

Orthoferrosilite: High-temperature crystal chemistry

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Abstract

The high-temperature crystal structure of orthoferrosilite (FeSiO_3 ; space group $Pbca$) has been examined using intensity data collected at 24°C, 400°C, 600°C, 800°C, 900°C, and 980°C. Structural changes between 24°C and 980°C were regular, and no transformations were observed. Mean Si-O bond lengths and tetrahedral volumes decrease slightly with increasing temperature, whereas mean Fe1-O and Fe2-O bonds show significant increases. Mean thermal expansion coefficients of the mean Fe1-O and Fe2-O distances in orthoferrosilite are larger than that observed for the Fe²⁺-O bond in the $C2/c$ hedenbergite structure. Both the *A* and *B* tetrahedral chains in orthoferrosilite straighten with increasing temperature and, at 980°C, the *A* chain is almost completely extended. The change in the O3-O3-O3 angle is much larger than in $C2/c$ pyroxenes for comparable temperature intervals. A new notation describing the tetrahedral chain rotation (*N* or *P*) and the configuration around the *M2* site is introduced to aid in understanding differences among the various pyroxene structures.

Introduction

Although a natural occurrence of pure ferrosilite (FeSiO_3) has not been reported and all polymorphs of this composition are stable only at high pressure (Lindsley, 1965), this material is of considerable interest because it is one of the end-members of the pyroxene quadrilateral (MgSiO_3 - $\text{CaMgSi}_2\text{O}_6$ - $\text{CaFeSi}_2\text{O}_6$ - FeSiO_3). In a study on the stability of ferrosilite, Lindsley, MacGregor, and Davis (1964) reported the occurrence of three polymorphs. Subsequent structural investigation of these polymorphs (Burnham, 1966) revealed that one, ferrosilite III (space group $P\bar{T}$), has a pyroxenoid structure and that the other two, clinoferrosilite (space group $P2_1/c$) and orthoferrosilite (space group $Pbca$), have pyroxene structures.

Because the metal sites in ferrosilite are occupied only by Fe^{2+} , the high-temperature diffraction experiments on orthoferrosilite discussed in this paper provide valuable information on structural thermal expansion and atomic vibrations, especially when combined with similar data for other end-member pyroxenes (Cameron, Sueno, Prewitt, and Papike, 1973). In particular, this work represents: (1) the first high-temperature structural investigation of an end-member $Pbca$ orthopyroxene, and (2) the first thermal expansion data on a pyroxene whose *M2* site is completely occupied by iron.

Experimental

X-ray intensity data collection

Single crystals of orthoferrosilite, synthesized hydrothermally at 800°C and 20 kbar for 16 days, were kindly supplied by Dr. D. H. Lindsley. A single crystal, $0.08 \times 0.08 \times 0.08$ mm, was selected for X-ray

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diffraction intensity measurement. It was mounted parallel to the *c* axis on a silica glass fiber using a high-temperature ceramic cement, and sealed in an evacuated silica glass capillary to prevent oxidation of iron. The details of the heater and the cement were described by Brown, Sueno, and Prewitt (1973).

The X-ray diffraction intensities ($\sin \theta/\lambda = 0.061 - 0.756$) were measured at several temperatures (24°C, 400°C, 600°C, 800°C, 900°C, and 980°C) on a PDP-15/35 computer-controlled Picker diffractometer in the $\omega-2\theta$ mode using MoK α radiation monochromatized with a graphite crystal. All the data were converted to structure factors by applying Lorentz and polarization corrections, but no absorption corrections were made. Just after the intensity data collection of each temperature, 20 independent 2θ values were measured for cell parameter determinations, and these data were used to refine the cell parameters in the PODEX-2 least-squares program written by Slicht. Final cell parameters are listed in Table 1.

Refinement

Full-matrix least-square structure refinements for each temperature were carried out using the RFIN program written by L. Finger (Geophysical Laboratory) and atomic scattering factors for neutral atoms (Doyle and Turner, 1968). Starting atom coordinates and temperature factors for the 24°C structure refinement were taken from the room-temperature orthoferrrosilite structure given by Burnham (1966). The starting atom coordinates for the high-temperature structure refinements were taken from those of the lower temperature structures.

All observations were weighted according to $w = 1/\sigma_i^2$ where σ_i is the standard error of the structure factor based on counting statistics (Prewitt and Slicht, 1968). All reflections which were indistinguishable from background or which had asymmetric backgrounds were rejected from the least-squares refinements. Table 2 lists the number of reflections collected at each temperature (excluding the standard reflection which was checked every 20 re-

flections), the number used for the final cycle of refinement, and the final weighted *R* factors.²

The results of the high-temperature structure refinements of orthoferrrosilite are reported as follows: positional parameters and isotropic temperature factors, Table 3; interatomic distances in tetrahedral chains, Table 4; interatomic angles in tetrahedral chains, Table 5; Fe-O interatomic distances and O-O distances in Fe coordination polyhedra, Table 6; selected interatomic angles in Fe-coordination polyhedra, Table 7; and magnitude and orientation of thermal ellipsoids, Table 8.

Throughout this paper the term mean thermal expansion coefficient (MTIC) is used to describe the expansion of cell dimensions and interatomic distances with increasing temperature. The MTIC was calculated using the following equation:

$$\alpha_x = \frac{1}{X_{24}} \frac{X_T - X_{24}}{T - 24} \circ C^{-1}$$

where X_{24} and X_T are the values of a parameter at 24°C and at some higher temperature. See Cameron et al (1973) for further explanation.

Discussion

The Phca orthopyroxene structure

A projection along a^* of part of the orthoferrrosilite structure is shown in Figure 1. The *M1* and *M2* sites are occupied by Fe²⁺, and at room temperature both are six-coordinated with the *M1* coordination polyhedron being the smaller and more regular of the two. There are two symmetrically independent tetrahedral sites, each of which is confined to one chain. The two distinct chains are designated *A* and *B*, following the notation of Burnham (1966). The *B* chain is the more kinked of the two, and the tetrahedra comprising this are both larger and more distorted than those of the *A* chain. The tetrahedra of both chains are completely occupied by silicon.

There are six crystallographically nonequivalent oxygen atoms in the structure. O1*A*, O2*A*, O1*B*, and O2*B* are nonbridging oxygens (each bonded only to one Si), and O3*A* and O3*B* are bridging oxygens (each bonded to two Si atoms). The nonbridging oxygens connect tetrahedral chains and *M1* octahedral strips vertically along a^* and laterally along b .

² To obtain observed structure factors and β_{ij} 's from the final cycle of each anisotropic refinement, order document AM-76-011 from the Business Office, Mineralogical Society of America, suite 1000 lower level, 1909 K Street, N.W., Washington, D.C. 20006. Please remit \$1.00 for the microfiche.

TABLE I. Unit-Cell Parameters of Orthoferrrosilite at Several Temperatures

	24°C	400°C	600°C	800°C	900°C	980°C
<i>a</i>	18.418(2)*	18.484(1)	18.527(1)	18.569(1)	18.596(1)	18.614(1)
<i>b</i>	9.076(1)	9.124(1)	9.145(1)	9.160(1)	9.188(1)	9.177(1)
<i>c</i>	10.175(1)	10.203(1)	10.223(1)	10.243(1)	10.263(1)	10.283(1)
<i>α</i>	97.5(1)	97.5(1)	97.5(1)	97.5(1)	97.5(1)	97.5(1)
<i>β</i>	97.5(1)	97.5(1)	97.5(1)	97.5(1)	97.5(1)	97.5(1)
<i>γ</i>	97.5(1)	97.5(1)	97.5(1)	97.5(1)	97.5(1)	97.5(1)
<i>V</i>	875.6(1)	886.9(1)	893.9(1)	901.1(1)	905.5(1)	908.2(1)

* Errors in parentheses represent one standard deviation.

TABLE 3. Final Positional Parameters and Equivalent Isotropic Temperature Factors (\AA) for Orthoferrosilite

Atom	Parameter	24°C	400°C	600°C	800°C	900°C	980°C
Fe1	x	0.37573(3)*	0.37554(4)	0.37517(5)	0.37499(6)	0.37492(6)	0.37467(7)
	y	0.65415(7)	0.65283(8)	0.65204(9)	0.65130(9)	0.6510(1)	0.6505(1)
	z	0.8746(1)	0.8823(2)	0.8869(2)	0.8926(2)	0.8968(2)	0.8992(2)
	B	0.46(1)	1.09(2)	1.42(2)	1.80(2)	1.98(2)	2.27(2)
Fe2	x	0.37766(4)	0.37724(5)	0.37714(6)	0.37666(7)	0.37641(8)	0.37637(8)
	y	0.48567(7)	0.48683(9)	0.4876(1)	0.4885(1)	0.4886(1)	0.4886(1)
	z	0.3667(1)	0.3748(2)	0.3805(2)	0.3879(2)	0.3926(2)	0.3964(3)
	B	0.62(1)	1.48(2)	2.01(2)	2.55(2)	2.83(3)	3.19(3)
SiA	x	0.27229(6)	0.27223(7)	0.27247(8)	0.27259(9)	0.27267(9)	0.2729(1)
	y	0.3387(1)	0.3384(2)	0.3376(2)	0.3369(2)	0.3371(2)	0.3374(3)
	z	0.0493(2)	0.0562(3)	0.0598(3)	0.0644(3)	0.0675(3)	0.0695(4)
	B	0.47(2)	0.86(2)	1.09(3)	1.33(3)	1.51(3)	1.64(4)
SiB	x	0.47310(6)	0.47356(7)	0.47411(8)	0.47462(9)	0.4752(1)	0.4755(1)
	y	0.33448(1)	0.3348(2)	0.3350(2)	0.3358(2)	0.3358(2)	0.3353(3)
	z	0.7891(2)	0.7862(3)	0.7827(3)	0.7783(3)	0.7742(3)	0.7725(4)
	B	0.42(2)	0.82(2)	1.09(3)	1.34(3)	1.47(3)	1.70(4)
O1A	x	0.1848(2)	0.1852(2)	0.1854(2)	0.1855(2)	0.1856(3)	0.1862(3)
	y	0.3396(3)	0.3386(4)	0.3393(5)	0.3390(5)	0.3386(6)	0.3394(7)
	z	0.0387(6)	0.0490(7)	0.0532(8)	0.0605(8)	0.0648(8)	0.0669(10)
	B	0.60(5)	1.18(6)	1.45(7)	1.77(8)	2.15(9)	2.26(10)
O2A	x	0.3118(2)	0.3113(2)	0.3112(3)	0.3115(3)	0.3115(3)	0.3120(3)
	y	0.4964(4)	0.4951(4)	0.4932(5)	0.4926(6)	0.4917(6)	0.4910(6)
	z	0.0582(6)	0.0695(7)	0.0756(8)	0.0832(9)	0.0856(10)	0.0921(11)
	B	0.68(5)	1.33(7)	1.92(8)	2.30(9)	2.54(10)	2.67(11)
O3A	x	0.3025(2)	0.3022(2)	0.3014(2)	0.3011(2)	0.3013(2)	0.3005(3)
	y	0.2363(4)	0.2406(5)	0.2434(5)	0.2450(6)	0.2470(7)	0.2491(7)
	z	0.8163(6)	0.8204(8)	0.8192(8)	0.8227(8)	0.8239(8)	0.8225(9)
	B	0.70(5)	1.44(7)	1.80(8)	2.45(10)	2.57(11)	2.87(13)
O1B	x	0.5610(2)	0.5613(2)	0.5613(2)	0.5617(2)	0.5622(2)	0.5623(3)
	y	0.3365(4)	0.3380(4)	0.3379(5)	0.3392(5)	0.3396(6)	0.3401(7)
	z	0.7868(6)	0.7838(7)	0.7812(8)	0.7771(9)	0.7731(9)	0.7727(10)
	B	0.71(5)	1.22(6)	1.72(7)	1.94(8)	2.20(9)	2.49(11)
O2B	x	0.4332(2)	0.4334(2)	0.4340(2)	0.4339(3)	0.4342(3)	0.4348(3)
	y	0.4805(3)	0.4806(4)	0.4825(5)	0.4832(6)	0.4846(6)	0.4847(7)
	z	0.6932(6)	0.6965(8)	0.7011(9)	0.7064(10)	0.7077(10)	0.7117(11)
	B	0.69(5)	1.39(7)	1.79(8)	2.24(10)	2.41(10)	3.13(13)
O3B	x	0.4476(2)	0.4481(2)	0.4487(2)	0.4488(3)	0.4500(3)	0.4493(3)
	y	0.2028(3)	0.2073(4)	0.2100(5)	0.2167(6)	0.2189(7)	0.2229(8)
	z	0.5865(6)	0.5882(7)	0.5719(8)	0.5604(9)	0.5521(9)	0.5455(10)
	B	0.60(5)	1.26(7)	1.76(8)	2.42(10)	2.71(11)	3.29(13)

* Errors in parentheses are one standard deviation.

TABLE 4. Interatomic Distances in Tetrahedral Chains in Orthofersilite at Several Temperatures

SIA	24°C	400°C	600°C	800°C	900°C	980°C	HTEC (x10 ⁻⁵)
S1(A)-O1A	1.613(3)*	1.608(4)	1.613(4)	1.617(5)	1.620(5)	1.615(5)	0.4358
O2A	1.607(3)	1.606(4)	1.596(5)	1.602(5)	1.605(5)	1.601(6)	-0.9377
O3A	1.652(3)	1.651(4)	1.656(4)	1.649(5)	1.653(5)	1.651(5)	-0.5356
O3A'	1.653(3)	1.652(4)	1.625(4)	1.621(5)	1.624(5)	1.621(5)	-0.4792
Mean	1.626	1.624	1.620	1.622	1.623	1.619	-0.3495
S1B-O1B	1.621(3)	1.622(4)	1.616(4)	1.618(5)	1.619(5)	1.616(5)	-0.2926
O2B	1.598(3)	1.595(4)	1.599(4)	1.594(5)	1.602(5)	1.599(6)	0.1358
O3B	1.666(3)	1.665(4)	1.663(5)	1.659(5)	1.662(5)	1.661(6)	-0.3682
O3B'	1.662(3)	1.651(4)	1.649(5)	1.642(5)	1.628(5)	1.622(6)	-2.3439
Mean	1.637	1.633	1.632	1.628	1.628	1.624	-0.7359
O1A-O2A	2.741(4)	2.734(5)	2.725(6)	2.733(6)	2.733(7)	2.727(7)	
O1A-O3A	2.700(4)	2.690(5)	2.676(6)	2.670(6)	2.673(7)	2.653(7)	
O1A-O3A'	2.634(4)	2.630(5)	2.629(5)	2.633(6)	2.641(7)	2.628(7)	
O2A-O3A	2.514(4)	2.529(6)	2.523(6)	2.526(7)	2.535(7)	2.529(8)	
O2A-O3A'	2.686(4)	2.671(6)	2.661(6)	2.662(7)	2.646(8)	2.650(8)	
O3A-O3A'	2.6309(6)	2.6352(6)	2.6406(4)	2.6503(4)	2.6562(3)	2.6600(1)	
Mean	2.651	2.648	2.642	2.646	2.647	2.641	
O1B-O2B	2.739(4)	2.738(5)	2.737(6)	2.742(6)	2.749(7)	2.738(8)	
O1B-O3B	2.635(4)	2.639(5)	2.635(6)	2.641(6)	2.639(7)	2.651(8)	
O1B-O3B'	2.638(4)	2.635(5)	2.627(6)	2.630(6)	2.616(7)	2.620(8)	
O2B-O3B	2.597(5)	2.584(6)	2.597(7)	2.575(8)	2.590(9)	2.573(10)	
O2B-O3B'	2.662(4)	2.654(5)	2.645(6)	2.636(6)	2.629(7)	2.618(8)	
O3B-O3B'	2.756(2)	2.743(2)	2.737(2)	2.718(2)	2.716(3)	2.708(3)	
Mean	2.671	2.662	2.663	2.657	2.657	2.651	

* Errors in parentheses are one standard deviation.

TABLE 5. Interatomic Angles (°) in Tetrahedral Chains of Orthofersilite at Several Temperatures

Atoms	24°C	400°C	600°C	800°C	900°C	980°C
O1A -S1A-O2A	116.71(18)*	116.73(23)	116.24(25)	116.20(29)	116.47(32)	116.64(34)
O1A -O2A	111.58(17)	110.71(21)	110.38(22)	109.67(24)	109.47(26)	108.94(29)
O1A - -O3A	108.50(17)	108.88(20)	106.58(22)	108.81(24)	108.99(26)	108.32(29)
O2A - -O3A	100.97(16)	101.56(21)	102.17(24)	102.03(27)	102.64(29)	102.87(32)
O2A - -O3A'	112.03(17)	111.69(22)	111.42(25)	111.37(28)	110.60(37)	110.95(32)
O3A - -O3A'	106.46(12)	106.67(15)	107.63(16)	108.36(18)	108.26(19)	108.79(20)
Mean	109.38	109.37	109.40	109.41	109.42	109.42
O1B -S1B-O2B	116.64(18)	116.65(22)	116.73(25)	117.21(28)	117.18(31)	116.76(35)
O1B -O2B	106.56(17)	106.95(21)	106.93(24)	107.42(27)	107.07(28)	108.10(32)
O1B - -O3B	106.94(17)	107.23(21)	107.13(23)	107.55(26)	107.34(28)	108.00(31)
O2B - -O3B	105.43(17)	104.88(23)	105.54(25)	104.68(29)	104.99(31)	104.21(35)
O2B - -O3B'	109.52(17)	109.65(21)	109.08(24)	109.07(27)	108.95(29)	108.72(33)
O3B - -O3B'	111.80(13)	111.61(16)	111.47(18)	110.87(19)	111.31(20)	111.00(23)
Mean	109.48	109.48	109.48	109.47	109.48	109.47
S1A -O3A-S1A	139.87(27)	139.76(25)	141.26(28)	141.98(32)	141.95(33)	143.39(36)
S1B -O3B-S1B	131.59(20)	133.97(26)	135.18(28)	137.83(34)	139.55(36)	140.08(40)
O3A -O3A-O3A'	190.89(28)	187.43(37)	185.26(41)	183.99(48)	182.37(52)	180.68(56)
O3B -O3B-O3B'	143.76(24)	146.97(31)	149.00(36)	154.07(45)	155.75(52)	158.85(60)

* Errors in parentheses are one standard deviation.

whereas the bridging oxygens connect individual tetrahedra in the silicate chains.

Thermal expansion mechanisms in pyroxenes

In recent years, numerous pyroxene structures have been refined using high-temperature data

(Brown *et al.*, 1972; Smyth and Burnham, 1972; Cameron *et al.*, 1973; Smyth, 1973; Smyth, 1974a). In all of these studies thermal expansion of the silicate tetrahedra was much less than that of the M1 and M2 polyhedra. Volumes of the tetrahedra changed only slightly with increasing temperature, and in addition,

TABLE 6. Fe-O and O-O Interatomic Distances in Fe Coordination Polyhedra in Orthoferrosilite at Several Temperatures

Atom	24°C	400°C	Fe-O distances (Å)	600°C	800°C	900°C	980°C	MTEC** (x10 ⁻⁵)
Fe1-01A	2.195(3)*	2.214(4)	2.228(4)	2.238(5)	2.241(5)	2.254(6)	2.657	
-01A'	2.085(3)	2.094(4)	2.090(4)	2.089(4)	2.093(5)	2.101(5)	0.665	
-01B	2.194(3)	2.231(4)	2.250(5)	2.269(5)	2.274(5)	2.289(6)	4.368	
-01B'	2.124(3)	2.110(4)	2.112(4)	2.109(5)	2.109(5)	2.105(5)	-0.817	
-02A	2.090(3)	2.110(4)	2.123(5)	2.127(5)	2.128(6)	2.134(6)	2.117	
-02B	2.124(3)	2.137(4)	2.134(5)	2.131(5)	2.133(5)	2.136(6)	0.378	
Mean	2.135	2.148	2.156	2.161	2.163	2.170	1.591	
Fe2-01A	2.158(3)	2.170(4)	2.164(4)	2.160(5)	2.162(5)	2.160(6)	-0.035	
-01B	2.129(3)	2.131(4)	2.139(5)	2.137(5)	2.135(5)	2.140(6)	0.477	
-02A	2.052(3)	2.018(4)	2.020(5)	2.018(5)	2.029(5)	2.014(6)	-0.149	
-02B	1.994(3)	1.985(4)	1.985(5)	1.994(5)	1.990(5)	2.000(6)	0.235	
-03A	2.460(3)	2.513(4)	2.556(5)	2.535(5)	2.598(6)	2.628(6)	6.879	
-03B	2.600(3)	2.699(4)	2.770(5)	2.807(5)	2.966(6)	3.016(7)	16.986	
-03B'	3.097(3)	3.060(4)	3.036(5)	2.971(6)	2.850(6)	2.900(7)	-6.314	
Mean (6)	2.228	2.253	2.274	2.296	2.311	2.326	4.592	
(7)	2.352	2.368	2.383	2.393	2.403	2.408	2.546	
Fe1 Octahedron								
			O-O distances (Å)					
	24°C	400°C	600°C	800°C	900°C	980°C		
O1A -01A'	3.083(3)	3.087(4)	3.103(5)	3.110(5)	3.113(6)	3.125(6)		
O1A -02A	3.119(4)	3.137(5)	3.154(6)	3.176(7)	3.183(8)	3.199(8)		
O1A'-02A	3.103(5)	3.131(6)	3.168(6)	3.170(7)	3.174(8)	3.198(8)		
O1A -01B	2.849(4)	2.883(5)	2.899(5)	2.912(6)	2.912(6)	2.929(7)		
O1A'-01B	2.932(4)	2.936(5)	2.946(5)	2.947(5)	2.946(6)	2.958(6)		
O1A -01B'	2.932(4)	2.936(5)	2.946(5)	2.947(5)	2.945(6)	2.958(6)		
O1A'-02B	2.838(4)	2.851(5)	2.857(5)	2.858(7)	2.857(7)	2.857(8)		
O2A -01B'	2.907(4)	2.909(6)	2.922(5)	2.909(7)	2.910(7)	2.897(6)		
O2A -02B	2.947(4)	2.993(6)	3.015(4)	3.025(7)	3.039(7)	3.045(4)		
O1B -01B'	3.058(3)	3.081(4)	3.089(5)	3.112(5)	3.123(6)	3.131(7)		
O1B -02B	3.235(4)	3.264(6)	3.253(4)	3.253(7)	3.257(8)	3.261(9)		
O1B'-02B	3.192(5)	3.197(6)	3.188(5)	3.184(7)	3.194(8)	3.180(9)		
Fe2 Polyhedron								
	24°C	400°C	600°C	800°C	900°C	980°C		
O1A-02A	2.925(5)	2.943(6)	2.949(6)	2.963(7)	2.983(8)	2.967(9)		
O1A-03A	2.634(5)	2.630(5)	2.629(5)	2.633(6)	2.641(7)	2.623(7)		
O2A-03A	2.514(4)	2.529(6)	2.523(6)	2.526(7)	2.536(7)	2.529(8)		
O1A-01B	2.849(4)	2.883(5)	2.889(5)	2.912(6)	2.912(6)	2.929(7)		
O1A-02B	2.838(4)	2.851(5)	2.857(5)	2.858(7)	2.857(7)	2.875(8)		
O2A-01B	2.908(5)	2.909(6)	2.922(6)	2.909(7)	2.910(7)	2.897(8)		
O2A-03B	3.093(5)	3.132(6)	3.153(6)	3.191(7)	3.223(8)	3.232(9)		
O3A-02B	3.339(4)	3.331(6)	3.346(6)	3.350(7)	3.352(7)	3.357(8)		
O3A-03B	2.960(5)	2.969(6)	3.033(6)	3.085(6)	3.129(6)	3.147(7)		
O1B-02B	3.105(5)	3.121(6)	3.134(7)	3.036(7)	3.021(8)	3.038(9)		
O1B-03B	3.396(5)	3.451(6)	3.495(7)					
O2B-03B	2.662(4)	2.654(5)	2.645(6)	2.635(7)	2.629(7)	2.618(8)		

* Error in parentheses represents one standard deviation.

** MTEC: Mean thermal expansion coefficient. See text of paper for explanation.

TABLE 7. Interatomic Angles ($^{\circ}$) in Fe Coordination Polyhedra in Orthoferrositite at Several Temperatures

Atom	24°C	400°C	600°C	800°C	900°C	980°C
O1A - M1-O1A'	92.19(12)*	91.77(14)	91.82(15)	91.84(17)	91.76(19)	91.62(20)
O1A - -O2A	92.19(12)	92.97(15)	93.44(16)	93.36(18)	93.49(20)	93.57(21)
O1A' - -O2A	96.03(12)	95.58(15)	96.95(17)	97.01(18)	97.50(19)	97.52(20)
O1A - -O1B	80.93(11)	80.51(13)	80.59(14)	80.39(16)	80.34(16)	80.29(17)
O1A - -O1B'	85.49(12)	85.46(14)	85.46(16)	85.31(16)	85.15(18)	85.42(20)
O1A' - -O1B	86.47(12)	85.66(14)	85.44(15)	84.97(17)	84.68(18)	84.62(20)
O1A' - -O2B	84.82(12)	84.96(16)	85.13(17)	85.23(19)	85.05(20)	85.47(23)
O2A - -O1B	87.29(12)	87.15(15)	87.25(17)	86.75(19)	86.75(20)	86.23(23)
O2A - -O2B	88.78(13)	89.63(15)	90.18(17)	90.57(19)	91.02(20)	91.33(22)
O1B - -O1B'	90.01(11)	90.35(14)	90.13(16)	90.51(17)	90.79(18)	90.82(20)
O1B - -O2B	97.03(12)	96.65(15)	95.79(17)	95.67(18)	95.24(19)	94.91(22)
O1B' - -O2B	97.45(13)	97.66(15)	97.34(18)	97.36(19)	97.72(20)	97.15(23)
O1A-H2-O2A	88.72(13)	89.24(15)	89.58(17)	90.27(19)	90.72(20)	90.53(22)
O1A - -O3A	110.27(11)	111.12(13)	111.34(14)	111.85(16)	112.45(17)	112.29(19)
O2A - -O3A	67.39(12)	66.83(14)	65.70(16)	65.30(17)	65.11(18)	64.46(20)
O1A - -O1B	83.29(11)	84.17(13)	84.70(15)	85.34(16)	85.34(17)	85.87(19)
O1A - -O2B	86.16(13)	86.53(16)	86.73(17)	86.83(18)	86.86(20)	87.37(22)
O2A - -O1B	88.88(13)	89.01(16)	89.20(17)	88.84(19)	88.65(20)	88.37(22)
O2A - -O3B	83.02(12)	81.83(15)	80.68(17)	79.00(18)	121.23(19)	120.48(21)
O3A - -O2B	111.26(12)	111.21(15)	112.21(16)	112.50(18)	113.15(19)	113.76(22)
O3A - -O3B	71.30(10)	70.14(12)	69.46(13)	68.43(14)	65.95(14)	66.12(16)
O1B - -O2B	93.95(12)	94.38(16)	94.25(18)	94.53(20)	94.11(22)	94.34(24)
O1B - -O3B	91.31(11)	90.41(13)	89.89(15)	89.25(16)	88.60(18)	88.39(20)
O2B - -O3B	102.38(11)	102.72(14)	103.33(16)	104.20(17)	104.65(19)	105.22(22)

Errors in parentheses are one standard deviation.

the volume of the $M2$ polyhedron (generally occupied by larger cations such as Ca, Na, Fe^{2+}) showed a higher rate of increase than the $M1$ polyhedron (occupied by atoms such as Mg, Al, Fe^{2+} , Fe^{3+}). This differential thermal expansion between the tetrahedra and polyhedra determines to a large degree how the structures behave with increasing temperature. Structural adaptations (Cameron *et al.*, 1973) necessary to maintain the fit between the tetrahedral chains and the octahedral strips include: (1) stretching of the silicate chains (increase of O3-O3-O3 angle), (2) distortion of the silicate tetrahedra, and (3) increase in out-of-plane tilting of tetrahedra as a result of movement of the O2 atoms farther from the bc plane which contains the O3 atoms.

