HIGH TEMPERATURE CRYSTAL CHEMISTRY OF HYDROUS Mg- AND Fe-RICH CORDIERITES

by

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TABLE OF CONTENTS

TABLE OF CONTENTS, continued

LIST OF TABLES

LIST OF FIGURES

LIST OF FIGURES, continued

INTRODUCTION

The expansion properties of the mineral cordierite, $(Mg,Fe)_2Al_4Si_5O_{18}.nH_2O$, have attracted the interests of ceramists because of its value as a thermal shock resistant material. It has also attracted the interests of mineralogists and petrologists because of its polymorphism and widespread occurrence in metamorphic terraines. The polymorphism of cordierite may not be as simple as once believed but may involve a two-step ordering process like that evinced by the alkali feldspars (Meagher and Gibbs, 1967). Apparently it can exist in all intermediate structural states between an hexagonal polymorph called indialite (Miyashiro and Iiyama, 1954; Meagher and Gibbs, 1977) and an orthorhombic form called low cordierite (Miyashiro *et al.*, 1955; Schreyer and Schairer, 1961; Gibbs, 1966; Meagher and Gibbs, 1966; Meagher, 1967; Cohen *et al.*, 1977). In low cordierite the Al and Si atoms are ordered in a tetrahedral framework of $Al_4Si_5O_{18}$ composition (Cohen *et al.*, 1977) whereas in indialite they are only partly ordered (Meagher and Gibbs, 1977). The existence of a completely disordered polymorph of cordierite has yet to be substantiated.

According to Newton (1973), cordierite plays a poorly understood yet important role in regionally metamorphosed rocks of the amphibolite and granulite facies. It is also a common constituent of thermally metamorphosed rocks, particularly those lacking well-developed foliation and derived from argillaceous sediments. In addition, it is frequently associated with anthophyllite or gedrite

in massive metamorphosed sulfide deposits and occurs in granitic pegmatites with quartz as micropegmatitic intergrowths. The Fe-Mg distribution for coexisting cordierite and garnet pairs has been measured experimentally by Hensen and Green (1971) and Currie (1971) and found to be potentially valuable to petrologists as a geobarometer-geothermometer.

Because of its unusually low thermal expansion, Mg-rich cordierite is an extremely important and valuable mineral in the ceramic industry. It is used as an insulator for spark plugs (Fessler, 1938), as a refractory coating on metals for internal combustion engines (Desmarquest, 1965), in the production of dolomitic types of refractories (Nagasaki *et al.*, 1970) and low expansion concrete (Magnan, 1971), and as a catalytic support for the treatment of waste gas (Soejima, 1974) and automobile exhaust emissions (Lachman and Lewis, 1973; Takao *et al.*, 1974). Perhaps its most important application in the future will be in the fabrication of turbine engines (Gostlow and Restall, 1972). Fe-rich cordierite has been produced in industry but only as a by-product in blast-furnace linings (Richardson, 1949), in "black cores" in stoneware pipes (Lach, 1974), and even in building-brick (Rathgeber and Fowler, 1966). Ceramists are not particularly interested in Fe-rich cordierite because it is much more difficult to synthesize and because it shows moderate oxidation at high temperatures.

In light of the increasing interest in this mineral, this study was undertaken to determine (1) the effect of heating upon the Al/Si

distribution in the tetrahedral framework, (2) the crystal structure of hydrous Mg- and Fe-rich low cordierite as a function of temperature in an attempt to clarify the unusual thermal expansion properties of the mineral, (3) the orientation of the water molecules in the channels of the structure, and (4) the effects of heating on water and the alkali atoms in these channels.

EXPERIMENTAL DETAIL AND OBSERVATIONS

Specimens

The Mg-rich cordierite used in our study, designated the White Well cordierite, was previously described and used in a combined X-ray and neutron diffraction study by Cohen *et al.* (1977). It is one of the most Mg-rich specimens ever to be reported in nature (see Table 1). We assumed that our crystal (0.30 × 0.22 × 0.22 mm) and those used by Cohen *et al.* (1977) had identical chemical compositions and crystal structures because they had statistically identical cell dimensions and were selected from the same specimen (approximately a 4 mm cube). The room temperature data (before heating) listed in Appendices D and E were taken from Cohen *et al.* (1977).

The Fe-rich cordierite used in our study (Table 1), designated the Dolni Bory cordierite, was collected from a pegmatite near Dolni Bory, Western Moravia, Czechoslovakia (Stanek and Miskovsky, 1964). Many of its single crystals were sector twinned; however, two exhibiting sharp and uniform extinction were found suitable for structure determination. Both crystals measured approximately 0.25 mm on a side. After orientation (see Appendix A) using the optical spindle stage techniques of Bloss (1977), crystals of the White Well and Dolni Bory cordierites were sealed in evacuated quartz capillaries to inhibit the oxidation of the iron. Each was then allowed to equilibrate for at least 12 hours at the temperature of the measurement before data collection was begun. The temperature fluctuations for the heater during the measurement were not more than ±10° at 375°C and ±15° at

TABLE 1

Cell parameters (24°C), distortion index (Δ), density (ρ) and composition of the White Well and Dolni Bory cordierites

	White Well	Dolni Bory
a	17.088(3) Å	17.230(5) Å
b	9.734(2)	9.835(3)
c	9.359(1)	9.314(3)
Δ	0.25°	0.21°
ρ	2.56 g/cm^3	2.78 g/cm^3
Formulas* (based on 18 oxygens)		
T cations	$Si_{5.01}Al_{3.95}$	$Si_{4.91}Al_{4.05}$
M cations	$Mn_{0.01}Mg_{1.91}Fe^{2+}_{0.08}$	$Mn_{0.08}Mg_{0.25}Fe^{2+}_{1.65}$
Alkalis	$Na_{0.05}K_{0.02}Ca_{0.02}$	$Na_{0.15}Ca_{0.05}$
Water	$(H_2O)_{0.56}$	$(H_2O)_{0.61}$

* White Well cordierite composition reported by Pryce (1973); Dolni Bory cordierite composition reported by Stanek and Miskovsky (1964).

775°C. Those interested in a detailed description of the crystal mounting techniques and the single crystal heater should consult Brown *et al.* (1973) and Appendix B of this thesis.

Data Collection and Refinements

The intensity data for the structural refinements were collected over a range of 5° to 60°2θ, the upper limit being imposed by the heater configuration. Three standard reflections measured every 30 reflections indicated that machine drift was within acceptable limits so no drift correction was applied. The observed intensities, corrected for Lorentz-polarization effects, were converted to $|F(obs)|$ with the program DATALIB.[1] Since the linear absorption coefficients for the White Well (9.1 cm^{-1}) and the Dolni Bory (25.2 cm^{-1}) cordierites were relatively small and since the crystal of the latter was lost, no absorption corrections were applied to the data sets. An approximate extinction correction was made and least-squares refinements were calculated first using isotropic and later using anisotropic temperature factor models. The $|F(obs)|$'s were weighted in the refinements according to the procedure described by Cohen (1975). In the refinement of each structure, reflections were automatically rejected at the $2\hat{\sigma}$ level for the White Well cordierite and at $3\hat{\sigma}$ for the Dolni Bory cordierite. In our refinement of the White Well cordierite, we neglected the channel constituents. On the other

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[1] Catalogued in the World List of Crystallography Computer Programs (3rd edition).

hand, while neglecting the water, we included the alkali atoms in our refinement for the Dolni Bory cordierite because of their greater abundance. The number of accepted reflections and the weighted and unweighted R-factors for the anisotropic refinements are given for both cordierites in Table 2. (See Appendix C for a complete listing of calculated and observed structure factors for each refinement.) The final positional parameters and anisotropic temperature factors, as well as the isotropic equivalent temperature factors for the non-equivalent atoms in the White Well and Dolni Bory cordierites, are listed in Appendix D. Selected interatomic distances and angles, calculated with the program ORFFE3,[1] are given in Appendix E. The bond distances and angles were not corrected for thermal motion because such corrections cannot be accurately or meaningfully made at this time.

Because the R-factors for the Dolni Bory cordierite were slightly higher than expected, an attempt was made to refine its structure within the constraints of subgroup symmetry *Ccc*2 (see Appendix D). During refinement, the parameters of the pairs of pseudo-symmetrically related atoms were not varied simultaneously but were varied alternately to avoid high correlation coefficients (Fang and Robinson, 1977). The results of the final anisotropic refinement on 1203 reflections recorded at 24°C yielded an unweighted R-factor of 0.067 and a weighted R of 0.058. Even though this drop in the R-factor was significant according to the statistics of Hamilton (1965), the lower symmetry space group was not accepted because (1) the fractional positional parameters were

TABLE 2

Results of the anisotropic refinements for the White Well and Dolni Bory cordierites

Cordierite	Temperature	# of accepted reflections	R-factor UNW	W
White Well	24°C (after Cohen *et al.*)	1057	0.033	0.041
	375°C	1077	0.041	0.066
	775°C	994	0.056	0.087
	24°C (after heating)	1176	0.038	0.061
Dolni Bory	24°C	1203	0.073	0.063
	375°C	716	0.061	0.063

statistically identical with those of the *Ccem* refinement except for the M site and (2) more than half of the atoms were calculated to have nonpositive-definite temperature factors.

Precession photographs of the White Well cordierite recorded following the heating experiment showed powder rings of weak intensity identified as the diffraction pattern of hematite. Later, when the Dolni Bory cordierite was heated above 600°C, the crystal changed from colorless to amber while the peak intensities dropped off drastically obviating the collection of additional data. A second crystal was selected and the measurements were repeated but again the peak intensities dropped off markedly at temperatures above 600°C. Precession photographs recorded after the second set of measurements showed the same faint powder rings of the hematite diffraction pattern. Rathgeber and Fowler (1966) have completed open air heating experiments at 1150°C on stoichiometric Fe-cordierite in which they noticed a reddening of the crystals, a 40% decrease in measured X-ray powder diffraction peak intensity, and the formation of hematite (see also Strunz *et al.*, 1971). On the other hand, hedenbergite, $CaFeSi_2O_6$, was successfully heated as high as 1000°C for data collection by Cameron *et al.* (1973) using the same heater and mounting techniques employed in our study. Also Brown and Prewitt (1973) heated an olivine (Fa_{31}) to 710°C in an evacuated capillary with no loss in the intensities of the diffraction data nor evidence of oxidation or breakdown. However, unlike cordierite, both of these minerals lack loosely bound water molecules and Fe atoms in the channels (Goldman *et al.*, 1977). Upon heating, these components apparently react even

in a thoroughly evacuated capillary to produce hematite. The decrease in the intensities of the diffraction data recorded for the Dolni Bory cordierite indicates that octahedral Fe is also involved in the reaction to form hematite which results in partial disruption of the Fe-cordierite structure.

Isotropic Temperature Factors

Isotropic equivalents of the anisotropic temperature factors for the White Well and Dolni Bory cordierites were calculated and are listed in Appendix D. Figure 1 shows the isotropic equivalent temperature factors for the cations in the White Well cordierite plotted against temperature. The Si atoms in the six-membered ring have the lowest temperature factors and increase at the slowest rate along with those outside the ring. The temperature factors for the Al atoms increase slightly faster, and at 24°C the M cations show the highest temperature factor and the greatest rate of increase to 775°C. The isotropic equivalents for the Dolni Bory cordierite are plotted against temperature in Figure 2. Despite the limited amount of data, the temperature factor variation with temperature for each cation has the same general trend as that observed for the White Well cordierite. These observations agree well with findings for the pyroxenes by Cameron *et al.* (1973) and for tremolite by Sueno *et al.* (1973). Both studies show that cations with higher charge and lower coordination have smaller temperature factors that increase more slowly with increasing temperature than cations with lower charge and higher coordination.

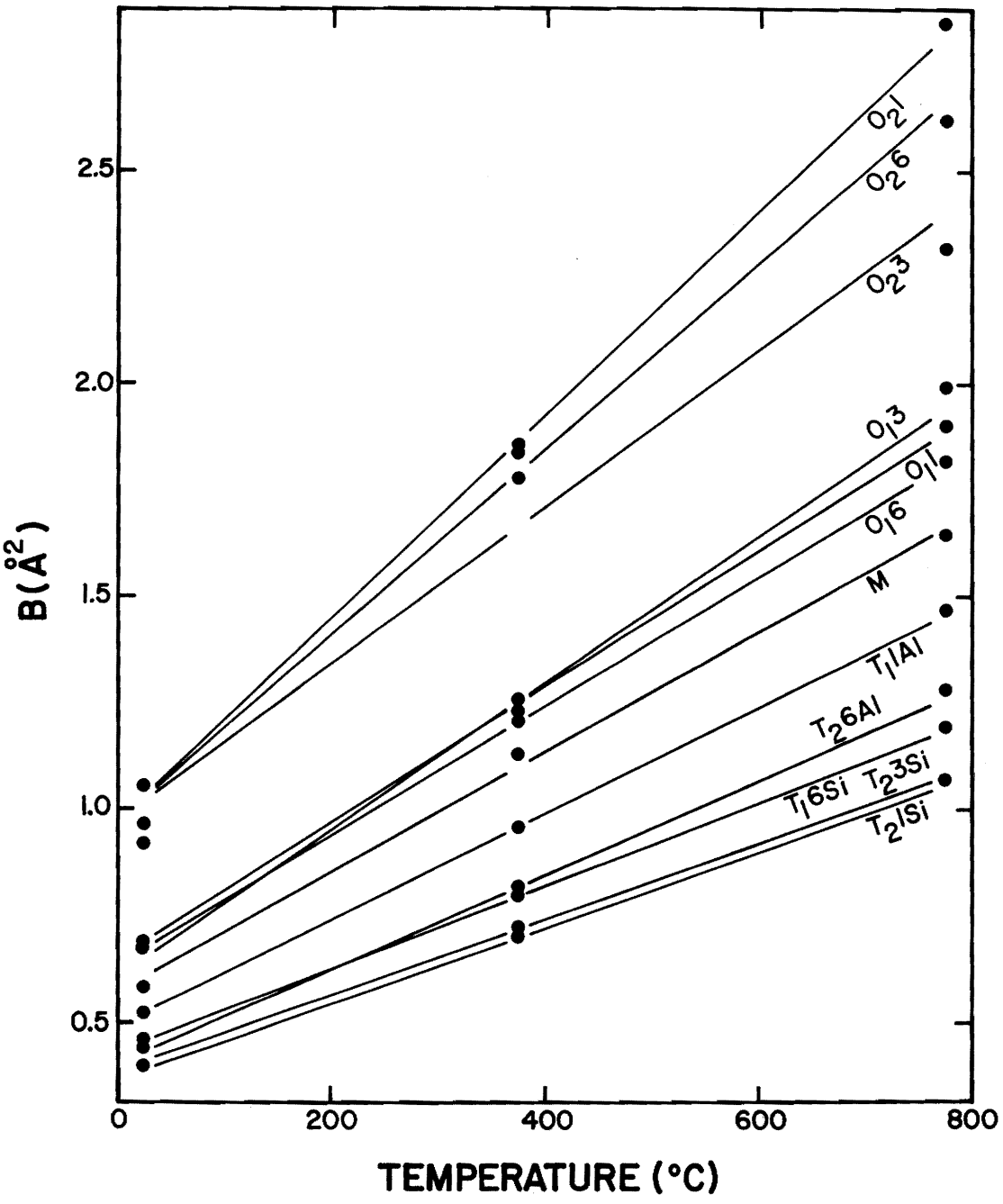

Figure 1. Isotropic equivalent temperature factors for the White Well cordierite plotted as a function of temperature from 24°C to 775°C. (The nomenclature of the atoms is the same as that in Fig. 4.)

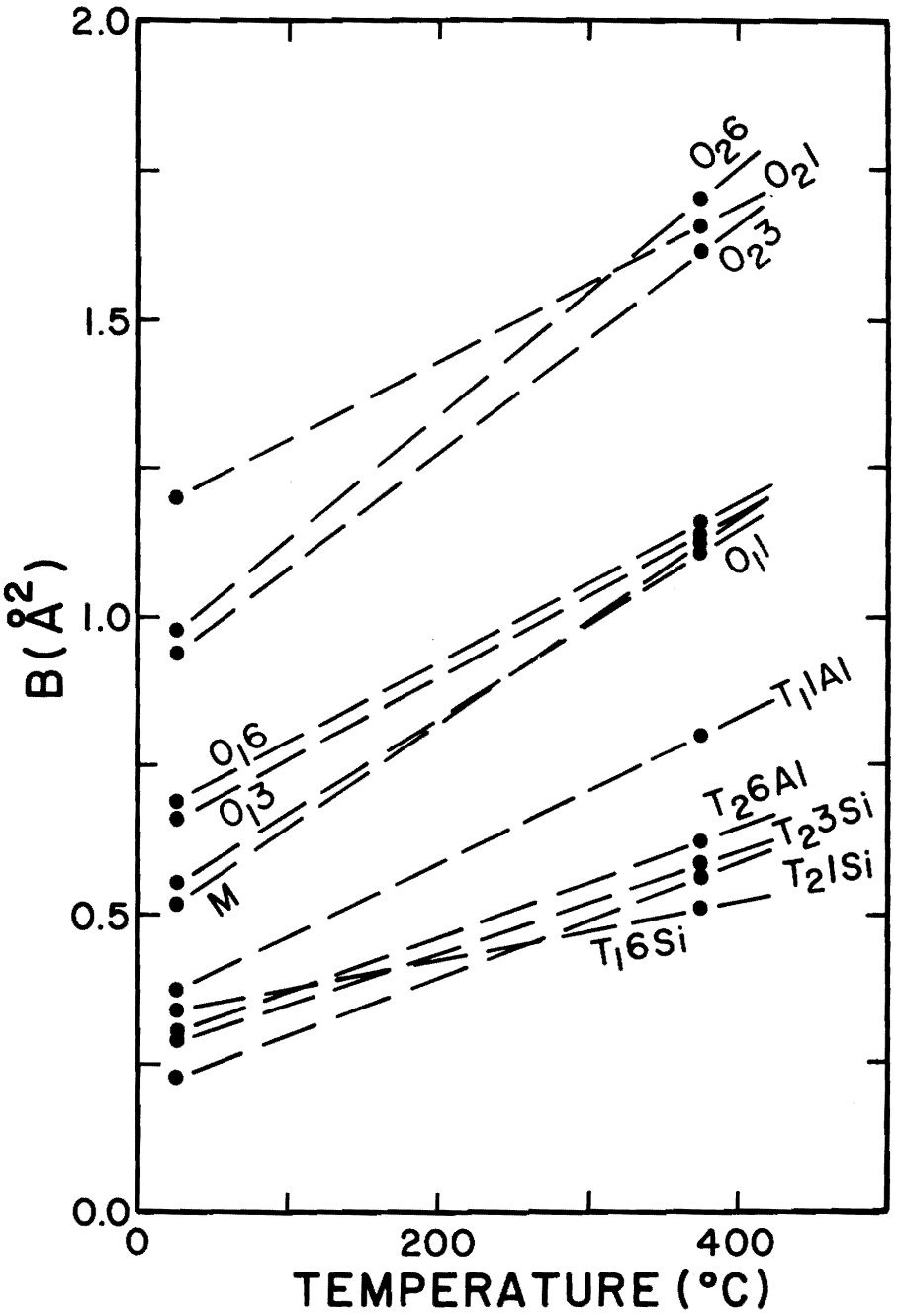

Figure 2. Isotropic equivalent temperature factors for the Dolni Bory cordierite plotted as a function of temperature from 24°C to 375°C. (The nomenclature of the atoms is the same as that in Fig. 4.)

The isotropic equivalent temperature factors of the oxygen atoms in the White Well cordierite are plotted against temperature in Figure 1. The six nonequivalent oxygens are clearly separated into two groups. The three distinct O_1 oxygens are three-coordinated and have smaller temperature factors which increase at a slower rate than the three independent O_2 oxygens in the ring which are only two-coordinated. Again, despite the limited data set, the oxygens in the Dolni Bory cordierite show the same general trends as evinced by the White Well cordierite (see Fig. 2). In general, oxygens with high coordination are more restricted in movement and display smaller temperature factors that increase slower with temperature. Oxygens with lower coordination seem to show the opposite trends as observed by Sueno *et al.* (1973) and Cohen *et al.* (1977).

Cell Parameters

The unit cell edges, obtained in a least-squares refinement of 28 computer centered reflections recorded at various temperatures up to 775°C for the White Well cordierite and up to 375°C for the Dolni Bory cordierite, are given in Table 3 along with their unit cell volumes and calculated distortion indices (Miyashiro, 1957).

The a cell edge of the White Well cordierite increases as a function of temperature at a rate slightly greater than that of b while c undergoes a slight but systematic shortening up to 775°C (Fig. 3). On the other hand, the c-cell edge of the Dolni Bory cordierite does not shorten upon heating but increases at about the same rate as the other axial directions. Because the changes in the

TABLE 3

Cell edges (Å), cell volume (Å^3), and calculated distortion index *vs* temperature for White Well cordierite

Temperature (°C)	*a*	*b*	*c*	V	Δ
24	17.088(3)	9.734(2)	9.359(1)	1556.7(4)	0.252
280	17.103(3)	9.737(2)	9.357(1)	1558.2(4)	0.262
375	17.113(3)	9.741(1)	9.358(1)	1560.0(3)	0.266
470	17.123(2)	9.745(1)	9.357(1)	1561.3(3)	0.268
590	17.132(2)	9.751(1)	9.357(1)	1563.1(3)	0.266
664	17.140(2)	9.755(1)	9.355(1)	1564.2(3)	0.267
775	17.149(2)	9.759(1)	9.352(1)	1565.1(3)	0.269
24*	17.119(2)	9.746(1)	9.361(1)	1561.8(3)	0.263

* After heating

Cell edges (Å), cell volume (Å^3), and calculated distortion index *vs* temperature for Dolni Bory cordierite

Temperature (°C)	*a*	*b*	*c*	V	Δ
24	17.230(5)	9.835(3)	9.314(3)	1578.3(8)	0.211
375	17.258(3)	9.847(2)	9.328(2)	1585.3(3)	0.218

cell volume of the Dolni Bory cordierite are not as well determined as those of the White Well cordierite, it is difficult to directly compare the rates of volume expansion for the two cordierites.

The thermal expansion data for synthetic indialite measured by Fischer *et al.* (1974) and by Lee and Pentecost (1976) are compared with those for the White Well cordierite in Figure 3. The expansion of the a-cell edge of the ordered White Well cordierite is about 1500 ppm greater at 775°C than that of indialite whereas the expansion along b is practically the same as that along a in the disordered polymorph. The contraction along c in the White Well cordierite is significantly less (∿800 ppm less at 775°C) than that along c in indialite. Moreover, the variation of c in the ordered polymorph is linear with temperature within the limits of error of the result. The two measurements for the disordered polymorph show a contraction along c with temperature, but Fischer *et al.* (1974) find that c begins to expand at temperatures greater than ∿400°C whereas Lee and Pentecost (1976) find that c continues to contract up to 1000°C. However, when Lee and Pentecost (1976) annealed their hexagonal specimen to produce an orthorhombic polymorph (with greater degree of order), they discovered that the contraction along c was increased over that of the hexagonal polymorph. Since the degree to which long-range order may develop in indialite is probably variable (Meagher and Gibbs, 1977) and since the contraction properties in the direction of c apparently depend on thermal history and structural state, we believe that the differences in the curves determined by Fischer *et al.* (1974) and Lee and Pentecost (1976) are real and

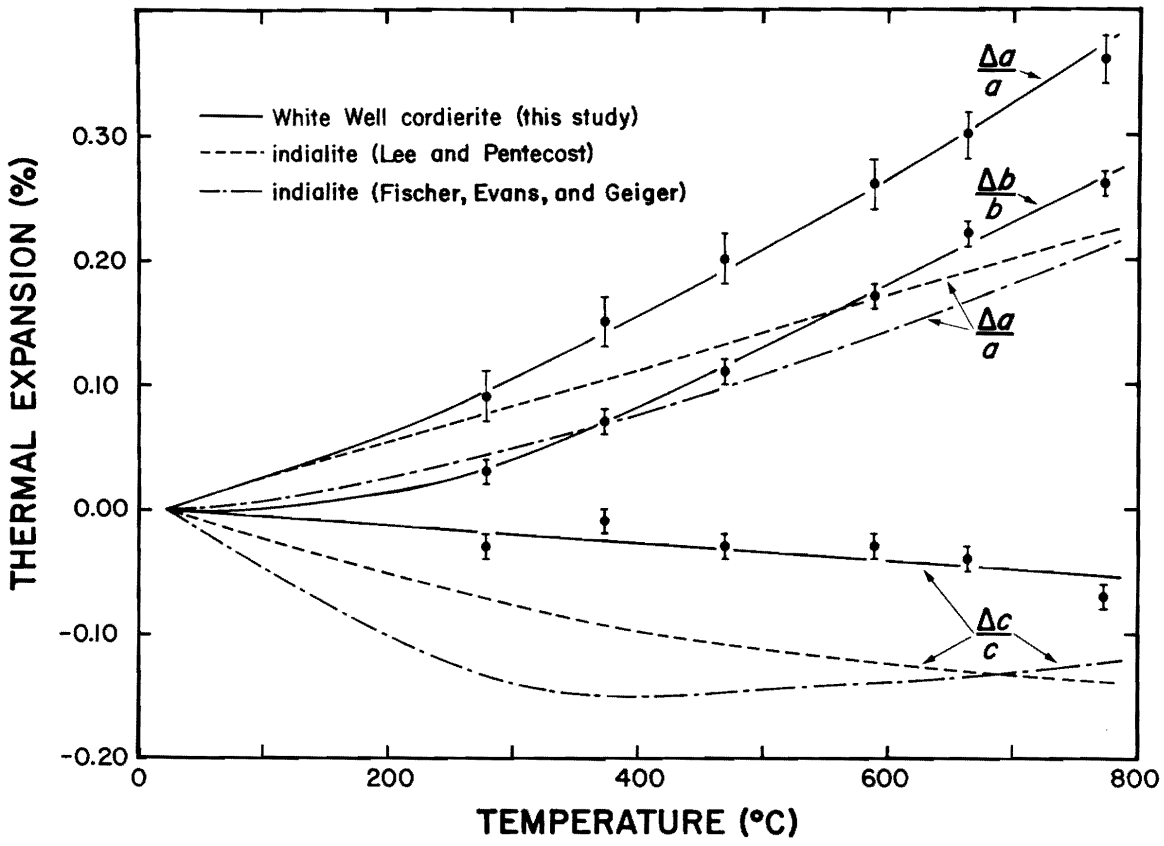

Figure 3. Axial expansion ($[(X_T - X_{24})/X_{24}]\cdot 100$ where X is a, b or c) *vs* temperature for two synthetic indialites and the White Well cordierite. The brackets for the White Well data are drawn at $1\hat{\sigma}$.

represent measurements on hexagonal polymorphs with different structural states.

STRUCTURE

The crystal structure of cordierite is described by Takane and Takeuchi (1936), Byström (1942), Gibbs (1966), Cohen *et al.* (1977) and Meagher and Gibbs (1977), and consists of a framework of four- and six-membered rings of tetrahedra. The six-membered rings lie in planes perpendicular to *c* and involve the three nonequivalent T_2 tetrahedra (see Fig. 4). The four-membered rings, consisting of alternating T_1 and T_2 tetrahedra, are linked into chains paralleling *c* which are further cross-linked to form the tetrahedral framework (see Fig. 5). A neutron site refinement by Cohen *et al.* (1977) has shown the White Well cordierite to be completely ordered ($t_16 = t_21 = t_23 = 0.0$ and $t_11 = t_26 = 1.0$ where t_xy represents the probability of finding an Al atom in T_xy) within the experimental error. On the other hand, an examination of the mean T-O bond lengths determined in an X-ray study of indialite indicates that the crystal has a long-range order of 0.38 with $t_1 = 0.72$ and $t_2 = 0.30$ (Meagher and Gibbs, 1977). The M-atoms (M = Mg, Fe) in cordierite reside within the framework in somewhat flattened octahedra that share two edges with AlO_4 tetrahedra and one with a SiO_4 tetrahedron. The large cavities, connected one to another by the openings of the six-membered rings, house the water molecules in hydrous cordierite with the alkali atoms residing at the origin and centering the six-membered rings of T_2-tetrahedra (Meagher, 1967).

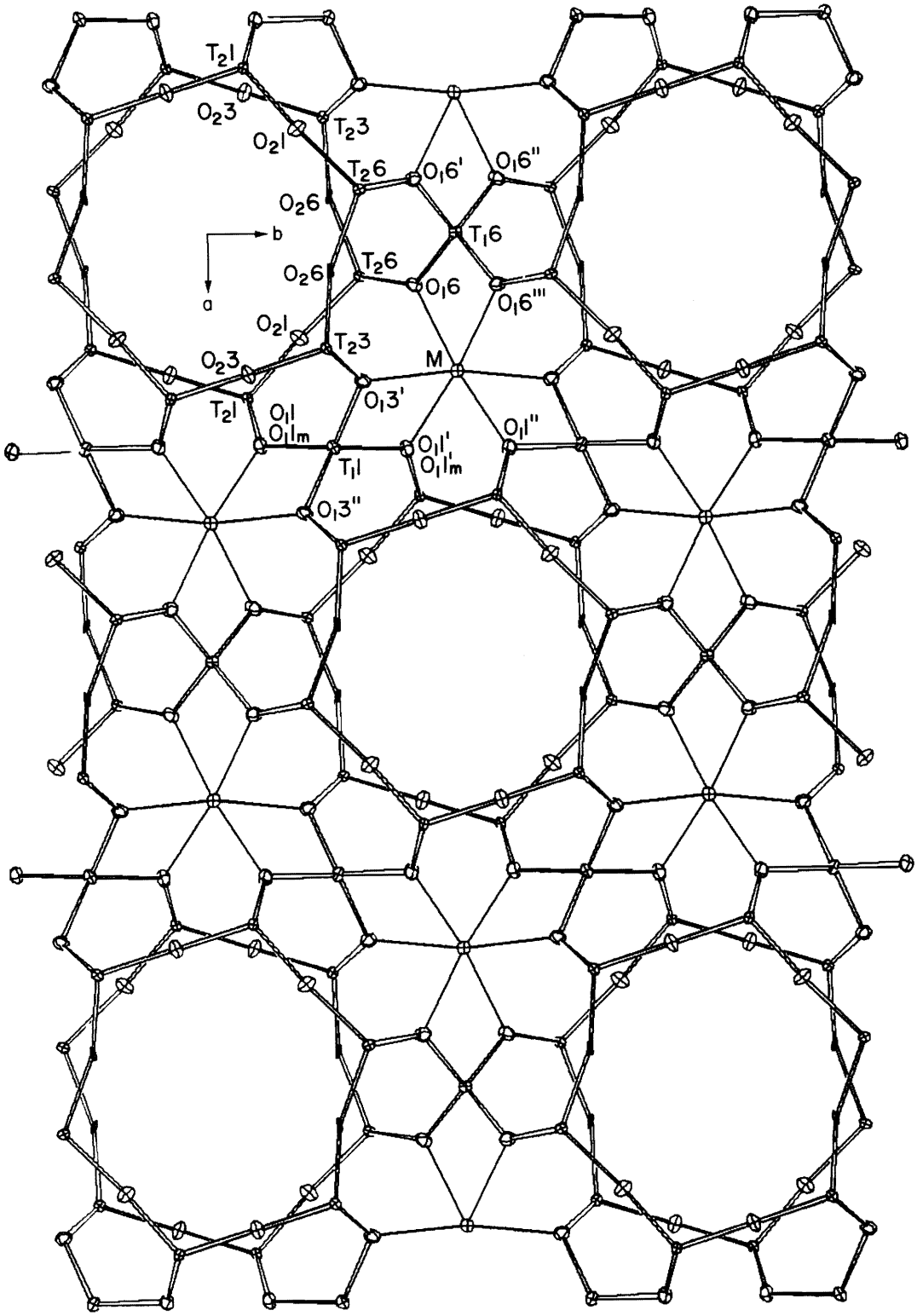

Figure 4. ORTEP (Johnson, 1965) drawing of the cordierite structure (between 0c and 1/2c) viewed down c. In ordered cordierite, $T_1$1 and $T_2$6 represent Al atoms, while $T_1$6, $T_2$1, and $T_2$3 represent Si atoms. The M octahedra houses Mg and Fe.

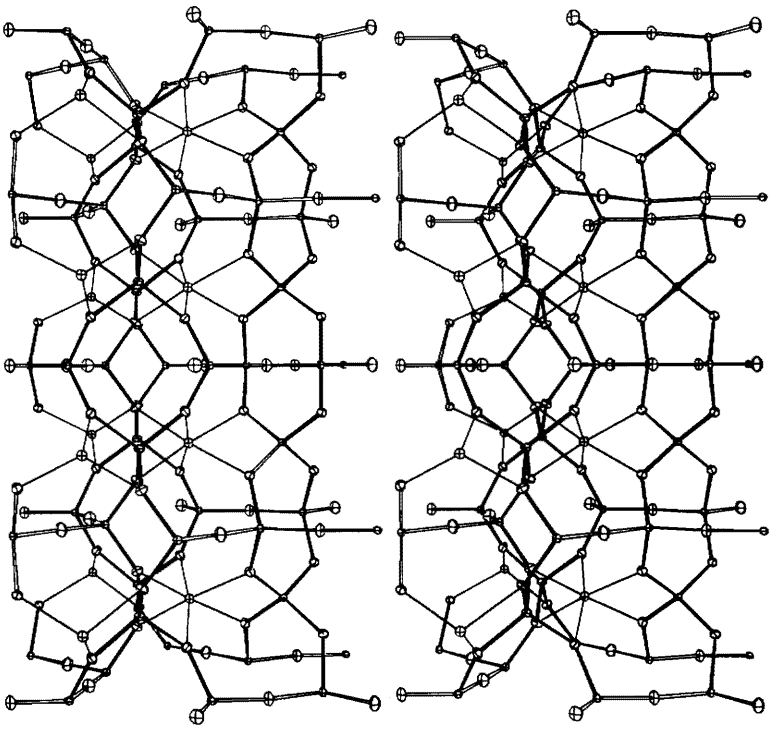

Figure 5. An ORTEP stereopair drawing showing the four-membered rings which are linked into chains paralleling *c*. The two symmetrically distinct chains are shown (the two overlying chains on the left are related by a c-glide) and have been highlighted by heavy-lined bonds. Note that the octahedron (single line bonds) shares three edges with tetrahedra. In this figure, *a* is horizontal and *c* is vertical.

DISCUSSION

Tetrahedral and Octahedral Bond Length Expansion

The mean T-O bond lengths for the individual tetrahedra in both the White Well and the Dolni Bory cordierites do not appear to change significantly with temperature, nor are they different after heating in the case of the White Well cordierite. Accordingly, we may conclude that the ordered configuration of Al and Si in the tetrahedral framework of low cordierite was unaffected by our heating experiments. On the other hand, the octahedral M-O bonds show a significant increase in length. The Mg-O bonds in the White Well cordierite increase 0.018 Å on the average when heated from 24°C to 775°C while the Fe-O bonds in the Dolni Bory cordierite increase by 0.007 Å when heated from 24°C to 375°C. Hence, in the temperature range 24°C to 375°C, the mean Fe-O bond length expansion (∿0.007(1) Å) is less than that of the mean Mg-O bond length expansion (∿0.011(1) Å). This result indicates that the Fe-O bond is stronger than the Mg-O bond, in agreement with similar results obtained by Skinner (1966) and Cameron *et al.* (1973).

Because the mean T-O bond lengths appear to remain unchanged, the volumes of the AlO_4 and SiO_4 tetrahedra show little change with heating (see Table 4). In contrast, the MgO_6 octahedra in the White Well cordierite exhibit a volume increase of 0.27 $Å^3$ when heated from 24°C to 775°C. Similarly, the FeO_6 octahedra in the Dolni Bory cordierite show a volume increase of 0.13 $Å^3$ when heated to 375°C.

