

CRYSTAL SYMMETRY AND ELASTIC CONSTANTS

by

MICHAEL WANDZILAK

S.B., Massachusetts Institute of Technology

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Signature of Author

[Handwritten signature]
Department of Geology and Geophysics
December 15, 1968

Certified by

[Handwritten signature]
Thesis Supervisor

Accepted by

[Handwritten signature]
Chairman, Departmental Committee of
Graduate Students

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Abstract

Techniques by which to obtain reliable estimates for both the single crystal and polycrystalline elastic properties of various low symmetry solids from a relatively few number of measurements on a given single crystal would be valuable. In this note, we consider two possible techniques: (1) the determination of single crystal elastic constants under an assumption of higher symmetry than the true symmetry of a given material, and (2) the estimation of aggregate properties from measurements made on a single crystal in several random directions. Neither method is very accurate.

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LIST OF SYMBOLS

α_L :	direction cosine
BETAV:	Voigt average of the compressibility, (Mbars) ⁻¹
BETAR:	Reuss average of the compressibility, (Mbars) ⁻¹
C_{ij} :	stiffnesses ($i=1,\dots,6; j=1,\dots,6$), Mbars
C_{ij}^{HEX} :	stiffnesses obtained under assumption of hexagonal symmetry, (Mbars)
C_{ij}^{CUB} :	stiffnesses obtained under assumption of cubic symmetry, (Mbars)
ER:	Reuss average of Young's modulus, Mbars
EV:	Voigt average of Young's modulus, Mbars
GR:	Reuss average of shear modulus, Mbars
GV:	Voigt average of shear modulus, Mbars
Γ_{ij} :	Christoffel constants ($i=1,\dots,6; j=1,\dots,6$)
KR:	Reuss average of bulk modulus, Mbars
KV:	Voigt average of bulk modulus, Mbars
PRR:	Reuss average of Poisson's ratio
PRV:	Voigt average of Poisson's ratio
ρ :	density
S_{ij} :	compliances ($i=1,\dots,6; j=1,\dots,6$), (Mbars) ⁻¹
σ :	standard deviation
V:	elastic velocity, km/sec
V_p :	compressional velocity in polycrystalline material, km/sec

- V_s : shear velocity in polycrystalline material,
km/sec
- V_L : longitudinal elastic velocity in single crystals,
km/sec
- V_T, V_t : elastic velocities of transverse modes, in single
crystals, km/sec

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The ultrasonic techniques for the determination of the single crystal elastic moduli of solids are difficult and time consuming for the materials with a low degree of symmetry. The triclinic class ($\bar{1}$ symmetry) has 21 independent elastic moduli. Thus it is not surprising that some investigators have looked for simpler ways to estimate elastic properties. Alexandrov and Ryzhova (1961) treated some crystals as though they possessed a higher symmetry and measured the elastic properties with reference to the higher symmetry. Perhaps the elastic properties measured under this assumption provide an adequate estimate of the single crystal elastic properties of the crystal, or at least constitute a set of data from which reliable estimates of the polycrystalline aggregate properties may be calculated by the Voigt-Reuss scheme. A second possible method to obtain estimates of the polycrystalline properties from a relatively few measurements on a single crystal might use averages of the velocities of elastic waves propagating along three orthogonal directions selected randomly in a given crystal.

In this note, we consider the errors in these schemes for representative materials of several symmetry classes (tetragonal, orthorhombic, monoclinic, hexagonal and trigonal). Our procedure may be illustrated for corundum. The true symmetry is trigonal ($\bar{3}m$) and requires six

independent elastic constants to specify completely the elastic properties. Because these six constants are known, the three velocities of elastic waves propagating in any direction in the crystal, with direction cosines (α_L), may be calculated (Hearmon, 1961) from

$$\begin{vmatrix} \Gamma_{11} - \rho v^2 & \Gamma_{12} & \Gamma_{13} \\ \Gamma_{12} & \Gamma_{22} - \rho v^2 & \Gamma_{23} \\ \Gamma_{13} & \Gamma_{23} & \Gamma_{33} - \rho v^2 \end{vmatrix} = 0$$