Topology of the $P\bar{h}ca$, $P2/c$ and $C2/c$ structures

Thompson (1970) discussed pyroxene architecture based on ideal close-packing of oxygen atoms, i.e., regular tetrahedra and octahedra with equal-length edges. In these "ideal" models, the basal triangle of an individual tetrahedron or octahedron is assumed to be parallel to the bc plane of the unit cell. Thompson (1970) pointed out that there are two possible orientations of a tetrahedral chain with re-

spect to the $M1$ octahedral strip to which it is connected through common O1 oxygen atoms. Thompson called these O or S rotations because in real silicate structures the orientations of the silicate chains are intermediate between the O and S extremes. In this paper, we use O or S orientation when speaking of ideal structures and O or S rotation to indicate the direction of rotation in real structures. In an O orientation or rotation, the basal triangles of the tetrahedra in the chain point in a direction opposite to the triangles on the top of the $M1$ octahedra to which they are linked (Fig. 2a). In an S orientation, the tetrahedral triangles are directed in the same way as the triangular faces of the octahedra (Fig. 2b). These two orientations correspond to cubic close packing (O orientations) or hexagonal close packing (S orientations) of the oxygen atoms.

Although the concept of O and S orientations is convenient for describing the two possibilities shown in Figure 2, additional relationships occur when larger segments of the structure are examined. Not only is it possible to attach tetrahedral chains to the tops and bottoms of octahedral strips in two different ways, but it is also possible to attach them laterally in different ways. Following the Thompson theme, we

TABLE 8. Amplitudes and Orientations of Major Axes of Thermal Ellipsoids

Atom	Ellipsoid axis (r_i)	24°C	400°C	600°C	800°C	900°C	980°C
Fe 1	rms	.064(2)**	.104(2)	.116(2)	.130(2)	.136(2)	.145(2)
r_1	a [†]	33 (5)	55 (5)	56 (5)	63 (2)	57 (5)	60 (3)
	b [†]	94 (5)	93 (5)	99 (5)	99 (3)	99 (5)	94 (3)
	c [†]	57 (7)	32 (5)	33 (3)	29 (3)	33 (2)	30 (3)
r_2	rms	.075(2)	.118(2)	.139(2)	.157(2)	.165(2)	.176(2)
	a	57 (8)	36 (6)	32 (3)	39 (8)	33 (2)	30 (5)
	b	79 (7)	70 (8)	86 (11)	114 (11)	89 (13)	89 (11)
r_3	c	144 (8)	119 (5)	122 (4)	119 (3)	123 (2)	120 (3)
	rms	.088(2)	.128(2)	.146(2)	.164(2)	.172(2)	.185(2)
	a	93 (5)	105 (7)	88 (10)	115 (10)	90 (25)	89 (10)
r_1	b	12 (7)	20 (8)	9 (5)	154 (11)	179 (26)	5 (4)
	c	79 (6)	78 (5)	81 (7)	87 (7)	89 (14)	86 (7)
Fe 2	rms	.067(2)	.106(2)	.124(2)	.141(2)	.149(2)	.156(2)
r_1	a	49 (3)	51 (3)	49 (3)	50 (3)	52 (1)	47 (1)
	b	86 (3)	90 (2)	90 (2)	85 (2)	92 (2)	83 (2)
	c	41 (3)	39 (2)	41 (1)	41 (1)	38 (1)	44 (1)
r_2	rms	.090(2)	.142(2)	.167(2)	.189(2)	.199(2)	.212(2)
	a	51 (3)	60 (3)	61 (3)	67 (4)	66 (5)	72 (2)
	b	59 (5)	40 (4)	40 (5)	34 (5)	30 (6)	32 (6)
r_3	c	126 (4)	114 (3)	115 (3)	114 (3)	107 (4)	116 (4)
	rms	.104(2)	.157(2)	.182(2)	.203(2)	.214(2)	.228(2)
	a	115 (4)	127 (3)	125 (3)	131 (3)	132 (3)	132 (3)
r_1	b	31 (5)	50 (4)	56 (5)	56 (5)	60 (6)	59 (6)
	c	73 (4)	61 (2)	60 (3)	60 (3)	57 (2)	57 (3)
Si A	rms	.061(2)	.090(3)	.104(4)	.110(4)	.117(3)	.124(4)
r_1	a	16 (18)	157 (31)	30 (22)	22 (14)	11 (6)	96 (25)
	b	89 (5)	105 (7)	71 (5)	75 (5)	79 (5)	73 (5)
	c	73 (18)	73 (31)	68 (26)	74 (16)	86 (9)	18 (6)
r_2	rms	.070(3)	.095(3)	.109(3)	.120(3)	.134(3)	.131(4)
	a	74 (18)	106 (29)	66 (25)	71 (15)	84 (9)	170 (16)
	b	91 (7)	109 (9)	91 (9)	100 (6)	101 (7)	99 (8)
r_3	c	164 (18)	162 (30)	156 (25)	156 (12)	168 (7)	94 (24)
	rms	.095(3)	.125(3)	.137(3)	.155(3)	.160(3)	.173(4)
	a	90 (5)	73 (5)	73 (5)	79 (4)	80 (4)	83 (5)
r_1	b	779 (7)	163 (5)	161 (5)	161 (4)	165 (5)	161 (4)
	c	89 (6)	86 (6)	81 (5)	75 (5)	78 (7)	73 (4)
Si B	rms	.057(4)	.084(3)	.100(3)	.109(4)	.115(4)	.125(4)
r_1	a	18 (7)	19 (6)	35 (9)	37 (6)	33 (6)	36 (7)
	b	104 (8)	94 (6)	95 (6)	110 (5)	104 (5)	102 (7)
	c	80 (8)	71 (7)	55 (10)	60 (6)	61 (5)	63 (6)
r_2	rms	.076(4)	.103(3)	.113(3)	.133(3)	.141(3)	.149(4)
	a	87 (10)	71 (8)	59 (10)	55 (7)	57 (6)	60 (7)
	b	118 (21)	68 (11)	108 (7)	81 (12)	76 (15)	60 (11)
r_3	c	152 (20)	150 (10)	143 (10)	143 (9)	144 (11)	135 (10)
	rms	.083(3)	.117(3)	.136(3)	.146(3)	.152(3)	.164(4)
	a	107 (7)	93 (6)	104 (5)	79 (9)	85 (10)	94 (8)
r_1	b	148 (19)	22 (11)	162 (7)	22 (7)	20 (11)	33 (10)
	c	64 (21)	68 (10)	76 (8)	71 (11)	70 (14)	57 (10)
OIA	rms	.059(10)	.090(8)	.107(8)	.091(10)	.128(9)	.126(10)
r_1	a	12 (18)	17 (10)	174 (5)	151 (5)	167 (7)	170 (11)
	b	83 (15)	85 (8)	96 (5)	98 (5)	102 (6)	95 (7)
	c	80 (11)	84 (10)	90 (6)	63 (6)	87 (12)	81 (10)
r_2	rms	.088(9)	.126(8)	.141(8)	.150(8)	.161(9)	.167(10)
	a	90 (16)	83 (10)	90 (11)	118 (7)	95 (12)	100 (11)
	b	35 (18)	107 (21)	96 (31)	85 (10)	83 (11)	73 (12)
r_3	c	125 (18)	161 (21)	174 (32)	151 (7)	171 (12)	160 (12)
	rms	.107(8)	.144(7)	.154(7)	.191(7)	.199(8)	.206(9)
	a	102 (8)	87 (8)	84 (9)	95 (6)	101 (6)	92 (6)
r_1	b	56 (18)	162 (20)	172 (24)	10 (6)	14 (8)	17 (11)
	c	37 (18)	72 (21)	84 (32)	82 (9)	82 (12)	73 (12)

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TABLE 8. Continued

Atom	Ellipsoid axis (r_1)	24°C	400°C	600°C	800°C	900°C	980°C
O2A	rms	.067(11)	.106(9)	.129(9)	.147(9)	.145(10)	.150(10)
	a	83 (15)	124 (8)	117 (7)	47 (6)	63 (6)	54 (7)
	b	116 (13)	136 (6)	153 (7)	44 (6)	34 (7)	37 (6)
	c	27 (13)	87 (16)	89 (16)	04 (18)	71 (17)	83 (17)
r ₁	rms	.087(9)	.129(8)	.150(8)	.170(8)	.171(9)	.170(10)
	a	131 (11)	104 (18)	99 (14)	94 (20)	88 (12)	80 (15)
	b	135 (16)	80 (16)	86 (18)	77 (17)	70 (16)	89 (15)
	c	105 (19)	163 (18)	171 (11)	167 (18)	160 (17)	170 (15)
r ₂	rms	.118(7)	.150(7)	.184(7)	.192(8)	.215(8)	.216(9)
	a	138 (10)	133 (9)	151 (7)	136 (8)	153 (6)	37 (7)
	b	56 (9)	47 (8)	63 (6)	49 (6)	64 (6)	127 (6)
	c	68 (8)	73 (17)	81 (10)	78 (19)	83 (9)	63 (12)
r ₃	rms	.071(10)	.090(10)	.092(11)	.105(11)	.116(11)	.115(14)
	a	44 (13)	66 (21)	76 (17)	114 (13)	63 (21)	91 (17)
	b	89 (22)	71 (6)	62 (4)	70 (6)	70 (6)	60 (3)
	c	48 (37)	31 (15)	32 (7)	32 (9)	34 (15)	30 (3)
O3A	rms	.080(9)	.110(8)	.119(8)	.140(9)	.137(10)	.144(10)
	a	49 (44)	24 (21)	14 (17)	156 (13)	27 (21)	176 (4)
	b	117 (12)	101 (8)	97 (9)	101 (5)	103 (8)	86 (9)
	c	127 (39)	111 (19)	102 (15)	111 (12)	113 (19)	93 (16)
r ₂	rms	.123(7)	.186(6)	.214(7)	.250(8)	.255(8)	.274(10)
	a	102 (7)	93 (4)	91 (4)	89 (3)	93 (3)	94 (3)
	b	151 (0)	158 (4)	151 (3)	157 (3)	156 (3)	150 (3)
	c	64 (8)	68 (4)	61 (3)	67 (3)	67 (3)	60 (3)
r ₃	rms	.054(12)	.085(9)	.113(9)	.103(10)	.116(10)	.145(10)
	a	29 (7)	8 (5)	16 (8)	15 (6)	24 (5)	25 (10)
	b	76 (7)	86 (5)	74 (4)	77 (5)	71 (5)	74 (8)
	c	66 (8)	83 (8)	79 (14)	82 (6)	76 (7)	71 (13)
O1B	rms	.099(8)	.132(7)	.140(7)	.166(7)	.175(8)	.179(8)
	a	74 (10)	83 (8)	82 (8)	60 (6)	72 (9)	74 (14)
	b	63 (9)	90 (26)	81 (10)	88 (12)	98 (12)	78 (18)
	c	148 (12)	173 (8)	167 (12)	168 (15)	160 (14)	150 (13)
r ₁	rms	.120(7)	.186(7)	.147(7)	.181(7)	.199(8)	.204(9)
	a	113 (12)	86 (5)	107 (6)	79 (6)	74 (6)	109 (9)
	b	31 (14)	176 (7)	18 (7)	165 (10)	159 (9)	21 (12)
	c	71 (15)	90 (26)	83 (10)	81 (18)	77 (18)	83 (18)
r ₂	rms	.082(9)	.088(10)	.111(10)	.123(10)	.125(11)	.171(10)
	a	51 (54)	56 (7)	56 (6)	54 (6)	58 (6)	125 (7)
	b	132 (21)	132 (5)	136 (7)	136 (5)	137 (6)	36 (11)
	c	67 (94)	70 (8)	65 (9)	69 (10)	64 (9)	84 (55)
r ₃	rms	.086(8)	.135(8)	.155(8)	.163(8)	.172(9)	.181(10)
	a	65 (65)	52 (10)	82 (10)	69 (10)	70 (10)	93 (31)
	b	97 (65)	94 (10)	114 (12)	100 (9)	107 (9)	84 (43)
	c	154 (87)	143 (10)	154 (10)	156 (11)	153 (9)	174 (51)
r ₁	rms	.109(7)	.163(7)	.178(7)	.209(8)	.216(8)	.238(9)
	a	49 (13)	55 (9)	145 (7)	44 (6)	39 (6)	35 (7)
	b	43 (13)	43 (5)	124 (9)	48 (5)	51 (5)	55 (7)
	c	78 (16)	69 (11)	83 (15)	81 (8)	84 (9)	69 (8)
r ₂	rms	.066(11)	.085(10)	.119(9)	.128(10)	.139(10)	.164(10)
	a	96 (23)	97 (9)	114 (21)	86 (19)	81 (17)	102 (11)
	b	80 (10)	63 (5)	74 (15)	55 (5)	61 (4)	72 (23)
	c	12 (16)	28 (5)	29 (11)	36 (7)	31 (3)	22 (17)
r ₃	rms	.085(8)	.127(7)	.135(8)	.150(9)	.162(9)	.171(10)
	a	173 (22)	167 (11)	164 (17)	15 (12)	17 (11)	160 (39)
	b	88 (23)	103 (11)	124 (10)	81 (12)	82 (11)	109 (22)
	c	97 (23)	91 (10)	102 (21)	101 (16)	105 (16)	95 (62)
r ₁	rms	.105(7)	.156(7)	.185(7)	.230(8)	.239(8)	.263(9)
	a	94 (16)	79 (11)	65 (6)	76 (4)	76 (5)	74 (5)
	b	170 (10)	150 (6)	142 (6)	143 (3)	150 (5)	153 (4)
	c	80 (10)	62 (5)	64 (5)	57 (3)	64 (4)	69 (4)

^{*}rms: root mean square amplitude (Å).^{**}Errors in parentheses are one standard deviation.[†]a, b, c represent angles (°) of r₁ with cell edges a, b, c, respectively.

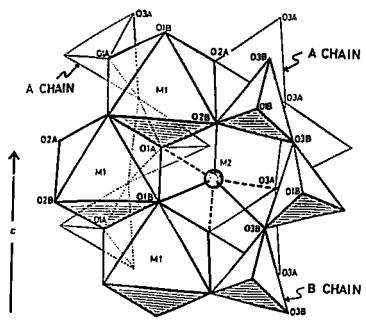


Fig. 1. Projection along a^* of part of the orthoferrosilite structure.

define N (negative) and P (positive) orientations as shown in Figure 3. In the N configuration (Fig. 3a), the basal triangles of the lateral tetrahedral chains point opposite to the triangles of the octahedra to which they are joined through common O2 oxygen atoms. In Figure 3c the orientations are both P , and in Figure 3b one of each type is shown.² One aspect of N and P orientations is that the combinations $\frac{N}{S}$, $\frac{P}{S}$, and $\frac{P}{P}$ result in different geometries and size limitations for the $M2$ site. Although in ideal structures the $M2$ site is octahedral, the $\frac{P}{P}$ configuration is the most stable because tetrahedra and octahedra do not share edges, and they adjust their shape and position relatively independently from each other. In the $\frac{P}{P}$ and $\frac{S}{S}$ configurations, one and two edges are shared, respectively. Each N occurring in this notation thus indicates an edge shared between an octahedron and a tetrahedron. Because of constraints due to edge-sharing, $M2$ sites in real structures with $\frac{P}{P}$ relationships are able to accept larger cations and, consequently, have larger volumes.

In order to preserve close-packing relationships in the ideal structures, only combinations of O with P and S with N are possible. For example, a chain with O orientation could not be attached to the upper side

of the octahedra in Figure 3a without violating the close packing arrangement [Thompson's (1970) parity violation]. However, in real silicate structures distortions permit parity violations to occur, and the $Pbca$ orthopyroxene structure has a combination of O and N rotations (Fig. 4c).

"I-beam" diagrams for $C2/c$, $P2_1/c$, and $Pbca$ silicate pyroxenes with S , O , P , and N symbolism for describing the rotational modes of tetrahedral chains and the coordination of $M2$ sites are shown in Figure 4. Each "I-beam" represents a tetrahedral-octahedral-tetrahedral unit in a real pyroxene structure. The (+) or (-) refers to the "skew" or "tilt" direction of the $M1$ octahedra. The $C2/c$ model has the octahedral sequence $+, +, +, \dots$ and the tetrahedral chains all have O and P rotations. $C2/e$ symmetry is also compatible with S and N rotations, but this results in the $M2$ octahedron sharing two edges. The octahedral stacking sequence in the $P2_1/c$ model is $+,-,+,-,\dots$ but there are two crystallographically distinct tetrahedral chains; these chains occur in combinations of $S-N$ and $O-P$ rotation. The octahedral stacking sequence of the $Pbca$ model is $+,-,-,+,\dots$ and two symmetrically distinct chains, the A and B chains, are O rotated with both P and N combinations.

Thermal structural expansion in orthoferrosilite

Mean Si-O bond lengths (Table 4, Fig. 5) and volumes (Table 9) of both the SiA and SiB tetrahedra decrease slightly with increasing temperature. The changes are regular, and over the temperature inter-

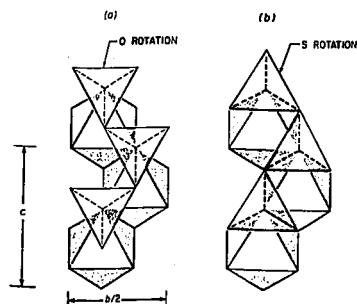
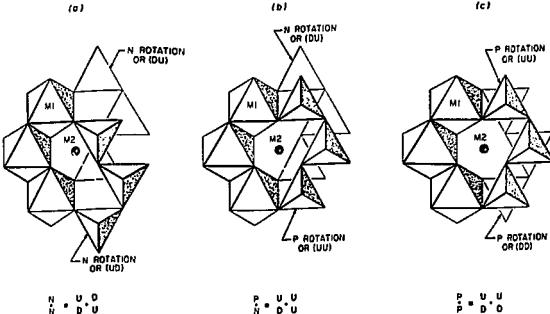


Fig. 2. Portion of the pyroxene structure showing O and S orientations of the tetrahedral chains (after Thompson, 1970).

²J. J. Papike, C. T. Prewitt, S. Sueno, and M. Cameron (1973) reviewed and discussed the topological differences of pyroxenes of several different space group symmetries using "ideal" models. In that paper symbols such as $\frac{N}{P}$, $\frac{O}{P}$ were introduced to describe the variation of the oxygen configuration around the $M2$ site in the various pyroxene structures.



a. $\frac{E}{X}$ tetrahedral chain configuration around the M2 site. Note that the tetrahedra and M2 octahedron share two edges.
b. $\frac{E}{X}$ tetrahedral chain configuration around the M2 site. Note that the tetrahedra and M2 octahedron share one edge.
c. $\frac{E}{X}$ tetrahedral chain configuration around the M2 site. Note that the tetrahedra and M2 octahedron do not share edges.

val studied the decreases are approximately equal to four times the standard deviation of the mean Si-O bond length at room temperature. The decrease observed is larger for the larger Si_2B tetrahedra (0.012\AA vs 0.007\AA), thus reducing the size difference between the two tetrahedra. This is consistent with other pyroxenes where the larger silicate tetrahedra occur in the more kinked chains. The O₃-O₃ dis-

tances behave differently in the two chains: a decrease of 0.05 Å is observed in the larger SiB tetrahedron and an increase of 0.029 Å occurs in the SiA tetrahedron. These contrasting changes, coupled with different rates of straightening of the A and B chains, are important in maintaining the fit between the silicate chains and octahedral strips with increasing temperature.

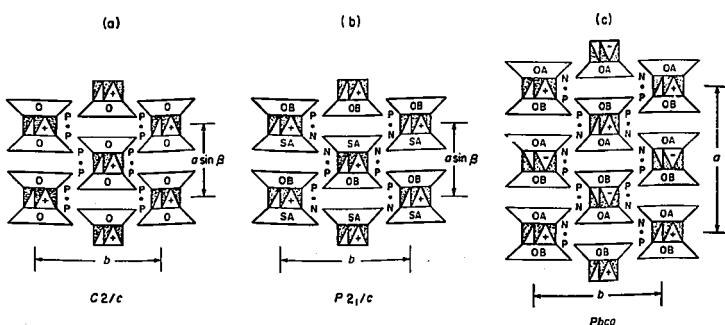


FIG. 4. "I-beam" diagrams of three pyroxene structural types with *N* and *P* symbolism. See text of paper for explanation.

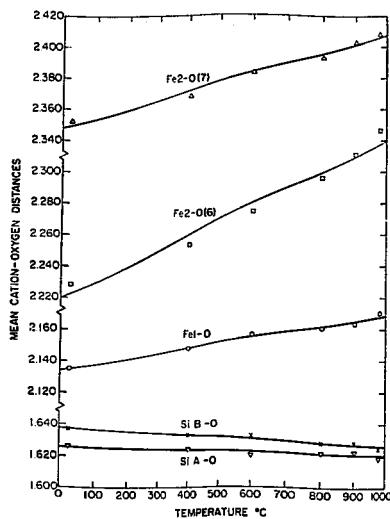


FIG. 5. Variation of mean cation-oxygen distances in orthoferrosilite with increasing temperature.

The Fe1 and Fe2 polyhedra both expand significantly with increasing temperature (Tables 6, 9, and Fig. 5). At room temperature Fe1 is coordinated by four oxygens within 2.125 Å and by two at approximately 2.195 Å. With increasing temperature this coordination is maintained, but the two longest bonds, Fe1-O1A and Fe1-O1B, exhibit slightly higher rates of increase (Fig. 6). Changes in individual bond lengths result in Fe1-O1A' and Fe1-O1B' becoming almost equivalent at temperatures close to 980°C.

TABLE 9. Cation Polyhedral Volume Expansion in Orthoferrosilite

	24°C	499°C	699°C	899°C	999°C	980°C	RTEC*
Fe1	12.800	13.039	13.189	13.237	13.318	13.432	5.0133
Fe2	16.851	17.240	17.569	17.937	18.074	18.175	8.4033
SiA	2.182	2.199	2.165	2.174	2.177	2.162	-0.671
SiB	2.233	2.221	2.216	2.199	2.193	2.187	-2.0736

* See text of paper for explanation.

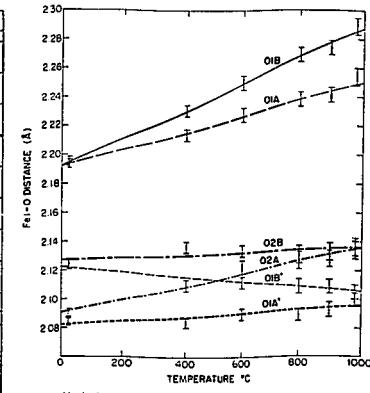


FIG. 6. Variation of individual Fe1-O distances in orthoferrosilite with increasing temperature.

The same is true for the Fe1-O2A and Fe1-O2B bonds.

At room temperature the Fe2 cation is coordinated by six oxygens in a very distorted octahedral arrangement: O1A, O1B, O2A, O2B are within 2.16 Å, O3A is at 2.46 Å, and O3B at 2.60 Å. The next nearest oxygen, O3B' is at 3.10 Å. With increasing temperature, the four short bonds remain relatively constant. However, as a result of the behavior of the three O3 atoms, the coordination number of the Fe2 cation (arbitrarily chosen as the number of oxygen atoms less than 3.00 Å distant) changes from six at 24°C to seven between 600° and 800°C, and back to six at higher temperatures. The change in coordination is related to the thermal expansion of the Fe2 polyhedron and the concomitant straightening of the tetrahedral chains with increasing temperature (Fig. 7). As the B tetrahedral chain straightens, O3B' moves closer to, and O3B farther from, Fe2. At approximately 675°C the two O3B oxygens are at an equal distance from Fe2, and angle O3B-O3B-O3B approximates 151°. Continued unkinking of the B chain moves O3B out of the coordination sphere of Fe2. The A chain, because of its configuration and disposition with respect to the Fe2 site at 24°C, behaves in a slightly different manner with increasing temperature. The same O3A atom remains bonded to Fe2 even at 980°C where the A chain becomes almost

fully extended; the second O₃/I atom does not enter the coordination sphere over the temperature range studied. In orthoferrosilite, the mean thermal expansion coefficient of the mean Fe₁-O distances (Table 6) is smaller than that of the Fe₂ polyhedron (both as six- and seven-coordinated). The values of the coefficients calculated for mean Fe₁-O and Fe₂-O bonds in orthoferrosilite are significantly larger than that obtained for the six-coordinated Fe²⁺-O bond in

the C2/c hedenbergite structure ($1.05 \times 10^{-6} \text{ C}^{-1}$; Cameron *et al.*, 1973).

Tetrahedral chain kinking and tilting

The variation with increasing temperature of the O₃-O₃-O₃ angles of six end-member clinopyroxenes and of the A and B chains in orthoferrosilite and pigeonite are plotted in Figure 7. Both chains in orthoferrosilite straighten with increasing temperature, and at 980°C the A chain is almost completely extended. Throughout the temperature range studied, the B chain (P rotated) remains more kinked than the A chain. The rate of straightening of both chains is greater at higher temperatures. In addition, the tetrahedral chains in orthoferrosilite show a much larger absolute change than those of the C2/c pyroxenes.

The O₃-O₃-O₃ angle in the A chain (Fig. 7) is plotted above 180° and that of the B chain below 180°, to maintain the analogy with the A and B chains in low clinopyroxene despite the fact that both chains are O-rotated in the *Pbca* pyroxene structure (Thompson, 1970; Papike *et al.*, 1973). Figure 7 helps to show how the A and B tetrahedral chains of the *Pbca* or P2/c pyroxenes approach symmetrically equivalent chain angles with increasing temperature and, therefore, the manner in which the M2 coordination changes from $\frac{p}{g}$ to $\frac{p}{f}$ above 980°C.

Thermal expansion of unit cell parameters

The unit-cell parameters of the *Pbca* orthoferrosilite of this study (Table 1) increase regularly with increasing temperature. Assuming linear expansion rates, the mean thermal expansion coefficients, MTEC, decrease in the order $\alpha_c > \alpha_a > \alpha_b$ (Table 10). This order differs from that determined for the C2/c and P2/c pyroxene structures: $\alpha_b > \alpha_{a10} > \alpha_c$ for C2/c clinopyroxenes (Cameron *et al.*, 1973) and $\alpha_c > \alpha_b > \alpha_{a10}$ for P2/c clinopyroxenes (Smyth, 1974a; Ohashi, 1973).⁴

The c axes of both the *Pbca* and the P2/c pyroxenes expand at higher rates than do the c axes of the C2/c pyroxenes. This behavior is related largely to the different magnitudes of straightening or extension of the tetrahedral chains in the three types of structures. The O₃-O₃-O₃ angles in the tetrahedral chains of *Pbca* orthopyroxenes and P2/c clinopyroxenes approach 180° at a rate of 0.6° to

⁴For direct comparison between the orthorhombic and monoclinic systems, the MTEC along a^* was used because this direction is perpendicular to the octahedral layers.

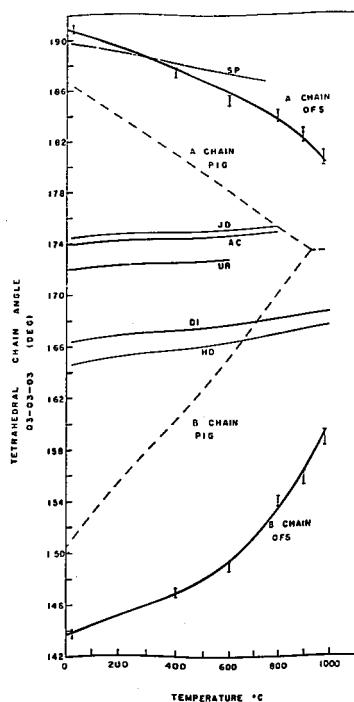


FIG. 7. Variation with increasing temperature of the O₃-O₃-O₃ angles of six end-member clinopyroxenes and of the A and B chains in orthoferrosilite and pigeonite.

TABLE 10. Mean Thermal Expansion Coefficients ($\times 10^{-6}$) of Pyroxene Cell Parameters

Orthoferrosilite**		Ferrhydrosilite***		Micas	
	(25°-980°C)	Ca _{0.015} Fe _{0.205} Al _{0.65} Si ₁₀ O ₂₀	(20°-100°C)	Ca _{0.015} Fe _{0.205} Al _{0.65} Si ₁₀ O ₂₀	(25°-1000°C)
a	0.112		0.136		0.164
b	0.103		0.145		0.145
c	0.168		0.155		0.168
v	0.393		0.438		0.377

C2/c		Retrograde**	
	Dissolve**	CafesO ₆	(25°-100°C)
	CaMgSi ₃ O ₈		
(25°-100°C)			
a	0.076		0.072
b	0.205		0.176
c	0.057		0.057
d _{2,01}	0.051		0.048
v	0.332		0.298

F2/c		Climohydsilite†	
	F _{0.95} Fe _{0.05} Al _{0.05} Si ₁₀ O ₂₀	Ca _{0.015} Fe _{0.10} Al _{0.65} Si ₁₀ O ₂₀	(20°-100°C)
	Ca _{0.1} Fe _{0.2} Al _{0.5} Si ₁₀ O ₂₀		
(25°-800°C)			
a	0.189		0.162
b	0.133		0.104
c	0.152		0.138
d _{2,01}	0.059		0.063
v	0.376		0.337

1.0° (mean of *A* and *B* chains) per 100°C temperature increase, but those of the *C2/c* pyroxenes change only about 0.1° to 0.2° per 100°C.