TABLE 4

Polyhedral volumes ($Å^3$) *vs* temperature for White Well cordierite

Polyhedra	24°C	375°C	775°C	24°C*
$T_1 1$	2.58	2.57	2.58	2.59
$T_1 6$	2.14	2.13	2.15	2.13
$T_2 1$	2.15	2.16	2.15	2.17
$T_2 6$	2.70	2.72	2.72	2.72
$T_2 3$	2.16	2.16	2.17	2.16
M	11.79	11.91	12.06	11.86

* After heating

Polyhedral volumes ($Å^3$) *vs* temperature for Dolni Bory cordierite

Polyhedra	24°C	375°C
$T_1 1$	2.61	2.63
$T_1 6$	2.16	2.17
$T_2 1$	2.18	2.17
$T_2 6$	2.73	2.72
$T_2 3$	2.16	2.17
M	12.42	12.55

The mean thermal expansion of the octahedron in the Mg-rich cordierite ($12.6 \times 10^{-6}°C^{-1}$) is significantly less than that observed for corresponding octahedra in periclase ($13.9 \times 10^{-6}°C^{-1}$), forsterite ($14.2 \times 10^{-6}°C^{-1}$) and diopside ($14.4 \times 10^{-6}°C^{-1}$) (Hazen and Prewitt, 1977). As indicated earlier, the octahedron in cordierite is isolated from other octahedra and shares three of its edges with tetrahedra. Since the dimensions of these tetrahedra show little or no change with heating, they act as rigid clamps and constrain the octahedron in its expansion upon heating. The octahedra in forsterite and diopside share edges with both tetrahedra and octahedra, those in periclase just sharing edges with other octahedra. The mutual expansion of the octahedra in these structures should not be as restricted. If this is true, then the mean thermal expansion of an M-containing polyhedron depends upon its environment as well as the strength of the M-O bond.

When trying to predict the thermal expansion of a crystalline material from its structure, which as Kahn (1976) points out, has "met with limited success," it may be inappropriate to assign a fixed rate of expansion to an M-O bond from one structure type to another.

A Structural Interpretation of the Thermal Expansion of Cordierite

The anisotropic thermal expansion of the unit cell of the White Well cordierite may be related to the thermal expansion of its Mg-rich octahedron and its accompanying effect on the tetrahedral framework. Figure 6 shows that the volume change of the octahedron correlates linearly with a and b, both axial directions increasing as the octahedral volume increases upon heating. On the other hand,

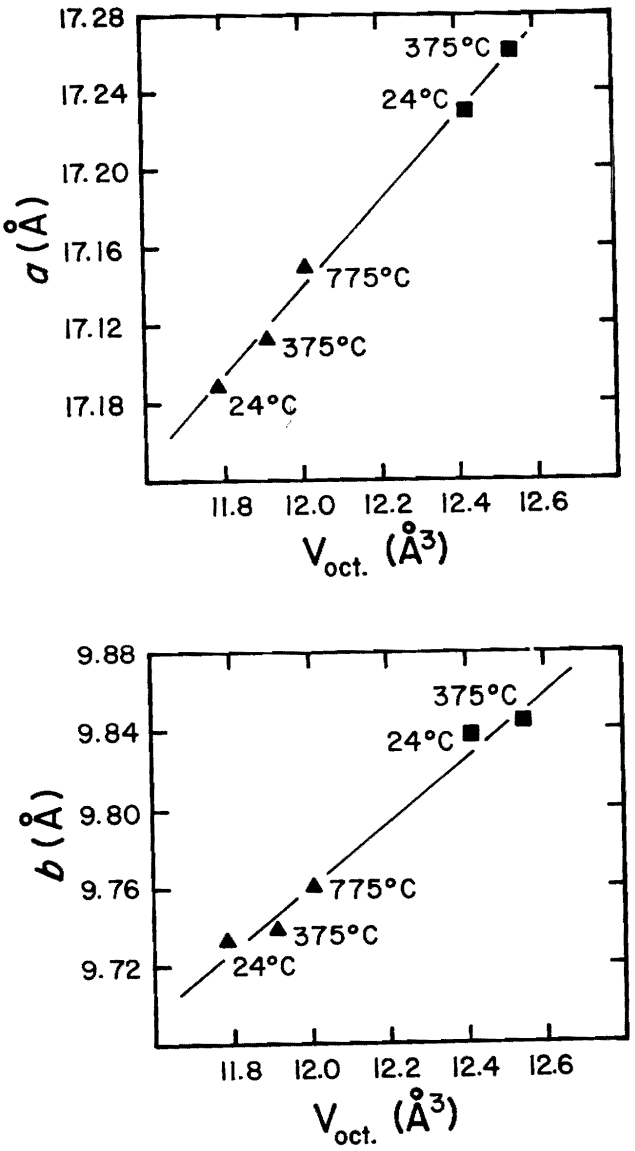

Figure 6. The a and b cell edges *vs* the octahedral volume for both the White Well (▲) and Dolni Bory (■) cordierites at various temperatures. The relationships between the cell edges and the octahedral volumes are similar for both cordierites and seem to be continuous as shown by the linearity of the data points.

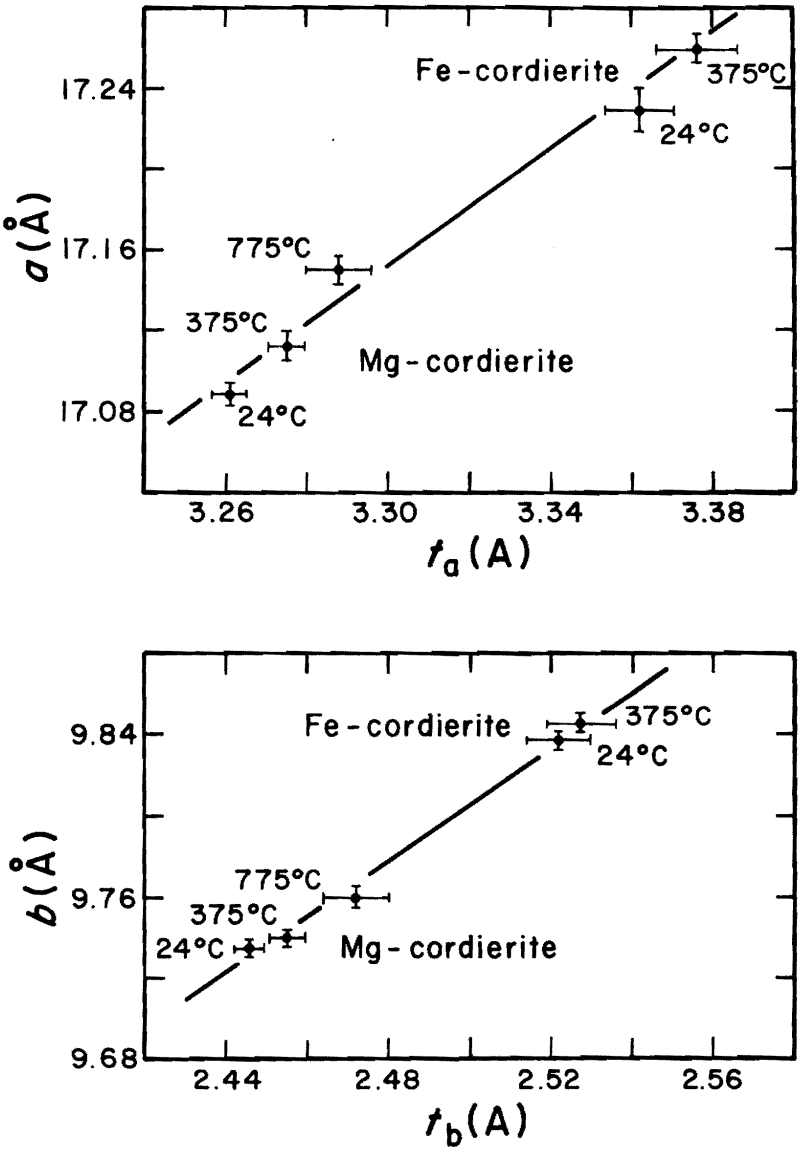

Figure 7. The a and b cell edges *vs* the thickness of the M-octahedron measured along a, t_a, and along b, t_b, for the White Well (Mg) and Dolni Bory (Fe) cordierites at various temperatures. The relationships between a and b and t_a and t_b are similar for both cordierites and seem to be continuous as shown by the linearity of the data points. The brackets are drawn at $1\hat{\sigma}$.

the c-cell edge appears to be independent of the volume change. In addition, the associated changes in the thickness of the octahedron measured along a and b correlate with changes in the lengths of a and b (Fig. 7) while the octahedral thickness measured along c is unaffected by the temperature change. This anisotropic expansion of the octahedron serves to rotate ($\sim$0.2°) the rigid six-membered rings clockwise and counterclockwise in alternate layers perpendicular to c (Fig. 8). Figure 9 shows the displacements of each of the tetrahedral cations in the rings accompanying this rotation. The twisting of the tetrahedral framework attending the rotation may be associated with a decrease in selected T-O-M and O-T-O angles which results in a more efficient packing of the structure and a concomitant contraction of the c-cell edge (Fig. 10).

As a test of the assertion that the thermal expansion of the octahedron is the driving force behind the thermal expansion of cordierite, we completed a *DLS* (Meier and Villiger, 1969) calculation (Meagher, Hochella and Gibbs, in preparation) for the White Well cordierite. The T-O bond lengths used in the calculation were initially set at the room temperature values (24°C) and the M-O bond lengths and the cell edges were initially set at the values measured at 775°C. The results of the calculation (Appendix E) show a close correspondence with the bond lengths and angles measured for the cordierite at 775°C, *i.e.*, almost all are within one or two estimated standard deviations of those recorded for the observed structure. This result agrees with the assertion that the anisotropic thermal expansion of the unit cell of cordierite is controlled in part by

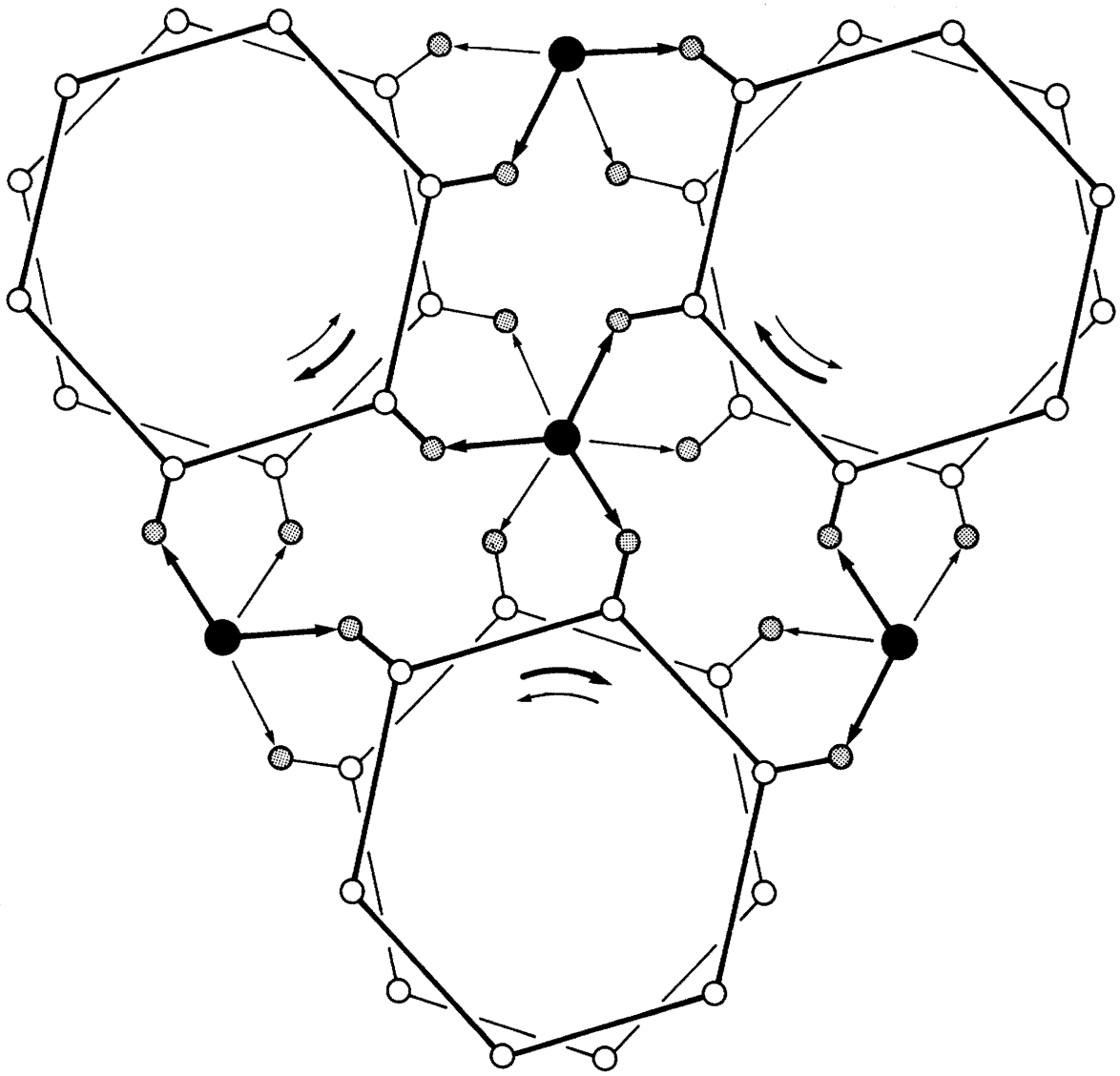

Figure 8. Rotation of the six-membered rings in the White Well cordierite. The open circles represent the tetrahedral cations in the ring, the dotted circles the O_1 oxygens, and the solid circles the octahedral cations (96% Mg). The vectors represent the expanding Mg-O bonds. The upper six-membered rings rotate upon heating in a clockwise direction whereas the lower ones rotate in a counterclockwise direction.

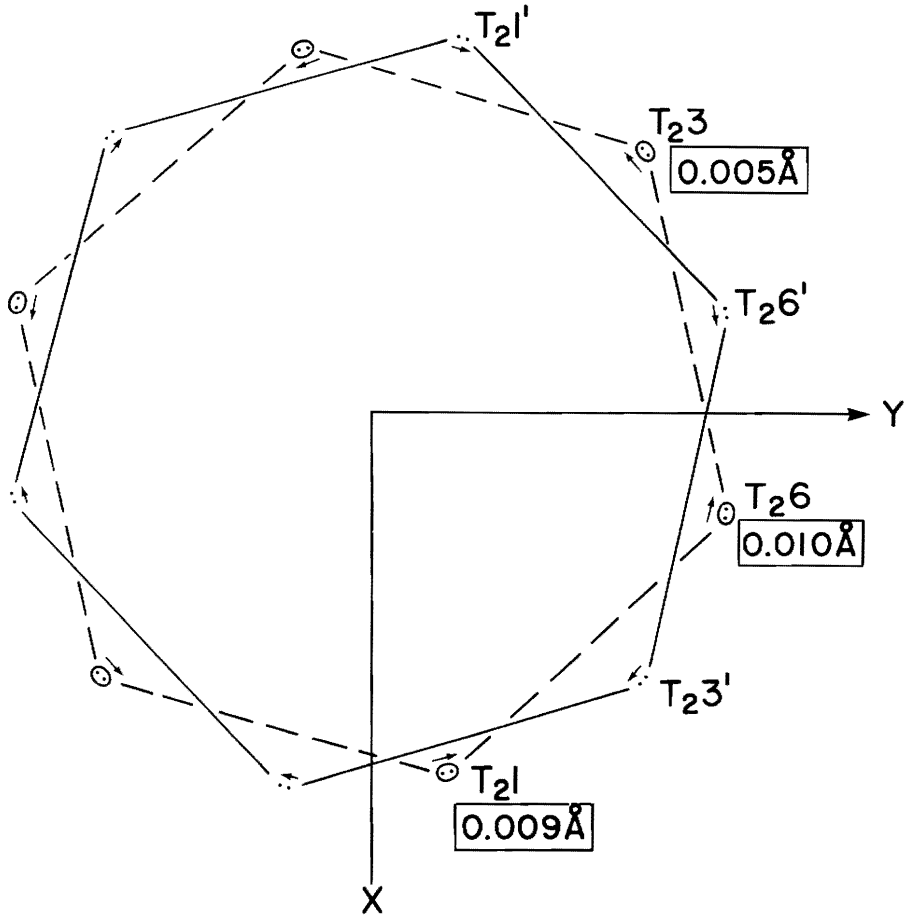

Figure 9. Stereographic projection of the actual displacements (boxes) of the independent tetrahedral ring cations from 24°C to 775°C in the White Well cordierite. The direction of rotation of these rings corresponds to the scheme shown in Figure 8, the upper ring rotating clockwise, the lower counterclockwise. The upper and lower rings are related by a 2-fold along Y as shown.

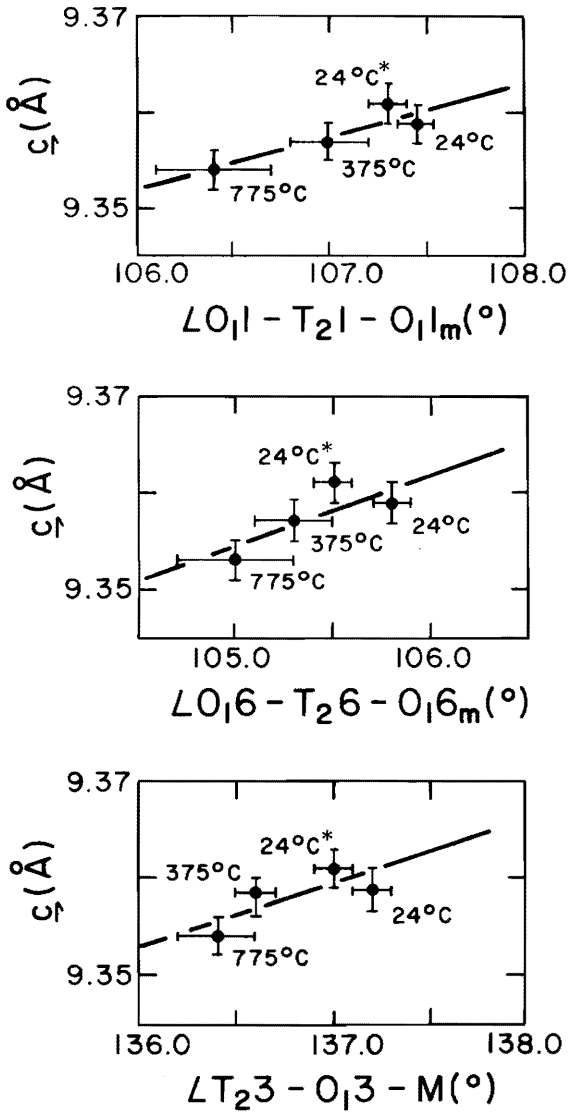

Figure 10. The length of the c-cell edge *vs* one T-O-M and two O-T-O angles at various temperatures for the White Well cordierite. These angles are oriented such that their change directly affects c. Their decrease is apparently related to the expansion of the octahedral bonds and slight rotation of the rings. Error bars are drawn at $1\hat{\sigma}$. (24°C* is after heating.)

the anisotropic thermal expansion properties of the octahedron.

The relationships between the thermal expansion of the Fe-rich octahedron and the *a*- and *b*-cell edges of the Dolni Bory cordierite is practically the same as that measured for the White Well cordierite (Figs. 6 and 7). The thickness of the octahedron measured along *a* and *b* is significantly greater than that measured for the White Well cordierite which conforms with the larger *a* and *b* cell dimensions of the Dolni Bory cordierite. Also, like the White Well cordierite, the change in the thickness of the octahedron measured along *a* and *b* correlates with the changes in these cell dimensions. However, despite the larger volume of the Fe-octahedron, the *c*-cell edge of the Dolni Bory cordierite is 0.05 Å shorter than that measured for the White Well cordierite. In addition, the thickness of the Fe-rich octahedron is significantly less than that of the Mg-rich octahedron, both measured along *c*. Unlike the White Well cordierite, both the thickness of the octahedron and the *c*-cell edge of the Dolni Bory cordierite increase with rising temperature. Also, evidence is lacking in support of a rotation of the six-membered rings associated with the expansion of the octahedron up to 375°C.

Orientation of the Water Molecules in the White Well Cordierite

A re-investigation of the water position in the channels of the White Well cordierite as proposed by Cohen *et al.* (1977) has led to a new, but not complete, interpretation using the X-ray and neutron diffraction data of Cohen (1975). X-ray $\Delta\rho$ maps show the oxygen of the water molecule (Ow) to be split into two positions along the x axis at ±0.027,0,1/4 as shown in Figure 11. Neutron $\Delta\rho$ maps (see

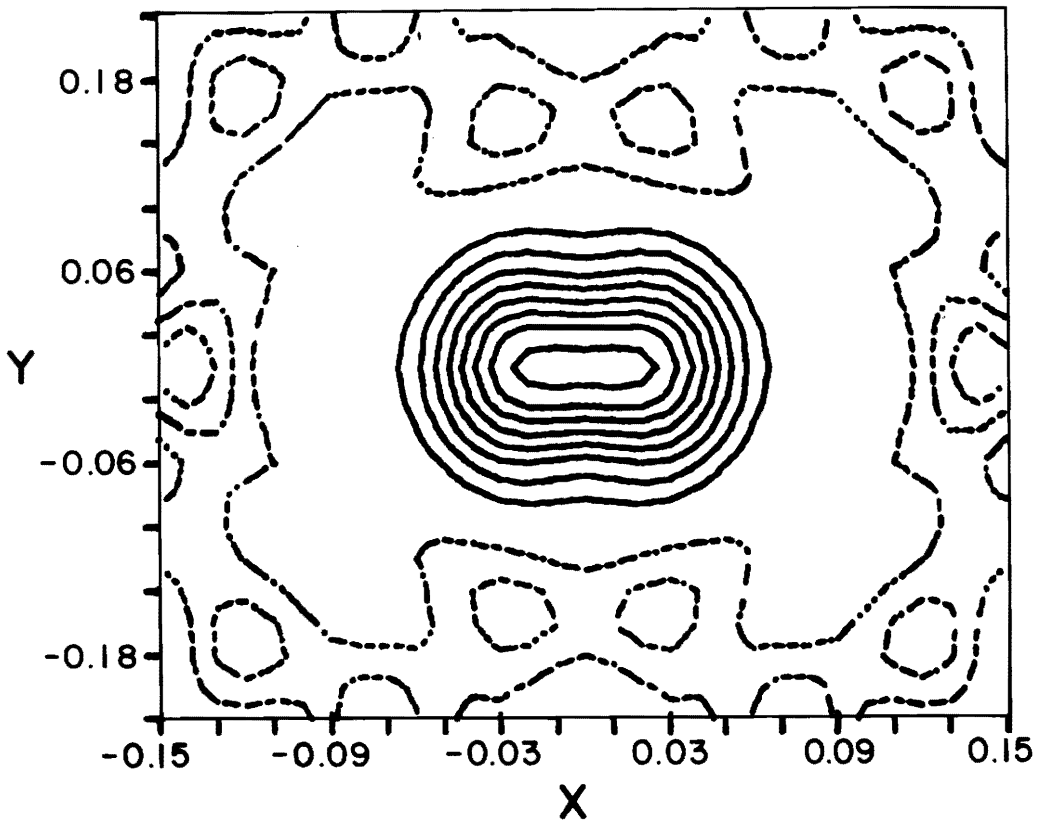

Figure 11. X-ray Δρ map (24°C) showing the elongated oxygen peak along the x axis. Section is the 001 plane at z = 1/4. The contour interval is .20$e^-/Å^3$ and the zero contour has been omitted. Subtraction of the peak was most complete when electron density was added at ±.027 on x.

Fig. 12) strongly suggest that there is an H-O-H position near the 100 plane with the H-H vector 23° from *c*. This H_2O position essentially agrees with the orientation of the water molecule proposed by Farrell and Newnham (1967), Tsang and Ghose (1972) and the type I water of Goldman *et al.* (1977), all based on spectroscopic methods. Problems arose when we attempted to completely subtract out the Ow peak using the multiplicity of H_2O from the chemical analysis of the White Well cordierite (Pryce, 1973). A negative residual was left at the Ow position indicating that the amount of H_2O in the formula should be $(H_2O)_{.36}$ instead of $(H_2O)_{.56}$. To further support the idea that less water is present, the amount of hydrogen needed to diminish the negative peaks of the $\Delta\rho$ map in Figure 12 fits with $(H_2O)_{.36}$. However, a thermal gravimetric weight loss curve for the White Well cordierite suggests that the amount of H_2O in the formula is correct. Despite this puzzling result, there is no evidence in these maps for the type II H_2O (H-O-H in the 100 plane with the H-H vector parallel to *b*) proposed by Goldman *et al.* (1977).

The Effects of Heating on Channel Constituents

The loosely bound channel constituents in cordierite undergo large anisotropic vibrations and positional changes upon heating. Four $\Delta\rho$ maps at each temperature of refinement (Figs. 13a-d) illustrate this in the White Well cordierite. The peak ascribed to the alkali atoms at 0,0,0 is elongated parallel to *c*, the channel axis, at 375°C, while the Ow peak seems to have become a single peak at 0,0,1/4 elongated further along *a* than the double peak at 24°C.

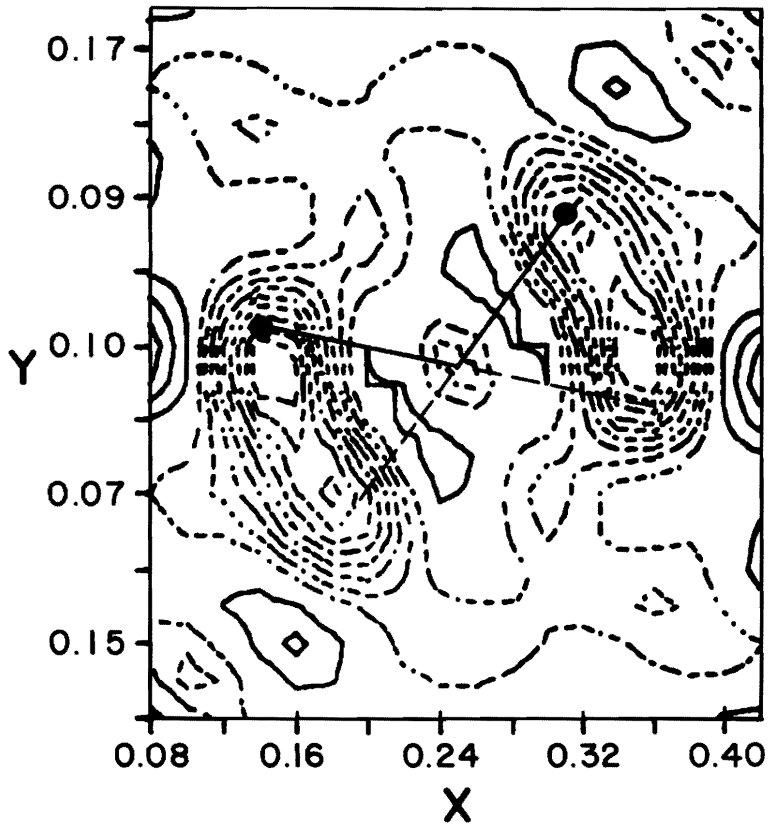

Figure 12. Neutron $\Delta\rho$ map (24°C) showing the negative scattering of the hydrogens (zero contour omitted) in the 100 plane at x = .01. The Ow peak has been subtracted out. The geometry of the 2 symmetry related water molecules shown is d(H1-Ow) = 0.99 Å, d(H2-Ow) = 1.01 Å and ∠H1-Ow-H2 = 105.1° with H1 at x = .010, y = .025, z = .150, H2 at x = .010, y = .078 and z = .311 and Ow at x = .027, y = 0, z = 1/4.

At 775°C in the White Well cordierite, the Ow peak is absent only to reappear in the 24°C (after heating) $\Delta\rho$ map as a single peak, less than half the size of the original Ow peak. This peak is no longer elongated parallel to a. The absence of the peak at 775°C is probably due to the water molecule's high temperature factors and seemingly complete disorder within the cavity. The Ow peak vanishes similarly in the Dolni Bory cordierite in the $\Delta\rho$ map computed from the 375°C data. On the other hand, the peak centering the six-membered ring has enlarged in the 775°C $\Delta\rho$ map for the White Well cordierite. Also, in the 24°C (after heating) $\Delta\rho$ map, it is clear that there is more electron density at 0,0,0 than the unheated sample, less electron density at 0,0,1/4, and an overall substantial drop in the original amount of channel constituents. It seems reasonable to suggest that some of the channel constituents have been driven out of the structure, while some of the remaining H_2O molecules have taken up positions centering the six-membered ring.

The State of the White Well Cordierite After Heating

The a- and b-cell edges of the White Well cordierite do not return to their original lengths after cooling to 24°C (Table 3). Observations such as these are usually attributed to a change in structural state with heating (see, for example, Karkhanavala and Hummel (1953) and Levien and Papike (1976)). However, this is not the case for the White Well cordierite since its completely ordered structure did not disorder at all during data collection at high temperatures. Possible explanations might include secondary

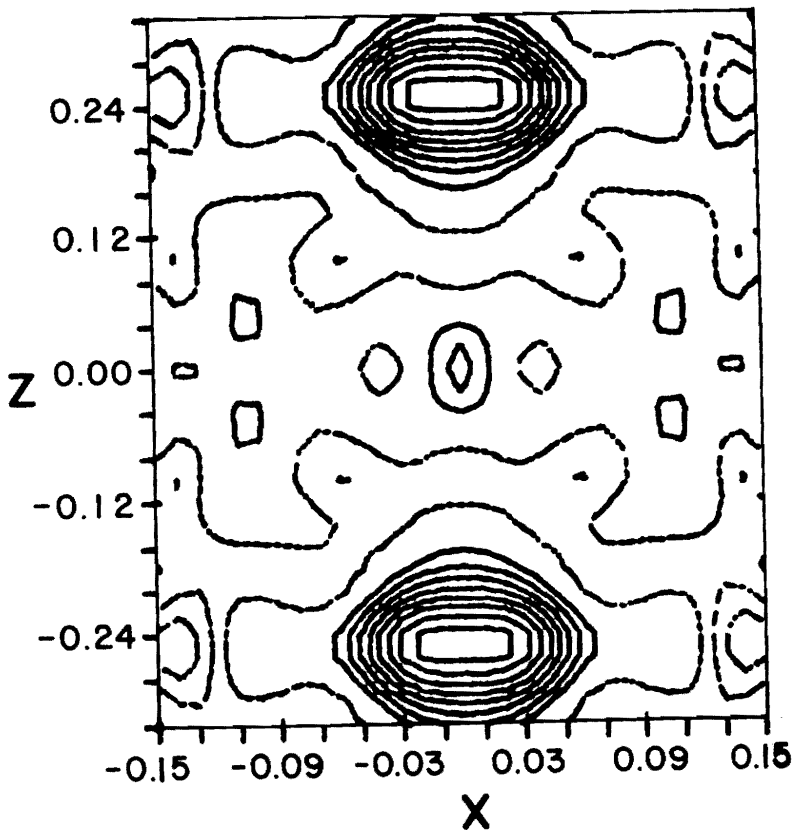

Figure 13a. X-ray $\Delta\rho$ map of the White Well cordierite showing the peaks ascribed to the channel constituents at 24°C. The zero contour is omitted and the contour interval is .20e$^-$/Å^3.

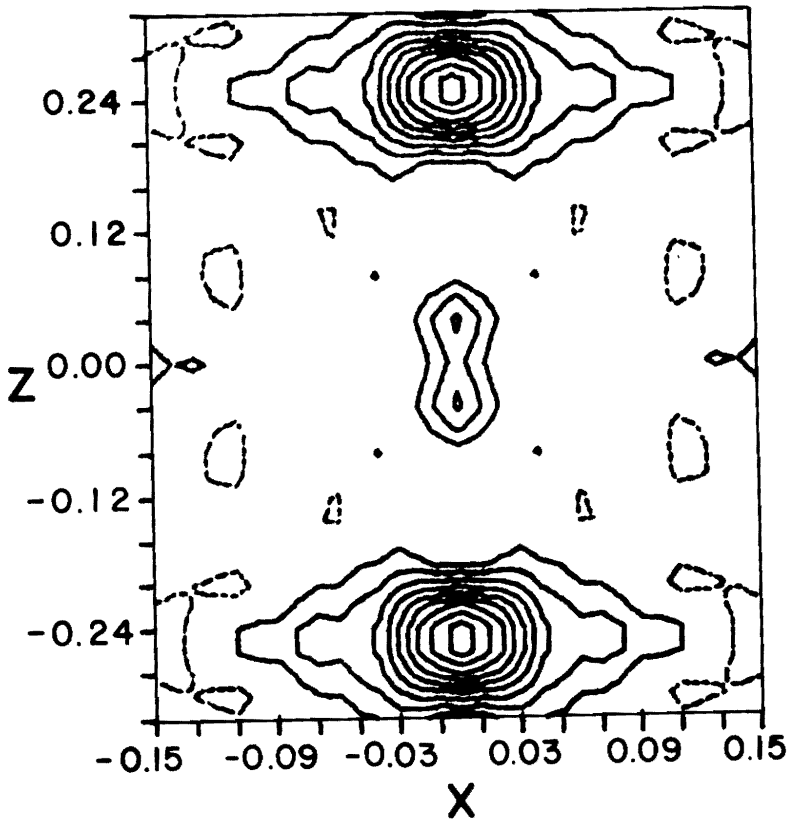

Figure 13b. X-ray $\Delta\rho$ map of the White Well cordierite showing the peaks ascribed to the channel constituents at 375°C. The zero contour is omitted and the contour interval is .20e$^-$/Å^3.

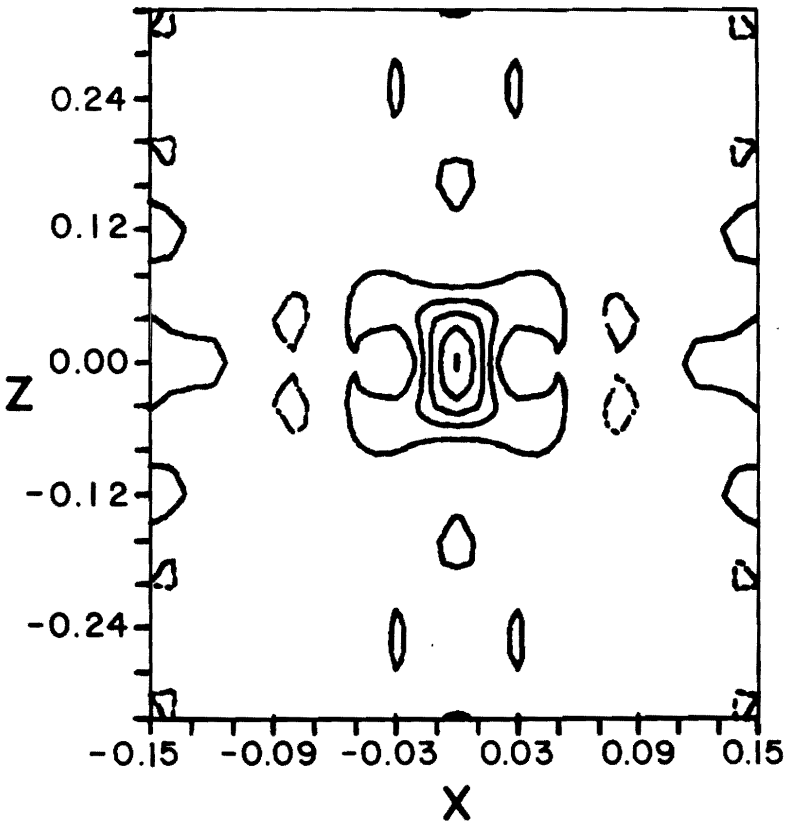

Figure 13c. X-ray $\Delta\rho$ map of the White Well cordierite showing the peaks ascribed to the channel constituents at 775°C. The zero contour is omitted and the contour interval is .20e$^-$/Å^3.