where the Γ_{ij} are the Christoffel stiffnesses and are given by $\Gamma_{ij} = C_{ijkl}\alpha_k\alpha_l$. Suppose that we wish to treat corundum as though the symmetry were hexagonal (6/mmm). From the velocities that one would measure for the directions often used to determine the elastic constants, we may use equation (1) to solve for the five independent C_{ij}^{HEX} . These values and the corresponding Voigt and Reuss averages may then be compared with the true values. In a similar way, the C_{ij}^{CUB} that result from the assumption of cubic symmetry could be obtained for corundum.

To obtain representative values, several materials in each symmetry class (for which data were available) were analyzed. Monoclinic and orthorhombic crystals were analyzed as though they were tetragonal and cubic, trigonal

crystals as though hexagonal and cubic, and hexagonal and tetragonal crystals as though cubic. Data on the true elastic properties were obtained from Simmons (1965). In table 1 we show the direction and the set of equations from which the values of the "pseudo elastic constants" were determined. Some of the relations that are used normally as a check on the consistency of experimental values are shown also in table 1.

For some simulated measurements the polarizations of the various modes of propagation were not those that would be expected in a crystal that actually possessed the assumed symmetry. In these cases the polarization that came closest to the expected value was chosen and its velocity was used in the relations of table 1 to determine the pseudo elastic constants.

The values of the single-crystal elastic constants obtained in this way are shown in table 2. As can be seen, the sets of elastic constants obtained under the assumption of higher symmetry do not provide an adequate description of the crystal's elastic properties. The polyaggregate elastic properties derived from these elastic moduli are presented in table 3, and here again we see that in general no reliable results are obtained. Attention is called in particular to the value of the

Reuss average of Young's modulus for staurolite, derived under the assumption of cubic symmetry ($m3m$). Its value is 8.109, while the true value for this material is 1.638. This example has been pointed out to show that there exists a certain instability in the values obtained assuming higher symmetry, which comes about because of the indirect way in which the C_{ij} were obtained, viz., as solutions to sets of equations. Two examples of the degree of internal consistency which were observed between the pseudo elastic constants obtained using this method are shown in table 4.

In table 5 the results have been examined in a somewhat different way. For a unit uni-axial stress, three of the resulting strain components are tabulated to show the extent of the errors introduced by assuming the crystals to possess a higher symmetry. In table 6 two measures of anisotropy, A as defined by Hearmon (1961) and A^* as defined by Chung (1967), have been calculated using the stiffnesses of table 1. For the tetragonal and hexagonal samples, because of the particular set of velocity measurements used, the anisotropy calculated under the assumption that the crystals are cubic agrees exactly with the true values for the crystals. But, in general, this method does not provide an adequate estimate of the anisotropy of the crystal.

The second method mentioned above, that of using the averages of the velocities of elastic waves propagating along three orthogonal directions selected randomly in a given crystal, was tested by simulating these measurements for ten random orientations in each of the materials examined. Table 7 shows the average velocities obtained in this way and compares them to the true Voigt-Reuss-Hill averages. In table 8 the bulk and shear moduli calculated from the velocity averages are shown along with the Voigt-Reuss-Hill averages of these quantities. As is seen there, while the majority of the values are within 1-2% of the average Voigt-Reuss values, there are several cases in which the error is about 10%, a figure which seems to define the reliability of this scheme.