The MTEC of the a cell edge ($\equiv d_{100}$) in *Pbca* orthopyroxenes is larger than those of d_{100} in *P2₁/c* and *C2/c* clinopyroxenes. It is conceivable that this difference is related to the different stacking sequences of pyroxene units in orthorhombic and monoclinic pyroxenes (Papike *et al.* 1973).

The MITE of the unit cell volume of ferrosilite was compared to that of two other orthopyroxenes (Table 10). Frisillo and Buljan (1972) obtained X-ray data

TABLE II. Rate of Increase of Isotropic Temperature Factors ($\times 10^{-3}$)

Atom	$\Delta B / \Delta T$	Atom	$\Delta B / \Delta T$
FeI	1.83	OIA	1.73
FeII	2.64	OIB	1.80
		O2A	2.14
SiIA	1.21	O2B	2.12
SiIB	1.29	O3A	2.26
		O3B	2.70

Assuming linear expansion rates.

from a powder of composition $Mg_{0.8}Fe_{0.2}SiO_4$. Smyth (1973) studied a single crystal having the composition $Ca_{0.15}Mg_{0.85}Fe_0.05SiO_4$. There is an inverse correlation between Fe/Mg ratio and MTEC of the unit cell volume for the three orthopyroxenes. The most Fe-rich orthopyroxene has the smallest MTEC and the most Mg-rich orthopyroxene has the largest MTEC coefficient. Similar observations have been reported for other minerals (Cameron *et al.* 1973).

Equivalent isotropic temperature factors

The rate of increase of the equivalent isotropic temperature factors (Table 11) of both cations and anions is shown in Figure 8. The rates of increase for the four-coordinated Si atoms are significantly lower than those for the six-coordinated FeI and Fe2. The temperature factor for Fe2, initially larger than that for FeI, also increases with increasing temperature at a significantly higher rate. Cameron *et al.* (1973) showed that the rate of increase of isotropic temperature factors of cations is proportional to coordination number and average $M-O$ distances, and inversely proportional to charge on the cation and to electronegativity. Because both M sites in

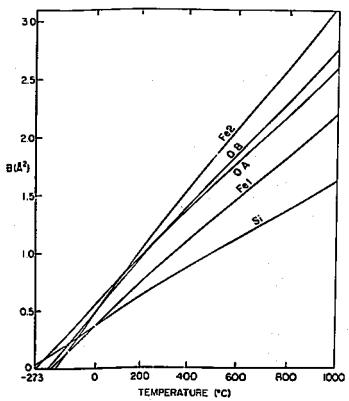


FIG. 8. Variation with increasing temperature of the equivalent isotropic temperature factors of cations and anions in orthorhombite. Values for oxygens of the *A* and *B* chains were averaged. The data points have been omitted to avoid overlap.

orthoferrosilite contain Fe^{2+} and because both are nominally six-coordinated, factors in addition to those listed above must be considered. The Fe^{2+} polyhedron is considerably more distorted than the Fe^{3+} polyhedron, and this distortion undoubtedly affects the rate of increased thermal vibration.

The rates of increase of the isotropic temperature factors of the oxygen atoms lie between those of Fe^{3+} and Fe^{2+} . The relative rates determined for orthoferrosilite ($\text{O}_3 > \text{O}_2 > \text{O}_1$) differ from those of the C_2/c pyroxenes ($\text{O}_2 > \text{O}_3 > \text{O}_1$). The high rates of increase for the O_3 atoms in the orthoferrosilite structure reflect their behavior as pivotal points during straightening of the tetrahedral chains. Furthermore, the rates of increase of the oxygens comprising the B chain, with one exception, are higher than those of the oxygens belonging to the A chain. This observation is probably related to the fact that the amount of straightening of the B chain is significantly greater than that of the A chain. Rates of increase of the isotropic temperature factors of Si atoms in the A and B chains and Fe^{2+} cations occupying M_1 and M_2 are greater than those in the C_2/c clinopyroxene structure (Cameron et al., 1973).

Thermal ellipsoids

All atoms in the orthoferrosilite structure are located on the general positions and thus their associate thermal ellipsoids are not constrained either in orientation or shape. The ellipsoids of vibration of the Fe^{3+} and Fe^{2+} atoms (Table 8; Fig. 9) are both triaxial, that for Fe^{2+} being larger. With increasing temperature, the rates of increase are similar for all axes with axes 2 and 3 of each ellipsoid increasing at slightly higher rates (Fig. 9). The short axes of both ellipsoids are oriented approximately parallel to the bonds involving apical oxygens, O_{2A} and O_{2B} of Fe^{2+} and $\text{O}_{1A'}$ and $\text{O}_{1B'}$ of Fe^{3+} .

The ellipsoids for the two Si atoms and the six oxygen atoms are also triaxial, and their orientation varies with increasing temperature. In general, the long axes of the ellipsoids of the bridging O_3 oxygens lie at large angles to the $\text{Si}-\text{O}-\text{Si}$ planes.

The possibility of a displacive transition in the orthopyroxene structure

Ohashi and Finger (1973) discussed the possibility that a high-low phase transition could occur in the orthopyroxene structure. Because orthopyroxene is in many ways similar to P_2/c clinopyroxene, one could infer that transformation to a "high" structure is possible at high temperature as was observed in

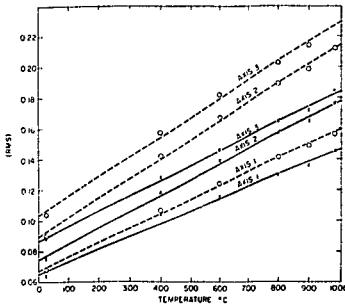


FIG. 9. Variation with increasing temperature of the magnitude of the three principal axes of the thermal ellipsoids of the Fe^{2+} cation (open circles) and the Fe^{3+} cation (crosses).

clinopyroxene ($P-C$ transition; Smyth, 1969; Prewitt, Brown, and Papike, 1971; Smyth and Burnham, 1972; Brown et al., 1972). However, Ohashi and Finger found no evidence for such a transformation and concluded only that the space group of the "high" orthopyroxene would be $Pbca$ as in the "low" orthopyroxene with "regional" symmetry imposing non-space-group extinction conditions for reflections. The two distinct silicate chains present in the "low" orthopyroxene structure would be equivalent by the symmetry operation of "regional" 2-fold axes which arise after the hypothetical transition to the high structure.

Although the present study indicates that at a temperature near 1050°C the $\text{O}_3-\text{O}_3-\text{O}_3$ angles of the A and B silicate chains (Fig. 7) and the volumes of the A and B tetrahedra (Tables 4 and 9) will be very similar, variations of individual $\text{Fe}^{3+}-\text{O}$ bond lengths with increasing temperature show that even the regional symmetry does not exist at high temperature. As shown in Figure 6, two sets of bonds, Fe^{3+} to $\text{O}_{1A'}$ and $\text{O}_{1A''}$ and Fe^{3+} to O_{2A} and O_{1B} , become almost equivalent at high temperature but another set, $\text{Fe}^{3+}-\text{O}_{1A}$ and $\text{Fe}^{3+}-\text{O}_{1B}$, diverge with increasing temperature. The divergence of the latter bond lengths violates the regional 2-fold axes in the hypothetical "high" orthopyroxene structure, and suggests that orthoferrosilite would not have this high-low transition even if the $\text{O}_3-\text{O}_3-\text{O}_3$ angles became equivalent.

Smyth (1974b) suggests another possibility for a phase transition in orthopyroxene. In a study of an

orthopyroxene crystal from lunar rock 76535, he noticed weak X-ray reflections which violated the *b* glide in space group *Pbcu*. His conclusion was that the true space group of this pyroxene is *P2₁ca* and that this resulted from the ordering of cations into twice as many crystallographically different octahedral sites as in the *Pbea* structure. The occurrence of this space group was predicted by Thompson (1970) in his study of close-packed ideal models. Smyth called these two possible structures low and high orthopyroxene and proposed that there would be a phase transformation between them. In order to test whether the orthofersilicate crystal used here might also have the *P2₁ca* space group, we refined the structure again using the 24°C data and a structure containing one set of atoms with the refined coordinates from Table 3 and one set related to the first set through an inversion center at 1/2 1/2 1/2. In the first few cycles of refinement the coordinates of set one were fixed and those of set two were allowed to vary. In subsequent cycles all coordinates were varied except for those of FeI in set one. The resulting model showed decreases in the weighted and unweighted *R*'s to 0.037 and 0.055, respectively. Although Hamilton's (1965) *R*-factor test indicates that this is a significant decrease in *R*, the temperature factors of twelve of the twenty atoms in the model refined to non-positive-definite values, and twenty correlation coefficients had magnitudes greater than 0.90. Furthermore, the refinement did not appear to be converging properly and the interatomic distances became unrealistic, with, e.g., Si-O distances greater than 1.80 Å or less than 1.57 Å.

From the experience related above, we conclude that it is not possible for us to either prove or disprove the existence of the space group *P2₁ca* within the scope of this investigation, even though our extensive effort to refine the structure in this space group using the normal criteria for acceptable results was unsuccessful. Perhaps further, more detailed work would provide a different answer.

Conclusions

1. The mean thermal expansion coefficients (MTEC) of the cell parameters of ferrosilite decrease in the order $\alpha_c > \alpha_a > \alpha_b$. The order for *C2/c* pyroxenes is $\alpha_b > \alpha_{a100} > \alpha_c$, and for *P2₁/c* pyroxenes, $\alpha_c > \alpha_b > \alpha_{a100}$.
2. A linear correlation exists between the MTEC of unit cell volume and Fe/Mg ratio in three orthopyroxenes of different compositions.
3. With increasing temperature, the mean Si-O bonds and tetrahedral volumes of both SiA and SiB tetrahedra decrease slightly. The observed decrease is larger for the larger SiB tetrahedron.

4. The FeI and Fe2 polyhedra both expand significantly with increasing temperature. The MTEC of the mean FeI-O distance is smaller than that of the mean Fe2-O distance, but both are significantly larger than that for Fe²⁺-O bonds in the *C2/c* pyroxenes.
5. A new notation describing the direction of rotation (*N* or *P*) of tetrahedral chains, and the orientation between the tetrahedra and the *M2* octahedron is introduced.
6. *A* and *B* tetrahedral chains in orthofersilite show a much larger magnitude of stretching than those of the *C2/c* pyroxenes. The rate of increase of the stretching is larger at higher temperature for both chains.
7. With increasing temperature, the rates of increase of equivalent isotropic temperature factors for Si atoms are significantly lower than those for six-coordinated Fe²⁺ atoms in the *M1* and *M2* sites. The temperature factor for Fe²⁺ in the *M2* site is larger than that of Fe²⁺ in the *M1* site, and it increases at a significantly higher rate with increasing temperature.
8. Ohashi and Finger's (1973) hypothetical "high orthopyroxene" cannot form in orthofersilite even if the O3-O3-O3 angles of both *A* and *B* chains become equivalent at high temperature.
9. Although refinement in space group *P2₁ca* was unsuccessful, the possibility that this space group exists for certain orthopyroxenes has not been ruled out.

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STRUCTURE FACTORS								PAGE 1	
	H	K	L	F(DPS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
4	0	0	100.011	195.631	-195.631	0.0	-5.620	-1.874	
6	0	0	32.281	33.592	-33.592	0.0	-1.311	-1.343	
0	0	0	103.60	113.901	-113.901	0.0	-10.342	-6.316	*
10	0	0	14.967	11.190	-11.190	0.0	3.777	2.003	
12	0	0	306.542	303.739	-303.739	0.0	2.802	0.535	
14	0	0	50.628	50.633	-50.633	0.0	-0.105	-0.081	
16	0	0	201.180	204.187	-204.187	0.0	-3.007	-0.921	
18	0	0	17.281	20.977	-20.977	0.0	-3.696	-1.337	
20	0	0	208.189	207.548	-207.548	0.0	0.641	0.188	
22	0	0	22.259	23.337	-23.337	0.0	-1.079	-0.441	
24	0	0	22.554	16.679	-16.679	0.0	5.915	2.539	
26	0	0	45.384	46.499	-46.499	0.0	-1.115	-0.664	
26	1	0	53.513	51.095	-51.095	0.0	2.418	1.502	
24	1	0	15.811	21.924	-21.924	0.0	-6.113	-1.694	
22	1	0	39.967	41.440	-41.440	0.0	-1.473	-0.856	
20	1	0	22.637	23.826	-23.826	0.0	-1.189	-0.527	
18	1	0	67.205	67.312	-67.312	0.0	-0.107	-0.079	
14	1	0	135.875	138.128	-138.128	0.0	-1.253	-0.567	
0	6	0	381.937	405.108	-405.108	0.0	-23.171	-3.343	*
10	1	0	41.747	40.617	-40.617	0.0	1.130	1.075	
6	1	0	250.563	266.756	-266.756	0.0	-7.123	-1.686	
4	1	0	14.734	9.414	-9.414	0.0	5.320	3.693	
2	1	0	84.745	84.967	-84.967	0.0	-0.223	-0.169	
0	2	0	15.171	13.245	-13.245	0.0	1.926	1.521	
2	2	0	8.261	2.908	-2.908	0.0	5.353	2.258	
4	2	0	191.760	195.744	-195.744	0.0	-3.784	-1.246	
6	2	0	20.031	19.206	-19.206	0.0	0.826	0.675	
8	2	0	86.151	88.484	-88.484	0.0	0.666	0.459	
10	2	0	32.499	33.532	-33.532	0.0	-1.033	-0.854	
12	2	0	15.374	14.244	-14.244	0.0	1.131	0.492	
14	2	0	0.311	3.666	-3.666	0.0	5.714	1.494	
16	2	0	86.337	86.980	-86.980	0.0	1.357	0.874	
18	2	0	10.588	19.876	-19.876	0.0	0.112	0.051	
20	2	0	32.762	30.800	-30.800	0.0	1.962	1.235	
22	2	0	23.448	25.493	-25.493	0.0	-1.546	-0.668	
24	2	0	42.915	46.811	-46.811	0.0	-3.906	-2.021	
26	2	0	19.202	17.982	-17.982	0.0	1.220	0.441	
26	3	0	12.450	18.044	-18.044	0.0	-5.594	-1.286	
0	6	0	380.192	405.108	-405.108	0.0	-24.917	-3.613	*
24	3	0	5.076	4.309	-4.309	0.0	0.767	0.109	
22	3	0	15.702	16.138	-16.138	0.0	-0.356	-0.113	
18	3	0	16.455	16.617	-16.617	0.0	-0.122	-0.045	
14	3	0	38.828	37.158	-37.158	0.0	1.671	1.169	
12	3	0	14.181	13.295	-13.295	0.0	0.887	0.324	
8	3	0	8.828	7.905	-7.905	0.0	0.923	0.330	
6	3	0	52.050	50.506	-50.506	0.0	1.564	1.552	
4	3	0	29.497	28.796	-28.796	0.0	0.701	0.740	
2	3	0	30.619	29.047	-29.047	0.0	1.572	1.636	
0	4	0	26.004	26.628	-26.628	0.0	0.276	0.278	
2	4	0	12.205	11.563	-11.563	0.0	0.741	0.411	
4	4	0	77.011	79.911	-79.911	0.0	-2.100	-1.638	
8	4	0	57.876	56.235	-56.235	0.0	1.661	1.400	
10	4	0	44.288	46.222	-46.222	0.0	-1.934	-1.576	

Fund cycle

24C. OPTODEFROSTITE, 6/18/73

STRUCTURE FACTORS

PAGE 2

H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA
12	4	0	6.385	16.013	-16.013	0.0	-9.629	-1.784
0	6	0	382.170	405.108	405.108	0.0	-22.938	-3.308 *
16	4	0	69.466	70.770	70.770	0.0	-1.274	-0.894
18	4	0	7.048	1.071	-1.071	0.0	5.997	1.231
20	4	0	40.056	45.296	49.296	0.0	-0.190	-0.134
22	4	0	30.754	30.573	-30.573	0.0	0.221	0.113
24	4	0	23.773	27.646	27.646	0.0	-3.873	-1.343
26	4	0	13.352	16.388	16.388	0.0	-3.036	-0.751
24	5	0	5.105	5.001	-5.001	0.0	-0.696	-0.102
22	5	0	44.639	43.659	-43.659	0.0	0.980	0.633
20	5	0	34.438	35.207	35.207	0.0	-0.769	-0.422
18	5	0	58.900	57.876	-57.876	0.0	1.014	0.574
14	5	0	239.600	237.257	-237.257	0.0	2.343	0.595
12	5	0	23.991	25.672	25.672	0.0	-1.680	-0.861
10	5	0	5.236	1.824	-1.824	0.0	3.512	0.609
8	5	0	20.323	21.033	-21.033	0.0	-0.711	-0.367
6	5	0	182.557	187.278	-187.278	0.0	-4.721	-1.626
4	5	0	14.283	9.116	-9.116	0.0	5.167	2.651
2	5	0	220.933	232.308	232.308	0.0	-11.375	-3.193 *
0	6	0	381.316	405.108	405.108	0.0	-23.792	-3.435 *
2	6	0	20.730	22.671	-22.671	0.0	-1.941	-1.034
0	6	0	380.075	405.108	405.108	0.0	-25.033	-3.631 *
4	6	0	106.732	110.608	-110.608	0.0	-3.876	-2.223
6	6	0	23.831	22.936	-22.936	0.0	0.896	0.496
8	6	0	143.825	142.951	-142.951	0.0	0.874	0.378
10	5	0	17.717	15.267	-15.267	0.0	2.450	1.033
12	6	0	164.488	164.606	-164.606	0.0	0.282	0.106
14	6	0	30.514	39.778	-39.778	0.0	-0.264	-0.186
16	6	0	106.345	107.692	-107.692	0.0	-1.347	-0.723
18	6	0	25.710	22.890	-22.890	0.0	2.820	1.456
20	6	0	170.157	179.462	-179.462	0.0	-0.305	-0.103
24	6	0	11.330	7.892	-7.892	0.0	3.438	0.783
22	7	0	22.346	24.539	-24.539	0.0	-2.193	-0.768
20	7	0	4.799	3.303	-3.303	0.0	1.406	0.201
18	7	0	17.310	16.924	-16.924	0.0	0.385	0.120
16	7	0	24.355	23.953	-23.953	0.0	0.403	0.200
14	7	0	61.907	60.238	-60.238	0.0	1.669	1.223
12	7	0	15.666	11.381	-11.381	0.0	4.284	1.636
10	7	0	84.553	85.031	-85.031	0.0	-0.478	-0.314
8	7	0	7.301	9.168	-9.168	0.0	-1.867	-0.415
6	7	0	39.149	30.810	-30.810	0.0	-0.661	-0.467
0	6	0	379.705	405.108	405.108	0.0	-25.323	-3.695 *
4	7	0	45.427	49.318	-49.318	0.0	-3.891	-2.895
2	7	0	20.774	23.270	-23.270	0.0	-2.496	-1.106
0	8	0	58.916	60.804	-60.804	0.0	-1.880	-1.431
2	8	0	34.001	36.005	-36.005	0.0	-2.004	-1.348
4	8	0	99.544	99.998	-99.998	0.0	-0.453	-0.265
8	8	0	43.602	42.250	-42.250	0.0	1.352	1.006
10	8	0	42.215	42.080	-42.080	0.0	0.134	0.095
12	8	0	48.306	48.285	-48.285	0.0	0.021	0.015
14	8	0	2.341	2.544	-2.544	0.0	-0.203	-0.026
16	8	0	80.907	80.352	-80.352	0.0	0.555	0.345
18	8	0	5.963	1.722	-1.722	0.0	4.241	0.667

24C. OPTHODERPOSILITE_6/18/73

STRUCTURE FACTORS

PAGE 3

H	K	L	F(OH)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
20	8	0	23.525	21.856	-21.856	0.0	1.669	0.659
22	8	0	17.368	14.288	-14.288	0.0	3.091	0.909
18	0	0	1.891	12.510	-12.510	0.0	-10.619	-1.054 *
12	9	0	8.043	3.728	3.728	0.0	4.315	0.913
10	9	0	13.047	7.326	7.326	0.0	5.720	1.937
0	6	0	380.618	405.108	405.108	0.0	-24.450	-3.550 *
8	9	0	25.185	28.128	-28.128	0.0	-2.942	-1.486
4	9	0	10.428	11.442	-11.442	0.0	-1.014	-0.262
2	9	0	9.032	12.670	-12.670	0.0	-3.638	-0.913
0	10	0	71.569	73.288	-73.288	0.0	-1.719	-1.135
2	10	0	13.119	17.590	-17.590	0.0	-4.870	-1.378
4	10	0	13.352	12.634	-12.634	0.0	0.718	0.207
6	10	0	8.174	0.778	-0.778	0.0	7.396	1.589
8	10	0	42.058	43.634	-43.634	0.0	-1.537	-0.975
12	10	0	30.022	29.807	-29.807	0.0	0.214	0.103
14	10	0	5.032	0.423	-0.423	0.0	4.609	0.653
18	10	0	13.803	9.009	-9.009	0.0	4.794	1.294
14	11	0	149.811	146.951	-146.951	0.0	2.861	1.109
10	11	0	14.647	12.873	-12.873	0.0	1.774	0.500
6	11	0	124.547	123.123	-123.123	0.0	1.425	0.662
4	11	0	22.026	24.591	-24.591	0.0	-2.966	-1.061
0	6	0	381.141	405.108	-405.108	0.0	-23.967	-3.471 *
2	11	0	118.586	116.392	-116.392	0.0	2.195	1.068
0	12	0	141.682	137.607	-137.607	0.0	4.075	1.699
2	12	0	9.541	12.218	-12.218	0.0	-2.677	-0.504
4	12	0	15.651	11.535	-11.535	0.0	4.115	1.224
6	12	0	5.890	9.126	-9.126	0.0	-3.236	-0.485
8	12	0	47.020	44.571	-44.571	0.0	2.449	1.496
10	12	0	12.348	13.220	-13.220	0.0	-0.872	-0.207
12	12	0	61.012	59.823	-59.823	0.0	1.189	0.744
6	13	0	16.189	13.412	-13.412	0.0	2.778	0.773
4	13	0	6.712	5.098	-5.098	0.0	3.613	0.668
2	13	0	53.615	50.105	-50.105	0.0	3.510	2.050
6	13	1	18.483	21.575	-21.575	0.0	-2.592	-0.758
5	13	1	6.443	4.049	-4.049	0.0	2.393	0.373
4	13	1	17.222	16.959	-16.959	0.0	0.264	0.077
3	13	1	23.933	19.863	-19.863	0.0	4.070	1.616
2	13	1	16.611	18.088	-18.088	0.0	-1.476	-0.409
1	13	1	20.512	18.008	-18.008	0.0	2.503	0.860
0	12	1	11.257	11.959	-11.959	0.0	-0.702	-0.162
1	12	1	14.007	7.783	-7.783	0.0	6.724	1.753
0	6	0	380.269	405.108	-405.108	0.0	-24.839	-3.602 *
3	12	1	8.334	8.079	-8.079	0.0	0.254	0.046
5	12	1	13.920	9.020	-9.020	0.0	4.899	1.331
7	12	1	14.734	7.869	-7.869	0.0	6.866	1.934
8	12	1	15.753	11.724	-11.724	0.0	4.029	1.306
10	12	1	8.683	1.133	-1.133	0.0	7.550	1.399
11	12	1	7.432	2.610	-2.610	0.0	4.821	0.839
15	11	1	3.839	16.201	-16.201	0.0	-12.362	-1.455 *
14	11	1	28.555	33.413	-33.413	0.0	-4.848	-1.849
13	11	1	15.127	14.462	-14.462	0.0	0.665	0.183
11	11	1	23.089	22.499	-22.499	0.0	0.589	0.219
10	11	1	20.177	19.977	-19.977	0.0	0.200	0.065

24C OTHOFFPOSILITE 6/18/73

STRUCTURE FACTORS

PAGE 4

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
9	11	1	23.380	23.450	-23.450	0.0	-0.070	-0.026
8	11	1	17.979	13.752	13.752	0.0	4.227	1.492
7	11	1	32.805	31.343	-31.343	0.0	1.463	0.766
6	11	1	52.371	49.912	49.912	0.0	2.459	1.616
0	6	0	380.508	405.108	405.108	0.0	-24.510	-3.553 *
5	11	1	43.529	42.318	42.318	0.0	1.211	0.740
4	11	1	11.126	3.633	3.633	0.0	7.493	2.094
3	11	1	12.188	14.265	14.265	0.0	-2.077	-0.506
2	11	1	32.383	32.240	-32.240	0.0	0.134	0.074
1	11	1	19.449	15.302	-15.302	0.0	4.147	1.759
0	10	1	55.342	55.256	55.256	0.0	0.086	0.062
1	10	1	47.502	47.026	-47.026	0.0	0.477	0.323
2	10	1	30.313	31.155	31.155	0.0	-0.841	-0.469
5	10	1	11.010	7.416	-7.416	0.0	3.594	0.976
6	10	1	24.486	21.240	-21.240	0.0	3.247	1.664
7	10	1	16.335	15.929	15.929	0.0	0.406	0.140
8	10	1	22.259	21.403	-21.403	0.0	0.856	0.367
9	10	1	12.756	13.655	-13.655	0.0	-0.829	-0.262
10	10	1	15.113	8.175	8.175	0.0	6.938	2.271
11	10	1	24.268	24.713	-24.713	0.0	-0.445	-0.182
12	10	1	42.492	40.485	-40.485	0.0	2.007	1.309
13	10	1	15.127	5.545	5.545	0.0	9.582	3.166
14	10	1	29.366	29.379	-29.379	0.0	-0.013	-0.006
0	6	0	380.367	405.108	-405.108	0.0	-24.761	-3.590 *
16	10	1	12.759	1.435	1.435	0.0	11.525	3.104 *
17	10	1	9.337	2.935	-2.935	0.0	6.402	1.294
18	10	1	16.248	18.616	-18.616	0.0	-2.358	-0.624
20	9	1	20.788	12.604	12.604	0.0	8.184	3.492
19	9	1	33.374	32.496	-32.496	0.0	0.877	0.421
18	9	1	41.893	42.277	-42.277	0.0	-0.384	-0.214
17	9	1	42.442	42.840	-42.840	0.0	-0.348	-0.189
16	9	1	14.676	14.305	-14.305	0.0	0.371	0.105
14	9	1	50.748	49.374	-49.374	0.0	1.373	0.886
13	9	1	6.472	3.220	3.220	0.0	3.252	0.565
12	9	1	75.749	75.053	-75.053	0.0	0.695	0.441
11	9	1	94.572	93.565	-93.565	0.0	1.007	0.375
10	9	1	98.311	100.617	-100.617	0.0	-2.306	-1.294
9	9	1	95.091	95.807	-95.807	0.0	-0.716	-0.413
8	9	1	61.236	39.929	-39.929	0.0	1.308	0.905
7	9	1	26.875	26.507	-26.507	0.0	0.368	0.204
6	9	1	48.175	46.978	-46.978	0.0	1.197	0.853
5	9	1	44.945	46.219	-46.219	0.0	-1.273	-0.908
0	6	0	380.482	405.108	-405.108	0.0	-24.626	-3.570 *
4	9	1	5.206	1.509	-1.509	0.0	3.698	0.652
3	9	1	36.115	37.017	-37.017	0.0	-0.902	-0.552
2	9	1	88.485	89.882	-89.882	0.0	-1.397	-0.866
1	9	1	66.490	60.340	-60.340	0.0	0.159	0.118
0	8	1	37.997	36.364	-36.364	0.0	1.633	1.204
1	8	1	8.464	9.731	-9.731	0.0	-1.266	-0.311
2	8	1	68.838	71.330	-71.330	0.0	-2.495	-1.807
3	8	1	128.386	131.496	-131.496	0.0	-3.110	-1.476
4	8	1	123.089	126.096	-126.097	0.0	-3.007	-1.482
5	8	1	77.796	77.032	-77.032	0.0	0.764	0.529