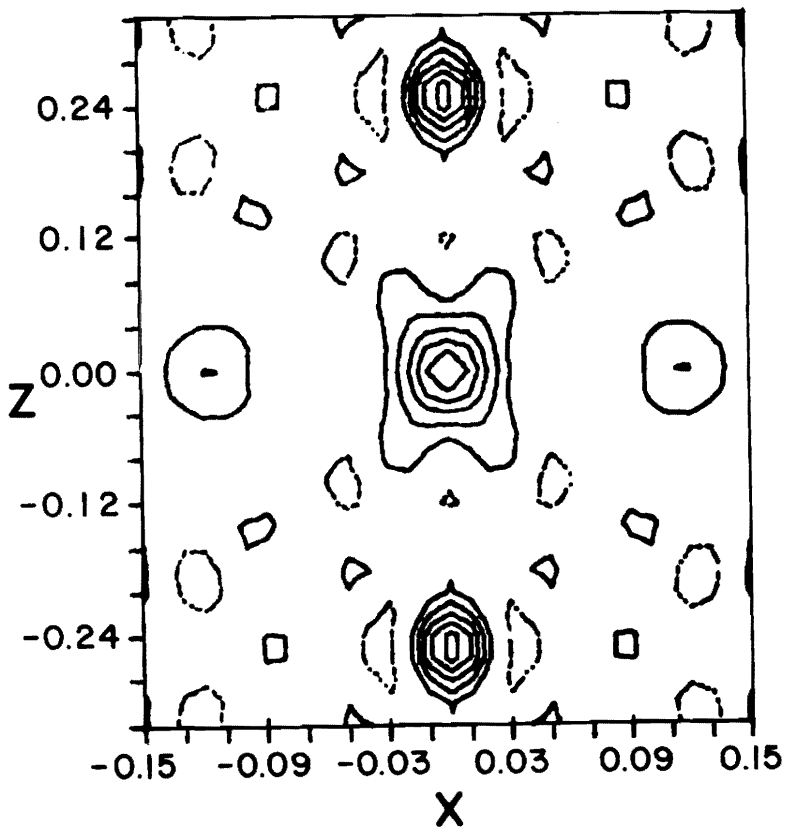

Figure 13d. X-ray $\Delta\rho$ map of the White Well cordierite showing the peaks ascribed to the channel constituents at 24°C (after heating). The zero contour is omitted and the contour interval is .20e$^-$/Å^3.

hematite forming upon heating or the channel constituents changing in amount and perhaps position with heating and cooling as shown in the previous section. It is not clear, though, how these changes might affect the $Al_4Si_5O_{18}$ framework, if at all (see Langer and Schreyer (1976) and Stout (1976)). Another, more plausible, explanation would seem to be that some of the iron in the framework was used to form the secondary hematite, and as a result some of the octahedra were left empty. Octahedral vacancies take up more space than filled octahedra, and a and b would be appropriately larger (see Table 4 and Fig. 6). If octahedral vacancies existed in the framework after heating, one would expect the isotropic temperature factors of the octahedra to be less after heating than before. But again this is not the case (see Appendix D). Thus, this question remains unresolved pending further study.

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APPENDIX A: THE PSEUDO-AXES OF CORDIERITE

INTRODUCTION

Cordierite is pseudo-hexagonal and has two zones, [110] and [310], that look remarkably similar to [100] and [010], respectively. Hence, care is required in distinguishing these zones in single crystal photographs of the mineral.

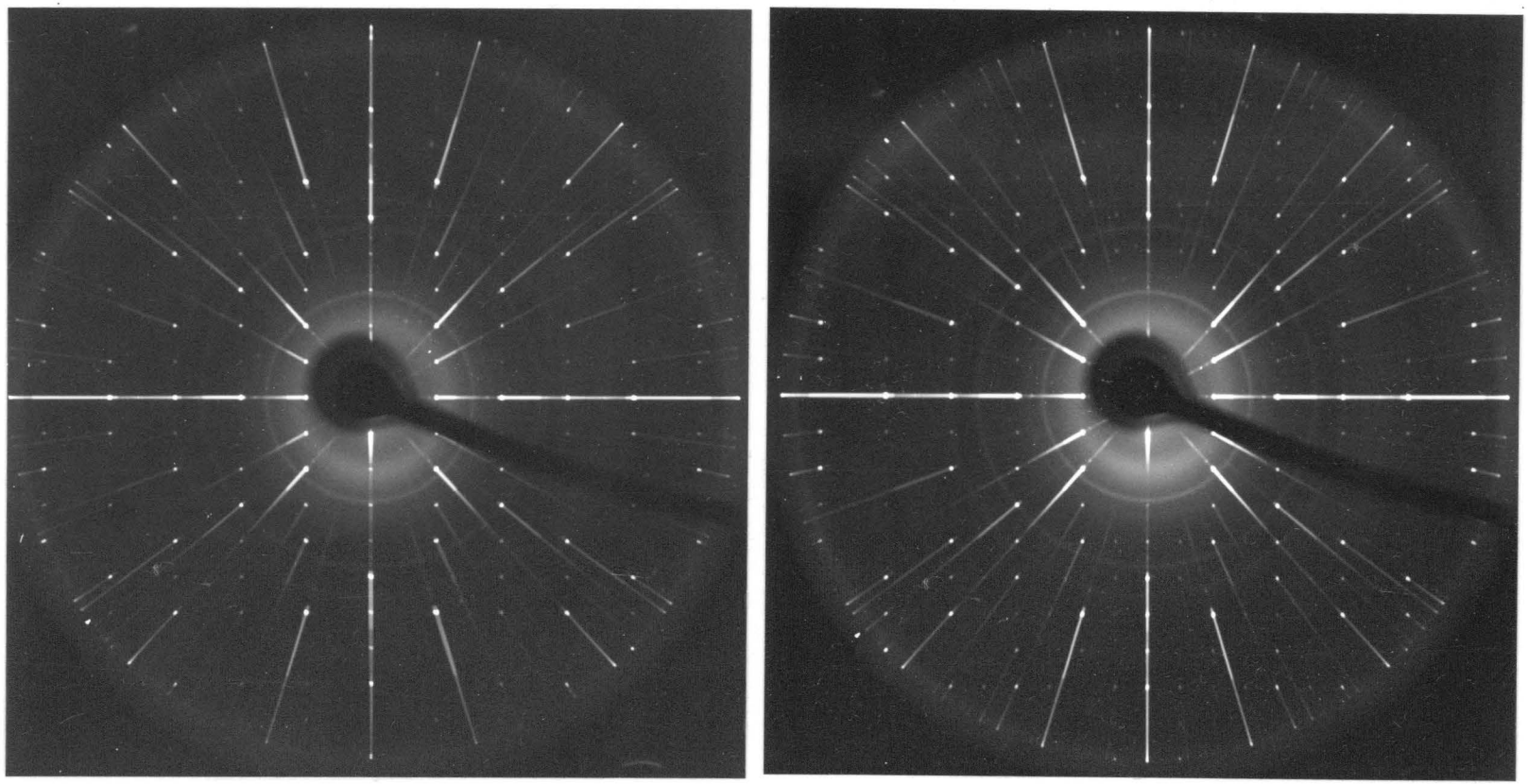
The first crystal structure determinations of cordierite were undertaken independently by Takane and Takeuchi (1936) and by Byström (1942). However, the results of these were slightly different and as Miyashiro *et al.* (1955) remarked, "Though all these investigations adopted the point group *mmm* (D_{2h}) and the space group *Cccm* (D_{2h}^{20}) as a basis of their structure studies, Takane and Takeuchi state that they observed, under favorable conditions, very weak reflections incompatible with this space group - such as (401), (601), (801), (10·0·1)." This led later investigators to wonder whether the true space group was *Cccm* or perhaps *Cccm*, the latter being consistent with the extra reflections observed by Takane and Takeuchi. Gibbs (1966) showed that by orienting the crystal on its pseudo-axes, the indexed peaks of the type (h0ℓ, h even, ℓ odd) were indeed present, but when oriented on the true axes, no peaks of this type were recorded. The author has also observed peaks of the type (0kℓ, k even, ℓ odd) when mounted on the pseudo-axes which also violates *Cccm*. But again, no such peaks are recorded when the crystal is oriented properly. Cohen (1975) has since confirmed the space group *Cccm* for cordierite.

The purpose of this note is to show the hazards of accidentally orienting cordierite on its pseudo-axes and how easy it is to do so. Suggestions are also made on how to avoid this problem. The crystal used for the precession photographs was White Well cordierite, $\underset{\rightarrow}{a}$ = 17.09, $\underset{\rightarrow}{b}$ = 9.73, $\underset{\rightarrow}{c}$ = 9.36, and was the same one previously used for the high temperature data collection.

CALCULATIONS

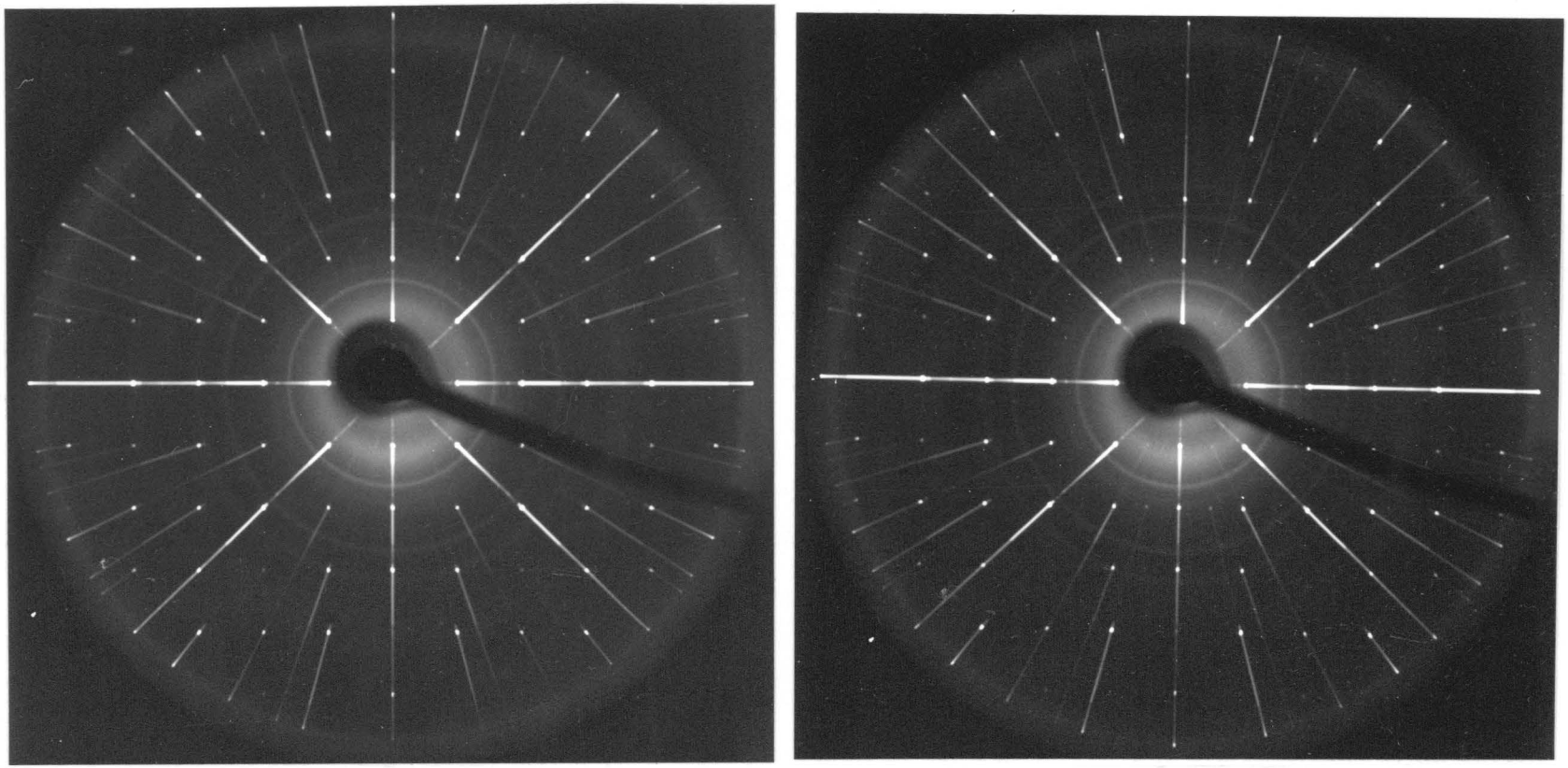
In order to show how similar the pseudo-axes are to the true ones, the following calculations were made.

We know that $x = F \cdot d^*$ where x is the distance in mm measured on the film along a zone, d^* is the spacing of reciprocal planes corresponding to x, and F is the crystal-to-film distance, which in our case is 60 mm. We also know that $d^* = \lambda/p$, where p is the period in the direct lattice. Combining these two equations, we have $x = 60 \cdot \lambda/p$. Now we can calculate the distance between peaks on a precession photograph. (Note: this equation does not take into account the possibility of systematic absences.) For $\underset{\rightarrow}{a}$ we have $x = 60 \cdot 0.7107/17.08 = 2.50$ mm. Because of the condition h00, h = 2n for *Ccem*, we would expect the distance between the peaks in the $\underset{\rightarrow}{a}^*$ direction to be 2x or 5.00 mm. For peaks on the [110] direction (pseudo-$\underset{\rightarrow}{a}$), we must first find d(110). We know that $\underset{\rightarrow}{r}^*(110) = 1/d(110)$ and that $\underset{\rightarrow}{r}^*(110) = \underset{\rightarrow}{a}^* + \underset{\rightarrow}{b}^*$. Also, $a^* = 1/a = 1/17.09 = 0.059$ and $b^* = 1/b = 1/9.73 = 0.103$. Then $r^*(110) = (a^{*2} + b^{*2})^{1/2} = 0.12$ and $d(110) = 8.45$ Å. Therefore, $x = 60 \cdot 0.7107/8.45 = 5.04$ mm. Since there are no systematic absences in this direction, the distance between peaks



(a) (b)

Figure 1. Precession photographs of the White Well cordierite after heating. The dial axis for both is c^*. (a) a^* is the vertical axis and the dial setting is 345°. (b) [110]* is the vertical axis and the dial setting is 45°. The powder rings in both photographs are from secondary hematite which formed during heating. (See main text.)



(a) (b)

Figure 2. Precession photographs of the White Well cordierite after heating. The dial axis for both is c^*. (a) b^* is the vertical axis and the dial setting is 75°. (b) [310]* is the vertical axis and the dial setting is 15°. The powder rings in both photographs are from secondary hematite which formed during heating. (See main text.)

on the film is 5.04 mm.

Similar calculations for $\underset{\rightarrow}{b}$* and [310]* show that distances between peaks on a photograph for these two directions are 8.76 mm and 8.68 mm, respectively.

DISCUSSION

When measuring from the center, the difference between the spacing of peaks on the real and pseudo-axes for lower order reflections is indistinguishable on x-ray film. Only out at higher order reflections (n > 10) can the differences start to be detected by simple ruler measurement. Figures 1 and 2 illustrate this point. The dial axis is $\underset{\rightarrow}{c}$ for all of these photographs. The precession photograph on the left of each figure shows the true axial direction as the vertical axis and the right has the pseudo-axis as the vertical axis. Dial settings are shown to give angular relationships. Note that all four photographs have Friedel symmetry *mm*2.

It is easy to see why picking [110] and [310] as axial directions is very easy unless caution is observed. This mistake leads to poor cell parameter measurements, peak intensity measurement errors, and indexed peaks that violate space group absences. Suggestions to avoid this dilemma are in order. (1) It is preferable to have $\underset{\rightarrow}{c}$ as the rotation axis of a precession or Weissenberg photograph. If this is the case, $\underset{\rightarrow}{a}$, $\underset{\rightarrow}{b}$, [110] and [310] are all in the same photograph and can be directly compared and axes properly assigned. (2) If the rotation axis is $\underset{\rightarrow}{a}$ or $\underset{\rightarrow}{b}$, it is suggested to find the two candidates for either the $\underset{\rightarrow}{a}$ or $\underset{\rightarrow}{b}$ axis and directly

compare the two photographs. Thus one can be sure of the real and pseudo-directions without having to accurately measure cell parameters which are known to vary with cation substitution. (3) Use optical means for orienting the crystal. Bloss (1977) has excellent optical techniques for orienting single crystals.

APPENDIX B: INSTALLATION, CALIBRATION, AND OPERATING PROCEDURES FOR A SINGLE-CRYSTAL HEATER IN CONJUNCTION WITH A FOUR-CIRCLE DIFFRACTOMETER

INTRODUCTION

The single crystal heater used in the cordierite study was designed and described by Brown, Sueno, and Prewitt (1973). The heater is relatively simple and convenient to use in that its geometry allows data collection up to 65°2θ and it is easily retracted for room temperature work. The maximum operating temperature of the heater is approximately 1200°C.

The purpose of this appendix is to review the procedure of furnace installation, specialized crystal mounting techniques, calibration procedures, and general operating procedures. A complete list of all essential starting materials and mailing addresses (when appropriate) of suppliers is also given.

INTEGRAL STARTING MATERIALS

1.* Crystal heater
2. Power supply
3. Voltage stabilizer
4. Digital voltmeter (covering up to approximately 15 mV)
5. Chart recorder (1 mV, 5 mV, and 10 mV ranges, full scale)
6. Short collimators (allows positioning of kapton shield)
7. Power and thermocouple leads for wiring
8. Binocular microscope
9. Micrometer occular
10. Crystal remounting device
11. Micro (small tip) soldering iron

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* Addresses are given for these items

12. Lakeside 70 resin
13.* Zircoa bond 6 and ZrO_2
14. Silica or mullite glass wool
15. Vacuum pump
16. Biological pipettes
17.* Silica glass capillaries (0.3 and 0.5 mm sizes)
18. Silica glass fibers
19. Small tube furnace for curing cement
20. Small lab vise with teflon covered jaws
21. Small tip acetylene-oxygen torch
22.* Pt and Pt-13% Rh thermocouple wire, 0.003", bare
23. Small diameter teflon tubing
24. Various compounds for melting point calibration
25.* Kapton (1 mil thickness)

ADDRESSES OF SELECTED SUPPLIERS

1. Blake Industries, Inc.
   P.O. Box 464
   52 Commerce Street
   Springfield, N.J. 07081

13. Zirconium Corporation of America
    P.O. Box 39217
    Solon, Ohio 44139

17. Uni-Mex Co.
    1829 N. Arborgast Ave., 1-G
    Griffen, Indiana 46319

22. Omega Engineering, Inc.
    Box 4047
    Stamford, Conn. 06907

25. DuPont
    Station Plaza Building
    20 Evergreen Place
    East Orange, N.J. 07018

INSTALLATION

The furnace as manufactured by Blake Industries is shown in Figures 1 and 2. It is a resistance heater with two ceramic prongs containing coils of Pt.-10% Rh. wire. Care must be taken not to bend or crack this ceramic. The furnace itself has 4 wire leads.

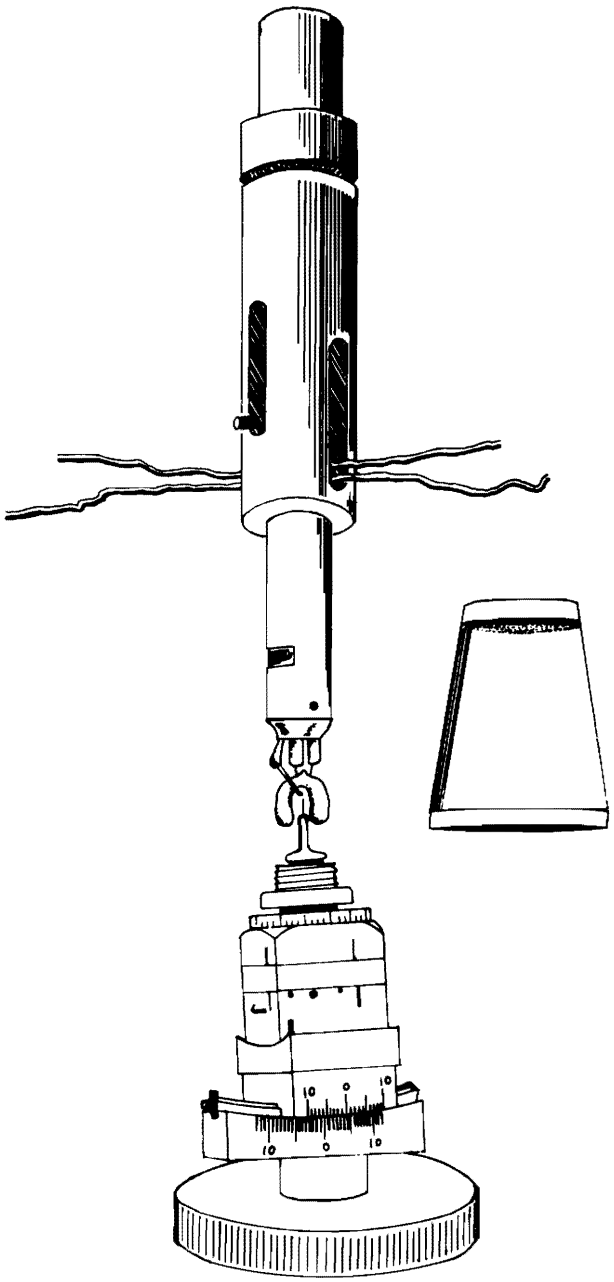

Figure 1. Single crystal heater with the aluminum post fully extended. The post can be retracted for room temperature data collection. The kapton shield, which covers the heater prongs and crystal to dampen temperature fluctuations, is shown on the right. (After Brown *et al.* (1973).)

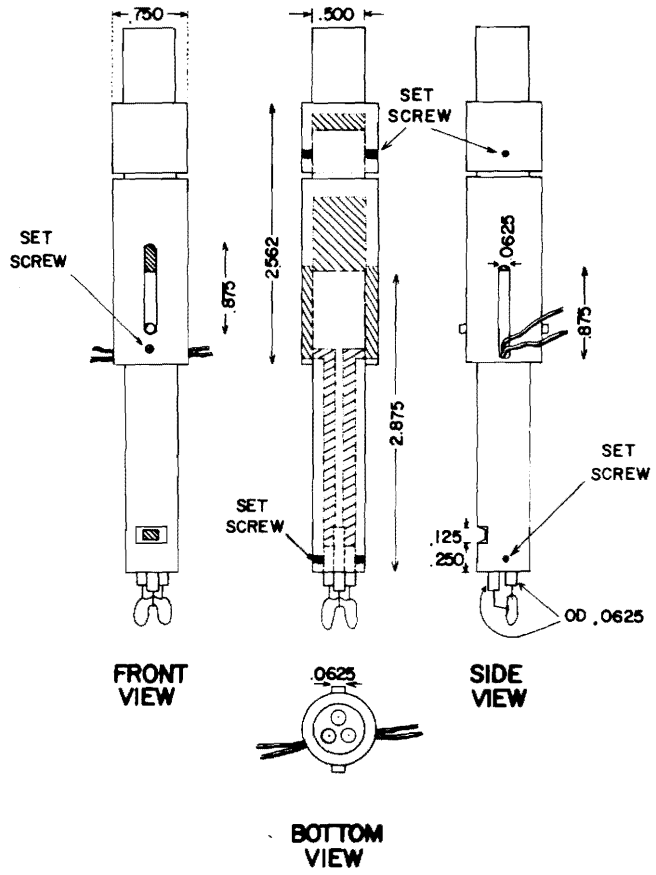

Figure 2. Plan view of the single crystal heater. (After Brown *et al.* (1973).)

The multi-strand wires are power leads whereas the single strand wires are Pt.-10% Rh. thermocouple leads. The heating element is mounted on an adjustable post that can be raised or lowered to the desired position. Because of this adjustable post, complete removal of the furnace is unnecessary for normal room temperature data collection. It is recommended that data collection be performed in the lower hemisphere dictating that the furnace be mounted "upside-down" in the upper hemisphere. The brass χ-circle of the Picker FACS-I is already drilled to receive the end post of the furnace. A set screw will be needed to hold the end post of the furnace in its pre-drilled hole.

A typical power supply for this furnace is described in Brown *et al.* (1973). The setup in our laboratory utilizes a 50 watt, 15 amp maximum power source with a 120 volt constant voltage transformer for line current stabilization. A thermocouple feed-back control, if obtainable, would be outstanding for a constant temperature maintenance at various χ settings. (See the operating procedures for more detail.)

Various wiring configurations have been used. Our setup is fairly simple and works quite well. All four leads from the furnace are run to one four-lead terminal that has been attached to the χ-circle (about 5" from the furnace) on a homemade bracket. Four extension wires (single strand copper wire will do for the thermocouple wire extensions) are run from the other side of the terminal up to a fine gauge extension spring (attached to the top of the glass cage) and then out the nearest top corner of the glass cage. The spring is specially placed so that it can give and take slack from the four extension wires at any data collection position without allowing the

wires to touch the hot X-ray collimator. (X-ray collimators can get hot enough to melt wire insulation.) The terminal, then, serves the purpose of keeping the extensions from tugging unnecessarily on the wire connections within the furnace.

CRYSTAL MOUNTING TECHNIQUE

1. Initial Mounting
   a. It is essential for high temperature work that the crystal is completely free of dirt, oil, and wax. It can usually be cleaned with a good acetone wash.
   b. Using a micro-soldering iron, melt a small amount of lakeside 70 on a glass fiber.
   c. Under the binocular microscope, bring the fiber up to the crystal and remelt the lakeside, attaching the crystal to the fiber. The cement should cover only a minimal area of the crystal; avoid coating the entire crystal with the cement.
   d. Mount the fiber on a goniometer head and align the crystal in the normal manner with a precession camera. For crystals that are mounted randomly, the Bloss spindle stage technique is an easy method for alignment (Bloss, 1977).
2. Remounting Crystal for High Temperature Work
   a. Place the goniometer head with aligned crystal on a crystal remounting device. Be sure to have the crystal in position so it can be remounted on a

desired crystallographic direction.

b. Make a careful sketch of the crystal at stage settings of 0° and 90° and indicate the dimensions of the crystal.

c. Place a 3 to 4 cm long silica glass fiber mounted in clay on another goniometer head and place it on the opposite end of the remounting device.

d. The high temperature cement must now be mixed. The first step is to grind either silica glass wool or mullite wool as fine as possible (this takes 3-5 minutes with a large mortar and pestle) wetting the wool with acetone before grinding. Dry the resulting powder. Place a very small amount on a glass slide and add a few drops of Zircoa Bond 6 and mix to a soupy consistency. The cement dries quickly and more Zircoa can be added to keep the cement from stiffening.

e. Using a needle or thin probe, place a small amount of the cement on the end of the long free fiber and immediately run the fiber tip up to the crystal.

f. Again, the amount of cement used is critical. If too little cement is used, the higher temperatures may affect the mount. More cement may be added with a needle. If too much cement is used,

a later mounting step may be impossible. Excess cement may be removed by coating a needle with a film of Zircoa and dissolving away the unwanted portion.

g. Let dry for about an hour. A drawing of the mounting procedure to this stage is shown in Figure 3.

h. Using the micro-soldering iron, melt the lakeside 70 on the original mount and retract that fiber. The crystal is now mounted in high temperature cement with a desired crystallographic direction approximately in line with the quartz fiber.

i. Carefully break the fiber away from the goniometer head and place it into either a 0.3 or 0.5 mm capillary, depending on the size of your mount. Let the crystal and fiber slide down to the end of the capillary.[1] The crystal should rest approximately 0.5 mm from the inner end of the glass capillary. Cement to this capillary a larger biological pipette with a good coating of Duco cement as shown in Figure 4a.

j. When the Duco is dry, place the large end of the pipette in a small table vise with teflon covered

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[1] If the crystal gets stuck along the way, an appropriate size fiber may be put down the capillary to gently shove the end of the fiber with mounted crystal farther along.

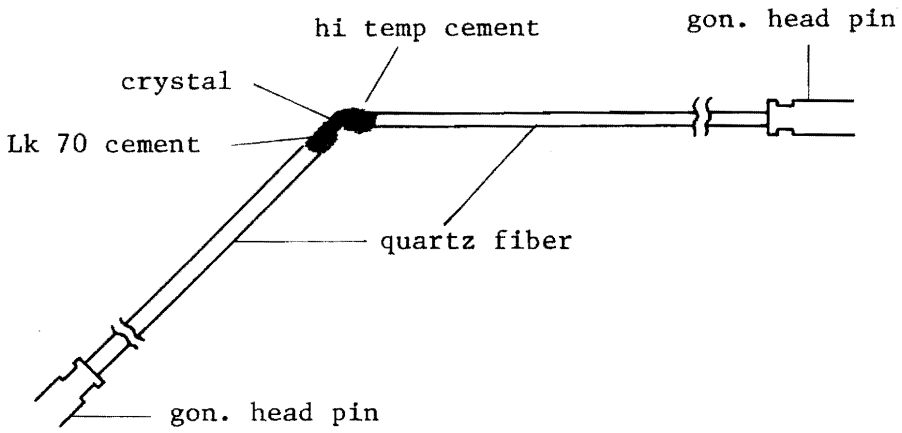

Figure 3. Remounting the crystal in high temperature cement along a known zone. The quartz fiber that the crystal is remounted on must be at least 3 to 4 cm long.

jaws and attach a vacuum hose to the pipette.

k. While the capillary is being evacuated, place it in a small tube furnace (or the equivalent) capable of 90-100°C and cure the cement in this temperature range for at least two hours (overnight if possible). This will properly prepare the cement for surviving extreme temperatures.

l. At this point make sure the crystal is still on the fiber and that the crystal is approximately 0.5 mm away from the inner end of the tube. Light taps on the vise may be used to position the crystal with attached fiber.[2] Also, the crystal should be no more than 1 mm away from the outer end of the capillary.

m. Next, using a small tip oxygen-acetylene torch, cut through the capillary at a point near the end of the quartz fiber. The result is shown in Figure 4b.

n. Finally, mix some fast drying epoxy and mount the evacuated tube in a brass goniometer head pin. Leave about 1.5 cm of the tube exposed. (Make sure you have the correct end of the capillary sticking out!) As a safeguard, it is usually advisable for the user

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[2] However, this is sometimes unsuccessful and it is best to position the crystal properly when it is initially slid down the capillary.

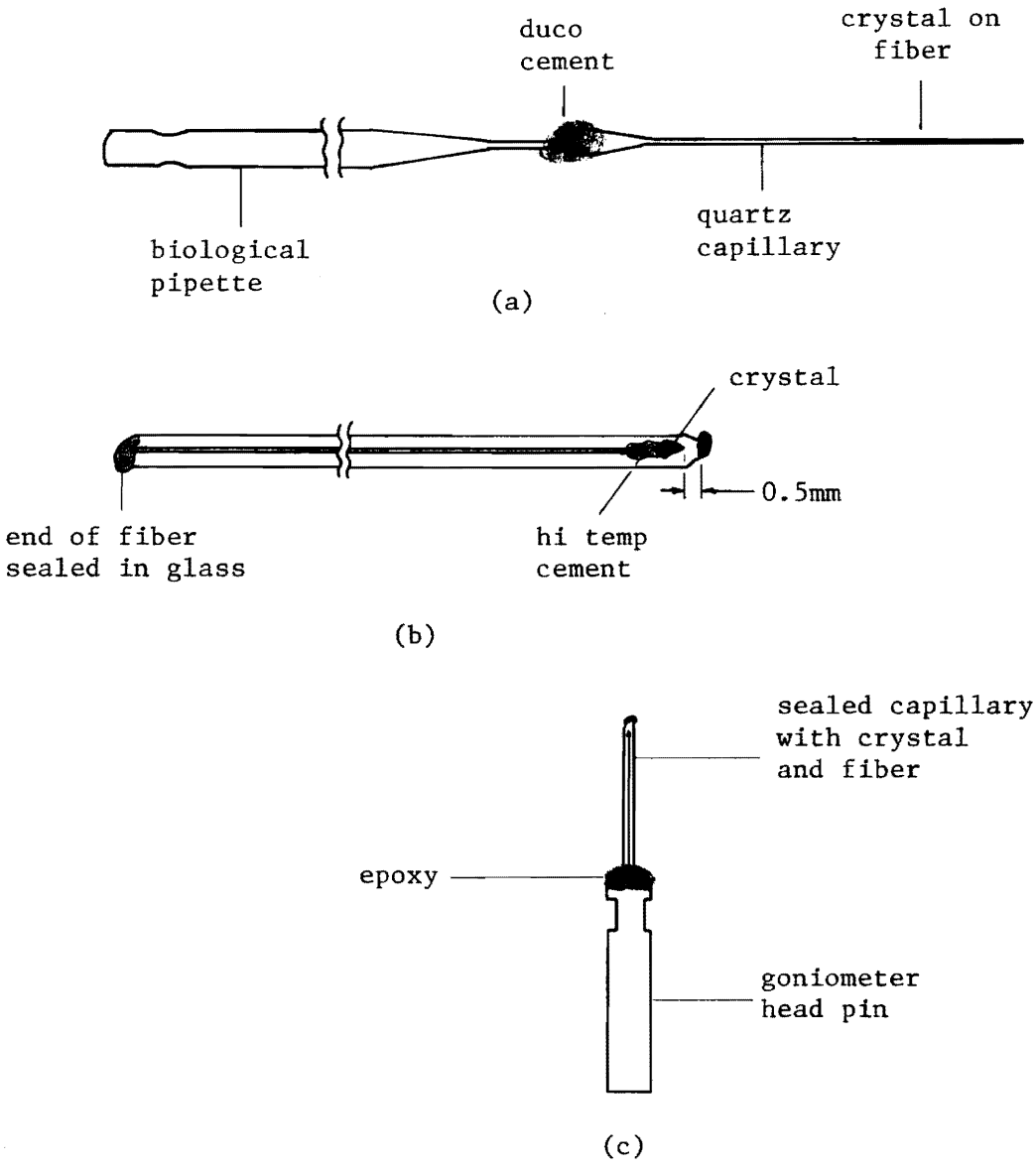

Figure 4. (a) Pipette, capillary configuration just before the vacuum hose is attached to the pipette. (b) Evacuated and sealed glass capillary. Note the distance from the crystal to the inner end of the capillary and that the quartz fiber is embedded in the opposite inner end. (c) The final product. The epoxy may be coated with high temperature cement so it will not soften during data collection at high temperatures.

to coat the dried epoxy with high temperature cement. The final mounting procedure is shown in Figure 4c.

NOTE: This mounting procedure is by far the most difficult procedure of the entire operation. Each step is essential and has a high potential for failure even when extreme care is taken. Patience and practice and a little luck are required.

FURNACE CALIBRATION

The furnace is calibrated using two independent methods. Even though only one method will provide the actual calibration curve for the furnace, the other also provides valuable information.

1. Calibration Thermocouple Method
   a. Figure 5 shows the calibration thermocouple and all its component parts. The setup is mounted in a copper pin which is attached to a goniometer head.
   b. The actual measuring technique involves monitoring both the calibration thermocouple and the permanent furnace thermocouple simultaneously. A switch can be rigged to permit a single voltmeter to be connected to either thermocouple depending on its position.
   c. Attach the goniometer head with calibrating thermocouple to the four-circle and center the connecting bead in the cross hairs of the telescope.