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TABLE #1

Elastic Waves and Velocity-Stiffness Relations for Cubic,
Tetragonal and Hexagonal Crystals

<u>Class</u>	<u>Direction of Propagation</u>	<u>Direction of Polarization</u>	<u>Velocity Relation</u>	<u>Note</u>
		(1, -1, 0)	$\rho V_T^2 = \frac{1}{2}(C_{11} - C_{12})$	*
	(1, 1, 0)	(1, 1, 0)	$\rho V_L^2 = \frac{1}{2}(C_{11} + C_{12}) + C_{44}$	*
		(0, 0, 1)	$\rho V_t^2 = C_{44}$	*
m3m		(0, 0, 1)	$\rho V_L^2 = C_{11}$	†
	(0, 0, 1)	transverse	$\rho V_T^2 = \rho V_t^2 = C_{44}$	†
	(1, 1, 1)	(1, 1, 1)	$\rho V_L^2 = \frac{1}{3}(C_{11} + 2C_{12} + 4C_{44})$	†
<hr/>				
		(1, 0, 0)	$\rho V_L^2 = C_{11}$	*
	(1, 0, 0)	(0, 1, 0)	$\rho V_T^2 = C_{44}$	*
		(0, 0, 1)	$\rho V_t^2 = C_{66}$	*
4/mmm	(1, 1, 0)	(-1, 1, 0)	$\rho V_t^2 = (C_{11} - C_{12})/2$	*
		(0, 1, -1)	$\rho V_T^2 = (C_{11} + C_{33})/4 - C_{13}/2$	*
	(0, 1, 1)	(0, 1, 1)	$\rho V_L^2 = (C_{11} + C_{33})/4 + C_{13}/2 + C_{44}$	*
		(1, 0, 0)	$\rho V_t^2 = (C_{44} + C_{66})/2$	†

Table #1--Cont.

<u>Class</u>	<u>Direction of Propagation</u>	<u>Direction of Polarization</u>	<u>Velocity Relation</u>	<u>Note</u>
	(0, 0, 1)	(0, 0, 1)	$\rho V_L^2 = C_{33}$	*
	(0, 0, 1)	transverse	$\rho V_T^2 = \rho V_t^2 = C_{44}$	*
	(1, 0, 0)	(0, 1, 0)	$\rho V_T^2 = \frac{1}{2}(C_{11} - C_{12})$	*
	(1, 0, 0)	(1, 0, 0)	$\rho V_L^2 = C_{11}$	*
		(0, 0, 1)	$\rho V_t^2 = C_{44}$	†
6/mmm		(0, 0, 1)	$\rho V_T^2 = \frac{1}{2}(C_{66} + C_{44})$	†
	(1, 2, $\sqrt{5}$)	(1, 2, $\sqrt{5}$)	$\rho V_L^2 = \frac{1}{4}(C_{11} + C_{33} + 2C_{44}) + \frac{1}{4}[(C_{11} - C_{33})^2 + 4(C_{13} + C_{44})^2]^{1/2}$	*
		quasi-transverse	$\rho V_t^2 = \frac{1}{4}(C_{11} + C_{33} + 2C_{44}) - \frac{1}{4}[(C_{11} - C_{33})^2 + 4(C_{13} + C_{44})^2]^{1/2}$	*

Note: * Used to solve for C_{ij} 's.

† Used as check on internal consistency.