24C ORTHOFEPOSILITE 6/18/73

STRUCTURE FACTORS

PAGE 5

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	8	1	13.148	13.807	-13.807	0.0	-0.659	-0.219
7	9	1	65.633	66.940	66.940	0.0	-1.306	-0.927
8	8	1	121.437	123.360	123.360	0.0	-1.923	-0.949
9	0	1	51.084	52.001	-52.001	0.0	-0.917	-0.660
10	8	1	25.447	26.244	26.244	0.0	-0.797	-0.405
11	8	1	39.266	39.438	-39.438	0.0	-0.172	-0.118
12	8	1	61.819	61.086	-61.086	0.0	0.733	0.495
13	8	1	65.501	65.009	65.009	0.0	0.492	0.335
14	8	1	5.512	3.925	-3.925	0.0	1.587	0.269
15	8	1	71.246	71.215	71.215	0.0	0.031	0.020
0	6	0	380.772	405.108	405.108	0.0	-24.335	-3.526 *
16	8	1	70.334	71.911	71.911	0.0	-1.576	-0.975
17	8	1	46.625	44.337	-44.337	0.0	2.288	1.374
18	8	1	37.603	38.356	38.356	0.0	-0.753	-0.410
19	8	1	30.357	34.482	-34.482	0.0	-4.125	-1.803
20	8	1	49.300	50.619	-50.619	0.0	-1.318	-0.812
21	8	1	10.923	7.707	-7.707	0.0	3.216	0.715
22	7	1	21.225	12.267	-12.267	0.0	8.959	3.620
21	7	1	9.541	2.332	-2.332	0.0	7.200	1.516
19	7	1	29.016	30.376	-30.376	0.0	-1.360	-0.580
17	7	1	5.628	2.111	-2.111	0.0	3.517	0.591
16	7	1	27.705	25.537	-25.537	0.0	2.168	1.191
15	7	1	12.465	12.802	-12.802	0.0	-0.337	-0.099
14	7	1	7.403	4.696	-4.696	0.0	2.707	0.571
13	7	1	17.761	15.993	-15.993	0.0	1.768	0.727
12	7	1	20.497	21.877	-21.877	0.0	-1.380	-0.561
11	7	1	29.060	26.382	-26.382	0.0	2.678	1.626
10	7	1	19.813	16.161	-16.161	0.0	3.652	1.818
0	6	0	381.490	405.108	405.108	0.0	-23.618	-3.409 *
2	7	1	48.131	48.382	-48.382	0.0	-0.251	-0.129
8	7	1	32.951	35.449	-35.449	0.0	-2.498	-1.558
6	7	1	24.420	22.844	-22.844	0.0	1.584	0.939
5	7	1	30.634	32.787	-32.787	0.0	-2.153	-1.285
4	7	1	23.613	23.643	-23.643	0.0	-0.030	-0.016
3	7	1	30.677	32.238	-32.238	0.0	-1.561	-0.965
2	7	1	18.823	21.335	-21.335	0.0	-2.512	-1.052
1	7	1	9.323	4.291	-4.291	0.0	5.031	1.305
0	6	1	17.353	15.173	-15.173	0.0	2.180	1.026
1	6	1	15.302	14.504	-14.504	0.0	0.798	0.343
3	6	1	20.526	23.421	-23.421	0.0	-2.895	-1.353
4	6	1	6.923	1.949	-1.949	0.0	4.974	1.147
6	6	1	6.472	9.355	-9.355	0.0	-2.883	-0.604
7	6	1	16.670	16.638	-16.638	0.0	0.032	0.013
9	6	1	7.941	10.482	-10.482	0.0	-2.541	-0.569
10	6	1	12.305	8.139	-8.139	0.0	4.165	1.344
0	6	0	379.708	405.108	405.108	0.0	-25.401	-3.697 *
11	6	1	9.003	10.367	-10.367	0.0	-1.365	-0.351
12	6	1	17.266	19.211	-19.211	0.0	-1.945	-0.805
13	6	1	1.614	11.468	-11.468	0.0	-9.856	-1.156
14	6	1	18.270	16.093	-16.093	0.0	2.177	0.984
15	6	1	9.046	11.536	-11.536	0.0	-2.489	-0.563
16	6	1	8.144	2.080	-2.080	0.0	6.064	1.315
18	6	1	8.508	4.145	-4.145	0.0	4.363	0.923

24C OPTHOEPPSILITE 6/18/73

STRUCTURE FACTORS

PAGE 6

H	K	I	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DFLT4/SIGMA
20	6	1	18.721	15.689	0.0	3.033	1.069	
21	6	1	2.036	4.550	4.550	0.0	-1.714	0.197
24	6	1	4.174	2.892	2.892	0.0	1.282	0.178
25	5	1	28.681	31.089	-31.089	0.0	-2.408	-0.930
23	5	1	11.315	9.239	-9.239	0.0	2.077	0.473
22	5	1	11.226	7.996	-7.996	0.0	3.232	0.758
21	5	1	40.332	40.464	-40.464	0.0	-0.133	-0.076
20	5	1	16.771	10.967	-10.967	0.0	5.804	2.078
0	6	0	381.702	405.108	-405.108	0.0	-23.326	-3.366 *
19	5	1	2.516	10.196	-10.196	0.0	-7.680	-0.922
18	5	1	25.782	29.588	-29.588	0.0	-3.805	-1.742
17	5	1	17.630	16.184	-16.184	0.0	1.464	0.571
16	5	1	28.040	29.433	-29.433	0.0	-1.393	-0.708
15	5	1	34.803	34.870	-34.870	0.0	-0.068	0.043
14	5	1	75.665	74.277	-74.277	0.0	1.368	0.948
13	5	1	32.193	32.562	-32.562	0.0	-0.349	-0.222
12	5	1	7.475	4.704	-4.704	0.0	2.771	0.417
10	5	1	38.478	39.523	-39.523	0.0	-1.044	-0.723
9	6	1	47.634	45.047	-45.047	0.0	1.687	1.358
8	5	1	36.246	35.593	-35.593	0.0	0.654	0.492
7	5	1	62.303	62.212	-62.212	0.0	0.091	0.073
6	5	1	62.215	61.805	-61.805	0.0	0.410	0.333
5	5	1	75.395	76.532	-76.532	0.0	-1.137	-0.849
4	5	1	30.511	31.128	-31.128	0.0	-0.218	0.182
3	5	1	40.156	40.464	-40.464	0.0	-0.307	-0.201
2	5	1	75.587	78.619	-78.619	0.0	-3.033	-2.314
1	5	1	11.226	11.351	-11.351	0.0	-0.123	-0.048
0	4	1	12.261	12.050	-12.050	0.0	0.211	0.108
0	6	0	380.831	405.108	-405.108	0.0	-24.277	-3.518 *
1	4	1	52.401	56.904	-56.904	0.0	-4.503	-4.275
2	4	1	77.000	79.865	-79.865	0.0	-2.865	-2.235
3	4	1	42.492	44.582	-44.582	0.0	-2.100	-2.115
4	4	1	52.470	55.226	-55.226	0.0	-1.348	-1.244
5	4	1	87.065	87.299	-87.299	0.0	-0.234	-0.163
6	4	1	27.953	28.655	-28.655	0.0	-0.702	-0.542
7	4	1	36.828	39.034	-39.034	0.0	-0.205	-0.178
8	4	1	78.759	8.134	-8.134	0.0	0.625	0.200
9	4	1	7.403	5.531	-5.531	0.0	1.871	0.466
10	4	1	5.000	8.319	-8.319	0.0	-3.228	-0.504
11	4	1	16.553	15.164	-15.164	0.0	1.389	0.561
12	4	1	9.774	10.664	-10.664	0.0	-0.891	-0.521
13	4	1	18.401	14.471	-14.471	0.0	3.930	1.875
14	4	1	31.610	33.070	-33.070	0.0	-1.460	-0.911
15	4	1	13.483	14.650	-14.650	0.0	-1.167	-0.363
16	4	1	48.072	49.554	-49.554	0.0	-1.481	-1.045
17	4	1	37.359	37.548	-37.548	0.0	-0.149	-0.097
18	4	1	31.043	32.726	-32.726	0.0	-0.883	-0.509
19	4	1	13.450	15.038	-15.038	0.0	-1.380	-0.302
20	4	1	2.614	9.715	-9.715	0.0	-0.101	-0.024
0	6	0	380.509	405.108	-405.108	0.0	-24.199	-3.506 *
21	4	1	17.295	18.651	-18.651	0.0	-1.356	-0.452
22	4	1	40.069	39.247	-39.247	0.0	0.822	0.361
23	4	1	45.252	44.331	-44.331	0.0	0.921	0.348

24C. O₂THOFEPPSILITE 6/18/73

STRUCTURE FACTORS

PAGE 7

H	K	L	F(NRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
24	4	1	24.763	28.620	-26.620	0.0	-1.857	-0.701
25	4	1	35.721	37.304	37.304	0.0	-1.583	-0.798
26	3	1	48.891	49.601	-49.601	0.0	-0.710	-0.398
25	3	1	45.851	49.624	-49.624	0.0	-3.773	-2.135
24	3	1	41.412	45.179	45.179	0.0	-3.767	-1.970
23	3	1	40.127	40.978	-40.978	0.0	-0.851	-0.474
22	3	1	113.496	117.996	117.996	0.0	-4.501	-2.213
21	3	1	90.364	91.155	91.155	0.0	-0.791	-0.461
20	3	1	14.196	15.433	15.433	0.0	-1.237	-0.362
19	3	1	45.661	47.115	47.115	0.0	-1.454	-0.948
18	3	1	90.438	91.219	-91.219	0.0	-0.381	-0.232
17	3	1	107.585	109.034	-109.034	0.0	-1.049	-0.567
16	3	1	6.152	8.220	-8.220	0.0	-2.068	-0.403
15	3	1	25.156	21.725	-21.725	0.0	3.431	2.031
14	3	1	86.296	84.998	-84.998	0.0	1.299	0.837
13	3	1	28.259	27.062	27.062	0.0	1.197	0.727
12	3	1	14.4975	145.272	-145.272	0.0	1.703	0.721
11	3	1	223.225	219.709	-219.709	0.0	3.515	0.972
10	3	1	238.485	235.027	-235.027	0.0	3.458	0.897
9	3	1	174.943	174.196	-174.196	0.0	0.747	0.269
8	3	1	63.711	64.350	-64.350	0.0	-0.639	-0.538
7	3	1	66.162	64.829	-64.829	0.0	1.333	1.135
6	3	1	210.759	200.652	-200.652	0.0	2.107	0.622
5	3	1	173.770	172.547	-172.547	0.0	1.031	0.375
4	3	1	44.084	41.045	41.045	0.0	3.039	3.105
3	3	1	43.981	50.524	50.524	0.0	-6.542	-6.892
2	3	1	149.937	182.192	-182.192	0.0	-12.255	-4.579 *
1	3	1	181.511	195.654	-195.654	0.0	-14.142	-4.926 *
0	2	1	63.227	67.777	-67.777	0.0	-4.551	-6.269
1	2	1	21.764	22.724	-22.724	0.0	-0.961	-0.815
2	2	1	125.480	128.312	-128.312	0.0	-2.832	-1.448
3	2	1	153.096	155.554	-155.554	0.0	-2.458	-1.030
4	2	1	156.250	159.168	-159.168	0.0	-2.918	-1.190
5	2	1	134.621	136.494	136.494	0.0	-1.874	-0.891
6	2	1	14.240	15.210	-15.210	0.0	-0.970	-0.635
7	2	1	108.820	105.878	-105.878	0.0	2.943	1.700
8	2	1	123.901	122.728	-122.728	0.0	1.173	0.600
0	6	1	380.424	405.108	405.108	0.0	-24.684	-3.579 *
1	2	1	56.148	55.401	-55.401	0.0	0.746	0.662
10	2	1	35.269	33.850	-33.850	0.0	1.419	1.202
11	2	1	55.752	55.350	-55.350	0.0	0.402	0.348
12	2	1	75.852	76.139	-76.139	0.0	-0.288	-0.206
13	2	1	61.042	61.316	61.316	0.0	-0.275	-0.213
15	2	1	61.452	60.910	-60.910	0.0	0.543	0.407
16	2	1	90.231	90.454	-90.454	0.0	-0.224	-0.141
17	2	1	66.074	63.595	-63.595	0.0	2.479	1.796
18	2	1	44.288	45.033	-45.033	0.0	-0.745	-0.510
19	2	1	18.387	18.004	-18.004	0.0	-0.617	-0.165
20	2	1	31.377	29.534	-29.534	0.0	1.843	1.119
21	2	1	11.781	12.799	-12.799	0.0	-1.019	-0.270
22	2	1	41.149	40.702	-40.702	0.0	0.446	0.264
23	2	1	76.765	79.340	-79.340	0.0	-2.575	-1.507

24C. DOPHOFERROSILITE-6/18/73

STRUCTURE FACTORS

PAGE 8

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
24	2	1	61.305	63.506	0.0	-2.201	-1.328	
25	2	1	54.874	58.237	0.0	-3.363	-1.868	
26	2	1	26.200	30.718	0.0	-2.517	-0.982	
26	1	1	29.973	30.521	0.0	-1.549	-0.699	
0	6	0	379.320	405.108	0.0	-25.798	-3.755 *	
25	1	1	22.142	21.098	0.0	1.053	0.402	
23	1	1	10.457	2.469	0.0	7.988	1.881	
22	1	1	10.690	2.643	0.0	8.047	2.072	
21	1	1	26.460	28.752	0.0	-1.892	-0.577	
20	1	1	5.425	11.457	-11.457	0.0	-6.032	-0.978
19	1	1	14.953	10.426	-10.426	0.0	4.527	1.620
18	1	1	20.832	15.535	-15.535	0.0	5.297	2.736
17	1	1	12.697	10.365	-10.365	0.0	2.332	0.778
16	1	1	39.310	40.949	40.949	0.0	-1.630	-1.208
15	1	1	33.661	33.660	33.660	0.0	-0.198	-0.127
14	1	1	51.289	52.667	52.667	0.0	-1.378	-1.047
13	1	1	34.832	34.378	34.378	0.0	0.454	0.318
12	1	1	12.145	7.173	7.173	0.0	4.972	1.818
11	1	1	21.851	19.158	-19.158	0.0	2.693	1.697
10	1	1	30.554	30.617	-30.617	0.0	0.337	0.293
0	1	1	0.130	4.496	-4.496	0.0	3.634	1.249
8	1'	1	46.406	47.556	47.556	0.0	-1.150	-1.157
7	1	1	54.591	54.470	-54.470	0.0	0.111	0.109
6	1'	1	64.415	65.044	65.044	0.0	-0.628	-0.571
0	6	0	340.773	405.108	405.108	0.0	-24.335	-3.526 *
5	1	1	92.600	91.521	91.521	0.0	1.079	0.736
4	1	1	56.675	54.701	54.701	0.0	1.973	1.953
3	1	1	11.766	7.640	7.640	0.0	4.126	2.233
2	1	1	46.859	47.606	-47.606	0.0	-0.767	-0.811
1	1	1	12.348	8.604	-8.604	0.0	3.745	2.361
0	0	2	33.826	32.556	-32.556	0.0	1.270	1.383
1	0	2	136.330	136.504	136.504	0.0	-0.174	-0.081
2	0	2	189.006	185.209	-185.209	0.0	3.797	1.267
3	0	2	205.323	207.345	207.345	0.0	-2.022	-0.617
4	0	2	14.298	14.861	14.861	0.0	-0.563	-0.349
5	0	2	266.786	260.968	-260.968	0.0	5.818	1.317
6	0	2	5.526	5.835	5.835	0.0	-0.308	-0.081
7	0	2	214.407	210.014	-210.014	0.0	4.393	1.275
8	0	2	7.330	2.725	2.725	0.0	4.605	1.353
0	0	2	200.071	197.018	197.018	0.0	3.053	0.950
10	0	2	22.768	20.326	20.326	0.0	2.442	1.497
11	0	2	253.341	246.752	-246.752	0.0	3.599	0.862
12	0	2	31.217	30.980	30.980	0.0	0.237	0.155
13	0	2	74.070	74.889	-74.889	0.0	-0.819	-0.586
14	0	2	8.426	1.908	1.908	0.0	6.716	1.576
0	6	0	380.463	405.108	405.108	0.0	-24.645	-3.573 *
15	0	2	112.150	111.572	-111.572	0.0	0.578	0.309
16	0	2	11.432	3.855	3.855	0.0	7.576	2.422
17	0	2	110.701	112.037	112.037	0.0	-1.246	-0.662
18	0	2	49.256	50.172	50.172	0.0	-0.916	-0.652
19	0	2	78.106	78.037	78.037	0.0	0.068	0.045
20	0	2	4.305	6.642	6.642	0.0	-2.337	-0.365
21	0	2	55.899	58.909	-58.909	0.0	3.010	1.939

24C-ORTHOFEROSILITE_6/18/73

STRUCTURE FACTORS

PAGE 6

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
22	0	2	99.529	99.685	99.685	0.0	-0.156	-0.045
23	0	2	154.718	157.189	-157.189	0.0	-2.471	-0.949
24	0	2	6.704	12.872	-12.872	0.0	-6.168	-0.904
25	0	2	58.477	61.190	61.190	0.0	-2.714	-1.610
26	0	2	31.494	32.793	32.793	0.0	-1.300	-0.534
26	1	2	19.463	13.237	13.237	0.0	6.256	2.589
25	1	2	30.517	28.992	28.992	0.0	1.525	0.748
24	1	2	37.136	35.220	35.220	0.0	1.917	1.133
23	1	2	52.723	54.947	54.947	0.0	-2.225	-1.334
22	1	2	20.177	17.804	17.804	0.0	2.373	0.926
21	1	2	23.685	20.832	-20.832	0.0	2.853	1.342
20	1	2	21.582	22.556	22.556	0.0	-0.574	-0.266
19	1	2	20.177	16.213	-16.213	0.0	3.964	1.918
0	6	0	380.909	405.108	405.108	0.0	-24.199	-3.506 *
18	1	2	11.432	10.409	10.409	0.0	1.023	0.278
17	1	2	87.449	88.318	88.318	0.0	-0.868	-0.549
14	1	2	56.865	57.045	-57.045	0.0	-0.180	-0.138
16	1	2	25.855	26.544	26.544	0.0	-0.688	-0.391
14	1	2	14.705	7.123	7.123	0.0	7.582	2.061
12	1	2	129.064	129.207	-129.207	0.0	-0.143	-0.068
11	1	2	112.509	111.785	-111.785	0.0	0.813	0.442
10	1	2	9.308	0.830	0.830	0.0	8.479	2.534
9	1	2	82.043	81.634	81.634	0.0	0.409	0.292
8	1	2	70.364	71.759	-71.759	0.0	-1.395	-1.104
7	1	2	44.200	43.903	43.903	0.0	0.298	0.283
6	1	2	16.046	13.422	-13.422	0.0	2.622	1.638
5	1	2	116.416	113.910	-113.910	0.0	2.503	1.359
4	1	2	44.712	39.010	39.010	0.0	5.693	5.996
3	1	2	63.007	65.442	-65.442	0.0	-2.435	-2.214
2	1	2	16.320	14.289	-14.289	0.0	2.031	1.501
1	1	2	62.367	62.875	62.875	0.0	-0.528	-0.487
0	2	2	6.574	2.727	2.727	0.0	3.847	1.303
1	2	2	32.047	35.887	35.887	0.0	-3.840	-3.874
0	6	0	379.862	405.108	405.108	0.0	-25.246	-3.663 *
3	2	2	76.323	74.918	74.918	0.0	1.405	1.109
4	2	2	24.581	23.521	-23.521	0.0	1.461	1.254
5	2	2	31.275	31.001	-31.001	0.0	0.274	0.248
6	2	2	68.582	65.561	65.561	0.0	3.421	2.839
7	2	2	100.599	100.523	-100.523	0.0	0.076	0.046
8	2	2	26.390	25.431	-25.431	0.0	0.949	0.686
9	2	2	76.470	76.115	76.115	0.0	0.355	0.259
10	2	2	33.161	33.136	-33.136	0.0	0.005	0.003
11	2	2	24.253	24.402	25.402	0.0	-1.148	-0.597
12	2	2	12.494	10.307	-10.307	0.0	2.187	0.703
13	2	2	46.509	44.564	-44.564	0.0	1.944	1.478
14	2	2	28.658	27.339	-27.339	0.0	1.619	0.993
15	2	2	52.825	54.492	-54.492	0.0	-1.667	-1.199
16	2	2	10.515	11.241	-11.241	0.0	-0.726	-0.195
17	2	2	22.885	22.775	-22.775	0.0	0.109	0.057
18	2	2	55.079	52.901	-52.901	0.0	2.178	1.653
19	2	2	56.250	55.738	58.738	0.0	-2.488	-1.666
20	2	2	13.105	13.376	13.376	0.0	-0.272	-0.080
21	2	2	23.089	20.123	-20.123	0.0	2.966	1.340

.24C OTHOFEEDSYLITE 6/18/72

STRUCTURE & FACTORS

PAGE 10

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	0	379.572	405.108	0.0	-25.536	-2.717 *	
22	2	2	22.754	22.684	-22.684	0.0	0.070	0.030
23	2	2	8.406	9.387	-9.387	0.0	-0.991	-0.184
25	2	2	23.870	23.771	23.771	0.0	-0.901	-0.342
25	3	2	7.679	5.713	5.713	0.0	1.966	0.348
24	3	2	11.141	6.220	-6.220	0.0	4.921	1.135
23	3	2	8.203	7.337	-7.337	0.0	0.865	0.159
22	3	2	5.192	5.365	5.365	0.0	-0.174	-0.026
20	3	2	9.308	7.782	-7.782	0.0	1.526	0.366
19	3	2	7.839	12.080	-12.000	0.0	-4.241	-0.819
18	3	2	13.267	5.758	-5.758	0.0	7.608	2.641
17	3	2	6.490	13.865	-13.865	0.0	-7.175	-1.330
16	3	2	8.043	7.954	7.954	0.0	0.089	0.020
15	3	2	5.352	14.261	14.261	0.0	-8.909	-1.587
12	3	2	18.314	11.465	11.465	0.0	6.449	2.180
11	3	2	13.963	13.317	13.317	0.0	0.646	0.227
10	6	0	379.901	405.108	405.108	0.0	-25.207	-3.657 *
10	3	2	8.857	5.315	5.315	0.0	3.542	0.922
9	3	2	7.534	12.222	12.222	0.0	-5.688	-1.053
8	3	2	14.021	15.133	-15.133	0.0	-1.112	-0.437
7	3	2	12.465	13.665	-13.665	0.0	-1.181	-0.443
6	3	2	9.221	12.127	12.127	0.0	-2.906	-0.908
5	3	2	26.190	26.078	26.078	0.0	0.113	0.087
4	3	2	43.324	40.993	-40.993	0.0	2.331	2.280
3	3	2	31.231	29.250	-29.250	0.0	1.981	1.812
2	3	2	5.017	1.930	-1.930	0.0	3.087	0.778
0	4	2	27.006	27.230	-27.230	0.0	-0.724	-0.183
1	4	2	35.655	36.388	36.388	0.0	-0.634	-0.397
2	4	2	66.867	69.656	69.656	0.0	-2.789	-2.288
3	4	2	34.438	33.437	-33.437	0.0	1.001	0.837
4	4	2	8.101	8.647	8.647	0.0	-0.547	-0.156
5	4	2	17.252	20.014	-20.014	0.0	-2.762	-1.309
6	4	2	37.238	35.589	35.589	0.0	1.650	1.346
7	4	2	45.647	47.070	-47.070	0.0	-1.424	-1.120
8	4	2	7.912	6.455	-6.455	0.0	1.056	0.253
9	4	2	7.655	5.507	-5.507	0.0	2.449	0.577
0	6	0	379.843	405.108	405.108	0.0	-25.265	-3.676 *
10	4	2	15.578	15.145	-15.145	0.0	0.433	0.158
11	4	2	25.229	23.779	-23.779	0.0	1.650	0.778
13	4	2	7.126	10.658	-10.658	0.0	-3.532	-0.734
14	4	2	20.075	27.402	-27.402	0.0	1.673	1.007
15	4	2	13.469	10.909	-10.909	0.0	2.559	0.867
16	4	2	12.537	13.991	-13.991	0.0	-1.453	-0.425
17	4	2	18.037	17.476	-17.476	0.0	0.561	0.223
18	4	2	29.113	27.511	-27.511	0.0	0.602	0.323
19	4	2	12.596	17.136	17.136	0.0	-4.541	-1.219
20	4	2	8.043	8.105	8.105	0.0	0.730	0.157
21	4	2	13.439	0.406	0.406	0.0	13.036	4.056 *
22	4	2	18.867	18.636	-18.636	0.0	0.231	0.073
24	4	2	12.625	1.504	1.504	0.0	11.031	2.950 *
25	4	2	9.512	8.392	-8.392	0.0	1.120	0.219
23	5	2	51.865	51.356	-51.356	0.0	0.489	0.288
22	5	2	22.594	20.903	-20.903	0.0	1.690	0.667

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA//SIGMA
21	5	2	51.381	48.541	48.541	0.0	3.040	2.018
0	6	0	301.025	405.108	405.108	0.0	-24.083	-3.489 *
20	5	2	26.977	21.625	21.625	0.0	5.352	2.916
19	5	2	40.404	42.874	42.874	0.0	-2.469	-1.352
18	5	2	11.577	14.142	14.142	0.0	-2.564	-0.627
17	5	2	92.334	91.007	91.007	0.0	1.326	0.799
16	5	2	29.424	28.458	28.458	0.0	0.966	0.930
15	5	2	56.441	58.875	58.875	0.0	-2.434	-1.462
14	5	2	12.759	10.775	10.775	0.0	2.024	0.647
13	5	2	66.811	65.691	65.691	0.0	1.220	0.874
12	5	2	97.480	96.383	96.383	0.0	1.097	0.649
11	5	2	104.021	100.997	100.997	0.0	3.024	1.522
10	5	2	10.558	11.148	11.148	0.0	9.440	2.840
9	5	2	157.262	155.469	155.469	0.0	1.293	0.514
8	5	2	90.038	89.635	89.635	0.0	0.363	0.232
7	5	2	73.967	75.100	75.100	0.0	-1.122	-0.802
6	5	2	4.104	6.669	6.669	0.0	2.435	0.629
5	5	2	99.546	99.199	99.199	0.0	0.345	0.205
4	5	2	7.432	11.681	11.681	0.0	-4.249	-0.981
3	5	2	152.179	156.681	156.681	0.0	-4.502	1.452
2	5	2	19.367	17.567	17.567	0.0	1.780	0.850
1	5	2	75.071	78.101	78.101	0.0	-3.029	-2.237
0	6	0	380.133	405.108	405.108	0.0	-24.975	-3.622 *
0	6	2	13.394	4.532	4.532	0.0	8.762	5.187
1	6	2	55.474	55.108	55.108	0.0	0.367	0.291
2	6	2	136.865	143.526	143.526	0.0	-6.681	-3.022
3	6	2	158.520	164.896	164.896	0.0	-6.074	-2.385
4	6	2	12.654	10.576	10.576	0.0	2.078	0.655
5	6	2	128.703	130.959	130.959	0.0	-2.256	-1.085
6	6	2	5.177	0.044	0.044	0.0	5.136	0.917
7	6	2	120.926	123.310	123.310	0.0	-2.392	-1.207
8	6	2	12.596	15.115	15.115	0.0	-2.519	-0.784
9	6	2	149.62	150.014	150.014	0.0	-1.692	-0.698
10	6	2	35.270	39.093	39.093	0.0	0.377	0.312
11	6	2	135.271	134.280	134.280	0.0	0.961	0.445
12	6	2	66.131	13.954	13.954	0.0	2.177	0.850
13	6	2	48.920	47.883	47.883	0.0	1.057	0.739
15	6	2	78.032	76.026	76.026	0.0	1.106	0.722
16	6	2	104.077	14.211	14.211	0.0	3.434	-0.423
17	6	2	62.552	62.782	62.782	0.0	0.230	0.151
18	6	2	26.326	22.631	22.631	0.0	3.705	1.817
19	6	2	57.485	68.234	68.234	0.0	-1.088	-0.679
0	6	0	380.734	405.108	405.108	0.0	-24.374	-3.532 *
21	6	2	51.347	50.123	50.123	0.0	1.224	0.782
22	6	2	71.060	69.313	69.313	0.0	1.756	1.076
23	6	2	100.020	110.122	110.122	0.0	-2.093	-1.032
22	7	2	23.744	23.438	23.438	0.0	0.306	0.120
21	7	2	17.135	21.376	21.376	0.0	-4.250	-1.147
19	7	2	5.675	5.791	5.791	0.0	0.885	0.142
17	7	2	18.401	12.787	12.787	0.0	5.615	2.031
16	7	2	23.496	24.119	24.119	0.0	-0.623	-0.259
15	7	2	12.494	12.801	12.801	0.0	-0.307	-0.085
14	7	2	10.486	5.821	5.821	0.0	4.665	1.197

