothermal compressibilities by the relation [Birch (1952)]

$$\beta_T = \beta_S \ (1 + \alpha\gamma T) \tag{2.9}$$

where α is the volumetric thermal expansion, T is the temperature in °K, γ is the thermal Gruneisen parameter, and β_T and β_S are the isothermal and adiabatic compressibilities, respectively. The Gruneisen parameter γ [Birch (1952)] is given as

$$\gamma = (\alpha K_S)/(\rho C_p)$$

where α is the volumetric thermal expansion, K_S is the adiabatic bulk modulus, ρ is the density, and C_p is the specific heat at constant pressure.

B. ELASTIC STIFFNESS CONSTANTS AT MODERATE PRESSURES. The stiffness constants at higher pressures are calculated over a small pressure increment from a lower pressure $[C_{ij}]$, the ratio of the prf at a higher pressure to the prf at a lower pressure, and the isothermal compressibility. If we assume linearity of the $[C_{ij}]$ values over this small pressure interval, then the ratio of the stiffness constant at a higher pressure to the elastic constant at 1 bar pressure can be written as

$$C_{ij}/(C_{ij})_o = (\rho V^2)/(\rho_o V_o^2) \tag{2.10}$$

where zero subscripts denote 1 bar values, V is the velocity, and ρ is the density. Using (2.1), (2.10) becomes

$$C_{ij}/(C_{ij})_o = (f/f_o)^2 \, (\ell/\ell_o)^2 \, (\rho/\rho_o) \tag{2.11}$$

However, the compressibility parallel to the c axis for a given pressure interval ΔP is

$$\beta_2 = -\frac{1}{c}\left(\frac{c - c_o}{\Delta P}\right)$$

or

$$(c_o/c) = 1 + \beta_2 \Delta P \tag{2.12}$$

Similarly, the compressibility perpendicular to the c axis is

$$(a_o/a) = 1 + \beta_1 \Delta P \tag{2.13}$$

For a wave propagated along the a, b crystallographic axes, the length and density changes of equation (2.11) are

$$(\ell/\ell_o) = (a/a_o)$$

and

$$(\rho/\rho_o) = (c_o/c)(a_o/a) \tag{2.14}$$

Equation (2.11) can then be written as

$$C_{ij} = (C_{ij})_o\ (f/f_o)^2\ (1 + \beta_2 \Delta P) \tag{2.15}$$

This equation gives the stiffness constants at a higher pressure and is used for those stiffness constants related to a wave propagated along the a, b axes. Table II gives these stiffness constants as C_{11}, C_{44A}, C_{66}, C_{PQ}, and C_{TU}. C_{12} is obtained by solving the velocity relation involving C_{PQ} or C_{TU}, for C_{12}.

Similarly, for a wave propagated parallel to the c axis, the length and density changes are

$$(\ell/\ell_o) = (c/c_o)$$

and

$$(\rho/\rho_o) = (c_o/c)(a_o/a)^2 \tag{2.16}$$

Equation (2.11) then has the form

$$C_{ij} = (C_{ij})_o\ (f/f_o)^2\ \ \frac{1 + 2(\beta_1 + \beta_2)\Delta P}{1 + (\beta_1 + \beta_2)\Delta P} \tag{2.18}$$

C. ELASTIC STIFFNESS CONSTANTS AT MODERATE TEMPERATURES. The stiffness constants at higher temperatures are obtained in a similar manner to those $[C_{ij}]$ obtained at higher pressures. The general formula for thermal expansion is given as

$$\ell = \ell_o (1 + \alpha \Delta t) \tag{2.19}$$

where α is the linear thermal expansion, Δt is the temperature difference, ℓ_o is the initial length of the specimen, and ℓ is the length of the expanded specimen.

Thermal expansion parallel and perpendicular to the c axis can be written as, respectively,

$$(c/c_o) = 1 + \alpha_2 \Delta t \tag{2.20}$$

and

$$(a/a_o) = 1 + \alpha_1 \Delta t \tag{2.21}$$

Equation (2.11) can then be written as

$$C_{ij} = (C_{ij})_o (f/f_o)^2 [1/(1 + \alpha_2 \Delta t)] \tag{2.22}$$

This equation is used to obtain stiffness constants C_{11}, C_{44A}, C_{66}, C_{PQ}, and C_{TU} at higher temperatures. C_{12} is obtained from the relationships involving C_{PQ} or C_{TU}.

Similarly, for C_{33} and C_{44} we have

$$C_{ij} = (C_{ij})_o (f/f_o)^2 (1 + \alpha_2 \Delta t)/(1 + \alpha_1 \Delta t)^2 \tag{2.23}$$

and for C_{13}

$$C_{ij} = (C_{ij})_o \, (f/f_o)^2 \, [(1 + \alpha_2 \Delta t) + (1 + \alpha_1 \Delta t)]^2 / [4(1 + \alpha_2 \Delta t)(1 + \alpha_1 \Delta t)^2] \tag{2.24}$$

D. COMPLIANCE CONSTANTS AND VELOCITIES FROM STIFFNESS CONSTANTS.

Having obtained the $[C_{ij}]$ at 1 bar and higher pressures, the velocities at the various pressures are then computed using the relation

$$V = (C_{ij}/\rho)^{\frac{1}{2}} \tag{2.25}$$

and the compliance constants at the various pressures are obtained from the relationships given in (1.79).

The velocities for an isotropic specimen are obtained from the general isotropic formuli

$$V_p^2 = \frac{K + \frac{4}{3}\mu}{\rho} \tag{2.26}$$

and

$$V_s^2 = \mu/\rho \tag{2.27}$$

E. DEBYE TEMPERATURE. The Debye temperature calculation is also included in the computer programs for the tetragonal system.

The Debye temperature was computed from the formula [Anderson (1963), Anderson et al. (1968)]

$$\theta = 251.45\ (\rho/\bar{M})^{\frac{1}{3}}\ V_m \tag{2.28}$$

where ρ is the density, $\bar{M}$ is the mean atomic weight, and V_m is the mean velocity given by

$$\frac{3}{V_m^3} = \frac{2}{V_s^3} + \frac{1}{V_p^3} \tag{2.29}$$

where V_p and V_s are the longitudinal and shear velocities.

F. ISOTROPIC POLYCRYSTALLINE SPECIMENS AND ANISOTROPY. For a single crystal, the stiffness constants and other related parameters are functions of crystal orientation. However, the isotropic stiffness constants of a polycrystalline specimen can be obtained from the single crystal stiffness constants of the specimen. For a random orientation of grains in the polycrystalline specimen, the parameters are macroscopically isotropic. Therefore, the stiffness constants (or compliance constants) of a single crystal specimen are used to determine isotropic bulk-(K) and shear-(U) moduli and these relationships [Meister and Peselnick (1966)] are given as

$$K_v = [2(C_{11} + C_{12}) + C_{33} + 4C_{13}]/9 \tag{2.30}$$

$$U_v = [2(C_{11} - C_{13} + 3C_{44}) + C_{33} - C_{12} + 3C_{66}]/15 \tag{2.31}$$

$$K_r = 1/(2S_{11} + S_{33} + 2S_{12} + 4S_{13}) \tag{2.32}$$

$$U_r = 15/(8S_{11} + 4S_{33} - 4S_{12} - 8S_{13} + 6S_{44} + 3S_{66}) \tag{2.33}$$

$$K_h = (K_v + K_r)/2 \tag{2.34}$$

$$U_h = (U_v + U_r)/2 \tag{2.35}$$

where K_v and U_v are the bulk and shear moduli calculated by Voigt (1928), K_r and U_r are the moduli calculated by Reuss (1929), and K_h and U_h are the moduli calculated by Hill (1952). The Hill modulus is the arithmetic average of the Voigt and Reuss moduli.

The anisotropy (A) is computed using the formula [Anderson (1963)]

$$A = \frac{2(U_v - U_h)}{(U_v + U_h)} \tag{2.36}$$

where U_v and U_h are the averaging schemes given in equations (2.31) and (2.35).

COMPUTER PROGRAMS

The purpose of including these programs is to eliminate a major portion of the programming necessary in computing elastic parameters of a material from the basic experimental data. From the crystalline systems, only the tetragonal system (422, 4mm, $\bar{4}$2m, 4/mmm) has been considered in detail. However, the bulk of this program can be used to obtain computer programs for the other crystalline systems.

The IBM 360/65 computer was used in performing the elastic moduli and related parameter computations. All programs are written in Fortran IV and are listed in the appendices along with sample input and output data. Appropriate comment and control cards are included with each main program. Appendix I and Appendix II each contain two programs and explanations for using them. The former includes those programs that are applicable to the isotropic system and the latter includes programs for computations within the tetragonal system. The first program in each appendix is for those elastic parameter computations concerning a specimen that is subjected to an increase in pressure. The second program performs those computations for a specimen that is in an increased temperature environment.

The programs were tested using current experimental data [Sokolowski and Manghnani (1969), Manghnani (1969), Fisher et al. (in press)].

CONCLUSIONS

This work has related the laboratory data, obtained at and above standard atmospheric conditions, to the elastic parameters of crystalline and non-crystalline materials. This was accomplished by deriving the set of elastic stiffness constants which characterizes each of the seven crystalline systems and the non-crystalline system and by consolidating from current literature various formulas which relate the stiffness constants to other elastic parameters. Using these formulas on a digital computer, computations which include most of those elastic parameters that are in the current literature are easily performed.

This work can be considered in its entirety for those who wish to begin general studies into pressure-temperature dependence of materials, or various sections of this work can be extracted for particular problems. The computer programs, for example, can be used as given or slightly modified to perform the computations required.

APPENDIX I

ISOTROPIC SYSTEM

A. INPUT-OUTPUT DATA. Two computer programs are included for the isotropic system. These programs are for computations of elastic and other associated parameters of a material subjected to increased temperature or pressure. The complete programs, with input data, and output results are listed. The deck sequence for the pressure or temperature computations is as follows:

1. Control cards
2. Main program
3. Control cards to input data
4. Parameter description cards
5. Specimen description card
6. Initial measurement card
7. Experimental pressure-prf data
8. Least squares indicator card
9. Data termination card
10. Control card

All control cards are those compatible with the IBM 360/65 computer. All input data must agree with the input format statements in the main program.

The parameter description cards are the first fifteen data cards and must be placed in the same order as those that are listed following the main program. Each parameter and its abbreviated form is punched on one card.

Example:

Longitudinal Frequency P Freq.

The specimen description card follows the last parameter description card and contains the necessary information to identify the specimen.

Example:

Pressure calculations for glass #111

The next card in the sequence of data cards is the initial measurements card. These measurements are made on the specimen at 1 bar pressure and room temperature. For the isotropic-pressure program, this card contains five variables.

Example:

Density (gm/cc)	P Velocity (km/sec)	S Velocity (km/sec)	P frequency (kc/s)	S frequency (kc/s)
2.9595	6.934	3.784	326.957	178.422

The initial P and S velocities are obtained from equation (2.1). The initial measurements card for the isotropic-temperature program must contain the linear coefficient of thermal expansion per degree centigrade in addition to the five aforementioned variables.

These programs will accommodate fifty pieces of experimental data. For the isotropic-pressure program, each card in this set of data contains pressure and the corresponding longitudinal and shear prf.

Example:

Pressure (k psi)	P frequency (kc/s)	S frequency (kc/s)
8.000	327.248	178.473

Similarly, each data card for the temperature program contains temperature and the corresponding longitudinal and shear prf. The number of pieces of prf data need not be counted, as this is done automatically within the program. However, to accomplish this automatic data-counting routine, a blank card must be placed at the end of the prf data.

The least squares indicator card follows the blank card. The least squares computations are between pressure (or temperature) and any of the fifteen parameters of the parameter description cards. A number 1 in any of the first fifteen columns of the least squares card indicates which parameter values will be used in the computation. The number sequence on the least squares card corresponds to the card sequence in the parameter description card set. A blank instead of a number will result in no least squares computation performed for a particular parameter.

The last card in the data set is the program termination card which contains only the number 1 punched in column 80.

Data sets for various specimens may be included for computation by repeating, for each specimen, deck sequence steps 5, 6, 7, and 8. Each set of these four sequence steps must follow the least squares indicator card of the previous specimen set.

The output is the elastic parameters as a function of pressure or temperature with the following units:

Density	g/cc
Longitudinal velocity	km/sec
Shear velocity	km/sec
Longitudinal prf	kc/sec
Shear prf	kc/sec
Volumetric thermal expansivity	$(°C)^{-1}$
Pressure	k psi
Temperature	°C
Bulk modulus	k bars
Shear modulus	k bars
Young's modulus	k bars
Compressibility	$(M\ bars)^{-1}$
Lame's constant	k bars

B. LISTING OF PRESSURE PROGRAM, INPUT AND OUTPUT DATA.

```
//ISOP  JOB (1242,1M,10F,190KB),'MILLER'
// EXEC  FORTCLG,RG=190K
//SYSIN  DD  *
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION P(50),PF(50),SF(50),PFR(50),SFR(50),XLR(50),DR(50),D(50)
     1,PV(50),SV(50),BMOD(50),SMOD(50),EMOD(50),SIG(50),COMP(50),M(15),X
     1(50),Y(50),DESC(20,20),YAX(20,20),AL(50)
      JJ = 1
C
C     INPUT PARAMETER AND SPECIMEN DESCRIPTION CARDS
C
    1 READ 2, (DESC(JJ,J1),J1=1,13),(YAX(JJ,J2),J2=1,3),IM
    2 FORMAT(13A4,3A4,15X,I11)
      IF(IM) 3,3,45
    3 JJ = JJ+1
      IF(JJ-16) 1,1,4
C
C     INPUT INITIAL MEASUREMENT CARD
C
    4 READ 5, RHO,PVI,SVI,PFI,SFI
    5 FORMAT(5F10.4)
      PRINT 6, (DESC(16,J3),J3=1,13),RHO,PVI,SVI,PFI,SFI
    6 FORMAT(1H1,13A4//1X,'RHO = DENSITY'/1X,'PV = LONGITUDINAL VELOCITY
     1'/1X,'SV = SHEAR VELOCITY'/1X,'P FREQ = LONGITUDINAL FREQUENCY'/1X
     1,'S FREQ = SHEAR FREQUENCY'/1X,'PRESS = PRESSURE'/1X,'PF RATIO = L
     1ONGITUDINAL FREQUENCY RATIO'/1X,'SF RATIO = SHEAR FREQUENCY RATIO'
     1/1X,'L RATIO = LENGTH RATIO'/1X,'BMOD = BULK MODULUS'/1X,'SMOD = S
     1HEAR MODULUS'/1X,'EMOD = YOUNGS MODULUS'/1X,'SIG = POISSONS RATIO'
     1/1X,'COMP = COMPRESSIBILITY'/1X,'L = LAME CONSTANT'///7X,'RHO',8X,
     1'PV',8X,'SV',5X,'P FREQ',4X,'S FREQ'/2X,5F10.4//4X,'PRESS',2X,'P F
     1REQ',3X,'S FREQ',4X,'PF RATIO',2X,'SF RATIO',3X,'L RATIO',4X,'DENS
     1ITY',5X,'PV',6X,'SV',4X,'BMOD', 3X,'SMOD',3X,'EMOD',4X,'SIG',4X,'C
     1OMP/MB',3X,'L')
      N = 1
C
C     INPUT EXPERIMENTAL PRESSURE-FREQUENCY DATA AND DETERMINE THE
C     NUMBER OF PIECES OF DATA
C
    7 READ 8, P(N),PF(N),SF(N)
    8 FORMAT(3F10.3)
      IF(PF(N)) 12,9,10
    9 IF(SF(N)) 12,14,7
   10 IF(SF(N)) 12,7,11
   11 N = N+1
      GO TO 7
   12 PRINT 13
   13 FORMAT('NEGATIVE FREQ IN DATA')
      GO TO 45
   14 N = N-1
C
C     COMPUTE SPECIMEN LENGTH AND CORRESPONDING VELOCITIES AT
C     VARIOUS PRESSURES
C
      DO 15 I = 1,N
      PFR(I) = PF(I)/PFI
      SFR(I) = SF(I)/SFI
```

```
      A = (PVI*PFR(I)*10.0**5)**2
      B = (SVI*SFR(I)*10.0**5)**2
      PX = (P(I)/1.4504*10.0**8)/(3.0*A-4.0*B)
      TT=1.0 + PX/RHO
      XLR(I)=1.0/TT
      DR(I)=TT**3
      D(I) = RHO*DR(I)
      PV(I) = PVI*PFR(I)*XLR(I)
      SV(I) = SVI*SFR(I)*XLR(I)
C
C     COMPUTE ELASTIC MODULI
C
      BMOD(I) = 10.0*D(I)*(PV(I)**2-4.0*SV(I)**2/3.0)
      SMOD(I) = 10.0*D(I)*SV(I)**2
      EMOD(I) = 9.0*BMOD(I)*SMOD(I)/(3.0*BMOD(I)+SMOD(I))
      SIG(I) = EMOD(I)/(2.0*SMOD(I))-1.0
      COMP(I) = (1.0/BMOD(I))*1000.0
      AL(I) = BMOD(I)-2.0*SMOD(I)/EMOD(I)
   15 PRINT 16, P(I),PF(I),SF(I),PFR(I),SFR(I),XLR(I),D(I),PV(I),SV(I)
     1,BMOD(I),SMOD(I),EMOD(I),SIG(I),COMP(I),AL(I)
   16 FORMAT(3F9.3,F11.6,F10.6,2F11.7,2F8.4,3F7.1,F8.4,F8.3,F7.1)
C
C     COMPUTE LEAST SQUARES FIT BETWEEN PRESSURE AND THE VARIOUS
C     PARAMETERS
C
      READ 17, (M(K),K = 1,15)
   17 FORMAT(15I1)
      LL = 6
      L = 59/(N+11)-1
      DO 44 K = 1,15
      IF(L-LL) 18,20,20
   18 PRINT 19
   19 FORMAT(1H1)
      LL = 0
   20 IF(M(K)) 21,44,21
   21 LL = LL+1
      DO 37 II = 1,N
      GO TO (22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37),K
   22 Y(II) =   PF(II)
      GO TO 37
   23 Y(II) =   SF(II)
      GO TO 37
   24 Y(II) =  PFR(II)
      GO TO 37
   25 Y(II) =  SFR(II)
      GO TO 37
   26 Y(II) =  XLR(II)
      GO TO 37
   27 Y(II) =    D(II)
      GO TO 37
   28 Y(II) =   DR(II)
      GO TO 37
   29 Y(II) =   PV(II)
      GO TO 37
   30 Y(II) =   SV(II)
      GO TO 37
```

```
   31 Y(II) = BMOD(II)
      GO TO 37
   32 Y(II) = SMOD(II)
      GO TO 37
   33 Y(II) = EMOD(II)
      GO TO 37
   34 Y(II) =  SIG(II)
      GO TO 37
   35 Y(II) = COMP(II)
      GO TO 37
   36 Y(II) = AL(II)
   37 CONTINUE
      PRINT 38,(DESC(16,J1),J1=1,13),(DESC(K,J2),J2=1,13)
   38 FORMAT(30X,13A4/30X,'LEAST SQUARES     PRESS VS ',13A4//)
      PRINT 39, (YAX(K,J1),J1=1,3)
   39 FORMAT(33X,'PRESS',16X,3A4,11X,'Y/Y0')
      SUMX  = 0.0
      SUMY  = 0.0
      SUMX2 = 0.0
      SUMXY = 0.0
      SUMY2 = 0.0
      C = N
      DO 40 J = 1,N
      X(J) = P(J)
      SUMX = SUMX+X(J)
      SUMY = SUMY+Y(J)
      SUMX2 = SUMX2 +X(J)**2
      SUMY2 = SUMY2 +Y(J)**2
   40 SUMXY = SUMXY+X(J)*Y(J)
C
C     COMPUTE SLOPE,INTERCEPT,CORRELATION COEFFICIENT,VARIANCE AND
C     STANDARD DEVIATION
C
      S = (SUMX*SUMY-C*SUMXY)/(SUMX**2-C*SUMX2)
      B = (SUMX2*SUMY-SUMX*SUMXY)/(C*SUMX2-SUMX**2)
      R = (C*SUMXY-SUMX*SUMY)/DSQRT((C*SUMX2-SUMX**2)*(C*SUMY2-SUMY**2))
      SXY = SUMXY-SUMX*SUMY/C
      SXX = SUMX2-SUMX*SUMX/C
      SYY = SUMY2-SUMY*SUMY/C
      VARS = (SYY-SXY**2/SXX)/(SXX*(C-2.0))
      DEVS =DSQRT(VARS)
      SPKB=S*14.504
      DO 41 J = 1,N
      YR = Y(J)/Y(1)
   41 PRINT 42, X(J),Y(J),YR
   42 FORMAT(19X,3(8X,F14.7))
      PRINT 43, S,VARS,DEVS,B,R,SPKB
   43 FORMAT(12HOSLOPE      =,F11.4/' VARIANCE  =',E13.2/' STD DEV   =',
     1F12.5/' INTERCEPT =',F11.4/' CORR. COEFF. = ',E12.5/' SLOPE PER KB
     1 =',F8.4//)
   44 CONTINUE
      JJ = 16
      GO TO 1
   45 STOP
      END
*
```

```
//GO.SYSIN DD *
 LONGITUDINAL FREQUENCY                                    P FREQ
 SHEAR FREQUENCY                                           S FREQ
 LONGITUDINAL FREQUENCY RATIO                              PF RATIO
 SHEAR FREQUENCY RATIO                                     SF RATIO
 LENGTH RATIO                                              L RATIO
 DENSITY                                                   DENSITY
 DENSITY RATIO                                             D RATIO
 LONGITUDINAL VELOCITY                                     P VEL
 SHEAR VELOCITY                                            S VEL
 BULK MODULUS                                              BMOD
 SHEAR MODULUS                                             SMOD
 YOUNGS MODULUS                                            EMOD
 POISSONS RATIO                                            SIG
 COMPRESSIBILITY PER MEGABAR                               COMP/MB
 LAME'S CONSTANT                                           L
PRESSURE CALCULATIONS FOR GLASS #111
2.9595    6.9340    3.7840    326.9570  178.4220
    00.015   326.957   178.422
     4.000   327.102   178.451
     8.000   327.248   178.473
    12.000   327.366   178.494
    16.000   327.529   178.518
    20.000   327.657   178.533
    24.000   327.812   178.554
    28.000   327.947   178.575
    32.000   328.086   178.594
    36.000   328.227   178.615
    40.000   328.363   178.632
    44.000   328.508   178.651
    48.000   328.630   178.670
    52.000   328.793   178.693

11   1 11111111

ISOP
```

PRESSURE CALCULATIONS FOR GLASS #111

RHO = DENSITY
PV = LONGITUDINAL VELOCITY
SV = SHEAR VELOCITY
P FREQ = LONGITUDINAL FREQUENCY
S FREQ = SHEAR FREQUENCY
PRESS = PRESSURE
PF RATIO = LONGITUDINAL FREQUENCY RATIO
SF RATIO = SHEAR FREQUENCY RATIO
L RATIO = LENGTH RATIO
BMOD = BULK MODULUS
SMOD = SHEAR MODULUS
EMOD = YOUNGS MODULUS
SIG = POISSONS RATIO
COMP = COMPRESSIBILITY
L = LAME CONSTANT

RHO	PV	SV	P FREQ	S FREQ
2.9595	6.9340	3.7840	326.9570	178.4220

PRESS	P FREQ	S FREQ	PF RATIO	SF RATIO	L RATIO	DENSITY	PV	SV	BMOD	SMOD	EMOD	SIG	COMP/48	L
0.015	326.957	178.422	1.000000	1.000000	0.9999996	2.9595036	6.9340	3.7840	857.9	423.8	1091.6	0.2879	1.166	857.1
4.000	327.102	178.451	1.000443	1.000163	0.9998930	2.9604503	6.9363	3.7842	859.1	423.9	1092.2	0.2881	1.164	858.3
8.000	327.248	178.473	1.000890	1.000286	0.9997863	2.9613982	6.9387	3.7843	860.3	424.1	1092.7	0.2883	1.162	859.5
12.000	327.366	178.494	1.001251	1.000404	0.9996798	2.9623447	6.9405	3.7843	861.3	424.2	1093.2	0.2885	1.161	860.5
16.000	327.529	178.518	1.001749	1.000538	0.9995737	2.9632877	6.9432	3.7844	862.7	424.4	1093.8	0.2887	1.159	861.9
20.000	327.657	178.533	1.002141	1.000622	0.9994679	2.9642296	6.9451	3.7843	863.8	424.5	1094.3	0.2889	1.158	863.0
24.000	327.812	178.554	1.002615	1.000740	0.9993624	2.9651681	6.9477	3.7844	865.1	424.7	1094.8	0.2891	1.156	864.3
28.000	327.947	178.575	1.003028	1.000858	0.9992571	2.9661054	6.9498	3.7844	866.2	424.8	1095.4	0.2892	1.154	865.5
32.000	328.086	178.594	1.003453	1.000964	0.9991522	2.9670403	6.9520	3.7844	867.4	424.9	1095.9	0.2894	1.153	866.6
36.000	328.227	178.615	1.003884	1.001082	0.9990475	2.9679730	6.9543	3.7845	868.6	425.1	1096.4	0.2896	1.151	867.8
40.000	328.363	178.632	1.004300	1.001177	0.9989431	2.9689038	6.9565	3.7844	869.8	425.2	1096.9	0.2898	1.150	869.0
44.000	328.508	178.651	1.004744	1.001283	0.9988390	2.9698316	6.9588	3.7845	871.0	425.3	1097.4	0.2900	1.148	870.2
48.000	328.630	178.670	1.005117	1.001390	0.9987350	2.9707597	6.9607	3.7845	872.1	425.5	1097.9	0.2902	1.147	871.3
52.000	328.793	178.693	1.005615	1.001519	0.9986317	2.9716814	6.9634	3.7846	873.4	425.6	1098.5	0.2904	1.145	872.7

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS LONGITUDINAL FREQUENCY

PRESS	P FREQ	Y/YO
0.0150000	326.9570000	1.0000000
4.0000000	327.1020000	1.0004435
8.0000000	327.2480000	1.0008900
12.0000000	327.3660000	1.0012509
16.0000000	327.5290000	1.0017495
20.0000000	327.6570000	1.0021410
24.0000000	327.8120000	1.0026150
28.0000000	327.9470000	1.0030279
32.0000000	328.0860000	1.0034531
36.0000000	328.2270000	1.0038843
40.0000000	328.3630000	1.0043003
44.0000000	328.5080000	1.0047437
48.0000000	328.6300000	1.0051169
52.0000000	328.7930000	1.0056154

SLOPE = 0.0351
VARIANCE = 0.18D-07
STD DEV = 0.00013
INTERCEPT = 326.9601
CORR. COEFF. = 0.99991D 00
SLOPE PER KB = 0.5093

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS SHEAR FREQUENCY

PRESS	S FREQ	Y/YO
0.0150000	178.4220000	1.0000000
4.0000000	178.4510000	1.0001625
8.0000000	178.4730000	1.0002858
12.0000000	178.4940000	1.0004035
16.0000000	178.5180000	1.0005381
20.0000000	178.5330000	1.0006221
24.0000000	178.5540000	1.0007398
28.0000000	178.5750000	1.0008575
32.0000000	178.5940000	1.0009640
36.0000000	178.6150000	1.0010817
40.0000000	178.6320000	1.0011770
44.0000000	178.6510000	1.0012835
48.0000000	178.6700000	1.0013900
52.0000000	178.6930000	1.0015189

SLOPE = 0.0050
VARIANCE = 0.38D-08
STD DEV = 0.00006
INTERCEPT = 178.4312
CORR. COEFF. = 0.99912D 00
SLOPE PER KB = 0.0732

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS. VS DENSITY

PRESS	DENSITY	Y/Y0
0.0150000	2.9595036	1.0000000
4.0000000	2.9604503	1.0003199
8.0000000	2.9613982	1.0006402
12.0000000	2.9623447	1.0009600
16.0000000	2.9632877	1.0012786
20.0000000	2.9642296	1.0015969
24.0000000	2.9651681	1.0019140
28.0000000	2.9661054	1.0022307
32.0000000	2.9670403	1.0025466
36.0000000	2.9679730	1.0028618
40.0000000	2.9689038	1.0031763
44.0000000	2.9698316	1.0034898
48.0000000	2.9707597	1.0038034
52.0000000	2.9716814	1.0041148

SLOPE = 0.0002
VARIANCE = 0.80D-13
STD DEV = 0.00000
INTERCEPT = 2.9595
CORR. COEFF. = 0.99999D 00
SLOPE PER KB = 0.0034

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS LONGITUDINAL VELOCITY

PRESS	P VEL	Y/Y0
0.0150000	6.9339972	1.0000000
4.0000000	6.9363328	1.0003368
8.0000000	6.9386883	1.0006765
12.0000000	6.9404509	1.0009307
16.0000000	6.9431700	1.0013229
20.0000000	6.9451477	1.0016081
24.0000000	6.9477000	1.0019762
28.0000000	6.9498289	1.0022832
32.0000000	6.9520442	1.0026027
36.0000000	6.9543034	1.0029285
40.0000000	6.9564578	1.0032392
44.0000000	6.9588048	1.0035777
48.0000000	6.9606641	1.0038458
52.0000000	6.9633965	1.0042399

SLOPE = 0.0006
VARIANCE = 0.81D-11
STD DEV = 0.00000
INTERCEPT = 6.9340
CORR. COEFF. = 0.99985D 00
SLOPE PER KB = 0.0081

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS SHEAR VELOCITY

PRESS	S VEL	Y/Y0
0.0150000	3.7839985	1.0000000
4.0000000	3.7842101	1.0000559
8.0000000	3.7842727	1.0000725
12.0000000	3.7843149	1.0000836
16.0000000	3.7844222	1.0001120
20.0000000	3.7843393	1.0000901
24.0000000	3.7843851	1.0001022
28.0000000	3.7844314	1.0001144
32.0000000	3.7844365	1.0001157
36.0000000	3.7844850	1.0001286
40.0000000	3.7844496	1.0001192
44.0000000	3.7844580	1.0001214
48.0000000	3.7844662	1.0001236
52.0000000	3.7845621	1.0001489

SLOPE = 0.0000
VARIANCE = 0.15D-11
STD DEV = 0.00000
INTERCEPT = 3.7842
CORR. COEFF. = 0.869090 00
SLOPE PER KB = 0.0001

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS BULK MODULUS

PRESS	BMOD	Y/Y0
0.0150000	857.9243148	1.0000000
4.0000000	859.0945923	1.0013641
8.0000000	860.3188040	1.0027910
12.0000000	861.3058710	1.0039416
16.0000000	862.6666268	1.0055277
20.0000000	863.7797944	1.0068252
24.0000000	865.0909783	1.0083535
28.0000000	866.2281711	1.0096790
32.0000000	867.4134492	1.0110606
36.0000000	868.6040240	1.0124483
40.0000000	869.7767683	1.0138153
44.0000000	871.0160194	1.0152597
48.0000000	872.0545909	1.0164703
52.0000000	873.4270247	1.0180700