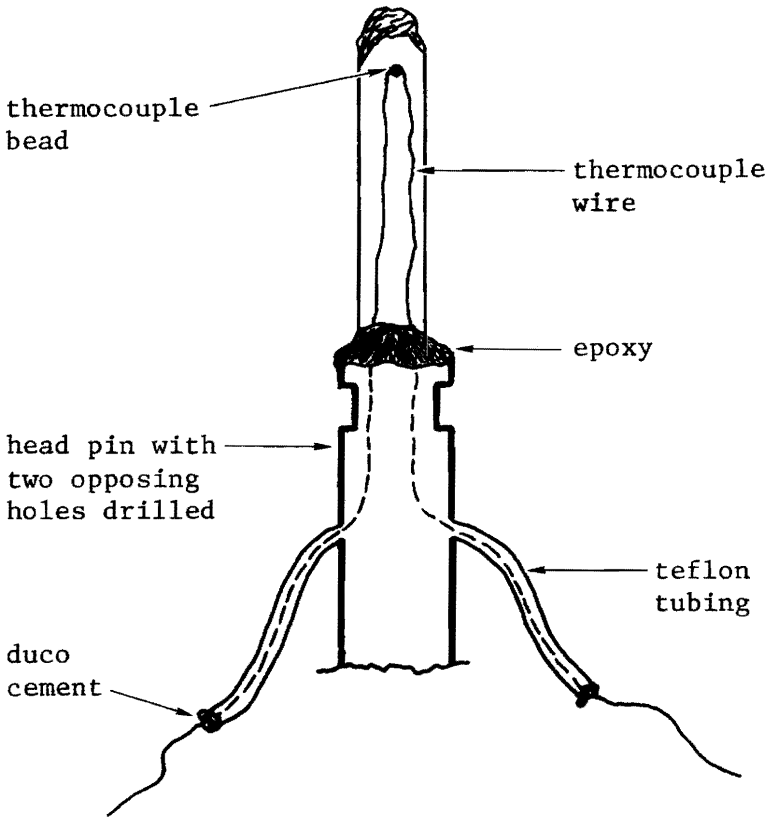

Figure 5. The calibration thermocouple shown mounted within a head pin and quartz capillary.

d. Adjust the furnace into its fully extended position. If the furnace is adjusted correctly, the calibrating thermocouple bead should be symmetrically between the two heater prongs and the measuring and calibration thermocouples should be separated by approximately 1 to 2 mm. If necessary, the furnace position can be adjusted slightly by carefully bending the supporting rods to the heater prongs.

e. The position that the bead of the calibration thermocouple has now assumed should be very close to the furnace hot spot. To check this, heat the furnace up to several hundred degrees (see operating instructions) and set $\chi = 0°$. After the temperature is stable, adjust the goniometer sledges and Z-translation until the highest temperature reading is obtained. If the starting position of the bead (step (c) above) is not the hot spot of the furnace, the furnace position must again be adjusted. Correct configuration is reached when the heater is fully extended and the thermocouple bead is centered in the cross hairs and also in the furnace hot spot.

f. Adjust the temperature of the furnace until the measuring thermocouple reads approximately 200°C. Make sure the furnace temperature is stabilized by waiting several minutes. Make a chart to record the χ setting, the calibration and furnace thermocouple readings in mV, and

the temperature at the calibration thermocouple tip.[3] Collect readings at χ settings of 0°, 45° and 90°. Notice that the temperature changes slightly with χ setting. This will be discussed later.

g. Repeat this procedure at approximately 400°C, 600°C, 800°C and 900°C.

h. Plot the furnace thermocouple mV readings *vs* temperature measured by the calibration thermocouple for a χ setting of 0°.

2. Crystal Melting Point Calibration

a. This method involves melting crystals with known melting points in the furnace. The procedure will provide the actual calibration curve for the furnace which will be used during experimental runs. The shape of this curve will be the approximate shape of the thermocouple curve, but this curve will be lower on the plot and accurate to an absolute degree. The calibration thermocouple acts as a heat sink of low thermal mass and thus is not solely accurate.

The melting point samples we used are shown in Table 1 along with their melting temperatures.

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[3] Remember that when using thermocouple mV-temperature equivalence charts, the cold junction is usually 0°C. mV readings must be corrected for room temperature data collection.

TABLE 1

Melting Point Crystals

Compound	Melting temperature*
Benzoic Acid	123°C
D-camphor	186-188°C
Anthracene	216°C
$NaNO_3$	307°C
B_2O_3	460°C
KIO_3	560°C
$Ba(NO_3)_2$	592°C
KCl	776°C
NaCl	801°C
$BaCl_2$	962°C

* Note that there is not a crystal listed that melts around 700°C. Any appropriate substance can be used if so desired to obtain data at this temperature.

b. Under a binocular microscope, pick an appropriate melting point crystal. The largest dimension should be no greater than 0.4 mm and the crystal must possess sharp (not rounded) corners.

c. Since crystal alignment is not relevant here, the crystal can be mounted arbitrarily with high temperature cement.

d. The crystal is put in a capillary, evacuated, *etc.*, exactly like the experimental crystal. This is to assure that the melting point crystal melts under the same conditions as the experimental crystal.

e. With the melting point crystal in the hot spot of the furnace and χ set to 0°, raise the furnace temperature very slowly while constantly watching the crystal through the telescope. The melting point mV value should be predicted beforehand from the thermocouple curve so that the observer can anticipate melting. Remember that the thermocouple curve will predict slightly higher mV readings at melting than will actually be observed.

f. Melting begins when the crystal edges start to round, and the voltmeter reading should be recorded at this point. Once a crystal is melted it should not be used again. Even if part of the crystal is still intact, its corners are rounded rendering it useless.

g. Plot temperature *vs* mV readings at each melting point. This is the final plot and the furnace is now calibrated (see Fig. 6).

FURNACE OPERATING PROCEDURE

1. Recalibrating the Furnace

   There are only two reasons for the furnace to ever be in need of recalibration. First, if the ceramic coating of the platinum heating coils cracks badly enough for platinum vapor to leak at high temperature or to cause a change in the hot spot, the furnace may have to be rebuilt and recalibrated. Second, any other catastrophe which brings damage to other parts of the furnace may slightly change its characteristics and it again will be in need of recalibration.

2. General Operation

   a. A schematic sketch of the entire setup is shown in Figure 7.

   b. Always keep the kapton film in place when collecting data. This greatly restricts temperature variation.

   c. It is necessary for the power supply to have a coarse and a fine adjustment. Also, an AC current stabilizer interconnected with the power supply is needed to dampen power, and thus temperature, fluctuations.

   d. A strip chart recorder is necessary to keep track of the temperature changes during data collection when

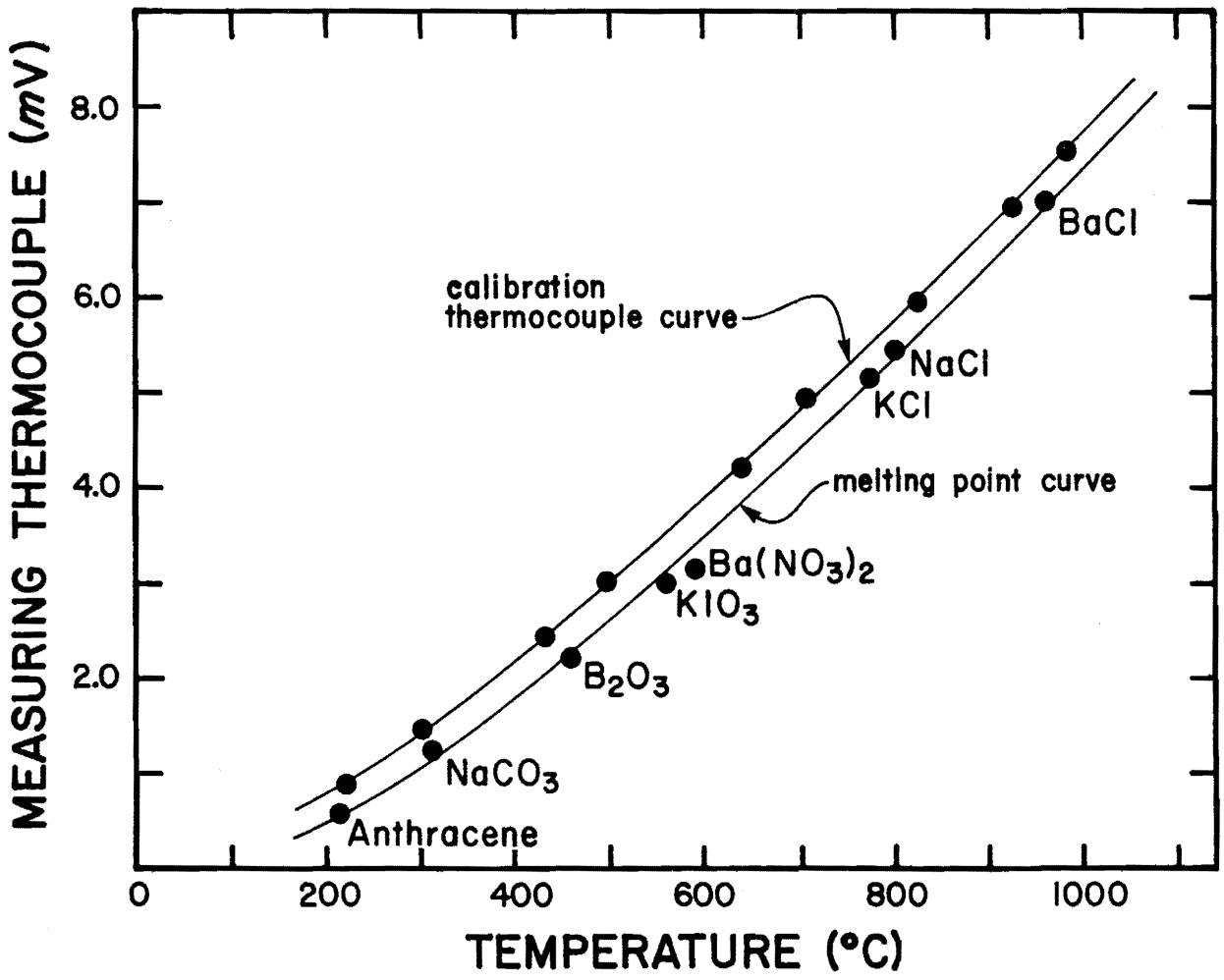

Figure 6. The final callibration plot for our furnace. This plot varies slightly from furnace to furnace.

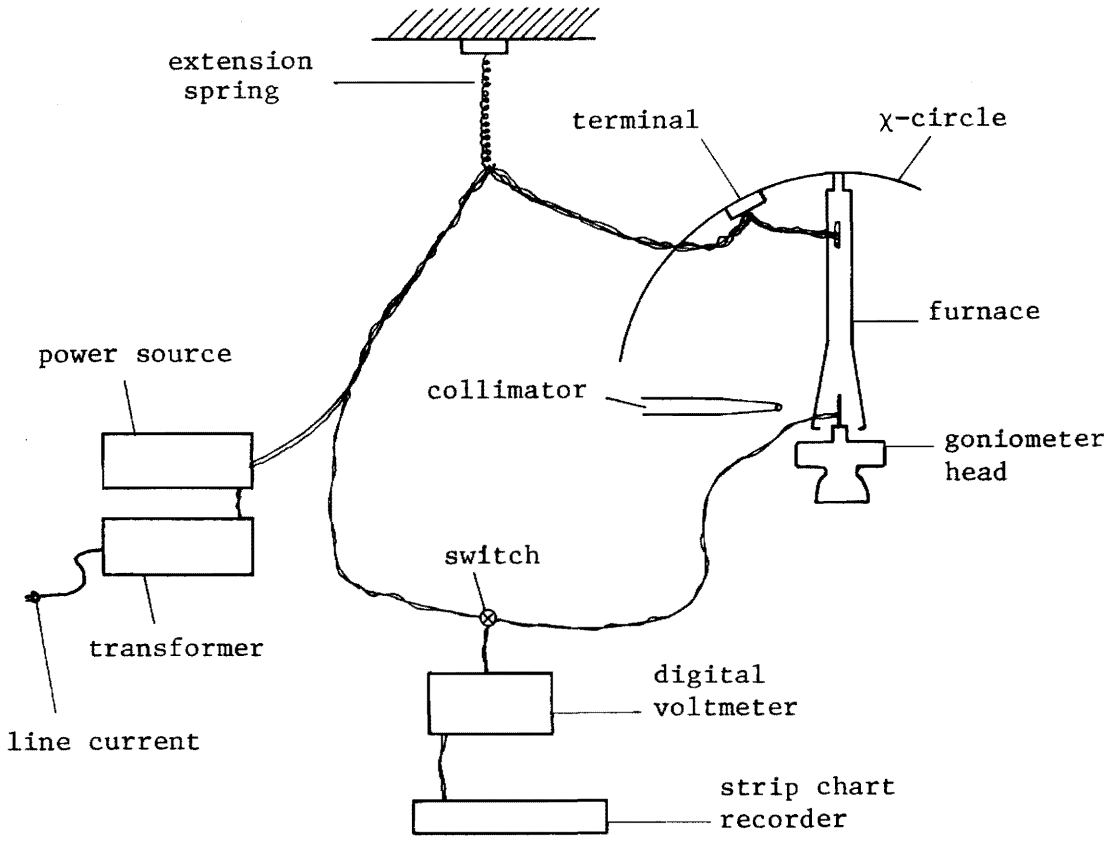

Figure 7. Schematic diagram of our high temperature data collecting setup.

the observer is not present.

e. When the furnace has been set at a certain temperature, it is a good idea to let the crystal equilibrate at this temperature for at least 12 hours. Also check for temperature fluctuation at this time.

f. Never raise the furnace temperature above 1200°C and to be completely safe, 1000°C. At temperatures above 1200°C the platinum heating coils start to vaporize.

g. Due to the configuration of the kapton shield and heat convection, there is a change in furnace temperature simply with a change in χ. The temperature change ranges from ±5° at low temperatures to as much as ±20° at 1000°C, depending on the position of χ between 0° and 90°. If these temperature changes cannot be tolerated, a thermocouple feedback controller may be installed.

h. After much testing, it has been shown that one should not attempt to collect data at a 2θ greater than 65°. At this point, the prongs start to interfere with diffracted radiation and will significantly affect the weaker reflections.

i. It is extremely advantageous and almost necessary to keep the goniometer head in the lower hemisphere and the heater in the upper hemisphere during data collection. This keeps the heat trapped within the shield and away from the goniometer head which could

show alignment deviations with temperature change.

j. As an alternative to (g) above, the χ temperature dependence can be removed by collecting data within small ranges (10° - 20°) of χ. The heater current can be adjusted for each segment of data collection to maintain a constant crystal temperature.

APPENDIX C: OBSERVED (FO) AND CALCULATED (FC) STRUCTURAL AMPLITUDES FOR THE WHITE WELL AND DOLNI BORY CORDIERITES AT VARIOUS TEMPERATURES

TABLE C-1. Structural Amplitudes for the White Well Cordierite at 375°C.

TABLE C-1, continued.

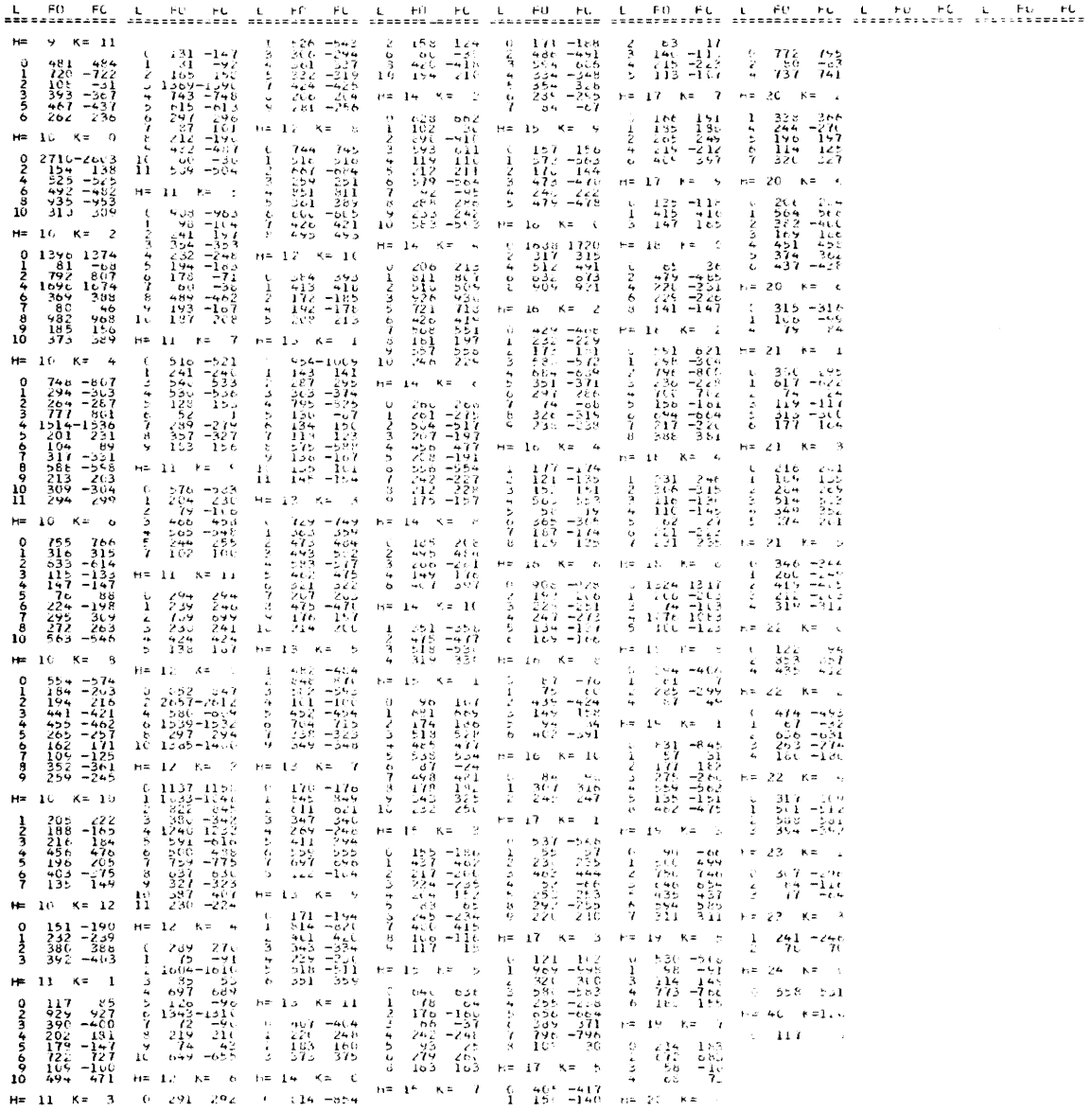

TABLE C-2. Structural Amplitudes for the White Well cordierite at 775°C.

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
			9	21	24	0	60	-63	H=	3	K= 11	2	161	171	12	80	81	3	10	10	10	24	25
H=	0	K= 0	11	22	21	1	48	-51				3	82	70				4	61	61	11	36	34
			12	39	-40	2	64	61	1	45	-44	4	8	-8	H=	6	K= 4	5	18	-14			
2	180	192				3	17	-18	2	48	-49	5	70	-71				6	118	117	H=	8	K= 8
4	406	391	H=	1	K= 7	4	35	-33	3	90	-91	6	137	137	0	154	150	7	43	-45			
6	295	295				5	29	-31	4	34	-32	7	175	-179	1	126	-125	9	23	-21	0	240	242
8	481	472	0	45	-48	6	36	-36	5	62	-65	9	53	-52	2	75	-75	10	113	114	1	49	-50
10	19	-20	1	10	-6	7	35	-35	6	36	-33	10	70	71	3	208	-208	11	9	-4	2	23	21
12	200	196	2	15	15	8	35	-35	7	25	-20	11	19	-16	4	43	-45				3	46	-44
			3	165	-170	9	14	-10				12	9	9	5	128	-131	H=	7	K= 7	4	60	60
H=	0	K= 2	4	132	-138	10	27	27	H=	3	K= 13				6	11	15				7	34	-34
			5	81	-84							H=	5	K= 3	7	66	-66	0	137	-143	8	147	146
0	149	-167	6	57	58	H=	2	K= 10	0	69	-70				8	44	45	1	19	-14	9	28	-26
2	293	-272	7	19	21				1	20	18	0	50	39	9	85	-87	2	36	38			
4	105	-114	8	50	-50	0	31	30	2	51	-52	1	73	-61	10	45	-46	3	13	-17	H=	8	K= 10
6	150	-150	9	45	-46	1	60	59				2	126	125	11	69	-70	4	73	-74			
8	71	-75	10	14	-10	2	33	-32	H=	4	K= 0	3	180	176				6	7	7	0	92	-91
10	84	-84	11	64	-66	3	64	64				4	67	-72	H=	6	K= 6	8	68	-68	1	15	-15
12	32	-31				4	100	99	0	75	56	5	67	67				9	10	-10	2	26	-24
			H=	1	K= 9	5	48	49	2	272	-253	6	110	109	0	189	185	10	31	30	3	27	-27
H=	0	K= 4				6	43	-45	4	79	-83	8	13	-5	1	24	24				4	80	-79
			0	33	-34	7	42	42	6	126	-123	9	76	75	2	311	-313	H=	7	K= 9	5	13	-19
0	194	191	1	104	102	8	27	25	8	25	27	10	36	36	3	31	34				6	30	-33
2	108	-108	2	72	74				10	104	-106	11	75	72	4	35	-39	0	26	-30	7	14	-6
4	379	365	3	98	101	H=	2	K= 12				12	24	-21	5	17	19	1	35	36			
6	151	-152	4	36	-37				H=	4	K= 2				6	158	-157	2	87	87	H=	8	K= 12
8	147	146	5	92	95	0	59	-55				H=	5	K= 5	7	16	10	3	86	85			
10	23	-25	6	53	56	1	40	-35	0	61	44				8	73	70	4	15	-17	1	8	-12
12	97	97	7	74	74	2	20	-19	1	237	230	0	277	-276	9	17	12	5	62	60	2	52	-52
			8	12	-12	4	80	-80	2	160	170	1	38	-38	10	177	-172	6	70	69	4	33	35
H=	0	K= 6	9	57	57				3	73	-61	2	26	-26				7	25	18			
						H=	3	K= 1	4	61	-65	3	18	-19	H=	6	K= 8	8	14	-17	H=	9	K= 1
0	203	-204	H=	1	K= 11				5	77	78	4	99	-102				9	40	38			
2	161	-161				0	161	-175	6	151	150	5	34	-33	0	23	-26				0	158	151
4	45	-47	0	105	-105	1	23	20	7	158	160	6	63	-64	1	51	50	H=	7	K= 11	1	70	70
6	174	-178	1	14	-14	2	256	-240	9	38	38	7	29	-30	2	19	-20				2	67	-68
8	177	-179	2	21	22	3	13	12	10	60	60	8	122	-124	3	79	79	0	48	-48	3	155	155
10	49	-50	3	9	-8	4	109	-115	11	22	20	10	18	10	4	59	59	1	28	27	4	42	-42
			4	37	-40	6	158	-152				11	14	-16	5	53	51	2	21	15	5	107	110
H=	0	K= 8	6	18	-13	7	10	10	H=	4	K= 4				6	37	-36	3	30	-33	6	33	33
						8	59	-62				H=	5	K= 7	7	36	33	4	63	-64	7	43	43
0	30	28	H=	1	K= 13	9	13	17	0	55	-61				8	13	-9	5	11	-7	8	36	35
2	211	-213				10	69	-70	1	34	-33	0	117	-118	9	45	46	6	24	25	9	59	60
4	105	106	0	33	31	12	48	-49	2	115	-114	1	25	23							10	39	-37
6	191	-192	2	99	99				3	23	-23	3	45	-44	H=	6	K= 10	H=	7	K= 13	11	68	69
8	31	32	3	29	29	H=	3	K= 3	4	91	86	4	101	-103									
10	80	-78	4	36	39				6	138	-139	7	23	24	0	76	78	0	20	-19	H=	9	K= 3
						0	42	36	7	8	-9	8	70	-69	1	26	-29	1	20	18			
H=	0	K= 10	H=	2	K= 0	1	12	13	8	10	-13	9	12	-12	2	114	-114				0	144	-142
						2	59	64	10	57	-55				4	95	94	H=	8	K= 0	1	16	-16
0	123	124	2	122	132	4	190	182	12	9	14	H=	5	K= 9	5	14	-18				2	117	-117
2	25	-24	4	39	24	5	14	-16				0	63	-64	6	105	-102	0	56	-57	3	25	26
4	33	-29	6	48	49	7	15	15	H=	4	K= 6	1	71	70	7	21	-24	2	157	-158	4	9	-15
6	42	43	8	89	-95	8	32	32				2	12	15	8	52	53	4	70	69	5	11	17
8	49	48	10	50	53	9	25	25	0	92	-97	3	50	-50				6	177	-182	6	116	-115
						10	45	48	1	90	94	4	71	-71	H=	6	K= 12	8	12	14	7	11	-11
H=	0	K= 12	H=	2	K= 2	12	33	34	2	134	138							10	66	-64	8	62	-63
									3	21	21	5	7	8	0	40	37				10	26	-24
0	188	186	0	32	13	H=	3	K= 5	4	29	28	6	8	15	1	81	80	H=	8	K= 2	11	15	16
2	13	-14	1	8	-4				5	40	39	7	67	63	2	36	39						
4	134	135	2	326	-304	0	164	157	6	71	72	8	47	-44	3	88	88	0	120	-124	H=	9	K= 5
6	16	8	3	6	-8	1	109	107	7	66	72	9	17	-13	4	69	66	1	84	82			
			4	75	-80	2	70	-68	8	26	-25				5	78	77	2	26	-23	0	145	148
H=	1	K= 1	5	13	14	3	157	158	9	35	33	H=	5	K= 11				3	103	105	1	160	162
			6	159	-154	4	51	-53	10	82	80				H=	7	K= 1	4	153	-153	2	99	98
1	11	12	7	9	-4	5	100	106				1	21	-20				5	78	76	3	114	114
2	219	226	9	12	-14	6	13	21	H=	4	K= 8	2	76	77	0	11	-23	6	10	-14	4	128	124
4	49	31	10	122	-122	7	58	57				3	12	14	1	72	62	7	41	41	5	111	110
6	48	50				8	35	36	3	13	9	4	8	14	2	104	104	8	69	-70	6	57	57
8	54	-57	H=	2	K= 4	9	65	66	4	9	-10	5	65	64	3	145	-142	9	39	40	7	113	112
10	85	87				10	44	-45	5	39	-39	7	22	-21	4	114	-121	10	24	-24	8	89	86
11	8	-1	0	59	46	11	54	56	6	64	-63				5	77	-77	11	37	37	9	79	76
12	25	-29	1	53	43	12	12	-2	7	60	-61	H=	5	K= 13	6	110	110	12	60	-56	10	48	48
			2	154	156				8	31	29				7	9	15				11	51	50
H=	1	K= 3	3	173	-173	H=	3	K= 7	9	12	-6	0	29	28	8	53	-55	H=	8	K= 4			
			4	46	-53				10	72	-72	1	27	-25	9	49	-48				H=	9	K= 7
1	261	-254	5	74	-75	0	176	176				2	55	52	10	25	22	0	140	141			
2	108	122	6	109	107	1	158	-159	H=	4	K= 10	3	16	18	11	74	-75	1	24	20	0	53	-53
3	71	61	7	9	7	2	119	123							12	32	-29	2	74	-18	1	92	-93
4	83	-90	9	70	-71	3	91	-91	0	12	12	H=	6	K= 0				3	60	-60	2	14	-13
5	68	-71	10	43	43	4	165	165	1	96	-93				H=	7	K= 3	4	177	181	3	116	-117
6	115	120	11	71	-74	5	81	-83	2	73	72	0	87	84				5	24	-24	4	44	46
7	171	-177	12	20	-19	6	90	92	3	23	-24	2	85	84	0	169	-176	6	16	-13	5	97	-95
8	18	-19				7	105	-109	4	26	-30	4	188	182	1	25	-24	7	14	14	6	57	-55
9	54	-56	H=	2	K= 6	8	97	95	5	49	-51	6	9	4	2	20	3	8	96	92	7	58	-58
10	52	52				9	70	-73	6	71	71	8	44	45	3	25	-29	9	22	-20	8	19	-19
11	21	-17	0	159	156	10	68	68	7	84	-82	10	30	35	4	180	-180	10	10	3	9	58	-57
12	14	-14	1	21	21	11	24	-26	8	15	10				5	33	-34	11	24	-27	10	11	17
			2	21	22							H=	6	K= 2	6	14	14						
H=	1	K= 5	3	85	85	H=	3	K= 9	H=	4	K= 12				7	99	-98	H=	8	K= 6	H=	9	K= 9
			4	172	173							0	144	145	9	9	-5						
0	119	-127	5	49	47	1	74	78	1	42	40	1	36	34	10	12	-3	0	33	-30	0	18	17
1	49	47	7	13	13	2	16	-19	2	63	-65	2	143	-144	11	15	-18	1	35	35	1	25	25
2	8	5	8	115	117	3	39	38	4	10	5	3	21	-24	12	57	-59	2	68	69	2	21	-18
3	79	79	9	37	38	4	20	20	5	23	19	4	343	336				3	83	81	4	19	17
4	146	-150	10	10	14	5	53	53				5	9	10	H=	7	K= 5	5	55	50	5	8	7
5	45	45	11	36	35	6	22	-19	H=	5	K= 1	6	182	-185				6	57	55	6	14	-4
6	31	31				7	54	56				8	118	115	0	37	-38	7	15	16	7	22	20
7	12	16	H=	2	K= 8	9	22	22	0	33	22	9	19	-19	1	46	-46	8	38	-35	8	11	1
8	95	-97							1	259	-252	10	44	-42	2	214	215	9	37	36			

TABLE C-2, continued.

L	FO	FC
H= 9 K= 11		
0	66	66
1	98	-99
2	15	-4
3	54	-50
5	64	-69
6	36	32
H= 10 K= 0		
0	370	-356
2	21	19
4	72	-72
6	67	-66
8	128	-130
10	42	42
H= 10 K= 2		
0	191	188
1	11	-9
2	108	110
4	232	229
6	58	53
7	11	6
8	134	132
9	25	21
10	51	53
H= 10 K= 4		
0	102	-110
1	40	-41
2	36	-39
3	106	109
4	207	-210
5	27	32
6	14	12
7	43	-45
8	80	-82
9	29	28
10	42	-42
11	40	41
H= 10 K= 6		
0	103	105
1	43	43
2	87	-84
3	16	-18
4	20	-20
5	10	12
6	31	-27
7	40	42
8	37	36
10	77	-75
H= 10 K= 8		
0	76	-78
1	25	-28
2	26	29
3	60	-57
4	62	-63
5	36	-35
6	22	23
7	15	-17
8	48	-49
9	35	-34
H= 10 K= 10		
1	28	30
2	26	-23
3	29	25
4	62	65
5	27	28
6	56	-51
7	18	20
H= 10 K= 12		
0	21	-26
1	32	-33
2	52	53
3	54	-55
H= 11 K= 1		
0	16	12
2	127	127
3	53	-55
4	28	25
5	24	-20
6	99	99
9	15	-14
10	67	64
H= 11 K= 3		
0	40	40
1	18	-20
1	11	-13
2	23	22
3	187	-190
4	101	-102
5	84	-84
6	41	40
7	12	14
8	29	-26
9	64	-67
10	8	-4
11	70	-69
H= 11 K= 5		
0	124	-132
1	13	-14
2	33	27
3	48	-48
4	32	-34
5	26	-25
6	24	-10
7	8	-9
8	67	-63
9	26	-23
10	26	28
H= 11 K= 7		
0	70	-71
1	33	-33
2	74	73
3	72	-73
5	17	21
6	7	6
7	39	-38
8	49	-45
9	25	21
H= 11 K= 9		
0	79	-80
1	28	31
2	11	-15
3	64	62
4	77	-75
5	33	35
7	14	14
H= 11 K= 11		
0	40	40
1	33	34
2	97	95
3	31	33
4	58	58
5	19	26
H= 12 K= 0		
0	116	116
2	363	-357
4	79	-83
6	210	-209
8	41	40
10	189	-191
H= 12 K= 2		
0	155	158
1	141	-143
2	112	115
3	52	-47
4	169	168
5	81	-84
6	63	67
7	104	-106
8	87	86
9	45	-44
10	53	56
11	31	-31
H= 12 K= 4		
0	39	37
1	10	-12
2	219	-220
3	12	7
4	95	94
5	17	-13
6	193	-179
7	10	-12
8	30	24
9	10	6
10	99	-89
H= 12 K= 6		
0	72	-74
3	42	-42
4	49	46
5	45	-44
7	58	-58
8	28	28
9	38	-35
H= 12 K= 8		
0	102	102
1	71	71
2	91	-93
3	35	34
4	116	111
5	49	53
6	82	-83
7	58	58
8	68	67
H= 12 K= 10		
0	92	94
1	56	57
2	24	-25
4	26	-24
5	28	29
H= 13 K= 1		
0	130	-138
1	19	19
2	39	40
3	56	-61
4	109	-113
5	18	-12
6	18	21
7	16	17
8	78	-80
9	19	-23
10	18	14
11	20	-21
H= 13 K= 3		
0	100	-102
1	50	46
2	65	66
3	67	69
4	80	-79
5	63	65
6	44	44
7	29	28
8	65	-64
9	24	21
10	29	27
H= 13 K= 5		
1	66	-66
2	116	115
3	80	-81
4	14	-14
5	62	-62
6	96	98
7	46	-44
9	48	-48
H= 13 K= 7		
0	23	-24
1	115	116
2	83	85
3	47	46
4	37	-34
5	56	54
6	76	76
7	95	95
8	17	-14
H= 13 K= 9		
0	23	-27
1	111	-112
2	55	57
3	47	-46
4	33	-31
5	71	-70
6	48	49
H= 13 K= 11		
0	56	-55
1	30	34
2	25	22
3	51	51
H= 14 K= 0		
0	111	-117
2	22	17
3	8	-4
4	57	-57
5	26	29
H= 14 K= 2		
0	86	90
1	14	4
2	122	-124
3	81	85
4	16	15
5	29	28
6	79	-77
7	13	-13
8	39	36
9	32	33
10	80	-81
H= 14 K= 4		
0	28	29
1	111	115
2	70	69
3	126	127
5	99	98
6	58	57
7	78	75
8	25	27
9	76	76
10	34	31
H= 14 K= 6		
0	35	37
1	36	-35
2	69	-71
3	28	-27
4	62	65
5	28	-26
6	76	-76
7	33	-31
8	29	31
9	24	-21
H= 14 K= 8		
0	25	28
2	68	66
3	36	-35
4	20	24
6	56	54
H= 14 K= 10		
1	48	-49
2	65	-65
3	71	-72
4	44	45
H= 15 K= 1		
0	13	15
1	93	91
2	24	25
3	71	72
4	66	65
5	73	73
6	12	-13
7	68	66
8	24	25
9	47	44
10	32	34
H= 15 K= 3		
0	21	-25
1	90	63
2	30	-27
3	51	-52
4	28	21
5	12	9
6	58	-52
7	55	57
8	14	-16
9	16	2
H= 15 K= 5		
0	87	87
1	11	9
2	24	-22
3	9	-5
4	33	-34
5	13	3
6	38	36
8	22	22
H= 15 K= 7		
0	55	-57
1	30	-19
2	23	-26
2	66	-67
3	81	82
4	46	-48
5	48	45
6	39	-40
7	11	-9
H= 16 K= 0		
0	231	235
2	42	43
4	70	67
6	86	92
8	124	127
H= 16 K= 2		
0	59	-64
1	32	-31
2	24	25
3	79	-78
4	93	-96
5	48	-51
6	41	39
7	10	-12
8	45	-44
9	33	-33
H= 16 K= 4		
1	24	-24
2	17	-18
3	21	21
4	77	76
5	8	3
6	50	-50
7	26	-24
8	18	17
H= 16 K= 6		
0	124	-127
2	28	28
3	31	-34
4	34	-37
5	18	-19
6	23	-23
H= 16 K= 8		
0	12	-10
1	10	-8
2	60	-56
3	20	22
5	13	11
6	55	-53
H= 16 K= 10		
0	12	12
1	42	43
2	33	34
H= 17 K= 1		
0	73	-75
1	8	9
2	31	32
3	65	61
4	7	-9
5	34	35
6	40	-35
9	30	29
H= 17 K= 3		
0	17	14
1	132	-134
2	44	41
3	79	-80
4	35	-32
5	90	-91
6	53	51
7	109	-109
8	15	4
H= 17 K= 5		
0	55	-57
1	30	-19
2	9	2
3	19	-15
4	29	-30
5	15	-15
H= 17 K= 7		
0	23	26
1	25	26
2	36	34
4	30	-29
6	56	54
H= 17 K= 9		
0	18	-16
1	57	57
2	20	22
H= 18 K= 0		
2	45	-46
4	31	-32
6	31	-31
8	19	-23
H= 18 K= 2		
0	81	86
1	41	-42
2	109	-109
3	32	-31
4	46	46
5	22	-25
6	95	-91
7	30	-30
8	53	52
H= 18 K= 4		
1	32	34
2	42	-43
3	16	-18
4	15	-20
5	8	4
6	30	-31
7	32	32
H= 18 K= 6		
0	181	180
1	28	-28
3	10	-14
4	147	148
5	14	-17
H= 18 K= 8		
0	54	-56
1	11	1
2	39	-41
4	12	9
H= 19 K= 1		
0	113	-115
1	8	4
2	24	20
3	36	-36
4	76	-77
5	18	-21
8	66	-65
H= 19 K= 3		
0	12	-6
1	68	65
2	102	102
3	88	88
5	59	60
7	43	42
H= 19 K= 5		
0	72	-69
1	13	-12
2	16	-20
4	106	-106
6	25	21
H= 19 K= 7		
0	29	25
2	96	93
3	8	-2
4	9	10
H= 20 K= 0		
0	106	109
2	11	-11
4	101	101
H= 20 K= 2		
1	46	50
4	33	-37
5	27	27
6	16	17
7	44	45
H= 20 K= 4		
0	28	28
1	77	78
2	52	-55
3	23	25
4	62	63
5	51	49
6	60	-60
H= 20 K= 6		
0	43	-43
1	14	-14
4	11	11
H= 21 K= 1		
0	41	40
1	84	-85
2	10	3
3	16	-16
5	43	-41
6	24	22
H= 21 K= 3		
0	29	27
1	15	15
2	39	37
3	70	69
4	48	48
5	37	36
H= 21 K= 5		
0	47	-47
1	36	-34
2	57	-55
3	29	-28
4	44	-43
H= 22 K= 0		
0	17	13
2	117	117
4	59	58
H= 22 K= 2		
0	65	-67
1	9	-4
2	87	-86
3	36	-37
4	25	-25
H= 22 K= 4		
0	43	42
1	69	-70
2	80	79
3	54	-54
H= 23 K= 1		
1	33	-34
2	10	12
H= 24 K= 0		
0	76	73
H= 40 K=120		
0	16	0

TABLE C-3. Structural Amplitudes for the White Well Cordierite at 24°C (after heating).