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STRUCTURE FACTORS

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H	K	I	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
13	7	2	30.721	30.919	0.0	-0.198	-0.116	
12	7	2	59.017	58.465	-58.465	0.0	0.553	0.389
11	7	2	15.127	16.524	-16.524	0.0	-1.397	-0.653
10	7	2	6.704	7.955	-7.955	0.0	-1.251	-0.245
9	7	2	13.061	3.708	3.708	0.0	9.353	3.402
8	7	2	55.137	56.770	-56.770	0.0	-1.633	-1.253
7	7	2	38.790	38.527	-38.527	0.0	0.272	0.196
0	6	0	382.112	405.108	405.108	0.0	-22.997	-3.317 *
5	7	2	12.901	11.794	11.794	0.0	1.107	0.368
4	7	2	28.215	33.416	-33.416	0.0	-5.201	-2.926
3	7	2	17.368	21.699	-21.699	0.0	-4.331	-1.644
2	7	2	13.978	7.370	-7.378	0.0	6.600	2.439
1	7	2	8.726	11.028	-11.028	0.0	-2.302	-0.851
0	8	2	12.014	4.178	-4.178	0.0	7.835	2.707
1	8	2	51.874	53.683	-53.683	0.0	-1.809	-1.330
2	8	2	21.574	10.849	10.849	0.0	1.725	0.953
3	8	2	44.405	43.636	43.636	0.0	0.769	0.566
4	8	2	8.857	10.073	10.073	0.0	-1.216	-0.298
5	8	2	35.517	36.391	-36.391	0.0	-0.874	-0.560
6	8	2	21.414	21.520	-21.520	0.0	-0.115	-0.054
7	8	2	55.386	56.816	-56.816	0.0	-1.430	-1.039
8	8	2	32.718	34.023	-34.023	0.0	-1.306	-0.740
10	8	2	5.366	0.594	0.594	0.0	4.772	0.827
11	8	2	38.639	38.911	-38.911	0.0	-0.273	-0.167
12	8	2	11.912	4.192	4.192	0.0	7.720	2.317
13	8	2	48.862	47.719	-47.719	0.0	1.142	0.766
0	6	0	381.258	405.108	405.108	0.0	-23.851	-3.444 *
14	6	2	13.911	16.313	-16.313	0.0	-2.598	0.956
15	6	2	46.815	45.980	-45.980	0.0	0.835	0.502
17	6	2	15.564	12.327	12.327	0.0	3.236	0.939
18	6	2	21.574	20.893	-20.893	0.0	0.682	0.237
19	6	2	35.809	36.606	-36.606	0.0	-0.797	-0.399
20	6	2	11.141	7.751	-7.751	0.0	3.390	0.769
19	9	2	12.857	16.847	-16.847	0.0	-3.989	-0.885
16	9	2	14.907	0.246	0.246	0.0	5.561	1.655
15	9	2	12.785	0.835	0.835	0.0	11.950	3.196 *
14	9	2	23.234	19.509	19.509	0.0	3.725	1.479
13	9	2	24.661	24.710	-24.710	0.0	-0.049	-0.022
12	9	2	9.177	8.332	-8.332	0.0	0.844	0.174
10	9	2	13.861	11.719	11.719	0.0	2.142	0.640
8	9	2	13.701	6.268	-6.268	0.0	7.433	2.456
0	6	0	375.456	405.108	405.108	0.0	-25.652	-3.734 *
5	9	2	10.399	2.996	-2.996	0.0	7.403	2.147
4	9	2	9.803	11.468	-11.468	0.0	-1.665	-0.399
2	9	2	19.595	17.702	-17.702	0.0	1.893	0.861
1	9	2	11.679	9.025	-9.025	0.0	2.654	0.815
0	10	2	7.795	8.366	8.366	0.0	-0.571	-0.124
1	10	2	20.512	15.872	-15.872	0.0	4.660	2.452
2	10	2	40.083	39.816	39.816	0.0	0.267	0.173
3	10	2	39.923	39.207	-39.207	0.0	0.716	0.442
4	10	2	8.188	3.389	3.389	0.0	4.799	1.030
5	10	2	18.353	14.272	14.272	0.0	4.071	1.589
6	10	2	23.584	21.381	21.381	0.0	2.202	1.058

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STRUCTURE_FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	10	2	15.811	12.655	-12.655	0.0	3.156	1.033
8	10	2	21.938	19.690	-19.690	0.0	2.249	0.984
9	10	2	11.170	15.458	-15.458	0.0	-4.288	-0.915
11	10	2	25.025	25.594	-25.594	0.0	-0.569	-0.231
12	10	2	15.345	11.340	-11.340	0.0	4.006	1.176
13	10	2	18.576	16.627	-16.627	0.0	1.949	0.687
0	6	0	378.915	405.108	405.108	0.0	-26.194	-3.816 *
14	10	2	11.781	13.443	-13.443	0.0	-1.662	-0.355
15	10	2	21.227	24.085	-24.085	0.0	-2.758	-0.831
14	11	2	10.748	4.174	-4.174	0.0	6.574	1.406
13	11	2	41.209	40.258	-40.258	0.0	1.052	0.534
12	11	2	63.329	62.544	-62.544	0.0	0.786	0.510
11	11	2	64.621	64.102	-64.102	0.0	0.519	0.315
10	11	2	15.098	2.031	-2.031	0.0	13.067	3.607 *
9	11	2	106.747	106.510	-106.510	0.0	1.238	0.626
8	11	2	48.005	48.361	-48.361	0.0	0.544	0.313
7	11	2	64.757	63.620	-63.620	0.0	1.177	0.729
6	11	2	11.635	13.407	-13.407	0.0	-1.772	-0.409
5	11	2	74.792	74.779	-74.779	0.0	0.013	0.008
3	11	2	87.316	86.370	-86.370	0.0	0.946	0.547
1	11	2	40.755	37.238	-37.238	0.0	3.517	2.042
0	12	2	13.949	8.278	-8.278	0.0	5.671	1.578
1	12	2	16.602	19.546	-19.546	0.0	-0.854	-0.261
2	12	2	52.249	59.922	-59.922	0.0	2.627	1.614
0	6	0	379.050	405.108	405.108	0.0	-26.058	-3.796 *
3	12	2	64.034	62.081	-62.081	0.0	1.952	1.177
4	12	2	10.254	3.677	-3.677	0.0	6.577	1.422
5	12	2	29.774	28.985	-28.985	0.0	0.789	0.326
6	12	2	15.273	8.694	-8.694	0.0	6.579	2.018
7	12	2	24.545	22.267	-22.267	0.0	2.277	0.874
8	12	2	6.283	1.499	-1.499	0.0	4.784	0.741
9	12	2	49.900	49.479	-49.479	0.0	0.420	0.244
10	12	2	16.961	14.990	-14.990	0.0	2.071	0.677
2	13	2	18.892	14.119	-14.119	0.0	4.763	1.750
1	13	2	40.740	38.802	-38.802	0.0	1.938	1.038
1	12	3	8.610	8.176	-8.176	0.0	0.434	0.074
2	12	3	0.843	10.083	-10.083	0.0	-9.239	-0.875
3	12	3	18.081	19.525	-19.525	0.0	-1.444	-0.413
4	12	3	13.381	2.657	-2.657	0.0	10.725	3.026 *
11	11	3	15.113	19.173	-19.173	0.0	-4.060	-1.028
10	11	3	32.033	32.894	-32.894	0.0	-0.861	-0.372
9	11	3	22.317	25.091	-25.091	0.0	-2.774	-0.894
0	6	0	380.598	405.108	405.108	0.0	-24.510	-3.553 *
7	11	3	24.894	21.379	-21.379	0.0	3.515	1.609
5	11	3	34.934	33.837	-33.837	0.0	1.097	0.557
4	11	3	8.886	5.338	-5.338	0.0	3.548	0.735
3	11	3	33.432	29.993	-29.993	0.0	3.440	1.934
2	11	3	41.733	40.542	-40.542	0.0	1.191	0.658
1	11	3	17.426	15.991	-15.991	0.0	1.436	0.427
0	10	3	25.302	26.223	-26.223	0.0	-0.921	-0.393
1	10	3	16.277	16.828	-16.828	0.0	1.448	0.481
3	10	2	42.331	41.319	-41.319	0.0	1.012	0.624
4	10	3	43.733	44.219	-44.219	0.0	-0.485	-0.282

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/STGMA
8	10	3	5.803	5.716	0.0	4.087	0.836	
9	10	3	15.535	18.138	0.0	-2.604	-0.707	
11	10	3	40.083	36.738	0.0	3.345	1.926	
0	6	0	380.017	405.108	405.100	0.0	-25.091	-3.640 *
13	10	3	10.850	0.323	-0.333	0.0	10.517	2.347 *
14	10	3	17.906	4.293	4.283	0.0	13.623	5.319 *
15	10	3	18.445	11.746	-11.766	0.0	6.699	2.171
17	9	3	25.185	25.616	25.616	0.0	-0.230	-0.084
15	9	3	47.429	48.021	48.021	0.0	-0.592	-0.329
14	9	3	106.656	105.429	105.429	0.0	1.527	0.764
13	9	3	89.654	99.079	98.079	0.0	1.575	0.902
12	9	3	13.323	7.267	-7.267	0.0	6.056	1.658
11	9	3	13.076	16.036	-16.036	0.0	-2.960	-0.756
10	9	3	6.472	13.315	13.315	0.0	-6.844	-1.030
9	9	3	19.751	19.335	19.335	0.0	0.415	0.153
7	9	3	48.131	47.894	47.894	0.0	0.236	0.163
6	9	3	78.165	78.197	78.197	0.0	-0.033	-0.021
5	9	3	34.657	32.153	-32.153	0.0	2.504	1.620
3	9	3	29.759	34.197	-34.197	0.0	-4.438	-2.072
2	9	3	69.158	70.415	-70.415	0.0	-1.257	-0.847
0	6	0	380.424	405.108	405.108	0.0	-24.684	-3.579 *
1	9	3	92.348	93.510	93.510	0.0	-1.162	-0.688
0	8	3	155.040	158.816	158.816	0.0	-3.776	-1.685
1	8	3	90.512	94.246	94.246	0.0	-3.736	-2.234
1	8	3	10.420	9.326	-9.326	0.0	1.102	0.271
3	8	3	51.581	51.930	51.930	0.0	-0.348	-0.250
4	8	3	32.062	34.502	-34.502	0.0	-2.440	-1.419
5	8	3	49.359	48.276	-48.276	0.0	1.003	0.760
6	8	3	11.417	6.007	-6.007	0.0	4.530	1.525
7	8	3	86.032	88.072	-88.072	0.0	-1.140	-0.699
8	8	3	71.687	73.838	-73.838	0.0	-2.151	-1.407
0	8	3	28.962	25.852	-25.852	0.0	1.011	0.532
11	8	3	20.410	21.516	-21.516	0.0	-1.507	-0.566
12	8	3	71.370	71.178	-71.178	0.0	0.200	0.126
13	8	3	68.444	68.541	-68.541	0.0	0.103	0.063
14	8	3	16.987	11.000	-11.000	0.0	5.596	1.204
15	8	3	29.150	70.066	-70.066	0.0	-0.807	-0.561
16	8	3	24.835	41.933	-41.933	0.0	-0.098	-0.057
17	8	3	25.043	27.858	-27.858	0.0	-1.915	-0.719
0	6	0	380.230	405.108	405.108	0.0	-24.878	-3.608 *
19	8	3	92.459	91.326	91.326	0.0	0.732	0.424
20	7	3	18.125	11.060	11.060	0.0	6.157	2.086
19	7	3	15.200	11.003	11.003	0.0	4.197	1.182
17	7	3	21.196	24.875	24.875	0.0	-3.679	-1.170
16	7	3	8.261	3.842	-3.842	0.0	4.419	0.830
15	7	3	2.220	10.166	-10.166	0.0	-6.938	-0.835
14	7	3	46.455	45.893	-45.893	0.0	0.761	0.478
13	7	2	29.572	28.960	-28.960	0.0	0.650	0.363
12	7	3	20.061	12.343	-12.343	0.0	7.718	3.699
11	7	3	4.075	10.229	-10.229	0.0	-1.154	0.267
10	7	3	27.760	25.138	-25.138	0.0	2.611	1.572
9	7	3	70.254	15.632	15.632	0.0	4.822	2.238
8	7	3	17.499	16.162	16.162	0.0	1.317	0.539

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	7	3	22.128	21.806	-21.806	0.0	0.321	0.145
6	7	3	36.057	37.273	-37.273	0.0	-1.216	-0.745
5	7	3	15.636	12.854	-12.854	0.0	2.781	1.079
4	7	3	22.437	24.700	-24.700	0.0	-2.062	-1.012
3	7	3	11.606	11.371	-11.371	0.0	0.236	0.068
0	6	0	380.385	405.108	-405.108	0.0	-24.723	-3.584 *
1	7	3	19.595	13.295	-13.295	0.0	6.300	3.254
0	6	3	3.723	7.086	-7.086	0.0	-4.163	-0.645
2	6	3	23.409	26.327	-26.327	0.0	-2.918	-1.464
3	6	3	14.327	16.218	-16.218	0.0	-1.891	-0.660
8	6	3	21.138	21.410	-21.410	0.0	-0.273	-0.123
9	6	3	14.007	12.496	-12.496	0.0	1.521	0.531
10	6	3	17.630	14.323	-14.323	0.0	3.307	1.377
11	6	3	11.825	7.636	-7.636	0.0	4.388	1.627
14	6	3	7.764	1.997	-1.997	0.0	5.769	1.232
15	5	3	6.421	6.196	-6.196	0.0	-1.775	-0.256
16	5	3	6.646	8.548	-8.548	0.0	-1.901	-0.321
17	6	3	6.763	10.366	-10.366	0.0	-3.584	-0.589
18	6	3	18.765	11.505	-11.505	0.0	7.260	2.034
0	6	0	381.219	405.108	-405.108	0.0	-23.889	-3.450 *
23	5	3	13.832	7.099	-7.099	0.0	6.733	1.794
22	5	3	12.305	13.681	-13.681	0.0	-1.676	-0.344
21	5	3	20.585	22.198	-22.198	0.0	-1.614	-0.525
20	5	3	4.552	2.077	-2.077	0.0	2.475	0.342
19	5	3	18.445	10.639	-10.639	0.0	7.806	2.963
18	5	3	32.791	32.808	-32.808	0.0	-0.017	-0.008
17	5	3	52.050	50.815	-50.815	0.0	1.235	0.893
16	5	3	13.221	17.969	-17.969	0.0	-4.748	-1.232
15	5	3	35.707	36.952	-36.952	0.0	-1.245	-0.715
14	5	3	28.215	29.347	-29.347	0.0	-1.132	-0.576
13	5	3	27.589	25.742	-25.742	0.0	1.847	0.660
12	5	3	10.166	4.404	-4.404	0.0	5.762	1.529
11	5	3	23.017	25.177	-25.177	0.0	-1.361	-0.617
10	5	3	53.366	52.912	-52.912	0.0	0.455	0.365
9	5	3	47.385	49.243	-49.243	0.0	-1.858	-1.353
8	5	3	6.123	7.098	-7.098	0.0	-0.965	-0.193
0	6	0	380.133	405.108	-405.108	0.0	-24.475	-3.622 *
7	5	3	7.688	4.905	-4.905	0.0	2.964	0.681
5	5	3	44.346	44.050	-44.050	0.0	0.296	0.221
4	5	3	15.666	15.490	-15.490	0.0	0.176	0.063
3	5	3	65.589	69.846	-69.846	0.0	-4.257	-3.052
2	5	3	73.938	77.440	-77.440	0.0	-3.502	-2.505
1	5	3	41.061	43.299	-43.299	0.0	-2.238	-1.549
0	4	3	134.122	144.255	-144.255	0.0	-10.134	-6.720 *
1	4	3	52.942	55.697	-55.697	0.0	-2.745	-2.156
2	4	3	17.092	18.431	-18.431	0.0	-1.330	-0.554
3	4	3	34.278	33.832	-33.832	0.0	0.446	0.315
4	4	3	29.861	32.928	-32.928	0.0	-3.064	-1.799
5	4	3	25.972	23.776	-23.776	0.0	2.196	1.300
6	4	3	12.436	10.739	-10.739	0.0	1.697	0.533
7	4	3	37.545	36.502	-36.502	0.0	0.952	0.673
8	4	3	17.857	15.962	-15.962	0.0	1.595	0.630
9	4	3	19.915	19.613	-19.613	0.0	0.302	0.140

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA SIGMA
10	4	3	33.455	30.729	30.729	0.0	3.126	2.257
11	4	3	14.618	9.383	9.383	0.0	5.615	1.955
12	4	3	48.394	49.999	49.999	0.0	-1.558	-1.086
0	6	0	379.443	405.108	405.108	0.0	-25.269	-3.676 *
13	4	3	41.767	40.854	40.854	0.0	0.914	0.624
14	4	3	14.691	11.678	11.678	0.0	-3.012	1.005
15	4	3	22.572	24.122	24.122	0.0	-1.150	-0.497
18	4	3	10.021	8.754	8.754	0.0	1.254	0.285
19	4	3	13.429	20.085	20.085	0.0	-6.427	-1.515
20	4	3	48.584	48.867	48.867	0.0	-0.253	-0.183
21	4	3	10.066	16.609	16.609	0.0	-5.503	-1.140
22	4	3	5.744	12.811	12.811	0.0	-7.066	-0.604
23	4	3	27.589	27.147	27.147	0.0	0.442	0.197
24	3	3	14.138	7.531	7.531	0.0	6.606	1.727
23	3	3	8.904	9.557	9.557	0.0	0.357	0.070
22	3	3	46.143	46.977	46.977	0.0	-0.833	-0.492
21	3	3	6.646	65.337	65.337	0.0	-6.692	-0.386
20	3	3	21.240	20.503	20.503	0.0	0.737	0.299
19	3	3	75.292	74.434	74.434	0.0	0.858	0.545
18	3	3	91.297	92.061	92.061	0.0	-0.764	-0.449
17	3	3	71.893	71.078	71.078	0.0	0.815	0.568
16	3	3	8.188	11.290	11.290	0.0	-3.102	-0.444
0	6	0	379.649	405.108	405.108	0.0	-25.459	-3.705 *
15	3	3	82.623	93.069	93.069	0.0	0.553	0.350
14	3	3	176.100	174.281	174.281	0.0	1.827	0.639
13	3	3	149.735	148.629	148.629	0.0	1.106	0.453
12	2	3	35.561	33.412	33.412	0.0	2.149	1.474
11	3	3	51.611	51.148	51.148	0.0	0.463	0.364
10	3	3	8.770	3.073	3.073	0.0	5.697	1.384
0	3	3	45.583	45.272	45.272	0.0	0.710	0.506
8	3	3	24.224	17.401	17.401	0.0	6.824	4.040
7	3	3	105.442	105.640	105.640	0.0	0.302	0.172
6	3	3	177.850	177.103	177.103	0.0	0.746	0.262
5	3	3	115.504	115.079	115.079	0.0	0.915	0.485
4	3	3	28.958	27.965	27.965	0.0	0.993	0.674
3	3	3	75.734	77.698	77.698	0.0	-1.964	-1.450
2	3	3	157.216	161.637	161.637	0.0	-4.421	-1.769
1	3	3	197.446	208.758	208.758	0.0	-11.312	-3.580 *
0	2	3	222.150	240.248	240.248	0.0	-18.089	-5.026 *
1	2	3	126.744	131.492	131.492	0.0	-4.768	-2.353
2	2	3	13.367	13.734	13.734	0.0	-0.367	-0.146
3	2	3	35.342	35.361	35.361	0.0	-0.016	-0.015
4	2	3	18.692	21.944	21.944	0.0	-3.252	-1.563
0	6	0	381.374	405.108	405.108	0.0	-23.734	-3.427 * -
5	2	3	56.958	57.566	57.566	0.0	-0.558	-0.492
6	2	3	15.229	18.557	18.557	0.0	-3.328	-1.257
7	2	3	91.371	90.246	90.246	0.0	1.125	0.717
8	2	3	66.038	64.055	64.055	0.0	2.753	2.130
9	2	3	10.777	8.643	8.643	0.0	2.135	0.592
10	2	3	23.758	23.259	23.259	0.0	0.500	0.258
11	2	3	21.793	23.279	23.279	0.0	-1.488	-0.690
12	2	3	94.142	92.700	92.700	0.0	1.442	0.876
13	2	3	81.350	80.869	80.869	0.0	0.481	0.323

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
14	2	3	13.252	14.931	-14.931	0.0	-1.570	-0.514
15	2	3	70.697	70.221	-70.221	0.0	0.466	0.300
16	2	3	40.638	39.367	-39.367	0.0	1.271	0.971
17	2	3	29.264	27.473	-27.473	0.0	1.791	0.991
18	2	3	8.730	14.177	-14.177	0.0	-4.357	-0.978
19	2	3	70.498	69.062	-69.062	0.0	1.056	0.724
20	2	3	93.489	92.139	-92.139	0.0	1.350	0.983
21	2	3	35.546	34.716	-34.716	0.0	0.831	0.498
22	2	3	15.213	14.981	-14.981	0.0	15.132	4.103 *
23	2	3	14.705	6.310	-6.310	0.0	8.355	2.308
24	2	3	379.591	405.108	-405.108	0.0	-25.517	-3.714 *
25	1	3	23.423	22.959	-22.959	0.0	0.425	0.155
26	1	3	15.185	16.377	-16.377	0.0	-1.192	-0.354
27	1	3	10.123	1.360	-1.360	0.0	8.014	1.880
28	1	3	9.483	7.811	-7.811	0.0	1.671	0.337
29	1	3	17.965	17.358	-17.358	0.0	0.606	0.203
30	1	3	12.169	5.402	-5.402	0.0	6.157	1.927
31	1	3	26.409	26.013	-26.013	0.0	0.396	0.211
32	1	3	53.571	52.176	-52.176	0.0	1.395	0.953
33	1	3	4.235	12.622	-12.622	0.0	-3.387	-0.556
34	1	3	18.405	22.174	-22.174	0.0	-3.569	-1.340
35	1	3	2.538	6.616	-6.616	0.0	-3.678	-0.517
36	1	3	4.058	7.844	-7.844	0.0	-3.137	-0.516
37	1	3	26.299	24.234	-24.234	0.0	3.924	2.471
38	1	3	75.270	50.512	-50.512	0.0	2.787	2.078
39	1	3	49.720	46.245	-46.245	0.0	-0.525	-0.307
40	1	3	5.221	8.048	-8.048	0.0	-2.897	-0.524
41	1	3	20.323	16.198	-16.198	0.0	4.125	2.147
42	1	3	25.196	35.120	-35.120	0.0	0.077	0.061
43	0	6	370.563	405.108	-405.108	0.0	-24.645	-3.573 *
44	1	2	47.283	45.646	-45.646	0.0	1.637	1.400
45	1	3	8.799	1.107	-1.107	0.0	7.691	2.329
46	1	3	50.500	58.436	-58.436	0.0	0.154	0.123
47	1	3	26.444	58.653	-58.653	0.0	0.234	0.205
48	1	3	148.423	146.956	-146.956	0.0	1.474	0.995
49	0	4	127.091	126.645	-126.645	0.0	1.468	0.617
50	0	4	56.045	56.329	-56.329	0.0	0.445	0.216
51	0	4	247.174	230.053	-230.053	0.0	-0.484	-0.268
52	0	4	27.596	25.940	-25.940	0.0	0.121	0.243
53	0	4	19.037	20.110	-20.110	0.0	2.056	1.237
54	0	4	51.537	42.876	-42.876	0.0	-2.072	-0.814
55	0	4	101.458	187.717	-187.717	0.0	-0.939	-0.696
56	0	4	35.196	33.401	-33.401	0.0	3.771	1.210
57	0	4	13.861	6.429	-6.429	0.0	1.795	1.282
58	0	4	68.231	60.136	-60.136	0.0	-2.567	-0.913
59	0	4	159.103	158.046	-158.046	0.0	0.185	0.103
60	0	4	29.557	30.582	-30.582	0.0	1.057	0.407
61	0	4	3.1291	9.753	-9.753	0.0	6.538	2.651
62	0	6	317.785	405.108	-405.108	0.0	-25.323	-5.685 *
63	0	4	6.166	9.720	-9.720	0.0	-3.953	-0.640
64	0	4	147.966	148.085	-148.085	0.0	-0.099	-0.040
65	0	4	4.145	3.281	-3.281	0.0	0.863	0.127

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
18	0	4	36.144	36.208	-36.208	0.0	-0.064	-0.036
19	0	4	14.472	4.384	-4.384	0.0	10.089	3.138 *
20	0	4	74.68	74.328	75.328	0.0	0.140	0.088
21	0	4	49.724	50.197	50.197	0.0	-0.473	-0.270
22	0	4	17.717	17.029	17.029	0.0	0.699	0.204
23	0	4	17.106	17.151	-17.151	0.0	-0.045	-0.012
23	1	4	28.929	24.267	-24.267	0.0	4.662	2.207
22	1	4	57.744	60.112	-60.112	0.0	-2.368	-1.406
21	1	4	8.877	7.249	-7.249	0.0	1.623	0.307
20	1	4	7.155	5.757	-5.757	0.0	1.399	0.228
19	1	4	14.953	15.305	-15.305	0.0	-0.353	-0.094
19	1	4	51.772	50.118	50.118	0.0	1.654	1.098
17	1	4	6.355	2.684	-2.684	0.0	3.671	0.668
15	1	4	32.412	30.137	-30.137	0.0	2.274	1.486
14	1	4	12.679	13.097	-13.097	0.0	-0.418	-0.169
13	1	4	10.446	5.516	-5.516	0.0	5.130	1.383
0	6	0	375.456	405.108	-405.108	0.0	-25.652	-3.734 *
12	1	4	9.133	15.265	-15.265	0.0	-6.132	-1.387
11	1	4	60.114	60.055	-60.055	0.0	0.059	0.042
10	1	4	116.339	114.965	114.965	0.0	1.373	0.705
0	1	4	27.603	24.556	-24.556	0.0	3.047	1.758
7	1	4	50.616	51.283	-51.283	0.0	-0.667	-0.512
6	1	4	69.247	67.406	-67.406	0.0	1.841	1.347
5	1	4	55.386	55.892	-55.892	0.0	-0.505	-0.376
4	1	4	11.534	1.548	-1.548	0.0	9.986	5.037
3	1	4	25.287	25.688	-25.688	0.0	-0.400	-0.208
22	1	4	67.322	66.766	-66.766	0.0	0.556	0.411
1	1	4	75.115	76.509	-76.509	0.0	-1.392	-0.695
0	2	4	72.443	76.930	-76.930	0.0	-4.287	-3.067
1	2	4	25.782	29.098	-29.098	0.0	-3.315	-1.686
2	2	4	9.163	2.516	-2.516	0.0	6.647	1.674
4	2	4	45.150	44.466	-44.466	0.0	0.504	0.352
3	2	4	68.997	71.186	-71.186	0.0	-2.100	-1.158
6	2	4	5.992	1.840	-1.840	0.0	4.152	0.786
7	2	4	33.811	35.365	-35.365	0.0	-1.553	-0.907
0	2	4	379.185	405.108	-405.108	0.0	-25.923	-3.775 *
8	2	4	63.990	62.723	-62.723	0.0	1.266	0.648
10	2	4	13.832	14.005	-14.005	0.0	-1.073	-0.356
12	2	4	46.382	44.815	-44.815	0.0	1.577	1.24
13	2	4	17.360	6.012	-6.012	0.0	10.456	5.050 *
14	2	4	24.093	19.222	-19.222	0.0	4.871	2.534
15	2	4	25.564	27.854	-27.854	0.0	-2.290	-1.100
16	2	4	22.550	24.369	-24.369	0.0	-1.820	-0.735
17	2	4	9.457	7.015	-7.015	0.0	2.643	0.624
18	2	4	12.072	5.512	-5.512	0.0	6.560	1.50
19	2	4	12.780	0.734	-0.734	0.0	12.065	5.202 *
20	2	4	50.865	47.789	-47.789	0.0	3.076	2.042
21	2	4	8.915	1.775	-1.775	0.0	7.140	1.435
22	2	4	23.321	19.661	-19.661	0.0	4.661	2.203
23	2	4	14.763	9.722	-9.722	0.0	5.042	1.632
22	3	4	10.792	2.169	-2.169	0.0	8.623	1.900
21	3	4	4.741	10.172	-10.172	0.0	-5.431	-0.685
19	3	4	9.890	6.709	-6.709	0.0	3.181	0.661