SLOPE = 0.2975
VARIANCE = 0.12D-05
STD DEV = 0.00111
INTERCEPT = 857.8862
CORR. COEFF. = 0.999920 00
SLOPE PER KB = 4.3149

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS SHEAR MODULUS

PRESS	SMOD	Y/Y0
0.0150000	423.7607946	1.0000000
4.0000000	423.9437530	1.0004317
8.0000000	424.0935461	1.0007852
12.0000000	424.2385393	1.0011274
16.0000000	424.3976571	1.0015029
20.0000000	424.5139455	1.0017773
24.0000000	424.6586262	1.0021187
28.0000000	424.8032768	1.0024601
32.0000000	424.9383148	1.0027787
36.0000000	425.0827860	1.0031197
40.0000000	425.2081433	1.0034155
44.0000000	425.3429004	1.0037335
48.0000000	425.4776933	1.0040516
52.0000000	425.6312505	1.0044139

SLOPE = 0.0352
VARIANCE = 0.90D-07
STD DEV = 0.00030
INTERCEPT = 423.8055
CORR. COEFF. = 0.99957D 00
SLOPE PER KB = 0.5106

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS YOUNGS MODULUS

PRESS	EMOD	Y/Y0
0.0150000	1091.5614265	1.0000000
4.0000000	1092.1764638	1.0005634
8.0000000	1092.7275477	1.0010683
12.0000000	1093.2252632	1.0015243
16.0000000	1093.8208574	1.0020699
20.0000000	1094.2770611	1.0024878
24.0000000	1094.8311412	1.0029954
28.0000000	1095.3538827	1.0034743
32.0000000	1095.8635926	1.0039413
36.0000000	1096.3948674	1.0044280
40.0000000	1096.8803129	1.0048727
44.0000000	1097.3980523	1.0053470
48.0000000	1097.8802135	1.0057888
52.0000000	1098.4625210	1.0063222

SLOPE = 0.1309
VARIANCE = 0.50D-06
STD DEV = 0.00071
INTERCEPT = 1091.6572
CORR. COEFF. = 0.99982D 00
SLOPE PER KB = 1.8987

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS POISSONS RATIO

PRESS	SIG	Y/YO
0.0150000	0.2879453	1.0000000
4.0000000	0.2881148	1.0005888
8.0000000	0.2883096	1.0012652
12.0000000	0.2884559	1.0017732
16.0000000	0.2886745	1.0025324
20.0000000	0.2888588	1.0031725
24.0000000	0.2890721	1.0039132
28.0000000	0.2892484	1.0045256
32.0000000	0.2894384	1.0051856
36.0000000	0.2896251	1.0058339
40.0000000	0.2898157	1.0064959
44.0000000	0.2900157	1.0071904
48.0000000	0.2901736	1.0077389
52.0000000	0.2903922	1.0084980

SLOPE = 0.0000
VARIANCE = 0.61D-13
STD DEV = 0.00000
INTERCEPT = 0.2879
CORR. COEFF. = 0.99983D 00
SLOPE PER KB = 0.0007

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS COMPRESSIBILITY PER MEGABAR

PRESS	COMP/MB	Y/YO
0.0150000	1.1656040	1.0000000
4.0000000	1.1640162	0.9986378
8.0000000	1.1623598	0.9972167
12.0000000	1.1610277	0.9960739
16.0000000	1.1591963	0.9945027
20.0000000	1.1577025	0.9932211
24.0000000	1.1559478	0.9917157
28.0000000	1.1544302	0.9904138
32.0000000	1.1528528	0.9890604
36.0000000	1.1512726	0.9877047
40.0000000	1.1497203	0.9863730
44.0000000	1.1480845	0.9849696
48.0000000	1.1467172	0.9837966
52.0000000	1.1449153	0.9822507

SLOPE = -0.0004
VARIANCE = 0.23D-11
STD DEV = 0.00000
INTERCEPT = 1.1656
CORR. COEFF. = -0.99991D 00
SLOPE PER KB = -0.0058

PRESSURE CALCULATIONS FOR GLASS #111
LEAST SQUARES PRESS VS LAME'S CONSTANT

PRESS	L	Y/Y0
0.0150000	857.1478843	1.0000000
4.0000000	858.3182640	1.0013654
8.0000000	859.5425930	1.0027938
12.0000000	860.5297482	1.0039455
16.0000000	861.8906356	1.0055332
20.0000000	863.0039142	1.0068320
24.0000000	864.3152265	1.0083619
28.0000000	865.4525254	1.0096887
32.0000000	866.6379178	1.0110716
36.0000000	867.8286049	1.0124608
40.0000000	869.0014638	1.0138291
44.0000000	870.2408350	1.0152750
48.0000000	871.2795014	1.0164868
52.0000000	872.6520666	1.0180881

SLOPE = 0.2975
VARIANCE = 0.12D-05
STD DEV = 0.00111
INTERCEPT = 857.1097
CORR. COEFF. = 0.99992D 00
SLOPE PER KB = 4.3154

C. LISTING OF TEMPERATURE PROGRAM, INPUT AND OUTPUT DATA.

```
//ISOT  JOB (1242,1M,10F,190K),'MILLER'
// EXEC  FORTCLG,RG=190K
//SYSIN  DD  *
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION T(50),PF(50),SF(50),PFR(50),SFR(50),XLR(50),DR(50),D(50)
     1,PV(50),SV(50),BMOD(50),SMOD(50),EMOD(50),SIG(50),COMP(50),M(15),X
     1(50),Y(50),DESC(20,20),YAX(20,20),AL(50)
      JJ = 1
C
C     INPUT PARAMETER AND SPECIMEN DESCRIPTION CARDS
C
    1 READ 2, (DESC(JJ,J1),J1=1,13),(YAX(JJ,J2),J2=1,3),IM
    2 FORMAT(13A4,3A4,15X,I1)
      IF(IM) 3,3,45
    3 JJ = JJ+1
      IF(JJ-16) 1,1,4
C
C     INPUT INITIAL MEASUREMENT CARD
C
    4 READ 5, RHO,PVI,SVI,PFI,SFI,ALPHA
    5 FORMAT(5F10.4,D10.3)
      PRINT 6, (DESC(16,J3),J3=1,13),RHO,PVI,SVI,PFI,SFI,ALPHA
    6 FORMAT(1H1,13A4//1X,'RHO = DENSITY'/1X,'PV = LONGITUDINAL VELOCITY
     1'/1X,'SV = SHEAR VELOCITY'/1X,'P FREQ = LONGITUDINAL FREQUENCY'/1X
     1,'S FREQ = SHEAR FREQUENCY'/1X,'ALPHA = VOLUMETRIC THERMAL EXPANSI
     1ON'/1X,'PRESS = PRESSURE'/1X,'PF RATIO = LONGITUDINAL FREQUENCY RA
     1TIO'/1X,'SF RATIO = SHEAR FREQUENCY RATIO'/1X,'L RATIO = LENGTH RA
     1TIO'/1X,'BMOD = BULK MODULUS'/1X,'SMOD = SHEAR MODULUS'/1X,'EMOD =
     1 YOUNGS MODULUS'/1X,'SIG = POISSONS RATIO'/1X,'COMP = COMPRESSIBIL
     1ITY'/1X,'L = LAME CONSTANT'///7X,'RHO',8X,'PV',8X,'SV',5X,'P FREQ'
     1,4X,'S FREQ',9X,'ALPHA'/2X,5F10.4,D14.3//4X,'T(C) ',2X,'P FREQ',3X
     1,'S FREQ',4X,'PF RATIO',2X,'SF RATIO',3X,'L RATIO',4X,'DENSITY',5X
     1,'PV',6X,'SV',4X,'BMOD',3X,'SMOD',3X,'EMOD',4X,'SIG',4X,'COMP/MB',
     13X,'L')
      N = 1
C
C     INPUT EXPERIMENTAL TEMPERATURE-FREQUENCY DATA AND DETERMINE THE
C     NUMBER OF PIECES OF DATA
C
    7 READ 8, T(N),PF(N),SF(N)
    8 FORMAT(3F10.3)
      IF(PF(N)) 12,9,10
    9 IF(SF(N)) 12,14,7
   10 IF(SF(N)) 12,7,11
   11 N = N+1
      GO TO 7
   12 PRINT 13
   13 FORMAT('NEGATIVE FREQ IN DATA')
      GO TO 45
   14 N = N-1
C
C
C     COMPUTE SPECIMEN LENGTH AND CORRESPONDING VELOCITIES AT
C     VARIOUS TEMPERATURES
C
      DO 16 I = 1,N
```

```
      PFR(I) = PF(I)/PFI
      SFR(I) = SF(I)/SFI
      XLR(I)=1.0+ALPHA*(T(I)-25.0)
      DR(I)=1.0/XLR(I)**3
      D(I) = RHO*DR(I)
      PV(I) = PVI*PFR(I)*XLR(I)
      SV(I) = SVI*SFR(I)*XLR(I)
C
C     COMPUTE ELASTIC MODULI
C
      BMOD(I) = 10.0*D(I)*(PV(I)**2-4.0*SV(I)**2/3.0)
      SMOD(I) = 10.0*D(I)*SV(I)**2
      EMOD(I) = 9.0*BMOD(I)*SMOD(I)/(3.0*BMOD(I)+SMOD(I))
      SIG(I) = EMOD(I)/(2.0*SMOD(I))-1.0
      COMP(I) = (1.0/BMOD(I))*1000.0
      AL(I) = BMOD(I)-2.0*SMOD(I)/EMOD(I)
      PRINT 15, T(I),PF(I),SF(I),PFR(I),SFR(I),XLR(I),D(I),PV(I),SV(I),
     1 BMOD(I),SMOD(I),EMOD(I),SIG(I),COMP(I),AL(I)
   15 FORMAT(3F9.3,F11.6,F10.6,2F11.7,2F8.4,3F7.1,F8.4,F8.3,F7.1)
   16 CONTINUE
C
C     COMPUTE LEAST SQUARES FIT BETWEEN TEMPERATURE AND THE VARIOUS
C     PARAMETERS
C
      READ 17, (M(K),K = 1,15)
   17 FORMAT(15I1)
      LL = 6
      L = 59/(N+11)-1
      DO 44 K = 1,15
      IF(L-LL) 18,20,20
   18 PRINT 19
   19 FORMAT(1H1)
      LL = 0
   20 IF(M(K)) 21,44,21
   21 LL = LL+1
      DO 37 II = 1,N
      GO TO (22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37),K
   22 Y(II) =   PF(II)
      GO TO 37
   23 Y(II) =   SF(II)
      GO TO 37
   24 Y(II) =  PFR(II)
      GO TO 37
   25 Y(II) =  SFR(II)
      GO TO 37
   26 Y(II) =  XLR(II)
      GO TO 37
   27 Y(II) =    D(II)
      GO TO 37
   28 Y(II) =   DR(II)
      GO TO 37
   29 Y(II) =   PV(II)
      GO TO 37
   30 Y(II) =   SV(II)
      GO TO 37
   31 Y(II) = BMOD(II)
```

```
      GO TO 37
   32 Y(II) = SMOD(II)
      GO TO 37
   33 Y(II) = EMOD(II)
      GO TO 37
   34 Y(II) =  SIG(II)
      GO TO 37
   35 Y(II) = COMP(II)
      GO TO 37
   36 Y(II) = AL(II)
   37 CONTINUE
      PRINT 38,(DESC(16,J1),J1=1,13),(DESC(K,J2),J2=1,13)
   38 FORMAT(30X,13A4/30X,'LEAST SQUARES     TEMP  VS ',13A4//)
      PRINT 39, (YAX(K,J1),J1=1,3)
   39 FORMAT(33X,'T(C)' ,17X,3A4,11X,'Y/Y0')
      SUMX  = 0.0
      SUMY  = 0.0
      SUMX2 = 0.0
      SUMXY = 0.0
      SUMY2 = 0.0
      C = N
      DO 40 J = 1,N
      X(J) = T(J)
      SUMX = SUMX+X(J)
      SUMY = SUMY+Y(J)
      SUMX2 = SUMX2 +X(J)**2
      SUMY2 = SUMY2 +Y(J)**2
   40 SUMXY = SUMXY+X(J)*Y(J)
C
C     COMPUTE SLOPE,INTERCEPT,CORRELATION COEFFICIENT,VARIANCE, AND
C     STANDARD DEVIATION
C
      S = (SUMX*SUMY-C*SUMXY)/(SUMX**2-C*SUMX2)
      B = (SUMX2*SUMY-SUMX*SUMXY)/(C*SUMX2-SUMX**2)
      R = (C*SUMXY-SUMX*SUMY)/DSQRT((C*SUMX2-SUMX**2)*(C*SUMY2-SUMY**2))
      SXY = SUMXY-SUMX*SUMY/C
      SXX = SUMX2-SUMX*SUMX/C
      SYY = SUMY2-SUMY*SUMY/C
      VARS = (SYY-SXY**2/SXX)/(SXX*(C-2.0))
      DEVS =DSQRT(VARS)
      DO 41 J = 1,N
      YR = Y(J)/Y(1)
   41 PRINT 42, X(J),Y(J),YR
   42 FORMAT(19X,3(8X,F14.7))
      PRINT 43, S,VARS,DEVS,B,R
   43 FORMAT(12HOSLOPE     =,F11.4,'/(C)'/' VARIANCE  =',E13.2/' STD DEV
     1   =',F12.5/' INTERCEPT =',F11.4/' CORR. COEFF. = ',E12.5//)
   44 CONTINUE
      JJ = 16
      GO TO 1
   45 STOP
      END
 *
//GO.SYSIN DD *
 LONGITUDINAL FREQUENCY                                  P FREQ
 SHEAR FREQUENCY                                         S FREQ
```

```
 LONGITUDINAL FREQUENCY RATIO                                    PF RATIO
 SHEAR FREQUENCY RATIO                                           SF RATIO
 LENGTH RATIO                                                    L RATIO
 DENSITY                                                         DENSITY
 DENSITY RATIO                                                   D RATIO
 LONGITUDINAL VELOCITY                                           P VEL
 SHEAR VELOCITY                                                  S VEL
 BULK MODULUS                                                    BMOD
 SHEAR MODULUS                                                   SMOD
 YOUNGS MODULUS                                                  EMOD
 POISSONS RATIO                                                  SIG
 COMPRESSIBILITY PER MEGABAR                                     COMP/MB
 LAME'S CONSTANT                                                 L
TEMPERATURE CALCULATIONS FOR GLASS #111
2.6360     5.9956     4.0554     526.116    363.326      .143D-04
    25.000    525.280    363.635
    50.000    524.300    363.375
    75.000    523.300    363.150
   100.000    522.210    362.925
   125.000    521.100    362.690
   150.000    519.920    362.460
   175.000    518.800    362.235
   200.000    517.560    362.000
   225.000    516.210    361.720
   250.000    514.800    361.540
   275.000    513.100    361.310
   300.000    511.380    361.075

11    1 11111111

ISOT
```

TEMPERATURE CALCULATIONS FOR GLASS #111

RHO = DENSITY
PV = LONGITUDINAL VELOCITY
SV = SHEAR VELOCITY
P FREQ = LONGITUDINAL FREQUENCY
S FREQ = SHEAR FREQUENCY
ALPHA = VOLUMETRIC THERMAL EXPANSION
PRESS = PRESSURE
PF RATIO = LONGITUDINAL FREQUENCY RATIO
SF RATIO = SHEAR FREQUENCY RATIO
L RATIO = LENGTH RATIO
BMOD = BULK MODULUS
SMOD = SHEAR MODULUS
EMOD = YOUNGS MODULUS
SIG = POISSONS RATIO
COMP = COMPRESSIBILITY
L = LAME CONSTANT

RHO	PV	SV	P FREQ	S FREQ	ALPHA
2.6360	5.9956	4.0554	526.1160	363.3260	0.143D-04

T(C)	P FREQ	S FREQ	PF RATIO	SF RATIO	L RATIO	DENSITY	PV	SV	BMOD	SMOD	EMOD	SIG	COMP/MB	L
25.000	525.280	363.635	0.998411	1.000850	1.0000000	2.6360000	5.9861	4.0588	365.5	434.3	933.2	0.0745	2.736	364.6
50.000	524.300	363.375	0.996548	1.000135	1.0003575	2.6331749	5.9770	4.0574	362.7	433.5	930.0	0.0727	2.757	361.8
75.000	523.300	363.150	0.994648	0.999516	1.0007150	2.6303539	5.9678	4.0563	359.7	432.8	926.7	0.0706	2.780	358.8
100.000	522.210	362.925	0.992576	0.998896	1.0010725	2.6275368	5.9575	4.0553	356.4	432.1	923.2	0.0683	2.806	355.5
125.000	521.100	362.690	0.990466	0.998250	1.0014300	2.6247238	5.9469	4.0541	353.1	431.4	919.6	0.0659	2.832	352.1
150.000	519.920	362.460	0.988223	0.997616	1.0017875	2.6219148	5.9356	4.0530	349.5	430.7	915.8	0.0632	2.861	348.5
175.000	518.800	362.235	0.986094	0.996997	1.0021450	2.6191099	5.9249	4.0519	346.1	430.0	912.2	0.0607	2.889	345.1
200.000	517.560	362.000	0.983737	0.996350	1.0025025	2.6163089	5.9129	4.0507	342.3	429.3	908.2	0.0578	2.921	341.4
225.000	516.210	361.720	0.981171	0.995580	1.0028600	2.6135119	5.8995	4.0490	338.3	428.5	903.9	0.0547	2.956	337.4
250.000	514.800	361.540	0.978491	0.995084	1.0032175	2.6107189	5.8855	4.0484	333.8	427.9	899.4	0.0509	2.996	332.9
275.000	513.100	361.310	0.975260	0.994451	1.0035750	2.6079298	5.8682	4.0473	328.5	427.2	894.0	0.0464	3.045	327.5
300.000	511.380	361.075	0.971991	0.993804	1.0039325	2.6051448	5.8506	4.0461	323.1	426.5	888.5	0.0416	3.095	322.1

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS LONGITUDINAL FREQUENCY

T(C)	P FREQ	Y/Y0
25.0000000	525.2800000	1.0000000
50.0000000	524.3000000	0.9981343
75.0000000	523.3000000	0.9962306
100.0000000	522.2100000	0.9941555
125.0000000	521.1000000	0.9920423
150.0000000	519.9200000	0.9897959
175.0000000	518.8000000	0.9876637
200.0000000	517.5600000	0.9853031
225.0000000	516.2100000	0.9827330
250.0000000	514.8000000	0.9800487
275.0000000	513.1000000	0.9768124
300.0000000	511.3800000	0.9735379

SLOPE = -0.0496/(C)
VARIANCE = 0.19D-05
STD DEV = 0.00140
INTERCEPT = 527.0635
CORR. COEFF. = -0.99607D 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS SHEAR FREQUENCY

T(C)	S FREQ	Y/Y0
25.0000000	363.6350000	1.0000000
50.0000000	363.3750000	0.9992850
75.0000000	363.1500000	0.9986662
100.0000000	362.9250000	0.9980475
125.0000000	362.6900000	0.9974012
150.0000000	362.4600000	0.9967687
175.0000000	362.2350000	0.9961500
200.0000000	362.0000000	0.9955037
225.0000000	361.7200000	0.9947337
250.0000000	361.5400000	0.9942387
275.0000000	361.3100000	0.9936062
300.0000000	361.0750000	0.9929600

SLOPE = -0.0093/(C)
VARIANCE = 0.29D-08
STD DEV = 0.00005
INTERCEPT = 363.8505
CORR. COEFF. = -0.99983D 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS DENSITY

T(C)	DENSITY	Y/YO
25.0000000	2.6360000	1.0000000
50.0000000	2.6331749	0.9989283
75.0000000	2.6303539	0.9978581
100.0000000	2.6275368	0.9967894
125.0000000	2.6247238	0.9957222
150.0000000	2.6219148	0.9946566
175.0000000	2.6191099	0.9935925
200.0000000	2.6163089	0.9925299
225.0000000	2.6135119	0.9914688
250.0000000	2.6107189	0.9904093
275.0000000	2.6079298	0.9893512
300.0000000	2.6051448	0.9882947

SLOPE = -0.0001/(C)
VARIANCE = 0.60D-14
STD DEV = 0.00000
INTERCEPT = 2.6388
CORR. COEFF. = -0.10000D 01

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS LONGITUDINAL VELOCITY

T(C)	P VEL	Y/YO
25.0000000	5.9860730	1.0000000
50.0000000	5.9770410	0.9984912
75.0000000	5.9677729	0.9969429
100.0000000	5.9574699	0.9952217
125.0000000	5.9469298	0.9934610
150.0000000	5.9355815	0.9915652
175.0000000	5.9249088	0.9897823
200.0000000	5.9128561	0.9877688
225.0000000	5.8995361	0.9855436
250.0000000	5.8855192	0.9832020
275.0000000	5.8681741	0.9803045
300.0000000	5.8505864	0.9773664

SLOPE = -0.0005/(C)
VARIANCE = 0.26D-09
STD DEV = 0.00002
INTERCEPT = 6.0044
CORR. COEFF. = -0.99445D 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS SHEAR VELOCITY

T(C)	S VEL	Y/YO
25.0000000	4.0588490	1.0000000
50.0000000	4.0573969	0.9996422
75.0000000	4.0563337	0.9993803
100.0000000	4.0552687	0.9991179
125.0000000	4.0540901	0.9988275
150.0000000	4.0529656	0.9985505
175.0000000	4.0518951	0.9982867
200.0000000	4.0507110	0.9979950
225.0000000	4.0490212	0.9975787
250.0000000	4.0484490	0.9974377
275.0000000	4.0473153	0.9971584
300.0000000	4.0461237	0.9968648

SLOPE = -0.0000/(C)
VARIANCE = 0.36D-12
STD DEV = 0.00000
INTERCEPT = 4.0598
CORR. COEFF. = -0.99915D 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS BULK MODULUS

T(C)	BMOD	Y/YO
25.0000000	365.5445536	1.0000000
50.0000000	362.7213907	0.9922768
75.0000000	359.7233897	0.9840754
100.0000000	356.4124587	0.9750178
125.0000000	353.0720350	0.9658796
150.0000000	349.4773386	0.9560458
175.0000000	346.0910837	0.9467822
200.0000000	342.3227792	0.9364735
225.0000000	338.3216247	0.9255277
250.0000000	333.8086966	0.9131820
275.0000000	328.4544920	0.8985348
300.0000000	323.0693457	0.8838029

SLOPE = -0.1515/(C)
VARIANCE = 0.23D-04
STD DEV = 0.00475
INTERCEPT = 371.2013
CORR. COEFF. = -0.99512D 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS SHEAR MODULUS

T(C)	SMOD	Y/YO
25.0000000	434.2613715	1.0000000
50.0000000	433.4856263	0.9982136
75.0000000	432.7942995	0.9966217
100.0000000	432.1037986	0.9950316
125.0000000	431.3903341	0.9933887
150.0000000	430.6896233	0.9917751
175.0000000	430.0016297	0.9901908
200.0000000	429.2907406	0.9885538
225.0000000	428.4741041	0.9866733
250.0000000	427.8952372	0.9853403
275.0000000	427.1987506	0.9837365
300.0000000	426.4912943	0.9821074

SLOPE = -0.0282/(C)
VARIANCE = 0.18D-07
STD DEV = 0.00013
INTERCEPT = 434.9189
CORR. COEFF. = -0.999890 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS YOUNGS MODULUS

T(C)	EMOD	Y/YO
25.0000000	933.2298312	1.0000000
50.0000000	929.9844053	0.9965224
75.0000000	926.7255423	0.9930303
100.0000000	923.2175997	0.9892714
125.0000000	919.6302474	0.9854274
150.0000000	915.8451434	0.9813715
175.0000000	912.2117307	0.9774781
200.0000000	908.2202572	0.9732011
225.0000000	903.8542779	0.9685227
250.0000000	899.3893385	0.9637383
275.0000000	894.0053143	0.9579691
300.0000000	888.4982192	0.9520680

SLOPE = -0.1597/(C)
VARIANCE = 0.18D-04
STD DEV = 0.00428
INTERCEPT = 938.8531
CORR. COEFF. = -0.996430 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS POISSONS RATIO

T(C)	SIG	Y/YO
25.0000000	0.0745025	1.0000000
50.0000000	0.0726819	0.9755642
75.0000000	0.0706305	0.9480288
100.0000000	0.0682822	0.9165093
125.0000000	0.0658911	0.8844152
150.0000000	0.0632310	0.8487105
175.0000000	0.0607073	0.8148360
200.0000000	0.0578149	0.7760128
225.0000000	0.0547362	0.7346895
250.0000000	0.0509457	0.6838125
275.0000000	0.0463576	0.6222290
300.0000000	0.0416370	0.5588673

SLOPE = -0.0001/(C)
VARIANCE = 0.28D-10
STD DEV = 0.00001
INTERCEPT = 0.0795
CORR. COEFF. = -0.98974D 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS COMPRESSIBILITY PER MEGABAR

T(C)	COMP/MB	Y/YO
25.0000000	2.7356446	1.0000000
50.0000000	2.7569369	1.0077833
75.0000000	2.7799138	1.0161823
100.0000000	2.8057381	1.0256223
125.0000000	2.8322832	1.0353257
150.0000000	2.8614159	1.0459750
175.0000000	2.8894128	1.0562091
200.0000000	2.9212196	1.0678359
225.0000000	2.9557673	1.0804646
250.0000000	2.9957278	1.0950720
275.0000000	3.0445618	1.1129230
300.0000000	3.0953107	1.1314740

SLOPE = 0.0013/(C)
VARIANCE = 0.29D-08
STD DEV = 0.00005
INTERCEPT = 2.6827
CORR. COEFF. = 0.99106D 00

TEMPERATURE CALCULATIONS FOR GLASS #111
LEAST SQUARES TEMP VS LAME'S CONSTANT

T(C)	L	Y/YO
25.0000000	364.6138903	1.0000000
50.0000000	361.7891479	0.9922528
75.0000000	358.7893606	0.9840255
100.0000000	355.4763765	0.9749392
125.0000000	352.1338528	0.9657719
150.0000000	348.5368092	0.9559066
175.0000000	345.1483165	0.9466132
200.0000000	341.3774342	0.9362711
225.0000000	337.3735203	0.9252898
250.0000000	332.8571727	0.9129032
275.0000000	327.4987957	0.8982071
300.0000000	322.1093183	0.8834258

SLOPE = -0.1516/(C)
VARIANCE = 0.23D-04
STD DEV = 0.00475
INTERCEPT = 370.2752
CORR. COEFF. = -0.99512D 00

APPENDIX II

CRYSTALLINE (TETRAGONAL) SYSTEM

A. INPUT-OUTPUT DATA. An attempt was made to obtain as much similarity as possible between the crystalline and isotropic program. Two computer programs are included for the tetragonal case. These programs provide ease of computation of elastic and other related parameters of a tetragonal crystal subjected to increased temperature or pressure. The complete programs with input data and output results are listed. The deck sequence is as follows:

1. Control cards
2. Main program
3. Control cards to input data
4. Parameter description cards
5. Specimen description card
6. Initial measurement card (1)
7. Initial measurement card (2)
8. Experimental pressure-prf data
9. Least squares indicator card
10. Data termination card
11. Control card

All input data must agree with the input format statements in the main program. The first 24 parameter description cards must be placed in the same order as those listed after the main program. As in the isotropic case, each parameter and its abbreviated form must be punched on one card.

Example:

C_{33} Velocity C_{33} Vel

The next data card following the last parameter description card is the specimen description card.

Example:

Pressure calculations for crystal #1111

Two initial measurement cards follow the specimen description card. These measurements are performed with the specimen at 1 bar pressure and room temperature. For the pressure program, measurement card (1) contains mean atomic weight, coefficient of volumetric thermal expansion, Gruneisen parameter, and room temperature in °K.

Example:

Mean Atomic Weight (gm)	Volumetric Expansion $(°C)^{-1}$	Gruneisen Parameter	Temperature (°K)
26.63	23.52×10^{-6}	1.28	298.15

Measurement card (2) contains the density (gm/cm^3) and initial elastic constants. The initial constants are calculated using equation (2.1), the relationships given in Table II, the length of the specimen and the initial prf data and have k bar units.

Example:

Density	C_{33}	C_{44}	C_{11}
4.264	4844.043	1245.463	2716.885
C_{66}	C_{PQ}	C_{TU}	C_{RS}
1949.548	467.794	4177.920	3984.370

In the temperature program, measurement card (1) contains thermal expansion coefficients parallel and perpendicular to the c axis, specific heat coefficients, and the mean atomic weight.

Example:

Thermal expansion parallel to c axis $(°C)^{-1}$	9.2×10^{-6} 2.875×10^{-9}
Thermal expansion perpendicular to c axis $(°C)^{-1}$	7.18×10^{-6} 1.25×10^{-9}
Specific heat at constant pressure (cal/mole deg.)	1.512×10^{-1} 2.45×10^{-4} 2.22×10^{-8}
Mean atomic weight (gm)	26.63

The second measurements card for the temperature program is the same as that card for the pressure program.

The next set of data following the initial measurement cards is the experimental pressure (or temperature) prf data. The input prf data for each particular pressure (temperature) must contain f_{33}, f_{11}, f_{44}, f_{66}, f_{RS}, and either f_{PQ} or f_{TU} or both. Table II indicates the crystal orientation to obtain the f_{ij} data. Either f_{44} or f_{44A} or both may be input data. The input units for the f_{ij} values are kc and must be in the same order as shown in data at the end of the main program.

Example:

Pressure	f_{33}	f_{44}	f_{11}	f_{44A}
0.015	476.719	241.682	460.900	0.0

f_{66}	f_{PQ}	f_{TU}	f_{RS}
453.534	163.067	487.327	595.771

The least squares indicator card and the program termination card function in the same way as the corresponding cards in the isotropic program.