L	FO	FC
H= 0 K= 0		
2	1458	1422
4	3003	2955
6	2330	2290
8	3843	3791
10	106	-131
12	1791	1759
H= 0 K= 2		
0	1199	-1219
2	2071	-2031
4	860	-869
6	1153	-1172
8	573	-598
10	744	-773
12	271	-264
H= 0 K= 4		
0	1363	1417
2	758	-794
4	2841	2797
6	1174	-1199
8	1198	1197
10	236	-186
12	866	878
H= 0 K= 6		
0	1527	-1509
2	1236	-1237
4	346	-369
6	1389	-1406
8	624	-636
10	458	-456
H= 0 K= 8		
0	234	206
2	1598	-1649
4	981	899
6	1562	-1581
8	285	286
10	708	-703
H= 0 K= 10		
0	975	956
2	194	-210
4	270	-259
6	308	303
8	439	426
H= 0 K= 12		
0	1642	1630
4	1141	1160
6	157	81
H= 1 K= 1		
1	88	97
2	1703	1663
3	131	38
4	306	235
6	419	388
8	427	-445
9	81	61
10	735	742
12	253	-255
H= 1 K= 3		
0	73	-190
1	1916	-1869
2	868	914
3	540	451
4	680	-697
5	506	-514
6	894	914
7	1319	-1344
9	416	-426
10	414	430
12	116	-155
H= 1 K= 5		
0	906	-955
1	373	334
2	127	34
3	618	627
4	1146	-1159
5	367	370
6	240	257
7	100	129
9	240	230
11	219	211
12	380	-361
H= 1 K= 7		
0	332	-343
2	122	132
3	1328	-1355
4	1041	-1069
5	661	-695
6	475	484
7	159	142
8	408	-421
9	473	-433
10	122	-76
11	609	-619
H= 1 K= 9		
0	224	-271
1	822	804
2	583	565
3	787	813
4	331	-321
5	755	761
6	449	470
7	614	600
8	171	-148
9	476	493
H= 1 K= 11		
0	869	-877
1	90	-99
2	235	217
3	111	-81
4	291	-291
6	74	-95
7	71	-67
H= 1 K= 13		
0	205	215
1	121	13
2	839	824
3	246	228
4	325	295
H= 2 K= 0		
2	997	971
4	225	174
6	411	392
8	731	-746
10	470	473
12	96	-32
H= 2 K= 2		
0	146	79
1	106	-37
2	2305	-2256
3	75	-56
4	621	-617
6	1184	-1193
7	83	-19
8	55	-23
10	994	-997
H= 2 K= 4		
0	408	347
1	421	347
2	1182	1174
3	1286	-1286
4	334	-380
5	520	-530
6	886	883
7	126	107
8	112	92
9	536	-526
10	394	379
11	565	-567
12	125	-149
H= 2 K= 6		
0	1154	1122
1	156	115
2	208	162
3	601	606
4	1303	1324
5	381	356
7	77	75
8	930	922
9	293	268
10	129	130
11	293	289
H= 2 K= 8		
0	432	-465
1	383	-413
2	511	531
3	81	-110
4	284	-279
5	229	-257
6	282	317
7	295	-316
8	246	-257
9	125	-94
10	258	280
H= 2 K= 10		
0	256	252
1	457	465
2	265	-272
3	488	492
4	795	769
5	396	379
6	377	-369
7	357	347
8	208	203
H= 2 K= 12		
0	436	-433
1	275	-274
2	99	-101
4	647	-665
6	89	71
H= 3 K= 1		
0	1265	-1264
1	170	146
2	1807	-1783
4	879	-869
5	131	-54
6	1193	-1193
7	56	85
8	471	-475
9	136	124
10	624	-619
12	379	-400
13	61	2
H= 3 K= 3		
2	500	481
4	1423	1402
5	179	-131
7	106	103
8	272	294
9	188	197
10	371	371
11	96	-83
12	356	337
H= 3 K= 5		
0	1236	1191
1	844	826
2	496	-518
3	1222	1220
4	387	-394
5	774	807
6	117	130
7	472	479
8	329	328
9	584	590
10	405	-402
11	495	490
12	60	7
H= 3 K= 7		
0	1307	1344
1	1225	-1228
2	893	888
3	734	-755
4	1262	1278
5	696	-706
6	725	715
7	898	-898
8	792	795
9	611	-624
10	544	551
11	299	-277
H= 3 K= 9		
0	96	84
1	632	665
2	124	-141
3	324	315
4	237	232
5	469	479
6	165	-165
7	499	521
9	201	203
H= 3 K= 11		
0	90	-56
1	404	-393
2	431	-458
3	783	-775
4	268	-293
5	546	-538
6	278	-309
7	194	-211
H= 3 K= 13		
0	557	-551
1	118	144
2	422	-408
3	82	76
H= 4 K= 0		
0	459	416
2	1915	-1871
4	655	-631
6	928	-937
8	97	178
10	870	-883
H= 4 K= 2		
0	380	351
1	1746	1703
2	1250	1287
3	552	-475
4	480	-495
5	544	563
6	1146	1164
7	1188	1221
9	302	279
10	518	510
11	152	132
H= 4 K= 4		
0	428	-409
1	269	-257
2	818	-836
3	216	-186
4	672	657
6	1035	-1045
8	97	-99
9	123	-155
10	424	-410
11	63	70
12	131	122
H= 4 K= 6		
0	748	-781
1	690	710
2	1024	1033
3	136	171
4	227	183
5	348	319
6	540	564
7	546	564
8	235	-262
9	285	272
10	682	681
11	104	81
H= 4 K= 8		
0	515	543
1	537	-508
2	748	-736
3	82	81
4	131	-54
5	284	-269
6	486	-471
7	467	-470
8	233	240
10	588	-581
H= 4 K= 10		
0	3	-2
1	750	-773
2	571	569
3	168	-153
4	286	-287
5	413	-420
7	703	-704
H= 4 K= 12		
0	168	112
1	356	341
2	535	-523
4	87	52
5	106	136
H= 5 K= 1		
0	164	168
1	1900	-1880
2	1272	1286
3	632	532
5	496	-518
6	1059	1070
7	1341	-1391
9	404	-404
10	570	584
11	76	-102
H= 5 K= 3		
0	340	291
1	577	-481
2	949	942
3	1331	1308
4	518	-533
5	447	460
6	874	861
7	190	-175
8	80	-40
9	555	558
10	323	325
11	557	573
12	143	-167
H= 5 K= 5		
0	2090	-2085
1	264	-265
2	212	-177
3	157	-146
4	776	-793
5	255	-243
6	481	-492
7	251	-224
8	1018	-1010
11	95	-140
H= 5 K= 7		
0	896	-929
1	159	153
3	351	-319
4	754	-819
5	68	-42
6	76	-21
7	180	134
8	573	-569
9	115	-99
H= 5 K= 9		
0	485	-491
1	592	608
2	123	127
3	395	-384
4	593	-594
5	93	92
6	190	149
7	557	586
8	370	-365
H= 5 K= 11		
0	61	-41
1	182	-190
2	612	593
3	87	51
4	91	76
5	151	-21
6	524	499
7	186	-190
H= 5 K= 13		
0	225	200
1	250	-197
2	474	459
3	211	188
H= 6 K= 0		
0	581	603
2	678	637
4	1409	1387
8	529	539
10	370	379
12	311	324
H= 6 K= 2		
0	1029	1079
1	290	267
2	1032	-1081
3	118	-172
4	2594	2561
5	94	84
6	1400	-1434
7	128	117
8	952	948
9	143	-128
10	367	-362
11	92	-44
12	746	742
H= 6 K= 4		
0	1131	1105
1	958	-946
2	563	-578
3	1613	-1602
4	352	-351
5	995	-1015
6	102	86
7	532	-537
8	367	376
9	746	-742
10	400	-417
11	617	-615
12	107	78
H= 6 K= 6		
0	1500	1492
1	179	206
2	2386	-2411
3	285	262
4	284	-296
5	176	180
6	1229	-1243
7	114	105
8	609	604
9	82	106
10	1526	-1510
11	68	84
H= 6 K= 8		
0	182	-195
1	373	378
2	95	-145
3	620	630
4	489	455
5	417	406
6	291	-302
7	264	250
8	69	-66
9	378	385
10	110	71
H= 6 K= 10		
0	607	659
1	246	-252
2	945	-962
4	606	787
5	145	-166
6	918	-893
7	209	-221
8	459	485
H= 6 K= 12		
0	308	298
1	685	662
2	335	320
3	750	741
4	627	600
5	660	652
H= 7 K= 1		
0	74	-171
1	569	491
2	777	759
3	1045	-1049
4	886	-916
5	519	-544
6	878	877
7	177	180
8	434	-442
9	349	-340
10	227	209
11	559	-572
12	231	-232
H= 7 K= 3		
0	1315	-1331
1	136	-166
2	118	-6
3	215	-248
4	1385	-1405
5	245	-249
6	63	99
8	805	-817
11	179	-163
12	545	-547
H= 7 K= 5		
0	324	-321
1	327	-326
2	1624	1633
3	114	138
4	480	488
5	161	-89
6	909	913
7	323	-332
9	159	-107
10	977	981
H= 7 K= 7		
0	1063	-1104
1	120	-117
2	375	346
3	150	-178
4	549	-564
5	90	-44
7	79	-66
8	566	-560
9	122	-96
10	271	283
H= 7 K= 9		
0	218	-225
1	295	280
2	693	702
3	694	688
4	150	-159
5	493	501
6	581	577
7	91	141
8	87	-143
9	315	292
H= 7 K= 11		
0	342	-342
1	187	191
2	179	181
3	278	-297
4	525	-510
5	94	-76
6	272	284
H= 7 K= 13		
0	127	-177
1	240	185
H= 8 K= 0		
0	443	-460
2	1169	-1190
4	521	562
6	1378	-1390
8	115	122
10	531	-526
H= 8 K= 2		
0	915	-951
1	612	606
2	198	-160
3	803	829
4	1192	-1191
5	593	601
6	95	-112
7	316	337
8	569	-561
9	364	353
10	171	-176
11	337	330
12	517	-513
H= 8 K= 4		
0	1054	1057
1	215	182
2	176	-156
3	431	-435
4	1331	1351
5	172	-174
6	131	-127
7	170	144
8	746	724
9	127	-122
11	202	-215
H= 8 K= 6		
0	271	-243
1	260	258
2	563	570
3	618	618
5	421	401
6	473	470
7	127	131
8	280	-288
9	299	284
10	263	254
11	298	302
H= 8 K= 8		
0	1884	1909
1	392	-392
2	167	134
3	346	-350
4	782	771
5	317	-319
6	498	498
7	273	-288
8	1178	1172
9	208	-229
H= 8 K= 10		
0	720	-755
1	110	-120
2	154	-135
3	254	-260
4	623	-610
5	175	-173
6	242	-225
H= 8 K= 12		
0	135	46
1	76	-105
2	410	-422
4	335	325
H= 9 K= 1		
0	1185	1151
1	527	530
2	505	-515
3	1161	1176
4	309	-315
5	806	849
6	218	239
7	359	335
8	323	304
9	499	496
10	344	-349
11	586	591
12	165	113
H= 9 K= 3		
0	1069	-1058
1	144	-154
2	890	-905
3	175	181
4	70	-88
5	59	116
6	968	-932
7	151	-127
8	511	-515
10	263	-250
11	78	137
H= 9 K= 5		
0	1113	1165
1	1247	1252
2	750	758
3	913	895
4	991	992
5	897	913
6	449	461
7	914	919
8	747	758
9	637	636
10	412	421
11	466	400
H= 9 K= 7		
0	402	-414
1	744	-772
2	51	-146
3	930	-937
4	342	371
5	777	-792
6	457	-474
7	511	-513
8	69	-135
9	516	-512
10	89	112
H= 9 K= 9		
0	111	101
1	194	222
2	127	-162
3	54	58

TABLE C-3, continued.

L	FO	FC
4	167	147
6	110	-102
7	201	190
8	70	27
H=	9	K= 11
0	630	623
1	801	-789
3	401	-419
5	523	-515
6	295	281
H=	10	K= 0
0	2808	-2713
2	144	153
4	538	-535
6	527	-534
8	1109	-1132
10	361	360
H=	10	K= 2
0	1431	1437
1	136	-107
2	838	841
4	1761	1772
6	415	430
7	56	1
8	1068	1069
9	131	135
10	467	482
H=	10	K= 4
0	771	-818
1	317	-326
2	254	-262
3	836	853
4	1619	-1637
5	243	242
6	152	132
7	373	-369
8	675	-672
9	210	-233
10	354	-348
11	346	342
H=	10	K= 6
0	811	819
1	312	310
2	662	-656
3	169	-188
4	151	-153
6	176	-194
7	311	321
8	320	329
10	618	-600
H=	10	K= 8
0	628	-658
1	165	-180
2	232	216
3	464	-456
4	545	-589
5	234	-251
6	176	194
7	118	-96
8	448	-458
9	294	-279
H=	10	K= 10
1	247	241
2	164	-196
3	236	242
4	595	545
5	238	261
6	423	-419
7	178	175
H=	10	K= 12
0	287	-316
1	258	-247
2	415	433
3	474	-481
H=	11	K= 1
0	154	75
1	138	-54
2	966	973
3	443	-440
4	192	182
5	180	-164
6	775	778
9	176	-152
10	546	540
11	73	-131
H=	11	K= 3
0	101	-128
1	79	-98
2	162	178
3	1484	-1516
4	793	-804
5	672	-685
6	365	349
7	109	110
8	196	-210
9	577	-581
11	640	-635
H=	11	K= 5
0	964	-1002
1	125	-103
2	259	224
3	382	-396
4	241	-245
5	203	-203
6	528	-527
7	196	-202
10	262	250
H=	11	K= 7
0	589	-614
1	289	-288
3	617	604
4	593	-601
5	161	174
6	167	-210
7	376	-361
8	382	-395
9	142	174
H=	11	K= 9
0	608	-625
1	273	265
2	123	-102
3	564	532
4	602	-610
5	316	304
6	124	-87
7	122	137
H=	11	K= 11
0	263	268
1	281	268
2	815	774
3	250	290
4	453	456
5	217	220
H=	12	K= 0
0	953	955
2	2788	-2776
4	639	-679
6	1670	-1665
8	345	347
10	1709	-1696
0	1179	1193
1	1065	-1085
2	868	883
3	354	-342
4	1315	1321
5	636	-655
6	553	550
7	852	-849
8	732	742
9	536	-551
10	488	485
11	270	-259
H=	12	K= 4
0	261	268
1	96	-65
2	1688	-1710
4	772	779
5	123	-89
6	1502	-1509
7	72	-92
8	265	263
9	81	78
10	806	-789
H=	12	K= 6
0	322	311
1	575	-578
2	106	-21
3	328	-314
4	576	553
5	576	-560
7	476	-473
8	249	235
9	286	-288
H=	12	K= 8
0	825	837
1	579	568
2	708	-772
3	269	272
4	555	561
5	449	436
6	717	-711
7	493	499
8	601	591
H=	12	K= 10
0	525	502
1	464	475
2	202	-172
4	185	-185
5	239	244
6	129	99
H=	13	K= 1
0	1025	-1071
1	188	182
2	338	322
3	360	-357
4	365	-374
5	65	-72
6	162	168
7	141	153
8	665	-653
9	150	-151
10	192	152
11	177	-159
H=	13	K= 3
0	782	-782
1	386	396
2	499	515
3	571	589
4	621	-637
5	526	557
6	378	364
7	255	248
8	519	-522
9	179	207
10	256	255
H=	13	K= 5
0	71	-148
1	498	-515
2	899	901
3	558	-620
4	171	-152
5	451	-471
6	785	-765
7	372	-367
8	82	-75
9	396	-407
H=	13	K= 7
0	155	-158
1	953	973
2	667	694
3	375	369
4	208	-274
5	475	473
6	647	655
7	828	846
8	134	-136
H=	13	K= 9
0	204	-223
1	943	-964
2	363	363
3	415	-383
4	269	-253
5	641	-619
6	448	439
H=	13	K= 11
0	474	-481
1	645	669
2	215	224
3	443	429
H=	14	K= 0
0	887	-934
2	212	175
4	499	-516
10	270	269
H=	14	K= 2
0	687	695
1	95	-21
2	973	-983
3	675	690
4	170	129
5	256	276
6	685	-616
7	121	-90
8	528	321
9	315	295
10	698	-675
H=	14	K= 4
0	208	208
1	871	877
2	546	544
3	975	988
4	84	-71
5	788	779
6	492	485
7	629	620
8	202	200
9	661	650
10	257	255
H=	14	K= 6
0	294	282
1	275	-296
2	568	-562
3	189	-192
4	544	540
5	203	-201
6	638	-640
7	621	-648
8	303	287
9	214	-169
H=	14	K= 8
0	454	266
1	17	-28
2	547	556
3	315	-311
4	172	141
6	453	461
H=	14	K= 10
0	105	-62
1	394	-395
2	543	-537
3	623	-630
4	429	414
H=	15	K= 1
0	142	126
1	736	737
2	184	194
3	570	570
4	520	524
5	569	581
6	95	-58
7	561	567
8	234	225
9	358	382
10	279	263
H=	15	K= 3
0	195	-206
1	480	482
2	266	-216
3	287	-299
4	432	189
6	284	-279
7	467	475
8	95	-118
9	89	17
H=	15	K= 5
0	736	729
2	147	-157
3	55	-83
4	293	-283
5	68	-11
6	262	289
8	253	242
H=	15	K= 7
0	161	-168
1	114	-69
2	526	-528
3	726	696
4	341	-339
5	397	388
6	311	-308
H=	15	K= 9
0	117	113
1	660	-659
2	114	92
3	549	-556
4	274	256
5	562	-565
H=	16	K= 0
0	1868	1901
2	303	319
4	518	521
6	751	774
8	1065	1067
H=	16	K= 2
0	504	-521
1	271	-261
2	175	188
3	670	-681
4	801	-812
5	451	-436
6	528	526
7	404	-406
9	328	-314
H=	16	K= 4
0	66	-27
1	214	-242
2	172	-136
3	115	151
4	662	666
5	86	5
6	430	-416
7	222	-247
8	159	153
9	84	-29
H=	16	K= 6
0	1031	-1047
2	279	291
3	287	-283
4	216	-264
5	196	-176
6	144	-139
7	79	2
H=	16	K= 8
0	103	-105
1	76	58
2	491	-514
3	186	196
5	106	89
6	476	-485
H=	16	K= 10
0	86	84
1	384	340
2	306	314
H=	17	K= 1
0	603	-614
1	113	-75
2	271	257
3	496	504
4	61	-77
5	248	272
8	307	-303
9	247	229
H=	17	K= 3
0	106	115
1	1103	-1124
2	355	351
3	593	-616
4	286	-281
5	735	-754
6	407	415
7	935	-940
8	98	34
H=	17	K= 5
0	468	-476
1	145	-144
2	54	42
3	116	-124
4	229	-244
5	125	-129
6	63	31
7	116	-98
8	395	-375
H=	17	K= 7
0	238	244
1	215	226
2	315	287
3	85	-57
4	248	-246
6	499	482
H=	17	K= 9
0	152	-131
1	496	490
3	176	151
H=	18	K= 0
2	492	-454
4	232	-230
6	258	-250
8	102	-130
H=	18	K= 2
0	681	681
1	336	-334
2	900	-903
3	650	-653
4	835	836
5	160	-147
6	864	-784
7	265	-261
8	474	459
H=	18	K= 4
0	322	319
2	341	-354
3	154	-125
4	163	-169
6	262	-244
7	323	316
H=	18	K= 6
0	1524	1532
1	229	-204
4	1216	1216
5	99	-119
H=	18	K= 8
0	489	-525
2	352	-338
3	115	75
4	124	71
H=	19	K= 1
0	892	-919
2	184	215
3	353	-329
4	592	-609
5	179	-202
6	80	37
8	570	-569
H=	19	K= 3
0	102	-64
1	602	611
2	857	852
3	768	761
5	538	537
6	699	694
7	408	427
H=	19	K= 5
0	602	-608
1	110	-93
2	93	-22
3	187	202
4	913	-909
5	59	51
6	171	149
H=	19	K= 7
0	166	171
1	67	117
2	761	769
H=	20	K= 0
0	906	899
2	105	-113
4	839	825
6	115	-102
H=	20	K= 2
1	422	423
4	335	-341
5	227	239
6	261	116
7	409	400
H=	20	K= 4
0	242	231
1	646	645
2	460	-470
3	167	188
4	560	552
5	414	416
6	522	-519
H=	20	K= 6
0	438	-446
1	123	-124
2	92	92
4	87	96
H=	21	K= 1
0	350	333
1	733	-731
2	57	-10
3	126	-112
5	350	-346
6	177	165
H=	21	K= 3
0	216	217
1	128	124
2	307	317
3	612	605
4	467	466
5	315	311
H=	21	K= 5
0	387	-385
1	333	-333
2	475	-464
3	281	-286
4	356	-357
H=	22	K= 0
2	979	974
4	473	456
H=	22	K= 2
0	565	-564
1	112	-75
2	755	-739
3	286	-316
4	195	-196
5	181	-149
H=	22	K= 4
0	368	372
1	658	-654
2	704	687
3	484	-483
H=	23	K= 1
0	357	-354
2	145	-124
3	79	-15
H=	23	K= 3
0	83	76
1	266	-263
H=	24	K= 0
0	745	733

TABLE C-4. Structural Amplitudes for the Dolni Bory Cordierite at 24°C (*Ccem*).

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
			8	1007	-994	1	566	550	6	914	-873	6	1128	1146	4	901	926	9	323	380						
H=	0	K= 0	9	288	227	3	590	661	10	432	-409	9	688	661	5	500	482	10	664	673	0	1850	1872			
			12	491	-531	4	701	670				10	488	525	7	317	351	11	535	511	1	574	574			
4	3965	3793	16	534	-531	5	529	508	H=	3	K= 15	11	636	642	8	294	210	14	395	404	2	1195	1150			
6	1921	1835				7	344	408				14	524	519	9	409	469				3	1242	1225			
8	4492	4378	H=	1	K= 7	9	441	502	2	360	-409				11	326	353	H=	7	K= 11	5	853	863			
12	2298	2297				11	336	348	3	390	466	H=	5	K= 5	12	360	428				7	385	352			
14	583	736	0	588	-648	12	400	334	8	429	331							0	556	-621	9	520	546			
18	457	-264	2	311	354				10	362	-405	0	2243	-2408	H=	6	K= 10	2	289	326	11	611	638			
			3	1314	-1295	H=	2	K= 12				1	254	-255				3	416	-396	12	434	381			
H=	0	K= 2	4	1388	-1385				H=	3	K= 17	4	966	-994	0	1083	1078	4	760	-797	15	403	154			
			5	644	-623	0	531	-531				6	377	-365	1	320	-333	5	296	-119	17	450	340			
6	1966	-1721	6	702	692	1	387	-369	0	357	256	8	1259	-1247	2	1268	-1311	6	366	426						
8	241	-172	9	471	-421	4	878	-913				12	639	-728	4	1156	1192	8	700	-595	H=	9	K= 3			
10	1125	-1081	11	630	-614	7	363	-355	H=	4	K= 0				6	1182	-1223	12	380	-384						
14	750	-737	12	489	-480	8	539	-517				H=	5	K= 7	8	861	839				0	527	-545			
18	357	-388	14	366	361				4	987	-1001				10	777	-804	H=	7	K= 13	2	1467	-1452			
			16	497	-479	H=	2	K= 14	6	760	-655	0	950	-998	12	546	624				3	278	228			
H=	0	K= 4										2	306	304	14	645	-673	0	364	-253	4	465	449			
			H=	1	K= 9	2	557	-538	H=	4	K= 2	3	502	-487				6	602	569	6	1404	-1420			
2	1597	-1488				4	325	-409				4	968	-1000	H=	6	K= 12	8	421	-298	10	532	-546			
4	3746	3431	0	513	-493	10	421	-502	1	1786	1742	7	323	204							11	288	185			
6	1850	-1749	2	862	900				2	1651	1719	8	722	-678	0	638	620	H=	7	K= 15	14	603	-698			
8	1775	1666	3	821	841	H=	2	K= 16	4	859	-863	9	279	-154	1	655	715									
10	626	-596	4	353	-402				5	605	613	10	387	140	3	813	785	0	499	-561	H=	9	K= 5			
12	1234	1231	5	789	774	2	472	507	6	1500	1505	12	636	-551	4	916	967	4	479	-494						
14	756	-820	6	723	702	6	448	382	9	292	286	16	371	-337	5	649	704	7	427	-337	0	1648	1676			
16	777	871	7	608	603	9	360	-216	10	724	735				7	535	547				1	1225	1216			
			9	572	522	10	465	383	12	336	-189	H=	5	K= 9	8	615	602	H=	7	K= 17	2	334	376			
H=	0	K= 6	10	584	567				13	621	655				9	477	525				3	913	879			
			11	431	553	H=	2	K= 18	14	693	678	0	691	-665	11	383	528	2	623	617	4	1629	1595			
0	929	-914	13	378	395							1	604	632	12	485	426	6	471	449	5	913	897			
2	1803	-1721	14	360	392	6	373	-120	H=	4	K= 4	2	263	343	13	416	367	7	362	-175	7	949	915			
4	364	262										3	332	-371							8	1171	1154			
6	1969	-1863	H=	1	K= 11	H=	3	K= 1	0	736	-784	4	731	-737	H=	6	K= 14	H=	8	K= 0	9	651	646			
8	316	-266							1	203	-232	6	358	315							11	570	482			
10	761	-742	0	1107	-1132	1	217	150	3	201	-176	8	481	-517	0	1257	1249	0	543	-563	12	639	605			
14	758	-863	4	506	-550	3	147	73	4	534	473	12	384	-418	1	548	-579	2	897	-838	13	411	492			
			8	693	-700	6	1892	-1765	6	849	-807				2	606	-592	4	411	371	16	525	587			
H=	0	K= 8	10	327	359	10	1022	-996	14	470	-515	H=	5	K= 11	3	778	-802	6	1282	-1226						
			11	353	25	14	495	-648							4	913	945	10	494	-425	H=	9	K= 7			
0	781	774	12	428	-518	18	403	-459	H=	4	K= 6	1	302	-330	6	425	-438	14	531	-510						
2	2196	-2199										2	775	809	7	377	-421				1	714	-740			
4	1286	1214	H=	1	K= 13	H=	3	K= 3	0	987	-1007	6	741	732	8	951	953	H=	8	K= 2	2	516	-461			
9	664	660							1	658	661	7	312	-360	9	540	-574				3	984	-984			
10	1124	-1153	2	1081	1133	2	238	-184	2	1385	1413	10	468	549	10	468	-512	0	1041	-1103	4	883	870			
12	483	518	3	290	212	4	2166	2055	5	337	307				11	424	-506	1	733	739	5	797	-814			
14	1065	-1047	6	841	906	5	197	-131	6	855	865	H=	5	K= 13	12	657	649	3	742	725	6	807	-802			
			7	352	-220	6	502	-460	7	566	550							4	1363	-1362	7	449	-494			
H=	0	K= 10	10	758	802	7	236	123	8	416	-425	2	538	593	H=	6	K= 16	5	601	600	9	556	-540			
						8	819	786	10	875	941	3	372	249				7	392	430	11	593	-580			
2	495	-527	H=	1	K= 15	12	662	661				4	301	-210	0	516	491	8	791	-728						
8	859	869				14	323	-257	H=	4	K= 8	6	659	647	2	526	-454	9	372	353	H=	9	K= 9			
10	711	-687	0	726	-726							7	334	-199	10	464	-484	11	291	307						
12	433	407	4	505	-498	H=	3	K= 5	0	415	429							12	710	-670	0	676	672			
			8	523	-590				1	674	-678	H=	5	K= 15	H=	6	K= 18	13	309	232	2	464	-517			
H=	0	K= 12				0	1964	1984	2	468	-431										4	406	386			
			H=	1	K= 17	1	826	810	4	295	-243	2	473	579	0	444	292	H=	8	K= 4	6	328	-284			
0	1849	1862				2	1168	-1122	6	332	-344	10	455	494	2	697	-667				8	340	401			
4	1567	1585	6	514	534	3	1275	1230	10	441	-482				4	664	574	0	884	842	10	335	-335			
8	1308	1290				4	196	121	13	498	-421	H=	5	K= 17	6	712	-683	3	628	-632	12	436	327			
12	1033	1051	H=	2	K= 0	5	857	811										4	1252	1246						
						6	304	-244	H=	4	K= 10	0	565	-538	H=	7	K= 1	5	343	-300	H=	9	K= 11			
H=	0	K= 14	0	2013	-2059	7	486	466				4	517	-506				8	638	654						
			2	1593	1539	8	748	738	3	290	-242	8	397	-428	1	512	431	9	298	-236	0	901	939			
0	460	261	6	681	721	9	578	598	4	440	-484				2	1260	1337	12	652	700	1	783	-781			
2	398	-318	8	914	-948	10	829	-795	5	396	-464	H=	6	K= 0	3	1121	-1084	15	361	-13	2	351	-347			
4	610	583	10	726	713	11	516	512	6	736	800				4	1053	-1099				3	313	-329			
6	503	383	12	280	-209	12	340	297	7	696	-656	0	1551	1500	5	631	-580	H=	8	K= 6	5	460	-476			
			18	389	397				10	383	416	2	195	-45	6	1247	1245				7	707	-717			
H=	0	K= 16				H=	3	K= 7	13	437	-426	6	466	-439	8	655	-682	0	327	-316	8	534	538			
			H=	2	K= 2	14	583	494	8	1051	1018	9	451	-439	1	346	277	9	426	-374						
0	982	935							12	628	651	10	420	505	2	753	791	13	374	-410						
2	422	-416	1	134	-24	0	1866	1879	14	328	-166	11	704	-674	3	794	792									
4	958	968	4	885	-882	1	1236	-1247	H=	4	K= 12	16	581	542	12	465	-392	6	703	691	H=	9	K= 13			
6	463	-477	5	208	221	2	481	-517							14	527	447	8	331	-384						
8	858	828	10	957	-909	3	774	-769	0	287	-65							9	423	374	2	674	-762			
						4	1924	1901	1	374	409	H=	6	K= 2	H=	7	K= 3	10	390	392	6	694	-700			
H=	0	K= 18	H=	2	K= 4	5	723	-728	2	356	-357							11	490	401	10	431	-473			
						6	415	374	6	339	-264	0	1873	1976												
2	681	-665	2	1524	1580	7	920	-929	7	457	419	1	269	218	0	1490	-1595									
6	761	-741	3	1422	-1347	8	1240	1212	12	379	-29	2	1672	-1653	1	227	-272	H=	8	K= 8	H=	9	K= 15			
			5	639	-579	9	612	-653				3	241	-153	3	215	-204									
H=	1	K= 1	6	1143	1149	10	451	385	H=	4	K= 14	6	1961	-1924	4	1666	-1692	0	1733	1751	0	342	363			
			9	647	-633	12	913	916				8	1485	1479	5	279	-281	1	364	-421	2	397	-277			
0	1985	-1963	10	563	595	16	605	588	0	522	-539	10	698	-692	8	1031	-1040	2	255	269						
2	2322	2252	11	664	-664	H=	3	K= 9	2	449	478	12	1053	1125	12	692	-754	3	330	-369	H=	10	K= 0			
4	164	-59	14	613	526				10	410	450	14	874	-940	16	458	-500	4	708	661						
6	747	761	17	378	-423	0	461	521	H=	4	K= 16	16	746	809				5	385	-337	0	2797	-3096			
8	668	-626				1	673	651							H=	7	K= 5	6	597	622	2	518	573			
10	999	1002	H=	2	K= 6	2	564	-582	1	336	430	H=	6	K= 4				8	1146	1124	4	852	-855			
12	456	-431				3	287	275	7	440	442	0	1853	1895	0	526	-606	12	535	576	6	271	-238			
14	301	317	0	1003	950	4	571	546				1	950	-959	1	336	-332	14	537	461	8	1406	-1399			
18	480	332	1	259	244	5	461	456	H=	4	K= 18	3	1594	-1561	2	1885	1969	16	393	372	12	705	-695			
			3	812	809	6	490	-523				5	1016	-989	6	1362	1226				14	366	-159			
H=	1	K= 3	4	1235	1138	7	526	519	3	386	94	10	1211	1225	10	605	609	H=	8	K= 10						
			5	494	493	8	322	324	4	534	-467	14	605	609							H=	10	K= 2			
1	2063	-1920	8	917	860	12	312	257							0	973	-925									
4	1023	-1040	9	442	401	13	374	321	H=	5	K= 1	8	772	785	7	676	-731	H=	7	K= 7	0	1067	1039			
5	573	-559	11	415	403	14	380	-305				10	802	-796	8	621	-592	2	1104	1136						
6	1220	1227	12	495	491				1	1881	-1906	11	522	-627	0	1466	-1446	12	471	-558	3	259	231			
7	1468	-1429				H=	3	K= 11	4	310	-375	12	342	346	2	553	546				4	1413	1392			
8	420	-385	H=	2	K= 8				5	556	-564	17	363	-360	4	927	-941	H=	8	K= 12	6	642	654			
9	404	-435				0	290	225	6	1317	1330				8	820	-837				8	915	871			
10	612	623	0	707	-742	1	295	-329	7	1482	-1497	H=	6	K= 6	10	330	410	6	457	-473	9	296	237			
13	653	-686	1	432	-449	2	718	-758	9	418	-413	0	1913	1933	12	618	-630				10	611	641			
14	550	561	2	731	732	5	504	-512	10	748	760	2	2857	-2952	H=	8	K= 14	H=	8	K= 14	12	415	407			
			4	484	-464	6	646	-641	13	634	-683	3	280	251							14	380	272			
H=	1	K= 5	5	318	-337	9	443	-390	14	556	558	6	1753	-1742	H=	7	K= 9	8	490	-522	16	432	440			
			6	469	469	10	473	-497	15	378	-494	8	902	930	0	528	-487	10	394	159						
0	1125	-1190	8	471	-477	11	465	-471				10	1886	-1926	1	334	378				H=	10	K= 4			
1	488	465	10	357	418	14	369	-294	H=	5	K= 3	12	440	447	2	956	989	H=	8	K= 18						
3	564	547	12	338	-308							14	775	-735	3	775	757				0	1028	-1095			
4	1402	-1377				H=	3	K= 13	3	1371	1335				4	265	-327	0	532	500	1	315	-322			
5	351	356	H=	2	K= 10				4	573	-660	H=	6	K= 8	5	476	562	2	446	466	3	855	862			
6	557	566				2	757	-778	5	525	510				6	828	805				4	1875	-1938			
															8	363	-334	H=	9	K= 1	5	268	224			

TABLE C-4, continued.