TABLE #2

 C_{ij} Obtained Assuming Higher Symmetry

<u>Material</u>	<u>Class</u>	<u>Assumed Class</u>	<u>C_{11}</u>	<u>C_{12}</u>	<u>C_{13}</u>	<u>C_{14}</u>	<u>C_{15}</u>
Rutile 3	4/mmm	-	2.7300	1.7600	1.4900	-	-
		m3m	3.4200	2.4500	2.4500	-	-
Olivine	mmm	-	3.2400	0.5900	0.7900	-	-
		4/mmm	3.2400	1.7630	0.5741	-	-
Staurolite	mmm	m3m	2.2582	0.7812	0.7812	-	-
		-	3.4300	0.6700	0.6100	-	-
Apatite 1	6/mmm	4/mmm	3.4300	2.2700	-0.3610	-	-
		m3m	2.3554	1.1954	1.1954	-	-
Magnesium 6	6/mmm	-	1.6670	0.1310	0.6550	-	-
		m3m	1.7720	0.2360	0.2360	-	-
Corundum 1	$\bar{3}m$	-	0.6332	0.2631	0.2165	-	-
		m3m	0.6375	0.2675	0.2675	-	-
Quartz 6	$\bar{3}m$	-	4.9700	1.6360	1.1090	-0.2350	-
		6/mmm	4.9700	2.3371	1.1509	0.0000	-
Diopside	2/m	m3m	5.3659	1.8448	1.8448	0.0000	-
		-	0.8674	0.0699	0.1191	-0.1791	-
Oligoclase	2/m	6/mmm	0.8674	0.2904	0.2204	0.0000	-
		m3m	0.6466	-0.0070	-0.0070	0.0000	-
Oligoclase	2/m	-	2.0400	0.8440	0.8830	-	-0.1930
		4/mmm	2.0652	1.0241	0.6892	-	0.0000
Oligoclase	2/m	m3m	2.0292	0.9881	0.9881	-	0.0000
		-	0.8060	0.4170	0.5380	-	0.1610
Oligoclase	2/m	4/mmm	0.8509	0.1425	0.3322	-	0.0000
		m3m	1.3932	0.6848	0.6848	-	0.0000

<u>C₂₂</u>	<u>C₂₃</u>	<u>C₂₅</u>	<u>C₃₃</u>	<u>C₃₅</u>	<u>C₄₄</u>	<u>C₄₆</u>	<u>C₅₅</u>	<u>C₆₆</u>
2.7300	1.4900	-	4.8400	-	1.2500	-	1.2500	1.9400
3.4200	2.4500	-	3.4200	-	1.2500	-	1.2500	1.2500
1.9800	0.7800	-	2.4900	-	0.6670	-	0.8100	0.7930
3.2400	0.5741	-	1.1143	-	0.8100	-	0.8100	2.4900
2.2582	0.7812	-	2.2582	-	0.9416	-	0.9416	0.9416
1.8500	0.1280	-	1.4700	-	0.4600	-	0.7000	0.9200
3.4300	-0.3610	-	-0.9121	-	0.9200	-	0.9200	1.4700
2.3554	1.1954	-	2.3554	-	0.8923	-	0.8923	0.8923
1.6670	0.6550	-	1.3960	-	0.6630	-	0.6630	0.7680
1.7720	0.2360	-	1.7720	-	0.6630	-	0.6630	0.6630
0.6332	0.2165	-	0.6561	-	0.1807	-	0.1807	0.1851
0.6375	0.2675	-	0.6375	-	0.1807	-	0.1807	0.1807
4.9700	1.1090	-	4.9800	-	1.4740	-	1.4740	1.6670
4.9700	1.1509	-	4.9800	-	1.4740	-	1.4740	1.3165
5.3659	1.8448	-	5.3659	-	1.3725	-	1.3725	1.3725
0.8674	0.1191	-	1.0720	-	0.5794	-	0.5794	0.3988
0.8674	0.2204	-	1.0720	-	0.5794	-	0.5794	0.2885
0.6466	-0.0070	-	0.6466	-	0.5994	-	0.5995	0.5995
1.7500	0.4832	-0.1960	2.3800	-0.3360	0.6750	-0.1130	0.5880	0.7050
2.0652	0.6892	0.0000	2.3988	0.0000	0.5628	0.0000	0.5628	0.4820
2.0292	0.9881	0.0000	2.0292	0.0000	0.6012	0.0000	0.6012	0.6012
1.6300	0.3740	0.1710	1.2420	-0.0740	0.1770	0.0100	0.2740	0.3620
0.8509	0.3322	0.0000	1.9786	0.0000	0.2291	0.0000	0.2291	0.3740
1.3932	0.6848	0.0000	1.3932	0.0000	0.2061	0.0000	0.2061	0.2061