The output of the elastic parameters, as a function of pressure or temperature, have the following units:

Temperature	°C
Pressure	k psi
Density	g/cc
Compressibility	$(\text{M bar})^{-1}$
Experimental prf data	kc/s
Stiffness constant data	k bar
Compliance constants	$(\text{M bar})^{-1}$
Velocities	km/sec
Bulk moduli (K)	k bar
Shear moduli (U)	k bar
Debye temperature	°K

B. LISTING OF PRESSURE PROGRAM, INPUT AND OUTPUT DATA.

```
//CRYP  JOB (1242,1M,10F,190KB),'MILLER'
// EXEC  FORTCLG,RG=190K
//SYSIN DD *
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION P(50),C(10,50),F(10,50),S(10,50),VL(10,50),PKB(50),BB1(5
     10),BB2(50),VCOMP(50),X(50),Y(50),R(50),PP(50),M(25),V(50,50),DESC(
     125,20),YAX(25,20)
      JJ=1
    1 I=1
C
C     INPUT PARAMETER AND SPECIMEN DESCRIPTION CARDS
C
    2 READ 3,(DESC(JJ,J1),J1=1,13),(YAX(JJ,J2),J2=1,3),IM
    3 FORMAT(13A4,3A4,15X,III)
      IF(IM) 4,4,78
    4 JJ=JJ+1
      IF(JJ-25)2,2,5
C
C     INPUT INITIAL MEASUREMENT CARD (1)
C
    5 READ 6,WGT,ALPHA,GAMA,TEMP
    6 FORMAT(F10.4,D10.5,2F10.5)
      AGT=1.0+ALPHA*GAMA*TEMP
C
C     INPUT INITIAL MEASUREMENT CARD (2)
C
      READ 7,R(1),(C(J,1),J=1,8)
    7 FORMAT(9F8.3)
C
C     INPUT EXPERIMENTAL PRESSURE-FREQUENCY DATA AND DETERMINE THE
C     NUMBER OF PIECES OF DATA
C
    8 READ 7,P(I),(F(J,I),J=1,8)
      P(I)=P(I)/14.5038
      IF(F(1,I))9,10,9
    9 I=I+1
      GO TO 8
   10 N=I-1
      I=1
      PRINT 11,(DESC(25,J1),J1=1,13)
   11 FORMAT(1H1,24X,13A4/25X,'ISOTHERMAL COMPRESSIBILITIES AS A FUNCTIO
     1N OF PRESSURE'//25X,'P = PRESSURE'/25X,'RHO = DENSITY'/25X,'I COMP
     1 PDTC = ISOTHERMAL COMPRESSIBILITY PERPENDICULAR TO C AXIS'/25X,'I
     1 COMP PLTC = ISOTHERMAL COMPRESSIBILITY PARALLEL TO C AXIS'/25X,'I
     1 VOL COMP = ISOTHERMAL VOLUMETRIC COMPRESSIBILITY'///25X,'  P(KPSI
     1)     P(KB)     RHO      I COMP PDTC  I COMP PLTC  I VOL COMP'/)
C
C     COMPUTE C12,C13 AND ALL COMPLIANCE CONSTANTS
C
   12 IF(F(6,I).LT.0.1) GO TO 14
      IF(F(7,I).LT.0.1)GO TO 13
      C(9,I)=C(7,I)-C(5,I)-C(6,I)
      GO TO 15
   13 C(9,I)=C(3,I)-2.0*C(6,I)
      C(7,I)=(C(3,I)+C(9,I)+2.0*C(5,I))/2.0
      GO TO 15
```

```
   14 C(9,I)=2.0*C(7,I)-2.0*C(5,I)-C(3,I)
      C(6,I)=(C(3,I)-C(9,I))/2.0
   15 IF(C(2,I))17,16,17
   16 J=4
      S(2,I)=0.0
      S(4,I)=1.0/C(4,I)
      GO TO 20
   17 J=2
      S(2,I)=1.0/C(2,I)
      IF(C(4,I))19,18,19
   18 S(4,I)=0.0
      GO TO 20
   19 S(4,I)=1.0/C(4,I)
   20 C(10,I)=DSQRT((4.0*C(8,I)-C(3,I)-C(1,I)-2.0*C(J,I))**2-(C(3,I)-
     1C(1,I))**2)/2.0-C(J,I)
      S(5,I)=1.0/C(5,I)
      XI=2.0*C(10,I)**2-C(1,I)*(C(9,I)+C(3,I))
      XXI=XI*(C(9,I)-C(3,I))
      S(3,I)=(C(3,I)*C(1,I)-C(10,I)**2)/XXI
      S(9,I)=(C(10,I)**2-C(9,I)*C(1,I))/XXI
      S(10,I)=C(10,I)/XI
      S(1,I)=-(C(3,I)+C(9,I))/XI
C
C     COMPUTE THE VELOCITIES FOR THE VARIOUS C(I,J)
C
      DO 21 J=1,10
   21 V1(J,I)=DSQRT(C(J,I)/(10.0*R(I)))
C
C     COMPUTE ADIABATIC AND ISOTHERMAL COMPRESSIBILITIES
C
      V(I,1)=S(3,I)+S(9,I)+S(10,I)
      V(I,2)=S(1,I)+2.0*S(10,I)
      V(I,3)=2.0*S(3,I)+S(1,I)+2.0*S(9,I)+4.0*S(10,I)
      BB1(I)=V(I,1)*AGT
      BB2(I)=V(I,2)*AGT
      VCOMP(I)=V(I,3)*AGT
      PP(I)=P(I)*14.5038
      PRINT 22,PP(I),P(I),R(I),BB1(I),BB2(I),VCOMP(I)
   22 FORMAT(25X,2F9.3,1X,F9.5,3(1X,E12.6))
      IF(I.GT.N-1) GO TO 27
C
C     COMPUTE ELASTIC CONSTANTS AT HIGHER PRESSURE
C
      DO 24 J=1,2
      IF(F(J,I).LT.0.1) GO TO 23
      C(J,I+1)=C(J,I)*(F(J,I+1)/F(J,I))**2*(1.0+BB1(I)*(P(I+1)-P(I)))**2
     1/(1.0+BB2(I)*(P(I+1)-P(I)))
      GO TO 24
   23 C(J,I+1) =0.0
   24 CONTINUE
      DO 26 J=3,7
      IF(F(J,I).LT.0.1) GO TO 25
      C(J,I+1)=C(J,I)*(F(J,I+1)/F(J,I))**2*(1.0+BB2(I)*(P(I+1)-P(I)))
      GO TO 26
   25 C(J,I+1)=0.0
   26 CONTINUE
```

```
      J=8
      C(J,I+1)= C(J,I)*(F(J,I+1)/F(J,I))**2*(1.0+(2.0*BB1(I)+BB2(I))*(P(
     1I+1)-P(I)))/(1.0+(BB1(I)+BB2(I))*(P(I+1)-P(I)))
      R(I+1)=R(I)*VCOMP(I)*(P(I+1)-P(I))+R(I)
      I=I+1
      GO TO 12
   27 PRINT 28,(DESC(25,J1),J1=1,13)
   28 FORMAT(1H1,24X,13A4/25X,'ADIABATIC COMPRESSIBILITIES AS A FUNCTION
     1 OF PRESSURE'//25X,'A COMP PDTC = ADIABATIC COMPRESSIBILITY PERPEN
     1DICULAR TO C AXIS'/ 25X,'A COMP PLTC = ADIABATIC COMPRESSIBILITY P
     1ARALLEL TO C AXIS'/25X,'A VOL COMP = ADIABATIC VOLUMETRIC COMPRESS
     1IBILITY'///26X,' P(KPSI)    P(KB)    RHO      A COMP PDTC  A COMP P
     1LTC  A VOL COMP'/)
      DO 29 I=1,N
   29 PRINT 22,PP(I),P(I),R(I),(V(I,J),J=1,3)
      PRINT 30,(DESC(25,J1),J1=1,13)
   30 FORMAT(1H1,14X,13A4/15X,'EXPERIMENTAL PRESSURE-FREQUENCY INPUT DAT
     1A'///16X,' P(KPSI)    P(KB)    F33      F44      F11      F44A
     1 F66      FPQ      FTU      FRS'/)
      DO 31 I=1,N
   31 PRINT 32,PP(I),P(I),(F(J,I),J=1,8)
   32 FORMAT(15X,10F9.3)
      PRINT 33,(DESC(25,J1),J1=1,13)
   33 FORMAT(1H1, 9X,13A4/10X,'ELASTIC CONSTANTS AS A FUNCTION OF PRESSU
     1RE'/10X,'C44 = PROPAGATION PARALLEL TO C AXIS'/10X,'C44A = PROPAGA
     1TION PERPENDICULAR TO C AXIS'/10X,'CPQ = (C11-C12)/2'/10X,'CRS = (
     1(C11+C33+2*C44+((C11-C33)**2+4*(C13+C44)**2)**1/2)/4'/10X,'CTU = (
     1C11+C12+2*C66)/2'///11X, 'P(KPSI)    P(KB)    C33      C44      C1
     11      C44A     C66      CPQ      CTU      CRS      C12      C13'/
     1)
      DO 34 I=1,N
   34 PRINT 35,PP(I),P(I),(C(J,I),J=1,10)
   35 FORMAT(9X,12F9.3)
      PRINT 36,(DESC(25,J1),J1=1,13)
   36 FORMAT(1H1, 9X,13A4/10X,'COMPLIANCE CONSTANTS AS A FUNCTION OF PRE
     1SSURE'///10X,' P(KPSI)    P(KB)     S33',10X,'S44',10X,'S11',10X,
     1'S44A',9X,'S66',10X,'S12',10X,'S13'/)
      DO 37 I=1,N
   37 PRINT 38,PP(I),P(I),(S(J,I),J=1,5),(S(J,I),J=9,10)
   38 FORMAT (9X,2F9.3,7(1X,E12.6))
      PRINT 39,(DESC(25,J1),J1=1,13)
   39 FORMAT(1H1,4X,13A4/5X,'VELOCITIES OF THE ELASTIC CONSTANTS AS A FU
     1NCTION OF PRESSURE'///7X,'P(KPSI)    P(KB)   V(C33)   V(C44)   V(C
     111)   V(C44A)  V(C66)   V(CPQ)   V(CTU)   V(CRS)   V(C12)   V(C13)
     1'/)
      DO 40 I=1,N
   40 PRINT 41, PP(I),P(I),(V1(J,I),J=1,10)
   41 FORMAT(5X,2F9.3,10F9.5)
      PRINT 42,(DESC(25,J1),J1=1,13)
   42 FORMAT(1H1,8X,13A4/9X,'VOIGT,REUSS,HILL MODULI AND CORRESPUNDING V
     1ELOCITIES'//9X,'K(V) = VOIGT BULK MODULUS'/9X,'U(V) = VOIGT SHEAR
     1MODULUS'/9X,'K(R) = REUSS BULK MODULUS'/9X,'U(R) = REUSS SHEAR MOD
     1ULUS'/9X,'K(H) = HILL BULK MODULUS'/9X,'U(H) = HILL SHEAR MODULUS'
     1/9X,'VS(V) = VOIGT SHEAR VELOCITY'/9X,'VS(R) = REUSS SHEAR VELOCIT
     1Y'/9X,'VS(VRH) = VOIGT,REUSS,HILL SHEAR VELOCITY'/9X,'VP(V) = VOIG
     1T LONGITUDINAL VELOCITY'/9X,'VP(R) = REUSS LONGITUDINAL VELOCITY'/
```

```
     19X,'VP(VRH) = VOIGT,REUSS,HILL LONGITUDINAL VELOCITY'//12X,'P     K
     1(V)      U(V)      K(R)      U(R)      K(H)      U(H)      VS(V)     VS(R
     1)    VS(VRH)    VP(V)     VP(R)    VP(VRH)'/)
C
C      COMPUTE ELASTIC MODULI AND COMPRESSIONAL- AND SHEAR-WAVE
C      VELOCITIES BY VOIGT,REUSS AND HILL AVERAGING SCHEMES
C
       DO 46 I=1,N
       IF(F(2,I).EQ. 0.0) GO TO 43
       L=2
       GO TO 44
   43  L=4
   44  V(I,4)=((2.0*C(3,I)+C(1,I))+2.0*(C(9,I)+2.0*C(10,I)))/9.0
       V(I,5)=(2.0*C(3,I)+C(1,I)-C(9,I)-2.0*C(10,I)+6.0*C(L,I)+3.0*C(5,I)
     1)/15.0
       V(I,6)=1.0/(2.0*S(3,I)+S(1,I)+2.0*(S(9,I)+2.0*S(10,I)))
       V(I,7)=15.0/(4.0*(2.0*S(3,I)+S(1,I))-4.0*(S(9,I)+2.0*S(10,I))+6.0*
     1S(L,I)+3.0*S(5,I))
       V(I,8)=0.5*(V(I,4)+V(I,6))
       V(I,9)=0.5*(V(I,5)+V(I,7))
       DO 45 K=3,5
       V(I,K+7)=DSQRT(V(I,2*K-1)/(10.0*R(I)))
   45  V(I,K+10)=DSQRT((V(I,2*K-2)+4.0*V(I,2*K-1)/3.0)/(10.0*R(I)))
   46  PRINT 47,PP(I),(V(I,J),J=4,15)
   47  FORMAT(9X,F5.1,6F9.3,6F9.4)
C
C      COMPUTE MEAN SOUND VELOCITIES ,DEBYE TEMPERATURE AND ANISOTROPY AS
C      A FUNCTION OF PRESSURE
C
       PRINT 48,(DESC(25,J1),J1=1,13)
   48  FORMAT(1H1,13X,13A4/14X,'VOIGT,REUSS AND HILL MEAN VELOCITIES AND
     1CORRESPONDING DEBYE TEMPERATURE'//14X,'VM(V) = MEAN VELOCITY'/14X,
     1'VM(R) = REUSS MEAN VELOCITY'/14X,'VM(VRH) = VOIGT,REUSS,HILL MEAN
     1 VELOCITY'/14X,'SIG(V) = POISSONS RATIO USING VOIGT VELOCITIES'/14
     1X,'SIG(R) = POISSONS RATIO USING REUSS VELOCITIES'/14X,'SIG(VRH) =
     1 POISSONS RATIO USING VRH VELOCITIES'/14X,'DT(V) = DEBYE TEMPERATU
     1RE USING VM(V)'/14X,'DT(R) = DEBYE TEMPERATURE USING VM(R)'/14X,'D
     1T(VRH) = DEBYE TEMPERATURE USING VM(VRH)'/14X,'A = SHEAR ANISOTROP
     1Y'/14X,'RHO = DENSITY'///17X,'P       VM(V)     VM(R)   VM(VRH)  SIG
     1(V)    SIG(R)  SIG(VRH)  DT(V)     DT(R)   DT(VRH)       A       RHO'/
     1)
       DO 51 I=1,N
       DO 49 K=16,18
       V(I,K)=((3.0*V(I,K-3)**3*V(I,K-6)**3)/(2.0*V(I,K-3)**3 +V(I,K-6)**
     13))**.33333333
       V(I,K+3)=0.5*(((V(I,K-3)/V(I,K-6))**2-2.0)/((V(I,K-3)/V(I,K-6))**2
     1-1.0))
   49  V(I,K+6)=251.2*(1.0/(WGT**.33333333))*(R(I)**.33333333)*V(I,K)
       V(I,25) = 2.0*(V(I,5)-V(I,9))/(V(I,5)+V(I,9))
       V(I,26)=R(I)
       PRINT 50,PP(I),(V(I,J),J=16,26)
   50  FORMAT(14X,F5.1,1X,11F9.4)
   51  CONTINUE
C
C      COMPUTE LEAST SQUARES FIT BETWEEN PRESSURE AND THE VARIOUS
C      PARAMETERS
```

```
C
      READ 52,(M(K),K=1,24)
   52 FORMAT(24I1)
      LL=6
      L=59/(N+1)-1
      DO 77 K=1,24
      IF(L-LL)53,55,55
   53 PRINT 54
   54 FORMAT(1H1)
      LL = 0
   55 IF(M(K)) 56,77,56
   56 LL = LL+1
      DO 67 II=1,N
      GO TO (57,58,59,60,61,61,61,61,61,62,62,63,63,63,63,63,64,64,65,65
     1,65,65,65,66),K
   57 Y(II)=R(II)
      GO TO 67
   58 Y(II)=BB1(II)
      GO TO 67
   59 Y(II)=BB2(II)
      GO TO 67
   60 Y(II)=VCOMP(II)
      GO TO 67
   61 Y(II)=C(K-4,II)
      GO TO 67
   62 Y(II)=C(K-1,II)
      GO TO 67
   63 Y(II)=V1(K-11,II)
      GO TO 67
   64 Y(II)=V1(K-8,II)
      GO TO 67
   65 Y(II)=F(K-18,II)
      GO TO 67
   66 Y(II)=F(8,II)
      GO TO 67
   67 CONTINUE
      PRINT 68, (DESC(25,J1),J1=1,13),(DESC(K,J2),J2=1,13)
   68 FORMAT(30X,13A4/30X,'LEAST SQUARES      PRESS VS ',13A4/)
      PRINT 69, (YAX(K,J1),J1=1,3)
   69 FORMAT(33X,'PRESS',12X,3A4,15X,'Y/Y0')
      SUMX  = 0.0
      SUMY  = 0.0
      SUMX2 = 0.0
      SUMXY = 0.0
      SUMY2 = 0.0
      CI=N
      DO 70 J=1,N
      X(J) = PP(J)
      SUMX = SUMX+X(J)
      SUMY = SUMY+Y(J)
      SUMX2 = SUMX2 +X(J)**2
      SUMY2 = SUMY2 +Y(J)**2
   70 SUMXY = SUMXY+X(J)*Y(J)
      IF(SUMXY) 73,71,73
   71 PRINT 72
      GO TO 77
```

```
   72 FORMAT(/////45X,'NO INPUT VALUES'/)
C
C      COMPUTE SLOPE,INTERCEPT,CORRELATION COEFFICIENT,VARIANCE AND
C      STANDARD DEVIATION
C
   73 SI=(SUMX*SUMY-CI*SUMXY)/(SUMX**2-CI*SUMX2)
      BI= (SUMX2*SUMY-SUMX*SUMXY)/(CI*SUMX2-SUMX**2)
      RI=(CI*SUMXY-SUMX*SUMY)/DSQRT((CI*SUMX2-SUMX**2)*(CI*SUMY2-SUMY**2
     1))
      SXY = SUMXY-SUMX*SUMY/CI
      SXX = SUMX2-SUMX*SUMX/CI
      SYY = SUMY2-SUMY*SUMY/CI
      VARS = (SYY-SXY**2/SXX)/(SXX*(CI-2.0))
      DEVS =DSQRT(VARS)
      SPKB=SI*14.504
      DO 74 J=1,N
      YR = Y(J)/Y(1)
   74 PRINT 75, X(J),Y(J),YR
   75 FORMAT(27X,F14.7,8X,E14.7,8X,F14.7)
      PRINT 76, SI,VARS,DEVS,BI,RI,SPKB
   76 FORMAT(12HOSLOPE      =,F11.4/' VARIANCE  =',E13.2/' STD DEV   =',
     1F12.5/' INTERCEPT =',F11.4/' CORR. COEFF. = ',E12.5/' SLOPE PER KB
     1 =',F8.4//)
   77 CONTINUE
      JJ=25
      GO TO 1
   78 STOP
      END
 *
//GO.SYSIN DD *
DENSITY                                                    DENSITY
COMP PERPENDICULAR TO C                                    COMP PDTC
COMP PARALLEL TO C                                         COMP PLTC
VOLUMETRIC COMP                                            VOL COMP
C33                                                        C33
C44                                                        C44
C11                                                        C11
C44A                                                       C44A
C66                                                        C66
C12                                                        C12
C13                                                        C13
C33 VELOCITY                                               C33 VEL
C44 VELOCITY                                               C44 VEL
C11 VELOCITY                                               C11 VEL
C44A VELOCITY                                              C44A VEL
C66 VELOCITY                                               C66 VEL
C12 VELOCITY                                               C12 VEL
C13 VELOCITY                                               C13 VEL
F33                                                        F33
F44                                                        F44
F11                                                        F11
F44A                                                       F44A
F66                                                        F66
FRS                                                        FRS
PRESSURE CALCULATIONS FOR CRYSTAL #1111
26.6329333 2.352D-05 1.28      298.15
```

```
4.264   4844.0431245.4632716.885
   0.015476.719 241.682 460.900
   4.000476.812 241.701 461.044
   8.000476.905 241.721 461.190
  12.000476.998 241.740 461.335
  16.000477.091 241.760 461.480
  20.000477.184 241.779 461.625
  24.000477.277 241.799 461.770
  28.000477.371 241.818 461.916
  32.000477.464 241.838 462.061
  36.000477.557 241.857 462.206
  40.000477.650 241.877 462.351
  44.000477.743 241.897 462.496
  48.000477.836 241.916 462.641
  52.000477.929 241.936 462.787
  56.000478.023 241.955 462.932
  60.000478.116 241.975 463.077
  64.000478.209 241.994 463.222
  68.000478.302 242.014 463.367
  72.000478.395 242.033 463.512
  76.000478.489 242.053 463.657
  80.000478.582 242.072 463.803
  84.000478.675 242.092 463.948
  92.000478.861 242.131 464.238
  96.000478.954 242.150 464.384
 100.000479.047 242.170 464.529
 104.000479.141 242.189 464.674
 108.000479.234 242.209 464.819
 112.000479.327 242.228 464.964
 116.000479.420 242.248 465.109
 120.000479.513 242.267 465.254

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CRYP
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1949.548 467.7944177.9203984.370
453.534 163.067 487.327 595.771
453.733 163.002 487.565 595.904
453.932 162.936 487.805 596.038
454.132 162.871 488.045 596.172
454.332 162.805 488.284 596.305
454.531 162.740 488.524 596.439
454.731 162.674 488.764 596.573
454.931 162.608 489.003 596.707
455.130 162.543 489.243 596.840
455.330 162.477 489.482 596.974
455.530 162.412 489.722 597.108
455.729 162.346 489.962 597.241
455.929 162.281 490.201 597.375
456.129 162.215 490.441 597.509
456.328 162.150 490.681 597.643
456.528 162.084 490.920 597.776
456.728 162.019 491.160 597.910
456.927 161.953 491.399 598.044
457.127 161.888 491.639 598.177
457.327 161.822 491.879 598.311
457.526 161.757 492.118 598.445
457.726 161.691 492.358 598.579
458.125 161.560 492.837 598.846
458.325 161.494 493.077 598.980
458.524 161.429 493.316 599.114
458.724 161.363 493.556 599.247
458.924 161.298 493.796 599.381
459.124 161.232 494.035 599.515
459.323 161.167 494.275 599.648
459.523 161.101 494.515 599.782
```

1

PRESSURE CALCULATIONS FOR CRYSTAL #1111
ISOTHERMAL COMPRESSIBILITIES AS A FUNCTION OF PRESSURE

P = PRESSURE
RHO = DENSITY
I COMP PDTC = ISOTHERMAL COMPRESSIBILITY PERPENDICULAR TO C AXIS
I COMP PLTC = ISOTHERMAL COMPRESSIBILITY PARALLEL TO C AXIS
I VOL COMP = ISOTHERMAL VOLUMETRIC COMPRESSIBILITY

P(KPSI)	P(KB)	RHO	I COMP PDTC	I COMP PLTC	I VOL COMP
0.015	0.001	4.26400	0.196276D-03	0.868621D-04	0.479414D-03
4.000	0.276	4.26456	0.196056D-03	0.868461D-04	0.478958D-03
8.000	0.552	4.26512	0.195832D-03	0.868323D-04	0.478497D-03
12.000	0.827	4.26569	0.195611D-03	0.868154D-04	0.478037D-03
16.000	1.103	4.26625	0.195390D-03	0.868025D-04	0.477582D-03
20.000	1.379	4.26681	0.195168D-03	0.867858D-04	0.477122D-03
24.000	1.655	4.26737	0.194947D-03	0.867709D-04	0.476666D-03
28.000	1.931	4.26793	0.194727D-03	0.867552D-04	0.476210D-03
32.000	2.206	4.26850	0.194507D-03	0.867428D-04	0.475756D-03
36.000	2.482	4.26906	0.194288D-03	0.867254D-04	0.475301D-03
40.000	2.758	4.26961	0.194069D-03	0.867103D-04	0.474848D-03
44.000	3.034	4.27017	0.193849D-03	0.866980D-04	0.474396D-03
48.000	3.309	4.27073	0.193632D-03	0.866804D-04	0.473944D-03
52.000	3.585	4.27129	0.193413D-03	0.866662D-04	0.473492D-03
56.000	3.861	4.27185	0.193195D-03	0.866502D-04	0.473040D-03
60.000	4.137	4.27241	0.192978D-03	0.866370D-04	0.472593D-03
64.000	4.413	4.27296	0.192761D-03	0.866199D-04	0.472142D-03
68.000	4.688	4.27352	0.192545D-03	0.866046D-04	0.471694D-03
72.000	4.964	4.27408	0.192328D-03	0.865899D-04	0.471247D-03
76.000	5.240	4.27463	0.192112D-03	0.865756D-04	0.470800D-03
80.000	5.516	4.27519	0.191897D-03	0.865589D-04	0.470353D-03
84.000	5.792	4.27574	0.191681D-03	0.865437D-04	0.469907D-03
92.000	6.343	4.27685	0.191252D-03	0.865135D-04	0.469018D-03
96.000	6.619	4.27740	0.191038D-03	0.864973D-04	0.468572D-03
100.000	6.895	4.27795	0.190824D-03	0.864816D-04	0.468130D-03
104.000	7.171	4.27851	0.190611D-03	0.864678D-04	0.467689D-03
108.000	7.446	4.27906	0.190398D-03	0.864524D-04	0.467248D-03
112.000	7.722	4.27961	0.190186D-03	0.864347D-04	0.466806D-03
116.000	7.998	4.28016	0.189973D-03	0.864220D-04	0.466368D-03
120.000	8.274	4.28071	0.189761D-03	0.864049D-04	0.465927D-03

PRESSURE CALCULATIONS FOR CRYSTAL #1111
ADIABATIC COMPRESSIBILITIES AS A FUNCTION OF PRESSURE

A COMP PDTC = ADIABATIC COMPRESSIBILITY PERPENDICULAR TO C AXIS
A COMP PLTC = ADIABATIC COMPRESSIBILITY PARALLEL TO C AXIS
A VOL COMP = ADIABATIC VOLUMETRIC COMPRESSIBILITY

P(KPSI)	P(KB)	RHO	A COMP PDTC	A COMP PLTC	A VOL COMP
0.015	0.001	4.26400	0.194530D-03	0.860894D-04	0.475149D-03
4.000	0.276	4.26456	0.194312D-03	0.860735D-04	0.474697D-03
8.000	0.552	4.26512	0.194090D-03	0.860599D-04	0.474240D-03
12.000	0.827	4.26569	0.193870D-03	0.860431D-04	0.473784D-03
16.000	1.103	4.26625	0.193651D-03	0.860303D-04	0.473333D-03
20.000	1.379	4.26681	0.193432D-03	0.860138D-04	0.472878D-03
24.000	1.655	4.26737	0.193213D-03	0.859990D-04	0.472425D-03
28.000	1.931	4.26793	0.192995D-03	0.859834D-04	0.471973D-03
32.000	2.206	4.26850	0.192776D-03	0.859711D-04	0.471524D-03
36.000	2.482	4.26906	0.192560D-03	0.859539D-04	0.471073D-03
40.000	2.758	4.26961	0.192342D-03	0.859389D-04	0.470624D-03
44.000	3.034	4.27017	0.192124D-03	0.859268D-04	0.470176D-03
48.000	3.309	4.27073	0.191909D-03	0.859093D-04	0.469728D-03
52.000	3.585	4.27129	0.191692D-03	0.858952D-04	0.469279D-03
56.000	3.861	4.27185	0.191476D-03	0.858793D-04	0.468832D-03
60.000	4.137	4.27241	0.191261D-03	0.858663D-04	0.468388D-03
64.000	4.413	4.27296	0.191046D-03	0.858494D-04	0.467942D-03
68.000	4.688	4.27352	0.190832D-03	0.858341D-04	0.467498D-03
72.000	4.964	4.27408	0.190617D-03	0.858196D-04	0.467054D-03
76.000	5.240	4.27463	0.190403D-03	0.858054D-04	0.466612D-03
80.000	5.516	4.27519	0.190190D-03	0.857888D-04	0.466168D-03
84.000	5.792	4.27574	0.189976D-03	0.857738D-04	0.465726D-03
92.000	6.343	4.27685	0.189551D-03	0.857439D-04	0.464846D-03
96.000	6.619	4.27740	0.189338D-03	0.857278D-04	0.464404D-03
100.000	6.895	4.27795	0.189127D-03	0.857123D-04	0.463966D-03
104.000	7.171	4.27851	0.188915D-03	0.856986D-04	0.463528D-03
108.000	7.446	4.27906	0.188704D-03	0.856833D-04	0.463091D-03
112.000	7.722	4.27961	0.188494D-03	0.856658D-04	0.462654D-03
116.000	7.998	4.28016	0.188283D-03	0.856531D-04	0.462219D-03
120.000	8.274	4.28071	0.188073D-03	0.856362D-04	0.461782D-03

PRESSURE CALCULATIONS FOR CRYSTAL #1111
EXPERIMENTAL PRESSURE-FREQUENCY INPUT DATA

P(KPSI)	P(KB)	F33	F44	F11	F44A	F66	FPQ	FTU	FRS
0.015	0.001	476.719	241.682	460.900	0.0	453.534	163.067	487.327	595.771
4.000	0.276	476.812	241.701	461.044	0.0	453.733	163.002	487.565	595.904
8.000	0.552	476.905	241.721	461.190	0.0	453.932	162.936	487.805	596.038
12.000	0.827	476.998	241.740	461.335	0.0	454.132	162.871	488.045	596.172
16.000	1.103	477.091	241.760	461.480	0.0	454.332	162.805	488.284	596.305
20.000	1.379	477.184	241.779	461.625	0.0	454.531	162.740	488.524	596.439
24.000	1.655	477.277	241.799	461.770	0.0	454.731	162.674	488.764	596.573
28.000	1.931	477.371	241.818	461.916	0.0	454.931	162.608	489.003	596.707
32.000	2.206	477.464	241.838	462.061	0.0	455.130	162.543	489.243	596.840
36.000	2.482	477.557	241.857	462.206	0.0	455.330	162.477	489.482	596.974
40.000	2.758	477.650	241.877	462.351	0.0	455.530	162.412	489.722	597.108
44.000	3.034	477.743	241.897	462.496	0.0	455.729	162.346	489.962	597.241
48.000	3.309	477.836	241.916	462.641	0.0	455.929	162.281	490.201	597.375
52.000	3.585	477.929	241.936	462.787	0.0	456.129	162.215	490.441	597.509
56.000	3.861	478.023	241.955	462.932	0.0	456.328	162.150	490.681	597.643
60.000	4.137	478.116	241.975	463.077	0.0	456.528	162.084	490.920	597.776
64.000	4.413	478.209	241.994	463.222	0.0	456.728	162.019	491.160	597.910
68.000	4.688	478.302	242.014	463.367	0.0	456.927	161.953	491.399	598.044
72.000	4.964	478.395	242.033	463.512	0.0	457.127	161.888	491.639	598.177
76.000	5.240	478.489	242.053	463.657	0.0	457.327	161.822	491.879	598.311
80.000	5.516	478.582	242.072	463.803	0.0	457.526	161.757	492.118	598.445
84.000	5.792	478.675	242.092	463.948	0.0	457.726	161.691	492.358	598.579
92.000	6.343	478.861	242.131	464.238	0.0	458.125	161.560	492.837	598.846
96.000	6.619	478.954	242.150	464.384	0.0	458.325	161.494	493.077	598.980
100.000	6.895	479.047	242.170	464.529	0.0	458.524	161.429	493.316	599.114
104.000	7.171	479.141	242.189	464.674	0.0	458.724	161.363	493.556	599.247
108.000	7.446	479.234	242.209	464.819	0.0	458.924	161.298	493.796	599.381
112.000	7.722	479.327	242.228	464.964	0.0	459.124	161.232	494.035	599.515
116.000	7.998	479.420	242.248	465.109	0.0	459.323	161.167	494.275	599.648
120.000	8.274	479.513	242.267	465.254	0.0	459.523	161.101	494.515	599.782