L	FO	FC
6	484	449
7	380	-378
8	859	-911
9	284	271
12	714	-764
14	394	274
16	598	-556
H= 10	K=	6
0	618	635
1	509	468
2	323	-310
3	155	-191
4	313	-339
7	465	488
10	482	-481
H= 10	K=	8
0	869	-867
1	308	-364
2	576	573
3	582	-586
4	707	-697
5	356	-398
6	409	467
7	312	-250
8	604	-627
9	383	-401
11	321	-302
H= 10	K=	10
1	308	261
4	385	413
6	292	-292
H= 10	K=	12
0	400	-412
2	611	684
3	451	-455
5	450	-408
6	435	474
7	341	-244
9	365	-280
10	622	551
H= 10	K=	14
0	415	419
3	406	563
11	361	367
H= 10	K=	16
0	438	-422
4	559	-632
H= 11	K=	1
2	1182	1216
3	407	-425
4	224	97
6	970	956
10	709	732
14	441	406
H= 11	K=	3
0	721	-277
2	297	371
3	1413	-1451
4	988	-947
5	568	-623
6	487	522
8	323	-334
9	526	-580
11	566	-640
17	439	-409
H= 11	K=	5
0	1121	-1126
4	412	-448
12	355	-397
H= 11	K=	7
0	646	-659
1	289	-321
4	669	-707
7	394	-393
8	460	-483
11	361	324
12	358	-405
H= 11	K=	9
0	926	-922
3	506	496
4	499	-734
8	646	-667
9	391	342
11	451	210
H= 11	K=	11
0	369	373
1	299	276
2	1036	1044
4	489	466
6	865	890
10	720	742
14	437	449
H= 11	K=	13
1	527	-527
2	1192	1228
3	663	-698
5	509	-529
6	971	1002
7	371	-376
9	441	-460
10	789	835
11	379	-375
14	481	494
16	408	-137
H= 11	K=	17
0	577	-596
4	689	-680
5	364	-86
6	365	-177
H= 12	K=	0
2	3047	-3182
6	2063	-2061
8	736	757
10	1994	-2039
12	359	194
14	779	-818
H= 12	K=	2
0	1698	1757
1	1128	-1115
2	514	512
3	544	-541
4	1873	1890
5	777	-786
7	871	-867
8	1112	1128
9	429	-431
11	306	-392
12	804	822
13	543	-504
16	459	561
H= 12	K=	4
0	865	855
2	2130	-2182
4	1156	1172
6	1858	-1866
8	679	636
10	1123	-1177
12	597	612
14	936	-971
16	405	366
H= 12	K=	6
0	694	666
1	651	-649
2	521	-479
3	328	-309
4	669	671
5	460	-398
6	402	-403
7	501	-556
8	410	490
12	443	383
H= 12	K=	8
0	1228	1232
1	486	477
2	1148	-1164
3	442	381
4	1305	1282
5	538	537
6	1055	-1062
7	497	583
8	914	936
10	687	-694
13	469	394
14	598	-597
H= 12	K=	10
0	615	762
1	524	496
2	578	-566
4	406	480
8	527	496
10	578	-597
H= 12	K=	12
0	675	696
2	905	-907
4	889	869
6	921	-894
8	511	579
10	649	-573
12	587	519
H= 12	K=	14
0	504	410
4	734	698
H= 12	K=	16
0	457	471
1	373	-228
4	371	364
6	657	-689
H= 13	K=	5
1	527	-527
2	1192	1228
3	663	-698
5	509	-529
6	971	1002
7	371	-376
9	441	-460
10	789	835
11	379	-375
14	481	494
16	408	-137
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0	393	-443
1	914	906
2	972	946
3	375	409
4	552	-529
5	423	470
6	850	882
7	767	807
9	480	496
10	506	583
13	373	369
14	575	486
15	540	484
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0	432	-436
1	866	-835
2	643	677
4	596	-591
5	526	-506
6	700	667
7	695	-769
8	423	-363
10	397	392
12	349	-322
13	529	-482
14	407	418
H= 13	K=	11
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1	366	308
2	501	424
3	456	403
4	678	-645
5	395	343
6	386	371
8	515	-502
11	393	282
12	446	-431
13	407	173
H= 13	K=	13
0	860	-859
4	677	-621
7	368	-122
8	662	-646
10	376	183
H= 13	K=	15
2	533	480
6	447	359
14	352	40
H= 13	K=	17
0	402	-249
1	435	322
4	374	-341
H= 14	K=	0
0	1199	-1176
2	241	203
14	369	-167
H= 14	K=	2
0	664	669
2	814	-807
3	727	733
6	513	-496
9	343	297
10	583	-669
H= 14	K=	4
1	855	881
2	689	707
3	1028	1050
5	794	816
7	605	643
10	384	398
11	504	547
12	323	-77
13	353	355
14	432	390
15	395	397
H= 14	K=	6
0	285	269
1	302	-343
2	467	-458
3	407	-358
4	482	450
5	330	-298
6	493	-548
7	297	-277
11	381	-206
14	366	-272
H= 14	K=	8
2	729	736
3	387	-343
6	664	628
10	400	468
H= 14	K=	10
1	429	-488
2	550	-482
3	655	-623
4	406	365
5	464	-482
6	481	-604
7	449	-363
9	452	-418
14	437	-468
H= 14	K=	12
4	549	-432
6	363	219
H= 14	K=	14
0	358	371
9	368	189
10	381	-341
H= 14	K=	16
3	405	331
5	359	282
H= 15	K=	1
0	474	451
2	258	-236
3	598	615
4	936	919
5	646	628
6	508	-457
7	599	631
8	459	489
9	382	457
11	448	366
13	347	361
15	357	288
16	426	394
H= 15	K=	3
1	584	607
2	620	-631
4	436	488
6	619	-606
7	575	581
10	332	-308
H= 15	K=	5
0	1247	1245
2	445	-513
8	610	604
10	643	-616
11	319	29
H= 15	K=	7
2	853	-827
3	756	702
5	356	378
6	644	-632
9	330	278
10	582	-577
11	463	425
H= 15	K=	9
0	533	514
1	785	-777
3	654	-661
4	747	685
8	349	431
9	475	-469
11	354	-420
12	461	374
13	535	-407
H= 15	K=	11
2	549	-435
4	319	239
H= 15	K=	13
0	519	401
4	684	676
7	355	226
H= 15	K=	15
2	471	-487
H= 15	K=	17
3	425	454
H= 16	K=	0
2	599	596
4	304	327
6	1004	999
8	814	870
12	435	475
14	637	606
H= 16	K=	2
0	811	-802
2	534	529
4	1038	-1047
5	269	-326
6	598	604
8	649	-637
12	370	-461
14	397	331
16	473	-384
H= 16	K=	4
3	270	211
4	453	413
6	285	-204
15	375	-73
H= 16	K=	6
0	1345	-1315
2	535	507
3	273	-215
4	590	-569
8	852	-821
10	454	461
12	557	-582
H= 16	K=	8
0	342	-233
2	388	-257
H= 16	K=	10
1	331	371
2	645	546
3	435	374
4	586	-588
5	365	348
6	740	723
7	464	310
H= 16	K=	12
0	333	355
3	474	-495
5	368	-348
9	351	-282
H= 16	K=	14
0	410	-431
2	366	427
3	403	398
5	394	275
H= 16	K=	16
3	374	-331
H= 17	K=	1
0	602	-528
2	401	423
3	542	560
4	288	-148
5	359	336
10	322	342
H= 17	K=	3
1	1095	-1097
2	447	413
3	751	-724
5	811	-813
6	481	478
7	936	-936
9	595	-626
10	385	198
11	541	-458
13	491	-549
14	364	302
H= 17	K=	5
0	573	-609
4	355	-267
8	372	-489
10	390	178
H= 17	K=	7
1	302	291
2	329	301
4	306	-392
6	517	529
H= 17	K=	9
1	473	419
4	466	-405
7	399	403
H= 17	K=	11
0	366	-363
3	531	439
10	421	324
11	366	312
H= 17	K=	15
0	381	-287
1	464	-270
H= 18	K=	0
0	506	518
2	747	-765
6	486	-444
10	679	-650
H= 18	K=	2
0	1083	1056
1	438	-499
2	1213	-1257
3	315	-268
4	1178	1174
5	357	-284
6	1078	-1113
7	434	-431
8	756	768
9	310	-278
12	618	683
14	601	-666
15	391	-252
H= 18	K=	4
0	517	392
1	262	144
7	296	168
8	327	318
10	448	-468
H= 18	K=	6
0	1801	1795
2	388	-307
4	1620	1597
12	841	903
H= 18	K=	8
0	318	-246
2	655	-658
9	325	68
H= 18	K=	10
0	1188	1152
1	353	344
2	562	-570
3	412	462
6	472	-396
8	812	831
10	451	-467
11	387	273
12	826	710
H= 18	K=	12
2	535	-567
6	516	-455
7	392	-343
9	385	-115
10	421	-467
H= 18	K=	14
0	466	566
2	779	-765
4	354	294
6	548	-600
8	400	436
H= 18	K=	16
0	577	440
4	391	349
H= 19	K=	1
0	1316	-1293
2	504	482
3	328	-328
8	871	-873
10	391	416
11	351	-245
H= 19	K=	3
0	305	-279
1	458	459
2	1078	1082
3	679	663
4	381	-309
5	472	421
6	989	953
9	471	481
10	683	687
14	526	534
15	374	278
H= 19	K=	5
0	675	-689
2	274	263
4	1145	-1167
6	574	498
8	631	-629
12	496	-550
H= 19	K=	7
2	1102	1083
6	1062	1020
10	698	714
H= 19	K=	9
0	904	-862
1	391	-441
2	428	421
4	481	-525
5	362	-291
7	491	-390
8	642	-624
9	454	-330
10	442	400
12	425	-433
H= 19	K=	11
0	599	-585
2	373	458
4	390	-376
7	341	282
8	405	-416
10	385	401
H= 19	K=	13
0	409	-523
4	418	-495
8	363	-440
H= 19	K=	15
0	377	-213
2	448	312
3	424	407
4	403	-407
H= 20	K=	0
0	806	837
4	720	766
8	644	625
12	469	416
14	362	-70
H= 20	K=	2
1	435	432
4	410	-432
7	532	444
8	326	-62
H= 20	K=	4
1	766	794
2	417	-420
3	285	305
4	491	549
5	578	573
6	507	-519
7	767	725
10	410	-187
13	445	471
14	373	-369
H= 20	K=	6
0	351	-386
2	343	-53
10	421	284
H= 20	K=	8
0	442	351
2	620	-623
6	451	-383
10	598	-574
H= 20	K=	10
1	509	-534
2	325	299
3	422	-393
5	349	-456
11	361	-309
H= 20	K=	12
4	342	203
H= 21	K=	1
0	659	672
1	711	-664
2	378	-284
5	349	-334
7	625	-648

TABLE C-5. Structural Amplitudes for the Dolni Bory Cordierite at 24°C (*Ccc2*).

L	FO	FC	AC	BC
H= 0 K= 0				
4	3892	3801	3798	135
6	1927	1853	1836	-248
8	4455	4331	4320	318
12	2306	2268	2264	122
14	587	741	720	-174
18	460	393	-188	-344
H= 0 K= 2				
6	1872	1719	-1700	-261
8	243	314	-188	251
10	1132	1068	-1041	-241
14	755	739	-705	-221
18	360	381	-340	-173
H= 0 K= 4				
2	1601	1489	-1486	-89
4	3720	3418	3409	249
6	1857	1734	-1726	-163
8	1783	1673	1646	300
10	630	627	-593	-202
12	1241	1225	1191	288
14	761	791	-770	-182
16	782	847	819	217
H= 0 K= 6				
0	934	902	-900	58
2	1809	1719	-1713	-137
4	266	309	254	176
6	1976	1854	-1832	-284
8	319	300	-260	149
10	766	760	-719	-245
14	762	854	-792	-317
H= 0 K= 8				
0	786	793	791	56
2	2202	2190	-2190	-64
4	1294	1244	1230	185
8	668	669	643	184
10	1130	1152	-1142	-151
12	486	536	481	237
14	1072	1050	-1011	-283
H= 0 K= 10				
2	498	555	-539	-135
8	865	878	833	277
10	716	692	-651	-235
12	436	433	380	208
H= 0 K= 12				
0	1858	1874	1873	51
4	1575	1591	1589	74
8	1316	1286	1281	114
12	1039	1040	1035	98
H= 0 K= 14				
0	463	295	291	48
2	401	336	-332	-51
4	614	575	555	152
12	506	418	332	254
H= 0 K= 16				
0	988	959	958	44
2	425	449	-443	-73
4	964	972	958	165
6	466	481	-465	-124
8	864	851	839	144
H= 0 K= 18				
2	686	653	-651	-44
6	766	755	-724	-213
H= 1 K= 1				
0	1957	1957	-1957	-28
2	2305	2258	2256	86
4	165	115	-52	-103
6	752	772	754	166
8	672	627	-617	-113
10	1095	991	984	120
12	459	421	-415	-72
14	303	324	301	120
18	483	340	317	125
H= 1 K= 3				
1	2060	1919	-1915	115
4	1028	1028	-1017	-152
5	577	576	-560	134
6	1227	1230	1227	81
7	1475	1430	-1424	-132
8	423	395	-376	-122
9	407	439	-431	80
10	616	616	610	81
13	658	674	-674	23
14	553	547	537	101
H= 1 K= 5				
0	1130	1201	-1201	-28
1	491	486	452	178
3	568	556	538	-141
4	1408	1372	-1372	-27
5	354	378	359	119
6	560	567	556	116
8	1013	991	-986	-101
9	290	249	231	93
12	494	527	-520	-88
16	538	507	-503	-66
H= 1 K= 7				
0	592	647	-647	-28
2	313	359	359	22
3	1320	1299	-1281	-211
4	1395	1381	-1379	-76
5	648	646	-616	197
6	707	698	692	94
9	474	427	-408	124
11	634	631	-619	-124
12	486	473	-459	-114
14	368	369	353	107
16	410	459	-453	-72
H= 1 K= 9				
0	516	484	-483	-27
2	867	912	912	5
3	826	863	838	-206
4	356	413	-404	-86
5	794	800	773	205
6	727	701	697	77
7	612	591	584	-87
9	575	569	538	185
10	588	544	542	45
11	434	584	560	-167
13	381	449	400	204
14	363	368	366	43
H= 1 K= 11				
0	1114	1139	-1139	-26
4	509	562	-558	-61
8	697	682	-682	-13
10	324	381	355	139
11	356	243	27	-242
12	431	491	-490	-31
H= 1 K= 13				
2	1088	1125	1123	65
3	292	264	216	-151
6	847	886	886	24
7	355	309	-210	-226
10	762	783	783	16
H= 1 K= 15				
0	731	720	-720	-23
4	509	575	-574	-41
8	527	590	-588	-46
H= 1 K= 17				
6	518	531	522	96
H= 2 K= 0				
0	1979	2037	-2037	-25
2	1592	1553	1545	154
6	685	723	720	58
8	920	942	-920	-198
10	730	706	668	230
12	282	257	-212	-145
18	392	356	320	156
H= 2 K= 2				
1	135	111	-22	-109
4	889	869	-865	-80
5	209	141	110	-89
10	963	939	-920	186
H= 2 K= 4				
2	1528	1583	1583	47
3	1427	1352	-1342	170
5	643	590	-586	-68
6	1149	1139	1125	177
9	651	639	-638	-11
10	566	595	579	136
11	668	661	-652	109
14	617	507	485	147
17	381	429	-428	-14
H= 2 K= 6				
0	1009	955	955	-25
1	261	335	234	-240
3	817	810	796	151
4	1242	1172	1153	-214
5	498	502	468	-182
8	922	876	867	-126
9	445	433	384	-201
11	418	408	400	83
12	499	550	517	-188
H= 2 K= 8				
0	711	742	-741	-24
1	435	454	-418	-176
2	736	740	735	87
4	488	484	-464	-137
5	321	369	-330	-165
6	472	483	461	145
8	474	477	-475	-41
10	359	416	409	74
12	340	322	-289	-141
H= 2 K= 10				
1	570	570	532	-204
3	594	669	637	204
4	706	667	666	-35
5	532	534	488	-217
7	346	448	409	183
9	444	524	497	-164
11	339	394	375	122
12	403	368	356	-95
H= 2 K= 12				
0	535	523	-522	-23
1	389	387	-336	-193
4	883	898	-898	-15
7	365	369	-345	129
8	542	545	-502	-213
H= 2 K= 14				
2	561	540	-540	-18
4	327	402	-402	-8
10	424	544	-529	126
H= 2 K= 16				
2	475	520	518	46
6	450	376	366	86
9	363	298	-203	-218
10	468	385	384	-29
H= 2 K= 18				
6	376	150	-141	50
H= 3 K= 1				
1	218	158	151	46
3	148	70	65	26
6	1898	1760	-1745	-233
10	1028	1013	-969	-296
14	499	648	-607	-228
18	405	472	-419	-218
H= 3 K= 3				
2	239	219	-167	-141
4	2169	2068	2055	236
5	198	152	-133	73
6	505	542	-437	-321
7	238	147	107	101
8	824	802	768	232
12	666	677	624	262
14	325	380	-217	-312
H= 3 K= 5				
0	1966	1987	1987	58
1	831	811	809	56
2	1174	1131	-1120	-157
3	1281	1231	1230	-51
4	197	212	120	175
5	862	823	820	-68
6	306	344	-231	-255
7	489	459	459	20
8	753	763	703	298
9	581	600	598	-45
10	834	817	-764	-290
11	520	530	520	-101
12	342	342	269	210
H= 3 K= 7				
0	1872	1883	1882	57
1	1242	1237	-1235	71
2	484	530	514	-128
3	778	767	-767	22
4	1931	1906	1891	239
5	727	722	-722	18
6	418	437	379	-217
7	926	922	-921	-43
8	1247	1209	1185	240
9	616	668	-661	95
10	454	453	408	-197
12	918	920	875	284
16	609	609	554	252
H= 3 K= 9				
0	464	532	529	54
1	677	645	644	-37
2	568	598	-588	-110
3	289	269	268	16
4	575	556	535	152
5	464	463	455	82
6	493	548	-503	-218
7	529	528	521	-84
8	324	377	311	214
12	314	330	239	227
13	377	336	334	-40
14	383	357	-258	-246
H= 3 K= 11				
0	292	249	244	52
1	297	327	-326	-27
2	723	758	-749	-119
5	507	506	-506	23
6	650	649	-631	-150
9	446	388	-381	-76
10	476	537	-485	-229
11	468	483	-478	-66
14	371	336	-264	-207
H= 3 K= 13				
2	761	777	-776	-37
6	920	872	-857	-161
10	435	406	-379	-147
H= 3 K= 15				
2	363	423	-405	-124
3	393	457	454	-52
8	432	339	318	117
10	365	474	-369	-297
H= 3 K= 17				
0	360	267	263	42
H= 4 K= 0				
4	992	990	-978	-158
6	764	682	-666	146
H= 4 K= 2				
1	1784	1731	1730	67
2	1653	1730	1724	148
4	864	864	-847	-173
5	609	624	622	46
6	1506	1510	1504	133
9	294	291	288	43
10	728	737	727	123
12	339	265	-165	-208
13	625	653	653	10
14	698	670	652	154
H= 4 K= 4				
0	740	782	-781	-31
1	204	271	-227	148
3	202	184	-174	-59
4	537	489	471	-130
6	855	821	-808	148
14	474	530	-510	144
H= 4 K= 6				
0	992	991	-991	-31
1	662	669	656	130
2	1391	1428	1425	91
5	339	345	304	164
6	861	875	866	127
7	570	548	538	-100
8	418	442	-406	-175
10	880	928	909	186
H= 4 K= 8				
0	417	417	416	-30
1	678	682	-657	181
2	472	447	-440	78
4	297	243	-238	-47
5	334	347	-328	113
10	444	539	-497	209
13	502	409	-407	47
H= 4 K= 10				
3	291	283	-249	-134
4	442	491	-479	-109
5	399	489	-465	151
6	741	788	778	121
7	701	676	-668	-103
10	386	415	411	55
13	440	439	-409	160
14	587	491	468	147
H= 4 K= 12				
0	289	37	-24	-28
1	377	427	393	167
2	358	359	-350	79
6	342	303	-278	120
7	460	442	405	-176
12	382	174	-21	-173
H= 4 K= 14				
0	525	544	-543	-26
2	452	464	457	80
10	413	483	461	145
H= 4 K= 16				
1	339	430	407	137
7	443	466	443	-144
H= 4 K= 18				
3	389	228	100	-204
4	537	453	-453	5
H= 5 K= 1				
1	1877	1901	-1900	-58
4	312	390	-359	-153
5	560	581	-572	107
6	1324	1325	1322	89
7	1489	1452	-1451	50
9	420	416	-415	26
10	753	744	742	49
13	638	688	-683	80
14	560	540	531	98
15	381	473	-473	-21
H= 5 K= 3				
3	1377	1329	1325	101
4	576	653	-649	-76
5	528	533	504	-174
6	1134	1146	1136	152
9	692	671	655	-148
10	491	523	517	80
11	640	635	632	57
14	528	511	495	124
H= 5 K= 5				
0	2241	2391	-2391	-21
1	256	287	-233	-167
4	972	995	-994	-50
6	380	362	-361	21
8	1265	1229	-1223	-115
12	643	723	-716	-97
H= 5 K= 7				
0	955	1000	-999	-21
2	308	317	310	62
3	506	528	-481	219
4	974	999	-999	-19
7	326	278	200	194
8	727	680	-678	-46
9	281	196	-155	-119
10	390	187	117	146
12	640	545	-542	-60
16	373	332	-330	-39
H= 5 K= 9				
0	696	687	-686	-21
1	608	671	631	-227
2	265	349	346	43
3	335	396	-371	138
4	736	735	-732	-68
6	361	325	315	80
8	484	513	-508	-76
12	387	393	-383	-89
H= 5 K= 11				
1	305	377	-292	-239
2	780	821	820	36
6	745	721	721	27
7	315	402	-340	215
10	471	520	519	8
H= 5 K= 13				
2	542	590	590	6
3	374	323	207	248
4	303	233	-232	-19
6	663	656	639	146
7	337	249	-186	166
H= 5 K= 15				
2	476	584	583	40
10	458	495	493	42
H= 5 K= 17				
0	568	534	-534	-18
4	520	504	-503	-20
8	399	432	-431	-30
H= 6 K= 0				
0	1554	1522	1520	59
2	196	161	-33	-158
6	469	489	-404	-277
8	1057	1042	1014	241
12	632	670	631	228
14	330	248	-99	-228
16	585	569	512	249
H= 6 K= 2				
0	1872	1980	1979	59
1	271	234	228	54
2	1676	1649	-1646	-111
3	243	163	-160	32
6	1967	1926	-1908	-261
8	1492	1468	1456	187
10	702	698	-676	-175
12	1059	1104	1074	256
14	879	947	-899	-299
16	751	794	771	187
H= 6 K= 4				
0	1856	1903	1902	58
1	955	949	-947	-60
3	1600	1549	-1547	-85
5	1022	983	-983	21
6	396	372	-290	-232
7	537	560	-548	-116
8	777	799	760	246
10	807	805	-757	-273
11	525	630	-629	-45
12	345	387	330	202
17	365	360	-360	-2
H= 6 K= 6				
0	1918	1934	1933	56
2	2852	2950	-2946	-150
3	282	236	235	20
6	1761	1746	-1744	-84
8	908	952	900	308
10	1894	1910	-1892	-261
12	442	476	416	231
14	780	730	-726	-78
H= 6 K= 8				
4	907	924	916	117
5	503	486	485	-24
7	319	367	358	-79
8	296	278	197	196
9	412	499	484	-120
11	328	400	366	-162
12	363	444	399	196
H= 6 K= 10				
0	1089	1115	1114	52
1	322	355	-341	100
2	1275	1323	-1320	-89
4	1163	1195	1186	143
6	1189	1222	-1206	-198
8	866	846	830	164
10	782	814	-794	-181
12	550	629	600	191
14	649	688	-642	-247
H= 6 K= 12				
0	642	624	622	49
1	659	707	703	75
3	818	784	784	-27
4	921	973	958	169
5	654	706	706	-8
7	538	557	550	-86
8	619	598	585	126
9	480	539	537	56
11	386	547	545	-42
12	488	457	394	232
13	419	388	386	-38
H= 6 K= 14				
0	1265	1234	1233	46
1	551	565	-565	-5
2	610	614	-610	-76
3	782	787	-784	-69
4	919	965	959	104
6	428	473	-449	-151
7	380	431	-416	-113
8	957	952	935	175
9	544	578	-577	-14
10	472	537	-500	-195
11	426	509	-507	-39
12	661	649	628	162
H= 6 K= 16				
0	519	497	495	43
2	530	464	-446	-128
10	468	509	-442	-253
H= 6 K= 18				
0	447	325	323	40
2	702	682	-681	-35
4	668	582	574	94
6	717	699	-688	-126
H= 7 K= 1				
1	515	428	427	-29
2	1264	1348	1346	64
3	1127	1085	-1083	-60
4	1059	1097	-1095	-68
5	635	579	-575	61
6	1253	1247	1239	133
8	659	678	-665	-133
9	454	430	-430	-3
10	423	511	493	137
11	708	657	-657	1
12	469	405	-389	-114
14	530	459	447	106
H= 7 K= 3				
0	1494	1589	-1588	-34
1	229	299	-280	104
3	217	295	-203	-214
4	1671	1692	-1690	-77
5	281	288	-287	22
8	1037	1035	-1033	-51
12	696	760	-755	-88
16	461	495	-493	-44
H= 7 K= 5				
0	530	604	-603	-34
1	338	357	-327	143
2	1889	1973	1973	-11
6	1369	1223	1218	117
10	1218	1224	1223	35
14	609	586	581	83
H= 7 K= 7				
0	1473	1444	-1444	-33
2	557	556	543	122
4	932	949	-937	-153
8	825	848	-843	-90
10	332	406	398	81
12	622	639	-617	-166
H= 7 K= 9				
0	532	486	-485	-32
1	336	398	370	146
2	962	995	993	73
3	780	752	750	-55
4	267	331	-323	-70
5	479	584	572	115
6	833	808	804	88
8	365	340	-325	-100
9	325	407	378	150
10	669	685	672	134
11	538	489	487	41
14	398	405	392	101
H= 7 K= 11				
0	559	628	-628	-31
2	291	328	327	33
3	418	421	-379	-183
4	765	789	-787	-51
5	298	268	-110	245
6	368	434	426	81
8	705	595	-581	-129
12	383	375	-359	-107
H= 7 K= 13				
0	367	261	-259	-29
6	606	571	564	93
8	424	316	-289	-128
H= 7 K= 15				
0	502	552	-551	-27
4	482	500	-500	-21
7	430	365	-337	-140
H= 7 K= 17				
2	627	611	606	80
6	474	430	430	16
7	364	214	-172	-127
H= 8 K= 0				
0	546	545	-545	-18
2	903	845	-831	156
4	414	394	378	-108
6	1289	1236	-1230	118
10	497	455	-428	153
14	534	558	-546	115
H= 8 K= 2				
0	1046	1104	-1104	-18
1	737	733	728	-86
3	746	725	719	98
4	1349	1353	-1351	-65
5	605	605	602	-57
7	395	427	426	33
8	796	728	-727	-37
9	375	349	349	-19
11	293	331	326	54
12	714	650	-647	-61
13	311	234	226	-59
H= 8 K= 4				

TABLE C-5, continued.

L	FO	FC	AC	BC
1	369	322	306	100
2	504	432	430	39
3	460	410	408	-38
4	682	641	-633	-98
5	397	362	349	98
6	388	377	370	72
8	519	511	-500	-110
11	396	299	296	-38
12	449	420	-415	-174
13	410	244	171	174
H= 13	K= 13			
0	866	856	-855	-32
4	682	606	-605	-39
7	351	316	-128	-289
8	666	641	-641	7
10	378	305	199	232
H= 13	K= 15			
2	536	459	458	20
6	450	363	356	72
9	354	122	35	-117
H= 13	K= 17			
0	405	245	-243	-27
1	438	313	309	53
4	377	321	-316	-54
H= 14	K= 0			
0	1206	1193	-1193	-10
2	243	260	184	183
14	371	234	-181	148
H= 14	K= 2			
0	668	651	651	-10
2	819	805	-805	-28
3	727	731	730	42
6	516	533	-504	173
9	345	332	325	-69
10	587	688	-685	71
H= 14	K= 4			
1	860	872	867	-92
2	693	718	713	46
3	1034	1046	1043	81
5	804	820	805	-153
7	608	649	648	37
10	386	401	379	130
11	507	554	554	12
12	326	133	-68	-115
13	356	379	363	-111
14	435	356	353	42
15	397	424	423	-22
H= 14	K= 6			
0	287	268	268	-11
1	304	358	-302	-157
2	470	455	-453	42
L	FO	FC	AC	BC
8	760	780	775	85
9	312	306	-304	-30
12	622	685	676	114
14	605	647	-589	-268
15	394	301	-283	-102
H= 18	K= 4			
0	520	387	385	46
1	264	154	150	-33
7	298	178	178	1
8	329	371	281	242
10	450	461	-450	-102
H= 18	K= 6			
0	1809	1810	1810	45
2	390	338	-307	-141
4	1628	1593	1592	63
12	846	872	858	157
H= 18	K= 8			
0	320	233	-229	44
2	660	656	-655	-34
9	327	191	84	171
H= 18	K= 10			
0	1195	1158	1158	42
1	385	389	347	94
2	566	588	-586	-51
3	415	475	463	-106
6	475	436	-393	-188
8	817	820	810	130
10	454	472	-450	-142
11	390	337	318	-113
12	831	723	715	107
H= 18	K= 12			
2	538	579	-571	-98
6	519	463	-423	-188
7	395	371	-362	-81
9	388	233	-141	186
10	423	454	-441	-109
H= 18	K= 14			
0	469	573	572	38
2	783	787	-782	-88
4	356	337	321	104
6	551	617	-605	-119
8	402	446	434	104
H= 18	K= 16			
0	581	447	445	36
4	393	341	331	82
H= 19	K= 1			
0	1323	1309	-1308	-40
2	507	476	476	15
3	330	337	-333	53

L	FO	FC	AC	BC
3	409	378	-347	150
4	486	476	-456	-135
5	332	295	-290	-53
6	497	556	-553	-53
7	299	314	-257	180
11	383	246	-190	156
14	368	314	-314	-9
H= 14	K= 8			
2	734	731	731	-4
3	390	385	-347	165
6	669	637	621	142
10	402	465	462	49
H= 14	K= 10			
1	432	483	-442	-196
2	553	480	-471	92
3	659	637	-613	175
4	409	389	376	-102
5	467	493	-467	-160
6	484	591	-588	156
7	452	378	-354	132
9	455	460	-434	-152
14	440	468	-467	-35
H= 14	K= 12			
4	553	461	-457	57
6	365	264	207	164
H= 14	K= 14			
0	360	361	361	-11
9	371	267	185	-192
10	383	344	-339	57
H= 14	K= 16			
3	408	366	318	182
5	361	331	275	-185
H= 15	K= 1			
0	477	464	462	51
2	260	254	-230	-108
3	602	635	615	159
4	962	930	902	226
5	650	651	634	-147
6	511	490	-455	-182
7	603	634	633	27
8	462	510	465	208
9	385	464	456	86
11	451	374	366	85
13	349	392	374	-118
15	360	312	294	104
16	429	448	364	261
H= 15	K= 3			
1	588	616	609	92
2	623	637	-628	-103
4	493	502	481	141
6	623	631	-594	-212
L	FO	FC	AC	BC
3	427	424	410	-110
4	406	426	-418	-80
H= 20	K= 0			
0	811	825	825	-3
4	724	762	760	58
8	649	671	658	130
12	472	448	448	-22
14	365	143	-68	127
H= 20	K= 2			
1	438	434	432	-45
4	412	437	-435	-48
7	535	468	464	61
8	328	149	-52	-139
H= 20	K= 4			
1	770	773	773	-1
2	419	434	-431	51
3	287	326	308	108
4	495	560	560	-14
5	582	565	552	-118
6	511	549	-528	147
7	772	747	737	123
10	413	225	-203	97
13	448	549	548	-27
14	376	437	-396	185
H= 20	K= 6			
0	353	390	-390	-4
9	345	181	-35	-177
10	424	309	264	-160
H= 20	K= 8			
0	445	361	361	-4
2	624	624	-622	-43
6	454	414	-381	161
10	601	585	-581	68
H= 20	K= 10			
1	512	519	-496	-152
2	327	304	297	65
3	424	418	-384	163
5	351	455	-441	-113
11	363	375	-329	181
H= 20	K= 12			
4	345	209	207	29
H= 21	K= 1			
0	664	667	666	43
1	716	709	-676	215
2	381	296	-285	-79
5	351	360	-326	153
7	629	673	-673	27

L	FO	FC	AC	BC
7	579	602	595	-88
10	334	371	-290	-231
H= 15	K= 5			
0	1253	1242	1241	49
2	448	515	-505	-101
8	614	630	579	248
10	647	649	-578	-294
11	321	76	21	73
H= 15	K= 7			
2	858	842	-834	-118
3	761	722	710	-128
5	358	393	388	65
6	649	637	-616	-163
9	332	290	280	76
10	586	602	-538	-271
11	466	448	432	-119
H= 15	K= 9			
0	536	519	517	46
1	790	762	-760	-43
3	658	665	-656	-106
4	752	686	674	125
8	351	442	411	161
9	478	497	-474	-150
11	356	460	-456	-55
12	464	382	335	185
13	538	438	-436	43
H= 15	K= 11			
2	553	455	-447	-81
4	321	289	227	179
H= 15	K= 13			
0	522	400	398	42
4	688	676	669	98
7	357	251	234	-89
H= 15	K= 15			
2	474	486	-481	-67
H= 15	K= 17			
3	428	448	448	-1
H= 16	K= 0			
2	603	611	611	-19
4	305	340	313	-133
6	1010	996	987	135
8	819	880	856	-204
12	438	495	446	-213
14	641	571	557	122
H= 16	K= 2			
0	816	807	-806	-39
2	538	550	529	150
L	FO	FC	AC	BC

L	FO	FC	AC	BC
4	1044	1043	-1032	-151
5	270	335	-318	105
6	602	609	607	51
8	653	638	-633	-79
12	372	480	-438	-195
14	395	375	340	159
16	477	402	-397	-66
H= 16	K= 4			
3	272	223	220	-34
4	456	412	409	-53
6	287	276	-209	180
15	377	106	-105	-5
H= 16	K= 6			
0	1352	1318	-1317	-38
2	538	497	496	31
3	275	225	-214	-68
4	594	574	-569	-77
8	857	816	-795	-186
10	457	508	492	129
12	561	562	-555	-89
H= 16	K= 8			
0	345	250	-248	-37
2	390	308	-267	152
H= 16	K= 10			
1	333	365	359	69
2	649	552	552	-13
3	438	393	385	-80
4	589	587	-582	-78
5	368	363	363	-3
6	745	739	721	163
7	467	373	308	-210
H= 16	K= 12			
0	413	401	-400	-31
2	368	432	430	42
3	406	419	409	-92
5	387	275	271	42
H= 16	K= 16			
3	377	330	-316	-94
H= 17	K= 1			
0	606	522	-522	-7
2	403	428	428	12
3	545	537	528	-96
4	289	155	-126	-91
5	361	325	317	75
L	FO	FC	AC	BC
1	1101	1087	-1080	-122
2	450	412	407	-61
3	756	745	-708	230
5	816	811	-796	-153
6	484	470	465	69
7	942	939	-935	89
9	599	632	-632	0
10	388	185	182	-35
11	545	502	-464	191
13	494	592	-569	-164
14	366	273	268	52
H= 17	K= 5			
0	576	623	-623	-7
4	357	270	-270	20
8	374	479	-475	65
10	393	292	134	259
H= 17	K= 7			
1	304	378	300	-230
2	331	298	298	-21
6	308	404	-403	27
6	521	535	528	83
H= 17	K= 9			
1	476	424	418	-67
4	469	409	-408	-26
7	395	427	405	135
H= 17	K= 11			
0	368	385	-385	-8
3	534	450	400	206
10	424	360	358	34
11	369	367	322	177
H= 17	K= 15			
0	384	323	-323	-8
1	467	345	-247	-242
H= 18	K= 0			
0	509	512	510	47
2	752	768	-767	-42
6	490	470	-416	-218
10	683	647	-633	-135
H= 18	K= 2			
0	1089	1064	1063	47
1	441	513	-507	76
2	1220	1262	-1258	-104
3	317	263	-261	-33
4	1185	1165	1161	99
5	359	302	-290	-85
6	1086	1112	-1087	-234
7	437	450	-441	-88
L	FO	FC	AC	BC
10	324	344	343	-27
H= 17	K= 5			
1	1101	1087	-1080	-122
2	450	412	407	-61
3	756	745	-708	230
5	816	811	-796	-153
6	484	470	465	69
7	942	939	-935	89
9	599	632	-632	0
10	388	185	182	-35
11	545	502	-464	191
13	494	592	-569	-164
14	366	273	268	52
H= 17	K= 7			
1	304	378	300	-230
2	331	298	298	-21
6	308	404	-403	27
6	521	535	528	83
H= 17	K= 9			
1	476	424	418	-67
4	469	409	-408	-26
7	395	427	405	135
H= 17	K= 11			
0	368	385	-385	-8
3	534	450	400	206
10	424	360	358	34
11	369	367	322	177
H= 17	K= 15			
0	384	323	-323	-8
1	467	345	-247	-242
H= 18	K= 0			
0	509	512	510	47
2	752	768	-767	-42
6	490	470	-416	-218
10	683	647	-633	-135
H= 18	K= 2			
0	1089	1064	1063	47
1	441	513	-507	76
2	1220	1262	-1258	-104
3	317	263	-261	-33
4	1185	1165	1161	99
5	359	302	-290	-85
6	1086	1112	-1087	-234
7	437	450	-441	-88

TABLE C-5, continued.