TABLE #3

Voigt-Reuss Averages Obtained Assuming Higher Symmetry

<u>Material</u>	<u>Class</u>	<u>Assumed Class</u>	<u>EV</u>	<u>ER</u>	<u>GV</u>	<u>GR</u>	<u>PRV</u>
Rutile	4/mmm	-	3.171	2.617	1.259	1.012	0.260
		m3m	2.543	2.105	0.944	0.766	0.347
Olivine	mmm	-	2.051	1.975	0.824	0.793	0.244
		4/mmm	2.714	1.944	1.134	0.827	0.197
		m3m	2.107	2.083	0.860	0.848	0.224
		-	1.865	1.638	0.772	0.692	0.208
Staurolite	mmm	4/mmm	2.176	8.109	0.955	1.439	0.139
		m3m	1.982	1.907	0.767	0.734	0.291
Apatite 1	6/mmm	-	1.530	1.404	0.638	0.575	0.199
		m3m	1.609	1.603	0.705	0.701	0.141
Magnesium 6	6/mmm	-	0.489	0.486	0.191	0.190	0.279
		m3m	0.474	0.474	0.182	0.182	0.298
Corundum 1	$\bar{3}m$	-	4.083	3.973	1.661	1.607	0.229
		6/mmm	3.876	3.769	1.538	1.491	0.260
		m3m	3.922	3.872	1.528	1.505	0.283
		-	1.011	0.903	0.478	0.411	0.057
Quartz 6	$\bar{3}m$	6/mmm	0.987	0.915	0.428	0.388	0.153
		m3m	0.829	0.788	0.490	0.449	-0.155
Diopside	2/m	-	1.663	1.544	0.658	0.615	0.264
		4/mmm	1.546	1.494	0.597	0.573	0.295
		m3m	1.494	1.488	0.569	0.566	0.313
		-	0.832	0.622	0.319	0.234	0.303
Oligoclase 1	2/m	4/mmm	0.893	0.761	0.358	0.308	0.247
		m3m	0.726	0.682	0.265	0.248	0.369

<u>PRR</u>	<u>KV</u>	<u>KR</u>	<u>Beta V</u>	<u>Beta R</u>	<u>V_s(Voigt)</u>	<u>V_s(Reuss)</u>	<u>V_p(Voigt)</u>	<u>V_p(Reuss)</u>
0.293	2.198	2.106	0.455	0.475	5.474	4.909	9.607	9.071
0.373	2.773	2.773	0.361	0.361	4.745	4.270	9.790	9.500
0.245	1.337	1.289	0.748	0.776	4.979	4.886	8.560	8.403
0.175	1.491	0.996	0.671	1.004	5.828	5.062	9.500	8.061
0.227	1.274	1.274	0.785	0.785	5.182	5.038	8.455	8.500
0.183	1.063	0.862	0.941	1.160	4.787	4.533	7.881	7.280
1.817	1.005	-1.026	0.995	-0.974	5.328	6.540	8.215	5.142
0.299	1.582	1.587	0.652	0.632	4.776	4.665	8.780	8.715
0.221	0.846	0.339	1.182	1.193	4.453	4.228	7.261	7.063
0.143	0.748	0.748	1.337	1.337	4.680	4.665	7.248	7.248
0.280	0.368	0.368	2.715	2.716	3.316	3.305	5.987	5.979
0.298	0.391	0.391	2.559	2.559	3.240	3.239	6.027	6.030
0.236	2.514	2.509	0.398	0.399	6.456	6.351	10.893	10.804
0.264	2.689	2.664	0.372	0.375	6.248	6.110	10.870	10.802
0.286	3.019	3.019	0.331	0.331	6.158	6.145	11.250	11.260
0.099	0.380	0.375	2.629	2.668	4.244	3.935	6.193	5.896
0.177	0.470	0.473	2.108	2.115	4.100	3.919	6.260	5.596
-0.123	0.211	0.211	4.742	4.742	4.300	4.101	5.720	5.298
0.255	1.176	1.051	0.850	0.951	4.457	4.310	7.876	7.519
0.302	1.259	1.259	0.794	0.794	4.244	4.150	7.865	7.835
0.314	1.335	1.335	0.749	0.794	4.149	4.132	7.953	7.842
0.329	0.704	0.607	1.420	1.648	3.477	2.978	6.541	5.900
0.237	0.588	0.482	1.700	2.076	3.683	3.419	6.350	5.820
0.377	0.921	0.921	1.086	1.086	3.161	3.064	6.946	6.878