PRESSURE CALCULATIONS FOR CRYSTAL #1111
ELASTIC CONSTANTS AS A FUNCTION OF PRESSURE
C44 = PROPAGATION PARALLEL TO C AXIS
C44A = PROPAGATION PERPENDICULAR TO C AXIS
CPQ = (C11-C12)/2
CRS = ((C11+C33+2*C44+((C11-C33)**2+4*(C13+C44)**2)**1/2)/4
CTU = (C11+C12+2*C66)/2

P(KPSI)	P(KB)	C33	C44	C11	C44A	C66	CPQ	CTU	CRS	C12	C13
0.015	0.001	4844.043	1245.463	2716.885	0.0	1949.548	467.794	4177.920	3984.370	1760.578	1498.430
4.000	0.276	4846.340	1245.763	2718.648	0.0	1951.306	467.432	4182.102	3986.364	1763.364	1499.804
8.000	0.552	4848.639	1246.075	2720.435	0.0	1953.065	467.065	4186.320	3988.373	1766.191	1501.177
12.000	0.827	4850.938	1246.375	2722.211	0.0	1954.833	466.704	4190.541	3990.382	1769.004	1502.577
16.000	1.103	4853.237	1246.686	2723.988	0.0	1956.602	466.337	4194.747	3992.378	1771.808	1503.926
20.000	1.379	4855.537	1246.987	2725.765	0.0	1958.363	465.975	4198.972	3994.387	1774.633	1505.327
24.000	1.655	4857.836	1247.297	2727.543	0.0	1960.134	465.609	4203.199	3996.398	1777.456	1506.707
28.000	1.931	4860.156	1247.598	2729.333	0.0	1961.905	465.242	4207.411	3998.408	1780.264	1508.090
32.000	2.206	4862.456	1247.908	2731.113	0.0	1963.669	464.881	4211.643	4000.405	1783.093	1509.442
36.000	2.482	4864.756	1248.208	2732.892	0.0	1965.442	464.515	4215.860	4002.417	1785.902	1510.845
40.000	2.758	4867.056	1248.519	2734.673	0.0	1967.216	464.155	4220.096	4004.428	1788.725	1512.227
44.000	3.034	4869.356	1248.829	2736.454	0.0	1968.983	463.788	4224.334	4006.427	1791.563	1513.581
48.000	3.309	4871.656	1249.129	2738.235	0.0	1970.758	463.428	4228.558	4008.439	1794.371	1514.986
52.000	3.585	4873.957	1249.439	2740.029	0.0	1972.535	463.062	4232.800	4010.452	1797.203	1516.366
56.000	3.861	4876.278	1249.739	2741.812	0.0	1974.303	462.702	4237.045	4012.465	1800.039	1517.757
60.000	4.137	4878.579	1250.049	2743.596	0.0	1976.082	462.337	4241.275	4014.465	1802.857	1519.114
64.000	4.413	4880.880	1250.348	2745.380	0.0	1977.861	461.977	4245.525	4016.478	1805.687	1520.521
68.000	4.688	4883.181	1250.658	2747.164	0.0	1979.632	461.612	4249.759	4018.492	1808.515	1521.907
72.000	4.964	4885.482	1250.957	2748.949	0.0	1981.413	461.253	4254.013	4020.493	1811.347	1523.287
76.000	5.240	4887.804	1251.267	2750.735	0.0	1983.194	460.888	4258.269	4022.508	1814.187	1524.659
80.000	5.516	4890.105	1251.566	2752.534	0.0	1984.968	460.528	4262.510	4024.523	1817.013	1526.065
84.000	5.792	4892.407	1251.875	2754.321	0.0	1986.751	460.164	4266.770	4026.539	1819.855	1527.453
92.000	6.343	4897.012	1252.484	2757.897	0.0	1990.311	459.440	4275.280	4030.558	1825.529	1530.225
96.000	6.619	4899.314	1252.783	2759.698	0.0	1992.097	459.076	4279.547	4032.575	1828.374	1531.633
100.000	6.895	4901.616	1253.092	2761.487	0.0	1993.875	458.717	4283.799	4034.592	1831.207	1533.024
104.000	7.171	4903.939	1253.390	2763.277	0.0	1995.662	458.353	4288.070	4036.596	1834.055	1534.393
108.000	7.446	4906.242	1253.699	2765.068	0.0	1997.450	457.995	4292.344	4038.613	1836.899	1535.785
112.000	7.722	4908.545	1253.998	2766.859	0.0	1999.239	457.631	4296.603	4040.631	1839.732	1537.199
116.000	7.998	4910.848	1254.307	2768.651	0.0	2001.021	457.273	4300.881	4042.636	1842.587	1538.564
120.000	8.274	4913.151	1254.605	2770.444	0.0	2002.811	456.910	4305.161	4044.655	1845.440	1539.979

PRESSURE CALCULATIONS FOR CRYSTAL #1111
COMPLIANCE CONSTANTS AS A FUNCTION OF PRESSURE

P(KPSI)	P(KB)	S33	S44	S11	S44A	S66	S12	S13
0.015	0.001	0.2603410-03	0.8029140-03	0.6636730-03	0.0	0.5129390-03	-.3820170-03	-.8712590-04
4.000	0.276	0.2602410-03	0.8027210-03	0.6641020-03	0.0	0.5124770-03	-.3827070-03	-.8708380-04
8.000	0.552	0.2601400-03	0.8025200-03	0.6644540-03	0.0	0.5120160-03	-.3834100-03	-.8704010-04
12.000	0.827	0.2600420-03	0.8023270-03	0.6649800-03	0.0	0.5115530-03	-.3841100-03	-.8699930-04
16.000	1.103	0.2599390-03	0.8021270-03	0.6654140-03	0.0	0.5110900-03	-.3848080-03	-.8695440-04
20.000	1.379	0.2598410-03	0.8019330-03	0.6658620-03	0.0	0.5106310-03	-.3855170-03	-.8691350-04
24.000	1.655	0.2597410-03	0.8017330-03	0.6663100-03	0.0	0.5101690-03	-.3862260-03	-.8687080-04
28.000	1.931	0.2596400-03	0.8015400-03	0.6667430-03	0.0	0.5097090-03	-.3869200-03	-.8682810-04
32.000	2.206	0.2595370-03	0.8013410-03	0.6671950-03	0.0	0.5092510-03	-.3876350-03	-.8678300-04
36.000	2.482	0.2594400-03	0.8011480-03	0.6676400-03	0.0	0.5087910-03	-.3883380-03	-.8674280-04
40.000	2.758	0.2593400-03	0.8009490-03	0.6680920-03	0.0	0.5083330-03	-.3890490-03	-.8670050-04
44.000	3.034	0.2592380-03	0.8007500-03	0.6685520-03	0.0	0.5078770-03	-.3897720-03	-.8665540-04
48.000	3.309	0.2591400-03	0.8005580-03	0.6690000-03	0.0	0.5074190-03	-.3904750-03	-.8661550-04
52.000	3.585	0.2590400-03	0.8003590-03	0.6694530-03	0.0	0.5069620-03	-.3911880-03	-.8657260-04
56.000	3.861	0.2589400-03	0.8001670-03	0.6699170-03	0.0	0.5065080-03	-.3919100-03	-.8653040-04
60.000	4.137	0.2588390-03	0.7999690-03	0.6703710-03	0.0	0.5060520-03	-.3926230-03	-.8648620-04
64.000	4.413	0.2587410-03	0.7997770-03	0.6708350-03	0.0	0.5055970-03	-.3933420-03	-.8644610-04
68.000	4.688	0.2586430-03	0.7995790-03	0.6712980-03	0.0	0.5051440-03	-.3940620-03	-.8640420-04
72.000	4.964	0.2585430-03	0.7993880-03	0.6717650-03	0.0	0.5046900-03	-.3947860-03	-.8636170-04
76.000	5.240	0.2584410-03	0.7991900-03	0.6722360-03	0.0	0.5042370-03	-.3955150-03	-.8631800-04
80.000	5.516	0.2583440-03	0.7989990-03	0.6726960-03	0.0	0.5037860-03	-.3962280-03	-.8627770-04
84.000	5.792	0.2582460-03	0.7988010-03	0.6731710-03	0.0	0.5033340-03	-.3969590-03	-.8623590-04
92.000	6.343	0.2580480-03	0.7984130-03	0.6741200-03	0.0	0.5024340-03	-.3984170-03	-.8615200-04
96.000	6.619	0.2579510-03	0.7982230-03	0.6745950-03	0.0	0.5019840-03	-.3991460-03	-.8611160-04
100.000	6.895	0.2578530-03	0.7980260-03	0.6750710-03	0.0	0.5015360-03	-.3998740-03	-.8607030-04
104.000	7.171	0.2577510-03	0.7978360-03	0.6755550-03	0.0	0.5010870-03	-.4006140-03	-.8602630-04
108.000	7.446	0.2576530-03	0.7976390-03	0.6760390-03	0.0	0.5006380-03	-.4013510-03	-.8598500-04
112.000	7.722	0.2575570-03	0.7974500-03	0.6765200-03	0.0	0.5001900-03	-.4020800-03	-.8594570-04
116.000	7.998	0.2574570-03	0.7972530-03	0.6770120-03	0.0	0.4997430-03	-.4028270-03	-.8590180-04
120.000	8.274	0.2573610-03	0.7970640-03	0.6775060-03	0.0	0.4992980-03	-.4035710-03	-.8586230-04

PRESSURE CALCULATIONS FOR CRYSTAL #1111
VELOCITIES OF THE ELASTIC CONSTANTS AS A FUNCTION OF PRESSURE

P(KPSI)	P(KB)	V(C33)	V(C44)	V(C11)	V(C44A)	V(C66)	V(CPQ)	V(CTU)	V(CRS)	V(C12)	V(C13)
0.015	0.001	10.65848	5.40452	7.98228	0.0	6.76174	3.31222	9.89855	9.66654	6.42568	5.92802
4.000	0.276	10.66031	5.40481	7.98434	0.0	6.76434	3.31072	9.90285	9.66833	6.43034	5.93035
8.000	0.552	10.66213	5.40513	7.98644	0.0	6.76694	3.30920	9.90719	9.67012	6.43506	5.93267
12.000	0.827	10.66396	5.40543	7.98852	0.0	6.76956	3.30770	9.91153	9.67192	6.43976	5.93504
16.000	1.103	10.66578	5.40574	7.99060	0.0	6.77217	3.30618	9.91584	9.67370	6.44444	5.93732
20.000	1.379	10.66760	5.40604	7.99268	0.0	6.77477	3.30468	9.92018	9.67550	6.44915	5.93969
24.000	1.655	10.66943	5.40636	7.99476	0.0	6.77739	3.30316	9.92452	9.67730	6.45385	5.94202
28.000	1.931	10.67127	5.40665	7.99686	0.0	6.78001	3.30165	9.92884	9.67909	6.45852	5.94435
32.000	2.206	10.67310	5.40697	7.99894	0.0	6.78261	3.30015	9.93318	9.68087	6.46323	5.94663
36.000	2.482	10.67492	5.40727	8.00102	0.0	6.78523	3.29863	9.93750	9.68267	6.46790	5.94900
40.000	2.758	10.67674	5.40758	8.00310	0.0	6.78784	3.29714	9.94184	9.68447	6.47258	5.95133
44.000	3.034	10.67857	5.40790	8.00518	0.0	6.79044	3.29562	9.94618	9.68625	6.47729	5.95361
48.000	3.309	10.68039	5.40820	8.00726	0.0	6.79306	3.29412	9.95050	9.68805	6.48194	5.95598
52.000	3.585	10.68221	5.40851	8.00936	0.0	6.79568	3.29261	9.95484	9.68985	6.48663	5.95830
56.000	3.861	10.68404	5.40881	8.01145	0.0	6.79828	3.29111	9.95918	9.69165	6.49132	5.96064
60.000	4.137	10.68586	5.40913	8.01353	0.0	6.80090	3.28960	9.96350	9.69343	6.49597	5.96292
64.000	4.413	10.68771	5.40942	8.01561	0.0	6.80351	3.28811	9.96784	9.69523	6.50065	5.96529
68.000	4.688	10.68953	5.40974	8.01769	0.0	6.80612	3.28659	9.97216	9.69703	6.50531	5.96762
72.000	4.964	10.69135	5.41004	8.01978	0.0	6.80873	3.28510	9.97650	9.69881	6.50998	5.96994
76.000	5.240	10.69320	5.41035	8.02186	0.0	6.81135	3.28358	9.98084	9.70061	6.51466	5.97224
80.000	5.516	10.69502	5.41065	8.02396	0.0	6.81395	3.28209	9.98516	9.70241	6.51931	5.97460
84.000	5.792	10.69684	5.41097	8.02605	0.0	6.81657	3.28058	9.98950	9.70421	6.52398	5.97693
92.000	6.343	10.70049	5.41158	8.03021	0.0	6.82179	3.27757	9.99817	9.70780	6.53330	5.98158
96.000	6.619	10.70231	5.41188	8.03232	0.0	6.82441	3.27606	10.00251	9.70960	6.53796	5.98394
100.000	6.895	10.70414	5.41219	8.03440	0.0	6.82702	3.27457	10.00683	9.71140	6.54260	5.98627
104.000	7.171	10.70598	5.41249	8.03648	0.0	6.82963	3.27306	10.01117	9.71318	6.54727	5.98856
108.000	7.446	10.70780	5.41281	8.03857	0.0	6.83225	3.27157	10.01551	9.71498	6.55192	5.99089
112.000	7.722	10.70963	5.41310	8.04066	0.0	6.83487	3.27006	10.01983	9.71678	6.55655	5.99326
116.000	7.998	10.71145	5.41342	8.04274	0.0	6.83747	3.26857	10.02418	9.71857	6.56121	5.99553
120.000	8.274	10.71327	5.41372	8.04483	0.0	6.84009	3.26706	10.02852	9.72037	6.56587	5.99790

PRESSURE CALCULATIONS FOR CRYSTAL #1111
VOIGT,REUSS,HILL MODULI AND CORRESPONDING VELOCITIES

K(V) = VOIGT BULK MODULUS
U(V) = VOIGT SHEAR MODULUS
K(R) = REUSS BULK MODULUS
U(R) = REUSS SHEAR MODULUS
K(H) = HILL BULK MODULUS
U(H) = HILL SHEAR MODULUS
VS(V) = VOIGT SHEAR VELOCITY
VS(R) = REUSS SHEAR VELOCITY
VS(VRH) = VOIGT,REUSS,HILL SHEAR VELOCITY
VP(V) = VOIGT LONGITUDINAL VELOCITY
VP(R) = REUSS LONGITUDINAL VELOCITY
VP(VRH) = VOIGT,REUSS,HILL LONGITUDINAL VELOCITY

P	K(V)	U(V)	K(R)	U(R)	K(H)	U(H)	VS(V)	VS(R)	VS(VRH)	VP(V)	VP(R)	VP(VRH)
0.0	2199.188	1256.120	2104.601	1004.546	2151.894	1130.333	5.4276	4.8537	5.1487	9.5317	8.9872	9.2635
4.0	2201.064	1256.611	2106.609	1004.350	2153.836	1130.480	5.4283	4.8529	5.1487	9.5342	8.9889	9.2655
8.0	2202.955	1257.107	2108.638	1004.150	2155.797	1130.629	5.4290	4.8521	5.1487	9.5367	8.9906	9.2677
12.0	2204.853	1257.537	2110.667	1003.945	2157.760	1130.771	5.4297	4.8513	5.1486	9.5392	8.9923	9.2698
16.0	2206.726	1258.098	2112.678	1003.750	2159.702	1130.924	5.4304	4.8505	5.1487	9.5417	8.9939	9.2719
20.0	2208.627	1258.586	2114.711	1003.537	2161.669	1131.062	5.4311	4.8497	5.1486	9.5442	8.9956	9.2740
24.0	2210.518	1259.042	2116.738	1003.330	2163.628	1131.206	5.4318	4.8489	5.1486	9.5467	8.9973	9.2761
28.0	2212.412	1259.579	2118.764	1003.131	2165.588	1131.355	5.4326	4.8481	5.1486	9.5492	8.9990	9.2782
32.0	2214.293	1260.077	2120.784	1002.921	2167.539	1131.499	5.4333	4.8473	5.1486	9.5517	9.0007	9.2803
36.0	2216.192	1260.568	2122.813	1002.712	2169.503	1131.640	5.4340	4.8464	5.1486	9.5542	9.0024	9.2824
40.0	2218.084	1261.066	2124.841	1002.500	2171.463	1131.783	5.4347	4.8456	5.1486	9.5568	9.0041	9.2845
44.0	2219.968	1261.564	2126.864	1002.283	2173.416	1131.924	5.4354	4.8448	5.1486	9.5593	9.0057	9.2866
48.0	2221.868	1262.055	2128.893	1002.072	2175.381	1132.064	5.4361	4.8439	5.1485	9.5618	9.0074	9.2887
52.0	2223.765	1262.555	2130.927	1001.860	2177.346	1132.207	5.4368	4.8431	5.1485	9.5643	9.0091	9.2908
56.0	2225.668	1263.046	2132.962	1001.636	2179.315	1132.341	5.4375	4.8422	5.1485	9.5668	9.0108	9.2929
60.0	2227.549	1263.548	2134.980	1001.424	2181.264	1132.486	5.4383	4.8414	5.1485	9.5693	9.0124	9.2950
64.0	2229.455	1264.035	2137.017	1001.199	2183.236	1132.619	5.4390	4.8406	5.1485	9.5718	9.0141	9.2971
68.0	2231.352	1264.535	2139.048	1000.978	2185.200	1132.756	5.4397	4.8397	5.1484	9.5743	9.0158	9.2992
72.0	2233.247	1265.029	2141.078	1000.752	2187.162	1132.891	5.4404	4.8389	5.1484	9.5768	9.0174	9.3013
76.0	2235.143	1265.530	2143.109	1000.526	2189.126	1133.028	5.4411	4.8380	5.1484	9.5793	9.0191	9.3034
80.0	2237.051	1266.022	2145.148	1000.305	2191.100	1133.163	5.4418	4.8371	5.1484	9.5818	9.0208	9.3055
84.0	2238.953	1266.520	2147.184	1000.074	2193.068	1133.297	5.4425	4.8363	5.1483	9.5843	9.0224	9.3076
92.0	2242.751	1267.511	2151.251	999.612	2197.001	1133.561	5.4439	4.8345	5.1481	9.5893	9.0257	9.3118
96.0	2244.665	1268.004	2153.298	999.378	2198.982	1133.691	5.4447	4.8336	5.1482	9.5918	9.0274	9.3139
100.0	2246.567	1268.501	2155.332	999.147	2200.949	1133.824	5.4454	4.8328	5.1482	9.5943	9.0290	9.3160
104.0	2248.464	1268.999	2157.365	998.909	2202.914	1133.954	5.4461	4.8319	5.1482	9.5968	9.0307	9.3180
108.0	2250.368	1269.497	2159.403	998.671	2204.886	1134.084	5.4468	4.8310	5.1481	9.5993	9.0323	9.3201
112.0	2252.281	1269.989	2161.444	998.433	2206.862	1134.211	5.4475	4.8301	5.1481	9.6018	9.0340	9.3222
116.0	2254.176	1270.489	2163.477	998.190	2208.826	1134.340	5.4482	4.8292	5.1480	9.6043	9.0356	9.3243
120.0	2256.093	1270.980	2165.525	997.941	2210.809	1134.461	5.4489	4.8283	5.1480	9.6068	9.0372	9.3264

PRESSURE CALCULATIONS FOR CRYSTAL #1111
VOIGT,REUSS AND HILL MEAN VELOCITIES AND CORRESPONDING DEBYE TEMPERATURE

VM(V) = MEAN VELOCITY
VM(R) = REUSS MEAN VELOCITY
VM(VRH) = VOIGT,REUSS,HILL MEAN VELOCITY
SIG(V) = POISSONS RATIO USING VOIGT VELOCITIES
SIG(R) = POISSONS RATIO USING REUSS VELOCITIES
SIG(VRH) = POISSONS RATIO USING VRH VELOCITIES
DT(V) = DEBYE TEMPERATURE USING VM(V)
DT(R) = DEBYE TEMPERATURE USING VM(R)
DT(VRH) = DEBYE TEMPERATURE USING VM(VRH)
A = SHEAR ANISOTROPY
RHO = DENSITY

P	VM(V)	VM(R)	VM(VRH)	SIG(V)	SIG(R)	SIG(VRH)	DT(V)	DT(R)	DT(VRH)	A	RHO
0.0	6.0328	5.4175	5.7341	0.2601	0.2941	0.2765	822.8873	738.9530	782.1455	0.1054	4.2640
4.0	6.0337	5.4167	5.7342	0.2602	0.2943	0.2766	823.0391	738.8837	782.1934	0.1057	4.2646
8.0	6.0345	5.4160	5.7343	0.2603	0.2945	0.2768	823.1927	738.8130	782.2416	0.1059	4.2651
12.0	6.0354	5.4152	5.7344	0.2604	0.2947	0.2769	823.3442	738.7405	782.2878	0.1062	4.2657
16.0	6.0363	5.4145	5.7345	0.2605	0.2949	0.2771	823.4991	738.6713	782.3375	0.1065	4.2663
20.0	6.0371	5.4137	5.7346	0.2606	0.2951	0.2772	823.6500	738.5963	782.3823	0.1067	4.2668
24.0	6.0380	5.4129	5.7347	0.2607	0.2953	0.2774	823.8035	738.5228	782.4292	0.1070	4.2674
28.0	6.0388	5.4122	5.7348	0.2607	0.2955	0.2775	823.9569	738.4525	782.4776	0.1073	4.2679
32.0	6.0397	5.4114	5.7349	0.2608	0.2957	0.2777	824.1109	738.3781	782.5244	0.1075	4.2685
36.0	6.0405	5.4106	5.7350	0.2609	0.2960	0.2778	824.2626	738.3040	782.5701	0.1078	4.2691
40.0	6.0414	5.4098	5.7351	0.2610	0.2962	0.2780	824.4162	738.2291	782.6166	0.1081	4.2696
44.0	6.0423	5.4090	5.7352	0.2611	0.2964	0.2781	824.5701	738.1522	782.6622	0.1083	4.2702
48.0	6.0431	5.4082	5.7352	0.2612	0.2966	0.2783	824.7219	738.0773	782.7077	0.1086	4.2707
52.0	6.0440	5.4074	5.7353	0.2613	0.2968	0.2784	824.8761	738.0021	782.7542	0.1089	4.2713
56.0	6.0448	5.4066	5.7354	0.2614	0.2970	0.2786	825.0279	737.9228	782.7977	0.1091	4.2718
60.0	6.0457	5.4058	5.7355	0.2615	0.2972	0.2787	825.1827	737.8477	782.8447	0.1094	4.2724
64.0	6.0465	5.4050	5.7356	0.2616	0.2974	0.2789	825.3342	737.7680	782.8879	0.1097	4.2730
68.0	6.0474	5.4042	5.7356	0.2617	0.2976	0.2790	825.4873	737.6896	782.9325	0.1099	4.2735
72.0	6.0483	5.4034	5.7357	0.2618	0.2978	0.2791	825.6399	737.6096	782.9761	0.1102	4.2741
76.0	6.0491	5.4026	5.7358	0.2618	0.2980	0.2793	825.7943	737.5296	783.0207	0.1105	4.2746
80.0	6.0500	5.4018	5.7359	0.2619	0.2982	0.2794	825.9461	737.4510	783.0645	0.1108	4.2752
84.0	6.0508	5.4009	5.7359	0.2620	0.2984	0.2796	826.0995	737.3692	783.1078	0.1110	4.2757
92.0	6.0526	5.3993	5.7361	0.2622	0.2988	0.2799	826.4051	737.2052	783.1936	0.1116	4.2768
96.0	6.0534	5.3984	5.7361	0.2623	0.2990	0.2800	826.5571	737.1224	783.2357	0.1118	4.2774
100.0	6.0543	5.3976	5.7362	0.2624	0.2992	0.2802	826.7102	737.0404	783.2788	0.1121	4.2780
104.0	6.0551	5.3967	5.7363	0.2625	0.2994	0.2803	826.8636	736.9557	783.3208	0.1124	4.2785
108.0	6.0560	5.3959	5.7363	0.2626	0.2996	0.2805	827.0172	736.8713	783.3631	0.1127	4.2791
112.0	6.0568	5.3950	5.7364	0.2627	0.2999	0.2806	827.1688	736.7867	783.4042	0.1130	4.2796
116.0	6.0577	5.3942	5.7364	0.2628	0.3001	0.2808	827.3227	736.7006	783.4459	0.1132	4.2802
120.0	6.0586	5.3933	5.7365	0.2629	0.3003	0.2809	827.4740	736.6122	783.4851	0.1135	4.2807

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS DENSITY

PRESS	DENSITY	Y/Y0
0.0150000	0.42640CCD 01	1.0000000
4.0000000	0.4264562D 01	1.0001317
8.0000000	0.4265125D 01	1.0002638
12.0000000	0.4265688D 01	1.0003958
16.0000000	0.4266250D 01	1.0005277
20.0000000	0.4266812D 01	1.0006595
24.0000000	0.4267374D 01	1.0007912
28.0000000	0.4267935D 01	1.0009227
32.0000000	0.4268495D 01	1.0010542
36.0000000	0.4269055D 01	1.0011855
40.0000000	0.4269615D 01	1.0013168
44.0000000	0.4270174D 01	1.0014479
48.0000000	0.4270733D 01	1.0015789
52.0000000	0.4271291D 01	1.0017098
56.0000000	0.4271849D 01	1.0018407
60.0000000	0.4272406D 01	1.0019714
64.0000000	0.4272963D 01	1.0021019
68.0000000	0.4273519D 01	1.0022324
72.0000000	0.4274075D 01	1.0023628
76.0000000	0.4274631D 01	1.0024931
80.0000000	0.4275186D 01	1.0026232
84.0000000	0.4275740D 01	1.0027533
92.0000000	0.4276848D 01	1.0030132
96.0000000	0.4277402D 01	1.0031430
100.0000000	0.4277954D 01	1.0032726
104.0000000	0.4278507D 01	1.0034021
108.0000000	0.4279058D 01	1.0035315
112.0000000	0.4279610D 01	1.0036609
116.0000000	0.4280161D 01	1.0037901
120.0000000	0.4280711D 01	1.0039192

SLOPE = 0.0001
VARIANCE = 0.75D-14
STD DEV = 0.00000
INTERCEPT = 4.264C
CORR. COEFF. = 0.99999D 00
SLOPE PER KB = 0.0020

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS COMP PERPENDICULAR TO C

PRESS	COMP PDTC	Y/Y0
0.0150000	0.1962761D-03	1.0000000
4.CC00000	0.1960557D-03	0.9988768
8.CC00000	0.1958321D-03	0.9977376
12.C000000	0.1956105D-03	0.9966089
16.0C00000	0.1953895D-03	0.9954828
20.C000000	0.1951683D-03	0.9943555
24.CCC0000	0.1949473D-03	0.9932298
28.0000000	0.1947272D-03	0.9921085
32.C000000	0.1945066D-03	0.9909845
36.0000000	0.1942879D-03	0.9898703
40.C000000	0.1940688D-03	0.9887539
44.0000000	0.1938490D-03	0.9876339
48.C000000	0.1936317D-03	0.9865270
52.C000000	0.1934127D-03	0.9854112
56.0000000	0.1931948D-03	0.9843009
60.0000000	0.1929778D-03	0.9831956
64.CC00000	0.1927611D-03	0.9820914
68.C0C0000	0.1925447D-03	0.9809888
72.0C00000	0.1923284D-03	0.9798870
76.CC00000	0.1921123D-03	0.9787858
80.C000000	0.1918968D-03	0.9776879
84.0000000	0.1916814D-03	0.9765904
92.C000000	0.1912523D-03	0.9744044
96.C000000	0.1910375D-03	0.9733100
100.C000000	0.1908243D-03	0.9722236
104.0000000	0.1906106D-03	0.9711350
108.0000000	0.1903977D-03	0.9700500
112.CC00000	0.1901859D-03	0.9689708
116.0000000	0.1899729D-03	0.9678858
120.C000000	0.1897609D-03	0.9668056

SLOPE = -C.C000
VARIANCE = 0.48D-20
STD DEV = 0.C0000
INTERCEPT = 0.0002
CORR. COEFF. = -0.99998D 00
SLOPE PER KB = -0.0C00

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS COMP PARALLEL TO C

PRESS	COMP PLTC	Y/Y0
0.0150000	0.8686213D-04	1.0000000
4.0000000	0.8684613D-04	0.9998157
8.0000000	0.8683234D-04	0.9996570
12.0000000	0.8681545D-04	0.9994625
16.0000000	0.8680248D-04	0.9993132
20.0000000	0.8678585D-04	0.9991218
24.0000000	0.8677055D-04	0.9989502
28.0000000	0.8675517D-04	0.9987686
32.0000000	0.8674281D-04	0.9986262
36.0000000	0.8672544D-04	0.9984263
40.0000000	0.8671027D-04	0.9982517
44.0000000	0.8669804D-04	0.9981108
48.0000000	0.8668043D-04	0.9979081
52.0000000	0.8666615D-04	0.9977438
56.0000000	0.8665020D-04	0.9975601
60.0000000	0.8663701D-04	0.9974083
64.0000000	0.8661993D-04	0.9972117
68.0000000	0.8660456D-04	0.9970347
72.0000000	0.8658989D-04	0.9968658
76.0000000	0.8657557D-04	0.9967009
80.0000000	0.8655889D-04	0.9965089
84.0000000	0.8654374D-04	0.9963345
92.0000000	0.8651355D-04	0.9959869
96.0000000	0.8649729D-04	0.9957997
100.0000000	0.8648160D-04	0.9956191
104.0000000	0.8646778D-04	0.9954600
108.0000000	0.8645235D-04	0.9952824
112.0000000	0.8643474D-04	0.9950796
116.0000000	0.8642157D-04	0.9949326
120.0000000	0.8640450D-04	0.9947361

SLOPE = -0.0000
VARIANCE = 0.35D-22
STD DEV = 0.00000
INTERCEPT = 0.0001
CORR. COEFF. = -0.99997D 00
SLOPE PER KB = -0.0000