L	FO	FC	AC	BC
0	889	856	855	-18
3	652	680	-652	184
4	1259	1270	1260	-155
5	345	336	-292	-166
8	643	695	670	-188
9	300	251	-248	-40
12	656	747	717	-212
15	364	113	-19	111
H=	8	K=	6	
0	329	330	-329	-18
1	348	332	266	-198
2	757	786	779	103
5	799	794	770	196
6	708	689	685	70
8	333	378	-364	-103
9	426	375	361	-102
10	393	339	364	245
11	494	446	404	187
H=	8	K=	8	
0	1741	1746	1745	-18
1	366	430	-385	-193
2	256	292	277	-94
3	352	384	-344	172
4	712	670	663	-98
5	388	399	-323	-224
6	601	612	611	33
8	1153	1172	1137	-283
12	538	611	584	-181
14	440	442	441	-28
16	396	442	394	-200
H=	8	K=	10	
0	979	933	-932	-17
4	680	728	-727	-35
8	625	574	-574	17
12	474	547	-547	-27
H=	8	K=	12	
6	460	496	-482	116
H=	8	K=	14	
8	493	541	-539	-38
10	397	168	145	85
H=	8	K=	18	
0	535	467	467	-15
2	449	474	461	-108
H=	9	K=	1	
0	1854	1882	1881	57
1	577	578	564	130
2	1200	1148	-1141	-124
3	1268	1218	1218	-37
5	888	887	865	-68
7	387	384	370	-101
9	523	546	545	23
11	615	640	635	-81
12	437	401	350	195
15	406	198	180	-81
17	453	327	327	5
H=	9	K=	3	
0	530	540	-537	56
2	1473	1453	-1448	-117
3	279	233	228	48
4	448	401	433	252
6	1411	1420	-1406	-201
10	536	555	-522	-187
11	290	286	189	131
14	607	699	-659	-232
H=	9	K=	5	
0	1654	1692	1692	55
1	1231	1211	1210	63
2	336	316	384	-160
3	919	889	884	-94
4	1636	1593	1585	151
5	918	900	895	97
7	955	933	926	-110
8	1178	1164	1148	196
9	655	663	663	31
11	574	490	488	-45
12	644	615	575	220
13	414	512	511	34
16	529	580	554	172
H=	9	K=	7	
1	719	737	-736	49
2	519	473	-458	-117
3	990	978	-978	4
4	888	875	862	151
5	802	815	-815	3
6	812	821	-785	-240
7	492	510	-509	-21
9	560	550	-547	57
11	597	603	-603	0
H=	9	K=	9	
0	680	666	664	52
2	447	525	-521	-60
4	409	422	393	154
6	330	327	-282	-166
8	343	363	366	283
10	387	413	-367	-191
12	439	378	301	228
H=	9	K=	11	
0	907	926	927	49
1	788	788	-782	95
2	383	385	-363	-129
3	315	332	-330	-36
5	463	475	-468	-82
7	712	727	-722	-83
8	537	556	515	210
9	329	343	-282	20
13	376	416	-408	-79
H=	9	K=	13	
2	678	760	-753	-103
6	698	713	-682	-209
10	434	507	-457	-219
H=	9	K=	15	
0	344	381	378	44
2	400	300	-290	-77
H=	10	K=	0	
0	2783	3087	-3086	-36
2	521	592	586	-80
4	857	854	-843	-136
6	273	315	-294	108
8	1414	1416	-1389	-275
12	710	714	-708	-92
14	368	206	-174	111

L	FO	FC	AC	BC
H=	10	K=	2	
0	1072	1035	1034	-36
2	1110	1153	1142	160
3	261	226	226	-7
4	1420	1398	1391	-130
6	647	668	657	115
8	921	886	877	-131
9	298	260	248	76
10	615	655	629	182
12	619	633	615	-147
14	383	311	279	137
16	434	469	449	-135
H=	10	K=	4	
0	1034	1081	-1081	-36
1	317	340	-312	134
3	860	861	861	29
4	1881	1928	-1923	-127
5	269	265	229	88
6	487	446	440	75
7	382	387	-373	-100
8	864	923	-903	-194
9	286	317	276	156
12	719	787	-758	-213
14	307	262	246	88
16	602	562	-544	-142
H=	10	K=	6	
0	623	620	619	-35
1	512	489	482	80
2	325	334	-319	98
3	257	251	-190	-165
4	315	334	-332	-38
7	468	477	468	-92
10	486	523	-465	239
H=	10	K=	8	
0	875	856	-856	-34
1	310	380	-356	134
2	579	576	570	86
3	586	576	-563	-120
4	712	706	-690	-148
5	359	407	-382	142
6	411	468	465	54
7	314	256	-254	-29
8	608	640	-624	-140
9	386	407	-391	112
11	323	312	-303	-75
H=	10	K=	10	
1	310	266	233	128
4	387	404	402	-39
6	294	345	-300	170
H=	10	K=	12	
0	403	430	-429	-31
2	615	674	667	98
3	454	473	-453	-138
5	453	447	-408	182
6	438	461	459	48
7	343	260	-236	-109
9	368	293	-270	113
10	626	540	519	149
H=	10	K=	14	
0	418	424	423	-30
3	610	564	558	-82
11	363	362	359	-47
H=	10	K=	16	
0	441	435	-434	-27
4	563	625	-620	-77
H=	11	K=	1	
2	1188	1227	1225	76
3	402	416	-415	-29
4	225	127	106	-71
6	976	961	957	-81
10	714	718	707	128
14	444	405	402	-51
H=	11	K=	3	
0	223	290	-290	-14
2	299	367	364	-48
3	1416	1445	-1442	95
4	893	943	-942	-39
5	571	629	-629	19
6	490	528	505	152
8	325	336	-326	-83
9	530	619	-608	112
11	570	641	-639	51
17	442	431	-431	17
H=	11	K=	5	
0	1128	1139	-1139	-14
4	414	449	-442	-79
12	358	371	-371	-23
H=	11	K=	7	
0	650	659	-659	-14
1	291	336	-310	-130
4	673	708	-705	-61
8	397	401	-398	98
8	463	477	-476	-28
11	363	340	314	130
12	360	388	-387	-17
H=	11	K=	9	
0	932	931	-931	-14
3	510	582	478	276
4	704	748	-748	-17
8	650	662	-662	-12
9	393	363	340	-128
11	454	337	231	245
H=	11	K=	11	
0	371	352	352	-14
1	291	335	278	-186
2	1042	1047	1045	48
4	492	459	456	-50
6	870	892	889	-73
10	725	729	715	106
14	440	441	431	-92
H=	11	K=	13	
4	653	702	-702	-8
5	361	261	-104	-240
H=	11	K=	15	
1	378	218	-95	-196
2	684	709	707	49
6	465	557	457	28
10	569	549	548	26

L	FO	FC	AC	BC
H=	11	K=	17	
0	581	586	-585	-13
4	694	484	-480	-66
5	367	283	-70	-274
6	367	168	-151	74
H=	12	K=	0	
2	3038	3173	-3169	-154
6	2070	2050	-2047	-105
8	740	770	726	256
10	2002	2021	-1997	-309
12	361	289	178	228
14	784	805	-801	-82
H=	12	K=	2	
0	1704	1765	1765	54
1	1134	1115	-1113	62
2	517	531	513	-135
3	547	531	-537	-30
4	1879	1893	1889	130
5	782	777	-777	-33
7	876	877	-876	-28
8	1119	1143	1129	183
9	431	435	-435	11
11	388	387	-385	-36
12	809	834	809	202
13	546	516	-516	2
16	462	558	546	118
H=	12	K=	4	
0	870	859	857	53
2	2135	2181	-2180	-71
4	1163	1173	1163	169
6	1866	1864	-1852	-214
8	683	642	603	222
10	1130	1177	-1166	-157
12	601	598	570	182
14	942	960	-940	-103
16	407	399	317	242
H=	12	K=	6	
0	698	681	679	52
1	655	659	-644	141
2	524	500	-493	-83
3	330	300	-299	-20
4	674	693	657	222
5	463	387	-385	-65
6	404	452	-399	-213
7	505	552	-548	-91
8	413	496	463	176
12	446	395	335	209
H=	12	K=	8	
0	1235	1243	1242	50
1	690	655	653	57
2	1154	1169	-1167	-72
3	445	385	384	-33
4	1311	1298	1283	196
5	541	542	520	153
6	1062	1068	-1054	-170
7	580	579	578	-30
8	919	929	914	168
10	692	688	-684	-77
13	473	418	409	85
14	602	621	-570	-245
H=	12	K=	10	
0	619	772	770	48
1	527	488	486	87
2	582	580	-560	-152
7	409	497	489	-88
8	531	505	491	120
10	582	666	-568	-349
H=	12	K=	12	
0	679	718	717	46
2	911	917	-914	-73
4	894	869	863	99
6	927	908	-907	-44
8	514	634	579	258
10	565	606	-564	-215
12	590	528	472	236
H=	12	K=	14	
0	507	420	418	43
4	739	705	703	53
H=	12	K=	16	
0	460	502	501	41
1	375	278	-233	152
4	373	391	362	146
6	662	709	-692	-157
H=	13	K=	5	
1	531	544	-529	125
2	1198	1237	1237	-33
3	667	703	-692	-121
5	512	532	-522	104
6	977	1004	990	169
7	373	414	-371	-186
9	444	461	-451	98
10	794	815	814	46
11	381	380	-378	-57
14	484	500	484	124
16	410	246	-140	-203
H=	13	K=	7	
0	395	453	-452	-36
1	920	900	900	-19
2	978	960	956	88
3	378	411	404	-76
4	556	536	-522	-124
5	426	476	466	97
6	855	876	-875	48
7	772	802	802	13
9	483	516	515	-26
10	509	554	551	76
13	375	378	371	68
14	479	497	486	76
15	543	490	490	-29
H=	13	K=	9	
0	435	445	-444	-35
1	811	860	-835	203
2	647	671	671	29
4	600	597	-593	-67
5	530	520	-510	104
6	704	668	659	114
7	699	782	-780	-52
8	426	364	-348	-108
10	400	404	391	102
12	351	329	-311	-106
13	532	532	-503	172
14	410	450	428	137
H=	13	K=	11	
0	680	646	-645	-34

TABLE C-6. Structural Amplitudes for the Dolni Bory Cordierite at 375°C.

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
			7	1416	-1357	6	1054	1054	7	868	-814	1	612	-649	0	1551	1550	2	1254	1364	H=	8	K=	4
H=	0	K= 0	8	339	-332	9	643	-585	8	1018	1043	2	716	704	4	2086	2002	3	1098	-1090				
			9	389	-458	10	551	503	9	558	-567	3	276	-241	6	316	-318	4	1033	-1045	0	878	836
4	3994	3691	10	549	536	11	588	-606	10	357	393	6	645	674	8	902	886	5	597	-602	3	625	-639
6	1957	1747	12	339	-223										12	522	526	6	1133	1137	4	1198	1217
8	4205	4025				H=	2	K= 6	H=	3	K= 9	H=	4	K= 12				8	589	-571	5	302	-275
10	385	-397	H=	1	K= 5													H=	6	K= 2	9	459	-413	8	622	635
12	1791	1881				0	962	935	0	405	440	1	407	358							10	439	419	9	340	-245
			0	1104	-1170	2	397	445	1	533	599	4	288	-76	0	1875	1912	11	579	-611	11	365	-273
H=	0	K= 2	1	489	463	3	801	752	2	515	-506				1	266	206	12	422	-332			
			2	380	438	4	1135	1094	3	286	263	H=	5	K= 1	2	1620	-1643				H=	8	K= 6
0	299	-304	3	532	534	5	484	452	4	478	423				3	196	-141	H=	7	K= 3			
2	2698	-2687	4	1366	-1322	8	796	808	5	344	394	2	1518	1585	4	3198	3155				2	692	708
6	1710	-1593	5	354	336	9	312	361	6	434	-431	4	339	-371	5	199	61	0	1467	-1568	3	713	755
8	247	-206	6	471	485				7	400	443	5	548	-540	6	1813	-1797	1	308	-296	4	249	-220
10	908	-880	8	889	-879	H=	2	K= 8	8	337	227	6	1241	1262	8	1318	1282	3	198	-205	5	459	449
			11	298	149							7	1408	-1367	9	245	-151	4	1586	-1616	6	564	585
H=	0	K= 4	12	433	-426	0	684	-713	H=	3	K= 11	9	391	-393	10	578	-584	6	376	402	8	332	-320
						1	366	-383				10	611	664	12	850	889	8	935	-922	9	325	338
0	2140	2218	H=	1	K= 7	2	668	653	1	377	-293							12	562	-587			
2	1557	-1442				4	428	-407	2	603	-641	H=	5	K= 3	H=	6	K= 4				H=	8	K= 8
4	3651	3272	0	562	-618	5	262	-283	3	657	-645							H=	7	K= 5			
6	1704	-1591	2	322	334	6	392	402	5	446	-455	1	468	-373	0	1785	1858				0	1580	1591
8	1566	1506	3	1184	-1168	7	326	-260	6	461	-513	2	1267	1310	1	902	-937	0	484	-551	1	399	-383
10	482	-485	4	1303	-1291							3	1324	1299	2	1144	-1125	1	301	-320	4	641	616
12	926	980	5	556	-551	H=	2	K= 10	H=	3	K= 13	4	623	-676	3	1497	-1488	2	1820	1902	5	277	-316
			6	589	589							5	538	530	5	951	-947	6	1136	1142	6	430	513
H=	0	K= 6	8	544	-555	1	499	448	2	656	-640	6	1041	1036	6	315	-259	9	292	-156	7	292	-279
			9	290	-342	3	553	570				9	631	607	7	437	-498	10	943	1024	8	977	1017
0	918	-917	11	368	-463	4	580	598	H=	4	K= 0	10	345	429	8	702	668						
2	1719	-1648				5	425	442				11	583	585	9	656	-641	H=	7	K= 7	H=	8	K= 10
4	257	223	H=	1	K= 9	9	364	385	4	967	-952				10	591	-600						
6	1736	-1688							6	757	-679	H=	5	K= 5	11	412	-521	0	1320	-1370	0	795	-808
8	303	-357	0	409	-449	H=	2	K= 12	10	671	-732							2	427	433	4	593	-655
10	552	-616	1	722	736				12	274	-106	0	2126	-2303	H=	6	K= 6	4	886	-880			
			2	777	801	0	465	-479				1	242	-279				8	718	-734	H=	9	K= 1
H=	0	K= 8	4	347	-366	4	734	-760	H=	4	K= 2	4	909	-920	0	1760	1786						
			5	677	686							5	299	-211	2	2704	-2798	H=	7	K= 9	0	1798	1838
0	466	693	6	619	598	H=	3	K= 1	2	1602	1662	6	316	-332	3	231	214				1	510	543
2	2078	-2065	7	581	556				4	823	-834	8	1108	-1103	6	1586	-1605	0	457	-477	2	1147	-1113
4	1138	1072	9	473	451	1	232	148	5	588	602	9	257	-91	8	750	765	1	344	367	3	1172	1170
6	1802	-1778				2	2398	-2489	6	1391	1403				10	1507	-1590	2	897	880	4	223	106
8	526	529	H=	1	K= 11	7	231	91	7	1262	1235	H=	5	K= 7				3	628	661	5	875	834
10	953	-909				10	824	-814	9	320	292				H=	6	K= 8	5	559	509	7	433	349
			0	967	-960				10	587	619	0	943	-965				6	693	686	8	544	548
H=	0	K= 10	2	393	397	H=	3	K= 3				2	329	300	0	234	195	8	292	-282	11	540	565
			4	490	-487				H=	4	K= 4	3	442	-459	1	457	433	9	401	327	12	298	228
0	1411	1363				0	1259	1196				4	891	-909	2	516	-545						
2	475	-426	H=	1	K= 13	2	320	-173	0	735	-765	7	260	163	3	594	620	H=	7	K= 11	H=	9	K= 3
8	609	639				6	400	-394	2	448	-378	8	630	-603	4	769	762						
			2	909	936	8	664	651	4	514	459	9	266	-128	5	433	423	0	559	-525	2	1348	-1367
H=	0	K= 12	4	312	250	12	495	467	6	943	-799	11	291	-132	6	614	-594	4	639	-660	4	356	376
									10	378	-294				7	389	312	6	324	308	6	1243	-1265
0	1628	1597	H=	2	K= 9	H=	3	K= 5				H=	5	K= 9				7	298	256	8	240	-205
2	375	-344							H=	4	K= 6				H=	6	K= 10				10	370	-388
4	1328	1247	2	1559	1529	0	1885	1980				0	585	-596				H=	8	K= 0			
6	366	-208	6	652	674	1	766	781	0	897	-916	3	305	-324	0	924	952				H=	9	K= 5
			8	835	-864	2	1119	-1073	1	622	619	4	628	-638	2	1097	-1131	0	535	-574			
H=	1	K= 1	12	325	-184	3	1195	1174	2	1329	1357	6	349	262	4	1010	1036	2	884	-823	0	1549	1601
						4	213	93	5	288	250	7	422	483	6	968	-1012	4	446	384	1	1143	1162
0	2014	-1953	H=	2	K= 2	5	816	787	6	784	800	8	449	-445	7	289	-247	6	1213	-1183	2	401	386
1	146	83				7	569	424	7	536	487				8	675	671	10	482	-423	3	809	831
2	2368	2222	4	864	-840	9	603	595	8	335	-305	H=	5	K= 11							4	1470	1478
6	692	718	5	177	92	9	502	511	10	773	787				H=	6	K= 12	H=	8	K= 2	5	850	820
8	553	-571	6	1007	-894	10	588	-593				1	293	-231							6	253	140
10	816	848	10	824	-847	11	475	448	H=	4	K= 8	2	705	713	1	597	634	0	1024	-1048	8	974	968
12	360	-316										6	625	635	3	716	689	1	702	687	9	570	585
			H=	2	K= 4	H=	3	K= 7	2	418	-401				4	788	780	3	639	653	11	418	408
H=	1	K= 3							5	309	-294	H=	5	K= 13	5	670	614	4	1293	-1278			
			0	131	16	0	1771	1822	7	532	-549							5	518	549	H=	9	K= 7
2	1280	1314	1	324	253	1	1137	-1171	10	405	-450	2	500	491	H=	7	K= 1	7	443	370			
4	981	-987	2	1507	1537	2	524	526										8	679	-653	0	236	12
5	562	-536	3	1357	-1283	3	702	-717	H=	4	K= 10	H=	6	K= 0	0	493	-543	12	545	-549	1	676	-683
6	1178	1162	5	619	-580	4	1811	1751							1	444	411				2	441	-386

TABLE C-6, continued.

L	FO	FC
3	971	-883
4	777	771
5	667	-721
6	658	-652
7	426	-447
9	448	-456
10	300	3
H=	9	K= 9
0	453	591
2	424	-450
4	344	351
8	296	287
H=	9	K= 11
0	751	734
1	728	-690
2	333	-271
5	396	-415
H=	10	K= 0
0	2870	-3039
2	457	468
4	924	-831
6	249	-303
8	1206	-1226
10	485	463
H=	10	K= 2
0	1007	1040
2	1039	1095
3	297	261
4	1366	1372
6	599	611
8	801	843
9	291	245
10	499	507
11	302	139
H=	10	K= 4
0	1018	-1060
1	333	-298
3	966	852
4	1735	-1778
5	275	246
6	327	329
11	339	332
H=	10	K= 6
0	570	608
1	288	449
2	324	-306
4	287	-298
10	434	-452
H=	10	K= 8
2	549	524
3	512	-566
4	564	-564
8	326	-472
H=	10	K= 10
0	349	-215
1	263	252
6	288	-273
H=	10	K= 12
0	340	-312
2	403	542
3	312	-370
H=	11	K= 1
2	1144	1192
3	490	-351
6	884	897
10	660	654
H=	11	K= 3
0	329	-284
2	296	343
3	1266	-1328
4	892	-926
5	588	-565
6	568	466
8	417	-297
9	474	-461
11	430	-523
H=	11	K= 5
0	1062	-1087
4	424	-453
8	551	-600
9	266	-146
H=	11	K= 7
0	623	-607
1	298	-267
3	467	502
4	616	-649
8	433	-401
H=	11	K= 9
2	787	-821
3	381	412
4	581	-653
8	507	-564
H=	11	K= 11
0	340	336
2	898	940
3	362	219
4	439	419
H=	12	K= 0
2	2966	-3041
4	283	-93
6	1911	-1939
8	787	663
10	1644	-1702
H=	12	K= 2
0	1634	1699
1	1021	-1066
2	527	488
3	585	-519
4	1746	1808
5	711	-703
6	781	193
7	777	-787
8	939	984
9	394	-417
H=	12	K= 4
1	788	797
2	2013	-2079
4	1004	1041
6	1630	-1671
8	428	503
10	942	-986
H=	12	K= 6
0	615	625
1	628	-587
2	471	-475
3	301	-274
4	611	616
5	390	-331
7	472	-480
8	320	381
H=	12	K= 8
0	1109	1113
1	548	562
2	998	-1026
4	1069	1102
5	450	440
6	876	-897
7	416	466
8	745	752
H=	12	K= 10
0	644	647
H=	13	K= 1
0	1124	-1159
2	588	652
3	522	-519
4	1128	-1137
7	298	81
8	780	-757
9	309	-258
11	285	-234
H=	13	K= 3
0	1048	-1051
2	846	841
3	452	403
4	795	-808
6	660	573
7	345	126
8	730	-680
10	384	387
H=	13	K= 5
0	444	-476
1	482	-524
2	1158	1185
3	680	-692
5	556	-536
9	473	-408
10	710	715
H=	13	K= 7
0	383	-467
1	824	851
2	932	838
3	573	411
4	618	-510
5	516	446
6	804	739
7	710	708
8	358	-299
H=	13	K= 9
0	387	-381
1	734	-751
2	584	576
4	564	-471
5	438	-427
6	431	527
7	587	-630
H=	13	K= 11
0	576	-561
2	350	334
3	416	365
H=	14	K= 0
0	1097	-1092
8	633	-582
H=	14	K= 2
1	286	-116
2	773	-762
3	640	672
6	486	-482
10	534	-615
H=	14	K= 4
1	733	776
2	644	630
3	469	947
5	741	730
6	515	517
7	523	551
9	623	596
10	355	332
H=	14	K= 6
0	382	264
1	364	-303
2	374	-390
3	260	-281
4	455	454
5	260	-243
6	503	-467
8	345	261
H=	14	K= 8
2	665	599
3	297	-328
6	558	508
H=	14	K= 10
1	387	-362
2	449	-462
3	507	-482
4	302	262
5	379	-358
H=	15	K= 1
0	378	383
1	750	749
3	562	598
4	825	814
5	569	603
6	425	-355
7	584	550
8	359	353
9	355	384
H=	15	K= 3
1	542	571
2	582	-553
3	258	-156
4	451	435
6	527	-509
7	476	509
H=	15	K= 5
0	1139	1130
2	406	-420
4	244	-4
8	492	456
H=	15	K= 7
2	704	-727
3	569	613
5	302	333
6	520	-534
H=	15	K= 9
0	392	423
1	702	-690
3	610	-589
4	579	513
5	564	-595
H=	16	K= 0
0	1377	1450
2	588	569
4	292	324
6	826	830
8	779	848
H=	16	K= 2
0	668	-666
2	516	446
3	493	-528
4	876	-875
5	324	-283
6	500	500
8	419	-470
H=	16	K= 4
0	260	-271
3	287	263
4	354	362
6	344	-234
H=	16	K= 6
0	1139	-1109
2	401	390
3	256	-200
4	521	-471
6	269	1
8	609	-649
H=	16	K= 8
2	355	-253
H=	16	K= 10
1	322	310
2	373	433
H=	17	K= 1
0	578	-528
2	378	408
3	508	508
5	310	311
H=	17	K= 3
2	560	445
3	728	-665
4	403	-314
5	695	-681
6	456	485
7	744	-790
H=	17	K= 5
0	717	-657
3	257	-123
4	285	-292
8	450	-470
H=	17	K= 7
1	309	253
2	293	317
4	352	-368
6	461	467
H=	17	K= 9
1	336	333
H=	18	K= 0
0	507	544
2	798	-789
6	473	-397
H=	18	K= 2
0	1929	949
1	480	-490
2	1086	-1130
3	269	-244
4	948	1055
5	256	-281
6	927	-963
7	460	-396
8	617	636
H=	18	K= 4
0	521	388
1	309	140
2	705	-608
3	263	-163
6	482	-481
0	1568	1571
1	405	-215
2	282	-246
4	1413	1400
5	336	-151
6	286	-240
H=	18	K= 8
2	549	-579
H=	19	K= 1
0	1208	-1250
2	479	417
3	381	-329
4	834	-784
7	288	115
8	692	-746
H=	19	K= 3
1	385	353
2	945	1009
3	630	580
5	374	347
6	868	853
H=	19	K= 5
0	709	-642
4	1050	-1043
6	401	425
H=	19	K= 7
2	1044	955
H=	20	K= 0
4	720	730
H=	20	K= 2
1	420	390
4	402	-383
7	396	386
H=	20	K= 4
1	707	691
4	466	499
5	396	448
6	491	-415
H=	20	K= 6
0	353	-263

APPENDIX D: FINAL FRACTIONAL COORDINATES AND THERMAL PARAMETERS FOR THE WHITE WELL AND DOLNI BORY CORDIERITES

Final fractional coordinates and thermal parameters ($\times 10^5$) for White Well cordierite at various temperatures

Atom		24°C*	375°C	775°C	24°C**
	x	1/4	1/4	1/4	1/4
	y	1/4	1/4	1/4	1/4
	z	0.2502(1)	0.2500(2)	0.2500(2)	0.2502(1)
	β_{11}	57(3)	93(4)	126(6)	51(3)
$T_1$1(Al)	β_{22}	133(8)	224(12)	363(19)	106(10)
	β_{33}	110(9)	272(14)	429(22)	174(12)
	β_{12}	15(3)	22(5)	35(8)	15(4)
	β_{13}	0	0	0	0
	β_{23}	0	0	0	0
	B_{eq}***	0.52	0.96	1.46	0.54
	x	0	0	0	0
	y	1/2	1/2	1/2	1/2
	z	1/4	1/4	1/4	1/4
	β_{11}	39(3)	60(5)	88(7)	33(4)
$T_1$6(Si)	β_{22}	146(10)	245(15)	352(22)	170(12)
	β_{33}	98(10)	228(17)	342(25)	136(15)
	β_{12}	0	0	0	0
	β_{13}	0	0	0	0
	β_{23}	0	0	0	0
	B_{eq}	0.45	0.81	1.19	0.50
	x	0.1926(1)	0.1920(1)	0.1917(1)	0.1924(1)
	y	0.0778(1)	0.0783(1)	0.0785(2)	0.0778(1)
	z	0	0	0	0
	β_{11}	38(2)	60(4)	87(5)	32(3)
$T_2$1(Si)	β_{22}	83(7)	155(11)	240(15)	91(9)
	β_{33}	118(8)	239(11)	373(20)	167(12)
	β_{12}	7(3)	11(5)	13(7)	1(4)
	β_{13}	0	0	0	0
	β_{23}	0	0	0	0
	B_{eq}	0.39	0.71	1.08	0.44

* All 24°C data from Cohen *et al.* (1977)

** After heating

*** B_{eq} is the isotropic equivalent of the anisotropic temperature factors calculated using the expression

$$B_{eq} = 4/3[\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^2 + 2\beta_{12}abcos\gamma + 2\beta_{23}bccos\alpha + 2\beta_{13}accos\beta]$$

Atom		24°C	375°C	775°C	24°C
	x	0.0508(1)	0.0506(1)	0.0500(1)	0.0508(1)
	y	0.3079(1)	0.3076(1)	0.3070(2)	0.3079(1)
	z	0	0	0	0
	β_{11}	31(3)	62(4)	91(6)	32(3)
$T_2 6$(Al)	β_{22}	121(8)	220(12)	335(18)	124(10)
	β_{33}	132(9)	268(15)	382(22)	153(13)
	β_{12}	8(3)	21(5)	27(8)	5(4)
	β_{13}	0	0	0	0
	β_{23}	0	0	0	0
	B_{eq}	0.43	0.83	1.23	0.46
	x	-0.1352(1)	-0.1351(1)	-0.1347(1)	-0.1352(1)
	y	0.2375(1)	0.2369(1)	0.2363(2)	0.2374(1)
	z	0	0	0	0
	β_{11}	37(2)	57(4)	86(5)	28(3)
$T_2 3$(Si)	β_{22}	99(7)	176(11)	273(16)	133(9)
	β_{33}	105(8)	247(13)	340(19)	141(11)
	β_{12}	-11(3)	-14(4)	-40(7)	-13(4)
	β_{13}	0	0	0	0
	β_{23}	0	0	0	0
	B_{eq}	0.39	0.73	1.08	0.44
	x	0.2474(1)	0.2470(1)	0.2468(2)	0.2473(1)
	y	0.1029(1)	0.1036(2)	0.1042(3)	0.1034(2)
	z	0.1410(2)	0.1407(3)	0.1398(4)	0.1409(2)
	β_{11}	74(5)	137(7)	217(12)	66(5)
$O_1 1$	β_{22}	153(13)	277(22)	414(36)	282(16)
	β_{33}	179(15)	308(25)	450(38)	153(20)
	β_{12}	9(5)	24(9)	16(16)	3(8)
	β_{13}	-31(6)	-40(11)	-122(19)	-31(8)
	β_{23}	-19(11)	-68(19)	-95(29)	-11(16)
	B_{eq}	0.69	1.25	1.90	0.79
	x	0.0620(1)	0.0620(1)	0.0619(2)	0.0623(1)
	y	0.4160(2)	0.4166(2)	0.4159(3)	0.4166(2)
	z	0.1512(2)	0.1512(3)	0.1510(4)	0.1513(2)
	β_{11}	54(5)	90(7)	122(10)	57(5)
$O_1 6$	β_{22}	211(13)	376(21)	550(33)	215(17)
	β_{33}	180(15)	331(25)	545(39)	198(21)
	β_{12}	17(6)	24(10)	23(16)	-3(8)
	β_{13}	-2(6)	-16(11)	-73(17)	10(8)
	β_{23}	-71(11)	-150(19)	-234(32)	-72(15)
	B_{eq}	0.69	1.21	1.81	0.73