TABLE #4

Internal Consistency of Data That Would Be Obtained Experimentally for
Crystals with Assumed Higher Symmetry

<u>Material</u>	<u>Class</u>	<u>Assumed Class</u>	<u>Relation</u>	<u>Value</u>
Oligoclase 1	2/m	4/mmm	$(C_{44}^{\text{TET}} + C_{66}^{\text{TET}})/2$	1.1664
			ρV^2	0.2872
		m3m	$(C_{11}^{\text{CUB}} + 2C_{12}^{\text{CUB}} + 4C_{44}^{\text{CUB}})/3$	1.1958
			ρV^2	1.1999
		m3m	C_{44}^{CUB}	0.2061
			ρV^2	0.8022
Quartz 6	$\bar{3}m$	6/mmm	C_{44}^{HEX}	0.5794
			ρV^2	0.6897
		6/mmm	$(C_{44}^{\text{HEX}} + C_{66}^{\text{HEX}})/2$	0.4339
			ρV^2	0.5051
		m3m	$(C_{11}^{\text{CUB}} + 2C_{12}^{\text{CUB}} + 4C_{44}^{\text{CUB}})/3$	1.0102
			ρV^2	0.9951
		m3m	C_{44}^{CUB}	0.5995
			ρV^2	0.0868

TABLE #5

Three Strain Components for a Unit Uni-Axial Stress in the (1, 0, 0) Direction
Assuming Higher Symmetry

<u>Material</u>	<u>Class</u>	Assumed <u>Class</u>	Strain		
			<u>S₁₁</u>	<u>S₂₂</u>	<u>S₃₃</u>
Rutile 3	4/mmm	-	0.6554	-0.3755	-0.0862
		m3m	0.7273	-0.3036	-0.3036
Olivine	mmm	-	0.3423	-0.0675	-0.0874
		4/mmm	0.4519	-0.2252	-0.1168
Staurolite	mmm	m3m	0.5386	-0.1384	-0.1384
		-	0.3367	-0.1130	-0.1299
Apatite	6/mmm	4/mmm	0.5146	-0.3475	-0.0661
		m3m	0.6449	-0.2171	-0.2171
Magnesium 6	6/mmm	-	0.7480	0.0970	-0.3965
		m3m	0.5826	-0.0685	-0.0685
Corundum 1	3m	-	2.0146	-0.6873	-0.4380
		m3m	2.0861	-0.6188	-0.6188
Quartz 6	3m	-	0.2352	-0.0716	-0.0364
		6/mmm	0.2637	-0.1161	-0.0341
Diopside	2/m	m3m	0.2261	-0.0579	-0.0579
		-	1.2770	-0.1791	-0.1220
Oligoclase	2/m	6/mmm	1.3351	-0.3980	-0.1927
		m3m	1.5469	0.0169	0.0169
Oligoclase	2/m	-	0.6925	-0.2771	-0.1977
		4/mmm	0.6659	-0.2946	-0.1067
Oligoclase	2/m	m3m	0.7239	-0.2370	0.2370
		-	2.3538	0.1990	-1.0516
Oligoclase	2/m	4/mmm	1.2728	-0.1388	-0.1904
		m3m	1.0617	-0.3499	-0.3499

TABLE #6

Elastic Anisotropy Assuming Higher Symmetry

See footnote a for explanation of symbols.