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS VOLUMETRIC COMP

PRESS	VOL COMP	Y/YO
0.0150000	0.4794144D-03	1.0000000
4.CCC0000	0.4789575D-03	0.9990469
8.CCC0000	0.4784965D-03	0.9980854
12.0000000	0.4780365D-03	0.9971259
16.C000000	0.4775815D-03	0.9961768
20.C000000	0.4771224D-03	0.9952191
24.C000000	0.4766656D-03	0.9942663
28.CCC0000	0.4762056D-03	0.9933152
32.C000000	0.4757560D-03	0.9923690
36.0000000	0.4753013D-03	0.9914205
40.CCC0000	0.4748479D-03	0.9904747
44.C000000	0.4743960D-03	0.9895322
48.C000000	0.4739439D-03	0.9885891
52.C000000	0.4734916D-03	0.9876456
56.C000000	0.4730398D-03	0.9867033
60.CC00000	0.4725927D-03	0.9857707
64.0000000	0.4721422D-03	0.9848310
68.C000000	0.4716940D-03	0.9838961
72.C000000	0.4712468D-03	0.9829633
76.CC00000	0.4708002D-03	0.9820318
80.0000000	0.4703525D-03	0.9810980
84.CC00000	0.4699065D-03	0.9801677
92.0000000	0.4690182D-03	0.9783148
96.CC00000	0.4685723D-03	0.9773848
100.CC00000	0.4681302D-03	0.9764625
104.C000000	0.4676891D-03	0.9755423
108.0000000	0.4672477D-03	0.9746217
112.CC00000	0.4668065D-03	0.9737013
116.C000000	0.4663677D-03	0.9727862
120.C000000	0.4659267D-03	0.9718662

SLOPE = -0.0000
VARIANCE = 0.18D-19
STD DEV = 0.CC000
INTERCEPT = 0.0005
CORR. COEFF. = -0.99998D 00
SLOPE PER KB = -0.CCC0

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C33

PRESS	C33	Y/Y0
0.0150000	0.4844043D 04	1.0000000
4.0000000	0.4846340D 04	1.0004742
8.0000000	0.4848639D 04	1.0009488
12.0000000	0.4850938D 04	1.0014234
16.0000000	0.4853237D 04	1.0018980
20.0000000	0.4855537D 04	1.0023727
24.0000000	0.4857836D 04	1.0028474
28.0000000	0.4860156D 04	1.0033263
32.0000000	0.4862456D 04	1.0038011
36.0000000	0.4864756D 04	1.0042759
40.0000000	0.4867056D 04	1.0047507
44.0000000	0.4869356D 04	1.0052256
48.0000000	0.4871656D 04	1.0057005
52.0000000	0.4873957D 04	1.0061754
56.0000000	0.4876278D 04	1.0066545
60.0000000	0.4878579D 04	1.0071295
64.0000000	0.4880880D 04	1.0076045
68.0000000	0.4883181D 04	1.0080796
72.0000000	0.4885482D 04	1.0085546
76.0000000	0.4887804D 04	1.0090340
80.0000000	0.4890105D 04	1.0095091
84.0000000	0.4892407D 04	1.0099843
92.0000000	0.4897012D 04	1.0109348
96.0000000	0.4899314D 04	1.0114101
100.0000000	0.4901616D 04	1.0118854
104.0000000	0.4903939D 04	1.0123649
108.0000000	0.4906242D 04	1.0128403
112.0000000	0.4908545D 04	1.0133157
116.0000000	0.4910848D 04	1.0137911
120.0000000	0.4913151D 04	1.0142666

SLOPE = 0.5760
VARIANCE = 0.20D-08
STD DEV = 0.00005
INTERCEPT = 4844.0204
CORR. COEFF. = 0.100000 01
SLOPE PER KB = 8.3547

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C44

PRESS	C44	Y/Y0
0.0150000	0.1245463D 04	1.0000000
4.0000000	0.1245763D 04	1.0002412
8.0000000	0.1246075D 04	1.0004910
12.0000000	0.1246375D 04	1.0007324
16.0000000	0.1246686D 04	1.0009820
20.0000000	0.1246987D 04	1.0012233
24.0000000	0.1247297D 04	1.0014728
28.0000000	0.1247598D 04	1.0017139
32.0000000	0.1247908D 04	1.0019633
36.0000000	0.1248208D 04	1.0022043
40.0000000	0.1248519D 04	1.0024535
44.0000000	0.1248829D 04	1.0027026
48.0000000	0.1249129D 04	1.0029434
52.0000000	0.1249439D 04	1.0031924
56.0000000	0.1249739D 04	1.0034330
60.0000000	0.1250049D 04	1.0036819
64.0000000	0.1250348D 04	1.0039223
68.0000000	0.1250658D 04	1.0041711
72.0000000	0.1250957D 04	1.0044114
76.0000000	0.1251267D 04	1.0046600
80.0000000	0.1251566D 04	1.0049002
84.0000000	0.1251875D 04	1.0051487
92.0000000	0.1252484D 04	1.0056372
96.0000000	0.1252783D 04	1.0058771
100.0000000	0.1253092D 04	1.0061253
104.0000000	0.1253390D 04	1.0063651
108.0000000	0.1253699D 04	1.0066131
112.0000000	0.1253998D 04	1.0068528
116.0000000	0.1254307D 04	1.0071007
120.0000000	0.1254605D 04	1.0073402

SLOPE = 0.0762
VARIANCE = 0.670-09
STD DEV = 0.00003
INTERCEPT = 1245.4665
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 1.1058

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C11

PRESS	C11	Y/Y0
0.0150000	0.2716885D 04	1.0000000
4.0000000	0.2718648D 04	1.0006488
8.0000000	0.2720435D 04	1.0013067
12.0000000	0.2722211D 04	1.0019604
16.0000000	0.2723988D 04	1.0026144
20.0000000	0.2725765D 04	1.0032685
24.0000000	0.2727543D 04	1.0039229
28.0000000	0.2729333D 04	1.0045819
32.0000000	0.2731113D 04	1.0052367
36.0000000	0.2732892D 04	1.0058918
40.0000000	0.2734673D 04	1.0065471
44.0000000	0.2736454D 04	1.0072026
48.0000000	0.2738235D 04	1.0078584
52.0000000	0.2740029D 04	1.0085187
56.0000000	0.2741812D 04	1.0091749
60.0000000	0.2743596D 04	1.0098313
64.0000000	0.2745380D 04	1.0104880
68.0000000	0.2747164D 04	1.0111448
72.0000000	0.2748949D 04	1.0118019
76.0000000	0.2750735D 04	1.0124592
80.0000000	0.2752534D 04	1.0131211
84.0000000	0.2754321D 04	1.0137789
92.0000000	0.2757897D 04	1.0150951
96.0000000	0.2759698D 04	1.0157580
100.0000000	0.2761487D 04	1.0164166
104.0000000	0.2763277D 04	1.0170755
108.0000000	0.2765068D 04	1.0177346
112.0000000	0.2766859D 04	1.0183940
116.0000000	0.2768651D 04	1.0190535
120.0000000	0.2770444D 04	1.0197133

SLOPE = 0.4464
VARIANCE = 0.13D-07
STD DEV = 0.00012
INTERCEPT = 2716.8328
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 6.4751

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C66

PRESS	C66	Y/Y0
0.0150000	0.1949548D 04	1.0000000
4.0000000	0.1951306D 04	1.0009016
8.0000000	0.1953065D 04	1.0018038
12.0000000	0.1954833D 04	1.0027108
16.0000000	0.1956602D 04	1.0036182
20.0000000	0.1958363D 04	1.0045216
24.0000000	0.1960134D 04	1.0054299
28.0000000	0.1961905D 04	1.0063386
32.0000000	0.1963669D 04	1.0072432
36.0000000	0.1965442D 04	1.0081528
40.0000000	0.1967216D 04	1.0090628
44.0000000	0.1968983D 04	1.0099687
48.0000000	0.1970758D 04	1.0108796
52.0000000	0.1972535D 04	1.0117908
56.0000000	0.1974303D 04	1.0126981
60.0000000	0.1976082D 04	1.0136102
64.0000000	0.1977861D 04	1.0145227
68.0000000	0.1979632D 04	1.0154312
72.0000000	0.1981413D 04	1.0163446
76.0000000	0.1983194D 04	1.0172584
80.0000000	0.1984968D 04	1.0181682
84.0000000	0.1986751D 04	1.0190829
92.0000000	0.1990311D 04	1.0209091
96.0000000	0.1992097D 04	1.0218250
100.0000000	0.1993875D 04	1.0227370
104.0000000	0.1995662D 04	1.0236538
108.0000000	0.1997450D 04	1.0245710
112.0000000	0.1999239D 04	1.0254887
116.0000000	0.2001021D 04	1.0264023
120.0000000	0.2002811D 04	1.0273208

SLOPE = 0.4439
VARIANCE = 0.25D-07
STD DEV = 0.00016
INTERCEPT = 1949.4795
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 6.4387

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C12

PRESS	C12	Y/Y0
0.0150000	0.1760578D 04	1.0000000
4.0000000	0.1763364D 04	1.0015822
8.0000000	0.1766151D 04	1.0031879
12.0000000	0.1769004D 04	1.0047862
16.0000000	0.1771808D 04	1.0063786
20.0000000	0.1774633D 04	1.0079832
24.0000000	0.1777456D 04	1.0095869
28.0000000	0.1780264D 04	1.0111815
32.0000000	0.1783053D 04	1.0127882
36.0000000	0.1785902D 04	1.0143841
40.0000000	0.1788725D 04	1.0159874
44.0000000	0.1791563D 04	1.0175994
48.0000000	0.1794371D 04	1.0191943
52.0000000	0.1797203D 04	1.0208029
56.0000000	0.1800039D 04	1.0224138
60.0000000	0.1802857D 04	1.0240140
64.0000000	0.1805687D 04	1.0256215
68.0000000	0.1808515D 04	1.0272280
72.0000000	0.1811347D 04	1.0288368
76.0000000	0.1814187D 04	1.0304496
80.0000000	0.1817013D 04	1.0320550
84.0000000	0.1819855D 04	1.0336692
92.0000000	0.1825529D 04	1.0368917
96.0000000	0.1828374D 04	1.0385080
100.0000000	0.1831207D 04	1.0401169
104.0000000	0.1834055D 04	1.0417346
108.0000000	0.1836899D 04	1.0433499
112.0000000	0.1839732D 04	1.0449591
116.0000000	0.1842587D 04	1.0465807
120.0000000	0.1845440D 04	1.0482013

SLOPE = 0.7073
VARIANCE = 0.57D-07
STD DEV = 0.00024
INTERCEPT = 1760.4734
CORR. COEFF. = 0.100000 01
SLOPE PER KB = 10.2581

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C13

PRESS	C13	Y/Y0
0.0150000	0.149843CD 04	1.0000000
4.CCC0000	0.14998C4D 04	1.0009169
8.CC00000	0.1501177D 04	1.0018334
12.C000000	0.1502577D 04	1.0027673
16.C000000	0.1503926D 04	1.0036682
20.CC00000	0.1505327D 04	1.0046030
24.CC00000	0.1506707D 04	1.0055238
28.C000000	0.1508090D 04	1.0064467
32.CCC0000	0.1509442D 04	1.0073492
36.C000000	0.1510845D 04	1.0082855
40.CC00000	0.1512227D 04	1.0092079
44.CC00000	0.1513581D 04	1.0101116
48.CC00000	0.1514966D 04	1.0110491
52.C000000	0.1516366D 04	1.0119700
56.CCC0000	0.1517757D 04	1.0128983
60.CC00000	0.1519114D 04	1.0138035
64.C000000	0.1520521D 04	1.0147426
68.CC00000	0.1521907D 04	1.0156678
72.C000000	0.1523287D 04	1.0165885
76.C000000	0.1524659D 04	1.0175045
80.C000000	0.1526065D 04	1.0184425
84.CC00000	0.1527453D 04	1.0193692
92.C000000	0.1530225D 04	1.0212188
96.CC00000	0.1531633D 04	1.0221584
100.C00C000	0.1533024D 04	1.0230867
104.CC00000	0.1534393D 04	1.0240005
108.CC00000	0.1535785D 04	1.0249296
112.C000000	0.1537199D 04	1.0258735
116.C000000	0.1538564D 04	1.0267841
120.CC00000	0.1539979D 04	1.0277287

SLOPE = 0.3462
VARIANCE = 0.17D-07
STD DEV = 0.00013
INTERCEPT = 1498.3876
CORR. COEFF. = 0.1C000D 01
SLOPE PER KB = 5.0209

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C33 VELOCITY

PRESS	C33 VEL	Y/Y0
0.0150000	0.1065848D 02	1.0000000
4.0000000	0.1066031D 02	1.0001712
8.0000000	0.1066213D 02	1.0003423
12.0000000	0.1066396D 02	1.0005135
16.0000000	0.1066578D 02	1.0006846
20.0000000	0.1066760D 02	1.0008557
24.0000000	0.1066943D 02	1.0010268
28.0000000	0.1067127D 02	1.0012000
32.0000000	0.1067310D 02	1.0013711
36.0000000	0.1067492D 02	1.0015422
40.0000000	0.1067674D 02	1.0017132
44.0000000	0.1067857D 02	1.0018843
48.0000000	0.1068039D 02	1.0020554
52.0000000	0.1068221D 02	1.0022265
56.0000000	0.1068404D 02	1.0023996
60.0000000	0.1068588D 02	1.0025707
64.0000000	0.1068771D 02	1.0027418
68.0000000	0.1068953D 02	1.0029128
72.0000000	0.1069135D 02	1.0030839
76.0000000	0.1069320D 02	1.0032570
80.0000000	0.1069502D 02	1.0034280
84.0000000	0.1069684D 02	1.0035991
92.0000000	0.1070049D 02	1.0039411
96.0000000	0.1070231D 02	1.0041122
100.0000000	0.1070414D 02	1.0042832
104.0000000	0.1070598D 02	1.0044563
108.0000000	0.1070780D 02	1.0046273
112.0000000	0.1070963D 02	1.0047983
116.0000000	0.1071145D 02	1.0049693
120.0000000	0.1071327D 02	1.0051403

SLOPE = 0.0005
VARIANCE = 0.11D-14
STD DEV = 0.00000
INTERCEPT = 10.6585
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 0.0066

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C44 VELOCITY

PRESS	C44 VEL	Y/Y0
0.0150000	0.5404516D 01	1.0000000
4.0000000	0.5404812D 01	1.0000548
8.0000000	0.5405130D 01	1.0001136
12.0000000	0.5405425D 01	1.0001682
16.0000000	0.5405743D 01	1.0002270
20.0000000	0.5406038D 01	1.0002817
24.0000000	0.5406356D 01	1.0003405
28.0000000	0.5406652D 01	1.0003952
32.0000000	0.5406970D 01	1.0004540
36.0000000	0.5407265D 01	1.0005086
40.0000000	0.5407583D 01	1.0005674
44.0000000	0.5407901D 01	1.0006262
48.0000000	0.5408196D 01	1.0006809
52.0000000	0.5408514D 01	1.0007397
56.0000000	0.5408809D 01	1.0007944
60.0000000	0.5409127D 01	1.0008532
64.0000000	0.5409423D 01	1.0009079
68.0000000	0.5409741D 01	1.0009667
72.0000000	0.5410036D 01	1.0010214
76.0000000	0.5410354D 01	1.0010802
80.0000000	0.5410650D 01	1.0011349
84.0000000	0.5410967D 01	1.0011937
92.0000000	0.5411581D 01	1.0013072
96.0000000	0.5411876D 01	1.0013619
100.0000000	0.5412194D 01	1.0014207
104.0000000	0.5412490D 01	1.0014754
108.0000000	0.5412808D 01	1.0015342
112.0000000	0.5413103D 01	1.0015889
116.0000000	0.5413421D 01	1.0016477
120.0000000	0.5413717D 01	1.0017024

SLOPE = 0.0001
VARIANCE = 0.11D-14
STD DEV = 0.00000
INTERCEPT = 5.4045
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 0.0011

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C11 VELOCITY

PRESS	C11 VEL	Y/YO
0.0150000	0.7982281D 01	1.0000000
4.0000000	0.7984345D 01	1.0002585
8.0000000	0.7986441D 01	1.0005212
12.0000000	0.7988521D 01	1.0007817
16.0000000	0.7990601D 01	1.0010422
20.0000000	0.7992681D 01	1.0013028
24.0000000	0.7994761D 01	1.0015634
28.0000000	0.7996859D 01	1.0018262
32.0000000	0.7998939D 01	1.0020869
36.0000000	0.8001020D 01	1.0023476
40.0000000	0.8003102D 01	1.0026083
44.0000000	0.8005183D 01	1.0028691
48.0000000	0.8007265D 01	1.0031299
52.0000000	0.8009364D 01	1.0033929
56.0000000	0.8011446D 01	1.0036537
60.0000000	0.8013529D 01	1.0039146
64.0000000	0.8015611D 01	1.0041755
68.0000000	0.8017694D 01	1.0044364
72.0000000	0.8019777D 01	1.0046974
76.0000000	0.8021861D 01	1.0049584
80.0000000	0.8023961D 01	1.0052216
84.0000000	0.8026045D 01	1.0054826
92.0000000	0.8030213D 01	1.0060048
96.0000000	0.8032315D 01	1.0062681
100.0000000	0.8034400D 01	1.0065293
104.0000000	0.8036485D 01	1.0067905
108.0000000	0.8038570D 01	1.0070517
112.0000000	0.8040655D 01	1.0073130
116.0000000	0.8042741D 01	1.0075742
120.0000000	0.8044827D 01	1.0078356

SLOPE = 0.0005
VARIANCE = 0.25D-14
STD DEV = 0.00000
INTERCEPT = 7.9823
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 0.0076

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C66 VELOCITY

PRESS	C66 VEL	Y/Y0
0.0150000	0.67617380 01	1.0000000
4.0000000	0.6764341D 01	1.0003848
8.0000000	0.6766941D 01	1.0007695
12.0000000	0.6769557D 01	1.0011563
16.0000000	0.6772173D 01	1.0015432
20.0000000	0.6774775D 01	1.0019279
24.0000000	0.6777391D 01	1.0023148
28.0000000	0.6780007D 01	1.0027018
32.0000000	0.6782609D 01	1.0030865
36.0000000	0.6785225D 01	1.0034735
40.0000000	0.6787842D 01	1.0038605
44.0000000	0.6790444D 01	1.0042452
48.0000000	0.6793061D 01	1.0046323
52.0000000	0.6795678D 01	1.0050193
56.0000000	0.6798280D 01	1.0054041
60.0000000	0.6800897D 01	1.0057912
64.0000000	0.6803514D 01	1.0061783
68.0000000	0.6806117D 01	1.0065632
72.0000000	0.6808734D 01	1.0069503
76.0000000	0.6811352D 01	1.0073374
80.0000000	0.6813955D 01	1.0077223
84.0000000	0.6816573D 01	1.0081095
92.0000000	0.6821794D 01	1.0088816
96.0000000	0.6824412D 01	1.0092688
100.0000000	0.6827015D 01	1.0096538
104.0000000	0.6829634D 01	1.0100411
108.0000000	0.6832252D 01	1.0104283
112.0000000	0.6834871D 01	1.0108156
116.0000000	0.6837475D 01	1.0112007
120.0000000	0.6840094D 01	1.0115880

SLOPE = 0.0007
VARIANCE = 0.94D-15
STD DEV = 0.00000
INTERCEPT = 6.7617
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 0.0095

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C12 VELOCITY

PRESS	C12 VEL	Y/YO
0.0150000	0.6425679D 01	1.0000000
4.CC00000	0.6430337D 01	1.0007249
8.CC00000	0.6435064D 01	1.0014606
12.0000000	0.6439764D 01	1.0021919
16.CC00000	0.6444440D 01	1.0029197
20.0CC0000	0.6449151D 01	1.0036528
24.CC00000	0.6453854D 01	1.0043848
28.C000000	0.6458524D 01	1.0051116
32.CC00000	0.6463229D 01	1.0058437
36.CC00000	0.6467895D 01	1.0065699
40.C000000	0.647258CD 01	1.0072990
44.0000000	0.6477289D 01	1.0080318
48.C000000	0.6481939D 01	1.0087555
52.C000000	0.6486628D 01	1.0094852
56.CC00000	0.6491321D 01	1.0102155
60.C000000	0.6495975D 01	1.0109398
64.CC00000	0.6500648D 01	1.0116670
68.C000000	0.6505313D 01	1.0123931
72.CC00000	0.6509982D 01	1.0131197
76.CC00000	0.6514660D 01	1.0138476
8C.CC00000	0.6519 3C9D 01	1.0145712
84.C000000	0.6523982D 01	1.0152985
92.C000000	0.6533297D 01	1.0167481
96.CC00000	0.6537964D 01	1.0174744
100.CC00000	0.6542604D 01	1.0181965
104.0000000	0.6547267D 01	1.0189222
108.CC00000	0.6551919D 01	1.0196461
112.CC00000	0.6556547D 01	1.0203664
116.C000000	0.6561210D 01	1.0210921
120.0000000	0.6565866D 01	1.0218166

SLOPE = 0.0012
VARIANCE = 0.14D-12
STD DEV = 0.C0000
INTERCEPT = 6.4258
CORR. COEFF. = 0.100000 01
SLOPE PER KB = 0.0169

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS C13 VELOCITY

PRESS	C13 VEL	Y/Y0
0.0150000	0.5928019D 01	1.0000000
4.0000000	0.5930346D 01	1.0003924
8.0000000	0.5932669D 01	1.0007843
12.0000000	0.5935042D 01	1.0011846
16.0000000	0.5937316D 01	1.0015682
20.0000000	0.5939689D 01	1.0019685
24.0000000	0.5942019D 01	1.0023617
28.0000000	0.5944355D 01	1.0027556
32.0000000	0.5946629D 01	1.0031392
36.0000000	0.5949002D 01	1.0035395
40.0000000	0.5951332D 01	1.0039327
44.0000000	0.5953606D 01	1.0043162
48.0000000	0.5955979D 01	1.0047165
52.0000000	0.5958301D 01	1.0051083
56.0000000	0.5960644D 01	1.0055035
60.0000000	0.5962918D 01	1.0058871
64.0000000	0.5965291D 01	1.0062873
68.0000000	0.5967621D 01	1.0066804
72.0000000	0.5969937D 01	1.0070711
76.0000000	0.5972238D 01	1.0074592
80.0000000	0.5974602D 01	1.0078580
84.0000000	0.5976932D 01	1.0082511
92.0000000	0.5981577D 01	1.0090347
96.0000000	0.5983941D 01	1.0094334
100.0000000	0.5986271D 01	1.0098265
104.0000000	0.5988557D 01	1.0102121
108.0000000	0.5990887D 01	1.0106052
112.0000000	0.5993259D 01	1.0110052
116.0000000	0.5995532D 01	1.0113888
120.0000000	0.5997904D 01	1.0117888

SLOPE = 0.0006
VARIANCE = 0.12D-13
STD DEV = 0.00000
INTERCEPT = 5.928C
CORR. COEFF. = 0.1C000D 01
SLOPE PER KB = 0.0084

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS F33

PRESS	F33	Y/Y0
0.0150000	0.4767190D 03	1.0000000
4.0000000	0.4768120D 03	1.0001951
8.0000000	0.4769050D 03	1.0003902
12.0000000	0.4769980D 03	1.0005853
16.0000000	0.4770910D 03	1.0007803
20.0000000	0.4771840D 03	1.0009754
24.0000000	0.4772770D 03	1.0011705
28.0000000	0.4773710D 03	1.0013677
32.0000000	0.4774640D 03	1.0015628
36.0000000	0.4775570D 03	1.0017578
40.0000000	0.4776500D 03	1.0019529
44.0000000	0.4777430D 03	1.0021480
48.0000000	0.4778360D 03	1.0023431
52.0000000	0.4779290D 03	1.0025382
56.0000000	0.4780230D 03	1.0027354
60.0000000	0.4781160D 03	1.0029304
64.0000000	0.4782090D 03	1.0031255
68.0000000	0.4783020D 03	1.0033206
72.0000000	0.4783950D 03	1.0035157
76.0000000	0.4784890D 03	1.0037129
80.0000000	0.4785820D 03	1.0039080
84.0000000	0.4786750D 03	1.0041030
92.0000000	0.4788610D 03	1.0044932
96.0000000	0.4789540D 03	1.0046883
100.0000000	0.4790470D 03	1.0048834
104.0000000	0.4791410D 03	1.0050806
108.0000000	0.4792340D 03	1.0052756
112.0000000	0.4793270D 03	1.0054707
116.0000000	0.4794200D 03	1.0056658
120.0000000	0.4795130D 03	1.0058609

SLOPE = 0.0233
VARIANCE = 0.22D-11
STD DEV = 0.00000
INTERCEPT = 476.7185
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 0.3378

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS F44

PRESS	F44	Y/Y0
0.0150000	0.2416820D 03	1.0000000
4.0000000	0.2417010D 03	1.0000786
8.0000000	0.2417210D 03	1.0001614
12.0000000	0.2417400D 03	1.0002400
16.0000000	0.2417600D 03	1.0003227
20.0000000	0.2417790D 03	1.0004014
24.0000000	0.2417990D 03	1.0004841
28.0000000	0.2418180D 03	1.0005627
32.0000000	0.2418380D 03	1.0006455
36.0000000	0.2418570D 03	1.0007241
40.0000000	0.2418770D 03	1.0008068
44.0000000	0.2418970D 03	1.0008896
48.0000000	0.2419160D 03	1.0009682
52.0000000	0.2419360D 03	1.0010510
56.0000000	0.2419550D 03	1.0011296
60.0000000	0.2419750D 03	1.0012123
64.0000000	0.2419940D 03	1.0012910
68.0000000	0.2420140D 03	1.0013737
72.0000000	0.2420330D 03	1.0014523
76.0000000	0.2420530D 03	1.0015351
80.0000000	0.2420720D 03	1.0016137
84.0000000	0.2420920D 03	1.0016964
92.0000000	0.2421310D 03	1.0018578
96.0000000	0.2421500D 03	1.0019364
100.0000000	0.2421700D 03	1.0020192
104.0000000	0.2421890D 03	1.0020978
108.0000000	0.2422090D 03	1.0021806
112.0000000	0.2422280D 03	1.0022592
116.0000000	0.2422480D 03	1.0023419
120.0000000	0.2422670D 03	1.0024205

SLOPE = 0.0049
VARIANCE = 0.23D-11
STD DEV = 0.00000
INTERCEPT = 241.6818
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 0.0708

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS F11

PRESS	F11	Y/Y0
0.C15C000	0.46090C0D 03	1.C000000
4.CC00000	0.4610440D 03	1.0003124
8.C000000	0.46119C0D 03	1.0006292
12.CC00000	0.461335CD 03	1.0009438
16.C0C0000	0.46148CCD 03	1.0012584
20.C000000	0.4616250D 03	1.0015730
24.C000000	0.46177C0D 03	1.0018876
28.C000000	0.4619160D 03	1.0022044
32.C000000	0.4620610D 03	1.0025190
36.CC00000	0.462206CD 03	1.0028336
40.C000000	0.4623510D 03	1.0031482
44.C000000	0.4624960D 03	1.0034628
48.CC00000	0.462641CD 03	1.0037774
52.C000000	0.462787CD 03	1.0040942
56.C000000	0.4629320D 03	1.0044088
60.C000000	0.463077CD 03	1.0047234
64.C000000	0.4632220D 03	1.0050380
68.C000000	0.4633670D 03	1.0053526
72.C000000	0.4635120D 03	1.0056672
76.CC00000	0.4636570D 03	1.0059818
80.CC00000	0.4638030D 03	1.0062985
84.C000000	0.4639480D 03	1.0066131
92.C000000	0.4642380D 03	1.0072424
96.C000000	0.4643840D 03	1.0075591
1C0.C000000	0.4645290D 03	1.0078737
104.C000000	0.4646740D 03	1.0081883
1C8.C000000	0.4648190D 03	1.0085029
112.C000000	0.464964CD 03	1.0088175
116.C000000	0.4651090D 03	1.0091321
120.CC00000	0.4652540D 03	1.0094467

SLOPE = 0.0363
VARIANCE = 0.27D-11
STD DEV = 0.C0000
INTERCEPT = 460.8994
CORR. COEFF. = 0.10000D 01
SLOPE PER KB = 0.5264

PRESSURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES PRESS VS F66

PRESS	F66	Y/Y0
0.C150000	0.4535340D 03	1.0000000
4.C000000	0.4537330D 03	1.0004388
8.C000000	0.4539320D 03	1.0008776
12.CC00000	0.4541320D 03	1.0013185
16.C000000	0.4543320D 03	1.0017595
20.C000000	0.4545310D 03	1.0021983
24.C000000	0.4547310D 03	1.0026393
28.C000000	0.4549310D 03	1.0030803
32.0000000	0.4551300D 03	1.0035190
36.CCC0000	0.4553300D 03	1.0039600
40.CCC0000	0.4555300D 03	1.0044010
44.0000000	0.4557290D 03	1.0048398
48.CC00000	0.4559290D 03	1.0052808
52.CC00000	0.4561290D 03	1.0057217
56.C000000	0.4563280D 03	1.0061605
60.CCC0000	0.4565280D 03	1.0066015
64.C000000	0.4567280D 03	1.0070425
68.CC00000	0.4569270D 03	1.0074812
72.CC00000	0.4571270D 03	1.0079222
76.CC00000	0.4573270D 03	1.0083632
80.CC00000	0.4575260D 03	1.0088020
84.CC00000	0.4577260D 03	1.0092430
92.C000000	0.4581250D 03	1.0101227
96.C000000	0.4583250D 03	1.0105637
100.C000000	0.4585240D 03	1.0110025
104.C000000	0.4587240D 03	1.0114435
108.CC00000	0.4589240D 03	1.0118844
112.CC00000	0.4591240D 03	1.0123254
116.CC00000	0.4593230D 03	1.0127642
120.CC00000	0.4595230D 03	1.0132052

SLOPE = 0.0499
VARIANCE = 0.210-11
STD DEV = 0.C0000
INTERCEPT = 453.5331
CORR. COEFF. = 0.100000 01
SLOPE PER KB = 0.7240