Atom		24°C	375°C	775°C	24°C
	x	-0.1732(1)	-0.1736(1)	-0.1734(2)	-0.1733(1)
	y	0.3101(2)	0.3090(2)	0.3082(4)	0.3102(2)
	z	0.1416(2)	0.1418(3)	0.1422(4)	0.1414(2)
	β_{11}	54(4)	111(7)	179(12)	60(5)
O_1^3	β_{22}	202(14)	342(22)	501(35)	174(17)
	β_{33}	199(15)	285(25)	549(42)	209(21)
	β_{12}	-11(6)	-26(10)	-55(17)	-20(8)
	β_{13}	20(6)	36(10)	95(18)	21(8)
	β_{23}	-29(11)	-90(19)	-140(32)	-39(15)
	B_{eq}	0.70	1.20	1.98	0.70
	x	0.1223(1)	0.1220(2)	0.1216(3)	0.1222(2)
	y	0.1839(2)	0.1846(4)	0.1843(6)	0.1844(3)
	z	0	0	0	0
	β_{11}	70(7)	135(12)	165(18)	73(8)
O_2^1	β_{22}	248(21)	368(35)	615(59)	178(25)
	β_{33}	386(25)	718(50)	1206(94)	401(36)
	β_{12}	51(9)	133(16)	217(27)	61(12)
	β_{13}	0	0	0	0
	β_{23}	0	0	0	0
	B_{eq}	1.04	1.83	2.83	0.98
	x	-0.0430(1)	-0.0434(2)	-0.0438(3)	-0.0432(2)
	y	0.2476(2)	0.2478(4)	0.2484(6)	0.2487(3)
	z	0	0	0	0
	β_{11}	53(7)	69(11)	122(17)	58(8)
O_2^6	β_{22}	301(21)	594(39)	883(69)	261(25)
	β_{33}	330(24)	711(49)	875(76)	360(34)
	β_{12}	-27(9)	-31(15)	-14(26)	-33(12)
	β_{13}	0	0	0	0
	β_{23}	0	0	0	0
	B_{eq}	0.97	1.85	2.62	0.98
	x	-0.1645(1)	-0.1641(2)	-0.1630(3)	-0.1646(2)
	y	0.0792(2)	0.0793(3)	0.0778(5)	0.0803(3)
	z	0	0	0	0
	β_{11}	91(7)	163(12)	243(20)	88(8)
O_2^3	β_{22}	144(19)	189(30)	298(45)	140(25)
	β_{33}	361(23)	779(50)	850(70)	412(35)
	β_{12}	-37(9)	-76(15)	-155(25)	-2(12)
	β_{13}	0	0	0	0
	β_{23}	0	0	0	0
	B_{eq}	0.96	1.79	2.32	1.00

Atom		24°C	375°C	775°C	24°C
	x	0.1625(1)	0.1622(1)	0.1626(1)	0.1624(1)
	y	1/2	1/2	1/2	1/2
	z	1/4	1/4	1/4	1/4
	β_{11}	48(3)	75(4)	109(7)	44(3)
M	β_{22}	142(9)	259(14)	385(20)	122(11)
	β_{33}	181(9)	436(16)	655(26)	225(13)
	β_{12}	0	0	0	0
	β_{13}	0	0	0	0
	β_{23}	0(7)	8(12)	30(20)	5(10)
	B_{eq}	0.58	1.13	1.68	0.59

Final fractional coordinates and thermal parameters ($\times 10^5$) for Dolni Bory cordierite at two temperatures

Atom		24°C (*Cccm*)	24°C (*Ccc*2)	375°C
	x	1/4	1/4	1/4
	y	1/4	1/4	1/4
	z	0.2502(3)	0.2494(5)	0.2501(4)
	β_{11}	41(6)	71(13)	94(9)
$T_1 1Al$	β_{22}	104(15)	129(29)	208(28)
	β_{33}	64(15)	64(32)	140(26)
	β_{12}	14(7)	29(14)	38(12)
	β_{13}	0	0	0
	β_{23}	0	0	0
	B_{eq}*	0.37		0.80
	x	-	3/4	-
	y	-	3/4	-
	z	-	0.7493(5)	-
	β_{11}	-	18(11)	-
$T_1 1_i Al$	β_{22}	-	72(26)	-
	β_{33}	-	72(31)	-
	β_{12}	-	-2(12)	-
	β_{13}	-	0	-
	β_{23}	-	0	-
	x	0	0	0
	y	1/2	1/2	1/2
	z	1/4	0.2486	1/4
	β_{11}	31(8)	32(8)	17(10)
$T_1 6Si$	β_{22}	122(20)	114(18)	219(34)
	β_{33}	44(20)	53(26)	144(35)
	β_{12}	0	0	0
	β_{13}	0	0	0
	β_{23}	0	0	0
	B_{eq}	0.33		0.52

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* B_{eq} is the isotropic equivalent of the anisotropic temperature factors calculated using the expression

$$B_{eq} = 4/3[\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^2 + 2\beta_{12}abcos\gamma + 2\beta_{23}bccos\alpha + 2\beta_{13}accos\beta].$$

Atom		24°C (*Ccem*)	24°C (*Ccc*2)	375°C
	x	0.1901(1)	0.1900(1)	0.1895(2)
	y	0.0794(2)	0.0792(2)	0.0795(3)
	z	0	0	0
	β_{11}	37(6)	38(6)	65(9)
$T_2$1Si	β_{22}	38(14)	61(14)	144(25)
	β_{33}	64(17)	57(17)	117(29)
	β_{12}	12(7)	12(7)	4(12)
	β_{13}	0	0	0
	β_{23}	0	0	0
	B_{eq}	0.31		0.58
	x	0.0501(1)	0.0501(1)	0.0499(2)
	y	0.3076(2)	0.3081(2)	0.3077(3)
	z	0	-0.0013(8)	0
	β_{11}	33(7)	30(7)	43(9)
$T_2$6Al	β_{22}	64(16)	85(16)	162(28)
	β_{33}	69(19)	97(22)	208(32)
	β_{12}	13(8)	7(8)	39(13)
	β_{13}	0	-62(27)	0
	β_{23}	0	-113(38)	0
	B_{eq}	0.29		0.62
	x	-0.1347(1)	-0.1347(1)	-0.1350(2)
	y	0.2343(2)	0.2343(2)	0.2344(3)
	z	0	-0.0023(8)	0
	β_{11}	34(7)	33(6)	59(9)
$T_2$3Si	β_{22}	43(15)	62(14)	151(26)
	β_{33}	73(16)	68(19)	140(28)
	β_{12}	-22(7)	-23(7)	-12(12)
	β_{13}	0	-45(22)	0
	β_{23}	0	78(30)	0
	B_{eq}	0.28		0.59
	x	0.2442(2)	0.2447(4)	0.2438(3)
	y	0.1052(3)	0.1053(0)	0.1049(5)
	z	0.1415(3)	0.1418(6)	0.1412(5)
	β_{11}	69(12)	89(23)	101(16)
$O_1$1	β_{22}	129(27)	217(56)	296(52)
	β_{33}	93(28)	102(54)	269(56)
	β_{12}	-15(14)	-36(27)	18(23)
	β_{13}	-44(16)	-106(32)	-80(26)
	β_{23}	-34(24)	-86(46)	-40(44)
	B_{eq}	0.55		1.10

Atom		24°C (*Cccm*)	24°C (*Ccc*2)	375°C
	x	-	0.7558(4)	-
	y	-	0.8948(6)	-
	x	-	0.8589(6)	-
	β_{11}	-	50(21)	-
$O_1 1_i$	β_{22}	-	107(48)	-
	β_{33}	-	162(55)	-
	β_{12}	-	2(24)	-
	β_{13}	-	13(30)	-
	β_{23}	-	48(43)	-
	x	0.0611(2)	0.0607(4)	0.0609(3)
	y	0.4144(4)	0.4145(7)	0.4151(5)
	z	0.1522(4)	0.1513(7)	0.1509(5)
	β_{11}	70(12)	90(24)	95(15)
$O_1 6$	β_{22}	207(29)	310(61)	324(48)
	β_{33}	134(33)	107(59)	285(60)
	β_{12}	30(14)	64(29)	23(23)
	β_{13}	23(16)	49(31)	-18(25)
	β_{23}	-58(26)	-114(50)	-131(46)
	B_{eq}	0.69		1.13
	x	-	0.9387(4)	-
	y	-	0.5850(6)	-
	z	-	0.8469(7)	-
	β_{11}	-	49(21)	-
$O_1 6_i$	β_{22}	-	144(48)	-
	β_{33}	-	195(61)	-
	β_{12}	-	9(24)	-
	β_{13}	-	19(29)	-
	β_{23}	-	33(46)	-
	x	-0.1729(2)	-0.1723(4)	-0.1729(3)
	y	0.3053(4)	0.3054(7)	0.3049(5)
	z	0.1428(4)	0.1429(7)	0.1427(5)
	β_{11}	80(13)	131(27)	65(17)
$O_1 3$	β_{22}	186(30)	272(61)	454(56)
	β_{33}	94(30)	14(53)	254(60)
	β_{12}	-21(14)	-46(28)	-45(23)
	β_{13}	3(15)	1(29)	46(22)
	β_{23}	-84(25)	-143(48)	-25(49)
	B_{eq}	0.67		1.14

Atom		24°C (*Cccm*)	24°C (*Ccc*2)	375°C
	x	-	0.1738(4)	-
	y	-	0.6942(6)	-
	z	-	0.8572(7)	-
	β_{11}	-	27(21)	-
$O_1^3{}_i$	β_{22}	-	155(51)	-
	β_{33}	-	160(58)	-
	β_{12}	-	5(23)	-
	β_{13}	-	11(26)	-
	β_{23}	-	-16(45)	-
	x	0.1188(3)	0.1189(3)	0.1200(5)
	y	0.1822(6)	0.1829(6)	0.1833(8)
	z	0	0.0019(18)	0
	β_{11}	72(20)	66(19)	137(27)
O_2^1	β_{22}	176(45)	282(51)	270(78)
	β_{33}	404(64)	373(68)	702(109)
	β_{12}	66(20)	100(25)	109(38)
	β_{13}	0	9(69)	0
	β_{23}	0	374(92)	0
	B_{eq}	0.97		1.71
	x	-0.0435(4)	-0.0433(4)	-0.0434(4)
	y	0.2449(6)	0.2461(6)	0.2462(9)
	z	0	0.0026(19)	0
	β_{11}	40(20)	54(20)	56(25)
O_2^6	β_{22}	363(56)	357(54)	579(94)
	β_{33}	494(66)	543(79)	607(101)
	β_{12}	-16(25)	-24(26)	-107(38)
	β_{13}	0	-261(62)	0
	β_{23}	0	-49(125)	0
	B_{eq}	1.20		1.67
	x	-0.1615(4)	-0.1618(4)	-0.1607(5)
	y	0.0778(5)	0.0780(5)	0.0766(7)
	z	0	-0.0016(15)	0
	β_{11}	90(19)	127(21)	190(29)
O_2^3	β_{22}	101(40)	112(40)	115(70)
	β_{33}	382(59)	462(74)	621(104)
	β_{12}	7(22)	-8(23)	-69(35)
	β_{13}	0	330(56)	0
	β_{23}	0	-53(78)	0
	B_{eq}	0.93		1.62

Atom		24°C (*Ccem*)	24°C (*Cmc*2)	375°C
M	x	0.1632(1)	0.1631(1)	0.1632(1)
	y	1/2	0.5054(3)	1/2
	z	1/4	0.2546(5)	1/4
	β_{11}	47(4)	48(3)	80(5)
	β_{22}	119(8)	49(9)	256(15)
	β_{33}	162(9)	130(9)	402(18)
	β_{12}	0	-22(9)	0
	β_{13}	0	25(11)	0
	β_{23}	12(10)	-94(11)	11(17)
	B_{eq}	0.53		1.11
NaCaFe	x	0	0	0
	y	0	0	0
	z	0	0	0
	B	3.5399(.84)	4.1322(.46)	4.8595(1.22)

APPENDIX E: INTERATOMIC DISTANCES AND ANGLES FOR THE WHITE WELL AND DOLNI BORY CORDIERITES AT VARIOUS TEMPERATURES

T-O and O-O interatomic distances (Å) and O-*T*-O angles (°) for the five tetrahedral sites *vs* temperature in White Well cordierite

		24°C	375°C	775°C	775°C* (*DLS*)	24°C**
$T_1 1$-$O_1 1$	[2]	1.760(2)	1.756(2)	1.758(3)	1.755	1.758(2)
-$O_1 3'$	[2]	1.757(2)	1.751(2)	1.751(3)	1.762	1.761(2)
Mean		1.758(1)	1.753(1)	1.754(2)	1.759	1.759(1)
$O_1 3''$-$O_1 3'$	[1]	2.873(3)	2.856(4)	2.862(7)	2.870	2.877(3)
$O_1 1$-$O_1 3''$	[2]	2.587(2)	2.591(3)	2.600(5)	2.601	2.591(2)
-$O_1 3'$	[2]	3.132(2)	3.119(3)	3.116(5)	3.125	3.134(3)
-$O_1 1'$	[1]	2.864(3)	2.875(5)	2.895(7)	2.863	2.859(4)
Mean		2.862(1)	2.859(2)	2.865(2)	2.864	2.864(1)
$O_1 3''$-$T_1 1$-$O_1 3'$	[1]	109.6(1)	109.3(2)	109.6(3)	109.0	109.6(1)
$O_1 1$-$T_1 1$-$O_1 3''$	[2]	94.7(1)	95.3(1)	95.6(2)	95.3	94.8(1)
-$O_1 3'$	[2]	125.9(1)	124.6(1)	125.2(2)	125.4	125.9(1)
-$O_1 1'$	[1]	109.0(1)	108.7(2)	108.2(2)	109.3	108.8(2)
Mean		110.0(1)	110.0(1)	109.9(1)	109.9	110.0(1)
$T_1 6$-$O_1 6$	[4]	1.626(2)	1.625(2)	1.631(3)	1.626	1.628(2)
Mean		1.626(2)	1.625(2)	1.631(3)	1.626	1.628(2)
$O_1 6$-$O_1 6'$	[2]	2.813(3)	2.815(5)	2.819(7)	2.828	2.821(4)
-$O_1 6'''$	[2]	2.676(3)	2.673(4)	2.684(6)	2.677	2.681(4)
-$O_1 6''$	[2]	2.467(3)	2.463(5)	2.475(6)	2.470	2.462(4)
Mean		2.652(1)	2.650(2)	2.659(2)	2.658	2.655(2)
$O_1 6$-$T_1 6$-$O_1 6'$	[2]	119.7(1)	120.0(2)	119.6(3)	119.5	120.0(1)
-$O_1 6'''$	[2]	110.7(1)	110.6(2)	110.7(3)	110.8	110.8(1)
-$O_1 6''$	[2]	98.7(1)	98.5(2)	98.7(2)	98.8	98.2(1)
Mean		109.7(1)	109.7(1)	109.7(1)	109.7	109.7(1)

* Simulated expansion by *DLS*. See text.

** After heating.

		24°C	375°C	775°C	775°C* (*DLS*)	24°C**
$T_2 1-O_1 1$	[2]	1.636(2)	1.638(3)	1.633(3)	1.637	1.638(2)
$-O_2 3'$	[1]	1.601(2)	1.607(3)	1.603(5)	1.602	1.613(3)
$-O_2 1$	[1]	1.583(2)	1.584(3)	1.585(5)	1.584	1.589(3)
Mean		1.614(1)	1.617(2)	1.614(2)	1.615	1.619(1)
$O_1 1-O_1 1m$	[1]	2.638(3)	2.633(5)	2.616(7)	2.626	2.638(4)
$-O_2 1$	[2]	2.632(2)	2.634(4)	2.634(6)	2.637	2.636(3)
$-O_2 3'$	[2]	2.624(2)	2.631(4)	2.633(5)	2.629	2.636(3)
$O_2 1-O_2 3'$	[1]	2.659(3)	2.670(5)	2.654(7)	2.661	2.679(4)
Mean		2.635(1)	2.639(2)	2.634(2)	2.637	2.644(1)
$O_1 1-T_2 1-O_1 1m$	[1]	107.4(1)	107.0(2)	106.4(3)	106.6	107.3(1)
$-O_2 1$	[2]	109.7(1)	109.7(1)	109.8(2)	109.9	109.5(1)
$-O_2 3'$	[2]	108.3(1)	108.4(1)	108.9(2)	108.5	108.3(1)
$O_2 1-T_2 1-O_2 3'$	[1]	113.3(1)	113.3(1)	113.2(2)	113.3	113.6(1)
Mean		109.4(1)	109.4(1)	109.5(1)	109.5	109.4(1)
$T_2 3-O_1 3$	[2]	1.634(2)	1.640(3)	1.644(4)	1.638	1.637(2)
$-O_2 3$	[1]	1.619(2)	1.614(3)	1.622(5)	1.620	1.613(3)
$-O_2 6$	[1]	1.578(2)	1.574(3)	1.563(5)	1.580	1.577(3)
Mean		1.617(1)	1.617(2)	1.618(2)	1.619	1.616(1)
$O_1 3-O_1 3m$	[1]	2.649(3)	2.654(5)	2.660(7)	2.645	2.647(4)
$-O_2 6$	[2]	2.659(2)	2.662(4)	2.655(6)	2.663	2.658(3)
$-O_2 3$	[2]	2.613(2)	2.607(4)	2.619(6)	2.617	2.607(3)
$O_2 6-O_2 3$	[1]	2.644(3)	2.640(5)	2.636(7)	2.647	2.648(4)
Mean		2.640(1)	2.639(2)	2.641(2)	2.643	2.638(1)
$O_1 3-T_2 3-O_1 3m$	[1]	108.2(1)	108.0(2)	108.0(3)	107.9	107.9(2)
$-O_2 6$	[2]	111.6(1)	111.8(1)	111.8(2)	111.7	111.6(1)
$-O_2 3$	[2]	106.8(1)	106.5(1)	106.6(2)	106.8	106.7(1)
$O_2 6-T_2 3-O_2 3$	[1]	111.5(1)	111.8(1)	111.7(1)	111.6	111.6(1)
Mean		109.4(1)	109.4(1)	109.4(1)	109.4	109.4(1)

		24°C	375°C	775°C	775°C* (*DLS*)	24°C**
$T_2$6-$O_1$6	[2]	1.773(2)	1.779(3)	1.779(4)	1.775	1.779(2)
-$O_2$1	[1]	1.716(2)	1.711(3)	1.715(5)	1.717	1.715(3)
-$O_2$6	[1]	1.706(2)	1.710(3)	1.707(5)	1.707	1.710(3)
Mean		1.742(1)	1.745(1)	1.746(2)	1.744	1.746(1)
$O_1$6-$O_1$6m	[1]	2.829(3)	2.829(5)	2.824(7)	2.828	2.821(4)
-$O_2$6	[2]	2.812(2)	2.819(4)	2.820(6)	2.814	2.818(3)
-$O_2$1	[2]	2.856(2)	2.857(4)	2.855(5)	2.858	2.860(3)
$O_2$1-$O_2$6	[1]	2.890(3)	2.896(5)	2.904(7)	2.895	2.901(4)
Mean		2.842(1)	2.846(2)	2.846(2)	2.845	2.846(1)
$O_1$6-$T_2$6-$O_1$6m	[1]	105.8(1)	105.3(2)	105.0(3)	105.6	105.5(1)
-$O_2$6	[2]	107.8(1)	107.8(1)	108.0(2)	107.8	107.7(1)
-$O_2$1	[2]	109.9(1)	109.8(1)	109.6(2)	109.8	109.8(1)
$O_2$1-$T_2$6-$O_2$6	[1]	115.2(1)	115.7(1)	116.1(1)	115.5	115.7(1)
Mean		109.4(1)	109.4(1)	109.4(1)	109.4	109.4(1)

Cation separation (Å) in White Well cordierite

		24°C	375°C	775°C	775°C* (*DLS*)	24°C**
Six-membered ring						
$T_2 1$–$T_2 6$	[2]	3.298(2)	3.293(2)	3.298(3)	3.300	3.302(2)
$T_2 6$–$T_2 3$	[2]	3.250(2)	3.252(2)	3.242(3)	3.255	3.256(2)
$T_2 3$–$T_2 1$	[2]	3.220(2)	3.221(2)	3.224(2)	3.222	3.225(2)
Mean		3.256(1)	3.255(1)	3.255(1)	3.259	3.261(1)
Four-membered ring						
$T_2 1$–$T_1 1$	[2]	3.042(1)	3.043(1)	3.045(2)	3.038	3.045(1)
$T_2 6$–$T_1 6$	[2]	3.117(1)	3.120(1)	3.123(1)	3.120	3.121(1)
$T_2 3$–$T_1 1$	[2]	3.053(1)	3.059(2)	3.066(2)	3.069	3.058(1)
Mean		3.071(1)	3.074(1)	3.078(1)	3.076	3.075(1)
d(M-T)						
M–$T_1 1$	[2]	2.855(1)	2.861(1)	2.864(1)	2.867	2.861(1)
M–$T_1 6$	[1]	2.776(1)	2.776(1)	2.789(2)	2.782	2.780(1)
Mean		2.829(1)	2.833(1)	2.839(1)	2.839	2.834(1)

* Simulated expansion by *DLS*. See text.

** After heating.

T-O-T and T-O-M angles (°) *vs* temperature
for White Well cordierite

		24°C	375°C	775°C	775°C* (*DLS*)	24°C**
$T_2$1-$O_2$1-$T_2$6	[2]	176.0(2)	176.3(3)	176.3(4)	176.3	176.3(2)
$T_2$1-$O_2$3-$T_2$3	[2]	179.5(2)	179.0(3)	179.5(4)	180.0	179.0(2)
$T_2$3-$O_2$6-$T_2$6	[2]	163.5(2)	164.3(3)	164.8(4)	164.0	164.3(2)
Mean		173.0(1)	173.2(1)	173.5(2)	173.4	173.2(1)
$T_2$1-$O_1$1-$T_1$1	[2]	127.2(1)	127.2(1)	127.7(2)	127.1	127.4(1)
$T_2$6-$O_1$6-$T_1$6	[2]	132.9(1)	132.8(1)	132.6(2)	132.9	132.6(1)
$T_2$3-$O_1$3-$T_1$1	[2]	128.2(1)	128.7(1)	129.1(2)	128.9	128.3(1)
Mean		129.4(1)	129.6(1)	129.8(1)	129.6	129.4(1)
$T_1$1-$O_1$1-M	[2]	94.9(1)	94.8(1)	94.6(2)	94.9	95.0(1)
$T_1$1-$O_1$3-M	[2]	94.6(1)	94.6(1)	94.5(2)	94.3	94.6(1)
$T_1$6-$O_1$6-M	[2]	95.0(1)	95.1(1)	95.0(2)	95.0	95.2(1)
$T_2$1-$O_1$1-M	[2]	137.7(1)	137.6(1)	137.6(2)	137.8	137.5(1)
$T_2$3-$O_1$3-M	[2]	137.1(1)	136.3(1)	136.2(2)	136.5	137.0(1)
$T_2$6-$O_1$6-M	[2]	131.9(1)	131.8(1)	132.0(2)	131.7	131.9(1)
Mean		115.3(1)	115.0(1)	115.0(1)	115.0	115.2(1)

* Simulated expansion by *DLS*. See text.

** After heating.

M-O and O-O interatomic distances (Å) and O-M-O angles (°) for the octahedral site in White Well cordierite

		24°C	375°C	775°C	775°C* (*DLS*)	24°C**
M_1-$O_1$6	[2]	2.113(2)	2.111(2)	2.124(4)	2.120	2.110(2)
-$O_1$1'	[2]	2.100(2)	2.116(2)	2.124(4)	2.121	2.110(2)
-$O_1$3'	[2]	2.115(2)	2.127(2)	2.135(4)	2.132	2.119(2)
Mean		2.108(1)	2.119(1)	2.128(2)	2.124	2.112(1)
$O_1$6-$O_1$6"	[1]	2.467(3)	2.463(4)	2.475(7)	2.470	2.462(4)
-$O_1$3'	[2]	2.902(2)	2.916(3)	2.917(5)	2.918	2.907(3)
$O_1$6"-$O_1$3'	[2]	3.272(2)	3.287(3)	3.304(5)	3.299	3.273(3)
$O_1$1"-$O_1$6"	[2]	3.261(2)	3.275(3)	3.288(5)	3.289	3.268(3)
$O_1$3'-$O_1$1'	[2]	2.587(2)	2.591(3)	2.600(5)	2.601	2.591(3)
-$O_1$1"	[2]	3.155(2)	3.175(3)	3.196(5)	3.184	3.165(3)
$O_1$1'-$O_1$1"	[1]	2.858(3)	2.875(5)	2.895(7)	2.877	2.859(4)
Mean		2.973(1)	2.986(1)	2.998(2)	2.994	2.977(1)
$O_1$6-M-$O_1$6"	[1]	71.4(1)	71.3(1)	71.3(1)	71.3	71.4(1)
-$O_1$3'	[2]	86.7(1)	86.9(1)	86.5(1)	86.6	86.8(1)
$O_1$6"-M-$O_1$3'	[2]	101.4(1)	101.7(1)	101.7(1)	101.7	101.4(1)
$O_1$1"-M-$O_1$6"	[2]	101.4(1)	101.6(1)	101.4(1)	101.7	101.5(1)
$O_1$3'-M-$O_1$1'	[2]	75.7(1)	75.3(1)	75.3(1)	75.4	75.6(1)
-$O_1$1"	[2]	96.9(1)	96.9(1)	97.3(1)	97.0	96.9(1)
$O_1$1"-M-$O_1$1'	[1]	85.8(1)	85.6(1)	85.9(2)	85.4	85.7(1)
Mean		90.1(1)	90.1(1)	90.1(1)	90.1	90.1(1)

* Simulated expansion by *DLS*. See text.

** After heating.

T-O and O-O interatomic distances (Å) and O-T-O angles (°) for the five tetrahedral sites in Dolni Bory cordierite

		24°C	375°C
$T_1 1-O_1 1$	[2]	1.748(4)	1.756(5)
$-O_1 3'$	[2]	1.748(4)	1.750(5)
Mean		1.748(2)	1.753(3)
$O_1 3''-O_1 3'$	[1]	2.870(7)	2.873(9)
$O_1 1-O_1 3''$	[2]	2.618(5)	2.631(7)
$-O_1 3'$	[2]	3.070(5)	3.072(6)
$-O_1 1'$	[1]	2.892(6)	2.898(9)
Mean		2.856(3)	2.863(3)
$O_1 3''-T_1 1-O_1 3'$	[1]	110.4(3)	110.3(4)
$O_1 1-T_1 1-O_1 3''$	[2]	96.9(2)	97.2(2)
$-O_1 3'$	[2]	122.7(2)	122.4(2)
$-O_1 1'$	[1]	109.3(2)	109.3(4)
Mean		109.8(1)	109.8(1)
$T_1 6-O_1 6$	[4]	1.627(4)	1.631(5)
Mean		1.627(2)	1.631(3)
$O_1 6-O_1 6'$	[2]	2.785(7)	2.801(9)
$-O_1 6'''$	[2]	2.697(7)	2.687(9)
$-O_1 6''$	[2]	2.487(7)	2.493(9)
Mean		2.656(3)	2.665(4)
$O_1 6-T_1 6-O_1 6'$	[2]	117.6(3)	118.3(4)
$-O_1 6'''$	[2]	111.9(3)	110.9(4)
$-O_1 6''$	[2]	99.3(3)	99.7(3)
Mean		109.6(1)	109.6(2)
$T_2 1-O_1 1$	[2]	1.634(4)	1.636(5)
$-O_2 3'$	[1]	1.623(6)	1.616(7)
$-O_2 1$	[1]	1.591(5)	1.576(7)
Mean		1.621(3)	1.616(3)

		24°C	375°C
$O_1 1$–$O_1 1m$	[1]	2.637(6)	2.633(9)
–$O_2 1$	[2]	2.642(6)	2.626(8)
–$O_2 3'$	[2]	2.647(6)	2.655(9)
$O_2 1$–$O_2 3'$	[1]	2.661(7)	2.655(9)
Mean		2.683(3)	2.680(4)
$O_1 1$–$T_2 1$–$O_1 1m$	[1]	107.6(3)	107.2(4)
–$O_2 1$	[2]	110.0(2)	109.7(3)
–$O_2 3'$	[2]	108.7(2)	108.7(3)
$O_2 1$–$T_2 1$–$O_2 3'$	[1]	111.8(3)	112.5(4)
Mean		109.5(1)	109.4(2)
$T_2 3$–$O_1 3$	[2]	1.641(3)	1.638(5)
–$O_2 3$	[1]	1.607(6)	1.615(7)
–$O_2 6$	[1]	1.575(6)	1.586(7)
Mean		1.616(2)	1.619(3)
$O_1 3$–$O_1 3m$	[1]	2.660(7)	2.663(9)
–$O_2 6$	[2]	2.664(7)	2.665(8)
–$O_2 3$	[2]	2.612(6)	2.621(8)
$O_2 6$–$O_2 3$	[1]	2.615(8)	2.624(9)
Mean		2.638(3)	2.643(3)
$O_1 3$–$T_2 3$–$O_1 3m$	[1]	108.3(3)	108.8(4)
–$O_2 6$	[2]	111.9(2)	111.5(3)
–$O_2 3$	[2]	107.0(2)	107.4(3)
$O_2 6$–$T_2 3$–$O_2 3$	[1]	110.5(3)	110.2(5)
Mean		109.4(1)	109.5(2)
$T_2 6$–$O_1 6$	[2]	1.773(4)	1.771(5)
–$O_2 1$	[1]	1.711(6)	1.721(7)
–$O_2 6$	[1]	1.726(6)	1.721(7)
Mean		1.746(3)	1.746(3)

		24°C	375°C
$O_1 6$-$O_1 6m$	[1]	2.832(7)	2.817(9)
-$O_2 6$	[2]	2.835(6)	2.826(8)
-$O_2 1$	[2]	2.866(6)	2.869(8)
$O_2 1$-$O_2 6$	[1]	2.864(8)	2.887(9)
Mean		2.850(3)	2.849(3)
$O_1 6$-$T_2 6$-$O_1 6m$	[1]	105.9(3)	105.3(4)
-$O_2 6$	[2]	108.2(2)	108.1(3)
-$O_2 1$	[2]	110.6(2)	110.5(2)
$O_2 1$-$T_2 6$-$O_2 6$	[1]	112.9(3)	114.0(4)
Mean		109.4(1)	109.4(1)

T-O-T and T-O-M angles (°) *vs* temperature for Dolni Bory cordierite

		24°C	375°C
$T_2 1$-$O_2 1$-$T_2 6$	[2]	173.3(4)	175.1(6)
$T_2 1$-$O_2 3$-$T_2 3$	[2]	179.0(4)	178.0(6)
$T_2 3$-$O_2 6$-$T_2 6$	[2]	162.9(4)	163.6(6)
Mean		171.7(2)	172.2(3)
$T_2 1$-$O_1 1$-$T_1 1$	[2]	128.7(2)	128.7(3)
$T_2 6$-$O_1 6$-$T_1 6$	[2]	133.2(2)	133.4(3)
$T_2 3$-$O_1 3$-$T_1 1$	[2]	129.4(2)	129.5(3)
Mean		130.4(1)	130.5(1)
$T_1 1$-$O_1 1$-M	[2]	94.4(2)	94.1(2)
$T_1 1$-$O_1 3$-M	[2]	94.1(2)	93.9(2)
$T_1 6$-$O_1 6$-M	[2]	94.1(2)	94.9(2)
$T_2 1$-$O_1 1$-M	[2]	136.6(2)	136.9(3)
$T_2 3$-$O_1 3$-M	[2]	136.0(2)	136.0(3)
$T_2 6$-$O_1 6$-M	[2]	131.1(2)	131.2(3)
Mean		114.4(1)	114.5(1)

Cation separation (Å) in Dolni Bory cordierite

		24°C	375°C
Six-membered ring			
$T_2 1$-$T_2 6$	[2]	3.296(3)	3.294(4)
$T_2 6$-$T_2 3$	[2]	3.264(3)	3.294(4)
$T_2 3$-$T_2 1$	[2]	3.230(3)	3.231(4)
Mean		3.263(2)	3.273(2)
Four-membered ring			
$T_2 1$-$T_1 1$	[2]	3.052(2)	3.058(3)
$T_2 6$-$T_1 6$	[2]	3.123(2)	3.125(2)
$T_2 3$-$T_1 1$	[2]	3.064(3)	3.065(3)
Mean		3.080(1)	3.083(2)
d(M-T)			
M-$T_1 1$	[2]	2.879(1)	2.881(1)
M-$T_1 6$	[1]	2.812(1)	2.817(2)
Mean		2.857(1)	2.860(1)

M-O and O-O interatomic distances (Å) and O-M-O angles (°) for the octahedral site in Dolni Bory cordierite

		24°C	375°C
M_1-$O_1$6	[2]	2.153(4)	2.161(5)
-$O_1$1'	[2]	2.154(4)	2.162(5)
-$O_1$3'	[2]	2.166(3)	2.173(5)
Mean		2.158(1)	2.165(3)
$O_1$6-$O_1$6"	[1]	2.482(7)	2.493(9)
-$O_1$3'	[2]	2.918(5)	2.936(7)
$O_1$6"-$O_1$3'	[2]	3.365(5)	3.368(7)
$O_1$1"-$O_1$6"	[2]	3.362(5)	3.377(6)
$O_1$3'-$O_1$1'	[2]	2.618(5)	2.631(6)
-$O_1$1"	[2]	3.277(5)	3.286(6)
$O_1$1'-$O_1$1"	[2]	2.856(6)	2.865(9)
Mean		3.035(2)	3.046(4)
$O_1$6-M-$O_1$6"	[1]	70.4(2)	70.4(3)
-$O_1$3'	[2]	85.0(1)	85.3(2)
$O_1$6"-M-$O_1$3'	[2]	102.4(1)	102.7(2)
$O_1$1"-M-$O_1$6"	[2]	102.7(1)	102.7(2)
$O_1$3'-M-$O_1$1'	[2]	74.6(1)	74.7(2)
-$O_1$1"	[2]	98.7(1)	98.6(2)
$O_1$1"-M-$O_1$1'	[1]	84.3(2)	84.2(3)
Mean		90.1(1)	90.2(1)

VITA

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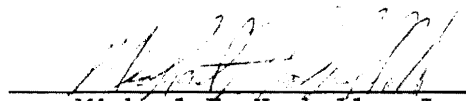

Michael F. Hochella, Jr.

HIGH TEMPERATURE CRYSTAL CHEMISTRY OF HYDROUS Mg- and Fe-RICH CORDIERITES

by

Michael F. Hochella, Jr.

(ABSTRACT)

Structural refinements have been completed using data recorded for a Mg-rich cordierite at 24°C, 375°C, 775°C and 24°C (after heating to 775°C) and for an Fe-rich cordierite at 24°C and 375°C. The mean T-O bond lengths in both cordierites remain unchanged but the mean octahedral bonds (M-O) lengthen upon heating. The unusually low thermal expansion of the Mg-cordierite is the result of its relatively "rigid" tetrahedral framework and the anisotropic expansion of octahedra isolated from each other. This anisotropic expansion leads to a slight rotation of the six-membered rings, a concomitant collapse of the structure parallel to c, and an expansion parallel to a and b. In the Fe-cordierite, the Fe-octahedron is more flattened, resulting in c being smaller and a and b being larger than the cell dimensions in the Mg-cordierite. Upon heating Fe-cordierite, there is no evidence for a rotation of the rings and a, b and c increase as the M-O bonds expand.

A re-examination of the water orientation in the cavities of the Mg-cordierite using neutron and X-ray $\Delta\rho$ maps confirms the orientation obtained previously by spectroscopic methods for type I water, *i.e.*, H-O-H near (100) with the H-H vector nearly parallel to c. However, no evidence was found in the $\Delta\rho$ maps for type II water. A peak ascribed to the alkali atoms that centers the six-membered ring

becomes elongated parallel to c upon heating through 375°C, while the peak ascribed to the oxygen associated with H_2O is absent in the Mg-cordierite at 775°C and in the Fe-cordierite at 375°C. After heating the Mg-cordierite to 775°C the peak reappeared in the $\Delta\rho$ maps computed from data recorded at 24°C, but it no longer showed an elongation parallel to a as it did before heating.