<u>Material</u>	<u>Class</u>	<u>Assumed Class</u>	<u>A</u>	<u>A*</u>
Rutile 3	4/mmm	-	2.588	0.105
		m3m	2.588	0.105
Olivine	mmm	-	0.504	0.055
		4/mmm	1.090	0.001
		m3m	1.275	0.006
		-	0.333	0.134
Staurolite	mmm	4/mmm	1.586	0.025
		m3m	1.539	0.021
Apatite 1	6/mmm	-	0.865	0.025
		m3m	0.865	0.025
Magnesium 6	6/mmm	-	0.975	0.00007
		m3m	0.975	0.00007
Corundum 1	$\bar{3}m$	-	0.884	0.0018
		6/mmm	1.121	0.0015
		m3m	0.778	0.0075
		-	1.453	0.017
Quartz 6	$\bar{3}m$	6/mmm	2.008	0.055
		m3m	1.835	0.045
Diopside	2/m	-	1.130	0.0017
		4/mmm	1.080	0.0006
		m3m	1.157	0.0024
		-	0.910	0.001
Oligoclase 1	2/m	4/mmm	0.647	0.188
		m3m	0.583	0.264

$$^a A = 2C_{44} / (C_{11} - C_{12}) \quad \text{Hearmon (1961)}$$

$$A^* = 3(A-1)^2 / [3(A-1)^2 + 25A] \quad \text{Chung (1967)}$$

TABLE #7

Comparison of the Voigt-Reuss-Hill Averages of Velocities with the Velocities Obtained Averaging Velocities in 3 Orthogonal Directions. The values of \bar{V}_s and \bar{V}_p are averages from ten different orientations selected randomly.

<u>Material</u>	<u>Class</u>	<u>V_s (VRH)</u>	<u>\bar{V}_s</u>	<u>V_p (VRH)</u>	<u>\bar{V}_p</u>
Rutile	4/mmm	5.191	5.365	9.339	9.679
Olivine	mmm	4.932	4.910	8.481	8.466
Staurolite	mmm	4.660	4.614	7.580	7.759
Apatite 1	6/mmm	4.341	4.564	7.162	7.106
Magnesium 6	6/mmm	3.310	3.313	5.983	5.985
Corundum 1	$\bar{3}m$	6.403	6.404	10.848	10.915
Quartz 6	$\bar{3}m$	4.089	4.195	6.044	6.181
Diopside	2/m	4.383	4.477	7.697	7.785
Oligoclase	2/m	3.227	3.340	6.220	6.632

TABLE #8

Bulk and Shear Moduli Calculated from \bar{V}_s and \bar{V}_p of Table 7

<u>Material</u>	<u>Class</u>	<u>(GV + GR)/2</u>	<u>G (Average)</u>	<u>Standard Deviation</u>	<u>Maximum Error</u>
Rutile 3	4/mmm	1.135	1.156	0.101	0.210
Olivine	mmm	0.809	0.798	0.018	0.039
Staurolite	mmm	0.732	0.722	0.025	0.052
Apatite 1	6/mmm	0.607	0.666	0.027	0.092
Magnesium 6	6/mmm	0.190	0.192	0.005	0.008
Corundum 1	$\bar{3}m$	1.634	1.653	0.092	0.165
Quartz 6	$\bar{3}m$	0.444	0.471	0.026	0.076
Diopside	2/m	0.636	0.646	0.025	0.060
Oligoclase 1	2/m	0.277	0.297	0.040	0.081

<u>Material</u>	<u>Class</u>	<u>(KV +KR)/2</u>	<u>K (Average)</u>	<u>Standard Deviation</u>	<u>Maximum Error</u>
Rutile 3	4/mmm	2.152	2.493	0.334	0.845
Olivine	mmm	1.313	1.332	0.107	0.163
Staurolite	mmm	0.963	1.061	0.112	0.311
Apatite 1	6/mmm	0.842	0.745	0.088	0.196
Magnesium 6	6/mmm	0.368	0.365	0.015	0.030
Corundum 1	$\bar{3}m$	2.512	2.530	0.307	0.464
Quartz 6	$\bar{3}m$	0.378	0.382	0.088	0.161
Diopside	2/m	1.114	1.182	0.089	0.240
Oligoclase 1	2/m	0.655	0.780	0.123	0.253