C LISTING OF TEMPERATURE PROGRAM, INPUT AND OUTPUT DATA.

```
//CRYT  JOB (1242,IM,10F,190KR),'MILLER'
// EXEC  FORTCLG,RG=190K
//SYSIN DD *
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION T(50),C(10,50),F(10,50),S(10,50),V1(10,50),BB1(50),BB2(5
     10),VCOMP(50),X(50),Y(50),R(50),M(25),V(50,50),DESC(25,20),YAX(25,2
     10),CP(50),GAMMA(50),ALPHAV(50)
      JJ=1
    1 I=1
C
C     INPUT PARAMETER AND SPECIMEN DESCRIPTION CARDS
C
    2 READ 3,(DESC(JJ,J1),J1=1,13),(YAX(JJ,J2),J2=1,3),IM
    3 FORMAT(13A4,3A4,15X,I1I)
      IF(IM) 4,4,83
    4 JJ=JJ+1
      IF(JJ-25)2,2,5
C
C     INPUT INITIAL MEASUREMENT CARD (1)
C
    5 READ 6, APL,BPL,APD,BPD,ACP,BCP,CCP,WGT
    6 FORMAT(7D10.5,F10.3)
C
C     INPUT INITIAL MEASUREMENT CARD (2)
C
      READ 7,R(1),(C(J,1),J=1,8)
    7 FORMAT(9F8.3)
C
C     INPUT EXPERIMENTAL TEMPERATURE-FREQUENCY DATA AND DETERMINE THE
C     NUMBER OF PIECES OF DATA
C
    8 READ 7,T(I),(F(J,I),J=1,8)
      IF(F(1,I))9,10,9
    9 I=I+1
      GO TO 8
   10 N=I-1
      I=1
      PRINT 11,(DESC(25,J1),J1=1,13)
   11 FORMAT(1H1,24X,13A4/25X,'COMPRESSIBILITY AS A FUNCTION OF TEMPERAT
     1URE'//25X,'T(C) = CENTIGRADE TEMPERATURE'/25X,'RHO = DENSITY'/25X,
     1'COMP PDTC = COMPRESSIBILITY PERPENDICULAR TO C AXIS'/25X,'COMP PL
     1TC = COMPRESSIBILITY PARALLEL TO C AXIS'/25X,'VOL COMP = VOLUMETRI
     1C COMPRESSIBILITY'///29X,'T(C)     RHO     COMP PDTC    COMP PLTC
     1   VOL COMP'/)
C
C     COMPUTE C12,C13 AND ALL COMPLIANCE CONSTANTS
C
   12 IF(F(6,I).LT.0.1) GO TO 14
      IF(F(7,I).LT.0.1)GO TO 13
      C(9,I)=C(7,I)-C(5,I)-C(6,I)
      GO TO 15
   13 C(9,I)=C(3,I)-2.0*C(6,I)
      C(7,I)=(C(3,I)+C(9,I)+2.0*C(5,I))/2.0
      GO TO 15
   14 C(9,I)=2.0*C(7,I)-2.0*C(5,I)-C(3,I)
      C(6,I)=(C(3,I)-C(9,I))/2.0
```

```
   15 IF(C(2,I))17,16,17
   16 J=4
      S(2,I)=0.0
      S(4,I)=1.0/C(4,I)
      GO TO 20
   17 J=2
      S(2,I)=1.0/C(2,I)
      IF(C(4,I))19,18,19
   18 S(4,I)=0.0
      GO TO 20
   19 S(4,I)=1.0/C(4,I)
   20 C(10,I)=DSQRT((4.0*C(8,I)-C(3,I)-C(1,I)-2.0*C(J,I))**2-(C(3,I)-
     1C(1,I))**2)/2.0-C(J,I)
      S(5,I)=1.0/C(5,I)
      XI=2.0*C(10,I)**2-C(1,I)*(C(9,I)+C(3,I))
      XXI=XI*(C(9,I)-C(3,I))
      S(3,I)=(C(3,I)*C(1,I)-C(10,I)**2)/XXI
      S(9,I)=(C(10,I)**2-C(9,I)*C(1,I))/XXI
      S(10,I)=C(10,I)/XI
      S(1,I)=-(C(3,I)+C(9,I))/XI
C
C     COMPUTE THE VELOCITIES FOR THE VARIOUS C(I,J)
C
      DO 21 J=1,10
   21 V1(J,I)=DSQRT(C(J,I)/(10.0*R(I)))
C
C     COMPUTE COMPRESSIBILITIES
C
      BB1(I)=S(3,I)+S(9,I)+S(10,I)
      BB2(I)=S(1,I)+2.0*S(10,I)
      VCOMP(I)=(2.0*C(1,I)+C(3,I)+C(9,I)-4.0*C(10,I))/(C(1,I)*C(3,I)+C(1
     1,I)*C(9,I)-2.0*C(10,I)**2)
      PRINT 22,T(I),R(I),BB1(I),BB2(I),VCOMP(I)
   22 FORMAT(25X, F9.3,1X,F9.5,3(1X,E12.6))
      PL=APL+BPL*(T(I)-25.0)
      PD=APD+BPD*(T(I)-25.0)
      ALPHAV(I)=PL+2*PD
      IF(I.GT.N-1) GO TO 27
C
C     COMPUTE ELASTIC CONSTANTS AT HIGHER TEMPERATURES
C
      DO 24 J=1,2
      IF(F(J,I).LT.0.1) GO TO 23
      C(J,I+1)=C(J,I)*(F(J,I+1)/F(J,I))**2*((1.0+PL*(T(I+1)-T(I)))/((1.0
     1+PD*(T(I+1)-T(I)))**2))
      GO TO 24
   23 C(J,I+1) =0.0
   24 CONTINUE
      DO 26 J=3,7
      IF(F(J,I).LT.0.1) GO TO 25
      C(J,I+1)=C(J,I)*(F(J,I+1)/F(J,I))**2 /(1.0+PL*(T(I+1)-T(I)))
      GO TO 26
   25 C(J,I+1)=0.0
   26 CONTINUE
      J=8
      C(J,I+1)=C(J,I)*(F(J,I+1)/F(J,I))**2*((1.0+PL*(T(I+1)-T(I)))+(1.0+
```

```
     1PD*(T(I+1)-T(I))))**2/((4.0*(1.0+PL*(T(I+1)-T(I))))*(1.0+PD*(T(I+1
     1)-T(I)))**2)
      R(I+1)=R(I)/((1.0+PD*(T(I+1)-T(I)))**2*(1.0+PL*(T(I+1)-T(I))))
      I=I+1
      GO TO 12
   27 PRINT 28,(DESC(25,J1),J1=1,13)
   28 FORMAT(1H1,14X,13A4/15X,'EXPERIMENTAL TEMPERATURE-FREQUENCY INPUT
     1DATA'///19X,'T(C)      F33       F44       F11       F44A      F66
     1FPQ       FTU       FRS'/)
      DO 29 I=1,N
   29 PRINT 30, T(I),(F(J,I),J=1,8)
   30 FORMAT(15X, 9F9.3)
      PRINT 31,(DESC(25,J1),J1=1,13)
   31 FORMAT(1H1,9X,13A4/10X,'ELASTIC CONSTANTS AS A FUNCTION OF TEMPERA
     1TURE'//10X,'C44 = PROPAGATION PARALLEL TO C AXIS'/10X,'C44A = PROP
     1AGATION PERPENDICULAR TO C AXIS'/10X,'CPQ = (C11-C12)/2'/10X,'CRS
     1= ((C11+C33+2*C44)+((C11-C33)**2+4(C13+C44)**2)**1/2)/4'/10X,'CTU
     1= (C11+C12+2*C66)/2'//13X,'T(C)      C33       C44       C11       C44
     1A      C66       CPQ       CTU       CRS       C12       C13'/)
      DO 32 I=1,N
   32 PRINT 33, T(I),(C(J,I),J=1,10)
   33 FORMAT(9X,11F9.3)
      PRINT 34,(DESC(25,J1),J1=1,13)
   34 FORMAT(1H1, 9X,13A4/10X,'COMPLIANCE CONSTANTS AS A FUNCTION OF TEM
     1PERATURE'///13X,'T(C)    S33',10X,'S44',10X,'S11',10X,'S44A',9X,'S6
     116',10X,'S12',10X,'S13'/)
      DO 35 I=1,N
   35 PRINT 36, T(I),(S(J,I),J=1,5),(S(J,I),J=9,10)
   36 FORMAT (9X, F9.3,7(1X,E12.6))
      PRINT 37,(DESC(25,J1),J1=1,13)
   37 FORMAT(1H1,9X,13A4/10X,'VELOCITIES OF THE ELASTIC CONSTANTS AS A F
     1UNCTION OF TEMPERATURE'///13X,'T(C)     V(C33)    V(C44)    V(C11)
     1V(C44A)  V(C66)    V(CPQ)    V(CTU)    V(CRS)    V(C12)    V(C13)'/)
      DO 38 I=1,N
   38 PRINT 39, T(I),(V1(J,I),J=1,10)
   39 FORMAT(9X,F9.3,10F9.5)
      PRINT 40,(DESC(25,J1),J1=1,13)
   40 FORMAT(1H1,8X,13A4/9X,'VOIGT,REUSS,HILL MODULI AND CORRESPONDING V
     1ELOCITIES'//9X,'K(V) = VOIGT BULK MODULUS'/9X,'U(V) = VOIGT SHEAR
     1MODULUS'/9X,'K(R) = REUSS BULK MODULUS'/9X,'U(R) = REUSS SHEAR MOD
     1ULUS'/9X,'K(H) = HILL BULK MODULUS'/9X,'U(H) = HILL SHEAR MODULUS'
     1/9X,'VS(V) = VOIGT SHEAR VELOCITY'/9X,'VS(R) = REUSS SHEAR VELOCIT
     1Y'/9X,'VS(VRH) = VOIGT,REUSS,HILL SHEAR VELOCITY'/9X,'VP(V) = VOIG
     1T LONGITUDINAL VELOCITY'/9X,'VP(R) = REUSS LONGITUDINAL VELOCITY'/
     19X,'VP(VRH) = VOIGT,REUSS,HILL LONGITUDINAL VELOCITY'//10X,'T(C)
     1  K(V)      U(V)      K(R)      U(R)      K(H)      U(H)      VS(V)     V
     1S(R)    VS(VRH)    VP(V)     VP(R)    VP(VRH)'/)
C
C     COMPUTE ELASTIC MODULI AND COMPRESSIONAL- AND SHEAR-WAVE
C     VELOCITIES BY VOIGT,REUSS AND HILL AVERAGING SCHEMES
C
      DO 44 I=1,N
      IF(F(2,I).EQ. 0.0) GO TO 41
      L=2
      GO TO 42
   41 L=4
```

```
   42 V(I,1)=S(3,I)+S(9,I)+S(10,I)
      V(I,2)=S(1,I)+2.0*S(10,I)
      V(I,3)=2.0*S(3,I)+S(1,I)+2.0*S(9,I)+4.0*S(10,I)
      V(I,4)=((2.0*C(3,I)+C(1,I))+2.0*(C(9,I)+2.0*C(10,I)))/9.0
      V(I,5)=(2.0*C(3,I)+C(1,I)-C(9,I)-2.0*C(10,I)+6.0*C(L,I)+3.0*C(5,I)
     1)/15.0
      V(I,6)=1.0/(2.0*S(3,I)+S(1,I)+2.0*(S(9,I)+2.0*S(10,I)))
      V(I,7)=15.0/(4.0*(2.0*S(3,I)+S(1,I))-4.0*(S(9,I)+2.0*S(10,I))+6.0*
     1S(L,I)+3.0*S(5,I))
      V(I,8)=0.5*(V(I,4)+V(I,6))
      V(I,9)=0.5*(V(I,5)+V(I,7))
      DO 43 K=3,5
      V(I,K+7)=DSQRT(V(I,2*K-1)/(10.0*R(I)))
   43 V(I,K+10)=DSQRT((V(I,2*K-2)+4.0*V(I,2*K-1)/3.0)/(10.0*R(I)))
   44 PRINT 45, T(I),(V(I,J),J=4,15)
   45 FORMAT(9X,F5.1,6F9.3,6F9.4)
C
C     COMPUTE MEAN SOUND VELOCITIES ,DEBYE TEMPERATURE AND ANISOTROPY AS
C     A FUNCTION OF TEMPERATURE
C
      PRINT 46,(DESC(25,J1),J1=1,13)
   46 FORMAT(1H1,13X,13A4/14X,'VOIGT,REUSS AND HILL MEAN VELOCITIES AND
     1CORRESPONDING DEBYE TEMPERATURE'//14X,'VM(V) = MEAN VELOCITY'/14X,
     1'VM(R) = REUSS MEAN VELOCITY'/14X,'VM(VRH) = VOIGT,REUSS,HILL MEAN
     1 VELOCITY'/14X,'SIG(V) = POISSONS RATIO USING VOIGT VELOCITIES'/14
     1X,'SIG(R) = POISSONS RATIO USING REUSS VELOCITIES'/14X,'SIG(VRH) =
     1 POISSONS RATIO USING VRH VELOCITIES'/14X,'DT(V) = DEBYE TEMPERATU
     1RE USING VM(V)'/14X,'DT(R) = DEBYE TEMPERATURE USING VM(R)'/14X,'D
     1T(VRH) = DEBYE TEMPERATURE USING VM(VRH)'/14X,'A = SHEAR ANISOTROP
     1Y'/14X,'RHO = DENSITY'///15X,'T(C)      VM(V)    VM(R)   VM(VRH)  S
     1IG(V)   SIG(R)  SIG(VRH)  DT(V)    DT(R)   DT(VRH)      A       RHO
     1'/)
      DO 49 I=1,N
      DO 47 K=16,18
      V(I,K)=((3.0*V(I,K-3)**3*V(I,K-6)**3)/(2.0*V(I,K-3)**3 +V(I,K-6)**
     13))**.33333333
      V(I,K+3)=0.5*(((V(I,K-3)/V(I,K-6))**2-2.0)/((V(I,K-3)/V(I,K-6))**2
     1-1.0))
   47 V(I,K+6)=251.2*(1.0/(WGT**.33333333))*(R(I)**.33333333)*V(I,K)
      V(I,25) = 2.0*(V(I,5)-V(I,9))/(V(I,5)+V(I,9))
      V(I,26)=R(I)
      PRINT 48, T(I),(V(I,J),J=16,26)
   48 FORMAT(14X,F5.1,1X,11F9.4)
   49 CONTINUE
C
C     COMPUTE THERMAL EXPANSION,SPECIFIC HEAT AND GRUNEISEN PARAMETER AS
C     A FUNCTION OF TEMPERATURE
C
      IF(ACP)50,56,50
   50 PRINT 51,(DESC(25,J1),J1=1,13)
   51 FORMAT(1H1,24X,13A4/25X,'THERMAL EXPANSION,SPECIFIC HEAT AND GRUNE
     1ISEN PARAMETER AS A FUNCTION OF TEMPERATURE'//25X,'ALPHA(V) = VOLU
     1METRIC EXPANSION'/25X,'CP = SPECIFIC HEAT  (CAL/G/DEG)'/25X,'GAMMA
     1 = GRUNEISEN PARAMETER'/25X,'RHO = DENSITY'///26X,'T(C)',6X,'ALPHA
     1(V)',7X,'RHO',7X,'CP',10X,'GAMMA'/)
      DO 55 I=1,N
```

```
   52 CP(I)=ACP+BCP*(T(I)+273.0)-CCP*(T(I)+273.0)**2
   53 GAMMA(I)=V(I,08)*ALPHAV(I)*100.0/(4.186*R(I)*CP(I))
      PRINT 54, T(I),ALPHAV(I),R(I),CP(I),GAMMA(I)
   54 FORMAT (21X,2(F10.3,D14.6),F10.5)
   55 CONTINUE
C
C     COMPUTE LEAST SQUARES FIT BETWEEN TEMPERATURE AND THE VARIOUS
C     PARAMETERS
C
   56 READ 57,(M(K),K=1,24)
   57 FORMAT(24I1)
      LL=6
      L=59/(N+1)-1
      DO 82 K=1,24
      IF(L-LL)58,60,60
   58 PRINT 59
   59 FORMAT(1H1)
      LL = 0
   60 IF(M(K)) 61,82,61
   61 LL = LL+1
      DO 72 II=1,N
      GO TO (62,63,64,65,66,66,66,66,66,67,67,68,68,68,68,68,69,69,70,70
     1,70,70,70,71),K
   62 Y(II)=R(II)
      GO TO 72
   63 Y(II)=BB1(II)
      GO TO 72
   64 Y(II)=BB2(II)
      GO TO 72
   65 Y(II)=VCOMP(II)
      GO TO 72
   66 Y(II)=C(K-4,II)
      GO TO 72
   67 Y(II)=C(K-1,II)
      GO TO 72
   68 Y(II)=V1(K-11,II)
      GO TO 72
   69 Y(II)=V1(K-8,II)
      GO TO 72
   70 Y(II)=F(K-18,II)
      GO TO 72
   71 Y(II)=F(8,II)
      GO TO 72
   72 CONTINUE
      PRINT 73, (DESC(25,J1),J1=1,13),(DESC(K,J2),J2=1,13)
   73 FORMAT(30X,13A4/30X,'LEAST SQUARES       TEMP VS ',13A4/)
      PRINT 74, (YAX(K,J1),J1=1,3)
   74 FORMAT(33X,'TEMP ',12X,3A4,15X,'Y/Y0')
      SUMX  = 0.0
      SUMY  = 0.0
      SUMX2 = 0.0
      SUMXY = 0.0
      SUMY2 = 0.0
      CI=N
      DO 75 J=1,N
      X(J) =  T(J)
```

```
      SUMX = SUMX+X(J)
      SUMY = SUMY+Y(J)
      SUMX2 = SUMX2 +X(J)**2
      SUMY2 = SUMY2 +Y(J)**2
   75 SUMXY = SUMXY+X(J)*Y(J)
      IF(SUMXY)78,76,78
   76 PRINT 77
      GO TO 82
   77 FORMAT(/////45X,'NO INPUT VALUES'/)
C
C     COMPUTE SLOPE,INTERCEPT,CORRELATION COEFFICIENT,VARIANCE AND
C     STANDARD DEVIATION
C
   78 SI=(SUMX*SUMY-CI*SUMXY)/(SUMX**2-CI*SUMX2)
      BI= (SUMX2*SUMY-SUMX*SUMXY)/(CI*SUMX2-SUMX**2)
      RI=(CI*SUMXY-SUMX*SUMY)/DSQRT((CI*SUMX2-SUMX**2)*(CI*SUMY2-SUMY**2
     1))
      SXY = SUMXY-SUMX*SUMY/CI
      SXX = SUMX2-SUMX*SUMX/CI
      SYY = SUMY2-SUMY*SUMY/CI
      VARS = (SYY-SXY**2/SXX)/(SXX*(CI-2.0))
      DEVS =DSQRT(VARS)
      DO 79 J=1,N
      YR = Y(J)/Y(1)
   79 PRINT 80, X(J),Y(J),YR
   80 FORMAT(27X,F14.7,8X,E14.7,8X,F14.7)
      PRINT 81, SI,VARS,DEVS,BI,RI
   81 FORMAT(12HOSLOPE     =,F11.4/' VARIANCE  =',E13.2/' STD DEV   =',
     1F12.5/' INTERCEPT =',F11.4/' CORR. COEFF. = ',E12.5//)
   82 CONTINUE
      JJ=25
      GO TO 1
   83 STOP
      END
 *
//GO.SYSIN DD *
DENSITY                                                    DENSITY
COMP PERPENDICULAR TO C                                    COMP PDTC
COMP PARALLEL TO C                                         COMP PLTC
VOLUMETRIC COMP                                            VOL COMP
C33                                                        C33
C44                                                        C44
C11                                                        C11
C44A                                                       C44A
C66                                                        C66
C12                                                        C12
C13                                                        C13
C33 VELOCITY                                               C33 VEL
C44 VELOCITY                                               C44 VEL
C11 VELOCITY                                               C11 VEL
C44A VELOCITY                                              C44A VEL
C66 VELOCITY                                               C66 VEL
C12 VELOCITY                                               C12 VEL
C13 VELOCITY                                               C13 VEL
F33                                                        F33
F44                                                        F44
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F11                                                    F11
F44A                                                   F44A
F66                                                    F66
FRS                                                    FRS
TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
   9.2D-06 2.875D-09  7.18D-06  1.25D-09 1.512D-01  2.45D-04  2.22D-08  26.63293
4.26    4839.499        2714.3361244.2951947.719 467.3554194.7003980.000
  25.000 498.910         460.600 317.460 388.600 163.120 495.150 595.880
  30.000 498.800         460.390 317.350 388.150 163.153 494.700 595.610
  40.000 498.310         459.950 317.120 387.220 163.220 493.880 595.100
  50.000 497.810         459.510 316.900 386.410 163.294 493.000 594.550
  60.000 497.300         459.100 316.670 385.500 163.325 492.180 594.040
  70.000 496.820         458.690 316.450 384.660 163.425 491.300 593.420
  80.000 496.310         458.250 316.220 383.800 163.490 490.500 592.890
  90.000 495.810         457.810 316.000 382.900 163.560 489.600 592.310
 100.000 495.400         457.300 315.770 382.100 163.620 488.700 591.800
 110.000 494.920         456.980 315.550 381.210 163.690 487.800 591.270
 120.000 494.450         456.520 315.320 380.340 163.758 486.910 590.720
 130.000 493.950         456.120 315.100 379.600 163.825 486.100 590.210
 140.000 493.580         455.700 314.890 378.800 163.890 485.240 589.700
 150.000 493.200         455.270 314.670 378.010 163.958 484.400 589.200
 160.000 492.730         454.880 314.450 377.260 164.019 483.600 588.690
 170.000 492.340         454.450 314.240 376.500 164.084 482.800 588.150
 180.000 491.900         454.000 314.010 375.700 164.150 481.920 587.600
 190.000 490.470         453.610 313.800 374.910 164.215 481.150 587.100
 200.000 491.000         453.170 313.670 374.110 164.284 480.390 586.600
 210.000 490.550         452.720 313.350 373.350 164.335 479.620 586.090
 220.000 490.080         452.310 313.120 372.610 164.400 478.900 585.590
 230.000 489.610         451.890 312.900 371.850 164.460 478.150 585.080
 240.000 489.120         451.450 312.670 371.100 164.517 477.400 584.530
 250.000 488.680         451.010 312.450 370.450 164.572 476.650 584.000
 260.000 488.200         450.600 312.230 369.700 164.630 475.930 583.500
 270.000 487.730         450.150 312.000 369.000 164.685 475.170 583.000
 280.000 487.280         449.750 311.770 368.250 164.734 474.450 582.500
 290.000 486.800         449.320 311.550 367.510 164.790 473.700 582.000
 300.000 486.350         448.900 311.320 366.800 164.833 472.950 581.550
 310.000 485.850         448.500 311.100 366.100 164.880 472.210 581.100

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CRYT
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TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
COMPRESSIBILITY AS A FUNCTION OF TEMPERATURE

T(C) = CENTIGRADE TEMPERATURE
RHO = DENSITY
COMP PDTC = COMPRESSIBILITY PERPENDICULAR TO C AXIS
COMP PLTC = COMPRESSIBILITY PARALLEL TO C AXIS
VOL COMP = VOLUMETRIC COMPRESSIBILITY

T(C)	RHO	COMP PDTC	COMP PLTC	VOL COMP
25.000	4.26000	0.193571D-03	0.869854D-04	0.474127D-03
30.000	4.25950	0.193846D-03	0.871443D-04	0.474835D-03
40.000	4.25849	0.194326D-03	0.872057D-04	0.475857D-03
50.000	4.25749	0.194919D-03	0.872957D-04	0.477134D-03
60.000	4.25648	0.195383D-03	0.873633D-04	0.478129D-03
70.000	4.25547	0.195934D-03	0.876710D-04	0.479539D-03
80.000	4.25446	0.196437D-03	0.877539D-04	0.480628D-03
90.000	4.25344	0.197000D-03	0.879393D-04	0.481940D-03
100.000	4.25242	0.197690D-03	0.879206D-04	0.483300D-03
110.000	4.25140	0.198194D-03	0.880840D-04	0.484472D-03
120.000	4.25038	0.198797D-03	0.881841D-04	0.485778D-03
130.000	4.24936	0.199365D-03	0.882205D-04	0.486951D-03
140.000	4.24834	0.199964D-03	0.883535D-04	0.488281D-03
150.000	4.24731	0.200564D-03	0.884383D-04	0.489566D-03
160.000	4.24628	0.201116D-03	0.885167D-04	0.490750D-03
170.000	4.24525	0.201686D-03	0.887256D-04	0.492098D-03
180.000	4.24422	0.202328D-03	0.888404D-04	0.493496D-03
190.000	4.24318	0.202835D-03	0.881301D-04	0.493800D-03
200.000	4.24214	0.203360D-03	0.891591D-04	0.495880D-03
210.000	4.24110	0.203947D-03	0.890806D-04	0.496975D-03
220.000	4.24006	0.204462D-03	0.891446D-04	0.498070D-03
230.000	4.23902	0.204999D-03	0.892319D-04	0.499229D-03
240.000	4.23797	0.205547D-03	0.893743D-04	0.500468D-03
250.000	4.23693	0.206159D-03	0.894865D-04	0.501805D-03
260.000	4.23588	0.206673D-03	0.895611D-04	0.502908D-03
270.000	4.23483	0.207290D-03	0.895542D-04	0.504135D-03
280.000	4.23377	0.207801D-03	0.896488D-04	0.505250D-03
290.000	4.23272	0.208373D-03	0.896839D-04	0.506429D-03
300.000	4.23166	0.208971D-03	0.895927D-04	0.507534D-03
310.000	4.23060	0.209552D-03	0.894889D-04	0.508593D-03

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
EXPERIMENTAL TEMPERATURE-FREQUENCY INPUT DATA

T(C)	F33	F44	F11	F44A	F66	FPQ	FTU	FRS
25.000	498.910	0.0	460.600	317.460	388.600	163.120	495.150	595.880
30.000	498.800	0.0	460.390	317.350	388.150	163.153	494.700	595.610
40.000	498.310	0.0	459.950	317.120	387.220	163.220	493.880	595.100
50.000	497.810	0.0	459.510	316.900	386.410	163.294	493.000	594.550
60.000	497.300	0.0	459.100	316.670	385.500	163.325	492.180	594.040
70.000	496.820	0.0	458.690	316.450	384.660	163.425	491.300	593.420
80.000	496.310	0.0	458.250	316.220	383.800	163.490	490.500	592.890
90.000	495.810	0.0	457.810	316.000	382.900	163.560	489.600	592.310
100.000	495.400	0.0	457.300	315.770	382.100	163.620	488.700	591.800
110.000	494.920	0.0	456.980	315.550	381.210	163.690	487.800	591.270
120.000	494.450	0.0	456.520	315.320	380.340	163.758	486.910	590.720
130.000	493.950	0.0	456.120	315.100	379.600	163.825	486.100	590.210
140.000	493.580	0.0	455.700	314.890	378.800	163.890	485.240	589.700
150.000	493.200	0.0	455.270	314.670	378.010	163.958	484.400	589.200
160.000	492.730	0.0	454.880	314.450	377.260	164.019	483.600	588.690
170.000	492.340	0.0	454.450	314.240	376.500	164.084	482.800	588.150
180.000	491.900	0.0	454.000	314.010	375.700	164.150	481.920	587.600
190.000	490.470	0.0	453.610	313.800	374.910	164.215	481.150	587.100
200.000	491.000	0.0	453.170	313.670	374.110	164.284	480.390	586.600
210.000	490.550	0.0	452.720	313.350	373.350	164.335	479.620	586.090
220.000	490.080	0.0	452.310	313.120	372.610	164.400	478.900	585.590
230.000	489.610	0.0	451.890	312.900	371.850	164.460	478.150	585.080
240.000	489.120	0.0	451.450	312.670	371.100	164.517	477.400	584.530
250.000	488.680	0.0	451.010	312.450	370.450	164.572	476.650	584.000
260.000	488.200	0.0	450.600	312.230	369.700	164.630	475.930	583.500
270.000	487.730	0.0	450.150	312.000	369.000	164.685	475.170	583.000
280.000	487.280	0.0	449.750	311.770	368.250	164.734	474.450	582.500
290.000	486.800	0.0	449.320	311.550	367.510	164.790	473.700	582.000
300.000	486.350	0.0	448.900	311.320	366.800	164.833	472.950	581.550
310.000	485.850	0.0	448.500	311.100	366.100	164.880	472.210	581.100

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
ELASTIC CONSTANTS AS A FUNCTION OF TEMPERATURE

C44 = PROPAGATION PARALLEL TO C AXIS
C44A = PROPAGATION PERPENDICULAR TO C AXIS
CPQ = (C11-C12)/2
CRS = ((C11+C33+2*C44)+((C11-C33)**2+4(C13+C44)**2)**1/2)/4
CTU = (C11+C12+2*C66)/2

T(C)	C33	C44	C11	C44A	C66	CPQ	CTU	CRS	C12	C13
25.000	4839.499	0.0	2714.336	1244.295	1947.719	467.355	4194.700	3980.000	1779.626	1495.667
30.000	4837.240	0.0	2711.737	1243.376	1943.121	467.523	4186.886	3976.251	1776.243	1492.070
40.000	4827.492	0.0	2706.307	1241.460	1933.643	467.864	4172.633	3969.160	1771.127	1489.805
50.000	4817.561	0.0	2700.882	1239.623	1925.384	468.245	4157.393	3961.541	1763.764	1486.378
60.000	4807.447	0.0	2695.814	1237.710	1916.148	468.379	4143.190	3954.462	1758.663	1484.279
70.000	4797.925	0.0	2690.751	1235.876	1907.629	468.909	4128.004	3945.927	1751.465	1478.458
80.000	4787.833	0.0	2685.341	1233.965	1898.932	469.238	4114.187	3938.597	1746.017	1475.916
90.000	4777.945	0.0	2679.936	1232.133	1889.859	469.596	4098.720	3930.610	1739.264	1471.649
100.000	4769.802	0.0	2673.717	1230.224	1881.794	469.897	4083.281	3923.559	1731.591	1468.555
110.000	4760.319	0.0	2669.725	1228.395	1872.862	470.255	4067.873	3916.250	1724.756	1464.958
120.000	4751.038	0.0	2664.101	1226.489	1864.147	470.601	4052.659	3908.682	1717.912	1461.377
130.000	4741.191	0.0	2659.183	1224.662	1856.724	470.942	4038.804	3901.651	1711.139	1458.955
140.000	4733.849	0.0	2654.036	1222.914	1848.731	471.271	4024.144	3894.627	1704.143	1454.633
150.000	4726.321	0.0	2648.777	1221.090	1840.852	471.617	4009.841	3887.740	1697.373	1450.939
160.000	4717.076	0.0	2643.988	1219.266	1833.379	471.923	3996.226	3880.728	1690.924	1448.067
170.000	4709.371	0.0	2638.739	1217.522	1825.825	472.252	3982.633	3873.327	1684.557	1443.229
180.000	4700.717	0.0	2633.262	1215.623	1817.899	472.586	3967.747	3865.802	1677.261	1439.214
190.000	4693.188	0.0	2628.487	1213.881	1810.087	472.915	3954.696	3858.941	1671.694	1449.829
200.000	4683.054	0.0	2623.136	1212.758	1802.196	473.267	3941.831	3852.087	1666.368	1432.095
210.000	4674.236	0.0	2617.675	1210.167	1794.707	473.514	3928.824	3845.107	1660.602	1430.801
220.000	4665.046	0.0	2612.682	1208.274	1787.426	473.843	3916.656	3838.265	1655.387	1428.469
230.000	4655.865	0.0	2607.577	1206.459	1779.968	474.143	3904.017	3831.298	1649.906	1425.736
240.000	4646.315	0.0	2602.247	1204.568	1772.622	474.425	3891.398	3823.813	1644.351	1422.400
250.000	4637.723	0.0	2596.922	1202.755	1766.244	474.696	3878.800	3816.598	1637.860	1418.774