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/STGMA
0	6	0	381.180	405.108	405.108	0.0	-23.928	-3.465 *
18	3	4	11.286	1.125	0.0	10.161	2.676 *	
17	3	4	7.769	5.133	5.133	0.0	-2.736	0.525
15	3	4	18.474	20.601	0.0	-2.127	-0.727	
14	3	4	12.756	3.341	0.0	9.415	3.252	
13	3	4	5.483	12.630	12.630	0.0	-7.147	-1.140
12	3	4	4.043	7.824	0.0	-3.781	-0.574	
11	3	4	8.915	6.501	0.0	2.414	0.550	
10	3	4	9.497	0.235	0.235	0.0	9.262	2.358
9	3	4	21.516	18.779	18.779	0.0	2.727	1.303
7	3	4	23.496	24.282	24.282	0.0	-0.786	-0.418
6	3	4	6.050	11.116	11.116	0.0	-5.066	-0.965
5	3	4	12.406	15.138	0.0	-2.732	-0.782	
3	3	4	9.541	4.790	4.790	0.0	4.751	1.247
2	3	4	9.614	3.086	3.086	0.0	5.628	1.460
1	3	4	13.556	17.636	0.0	-4.080	-1.258	
0	4	4	49.271	52.285	52.285	0.0	-3.014	-2.265
0	6	0	378.663	405.108	405.108	0.0	-26.445	-3.854 *
2	4	4	11.432	7.819	7.819	0.0	3.613	1.114
3	4	4	15.476	11.508	11.508	0.0	3.969	1.507
4	4	4	6.137	7.489	7.489	0.0	-1.352	-0.260
5	4	4	48.970	49.833	49.833	0.0	-0.855	-0.236
7	4	4	7.315	5.958	5.958	0.0	1.357	0.299
6	4	4	4.028	7.749	7.749	0.0	-2.921	-0.496
9	4	4	33.469	35.134	35.134	0.0	-1.565	-0.898
11	4	4	13.861	17.104	17.104	0.0	-3.242	-1.046
12	4	4	19.973	18.540	18.540	0.0	-1.436	0.619
13	4	4	18.492	20.017	20.017	0.0	-1.325	-0.523
14	4	4	16.771	15.580	15.580	0.0	1.191	0.438
15	4	4	43.529	45.268	45.268	0.0	-1.739	-1.063
17	4	4	10.900	18.422	18.422	0.0	1.478	0.505
18	4	4	11.897	8.780	8.780	0.0	3.117	0.734
19	4	4	21.167	25.681	25.681	0.0	-4.516	-1.442
20	4	4	17.469	14.717	14.717	0.0	2.782	0.869
21	4	4	28.049	30.002	30.002	0.0	-1.933	-0.824
0	6	0	379.708	405.108	405.108	0.0	-25.401	-3.697 *
22	4	4	2.356	10.751	10.751	0.0	-8.395	-0.867
21	5	4	24.821	25.121	25.121	0.0	-0.300	-0.119
20	5	4	11.883	6.978	6.978	0.0	4.905	1.200
19	5	4	21.851	21.663	21.663	0.0	0.168	0.059
18	5	4	76.063	75.179	75.179	0.0	0.864	0.515
17	5	4	11.243	0.557	0.557	0.0	10.646	2.472 *
16	5	4	14.792	10.103	10.103	0.0	4.650	1.402
15	5	4	47.040	47.290	47.290	0.0	-0.341	-0.218
14	5	4	58.660	59.992	59.992	0.0	-1.032	-0.677
13	5	4	50.353	50.621	50.621	0.0	-0.268	-0.175
12	5	4	15.360	16.319	16.319	0.0	-0.959	-0.320
11	5	4	63.609	63.519	63.519	0.0	0.089	0.063
10	5	4	148.896	149.151	149.151	0.0	-0.255	-0.104
9	5	4	21.167	18.795	18.795	0.0	2.372	1.031
7	5	4	24.224	27.855	27.855	0.0	-3.630	-1.598
6	5	4	97.866	97.584	97.584	0.0	0.281	0.165
5	5	4	21.021	19.475	19.475	0.0	1.546	0.743

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STRUCTURE FACTORS

PAGE 20

H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA
3	5	4	49.818	52.390	-52.390	0.0	-3.572	-2.599
0	6	0	370.979	405.108	405.108	0.0	-25.129	-3.645
2	5	4	114.722	119.816	-119.816	0.0	-5.053	-2.687
1	5	4	39.858	40.641	-40.641	0.0	-1.783	-1.234
0	6	4	70.956	79.566	-79.566	0.0	-2.610	-1.737
1	6	4	62.000	60.342	-60.342	0.0	-1.667	-1.197
2	6	4	59.512	59.374	-59.374	0.0	0.138	0.023
3	6	4	30.546	30.268	-30.268	0.0	0.278	0.151
4	6	4	150.826	162.501	-162.501	0.0	-2.576	-1.025
5	6	4	19.505	20.977	-20.977	0.0	1.402	0.554
6	6	4	12.018	12.273	-12.273	0.0	0.744	0.230
8	6	4	120.667	130.828	-130.828	0.0	-1.161	-0.534
9	6	4	49.774	47.752	-47.752	0.0	1.022	0.714
10	6	4	16.335	14.049	-14.049	0.0	2.286	0.610
11	6	4	56.270	54.350	-54.350	0.0	1.520	1.304
12	6	4	102.845	102.810	-102.810	0.0	0.035	0.019
13	6	4	37.734	39.518	-39.518	0.0	-1.783	-0.963
14	6	4	10.528	4.428	-4.428	0.0	2.520	1.392
15	6	4	9.410	7.152	-7.152	0.0	2.258	0.447
16	6	4	109.346	104.891	-104.891	0.0	0.456	0.235
17	6	4	5.894	10.953	-10.953	0.0	-5.059	-0.593
0	6	0	340.366	405.108	-405.108	0.0	-24.742	-3.587
18	6	4	25.113	24.233	-24.233	0.0	0.879	0.339
19	6	4	20.963	20.973	-20.973	0.0	-0.010	-0.005
20	6	4	59.253	57.867	-57.867	0.0	1.386	0.830
18	7	4	11.450	1.213	-1.213	0.0	10.438	2.509
17	7	4	12.130	5.973	-5.973	0.0	9.158	1.249
16	7	4	15.411	11.455	-11.455	0.0	4.256	1.212
15	7	4	38.828	43.265	-43.265	0.0	-4.436	-2.172
14	7	4	30.765	27.680	-27.680	0.0	3.085	1.460
13	7	4	0.046	6.775	-6.775	0.0	2.271	0.586
12	7	4	6.777	3.625	-3.625	0.0	3.152	0.539
11	7	4	46.976	50.529	-50.529	0.0	-3.553	-2.026
10	7	4	28.739	27.597	-27.597	0.0	1.143	0.577
9	7	6	29.089	28.010	-28.010	0.0	1.079	0.593
6	7	6	5.661	17.154	-17.154	0.0	-11.293	-1.718
5	7	4	13.410	14.106	-14.106	0.0	-0.776	-0.247
3	7	4	24.207	24.980	-24.980	0.0	-0.174	-0.086
2	7	4	7.752	5.884	-5.884	0.0	1.867	0.386
0	6	0	379.443	405.108	-405.108	0.0	-23.265	-3.576
1	7	4	31.404	36.172	-36.172	0.0	-6.678	-2.432
0	6	4	62.493	62.868	-62.868	0.0	-0.375	-0.248
1	8	4	14.269	11.183	-11.183	0.0	3.085	1.024
3	8	4	15.527	10.303	-10.303	0.0	5.624	2.034
4	8	4	21.382	44.915	-44.915	0.0	-3.333	-2.142
5	8	4	35.026	37.178	-37.178	0.0	-2.142	-1.323
7	8	4	11.007	6.611	-6.611	0.0	4.486	1.086
8	8	4	52.840	54.555	-54.555	0.0	-1.715	-1.056
9	8	4	28.667	26.770	-26.770	0.0	1.897	0.986
10	8	4	4.305	9.219	-9.219	0.0	-4.914	-0.673
11	8	4	14.836	14.304	-14.304	0.0	0.532	0.149
12	8	4	48.058	45.763	-45.763	0.0	2.295	-1.454
13	8	4	11.374	3.700	-3.700	0.0	7.674	1.836

25C. ORTHOFEPOSILITE 6/18/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
14	8	4	16.320	10.699	10.699	0.0	5.621	1.680
15	8	4	20.759	20.260	20.260	0.0	0.499	0.174
16	8	4	30.823	31.570	-31.570	0.0	-0.767	-0.335
14	9	4	3.739	1.693	-1.693	0.0	2.055	0.249
13	9	4	10.864	7.891	-7.891	0.0	2.974	0.649
0	6	0	379.998	405.108	405.108	0.0	-25.110	-3.663 *
12	9	4	13.047	11.505	-11.505	0.0	1.542	0.365
9	9	4	26.394	29.933	29.933	0.0	-3.439	-1.327
9	9	4	10.675	4.643	-4.643	0.0	6.033	1.330
7	9	4	13.847	6.230	-6.230	0.0	7.616	2.237
6	9	4	11.795	8.712	-8.712	0.0	3.083	0.803
5	9	4	11.083	12.364	12.364	0.0	-1.281	-0.281
3	9	4	15.826	19.340	-19.340	0.0	-3.514	-0.974
1	9	4	10.821	4.713	-4.713	0.0	6.108	1.521
0	10	4	9.279	7.088	-7.088	0.0	2.191	0.435
1	10	4	20.978	18.421	18.421	0.0	2.556	0.965
2	10	4	6.995	6.723	-6.723	0.0	0.272	0.048
3	10	4	27.370	25.650	-25.650	0.0	1.720	0.747
4	10	4	36.757	36.592	-36.592	0.0	0.175	0.096
5	10	4	19.376	18.543	-18.543	0.0	0.833	0.276
0	6	0	379.746	405.108	405.108	0.0	-25.362	-3.691 *
8	10	4	27.691	26.932	-26.932	0.0	0.758	0.321
11	10	4	8.130	13.325	13.325	0.0	-5.196	-0.827
7	11	4	17.703	25.401	25.401	0.0	-7.698	-1.805
6	11	4	70.893	68.643	-68.643	0.0	2.250	1.378
5	11	4	21.070	25.223	-25.223	0.0	-4.144	-1.222
3	11	4	16.087	19.678	-19.678	0.0	-3.590	-0.928
2	11	4	86.725	86.316	-86.316	0.0	0.400	0.221
1	11	4	23.220	21.436	-21.436	0.0	1.784	0.681
0	10	5	37.034	33.176	-33.176	0.0	3.858	2.320
1	10	5	10.617	6.764	-6.764	0.0	3.853	0.825
2	10	5	31.552	29.984	-29.984	0.0	1.568	0.732
4	10	5	10.806	13.560	-13.560	0.0	-2.754	-0.546
5	10	5	24.399	22.034	-22.034	0.0	2.365	0.955
10	0	5	70.049	78.657	78.657	0.0	0.292	0.225
9	9	5	43.280	43.617	43.617	0.0	-0.336	-0.181
8	9	5	38.566	40.151	-40.151	0.0	-1.585	-0.739
0	6	0	380.889	405.108	405.108	0.0	-24.219	-3.509 *
7	9	5	39.967	39.603	-39.603	0.0	0.364	0.198
6	9	5	55.664	54.112	-54.112	0.0	1.552	0.973
5	9	5	51.581	51.092	-51.092	0.0	0.490	0.302
4	9	5	52.628	2.262	-2.262	0.0	7.366	1.485
3	9	5	60.426	69.335	-69.335	0.0	1.001	0.676
2	9	5	53.220	52.927	-52.927	0.0	0.293	0.167
0	8	5	41.601	42.489	-42.489	0.0	-0.888	-0.515
1	8	5	49.154	50.396	50.396	0.0	-1.242	-0.745
2	8	5	51.684	55.311	-55.311	0.0	-3.627	-1.990
3	8	5	38.522	39.381	-39.381	0.0	-0.858	-0.460
4	8	5	84.302	89.187	-89.187	0.0	-4.885	-2.734
5	8	5	29.876	30.040	-30.040	0.0	-0.164	-0.070
6	8	5	6.239	6.223	-6.223	0.0	0.016	0.003
7	8	5	18.299	11.459	-11.459	0.0	6.840	2.293
8	8	5	69.188	68.618	-68.618	0.0	0.570	0.352

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
9	8	5	61.349	60.786	60.786	0.0	0.563	0.331
11	8	5	76.338	78.464	78.464	0.0	-2.127	-1.203
12	8	5	65.340	65.855	65.855	0.0	-0.515	-0.322
0	6	0	379.185	405.108	405.108	0.0	-25.923	-3.775 *
13	P	5	11.505	8.098	8.098	0.0	3.407	0.768
15	7	5	18.056	18.425	18.425	0.0	-0.329	-0.097
12	7	5	26.077	25.189	25.189	0.0	1.788	0.758
11	7	5	11.214	7.230	7.230	0.0	3.984	0.901
8	7	5	27.326	27.570	27.570	0.0	-0.244	-0.110
7	7	5	6.574	9.468	9.468	0.0	-2.895	-0.458
6	7	5	20.046	18.569	18.569	0.0	1.477	0.546
5	7	5	17.353	22.029	22.029	0.0	-4.676	-1.403
4	7	5	26.554	26.262	26.262	0.0	0.292	0.135
3	7	5	26.278	31.470	31.470	0.0	-5.192	-2.095
1	7	5	13.803	15.254	15.254	0.0	-1.451	-0.396
0	6	5	12.654	10.488	10.488	0.0	2.166	0.667
1	6	5	17.179	15.747	15.747	0.0	1.432	0.494
2	6	5	16.466	16.607	16.607	0.0	-0.141	-0.047
3	6	5	15.418	17.245	17.245	0.0	-1.827	-0.587
0	6	0	380.618	405.108	405.108	0.0	-24.490	-3.550 *
5	6	5	8.668	13.761	13.761	0.0	-5.093	-1.048
7	6	5	6.268	10.448	10.448	0.0	-4.180	-0.653
8	6	5	7.679	11.199	11.199	0.0	-3.521	-0.627
9	6	5	11.432	2.027	2.027	0.0	9.404	2.317
10	6	5	14.050	12.928	12.928	0.0	1.123	0.290
11	6	5	12.727	3.420	3.420	0.0	9.307	2.414
12	6	5	11.374	4.573	4.573	0.0	6.800	1.629
13	6	5	21.647	16.763	16.763	0.0	4.884	1.917
15	6	5	10.166	9.478	9.478	0.0	0.688	0.136
17	6	5	9.788	7.248	7.248	0.0	2.560	0.498
18	5	5	20.439	19.085	19.085	0.0	0.454	0.137
16	5	5	7.941	2.428	2.428	0.0	5.513	1.005
15	5	5	21.822	12.797	12.797	0.0	9.025	4.052
14	5	5	33.913	33.527	33.527	0.0	0.386	0.187
13	5	5	23.962	16.088	16.088	0.0	6.974	3.012
0	6	0	379.050	405.108	405.108	0.0	-26.058	-3.796 *
12	5	5	26.846	27.347	27.347	0.0	-0.502	-0.200
11	5	5	11.577	14.678	14.678	0.0	-3.100	-0.687
10	5	5	44.157	43.974	43.974	0.0	0.182	0.114
9	5	5	33.899	33.887	33.887	0.0	0.011	0.006
8	5	5	8.872	6.074	6.074	0.0	1.897	0.413
7	5	5	43.266	40.577	40.577	0.0	2.689	1.805
6	5	5	58.828	62.570	62.570	0.0	-3.741	-2.503
5	5	5	15.462	11.532	11.532	0.0	3.930	1.392
4	5	5	10.966	10.844	10.844	0.0	0.122	0.032
3	5	5	9.454	1.707	1.707	0.0	3.746	0.630
2	5	5	36.903	35.029	35.029	0.0	1.874	1.247
1	5	5	14.400	13.659	13.659	0.0	0.741	0.227
0	4	5	9.119	13.220	13.220	0.0	-4.101	-0.972
1	4	5	19.129	17.508	17.508	0.0	1.621	0.671
2	4	5	45.121	46.031	46.031	0.0	-0.910	-0.656
3	4	5	13.730	19.037	19.037	0.0	-5.306	-1.501
4	4	5	32.412	32.336	32.336	0.0	0.075	0.047

STRUCTURE FACTORS						PAGE 23		
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	4	5	1.847	9.576	9.576	0.0	-7.729	-0.898
6	4	5	22.128	21.373	21.373	0.0	0.754	0.343
7	4	5	0.090	2.265	2.265	0.0	2.155	0.455
0	6	0	-370.746	405.108	405.108	0.0	-25.362	-3.691 *
14	7	5	10.195	8.004	8.004	0.0	2.191	0.430
8	4	5	7.606	6.533	6.533	0.0	1.074	0.212
9	4	5	43.368	43.298	43.298	0.0	0.070	0.043
11	4	5	46.766	47.489	47.489	0.0	-0.703	-0.445
12	4	5	11.606	12.613	12.613	0.0	-1.007	-0.735
13	4	5	20.162	24.491	24.491	0.0	4.671	2.357
14	4	5	9.327	2.554	2.554	0.0	6.783	1.417
15	4	5	17.237	13.518	13.518	0.0	3.719	1.259
16	4	5	18.547	15.785	15.785	0.0	2.762	0.912
17	4	5	26.234	26.108	26.108	0.0	0.126	0.051
18	4	5	30.881	30.053	30.053	0.0	0.708	0.395
20	3	5	32.228	32.773	32.773	0.0	0.495	0.210
19	3	5	16.531	10.401	10.401	0.0	6.531	2.158
18	3	5	70.692	81.221	81.221	0.0	-5.526	-1.477
17	3	5	66.573	66.942	66.942	0.0	-2.369	-1.356
16	3	5	40.900	50.989	50.989	0.0	-1.090	-0.611
15	3	5	55.287	55.736	55.736	0.0	-0.251	0.156
14	3	5	57.671	56.196	56.196	0.0	1.525	-0.938
13	3	5	52.635	53.741	53.741	0.0	-1.106	-0.657
0	6	0	380.501	405.108	405.108	0.0	-24.607	-3.567 *
12	3	5	63.320	62.028	62.028	0.0	0.692	0.445
11	3	5	40.945	40.254	40.254	0.0	0.491	0.426
10	3	5	128.501	147.151	147.151	0.0	-1.509	0.570
9	3	5	69.923	70.223	70.223	0.0	-0.300	-0.198
8	3	5	50.708	58.046	58.046	0.0	0.761	0.519
7	3	5	61.731	60.738	60.738	0.0	0.923	0.713
6	3	5	111.971	110.774	110.774	0.0	1.196	0.625
5	3	5	79.241	78.607	78.607	0.0	0.634	0.410
4	3	5	13.890	13.366	13.366	0.0	0.594	0.172
3	3	5	106.807	107.267	107.267	0.0	-0.460	-0.247
2	3	5	10.417	112.178	112.178	0.0	-2.761	-1.468
1	3	5	10.864	12.534	12.534	0.0	-1.670	-0.427
0	2	5	29.453	29.949	29.949	0.0	-0.496	-0.283
1	2	5	44.011	44.711	44.711	0.0	-0.160	-0.112
2	2	5	53.007	61.836	61.836	0.0	1.171	0.840
3	2	5	37.253	38.051	38.051	0.0	-0.799	-0.532
4	2	5	91.341	91.221	91.221	0.0	0.120	0.073
5	2	5	40.521	38.121	38.121	0.0	1.500	0.950
6	2	5	22.797	18.284	18.284	0.0	4.513	2.385
7	2	5	19.173	18.994	18.994	0.0	0.17R	0.068
0	6	0	380.405	405.108	405.108	0.0	-24.704	-3.582 *
8	2	5	60.510	59.438	59.438	0.0	1.471	1.079
9	2	5	74.968	72.792	72.792	0.0	2.176	1.421
10	2	5	4.014	5.373	5.373	0.0	-1.350	-0.193
11	2	5	85.543	86.457	86.457	0.0	1.0R	0.668
12	2	5	57.598	58.447	58.447	0.0	-0.849	-0.552
13	2	5	1.105	11.458	11.458	0.0	-10.353	-1.045 *
14	2	5	12.610	13.495	13.495	0.0	-0.885	-0.229
15	2	5	9.279	10.418	10.418	0.0	-1.139	-0.226

STRUCTURE FACTORS							PAGE 24	
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
16	2	5	48.160	51.945	-51.945	0.0	-3.705	-2.039
17	2	5	33.859	36.481	36.481	0.0	-2.582	-1.173
18	2	5	20.250	20.708	20.708	0.0	-0.458	-0.152
19	2	5	18.460	21.410	21.410	0.0	-2.950	-0.874
20	2	5	23.715	24.627	24.627	0.0	-0.912	-0.330
20	1	5	19.420	17.705	17.705	0.0	1.715	0.598
19	1	5	13.265	9.467	-9.467	0.0	3.797	0.913
17	1	5	12.217	14.049	-14.049	0.0	-1.832	-0.427
16	1	5	13.323	2.237	2.237	0.0	11.086	2.931 *
15	1	5	21.662	23.080	-23.080	0.0	-1.418	-0.535
14	1	5	34.147	20.097	-30.097	0.0	4.049	2.458
0	6	0	380.172	405.108	405.108	0.0	-25.936	-3.616 *
13	1	5	18.295	15.267	-15.267	0.0	3.018	1.185
12	1	5	39.398	38.318	38.318	0.0	1.079	0.732
11	1	5	6.050	12.514	-12.514	0.0	-6.564	-1.066
10	1	5	24.055	24.840	24.840	0.0	-0.805	-0.359
9	1	5	17.179	18.371	18.371	0.0	-1.192	-0.443
8	1	5	22.870	20.126	20.126	0.0	2.764	1.318
7	1	5	26.598	25.983	25.983	0.0	0.615	0.327
6	1	5	59.517	57.912	-57.912	0.0	1.605	1.217
5	1	5	54.456	6.168	6.168	0.0	-6.714	-0.622
4	1	5	20.861	21.161	21.161	0.0	-0.280	-0.153
3	1	5	17.572	16.994	-16.994	0.0	0.578	0.236
2	1	5	20.366	21.833	21.833	0.0	-1.667	-0.630
1	1	5	14.734	12.194	12.194	0.0	2.540	0.909
1	0	6	152.362	149.630	-149.630	0.0	2.732	1.083
3	0	6	63.271	62.491	-62.491	0.0	0.780	0.321
4	0	6	36.465	35.717	-35.717	0.0	0.748	0.468
5	0	6	78.813	78.420	78.420	0.0	0.393	0.247
6	0	6	11.272	1.898	1.898	0.0	9.374	2.907
0	6	0	378.470	405.108	405.108	0.0	-26.638	-3.894 *
7	0	6	129.848	127.337	127.337	0.0	2.512	1.133
8	0	6	10.242	18.637	18.637	0.0	1.205	0.470
9	0	6	34.876	34.034	-34.034	0.0	0.841	0.471
10	0	6	25.896	24.297	24.297	0.0	1.609	0.773
11	0	6	41.704	40.798	-40.798	0.0	0.904	0.525
12	0	6	18.343	12.104	-12.104	0.0	6.239	2.317
13	0	6	107.865	105.192	105.192	0.0	2.673	1.358
14	0	6	11.400	1.890	-1.890	0.0	9.610	2.124
15	0	6	106.360	106.033	106.033	0.0	0.326	0.187
16	0	6	21.487	18.863	18.863	0.0	2.625	0.875
17	0	6	48.730	50.065	-50.065	0.0	-1.335	-0.702
17	1	6	7.854	1.041	-1.041	0.0	6.812	1.125
16	1	6	18.911	21.203	21.203	0.0	-2.292	-0.653
15	1	6	43.397	41.608	-41.608	0.0	1.786	1.175
13	1	6	83.268	84.795	84.795	0.0	-1.527	-0.869
12	1	6	16.611	15.988	15.988	0.0	0.723	0.214
10	1	6	12.436	10.996	-10.996	0.0	1.540	0.346
9	1	6	12.785	4.815	4.815	0.0	7.970	2.099
0	6	0	378.934	405.108	405.108	0.0	-26.175	-3.613 *
8	1	6	3.272	6.291	-6.291	0.0	-3.019	-0.377
7	1	6	53.440	53.910	-53.910	0.0	-0.470	-0.300
6	1	6	13.294	12.167	-12.167	0.0	1.127	0.330

STRUCTURE FACTORS						PAGE 25		
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DFLT& F	DELTA/SIGMA
5	1	6	21.735	21.893	0.0	-0.159	-0.065	
4	1	6	8.435	8.450	-15.850	0.0	-7.415	-1.370
3	1	6	5.715	6.640	6.640	0.0	-0.975	-0.157
2	1	6	7.228	7.764	-2.764	0.0	4.464	0.857
1	1	6	80.573	81.551	-81.551	0.0	-1.028	-0.633
0	2	6	26.015	27.334	27.334	0.0	-1.318	-0.416
1	2	6	25.535	28.699	-28.699	0.0	-3.164	-1.530
2	2	6	26.409	26.812	26.812	0.0	-0.404	-0.702
3	2	6	48.058	50.986	-50.986	0.0	-2.929	-1.758
4	2	6	19.027	15.436	-15.436	0.0	3.591	1.443
5	2	6	17.324	16.353	16.353	0.0	-2.029	-0.655
6	2	6	27.559	25.329	-25.329	0.0	2.231	1.086
7	2	6	6.065	5.750	-5.750	0.0	0.314	0.052
8	2	6	14.938	20.606	20.606	0.0	-5.668	-1.459
0	2	6	16.771	15.502	-15.502	0.0	1.269	0.391
10	2	6	22.506	23.715	-23.715	0.0	-1.209	-0.454
11	2	6	47.298	46.630	-46.630	0.0	0.668	0.394
0	6	0	378.412	405.108	405.108	0.0	-26.626	-3.903 *
12	2	6	17.397	14.156	-14.156	0.0	3.241	1.008
13	2	6	12.261	3.039	3.039	0.0	8.322	1.973
15	2	6	28.045	28.499	28.499	0.0	0.556	0.245
16	2	6	12.843	10.254	10.254	0.0	2.589	0.607
16	3	6	17.208	12.407	-12.407	0.0	4.801	1.416
15	3	6	13.512	4.242	4.242	0.0	9.270	2.351
12	3	6	12.959	10.769	-10.769	0.0	2.190	0.525
11	3	6	2.880	0.839	0.839	0.0	2.041	0.237
10	3	6	3.272	1.252	1.252	0.0	2.020	0.247
0	3	6	11.054	2.892	2.892	0.0	8.162	1.908
7	3	6	17.105	12.272	-12.272	0.0	4.834	1.721
5	3	6	14.516	5.547	5.547	0.0	8.969	2.964
4	3	6	18.649	20.768	20.768	0.0	-2.119	-0.707
3	3	6	8.712	6.711	-6.711	0.0	2.000	0.417
2	3	6	11.315	5.906	5.906	0.0	5.610	1.436
0	6	0	386.095	405.108	405.108	0.0	-24.013	-3.629 *
0	4	6	26.817	27.795	27.795	0.0	-0.979	0.454
1	4	6	15.447	15.205	15.205	0.0	0.242	0.074
3	4	6	33.826	38.580	-38.580	0.0	-4.754	-2.346
4	4	6	8.014	9.723	9.723	0.0	-1.709	0.304
5	4	6	13.047	3.550	3.550	0.0	0.496	2.731
6	4	6	8.843	10.786	-10.786	0.0	-1.943	-0.369
7	4	6	8.552	15.604	-15.604	0.0	-7.053	-1.243
8	4	6	18.902	16.141	16.141	0.0	0.761	0.231
0	4	6	12.974	11.715	-11.715	0.0	1.259	0.303
10	4	6	9.846	6.956	6.956	0.0	2.890	0.598
11	4	6	11.417	17.425	-17.425	0.0	-6.008	-1.170
12	4	6	10.694	13.961	-13.961	0.0	-3.868	-0.715
13	4	6	18.583	19.164	-19.164	0.0	-0.181	0.057
14	4	6	10.515	5.625	5.625	0.0	4.891	0.995
15	4	6	7.039	3.818	3.818	0.0	3.221	0.540
13	5	6	94.349	92.140	-92.140	0.0	2.209	1.221
12	5	6	15.605	3.004	3.004	0.0	11.700	3.689 *
0	6	0	377.524	405.108	405.108	0.0	-27.584	-4.028 *
11	5	6	27.953	26.712	-26.712	0.0	1.241	0.539