260.000	4628.382	0.0	2591.947	1200.944	1758.926	474.983	3866.710	3809.781	1632.800	1416.431
270.000	4619.241	0.0	2586.518	1199.057	1752.099	475.254	3853.990	3802.971	1626.637	1414.266
280.000	4610.487	0.0	2581.667	1197.171	1744.811	475.490	3841.939	3796.166	1621.638	1411.631
290.000	4601.175	0.0	2576.477	1195.363	1737.633	475.766	3829.421	3789.368	1616.022	1409.371
300.000	4592.440	0.0	2571.406	1193.480	1730.753	475.967	3816.925	3783.226	1610.205	1408.214
310.000	4582.771	0.0	2566.569	1191.675	1723.981	476.191	3804.610	3777.089	1604.438	1407.508

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
COMPLIANCE CONSTANTS AS A FUNCTION OF TEMPERATURE

T(C)	S33	S44	S11	S44A	S66	S12	S13
25.000	0.260150D-03	0.0	0.675002D-03	0.803668D-03	0.513421D-03	-.394849D-03	-.865824D-04
30.000	0.260069D-03	0.0	0.674631D-03	0.804262D-03	0.514636D-03	-.394323D-03	-.864622D-04
40.000	0.260684D-03	0.0	0.675189D-03	0.805503D-03	0.517159D-03	-.394124D-03	-.867390D-04
50.000	0.261242D-03	0.0	0.674497D-03	0.806697D-03	0.519377D-03	-.392605D-03	-.869732D-04
60.000	0.261897D-03	0.0	0.674857D-03	0.807944D-03	0.521880D-03	-.392207D-03	-.872670D-04
70.000	0.262205D-03	0.0	0.673920D-03	0.809143D-03	0.524211D-03	-.390719D-03	-.872672D-04
80.000	0.262833D-03	0.0	0.674286D-03	0.810396D-03	0.526612D-03	-.390310D-03	-.875398D-04
90.000	0.263311D-03	0.0	0.673878D-03	0.811601D-03	0.529140D-03	-.389192D-03	-.876859D-04
100.000	0.263805D-03	0.0	0.673530D-03	0.812860D-03	0.531408D-03	-.387899D-03	-.879420D-04
110.000	0.264299D-03	0.0	0.672269D-03	0.814070D-03	0.533942D-03	-.385967D-03	-.881075D-04
120.000	0.264808D-03	0.0	0.671990D-03	0.815335D-03	0.536438D-03	-.384881D-03	-.883121D-04
130.000	0.265456D-03	0.0	0.671393D-03	0.816552D-03	0.538583D-03	-.383410D-03	-.886179D-04
140.000	0.265758D-03	0.0	0.670708D-03	0.817719D-03	0.540912D-03	-.382042D-03	-.887023D-04
150.000	0.266131D-03	0.0	0.670244D-03	0.818941D-03	0.543227D-03	-.380834D-03	-.888465D-04
160.000	0.266693D-03	0.0	0.669726D-03	0.820165D-03	0.545441D-03	-.379521D-03	-.890881D-04
170.000	0.266966D-03	0.0	0.669412D-03	0.821341D-03	0.547698D-03	-.378606D-03	-.891202D-04
180.000	0.267404D-03	0.0	0.668817D-03	0.822623D-03	0.550086D-03	-.377207D-03	-.892819D-04
190.000	0.270596D-03	0.0	0.669613D-03	0.823804D-03	0.552460D-03	-.375545D-03	-.912327D-04
200.000	0.268326D-03	0.0	0.669065D-03	0.824567D-03	0.554878D-03	-.376121D-03	-.895833D-04
210.000	0.269018D-03	0.0	0.669384D-03	0.826332D-03	0.557194D-03	-.375468D-03	-.899689D-04
220.000	0.269624D-03	0.0	0.669656D-03	0.827627D-03	0.559464D-03	-.374954D-03	-.902398D-04
230.000	0.270199D-03	0.0	0.669841D-03	0.828872D-03	0.561808D-03	-.374358D-03	-.904838D-04
240.000	0.270750D-03	0.0	0.670095D-03	0.830173D-03	0.564136D-03	-.373860D-03	-.906877D-04
250.000	0.271219D-03	0.0	0.669855D-03	0.831424D-03	0.566173D-03	-.372830D-03	-.908661D-04
260.000	0.271842D-03	0.0	0.670203D-03	0.832678D-03	0.568529D-03	-.372389D-03	-.911404D-04
270.000	0.272497D-03	0.0	0.670279D-03	0.833989D-03	0.570744D-03	-.371517D-03	-.914715D-04
280.000	0.273050D-03	0.0	0.670568D-03	0.835303D-03	0.573128D-03	-.371067D-03	-.917008D-04
290.000	0.273702D-03	0.0	0.670778D-03	0.836566D-03	0.575495D-03	-.370396D-03	-.920089D-04
300.000	0.274426D-03	0.0	0.670876D-03	0.837886D-03	0.577783D-03	-.369488D-03	-.924166D-04
310.000	0.275267D-03	0.0	0.670900D-03	0.839155D-03	0.580053D-03	-.368459D-03	-.928888D-04

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
VELOCITIES OF THE ELASTIC CONSTANTS AS A FUNCTION OF TEMPERATURE

T(C)	V(C33)	V(C44)	V(C11)	V(C44A)	V(C66)	V(CPQ)	V(CTU)	V(CRS)	V(C12)	V(C13)
25.000	10.65848	0.0	7.98228	5.40452	6.76174	3.31222	9.92306	9.66578	6.46338	5.92533
30.000	10.65662	0.0	7.97893	5.40284	6.75415	3.31300	9.91440	9.66179	6.45761	5.91855
40.000	10.64714	0.0	7.97188	5.39931	6.73845	3.31460	9.89868	9.65431	6.44907	5.91476
50.000	10.63744	0.0	7.96482	5.39595	6.72484	3.31635	9.88175	9.64618	6.43641	5.90865
60.000	10.62752	0.0	7.95829	5.39243	6.70949	3.31721	9.86602	9.63870	6.42786	5.90517
70.000	10.61825	0.0	7.95176	5.38907	6.69535	3.31948	9.84910	9.62944	6.41545	5.89428
80.000	10.60834	0.0	7.94470	5.38554	6.68087	3.32105	9.83377	9.62163	6.40623	5.88991
90.000	10.59865	0.0	7.93765	5.38218	6.66568	3.32271	9.81644	9.61302	6.39459	5.88209
100.000	10.59088	0.0	7.92938	5.37866	6.65224	3.32417	9.79910	9.60554	6.38123	5.87661
110.000	10.58161	0.0	7.92441	5.37530	6.63723	3.32583	9.78177	9.59774	6.36939	5.87011
120.000	10.57256	0.0	7.91701	5.37177	6.62256	3.32746	9.76463	9.58961	6.35750	5.86364
130.000	10.56287	0.0	7.91065	5.36842	6.61016	3.32906	9.74910	9.58214	6.34572	5.85948
140.000	10.55596	0.0	7.90395	5.36523	6.59671	3.33063	9.73257	9.57466	6.33350	5.85150
150.000	10.54884	0.0	7.89707	5.36188	6.58343	3.33225	9.71643	9.56735	6.32167	5.84477
160.000	10.53979	0.0	7.89088	5.35852	6.57085	3.33374	9.70109	9.55988	6.31041	5.83969
170.000	10.53246	0.0	7.88400	5.35534	6.55810	3.33530	9.68576	9.55192	6.29928	5.83064
180.000	10.52406	0.0	7.87677	5.35181	6.54465	3.33689	9.66881	9.54379	6.28639	5.82323
190.000	10.49448	0.0	7.87059	5.34863	6.53137	3.33846	9.65408	9.53649	6.27672	5.84538
200.000	10.50683	0.0	7.86353	5.34681	6.51791	3.34011	9.63954	9.52918	6.26748	5.81023
210.000	10.49822	0.0	7.85631	5.34175	6.50515	3.34139	9.62480	9.52171	6.25739	5.80832
220.000	10.48919	0.0	7.84977	5.33822	6.49274	3.34296	9.61107	9.51440	6.24832	5.80429
230.000	10.48015	0.0	7.84307	5.33487	6.47998	3.34443	9.59673	9.50693	6.23874	5.79945
240.000	10.47069	0.0	7.83601	5.33134	6.46739	3.34584	9.58239	9.49881	6.22900	5.79338
250.000	10.46229	0.0	7.82896	5.32799	6.45654	3.34720	9.56804	9.49102	6.21746	5.78670
260.000	10.45305	0.0	7.82242	5.32463	6.44395	3.34863	9.55430	9.48371	6.20862	5.78264
270.000	10.44401	0.0	7.81570	5.32111	6.43223	3.35000	9.53976	9.47641	6.19766	5.77893
280.000	10.43541	0.0	7.80884	5.31758	6.41964	3.35125	9.52602	9.46910	6.18890	5.77427
290.000	10.42617	0.0	7.80196	5.31423	6.40722	3.35264	9.51167	9.46180	6.17894	5.77036
300.000	10.41757	0.0	7.79525	5.31070	6.39532	3.35377	9.49733	9.45531	6.16858	5.76871
310.000	10.40790	0.0	7.78889	5.30735	6.38359	3.35498	9.48318	9.44882	6.15829	5.76799

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
VOIGT,REUSS,HILL MODULI AND CORRESPONDING VELOCITIES

K(V) = VOIGT BULK MODULUS
U(V) = VOIGT SHEAR MODULUS
K(R) = REUSS BULK MODULUS
U(R) = REUSS SHEAR MODULUS
K(H) = HILL BULK MODULUS
U(H) = HILL SHEAR MODULUS
VS(V) = VOIGT SHEAR VELOCITY
VS(R) = REUSS SHEAR VELOCITY
VS(VRH) = VOIGT,REUSS,HILL SHEAR VELOCITY
VP(V) = VOIGT LONGITUDINAL VELOCITY
VP(R) = REUSS LONGITUDINAL VELOCITY
VP(VRH) = VOIGT,REUSS,HILL LONGITUDINAL VELOCITY

T(C)	K(V)	U(V)	K(R)	U(R)	K(H)	U(H)	VS(V)	VS(R)	VS(VRH)	VP(V)	VP(R)	VP(VRH)
25.0	2201.121	1253.743	2109.142	995.029	2155.131	1124.386	5.4250	4.8330	5.1375	9.5347	8.9807	9.2619
30.0	2197.942	1252.663	2105.993	994.973	2151.968	1123.818	5.4230	4.8331	5.1365	9.5296	8.9771	9.2574
40.0	2193.509	1249.270	2101.471	993.433	2147.490	1121.352	5.4163	4.8299	5.1315	9.5196	8.9695	9.2487
50.0	2188.041	1246.446	2095.846	993.018	2141.943	1119.732	5.4108	4.8295	5.1284	9.5094	8.9625	9.2400
60.0	2183.724	1243.104	2091.486	991.623	2137.605	1117.363	5.4042	4.8267	5.1236	9.4997	8.9554	9.2315
70.0	2177.354	1240.612	2085.334	991.494	2131.344	1116.053	5.3994	4.8269	5.1212	9.4888	8.9481	9.2224
80.0	2172.690	1237.417	2080.612	990.139	2126.651	1113.778	5.3931	4.8242	5.1166	9.4789	8.9406	9.2137
90.0	2166.993	1234.509	2074.946	989.475	2120.970	1111.992	5.3874	4.8232	5.1131	9.4681	8.9331	9.2045
100.0	2161.626	1231.684	2069.108	988.796	2115.367	1110.240	5.3818	4.8221	5.1096	9.4579	8.9253	9.1954
110.0	2156.568	1228.937	2064.101	988.773	2110.335	1108.855	5.3765	4.8226	5.1071	9.4482	8.9197	9.1877
120.0	2151.175	1225.997	2058.556	987.980	2104.865	1106.988	5.3707	4.8213	5.1034	9.4377	8.9121	9.1787
130.0	2146.406	1223.244	2053.595	987.452	2100.001	1105.348	5.3653	4.8205	5.1002	9.4283	8.9057	9.1707
140.0	2140.971	1220.813	2048.000	987.132	2094.486	1103.973	5.3606	4.8203	5.0976	9.4186	8.8988	9.1624
150.0	2135.819	1218.248	2042.624	986.588	2089.222	1102.418	5.3556	4.8196	5.0947	9.4090	8.8918	9.1541
160.0	2131.018	1215.582	2037.699	986.019	2084.359	1100.801	5.3504	4.8188	5.0916	9.3997	8.8853	9.1461
170.0	2125.431	1213.229	2032.116	985.436	2078.774	1099.333	5.3459	4.8180	5.0888	9.3899	8.8780	9.1375
180.0	2119.847	1210.599	2026.357	984.948	2073.102	1097.774	5.3407	4.8173	5.0858	9.3797	8.8705	9.1286
190.0	2119.207	1204.824	2025.112	982.220	2072.160	1093.522	5.3286	4.8113	5.0765	9.3703	8.8651	9.1212
200.0	2110.049	1205.460	2016.617	983.026	2063.333	1094.243	5.3307	4.8138	5.0788	9.3610	8.8563	9.1122
210.0	2105.999	1202.167	2012.172	981.525	2059.086	1091.846	5.3241	4.8107	5.0739	9.3515	8.8488	9.1037
220.0	2101.673	1199.334	2007.752	980.287	2054.712	1089.811	5.3184	4.8083	5.0698	9.3424	8.8418	9.0956
230.0	2097.086	1196.553	2003.087	979.145	2050.087	1087.849	5.3129	4.8061	5.0658	9.3331	8.8347	9.0873
240.0	2092.123	1193.795	1998.131	977.954	2045.127	1085.875	5.3074	4.8037	5.0619	9.3233	8.8270	9.0786
250.0	2086.932	1191.428	1992.807	977.260	2039.869	1084.344	5.3028	4.8026	5.0589	9.3139	8.8198	9.0702
260.0	2082.622	1188.604	1988.436	975.970	2035.529	1082.287	5.2972	4.8001	5.0547	9.3048	8.8127	9.0621
270.0	2078.068	1185.850	1983.596	974.898	2030.832	1080.374	5.2917	4.7980	5.0509	9.2956	8.8054	9.0538
280.0	2073.736	1183.092	1979.219	973.658	2026.477	1078.375	5.2862	4.7956	5.0469	9.2865	8.7984	9.0458
290.0	2069.295	1180.296	1974.610	972.475	2021.953	1076.386	5.2806	4.7932	5.0428	9.2773	8.7912	9.0375
300.0	2065.391	1177.451	1970.311	971.335	2017.851	1074.393	5.2749	4.7910	5.0388	9.2686	8.7844	9.0298
310.0	2061.646	1174.563	1966.208	970.227	2013.927	1072.395	5.2691	4.7889	5.0347	9.2601	8.7780	9.0223

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
VOIGT,REUSS AND HILL MEAN VELOCITIES AND CURRESPONDING DEBYE TEMPERATURE

VM(V) = MEAN VELOCITY
VM(R) = REUSS MEAN VELOCITY
VM(VRH) = VOIGT,REUSS,HILL MEAN VELOCITY
SIG(V) = POISSONS RATIO USING VOIGT VELOCITIES
SIG(R) = POISSONS RATIO USING REUSS, VELOCITIES
SIG(VRH) = POISSONS RATIO USING VRH VELOCITIES
DT(V) = DEBYE TEMPERATURE USING VM(V)
DT(R) = DEBYE TEMPERATURE USING VM(R)
DT(VRH) = DEBYE TEMPERATURE USING VM(VRH)
A = SHEAR ANISOTROPY
RHO = DENSITY

T(C)	VM(V)	VM(R)	VM(VRH)	SIG(V)	SIG(R)	SIG(VRH)	DT(V)	DT(R)	DT(VRH)	A	RHO
25.0	6.0304	5.3957	5.7226	0.2606	0.2962	0.2778	822.2915	735.7504	780.3300	0.1088	4.2600
30.0	6.0280	5.3957	5.7214	0.2605	0.2959	0.2776	821.9422	735.7206	780.1309	0.1084	4.2595
40.0	6.0207	5.3921	5.7158	0.2607	0.2958	0.2776	820.8741	735.1704	779.3071	0.1079	4.2585
50.0	6.0145	5.3913	5.7122	0.2606	0.2954	0.2774	819.9735	735.0087	778.7542	0.1071	4.2575
60.0	6.0073	5.3881	5.7068	0.2608	0.2953	0.2774	818.9196	734.5103	777.9624	0.1065	4.2565
70.0	6.0018	5.3880	5.7039	0.2606	0.2948	0.2771	818.1131	734.4455	777.5051	0.1057	4.2555
80.0	5.9949	5.3849	5.6988	0.2607	0.2946	0.2771	817.0996	733.9578	776.7400	0.1052	4.2545
90.0	5.9885	5.3835	5.6947	0.2606	0.2943	0.2769	816.1660	733.7074	776.1286	0.1044	4.2534
100.0	5.9823	5.3820	5.6908	0.2606	0.2939	0.2767	815.2607	733.4497	775.5286	0.1037	4.2524
110.0	5.9764	5.3823	5.6878	0.2606	0.2935	0.2764	814.3813	733.4311	775.0552	0.1027	4.2514
120.0	5.9699	5.3806	5.6835	0.2605	0.2931	0.2763	813.4369	733.1354	774.4172	0.1020	4.2504
130.0	5.9639	5.3796	5.6799	0.2605	0.2928	0.2761	812.5563	732.9382	773.8593	0.1013	4.2494
140.0	5.9586	5.3790	5.6769	0.2604	0.2924	0.2758	811.7705	732.8096	773.3839	0.1005	4.2483
150.0	5.9531	5.3780	5.6734	0.2604	0.2920	0.2756	810.9441	732.6031	772.8505	0.0998	4.2473
160.0	5.9472	5.3768	5.6698	0.2604	0.2917	0.2755	810.0878	732.3911	772.2990	0.0991	4.2463
170.0	5.9421	5.3756	5.6665	0.2602	0.2913	0.2752	809.3229	732.1688	771.7909	0.0985	4.2452
180.0	5.9363	5.3747	5.6630	0.2601	0.2909	0.2750	808.4691	731.9785	771.2510	0.0978	4.2442
190.0	5.9235	5.3681	5.6532	0.2610	0.2912	0.2756	806.6576	731.0292	769.8487	0.0969	4.2432
200.0	5.9251	5.3704	5.6551	0.2600	0.2903	0.2747	806.8096	731.2763	770.0455	0.0967	4.2421
210.0	5.9178	5.3669	5.6496	0.2602	0.2902	0.2747	805.7554	730.7364	769.2354	0.0962	4.2411
220.0	5.9116	5.3640	5.6450	0.2603	0.2900	0.2746	804.8441	730.2902	768.5448	0.0957	4.2401
230.0	5.9055	5.3614	5.6406	0.2603	0.2898	0.2746	803.9462	729.8754	767.8763	0.0952	4.2390
240.0	5.8994	5.3587	5.6361	0.2603	0.2896	0.2744	803.0510	729.4405	767.1998	0.0947	4.2380
250.0	5.8942	5.3572	5.6326	0.2602	0.2893	0.2742	802.2778	729.1796	766.6697	0.0941	4.2369
260.0	5.8880	5.3542	5.6280	0.2602	0.2891	0.2742	801.3654	728.7136	765.9695	0.0936	4.2359
270.0	5.8819	5.3518	5.6236	0.2603	0.2889	0.2741	800.4719	728.3215	765.3142	0.0931	4.2348
280.0	5.8759	5.3489	5.6191	0.2603	0.2887	0.2740	799.5785	727.8730	764.6324	0.0926	4.2338
290.0	5.8697	5.3462	5.6145	0.2604	0.2885	0.2739	798.6706	727.4424	763.9516	0.0921	4.2327
300.0	5.8634	5.3436	5.6100	0.2605	0.2883	0.2739	797.7506	727.0298	763.2727	0.0915	4.2317
310.0	5.8570	5.3411	5.6055	0.2606	0.2881	0.2739	796.8173	726.6297	762.5931	0.0909	4.2306

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
THERMAL EXPANSION,SPECIFIC HEAT AND GRUNEISEN PARAMETER AS A FUNCTION OF TEMPERATURE

ALPHA(V) = VOLUMETRIC EXPANSION
CP = SPECIFIC HEAT (CAL/G/DEG)
GAMMA = GRUNEISEN PARAMETER
RHO = DENSITY

T(C)	ALPHA(V)	RHO	CP	GAMMA
25.000	0.2356000-04	4.260	0.222239D 00	1.28121
30.000	0.2358690-04	4.259	0.223397D 00	1.27430
40.000	0.2364060-04	4.258	0.225710D 00	1.26178
50.000	0.2369440-04	4.257	0.228019D 00	1.24891
60.000	0.2374810-04	4.256	0.230323D 00	1.23700
70.000	0.2380190-04	4.255	0.232623D 00	1.22424
80.000	0.2385560-04	4.254	0.234919D 00	1.21262
90.000	0.2390940-04	4.253	0.237210D 00	1.20069
100.000	0.2396310-04	4.252	0.239496D 00	1.18904
110.000	0.2401690-04	4.251	0.241779D 00	1.17793
120.000	0.2407060-04	4.250	0.244056D 00	1.16679
130.000	0.2412440-04	4.249	0.246330D 00	1.15621
140.000	0.2417810-04	4.248	0.248598D 00	1.14547
150.000	0.2423190-04	4.247	0.250863D 00	1.13507
160.000	0.2428560-04	4.246	0.253123D 00	1.12508
170.000	0.2433940-04	4.245	0.255378D 00	1.11489
180.000	0.2439310-04	4.244	0.257629D 00	1.10483
190.000	0.2444690-04	4.243	0.259876D 00	1.09746
200.000	0.2450060-04	4.242	0.262118D 00	1.08609
210.000	0.2455440-04	4.241	0.264356D 00	1.07730
220.000	0.2460810-04	4.240	0.266589D 00	1.06860
230.000	0.2466190-04	4.239	0.268818D 00	1.05992
240.000	0.2471560-04	4.238	0.271043D 00	1.05123
250.000	0.2476940-04	4.237	0.273263D 00	1.04253
260.000	0.2482310-04	4.236	0.275478D 00	1.03444
270.000	0.2487690-04	4.235	0.277689D 00	1.02630
280.000	0.2493060-04	4.234	0.279896D 00	1.01848
290.000	0.2498440-04	4.233	0.282098D 00	1.01070
300.000	0.2503810-04	4.232	0.284296D 00	1.00325
310.000	0.2509190-04	4.231	0.286489D 00	0.99602

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS DENSITY

TEMP	DENSITY	Y/Y0
25.0000000	0.42600000 01	1.0000000
30.0000000	0.4259498D 01	0.9998822
40.0000000	0.4258494D 01	0.9996464
50.0000000	0.4257487D 01	0.9994101
60.0000000	0.4256478D 01	0.9991734
70.0000000	0.4255468D 01	0.9989361
80.0000000	0.4254455D 01	0.9986984
90.0000000	0.4253440D 01	0.9984602
100.0000000	0.4252424D 01	0.9982215
110.0000000	0.4251405D 01	0.9979823
120.0000000	0.4250384D 01	0.9977427
130.0000000	0.4249361D 01	0.9975025
140.0000000	0.4248336D 01	0.9972619
150.0000000	0.4247309D 01	0.9970209
160.0000000	0.4246280D 01	0.9967793
170.0000000	0.4245249D 01	0.9965373
180.0000000	0.4244216D 01	0.9962948
190.0000000	0.4243181D 01	0.9960518
200.0000000	0.4242143D 01	0.9958083
210.0000000	0.4241104D 01	0.9955644
220.0000000	0.4240063D 01	0.9953200
230.0000000	0.4239020D 01	0.9950751
240.0000000	0.4237975D 01	0.9948297
250.0000000	0.4236927D 01	0.9945839
260.0000000	0.4235878D 01	0.9943376
270.0000000	0.4234827D 01	0.9940908
280.0000000	0.4233773D 01	0.9938435
290.0000000	0.4232718D 01	0.9935958
300.0000000	0.4231661D 01	0.9933476
310.0000000	0.4230601D 01	0.9930989

SLOPE = -0.0001
VARIANCE = 0.22D-13
STD DEV = 0.00000
INTERCEPT = 4.2627
CORR. COEFF. = -0.99997D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS COMP PERPENDICULAR TO C

TEMP	COMP PDTC	Y/Y0
25.0000000	0.1935706D-03	1.0000000
30.0000000	0.1938455D-03	1.0014203
40.0000000	0.1943257D-03	1.0039011
50.0000000	0.1949193D-03	1.0069675
60.0000000	0.1953829D-03	1.0093624
70.0000000	0.1959342D-03	1.0122106
80.0000000	0.1964370D-03	1.0148081
90.0000000	0.1970005D-03	1.0177190
100.0000000	0.1976897D-03	1.0212796
110.0000000	0.1981942D-03	1.0238860
120.0000000	0.1987967D-03	1.0269986
130.0000000	0.1993653D-03	1.0299357
140.0000000	0.1999638D-03	1.0330280
150.0000000	0.2005641D-03	1.0361289
160.0000000	0.2011164D-03	1.0389823
170.0000000	0.2016861D-03	1.0419255
180.0000000	0.2023280D-03	1.0452416
190.0000000	0.2028349D-03	1.0478600
200.0000000	0.2033605D-03	1.0505754
210.0000000	0.2039474D-03	1.0536073
220.0000000	0.2044625D-03	1.0562683
230.0000000	0.2049988D-03	1.0590391
240.0000000	0.2055467D-03	1.0618693
250.0000000	0.2061591D-03	1.0650333
260.0000000	0.2066734D-03	1.0676902
270.0000000	0.2072904D-03	1.0708777
280.0000000	0.2078005D-03	1.0735129
290.0000000	0.2083726D-03	1.0764685
300.0000000	0.2089707D-03	1.0795584
310.0000000	0.2095522D-03	1.0825621

SLOPE = 0.0000
VARIANCE = 0.17D-19
STD DEV = 0.00000
INTERCEPT = 0.0002
CORR. COEFF. = 0.99993D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS COMP PARALLEL TO C

TEMP	COMP PLTC	Y/YO
25.0000000	0.8698539D-04	1.0000000
30.0000000	0.8714432D-04	1.0018271
40.0000000	0.8720574D-04	1.0025332
50.0000000	0.8729574D-04	1.0035678
60.0000000	0.8736330D-04	1.0043446
70.0000000	0.8767102D-04	1.0078822
80.0000000	0.8775392D-04	1.0088352
90.0000000	0.8793926D-04	1.0109659
100.0000000	0.8792059D-04	1.0107513
110.0000000	0.8808396D-04	1.0126293
120.0000000	0.8818411D-04	1.0137807
130.0000000	0.8822046D-04	1.0141986
140.0000000	0.8835351D-04	1.0157282
150.0000000	0.8843826D-04	1.0167025
160.0000000	0.8851674D-04	1.0176047
170.0000000	0.8872556D-04	1.0200053
180.0000000	0.8884038D-04	1.0213253
190.0000000	0.8813005D-04	1.0131593
200.0000000	0.8915908D-04	1.0249891
210.0000000	0.8908060D-04	1.0240869
220.0000000	0.8914459D-04	1.0248225
230.0000000	0.8923186D-04	1.0258258
240.0000000	0.8937427D-04	1.0274631
250.0000000	0.8948647D-04	1.0287528
260.0000000	0.8956108D-04	1.0296106
270.0000000	0.8955416D-04	1.0295311
280.0000000	0.8964883D-04	1.0306194
290.0000000	0.8968392D-04	1.0310228
300.0000000	0.8959270D-04	1.0299741
310.0000000	0.8948893D-04	1.0287812

SLOPE = 0.0000
VARIANCE = 0.16D-18
STD DEV = 0.00000
INTERCEPT = 0.0001
CORR. COEFF. = 0.97632D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS VOLUMETRIC COMP

TEMP	VOL COMP	Y/YO
25.0000000	0.4741265D-03	1.0000000
30.0000000	0.4748353D-03	1.0014949
40.0000000	0.4758572D-03	1.0036501
50.0000000	0.4771343D-03	1.0063438
60.0000000	0.4781290D-03	1.0084418
70.0000000	0.4795394D-03	1.0114165
80.0000000	0.4806279D-03	1.0137123
90.0000000	0.4819402D-03	1.0164800
100.0000000	0.4832999D-03	1.0193480
110.0000000	0.4844724D-03	1.0218208
120.0000000	0.4857775D-03	1.0245736
130.0000000	0.4869510D-03	1.0270485
140.0000000	0.4882812D-03	1.0298541
150.0000000	0.4895664D-03	1.0325649
160.0000000	0.4907495D-03	1.0350603
170.0000000	0.4920978D-03	1.0379039
180.0000000	0.4934964D-03	1.0408538
190.0000000	0.4937998D-03	1.0414936
200.0000000	0.4958800D-03	1.0458812
210.0000000	0.4969754D-03	1.0481914
220.0000000	0.4980695D-03	1.0504991
230.0000000	0.4992295D-03	1.0529456
240.0000000	0.5004676D-03	1.0555570
250.0000000	0.5018047D-03	1.0583771
260.0000000	0.5029079D-03	1.0607040
270.0000000	0.5041350D-03	1.0632921
280.0000000	0.5052499D-03	1.0656435
290.0000000	0.5064292D-03	1.0681308
300.0000000	0.5075342D-03	1.0704614
310.0000000	0.5085933D-03	1.0726952

SLOPE = 0.0000
VARIANCE = 0.18D-18
STD DEV = 0.00000
INTERCEPT = 0.0005
CORR. COEFF. = 0.99983D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C33

TEMP	C33	Y/YO
25.0000000	0.4839499D 04	1.0000000
30.0000000	0.4837240D 04	0.9995333
40.0000000	0.4827492D 04	0.9975190
50.0000000	0.4817561D 04	0.9954669
60.0000000	0.4807447D 04	0.9933771
70.0000000	0.4797925D 04	0.9914094
80.0000000	0.4787833D 04	0.9893241
90.0000000	0.4777945D 04	0.9872810
100.0000000	0.4769802D 04	0.9855982
110.0000000	0.4760319D 04	0.9836388
120.0000000	0.4751038D 04	0.9817211
130.0000000	0.4741191D 04	0.9796864
140.0000000	0.4733849D 04	0.9781692
150.0000000	0.4726321D 04	0.9766136
160.0000000	0.4717076D 04	0.9747033
170.0000000	0.4709371D 04	0.9731112
180.0000000	0.4700717D 04	0.9713231
190.0000000	0.4673188D 04	0.9656346
200.0000000	0.4683054D 04	0.9676733
210.0000000	0.4674236D 04	0.9658512
220.0000000	0.4665046D 04	0.9639522
230.0000000	0.4655865D 04	0.9620552
240.0000000	0.4646315D 04	0.9600818
250.0000000	0.4637723D 04	0.9583065
260.0000000	0.4628382D 04	0.9563763
270.0000000	0.4619241D 04	0.9544874
280.0000000	0.4610487D 04	0.9526786
290.0000000	0.4601175D 04	0.9507545
300.0000000	0.4592440D 04	0.9489495
310.0000000	0.4582771D 04	0.9469515

SLOPE = -0.8970
VARIANCE = 0.58D-04
STD DEV = 0.00759
INTERCEPT = 4860.5693
CORR. COEFF. = -0.99900D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C11

TEMP	C11	Y/YO
25.0000000	0.2714336D 04	1.0000000
30.0000000	0.2711737D 04	0.9990424
40.0000000	0.2706307D 04	0.9970418
50.0000000	0.2700882D 04	0.9950432
60.0000000	0.2695814D 04	0.9931762
70.0000000	0.2690751D 04	0.9913109
80.0000000	0.2685341D 04	0.9893177
90.0000000	0.2679936D 04	0.9873264
100.0000000	0.2673717D 04	0.9850354
110.0000000	0.2669725D 04	0.9835647
120.0000000	0.2664101D 04	0.9814928
130.0000000	0.2659183D 04	0.9796808
140.0000000	0.2654036D 04	0.9777846
150.0000000	0.2648777D 04	0.9758471
160.0000000	0.2643988D 04	0.9740829
170.0000000	0.2638739D 04	0.9721489
180.0000000	0.2633262D 04	0.9701313
190.0000000	0.2628487D 04	0.9683719
200.0000000	0.2623136D 04	0.9664006
210.0000000	0.2617675D 04	0.9643887
220.0000000	0.2612682D 04	0.9625491
230.0000000	0.2607577D 04	0.9606686
240.0000000	0.2602247D 04	0.9587048