24C ORTHOPEROVOSILITE 6/18/73

STRUCTURE FACTORS

PAGE 26

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
10	5	6	20.090	15.828	15.828	0.0	4.262	1.541
9	5	6	16.655	15.695	15.695	0.0	0.960	0.277
8	5	6	11.926	12.641	-12.641	0.0	-0.715	-0.160
7	5	6	74.482	75.943	75.943	0.0	-1.461	-0.870
6	5	6	10.326	7.405	7.405	0.0	2.821	0.608
5	5	6	60.616	63.230	-63.230	0.0	-2.614	-1.578
4	5	6	7.155	8.049	-8.049	0.0	-1.793	-0.288
3	5	6	21.458	21.037	-21.037	0.0	0.421	0.155
2	5	6	20.283	19.071	19.071	0.0	1.223	0.431
1	5	6	101.135	102.116	102.116	0.0	-0.981	-0.528
0	6	6	11.345	9.443	-9.443	0.0	1.902	0.408
1	6	6	118.332	121.486	-121.486	0.0	-3.155	-1.514
2	6	6	17.401	15.953	15.953	0.0	1.648	0.508
3	6	6	31.537	33.756	-33.756	0.0	-2.219	-0.970
4	6	6	25.666	26.983	-26.983	0.0	-1.317	-0.497
5	6	6	60.235	59.007	59.007	0.0	1.228	0.791
6	6	6	12.785	6.083	-6.083	0.0	6.702	1.572
7	6	6	85.206	85.844	-85.844	0.0	-0.637	-0.303
8	6	6	19.799	19.346	19.346	0.0	0.453	0.150
9	6	6	12.610	10.692	-10.692	0.0	1.918	0.450
10	6	6	14.260	2.842	-2.842	0.0	11.397	3.278 *
11	6	6	36.261	36.440	-36.440	0.0	-0.179	-0.089
10	7	6	5.396	0.358	-0.358	0.0	5.037	0.705
9	7	6	28.462	25.856	25.856	0.0	2.606	1.139
8	7	6	6.312	0.040	-0.040	0.0	6.271	0.987
7	7	6	26.715	25.976	-25.976	0.0	0.789	0.320
6	7	6	23.016	23.815	-23.815	0.0	-0.800	0.293
4	7	6	14.472	10.973	10.973	0.0	3.499	1.032
3	7	6	32.966	31.652	-31.652	0.0	1.314	0.430
1	7	6	23.278	20.809	-20.809	0.0	2.469	0.942
0	8	6	21.473	23.645	23.645	0.0	-2.172	-0.739
1	8	6	29.075	25.934	-25.934	0.0	3.140	1.400
2	8	6	15.505	8.155	8.155	0.0	7.310	2.076
3	8	6	40.857	43.338	-43.338	0.0	-2.481	-1.141
5	8	6	20.759	21.015	21.015	0.0	-0.256	-0.085
6	8	6	16.349	10.452	-10.452	0.0	5.897	1.894
6	5	7	18.081	13.106	-13.106	0.0	4.975	1.590
5	5	7	3.170	8.100	8.100	0.0	-4.920	-0.562
4	5	7	21.312	24.368	-24.368	0.0	-3.056	-1.029
3	5	7	15.564	18.790	18.790	0.0	-3.227	-0.821
2	5	7	14.923	16.096	16.096	0.0	-1.173	-0.291
1	5	7	47.824	49.349	-49.349	0.0	-1.525	-0.869
1	4	7	23.831	24.363	24.363	0.0	-0.532	-0.197
2	4	7	27.195	31.250	31.250	0.0	-4.055	-1.521
3	4	7	10.326	7.745	7.745	0.0	2.581	0.525
4	4	7	30.545	29.631	-29.631	0.0	0.915	0.400
5	4	7	25.812	22.937	22.937	0.0	2.975	1.253
7	4	7	15.360	11.778	11.778	0.0	3.582	0.940
8	4	7	17.514	17.395	17.395	0.0	0.118	0.033
10	3	7	79.182	78.332	78.332	0.0	0.849	0.480
9	3	7	63.447	63.058	-63.058	0.0	0.389	0.230
8	3	7	31.071	32.208	-32.208	0.0	-1.137	-0.482
7	3	7	69.511	70.224	-70.224	0.0	-0.713	-0.407

24C. ORTHOFERROPSILITE 6/18/73

STRUCTURE FACTORS

PAGE 27

H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA
6	3	7	51.625	50.742	-50.742	0.0	0.884	0.508
5	3	7	79.123	77.164	-77.164	0.0	1.058	1.135
3	3	7	92.880	95.676	-95.676	0.0	-1.786	-0.972
2	3	7	59.429	57.798	-57.798	0.0	1.631	1.012
1	3	7	17.775	14.472	-14.472	0.0	3.303	1.031
0	2	7	14.530	17.414	-17.414	0.0	-2.476	-0.617
1	2	7	50.294	52.702	-52.702	0.0	-2.408	-1.395
2	2	7	39.879	38.829	-38.829	0.0	1.050	0.605
3	2	7	30.736	27.216	-27.216	0.0	3.520	1.816
4	2	7	56.272	55.757	-55.757	0.0	0.523	0.305
6	2	7	11.286	4.832	-4.832	0.0	6.454	1.445
7	2	7	23.846	19.197	-19.197	0.0	4.639	1.959
8	2	7	34.671	34.738	-34.738	0.0	-0.067	-0.030
9	2	7	62.200	60.060	-60.060	0.0	2.140	1.292
10	2	7	3.374	8.466	-8.466	0.0	-5.092	-0.561
11	2	7	60.367	60.753	-60.753	0.0	-0.386	-0.221
11	1	7	18.503	19.626	-19.626	0.0	-1.123	-0.323
10	1	7	16.640	17.372	-17.372	0.0	-0.731	-0.187
9	1	7	25.025	26.428	-26.428	0.0	-1.403	-0.518
8	1	7	19.537	13.290	-13.290	0.0	6.247	2.212
6	1	7	13.947	3.286	-3.286	0.0	10.561	2.813 *
4	1	7	26.161	20.830	-20.830	0.0	5.332	2.525
3	1	7	13.776	14.177	-14.177	0.0	-0.403	-0.106
1	1	7	38.931	41.092	-41.092	0.0	-2.161	-1.073

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	0	356.742	372.296	372.296	0.0	-15.554	-2.431 *
4	0	0	187.367	190.262	-190.262	0.0	-2.875	-0.972
6	0	0	28.950	28.651	-28.651	0.0	0.098	0.098
8	3	0	101.455	110.064	110.064	0.0	-8.628	-5.342
10	0	0	12.912	8.523	8.523	0.0	3.989	1.723
12	0	3	290.188	283.575	-283.575	0.0	6.614	1.340
14	0	3	40.104	39.573	-39.573	0.0	0.536	0.393
16	0	0	174.718	177.929	177.929	0.0	-3.211	-1.139
18	0	0	11.250	9.141	9.141	0.0	2.149	0.559
20	0	0	173.138	173.073	-173.073	0.0	0.065	0.023
22	0	0	16.287	15.709	-15.709	0.0	0.578	0.193
26	0	0	22.762	23.475	23.475	0.0	-6.713	-2.186
26	1	0	34.603	37.778	-37.778	0.0	-3.178	-1.382
24	1	0	17.645	19.752	-19.752	0.0	-2.105	-0.640
22	1	0	29.316	30.531	30.531	0.0	-1.216	-0.543
20	1	0	20.555	19.436	-19.436	0.0	1.162	0.510
18	1	0	57.355	56.717	-56.717	0.0	1.179	0.880
16	1	2	11.345	2.756	-2.756	0.0	9.049	2.693
14	1	0	131.508	131.918	131.918	0.0	-0.409	-0.192
12	1	0	8.778	4.361	-4.361	0.0	4.417	1.209
0	6	0	355.053	372.296	372.296	0.0	-17.233	-2.769 *
10	1	0	42.958	42.891	42.891	0.0	0.137	0.095
6	1	0	258.269	262.748	262.748	0.0	-4.479	-1.049
4	1	0	19.253	9.199	9.199	0.0	1.054	0.565
2	1	0	64.780	65.143	-65.143	0.0	-0.363	-0.278
0	2	0	13.233	11.554	-11.554	0.0	1.279	0.376
2	2	0	7.624	2.339	2.339	0.0	5.285	2.110
4	2	0	193.047	156.133	-156.133	0.0	-3.086	-1.006
6	2	0	16.057	18.043	-18.043	0.0	-1.966	-1.246
8	2	0	86.667	85.861	85.861	0.0	0.806	0.571
10	2	0	27.382	28.256	28.256	0.0	-0.375	-0.285
12	2	0	11.173	12.710	-12.710	0.0	-1.536	-0.667
16	2	0	76.344	77.159	77.159	0.0	-0.814	-0.556
18	2	0	7.823	13.915	13.915	0.0	-6.087	-1.171
20	2	0	15.396	20.487	-20.487	0.0	-5.091	-1.535
22	2	0	19.027	16.037	-16.037	0.0	2.983	1.057
24	2	0	33.257	36.801	36.801	0.0	-3.504	-1.554
26	2	0	15.381	15.860	-15.860	0.0	-0.479	-0.111
0	6	0	355.823	372.296	372.296	0.0	-16.473	-2.578 *
24	3	0	13.350	2.695	-2.695	0.0	10.655	2.784 *
22	3	0	13.467	10.513	-10.513	0.0	2.954	0.787
20	3	0	6.835	4.048	4.048	0.0	2.787	0.533
18	3	0	12.561	12.547	12.547	0.0	0.014	0.004
16	3	0	12.655	7.553	-7.553	0.0	4.451	1.553
14	3	0	36.420	40.466	-40.466	0.0	-1.955	-0.665
12	3	0	15.220	10.323	-10.323	0.0	4.897	1.082
10	3	0	6.674	2.419	2.419	0.0	4.255	1.022
8	3	0	9.493	6.220	-6.220	0.0	3.274	1.186
6	3	0	46.945	45.208	-45.208	0.0	1.737	1.793
4	3	0	27.631	22.583	22.583	0.0	-0.352	-0.309
2	3	0	37.911	36.970	-36.970	0.0	0.941	1.004
0	4	0	25.469	25.366	25.366	0.0	0.043	0.040
2	4	0	12.079	10.667	-10.667	0.0	1.212	0.643

F.Mel.

400G ORTHOPHOSPHITE 6/29/73

STRUCTURE FACTORS PAGE 2

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
4	4	0	68.317	72.497	-72.097	0.0	-3.780	-3.201
6	4	1	6.441	2.645	2.845	0.0	3.595	0.989
8	4	0	61.002	66.159	-60.159	0.0	6.843	0.658
10	4	0	38.653	39.765	39.765	0.3	-1.107	-0.339
12	4	0	3.450	15.548	-15.548	0.3	-12.058	-1.661 *
0	6	0	351.579	372.296	372.296	0.0	-17.720	-2.302 *
16	4	0	57.321	58.145	59.145	0.0	-0.826	-0.556
18	4	0	8.652	2.343	2.348	0.0	6.256	1.301
20	4	0	45.903	46.654	-46.054	0.3	-3.151	-1.917
22	4	0	19.312	19.295	-19.295	0.0	0.017	0.006
24	4	0	23.318	22.597	22.597	0.0	0.721	0.259
26	4	0	2.789	8.617	8.617	0.3	-6.028	-0.641
24	5	C	0.847	0.993	0.993	0.0	0.754	0.268
22	5	0	27.940	28.214	-28.214	0.0	-0.276	-0.118
20	5	0	22.324	26.660	26.660	0.0	-4.262	-1.542
12	5	0	73.153	74.766	74.766	0.0	-1.513	0.765
16	5	0	12.532	d.111	5.111	0.0	4.421	1.339
14	5	0	211.057	210.337	-210.167	0.0	0.350	0.246
12	5	C	14.665	18.094	18.094	0.0	-3.429	-1.052
10	5	0	8.223	s.644	-5.064	0.0	0.159	0.035
8	5	2	19.437	18.300	-18.200	0.0	0.197	0.598
6	5	0	168.042	168.383	-168.200	0.0	-2.239	0.847
4	5	0	6.572	5.620	-5.800	0.0	0.772	0.192
9	0	21.759	220.341	220.341	0.0	-9.547	-2.802	
6	0	356.723	372.226	372.226	0.0	-15.573	-2.434 *	
2	6	0	15.855	16.596	16.596	0.0	-0.892	0.363
0	6	0	356.622	372.296	372.296	0.0	-13.676	-2.119 *
4	6	0	92.556	96.559	-96.559	0.0	-3.163	1.983
6	6	0	16.345	16.636	-16.636	0.0	-0.291	0.111
8	6	0	131.372	130.596	130.596	0.0	0.774	0.362
10	6	0	17.821	13.571	-13.571	0.0	4.251	1.701
12	6	0	139.874	139.728	-139.728	0.0	0.145	0.063
14	6	0	26.901	26.338	-26.338	0.0	-2.435	-1.233
16	6	0	79.277	83.396	83.396	0.0	-4.119	2.550
18	6	0	19.531	12.623	12.623	0.0	-4.492	0.333
20	6	0	139.522	141.365	-141.365	0.3	-1.942	0.713
24	6	0	10.121	7.224	-7.224	0.0	2.847	0.514
22	7	0	23.639	20.761	-20.761	0.0	2.337	0.850
20	7	0	11.029	11.534	11.534	0.0	11.496	2.947 *
18	7	0	16.345	15.533	15.533	0.0	2.483	0.841
16	7	0	13.847	16.745	-16.745	0.0	-2.898	0.806
14	7	0	60.914	58.691	58.691	0.0	2.222	1.572
12	7	0	12.313	7.001	-7.001	0.0	5.312	1.574
10	7	0	14.979	74.855	74.855	0.0	0.044	0.030
6	7	0	32.492	35.553	35.553	0.0	-3.051	-1.730
0	6	0	257.263	372.296	372.296	0.0	-15.037	-2.442 *
4	7	0	38.468	39.580	39.580	0.0	-1.112	-0.791
2	7	0	19.152	19.581	19.581	0.0	-0.935	-0.330
0	9	C	59.912	61.147	61.147	0.0	-1.234	-0.911
2	8	0	21.753	27.638	-27.638	0.0	-5.855	-2.472
4	3	0	92.643	91.642	-91.642	0.0	0.006	0.456
8	8	0	38.629	36.620	36.620	0.0	2.009	1.357
10	8	0	27.955	29.529	29.529	0.0	-1.574	-0.834

400C ORTHOFEPROSILITE 6/28/73				STRUCTURE FACTORS				PAGE 3	
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	S0
12	8	0	44.216	44.514	-44.914	0.0	-0.498	-0.441	
14	8	0	6.324	6.588	-6.588	0.0	6.735	0.421	
16	8	0	70.222	68.551	68.991	0.0	1.231	0.758	
13	8	0	12.444	1.554	-1.556	0.0	10.888	2.615 *	
20	8	0	8.577	11.078	-11.078	0.0	-3.001	-0.462	
20	9	0	9.800	1.074	1.074	0.0	8.727	1.512	
13	9	0	8.164	3.254	-3.254	0.0	4.911	1.010	
0	6	0	355.603	372.256	372.256	0.0	-14.694	-2.122 *	
8	9	0	21.373	19.544	-19.944	0.0	1.439	0.423	
6	9	0	20.131	15.433	19.433	0.0	0.698	0.255	
4	9	0	14.168	10.178	-10.178	0.0	3.990	1.3C7	
2	9	0	5.258	3.283	3.293	0.0	1.964	0.339	
0	10	0	66.653	64.624	-64.824	0.0	1.865	1.431	
2	13	0	11.845	12.739	12.769	0.0	-0.943	-0.237	
4	10	0	16.582	16.670	-16.870	0.0	5.311	2.185	
8	10	0	37.319	36.468	-36.668	0.0	0.702	0.420	
10	10	0	9.362	1.348	-1.348	0.0	8.013	1.653	
12	10	0	21.125	22.767	22.767	0.0	-1.582	-0.513	
16	11	0	7.387	5.449	-5.449	0.0	-1.563	-0.242	
14	11	0	125.782	103.240	-103.240	0.0	3.742	1.876	
10	11	0	4.873	1.429	-1.629	0.0	3.249	0.434	
8	11	0	12.883	C.034	0.034	0.0	12.048	3.355 *	
6	11	0	54.552	91.514	-91.514	0.0	2.933	1.629	
0	6	0	357.651	372.296	372.296	0.0	-14.865	-2.311 *	
4	11	0	21.667	18.630	18.630	0.0	2.977	1.219	
2	11	0	84.409	63.564	83.504	0.0	0.995	0.646	
0	12	0	105.647	103.335	103.335	0.0	2.263	1.127	
2	12	0	9.501	10.519	-10.519	0.0	-0.934	-0.182	
4	12	0	12.959	1.566	-1.546	0.0	11.053	2.582 *	
6	12	0	15.030	7.684	7.684	0.0	7.347	2.061	
8	12	0	33.648	21.412	31.412	0.0	2.237	1.022	
12	12	0	42.115	41.567	-41.567	0.0	1.149	0.647	
2	13	0	40.285	36.770	36.000	0.0	4.285	2.118	
7	13	1	13.365	0.153	0.153	0.0	13.212	3.207 *	
6	13	1	16.872	12.417	-12.417	0.0	4.454	1.151	
5	13	1	6.674	1.588	-1.588	0.0	5.087	0.744	
4	13	1	8.752	10.287	10.287	0.0	-1.494	-0.247	
3	13	1	24.409	14.351	-14.351	0.0	6.058	2.125	
2	13	1	9.464	12.123	12.123	0.0	-2.659	-0.470	
1	13	1	14.300	15.780	15.780	0.0	-1.483	-0.342	
0	5	0	355.996	372.256	372.256	0.0	-14.301	-2.551 *	
1	12	1	3.158	2.414	-2.414	0.0	0.784	0.091	
3	12	1	10.472	8.398	8.396	0.0	2.076	0.419	
5	12	1	17.354	13.493	-13.693	0.0	3.661	1.118	
6	12	1	9.817	9.129	5.109	0.0	4.898	0.380	
7	12	1	10.943	1.412	1.412	0.0	9.527	2.013	
9	12	1	12.415	1.652	1.652	0.0	10.763	2.352 *	
10	12	1	14.767	1.299	1.299	0.0	13.463	2.047 *	
11	12	1	6.631	6.668	6.696	0.0	-0.066	-0.010	
12	12	1	4.075	2.419	2.419	0.0	1.655	0.201	
15	11	1	2.088	12.154	-13.954	0.0	-11.865	-1.124 *	
14	11	1	28.540	25.446	25.666	0.0	2.894	1.150	
12	11	1	14.387	5.636	5.636	0.0	8.751	2.312	

4000 ORTHOPHOSPHATE 6/28/73				STRUCTURE FACTORS				PAGE 4	
H	K	L	F(OHS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	3)
11	11	1	14.139	20.135	0.0	-5.996	-1.299		
10	11	1	18.903	16.167	-16.167	0.0	2.736	0.936	
9	11	1	22.631	16.414	-16.414	0.0	6.217	2.446	
8	11	1	10.823	13.478	13.478	0.0	-2.655	-0.520	
0	6	0	356.761	372.296	372.296	0.0	-19.535	-2.428 *	
7	11	1	25.516	26.594	-26.594	0.0	-1.567	-0.580	
6	11	1	38.057	38.274	38.274	0.0	-0.217	-0.112	
5	11	1	36.543	35.267	35.267	0.0	1.276	0.555	
3	11	1	17.032	13.410	13.410	0.0	3.623	1.164	
2	11	1	28.2C3	27.484	-27.484	0.0	0.720	0.321	
1	11	1	21.233	18.299	-18.299	0.0	1.934	0.719	
0	10	1	41.207	46.135	46.135	0.0	1.074	0.678	
1	10	1	18.698	37.437	-37.437	0.0	1.251	0.758	
2	10	1	27.604	30.365	30.365	0.0	-2.762	-1.284	
3	10	1	13.321	5.540	5.540	0.0	7.381	2.429	
6	10	1	14.037	18.440	18.440	0.0	-4.403	-1.190	
7	10	1	16.658	16.367	16.367	0.0	2.332	0.822	
8	10	1	19.078	19.130	19.130	0.0	0.969	0.349	
11	10	1	19.502	20.044	-20.044	0.0	-0.502	-0.163	
12	10	1	25.477	27.552	-27.552	0.0	-1.075	-0.430	
0	6	0	355.653	372.356	372.356	0.0	-19.688	-2.453 *	
13	10	1	16.769	4.571	4.571	0.0	12.198	3.554 *	
14	10	1	24.181	23.754	-23.754	0.0	0.427	0.165	
15	10	1	9.128	5.579	-5.579	0.0	6.149	1.484	
17	10	1	10.326	0.532	-0.532	0.0	9.424	1.757	
18	10	1	13.599	13.698	-13.698	0.0	-0.399	-0.023	
20	9	1	18.421	11.911	11.911	0.0	6.510	2.134	
19	9	1	28.862	26.505	26.505	0.0	2.357	0.954	
18	9	1	30.428	28.282	-28.282	0.0	2.146	0.952	
17	9	1	25.953	31.133	-31.133	0.0	-1.176	-0.480	
16	9	1	9.318	15.310	-15.310	0.0	-5.992	-1.052	
15	9	1	6.382	C.658	-0.858	0.0	5.524	0.828	
14	9	1	33.517	30.535	30.535	0.0	2.982	1.591	
13	9	1	10.370	1.801	-1.801	0.0	8.569	1.880	
12	9	1	63.880	62.229	62.229	0.0	0.851	0.550	
11	9	1	17.252	76.475	-76.475	0.0	0.747	0.452	
10	9	1	74.805	75.648	-75.648	0.0	-0.843	-0.527	
9	9	1	80.243	FC.583	-80.583	0.0	0.323	-0.202	
8	9	1	35.391	38.223	-38.223	0.0	-2.831	-1.585	
7	9	1	27.125	25.120	-25.120	0.0	2.805	1.565	
0	6	0	257.375	372.296	372.296	0.0	-14.922	-2.323 *	
6	9	1	24.652	35.801	-35.801	0.0	-0.850	-0.483	
5	9	1	35.916	37.303	37.303	0.0	-1.487	-0.868	
4	9	1	16.419	4.371	-4.371	0.0	12.047	4.337 *	
3	9	1	35.865	35.027	35.027	0.0	0.013	0.512	
2	9	1	64.467	69.523	-69.523	0.0	-3.036	-1.558	
1	9	1	48.045	48.643	-48.643	0.0	-0.597	0.407	
0	8	1	30.252	28.157	-28.157	0.0	2.095	1.290	
2	8	1	66.413	7C.434	-70.434	0.0	-4.021	-2.899	
3	8	1	112.553	116.435	-116.435	0.0	-3.882	-2.049	
4	8	1	98.272	55.566	-59.366	0.0	-1.676	-0.933	
5	8	1	67.446	66.148	66.148	0.0	1.298	0.946	
6	8	1	12.653	19.618	-10.618	0.0	2.235	0.692	

STRUCTURE FACTORS							PAGE 5	
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	8	1	54.041	53.567	53.567	0.0	0.474	0.355
8	9	1	53.349	53.892	53.892	0.0	-0.534	-0.320
9	8	1	42.929	43.424	43.424	0.0	-0.485	-0.303
10	8	1	21.544	23.113	23.113	0.0	-1.175	-0.502
11	8	1	33.223	31.401	31.401	0.0	1.852	1.160
12	8	1	46.754	45.167	45.167	0.0	1.587	1.055
13	8	1	56.012	55.620	55.620	0.0	0.392	0.272
0	6	0	358.255	372.296	372.296	0.0	-14.001	-2.171 *
14	8	1	10.910	11.531	11.531	0.0	9.233	2.314
15	8	1	54.379	55.262	55.262	0.0	-0.882	-0.566
16	8	1	50.866	51.571	51.571	0.0	-1.104	-0.990
17	8	1	36.724	34.803	34.803	0.0	1.921	0.371
18	8	1	28.950	28.758	28.758	0.0	0.192	0.083
19	8	1	22.163	21.611	21.611	0.0	0.552	0.190
20	9	1	32.446	28.288	28.288	0.0	4.116	2.023
21	9	1	17.076	7.898	7.898	0.0	9.173	2.661
23	7	1	5.521	1.650	1.650	0.0	3.823	0.527
22	7	1	10.165	13.001	13.001	0.0	-2.836	-0.533
21	7	1	6.360	3.955	3.955	0.0	2.413	0.358
20	7	1	17.123	3.992	3.992	0.0	9.030	2.117
19	7	1	26.362	26.551	26.551	0.0	-0.255	-0.058
18	7	1	6.693	2.359	2.359	0.0	6.331	1.214
17	7	1	1.923	4.969	4.969	0.0	-3.362	-0.520
16	7	1	19.429	18.451	18.451	0.0	C.979	0.362
15	7	1	16.419	11.293	11.293	0.0	5.125	1.719
13	7	1	9.736	13.412	13.412	0.0	-3.627	-0.911
12	7	1	21.447	21.033	21.033	0.0	0.413	0.178
0	6	0	357.777	372.296	372.296	0.0	-14.519	-2.259 *
11	7	1	21.520	22.132	22.132	0.0	-0.672	-0.283
10	7	1	14.417	18.339	18.339	0.0	-3.922	-1.204
9	7	1	43.365	45.513	45.513	0.0	-2.148	-1.494
8	7	1	33.414	35.654	35.654	0.0	-2.283	-1.403
7	7	1	12.161	8.247	8.247	0.0	3.934	1.218
6	7	1	14.285	14.579	14.579	0.0	-0.293	-0.093
5	7	1	23.406	26.050	26.050	0.0	-2.644	-1.182
4	7	1	25.219	26.229	26.229	0.0	-0.990	-0.501
3	7	1	31.613	30.488	30.488	0.0	1.125	0.680
2	7	1	16.550	17.374	17.374	0.0	-0.824	-0.291
0	6	1	12.256	4.873	4.873	0.0	7.382	2.514
1	6	1	11.241	5.088	5.088	0.0	6.173	1.974
2	6	1	12.649	3.685	3.685	0.0	8.964	3.115
3	6	1	26.199	26.019	26.019	0.0	0.180	0.103
4	6	1	10.677	7.590	7.590	0.0	3.087	0.866
5	6	1	11.904	8.887	8.887	0.0	3.317	0.910
7	6	1	13.964	13.670	13.670	0.0	0.894	0.275
8	5	1	3.636	7.349	7.349	0.0	-3.712	-0.518
0	6	0	357.565	372.296	372.296	0.0	-14.327	-2.229 *
11	6	1	5.325	3.019	3.019	0.0	2.327	0.413
13	6	1	15.571	11.692	11.692	0.1	1.879	0.643
14	6	1	11.509	11.300	11.300	0.0	-1.883	-0.699
15	6	1	10.576	14.253	14.253	0.0	-3.688	-0.136
17	6	1	8.515	1.170	1.170	0.0	7.345	1.515
20	6	1	14.664	19.665	19.665	0.0	1.219	0.330