250.0000000	0.2596922D 04	0.9567430
260.0000000	0.2591947D 04	0.9549103
270.0000000	0.2586518D 04	0.9529099
280.0000000	0.2581667D 04	0.9511229
290.0000000	0.2576477D 04	0.9492108
300.0000000	0.2571406D 04	0.9473427
310.0000000	0.2566569D 04	0.9455607

SLOPE = -0.5187
VARIANCE = 0.50D-06
STD DEV = 0.00071
INTERCEPT = 2726.7992
CORR. COEFF. = -0.99997D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C44A

TEMP	C44A	Y/YO
25.0000000	0.1244295D 04	1.0000000
30.0000000	0.1243376D 04	0.9992612
40.0000000	0.1241460D 04	0.9977213
50.0000000	0.1239623D 04	0.9962454
60.0000000	0.1237710D 04	0.9947076
70.0000000	0.1235876D 04	0.9932336
80.0000000	0.1233965D 04	0.9916978
90.0000000	0.1232133D 04	0.9902257
100.0000000	0.1230224D 04	0.9886920
110.0000000	0.1228395D 04	0.9872218
120.0000000	0.1226489D 04	0.9856901
130.0000000	0.1224662D 04	0.9842219
140.0000000	0.1222914D 04	0.9828171
150.0000000	0.1221090D 04	0.9813507
160.0000000	0.1219266D 04	0.9798853
170.0000000	0.1217522D 04	0.9784831
180.0000000	0.1215623D 04	0.9769574
190.0000000	0.1213881D 04	0.9755570
200.0000000	0.1212758D 04	0.9746546
210.0000000	0.1210167D 04	0.9725726
220.0000000	0.1208274D 04	0.9710508
230.0000000	0.1206459D 04	0.9695921
240.0000000	0.1204568D 04	0.9680725
250.0000000	0.1202755D 04	0.9666158
260.0000000	0.1200944D 04	0.9651600
270.0000000	0.1199057D 04	0.9636434
280.0000000	0.1197171D 04	0.9621279
290.0000000	0.1195363D 04	0.9606751
300.0000000	0.1193480D 04	0.9591616
310.0000000	0.1191675D 04	0.9577108

SLOPE = -0.1840
VARIANCE = 0.13D-06
STD DEV = 0.00037
INTERCEPT = 1248.7669
CORR. COEFF. = -0.99994D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C66

TEMP	C66	Y/Y0
25.0000000	0.1947719D 04	1.0000000
30.0000000	0.1943121D 04	0.9976394
40.0000000	0.1933643D 04	0.9927730
50.0000000	0.1925384D 04	0.9885326
60.0000000	0.1916148D 04	0.9837908
70.0000000	0.1907629D 04	0.9794171
80.0000000	0.1898932D 04	0.9749516
90.0000000	0.1889859D 04	0.9702937
100.0000000	0.1881794D 04	0.9661527
110.0000000	0.1872862D 04	0.9615666
120.0000000	0.1864147D 04	0.9570922
130.0000000	0.1856724D 04	0.9532813
140.0000000	0.1848731D 04	0.9491773
150.0000000	0.1840852D 04	0.9451322
160.0000000	0.1833379D 04	0.9412956
170.0000000	0.1825825D 04	0.9374170
180.0000000	0.1817899D 04	0.9333477
190.0000000	0.1810087D 04	0.9293370
200.0000000	0.1802196D 04	0.9252856
210.0000000	0.1794707D 04	0.9214406
220.0000000	0.1787426D 04	0.9177022
230.0000000	0.1779968D 04	0.9138733
240.0000000	0.1772622D 04	0.9101014
250.0000000	0.1766244D 04	0.9068270
260.0000000	0.1758926D 04	0.9030699
270.0000000	0.1752099D 04	0.8995645
280.0000000	0.1744811D 04	0.8958228
290.0000000	0.1737633D 04	0.8921374
300.0000000	0.1730753D 04	0.8886052
310.0000000	0.1723981D 04	0.8851284

SLOPE = -0.7833
VARIANCE = 0.40D-04
STD DEV = 0.00631
INTERCEPT = 1961.5737
CORR. COEFF. = -0.99909D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C12

TEMP	C12	Y/YO
25.0000000	0.1779626D 04	1.0000000
30.0000000	0.1776243D 04	0.9980988
40.0000000	0.1771127D 04	0.9952242
50.0000000	0.1763764D 04	0.9910871
60.0000000	0.1758663D 04	0.9882206
70.0000000	0.1751465D 04	0.9841761
80.0000000	0.1746017D 04	0.9811147
90.0000000	0.1739264D 04	0.9773199
100.0000000	0.1731591D 04	0.9730081
110.0000000	0.1724756D 04	0.9691678
120.0000000	0.1717912D 04	0.9653217
130.0000000	0.1711139D 04	0.9615160
140.0000000	0.1704143D 04	0.9575848
150.0000000	0.1697373D 04	0.9537805
160.0000000	0.1690924D 04	0.9501568
170.0000000	0.1684557D 04	0.9465791
180.0000000	0.1677261D 04	0.9424797
190.0000000	0.1671694D 04	0.9393512
200.0000000	0.1666368D 04	0.9363587
210.0000000	0.1660602D 04	0.9331185
220.0000000	0.1655387D 04	0.9301879
230.0000000	0.1649906D 04	0.9271080
240.0000000	0.1644351D 04	0.9239869
250.0000000	0.1637860D 04	0.9203395
260.0000000	0.1632800D 04	0.9174961
270.0000000	0.1626637D 04	0.9140330
280.0000000	0.1621638D 04	0.9112240
290.0000000	0.1616022D 04	0.9080686
300.0000000	0.1610205D 04	0.9047995
310.0000000	0.1604438D 04	0.9015589

SLOPE = -0.6223
VARIANCE = 0.24D-04
STD DEV = 0.00494
INTERCEPT = 1793.5702
CORR. COEFF. = -0.99912D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C13

TEMP	C13	Y/Y0
25.0000000	0.1495667D 04	1.0000000
30.0000000	0.1492070D 04	0.9975947
40.0000000	0.1489805D 04	0.9960808
50.0000000	0.1486378D 04	0.9937893
60.0000000	0.1484279D 04	0.9923862
70.0000000	0.1478458D 04	0.9884942
80.0000000	0.1475916D 04	0.9867942
90.0000000	0.1471649D 04	0.9839415
100.0000000	0.1468555D 04	0.9818727
110.0000000	0.1464958D 04	0.9794678
120.0000000	0.1461377D 04	0.9770738
130.0000000	0.1458955D 04	0.9754545
140.0000000	0.1454633D 04	0.9725644
150.0000000	0.1450939D 04	0.9700947
160.0000000	0.1448067D 04	0.9681743
170.0000000	0.1443229D 04	0.9649398
180.0000000	0.1439214D 04	0.9622553
190.0000000	0.1449829D 04	0.9693527
200.0000000	0.1432095D 04	0.9574961
210.0000000	0.1430801D 04	0.9566307
220.0000000	0.1428469D 04	0.9550712
230.0000000	0.1425736D 04	0.9532444
240.0000000	0.1422400D 04	0.9510135
250.0000000	0.1418774D 04	0.9485897
260.0000000	0.1416431D 04	0.9470226
270.0000000	0.1414266D 04	0.9455757
280.0000000	0.1411631D 04	0.9438135
290.0000000	0.1409371D 04	0.9423024
300.0000000	0.1408214D 04	0.9415288
310.0000000	0.1407508D 04	0.9410570

SLOPE = -0.3212
VARIANCE = 0.39D-04
STD DEV = 0.00628
INTERCEPT = 1501.0441
CORR. COEFF. = -0.99469D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C33 VELOCITY

TEMP	C33 VEL	Y/Y0
25.0000000	0.1065848D 02	1.0000000
30.0000000	0.1065662D 02	0.9998255
40.0000000	0.1064714D 02	0.9989354
50.0000000	0.1063744D 02	0.9980253
60.0000000	0.1062752D 02	0.9970953
70.0000000	0.1061825D 02	0.9962255
80.0000000	0.1060834D 02	0.9952957
90.0000000	0.1059865D 02	0.9943860
100.0000000	0.1059088D 02	0.9936570
110.0000000	0.1058161D 02	0.9927877
120.0000000	0.1057256D 02	0.9919386
130.0000000	0.1056287D 02	0.9910294
140.0000000	0.1055596D 02	0.9903811
150.0000000	0.1054884D 02	0.9897130
160.0000000	0.1053979D 02	0.9888643
170.0000000	0.1053246D 02	0.9881764
180.0000000	0.1052406D 02	0.9873882
190.0000000	0.1049448D 02	0.9846127
200.0000000	0.1050683D 02	0.9857721
210.0000000	0.1049822D 02	0.9849642
220.0000000	0.1048919D 02	0.9841162
230.0000000	0.1048015D 02	0.9832684
240.0000000	0.1047069D 02	0.9823805
250.0000000	0.1046229D 02	0.9815931
260.0000000	0.1045305D 02	0.9807256
270.0000000	0.1044401D 02	0.9798781
280.0000000	0.1043541D 02	0.9790710
290.0000000	0.1042617D 02	0.9782037
300.0000000	0.1041757D 02	0.9773968
310.0000000	0.1040790D 02	0.9764896

SLOPE = -0.0009
VARIANCE = 0.69D-10
STD DEV = 0.00001
INTERCEPT = 10.6794
CORR. COEFF. = -0.99874D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C11 VELOCITY

TEMP	C11 VEL	Y/Y0
25.0000000	0.79822810 01	1.0000000
30.0000000	0.79789280 01	0.9995800
40.0000000	0.79718750 01	0.9986964
50.0000000	0.79648220 01	0.9978129
60.0000000	0.79582900 01	0.9969944
70.0000000	0.79517570 01	0.9961760
80.0000000	0.79447040 01	0.9952925
90.0000000	0.79376510 01	0.9944089
100.0000000	0.79293840 01	0.9933732
110.0000000	0.79244120 01	0.9927503
120.0000000	0.79170120 01	0.9918233
130.0000000	0.79106520 01	0.9910266
140.0000000	0.79039460 01	0.9901864
150.0000000	0.78970660 01	0.9893245
160.0000000	0.78908800 01	0.9885495
170.0000000	0.78840000 01	0.9876876
180.0000000	0.78767730 01	0.9867823
190.0000000	0.78705870 01	0.9860073
200.0000000	0.78635330 01	0.9851236
210.0000000	0.78563060 01	0.9842182
220.0000000	0.78497730 01	0.9833997
230.0000000	0.78430660 01	0.9825595
240.0000000	0.78360120 01	0.9816758
250.0000000	0.78289580 01	0.9807921
260.0000000	0.78224240 01	0.9799736
270.0000000	0.78151960 01	0.9790681
280.0000000	0.78088360 01	0.9782713
290.0000000	0.78019560 01	0.9774093
300.0000000	0.77952480 01	0.9765690
310.0000000	0.77888880 01	0.9757722

SLOPE = -0.0007
VARIANCE = 0.81D-12
STD DEV = 0.00000
INTERCEPT = 7.9989
CORR. COEFF. = -0.99998D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C44A VELOCITY

TEMP	C44A VEL	Y/YO
25.0000000	0.5404517D 01	1.0000000
30.0000000	0.5402838D 01	0.9996894
40.0000000	0.5399310D 01	0.9990366
50.0000000	0.5395953D 01	0.9984154
60.0000000	0.5392426D 01	0.9977628
70.0000000	0.5389069D 01	0.9971416
80.0000000	0.5385541D 01	0.9964890
90.0000000	0.5382185D 01	0.9958679
100.0000000	0.5378658D 01	0.9952153
110.0000000	0.5375301D 01	0.9945943
120.0000000	0.5371775D 01	0.9939417
130.0000000	0.5368419D 01	0.9933208
140.0000000	0.5365233D 01	0.9927313
150.0000000	0.5361877D 01	0.9921104
160.0000000	0.5358522D 01	0.9914895
170.0000000	0.5355337D 01	0.9909002
180.0000000	0.5351811D 01	0.9902478
190.0000000	0.5348626D 01	0.9896585
200.0000000	0.5346805D 01	0.9893216
210.0000000	0.5341746D 01	0.9883854
220.0000000	0.5338220D 01	0.9877331
230.0000000	0.5334866D 01	0.9871124
240.0000000	0.5331341D 01	0.9864602
250.0000000	0.5327986D 01	0.9858395
260.0000000	0.5324632D 01	0.9852189
270.0000000	0.5321108D 01	0.9845667
280.0000000	0.5317583D 01	0.9839146
290.0000000	0.5314229D 01	0.9832940
300.0000000	0.5310705D 01	0.9826419
310.0000000	0.5307351D 01	0.9820214

SLOPE = -0.0003
VARIANCE = 0.680-12
STD DEV = 0.00000
INTERCEPT = 5.4129
CORR. COEFF. = -0.99992D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C66 VELOCITY

TEMP	C66 VEL	Y/Y0
25.0000000	0.6761738D 01	1.0000000
30.0000000	0.6754151D 01	0.9988779
40.0000000	0.6738452D 01	0.9965562
50.0000000	0.6724840D 01	0.9945431
60.0000000	0.6709487D 01	0.9922725
70.0000000	0.6695351D 01	0.9901819
80.0000000	0.6680865D 01	0.9880396
90.0000000	0.6665682D 01	0.9857941
100.0000000	0.6652238D 01	0.9838059
110.0000000	0.6637226D 01	0.9815858
120.0000000	0.6622561D 01	0.9794170
130.0000000	0.6610159D 01	0.9775827
140.0000000	0.6596710D 01	0.9755938
150.0000000	0.6583434D 01	0.9736305
160.0000000	0.6570854D 01	0.9717700
170.0000000	0.6558099D 01	0.9698836
180.0000000	0.6544646D 01	0.9678940
190.0000000	0.6531366D 01	0.9659300
200.0000000	0.6517910D 01	0.9639401
210.0000000	0.6505151D 01	0.9620530
220.0000000	0.6492738D 01	0.9602173
230.0000000	0.6479976D 01	0.9583300
240.0000000	0.6467387D 01	0.9564682
250.0000000	0.6456540D 01	0.9548640
260.0000000	0.6443949D 01	0.9530019
270.0000000	0.6432229D 01	0.9512686
280.0000000	0.6419636D 01	0.9494062
290.0000000	0.6407216D 01	0.9475694
300.0000000	0.6395318D 01	0.9458098
310.0000000	0.6383594D 01	0.9440758

SLOPE = -0.0013
VARIANCE = 0.82D-10
STD DEV = 0.00001
INTERCEPT = 6.7867
CORR. COEFF. = -0.99935D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C12 VELOCITY

TEMP	C12 VEL	Y/Y0
25.0000000	0.6463378D 01	1.0000000
30.0000000	0.6457612D 01	0.9991078
40.0000000	0.6449066D 01	0.9977857
50.0000000	0.6436409D 01	0.9958273
60.0000000	0.6427855D 01	0.9945040
70.0000000	0.6415450D 01	0.9925846
80.0000000	0.6406226D 01	0.9911576
90.0000000	0.6394588D 01	0.9893569
100.0000000	0.6381229D 01	0.9872901
110.0000000	0.6369387D 01	0.9854579
120.0000000	0.6357500D 01	0.9836187
130.0000000	0.6345719D 01	0.9817960
140.0000000	0.6333497D 01	0.9799050
150.0000000	0.6321668D 01	0.9780749
160.0000000	0.6310412D 01	0.9763334
170.0000000	0.6299285D 01	0.9746118
180.0000000	0.6286395D 01	0.9726175
190.0000000	0.6276718D 01	0.9711203
200.0000000	0.6267478D 01	0.9696908
210.0000000	0.6257391D 01	0.9681301
220.0000000	0.6248324D 01	0.9667273
230.0000000	0.6238739D 01	0.9652443
240.0000000	0.6228997D 01	0.9637370
250.0000000	0.6217459D 01	0.9619518
260.0000000	0.6208615D 01	0.9605836
270.0000000	0.6197656D 01	0.9588881
280.0000000	0.6188895D 01	0.9575326
290.0000000	0.6178941D 01	0.9559924
300.0000000	0.6168579D 01	0.9543893
310.0000000	0.6158293D 01	0.9527979

SLOPE = -0.0011
VARIANCE = 0.62D-10
STD DEV = 0.00001
INTERCEPT = 6.4888
CORR. COEFF. = -0.99926D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS C13 VELOCITY

TEMP	C13 VEL	Y/Y0
25.0000000	0.5925332D 01	1.0000000
30.0000000	0.5918550D 01	0.9988555
40.0000000	0.5914755D 01	0.9982150
50.0000000	0.5908646D 01	0.9971840
60.0000000	0.5905173D 01	0.9965978
70.0000000	0.5894282D 01	0.9947597
80.0000000	0.5889912D 01	0.9940223
90.0000000	0.5882094D 01	0.9927028
100.0000000	0.5876609D 01	0.9917772
110.0000000	0.5870111D 01	0.9906806
120.0000000	0.5863637D 01	0.9895880
130.0000000	0.5859481D 01	0.9888866
140.0000000	0.5851500D 01	0.9875397
150.0000000	0.5844773D 01	0.9864043
160.0000000	0.5839692D 01	0.9855468
170.0000000	0.5830637D 01	0.9840187
180.0000000	0.5823230D 01	0.9827685
190.0000000	0.5845378D 01	0.9865065
200.0000000	0.5810230D 01	0.9805746
210.0000000	0.5808315D 01	0.9802514
220.0000000	0.5804291D 01	0.9795723
230.0000000	0.5799451D 01	0.9787555
240.0000000	0.5793375D 01	0.9777301
250.0000000	0.5786703D 01	0.9766040
260.0000000	0.5782637D 01	0.9759178
270.0000000	0.5778935D 01	0.9752930
280.0000000	0.5774266D 01	0.9745050
290.0000000	0.5770361D 01	0.9738460
300.0000000	0.5768712D 01	0.9735678
310.0000000	0.5767989D 01	0.9734457

SLOPE = -0.0006
VARIANCE = 0.16D-09
STD DEV = 0.00001
INTERCEPT = 5.9349
CORR. COEFF. = -0.99354D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS F33

TEMP	F33	Y/Y0
25.0000000	0.4989100D 03	1.0000000
30.0000000	0.4988000D 03	0.9997795
40.0000000	0.4983100D 03	0.9987974
50.0000000	0.4978100D 03	0.9977952
60.0000000	0.4973000D 03	0.9967730
70.0000000	0.4968200D 03	0.9958109
80.0000000	0.4963100D 03	0.9947886
90.0000000	0.4958100D 03	0.9937865
100.0000000	0.4954000D 03	0.9929647
110.0000000	0.4949200D 03	0.9920026
120.0000000	0.4944500D 03	0.9910605
130.0000000	0.4939500D 03	0.9900583
140.0000000	0.4935800D 03	0.9893167
150.0000000	0.4932000D 03	0.9885551
160.0000000	0.4927300D 03	0.9876130
170.0000000	0.4923400D 03	0.9868313
180.0000000	0.4919000D 03	0.9859494
190.0000000	0.4904700D 03	0.9830831
200.0000000	0.4910000D 03	0.9841454
210.0000000	0.4905500D 03	0.9832435
220.0000000	0.4900800D 03	0.9823014
230.0000000	0.4896100D 03	0.9813594
240.0000000	0.4891200D 03	0.9803772
250.0000000	0.4886800D 03	0.9794953
260.0000000	0.4882000D 03	0.9785332
270.0000000	0.4877300D 03	0.9775911
280.0000000	0.4872800D 03	0.9766892
290.0000000	0.4868000D 03	0.9757271
300.0000000	0.4863500D 03	0.9748251
310.0000000	0.4858500D 03	0.9738229

SLOPE = -0.0456
VARIANCE = 0.15D-06
STD DEV = 0.00039
INTERCEPT = 500.0091
CORR. COEFF. = -0.99899D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS F11

TEMP	F11	Y/Y0
25.0000000	0.4606000D 03	1.0000000
30.0000000	0.4603900D 03	0.9995441
40.0000000	0.4599500D 03	0.9985888
50.0000000	0.4595100D 03	0.9976335
60.0000000	0.4591000D 03	0.9967434
70.0000000	0.4586900D 03	0.9958532
80.0000000	0.4582500D 03	0.9948980
90.0000000	0.4578100D 03	0.9939427
100.0000000	0.4573000D 03	0.9928354
110.0000000	0.4569800D 03	0.9921407
120.0000000	0.4565200D 03	0.9911420
130.0000000	0.4561200D 03	0.9902736
140.0000000	0.4557000D 03	0.9893617
150.0000000	0.4552700D 03	0.9884281
160.0000000	0.4548800D 03	0.9875814
170.0000000	0.4544500D 03	0.9866479
180.0000000	0.4540000D 03	0.9856709
190.0000000	0.4536100D 03	0.9848241
200.0000000	0.4531700D 03	0.9838689
210.0000000	0.4527200D 03	0.9828919
220.0000000	0.4523100D 03	0.9820017
230.0000000	0.4518900D 03	0.9810899
240.0000000	0.4514500D 03	0.9801346
250.0000000	0.4510100D 03	0.9791793
260.0000000	0.4506000D 03	0.9782892
270.0000000	0.4501500D 03	0.9773122
280.0000000	0.4497500D 03	0.9764438
290.0000000	0.4493200D 03	0.9755102
300.0000000	0.4489000D 03	0.9745983
310.0000000	0.4485000D 03	0.9737299

SLOPE = -0.0425
VARIANCE = 0.27D-08
STD DEV = 0.00005
INTERCEPT = 461.6441
CORR. COEFF. = -0.99998D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS F44A

TEMP	F44A	Y/Y0
25.0000000	0.31746000D 03	1.0000000
30.0000000	0.31735000D 03	0.9996535
40.0000000	0.31712000D 03	0.9989290
50.0000000	0.31690000D 03	0.9982360
60.0000000	0.31667000D 03	0.9975115
70.0000000	0.31645000D 03	0.9968185
80.0000000	0.31622000D 03	0.9960940
90.0000000	0.31600000D 03	0.9954010
100.0000000	0.31577000D 03	0.9946765
110.0000000	0.31555000D 03	0.9939835
120.0000000	0.31532000D 03	0.9932590
130.0000000	0.31510000D 03	0.9925660
140.0000000	0.31489000D 03	0.9919045
150.0000000	0.31467000D 03	0.9912115
160.0000000	0.31445000D 03	0.9905185
170.0000000	0.31424000D 03	0.9898570
180.0000000	0.31401000D 03	0.9891325
190.0000000	0.31380000D 03	0.9884710
200.0000000	0.31367000D 03	0.9880615
210.0000000	0.31335000D 03	0.9870535
220.0000000	0.31312000D 03	0.9863290
230.0000000	0.31290000D 03	0.9856360
240.0000000	0.31267000D 03	0.9849115
250.0000000	0.31245000D 03	0.9842185
260.0000000	0.31223000D 03	0.9835255
270.0000000	0.31200000D 03	0.9828010
280.0000000	0.31177000D 03	0.9820765
290.0000000	0.31155000D 03	0.9813835
300.0000000	0.31132000D 03	0.9806590
310.0000000	0.31110000D 03	0.9799660

SLOPE = -0.0222
VARIANCE = 0.23D-08
STD DEV = 0.00005
INTERCEPT = 318.0090
CORR. COEFF. = -0.99993D 00

TEMPERATURE CALCULATIONS FOR CRYSTAL #1111
LEAST SQUARES TEMP VS F66

TEMP	F66	Y/Y0
25.0000000	0.3886000D 03	1.0000000
30.0000000	0.3881500D 03	0.9988420
40.0000000	0.3872200D 03	0.9964488
50.0000000	0.3864100D 03	0.9943644
60.0000000	0.3855000D 03	0.9920226
70.0000000	0.3846600D 03	0.9898610
80.0000000	0.3838000D 03	0.9876480
90.0000000	0.3829000D 03	0.9853320
100.0000000	0.3821000D 03	0.9832733
110.0000000	0.3812100D 03	0.9809830
120.0000000	0.3803400D 03	0.9787442
130.0000000	0.3796000D 03	0.9768399
140.0000000	0.3788000D 03	0.9747813
150.0000000	0.3780100D 03	0.9727483
160.0000000	0.3772600D 03	0.9708183
170.0000000	0.3765000D 03	0.9688626
180.0000000	0.3757000D 03	0.9668039
190.0000000	0.3749100D 03	0.9647710
200.0000000	0.3741100D 03	0.9627123
210.0000000	0.3733500D 03	0.9607566
220.0000000	0.3726100D 03	0.9588523
230.0000000	0.3718500D 03	0.9568966
240.0000000	0.3711000D 03	0.9549665
250.0000000	0.3704500D 03	0.9532939
260.0000000	0.3697000D 03	0.9513639
270.0000000	0.3690000D 03	0.9495625
280.0000000	0.3682500D 03	0.9476325
290.0000000	0.3675100D 03	0.9457283
300.0000000	0.3668000D 03	0.9439012
310.0000000	0.3661000D 03	0.9420998

SLOPE = -0.0788
VARIANCE = 0.27D-06
STD DEV = 0.00052
INTERCEPT = 390.0959
CORR. COEFF. = -0.99938D 00

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BIBLIOGRAPHY

Anderson, O. L., 1963. A simplified method for calculating Debye temperature from elastic constants, J. Phys. Chem. Solids, 24, 909.

Anderson, O. L., Edward Schrieber, Robert C. Libermann, and Naohiro Soga, 1968. Some elastic constant data on minerals relevant to geophysics, Rev. Geophys., 6, 4, 491.

Birch, F., 1952. Elasticity and constitution of the earth's interior, J. Geophys. Res., 57, 227.

Birch, F., 1960. Elastic constants of rutile: a correction to a paper by R. K. Verma, 'Elasticity of some high-density crystals,' J. Geophys. Res., 65, 3855.

Birch, F., 1961. The velocity of compressional waves in rocks to 10 kilobars, Part 2, J. Geophys. Res., 66, 7, 2206.

Cook, R. K., 1957. Variation of elastic constants and static strains with hydrostatic pressure: a method for calculation from ultrasonic measurements, J. Acoust. Soc., 29, 4, 445.

Federov, F. I., 1968. Theory of elastic waves in crystals, Plenum Press, New York, 367 pp.

Fisher, E. S., 1964. Single crystal elastic moduli and the hcp → bcc transformation in Ti, Zr, and Hf, Phys. Rev., 135, 2A, A482.

Fisher, F. S., M. H. Manghnani, and T. J. Sokolowski, 1971. Hydrostatic pressure derivatives of the single crystal elastic moduli of zirconium, J. App. Phys., (in press).

Frederick, D. and T. S. Chang, 1965. Continuum mechanics, Allyn and Bacon, Inc., Boston, 218 pp.

Hill, R., 1952. The elastic behavior of a crystalline aggregate, Proc. Phys. Soc. London, 65A, 349.

Johnson, D. P., J. L. Cross, J. K. Hill, and H. A. Bowman, 1957. Elastic distortion error in the dead-weight piston gage, Ind. and Eng. Chem., 49, 12, 2046.

Johnson, D. P. and D. H. Newhall, 1953. The piston gage as a precise pressure-measuring instrument, Trans. ASME, 301.

Kittel, C., 1960. Introduction to solid state physics, John Wiley and Sons, Inc., Second Edition, New York, 85 pp.

Love, A. E. H., 1944. The mathematical theory of elasticity, Dover Publications, Inc., New York, 154 pp.

Manghnani, M. H., 1969. Elastic constants of single-crystal rutile under pressures to 7.5 kilobars, J. Geophys. Res., 74, 17, 4317.

Mason, B. and L. G. Berry, 1968. Elements of mineralogy, W. H. Freeman and Company, San Francisco, 550 pp.

Meister, R. and Louis Peselnick, 1966. Variational method of determining effective moduli of polycrystals with tetragonal symmetry, J. App. Phys., 37, 11, 4121.

McSkimin, H. J., 1950. Ultrasonic measurement techniques applicable to small solid specimens, J. Acoust. Soc. Am., 22, 413.

McSkimin, H. J., 1961. Pulse superposition method for measuring ultrasonic wave velocities in solids, J. Acoust. Soc. Am., 33, 12.

McSkimin, H. J. and P. Andreatch, 1962. Analysis of the pulse superposition method for measuring ultrasonic wave velocities as a function of temperature and pressure, J. Acoust. Soc. Am., 34, 5, 609.

Newhall, D. H., 1962. Manganin high-pressure sensors, instruments and control systems, Harwood Engineering Co., Inc.

Nye, J. F., 1967. Physical properties of crystals, Oxford at the Clarendon Press, 315 pp.

Reuss, A., 1929. Berechnung de fliessgrenze von mischkristallen auf grund der plastizita-tsbedingung fur einkristalle, Z. Angew, Math. Mech., 9, 49.

Schrieber, E. and O. L. Anderson, 1966. Pressure derivatives of the sound velocities of polycrystalline alumina, J. Am. Cer. Soc., 49, 4, 184.

Sokolnikoff, I. S., 1946. Mathematical theory of elasticity, McGraw-Hill Book Company, Inc., New York, 59.

Sokolowski, T. J. and M. H. Manghnani, 1969. Adiabatic elastic moduli of vitreous calcium aluminates to 3.5 kilobars, J. Am. Cer. Soc., 52, 10, 539.

Verma, R. K., 1960. Elasticity of some high density crystals, J. Geophys. Res., 62, 2, 757.

Voigt, W., 1928. Lehrbuch der kristallphysik, B. B. Teubner, Leipzig.

Wooster, W. A., 1938. Crystal physics, Cambridge University Press, London, 282 pp.