400C UORTHOFERROSILITE 6/29/73

STRUCTURE FACTORS

PAGE 6

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
21	6	1	8.477	1.309	1.309	0.0	6.768	1.151
22	6	1	15.729	1.172	-1.172	0.0	11.557	2.858 *
23	6	1	11.971	1.728	1.728	0.0	13.249	2.241 *
24	6	1	12.152	1.523	-1.523	0.0	10.629	2.365 *
25	6	1	22.392	21.205	-21.205	0.0	1.398	0.359
21	5	1	7.939	5.057	-5.057	0.0	2.374	0.462
23	5	1	16.444	9.132	-9.132	0.0	8.302	2.556
20	6	0	357.354	372.236	372.236	0.0	-14.903	2.320 *
21	5	1	25.769	29.653	29.653	0.0	0.071	0.032
15	5	1	23.991	21.551	-21.551	0.0	2.439	1.097
17	5	1	11.626	12.176	-15.176	0.0	-3.550	1.889
16	5	1	23.260	26.071	26.071	0.0	-2.742	1.194
19	5	1	31.701	32.249	-32.249	0.0	-0.544	0.257
14	5	1	55.383	60.656	60.656	0.0	-0.775	0.566
13	5	1	20.043	34.231	30.731	0.0	-2.689	1.425
11	5	1	10.253	4.563	4.563	0.0	5.690	1.432
10	5	1	37.050	36.177	-36.177	0.0	0.714	0.468
9	5	1	41.531	42.048	-42.048	0.0	-0.517	0.371
8	5	1	25.447	32.842	32.842	0.0	-3.393	1.901
7	5	1	64.171	68.254	-64.254	0.0	-0.983	0.966
6	5	1	61.342	60.567	60.567	0.0	1.275	1.053
9	5	1	75.929	75.833	75.833	0.0	0.097	0.071
4	5	1	30.051	29.926	29.926	0.0	0.165	0.119
3	5	1	41.370	42.476	-42.476	0.0	-1.105	0.919
2	5	1	67.669	70.714	-70.714	0.0	-3.106	2.305
0	6	0	356.321	372.296	372.296	0.0	-15.976	2.499 *
1	4	1	13.876	15.994	-15.994	0.0	-2.118	0.903
0	4	1	12.444	8.265	-8.265	0.0	4.179	2.218
1	4	1	49.339	53.032	-53.032	0.0	-3.693	3.592
2	4	1	76.303	79.001	79.001	0.0	-2.701	2.121
3	4	1	42.822	45.674	-45.674	0.0	-2.952	2.138
4	4	1	51.087	52.507	-52.507	0.0	-1.421	1.325
5	4	1	83.954	84.920	-84.920	0.0	-1.315	0.720
6	4	1	25.140	30.023	30.023	0.0	-0.883	0.556
7	4	1	35.169	36.502	-36.502	0.0	-0.613	0.492
8	4	1	7.857	10.330	-10.330	0.0	-2.523	0.517
9	4	1	9.596	7.625	7.625	0.0	1.971	0.555
11	4	1	17.076	13.292	13.292	0.0	3.785	1.439
12	4	1	11.188	7.846	7.846	0.0	3.342	0.911
13	4	1	12.156	13.033	-13.033	0.0	-0.807	-0.217
14	4	1	29.345	29.425	-29.425	0.0	-0.281	-0.163
15	4	1	17.558	15.440	-15.440	0.0	2.119	0.810
16	4	1	42.353	40.034	-40.034	0.0	2.318	1.664
17	4	1	34.732	33.355	33.355	0.0	1.377	0.197
18	4	1	30.091	29.468	-29.468	0.0	0.623	0.302
0	6	1	258.603	372.236	372.236	0.0	-13.694	-2.122 *
10	4	1	14.124	12.225	-12.225	0.0	1.898	0.539
20	4	1	7.069	7.072	-7.072	0.0	-0.004	-0.001
21	4	1	16.488	15.857	15.857	0.0	1.132	0.347
22	4	1	36.094	35.737	-35.737	0.0	-0.643	-0.343
23	4	1	32.667	35.407	-35.407	0.0	-2.739	-1.184
24	4	1	24.751	22.766	-22.766	0.0	1.986	0.823
25	4	1	28.394	30.253	30.253	0.0	-1.859	-0.698

400C ORTHOFERROSILITE 6/28/73				STRUCTURE FACTORS		PAGE 7			
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	34
26	4	1	22.645	16.957	-16.967	0.0	5.679	2.271	
26	3	1	30.867	29.976	-28.996	0.0	1.873	0.810	
25	3	1	36.035	32.638	-32.838	0.0	3.197	1.562	
24	3	1	27.925	33.115	33.515	0.0	-5.590	-2.088	
23	3	1	33.151	35.218	-35.218	0.0	-2.067	-0.971	
22	3	1	63.919	85.309	85.309	0.0	-1.390	-0.521	
21	3	1	72.173	71.689	71.689	0.0	0.484	0.315	
20	3	1	20.657	17.156	17.156	0.0	3.493	1.593	
19	3	1	46.666	44.275	44.275	0.0	2.391	1.733	
18	3	1	71.321	79.651	-70.861	0.0	0.469	0.317	
17	3	1	91.300	93.238	-93.238	0.0	-1.929	-1.167	
16	3	1	18.333	16.261	-16.261	0.0	2.072	0.854	
15	3	1	18.351	21.276	-21.206	0.0	-2.814	-1.076	
0	6	0	355.211	372.256	372.256	0.0	-17.035	-2.684 *	
14	3	1	71.448	70.137	70.137	0.0	1.312	0.934	
13	3	1	24.473	22.992	22.992	0.0	1.481	0.763	
12	3	1	140.007	163.153	-140.185	0.0	-0.099	-0.043	
11	3	1	212.815	209.576	238.576	0.0	4.233	1.224	
10	3	1	210.044	226.539	-206.839	0.0	3.165	0.923	
9	3	1	168.860	167.289	-167.289	0.0	1.571	0.583	
8	3	1	65.749	65.828	-65.826	0.0	-0.071	-0.063	
7	3	1	73.104	71.847	-71.847	0.0	1.257	0.988	
6	3	1	186.232	184.512	184.512	0.0	1.320	0.444	
5	3	1	170.052	169.141	169.141	0.0	0.951	0.395	
4	3	1	50.569	46.405	46.405	0.0	4.564	4.626	
3	3	1	55.615	61.233	61.233	0.0	-5.668	-5.305	
2	3	1	162.329	172.536	-172.536	0.0	-10.207	-3.798 *	
1	3	1	180.588	194.817	-194.817	0.0	-14.223	-4.970 *	
0	2	1	55.423	59.607	59.607	0.0	-4.184	-4.153	
1	2	1	14.811	17.376	17.376	0.0	-2.567	-1.469	
2	2	1	130.161	132.313	-132.313	0.0	-2.172	-1.067	
3	2	1	155.357	157.634	-157.634	0.0	-2.237	-0.917	
4	2	1	147.055	148.011	-148.011	0.0	-0.956	-0.115	
5	2	1	134.673	135.723	135.723	0.0	-1.050	-0.496	
0	6	0	355.657	372.256	372.256	0.0	-16.339	-2.557 *	
6	2	1	11.378	14.133	-14.133	0.0	-2.755	-1.338	
7	2	1	1C5.432	163.680	163.680	0.0	2.252	1.342	
8	2	1	112.466	112.735	112.735	0.0	0.753	0.416	
9	2	1	56.926	56.446	56.446	0.0	2.480	2.105	
10	2	1	31.452	30.241	30.241	0.0	1.211	0.930	
11	2	1	52.130	52.083	-52.083	0.0	0.047	0.039	
12	2	1	65.469	65.350	-65.350	0.0	0.119	0.089	
13	2	1	56.543	59.741	59.741	0.0	-1.193	-0.854	
14	2	1	12.970	7.874	7.874	0.0	5.096	1.571	
15	2	1	56.962	54.313	54.313	0.0	1.665	1.230	
16	2	1	74.968	74.460	74.460	0.0	0.508	0.357	
17	2	1	58.808	56.790	-56.790	0.0	2.018	1.458	
18	2	1	41.473	40.263	40.263	0.0	1.209	0.425	
19	2	1	18.523	15.322	-15.322	0.0	3.201	1.222	
20	2	1	16.041	19.932	-19.932	0.0	-1.891	-0.637	
21	2	1	16.342	11.119	-11.119	0.0	8.222	3.472	
22	2	1	40.652	41.275	41.275	0.0	-0.623	-0.354	
23	2	1	60.560	63.431	63.431	0.0	-2.871	-1.756	

STRUCTURE FACTORS							PAGE 8		
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	35
24	2	1	46.441	47.637	47.637	0.0	-1.176	-0.673	
25	2	1	45.316	47.138	-47.730	0.0	-2.423	-1.241	
0	6	0	357.047	372.296	372.296	0.0	-15.209	-2.369 *	
2	2	1	22.782	26.723	26.723	0.0	-3.741	-1.163	
26	1	1	17.602	19.631	-19.631	0.0	-2.079	-0.574	
24	1	1	5.917	7.603	-7.908	0.0	2.009	0.387	
22	1	1	14.870	5.897	-5.897	0.0	8.973	3.025	
21	1	1	15.600	20.495	20.495	0.0	-4.895	-1.438	
19	1	1	13.628	6.713	-8.718	0.0	4.910	1.521	
18	1	1	8.719	13.713	-10.713	0.0	-1.994	-0.420	
17	1	1	3.570	6.756	-6.756	0.0	-3.173	-0.443	
16	1	1	37.466	36.233	36.233	0.0	1.203	0.338	
15	1	1	32.565	31.711	-31.711	0.0	0.854	0.556	
14	1	1	43.277	44.712	44.712	0.0	-1.435	-1.041	
13	1	1	29.769	31.666	31.666	0.0	-1.296	-0.744	
12	1	1	9.026	11.101	11.101	0.0	-2.155	-0.537	
11	1	1	11.948	15.933	-15.933	0.0	-3.355	-1.200	
10	1	1	26.053	24.813	-24.813	0.0	1.243	0.911	
0	6	0	355.613	372.296	372.296	0.0	-16.683	-2.612 *	
8	1	1	48.061	47.190	-7.180	0.0	0.880	0.882	
7	1	1	55.350	55.654	-55.654	0.0	0.296	0.278	
6	1	1	55.132	55.403	55.403	0.0	-0.268	-0.256	
5	1	1	90.727	83.492	88.452	0.0	-2.235	1.548	
4	1	1	57.513	56.664	56.664	0.0	0.848	0.824	
3	1	1	11.327	9.541	9.541	0.0	1.487	0.722	
2	1	1	44.358	43.754	-43.754	0.0	0.344	0.391	
1	1	1	13.783	11.347	-11.347	0.0	2.441	1.667	
0	2	2	5.623	9.907	-9.907	0.0	-4.284	-1.155	
1	0	2	121.794	123.132	123.132	0.0	-1.368	-0.718	
2	0	2	178.246	172.569	-174.569	0.0	3.678	1.301	
3	0	2	210.536	211.573	211.573	0.0	-1.036	-0.306	
4	0	2	14.932	17.199	-17.199	0.0	1.733	1.235	
5	0	2	258.556	252.143	-252.143	0.0	5.763	1.345	
7	0	2	207.039	201.010	-201.010	0.0	6.329	1.010	
8	0	2	26.389	29.373	29.373	0.0	-1.334	-0.946	
9	0	2	192.189	186.528	186.528	0.0	3.561	1.183	
10	0	2	16.214	13.631	13.631	0.0	2.583	1.112	
11	0	2	225.901	222.723	222.723	0.0	3.178	0.862	
0	6	0	356.359	372.295	372.295	0.0	-15.931	-2.492 *	
12	0	2	6.163	5.473	5.473	0.0	0.490	0.308	
13	0	2	73.341	72.344	-72.344	0.0	0.997	0.717	
15	0	2	92.961	92.014	-92.014	0.0	0.948	0.583	
16	0	2	21.242	19.054	19.054	0.0	2.188	1.069	
17	0	2	58.406	56.544	56.544	0.0	0.362	0.209	
18	0	2	43.218	43.515	43.515	0.0	-0.297	-0.183	
19	0	2	57.395	57.193	57.193	0.0	0.793	0.539	
21	0	2	41.092	41.167	-41.167	0.0	-0.076	-0.044	
22	0	2	96.270	85.313	85.313	0.0	5.043	-2.793	
23	0	2	115.369	120.942	-120.942	0.0	-1.353	-0.645	
25	0	2	50.273	51.015	51.015	0.0	-0.942	-0.549	
26	0	2	23.064	28.459	28.459	0.0	-5.375	-1.634	
26	1	2	9.084	8.394	8.394	0.0	0.690	0.118	
25	1	2	18.786	23.662	20.862	0.0	-2.076	-0.577	

400C ORTHOFERROSILITE 6/28/73				STRUCTURE FACTORS			PAGE 5	
H	K	L	F(OHRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
24	1	2	30.891	28.537	28.997	0.0	1.884	0.900
23	1	2	44.421	45.680	45.680	0.0	-1.259	-0.715
22	1	2	18.454	19.280	19.280	0.0	-0.786	-0.254
0	6	0	356.455	372.236	372.236	0.0	-15.841	-2.477 *
21	1	2	15.746	16.119	16.119	0.0	-0.373	-0.111
20	1	2	17.807	16.779	16.779	0.0	-0.972	-0.321
19	1	2	3.441	14.467	14.467	0.0	-11.005	-1.403 *
17	1	2	74.820	76.158	76.158	0.0	-1.374	-0.513
16	1	2	59.982	57.535	57.535	0.0	1.448	1.562
15	1	2	17.642	17.331	17.331	0.0	-0.269	-0.068
14	1	2	6.853	6.300	6.300	0.0	0.893	0.113
13	1	2	3.768	2.899	2.899	0.0	0.870	0.125
12	1	2	119.645	121.210	121.210	0.0	-1.516	-0.772
11	1	2	111.413	110.561	110.561	0.0	0.449	0.245
10	1	2	16.166	13.199	13.199	0.0	2.385	1.238
9	1	2	81.423	81.079	81.079	0.0	0.184	0.130
8	1	2	64.825	66.148	66.148	0.0	-1.334	-1.076
7	1	2	43.937	42.333	42.333	0.0	1.584	1.459
5	1	2	112.342	110.244	110.244	0.0	2.098	1.183
4	1	2	44.039	39.619	39.619	0.0	4.220	4.230
3	1	2	56.677	60.010	60.010	0.0	-0.333	-0.310
2	1	2	21.313	20.499	20.499	0.0	0.875	0.656
0	6	0	355.125	372.306	372.306	0.0	-17.161	-1.693 *
1	1	2	59.927	61.566	61.566	0.0	-1.939	-1.903
0	2	2	6.514	4.552	4.552	0.0	1.952	0.625
1	2	2	31.443	36.834	36.834	0.0	-3.390	-3.405
2	1	2	1.972	0.437	0.437	0.0	1.865	0.253
3	2	2	74.317	73.342	73.342	0.0	0.975	0.765
4	2	2	14.113	14.457	14.457	0.0	-0.347	-0.177
5	2	2	26.569	29.711	29.711	0.0	-2.722	-2.045
6	2	2	67.938	63.231	63.231	0.0	1.717	1.419
7	2	2	97.764	97.330	97.330	0.0	0.634	0.272
8	2	2	5.357	8.157	8.157	0.0	-2.133	-0.463
9	2	2	75.427	76.000	76.000	0.0	-0.574	-0.422
10	2	2	31.745	31.031	31.031	0.0	0.714	0.469
11	2	2	19.809	20.695	20.695	0.0	-1.375	-0.745
12	2	2	15.644	14.257	14.257	0.0	1.387	0.494
13	2	2	38.585	40.335	40.335	0.0	-1.750	-1.066
14	2	2	20.657	22.374	22.374	0.0	1.436	0.512
15	2	2	42.602	43.179	43.179	0.0	-0.577	-0.402
16	2	2	15.667	17.250	17.250	0.0	5.837	1.341
17	2	2	21.201	20.822	20.822	0.0	2.379	1.214
18	2	2	44.201	47.117	47.117	0.0	-2.916	-1.911
0	6	0	355.441	372.296	372.296	0.0	-16.355	-2.647 *
19	2	2	46.950	48.598	48.598	0.0	-1.628	-1.376
21	2	2	23.026	20.852	20.852	0.0	2.174	0.912
22	2	2	13.716	21.133	21.133	0.0	-7.417	-1.612
24	2	2	4.221	0.830	-0.860	0.0	3.340	0.428
25	2	2	11.290	16.318	16.318	0.0	-9.028	-0.972
26	2	2	13.452	8.931	8.931	0.0	4.361	1.019
24	3	2	17.368	5.604	-5.604	0.0	11.765	3.719 *
23	3	2	14.626	5.591	-5.591	0.0	9.235	2.555
22	3	2	5.260	5.079	5.079	0.0	4.189	0.752

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
21	3	2	10.209	0.805	-0.805	0.0	9.404	2.044
20	3	2	10.954	6.181	-5.181	0.0	4.773	1.138
19	3	2	4.863	11.092	-11.092	0.0	-7.029	-0.990
18	3	2	9.917	2.976	-2.976	0.0	6.941	1.644
17	3	2	5.768	7.957	-7.957	0.0	-2.159	-0.368
16	3	2	9.990	7.468	-7.468	0.0	2.522	0.600
15	3	2	10.706	15.347	-15.347	0.0	-4.641	-1.147
14	3	2	7.362	0.520	-0.520	0.0	6.775	1.472
0	6	0	355.288	372.276	372.296	0.0	-17.508	-2.672
10	3	2	11.811	3.755	3.755	0.0	9.047	2.416
9	3	2	14.066	15.745	15.745	0.0	-1.680	-0.361
8	3	2	16.479	14.316	-14.316	0.0	4.163	1.978
7	3	2	2.600	10.447	-10.447	0.0	-8.347	-1.203
6	3	2	3.636	8.415	-8.415	0.0	-4.808	-0.844
5	3	2	22.470	21.814	-21.814	0.0	0.656	0.412
4	3	2	43.750	41.055	-41.055	0.0	2.785	2.637
3	3	2	35.464	35.228	-35.228	0.0	0.237	0.207
1	3	2	1.972	2.566	-2.566	0.0	-0.934	-0.159
0	4	2	13.146	17.395	-17.395	0.0	-4.250	-1.643
1	4	2	34.014	34.920	-34.920	0.0	-0.905	-0.782
2	4	2	66.358	68.821	-68.821	0.0	-2.422	-1.378
3	4	2	36.552	36.596	-36.596	0.0	-0.103	-0.087
4	5	2	8.580	8.273	-8.273	0.0	0.313	0.090
5	4	2	17.705	15.678	-15.678	0.0	2.027	0.970
6	4	2	31.628	31.852	-31.852	0.0	-0.224	-0.147
0	6	0	355.862	372.296	372.296	0.0	-16.435	-2.572
7	4	2	44.201	44.036	-44.036	0.0	0.165	0.130
9	4	2	14.303	6.152	-6.152	0.0	8.147	2.889
10	4	2	12.254	16.376	-16.376	0.0	-4.121	-1.093
11	4	2	15.980	16.314	-16.314	0.0	-0.333	-0.112
12	4	2	7.916	5.489	-5.489	0.0	2.427	0.528
13	4	2	12.722	9.191	-9.191	0.0	3.541	1.154
14	4	2	21.710	21.573	-21.573	0.0	0.137	0.061
16	4	2	6.076	11.497	-11.497	0.0	-5.421	-0.919
17	4	2	17.283	15.049	-15.049	0.0	2.159	0.757
18	4	2	19.809	22.142	-22.142	0.0	-2.733	-0.939
20	4	2	2.906	3.771	-3.771	0.0	-0.865	-0.101
21	4	2	14.055	0.931	-0.931	0.0	13.165	3.900
22	4	2	19.924	16.517	-16.517	0.0	3.307	1.143
23	4	2	11.246	5.052	-5.052	0.0	6.195	1.329
25	4	2	12.079	7.940	-7.940	0.0	4.139	0.880
24	5	2	11.553	5.253	-5.253	0.0	6.300	1.442
0	6	0	355.919	372.296	372.296	0.0	-16.377	-2.563
23	5	2	35.374	37.590	-37.590	0.0	-2.116	-0.944
22	5	2	21.227	21.926	-21.926	0.0	-0.698	-0.244
21	5	2	25.453	32.602	-32.602	0.0	-7.148	-2.295
20	5	2	7.668	16.647	-16.647	0.0	-8.979	-1.453
19	5	2	32.331	32.120	-32.120	0.0	0.211	0.100
17	5	2	69.424	70.772	-70.772	0.0	-1.347	-0.903
16	5	2	26.389	24.947	-24.947	0.0	1.144	0.705
15	5	2	45.756	45.327	-45.327	0.0	0.729	0.452
14	5	2	5.126	0.998	-0.998	0.0	4.128	0.698
13	5	2	47.767	48.061	-48.061	0.0	-0.294	-0.211

STRUCTURE FACTORS						PAGE 11			
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	38
12	5	2	84.765	84.925	84.925	0.0	-0.159	-0.103	
11	5	2	95.869	96.092	96.092	0.0	1.776	1.354	
10	5	2	20.102	17.077	17.077	0.0	3.025	1.370	
9	5	2	142.763	142.763	142.763	0.0	0.001	0.000	
8	5	2	81.486	83.896	83.896	0.0	-2.410	-1.578	
7	5	2	66.487	64.856	64.856	0.0	1.591	1.172	
6	5	2	14.665	14.905	14.905	0.0	-0.241	-0.081	
5	5	2	80.351	86.785	86.785	0.0	1.606	1.059	
4	5	2	10.052	13.334	13.334	0.0	-3.242	-0.860	
0	6	0	354.275	372.256	372.256	0.0	-18.021	-2.444 *	
3	5	2	137.446	142.338	142.338	0.0	-4.992	-2.212	
1	5	2	65.572	68.459	68.459	0.0	-2.087	-2.250	
0	6	2	8.303	10.122	10.122	0.0	-2.119	-0.453	
1	6	2	42.011	41.182	41.182	0.0	0.819	0.588	
2	6	2	125.289	131.816	131.816	0.0	-6.528	-3.193	
3	6	2	150.112	155.915	155.915	0.0	-5.803	-2.403	
5	6	2	115.866	116.874	116.874	0.0	-1.010	-0.524	
6	6	2	12.269	1.918	1.918	0.0	10.351	3.149 *	
7	6	2	105.812	106.571	106.571	0.0	-1.158	-0.450	
9	6	2	133.915	133.124	133.124	0.0	-2.209	-1.031	
10	6	2	32.126	33.983	33.983	0.0	-1.057	-1.123	
11	6	2	109.217	106.998	106.998	0.0	2.319	1.256	
13	6	2	34.332	41.044	41.044	0.0	-1.712	-1.062	
14	6	2	5.827	11.218	11.218	0.0	-5.391	-0.889	
15	6	2	57.426	58.547	58.547	0.0	0.879	0.551	
16	6	2	24.956	19.614	19.614	0.0	5.342	2.954	
0	6	0	354.314	372.296	372.296	0.0	-17.982	-2.829 *	
17	6	2	52.453	56.118	56.118	0.0	1.635	1.063	
18	6	2	17.690	17.575	17.575	0.0	0.015	0.036	
19	6	2	47.297	47.017	47.017	0.0	0.280	0.164	
20	6	2	11.889	5.559	5.559	0.0	6.830	1.667	
21	6	2	31.203	33.908	33.908	0.0	-2.705	-1.170	
22	6	2	57.336	55.324	55.324	0.0	2.012	1.199	
23	6	2	90.640	77.575	77.575	0.0	2.665	1.536	
22	7	2	21.095	16.120	16.120	0.0	4.976	1.782	
21	7	2	11.916	13.516	13.516	0.0	-1.593	-0.336	
19	7	2	4.966	2.787	2.787	0.0	2.178	0.297	
17	7	2	8.237	10.396	10.396	0.0	-2.159	-0.365	
16	7	2	20.379	21.771	21.771	0.0	-1.392	-0.406	
14	7	2	10.238	7.266	7.266	0.0	2.972	0.599	
13	7	2	30.501	27.622	27.622	0.0	2.879	1.667	
12	7	2	50.940	50.305	50.305	0.0	0.935	0.649	
11	7	2	17.251	17.009	17.009	0.0	0.243	0.087	
10	7	2	12.342	7.577	7.577	0.0	4.365	1.305	
0	6	0	357.116	372.296	372.296	0.0	-15.190	-2.366 *	
9	7	2	7.624	8.371	8.371	0.0	-0.747	-0.153	
8	7	2	50.763	56.262	56.262	0.0	0.501	0.383	
7	7	2	35.684	34.826	34.826	0.0	0.853	0.391	
5	7	2	9.266	12.728	12.728	0.0	-4.462	-0.958	
4	7	2	24.991	33.183	33.183	0.0	-4.291	-2.328	
3	7	2	15.869	21.204	21.204	0.0	-1.394	-0.565	
2	7	2	3.812	7.070	7.070	0.0	-3.259	-0.473	
1	7	2	15.220	5.115	5.115	0.0	6.105	2.199	

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STRUCTURE FACTORS

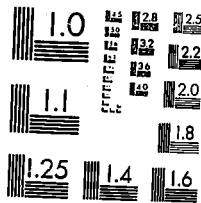
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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	3	2	8.559	1.917	1.917	0.0	6.641	1.536
1	0	2	51.586	50.975	50.975	0.0	0.611	0.462
2	8	2	17.675	18.781	18.781	0.0	-1.105	-0.425
3	9	2	30.468	38.453	38.453	0.0	0.015	0.010
4	8	2	4.264	3.025	3.025	0.0	1.239	0.157
5	4	2	32.662	34.424	34.424	0.0	-1.742	-0.937
6	8	2	20.248	18.638	18.638	0.0	1.610	0.663
7	8	2	53.556	51.103	51.103	0.0	2.453	1.756
9	9	2	32.916	30.959	30.959	0.0	1.917	1.065
10	8	2	4.9C7	0.621	0.621	0.0	4.286	0.670
0	6	0	357.183	372.296	372.296	0.0	-15.114	-2.354 *
11	9	2	37.754	35.300	35.300	0.0	2.494	1.533
13	8	2	36.573	39.475	39.475	0.0	-2.898	-1.545
14	8	2	10.443	13.461	13.461	0.0	-3.318	-0.644
15	9	2	30.647	32.795	32.795	0.0	-2.152	-0.913
17	3	2	8.456	10.232	10.232	0.0	-1.776	-0.302
18	8	2	20.876	17.586	17.586	0.0	2.892	0.984
19	3	2	32.814	27.757	27.757	0.0	5.057	2.617
20	8	2	11.480	8.962	8.962	0.0	2.518	0.524
21	8	2	15.089	13.212	13.212	0.0	1.877	0.483
16	9	2	13.354	15.217	15.217	0.0	-1.823	-0.371
18	0	2	13.558	0.555	0.555	0.0	13.013	3.211 *
17	9	2	7.113	7.919	7.919	0.0	-9.836	-0.126
14	9	2	7.452	14.142	14.142	0.0	-6.650	-1.037
13	9	2	14.586	13.597	13.597	0.0	1.430	0.399
11	9	2	10.618	7.975	7.975	0.0	2.643	0.609
0	5	0	356.455	372.296	372.296	0.0	-15.841	-2.477 *
10	9	2	7.098	6.742	6.742	0.0	7.356	0.062
3	9	2	14.300	3.860	3.860	0.0	10.439	3.323 *
6	6	2	12.258	3.684	3.684	0.0	4.814	2.621
5	9	2	1C.151	8.689	8.689	0.0	1.462	0.342
4	9	2	6.C76	8.566	8.566	0.0	-2.490	-0.499
3	9	2	11.188	7.966	7.966	0.0	3.222	0.355
2	0	2	13.788	13.869	13.869	0.0	-0.080	-0.024
0	10	2	1.942	6.844	6.844	0.0	-4.921	-0.575
1	10	2	12.152	11.662	11.662	0.0	0.490	0.127
2	10	2	32.931	32.715	32.715	0.0	0.215	0.114
3	10	2	25.140	32.287	32.287	0.0	-3.147	-1.415
4	10	2	10.545	4.769	4.769	0.0	5.776	1.373
5	10	2	14.563	14.456	14.456	0.0	0.076	0.021
6	10	2	17.699	17.642	17.642	0.0	0.048	0.016
7	10	2	8.968	11.516	11.516	0.0	-2.548	-0.456
8	10	2	6.656	16.925	16.925	0.0	-7.271	-1.368
9	10	2	14.003	12.127	12.127	0.0	1.881	0.484
0	6	0	356.455	372.296	372.296	0.0	-15.401	-2.467 *
10	10	2	4.484	0.732	0.732	0.0	3.752	0.502
11	10	2	21.958	24.269	24.269	0.0	-2.310	-0.775
13	10	2	13.558	11.733	11.733	0.0	1.866	0.450
15	10	2	15.323	19.125	19.125	0.0	-3.803	-0.929
16	10	2	11.612	3.808	3.808	0.0	10.803	2.393 *
17	10	2	22.854	20.549	20.549	0.0	2.346	0.814
13	11	2	15.590	19.153	19.153	0.0	0.437	0.133
12	11	2	43.775	47.561	47.561	0.0	-3.786	-1.732

STRUCTURE FACTORS							PAGE 13	
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
11	11	2	47.958	48.299	0.0	-0.341	-0.181	
10	11	2	13.223	7.445	7.445	0.0	5.789	1.376
9	11	2	75.427	75.229	-75.229	0.0	3.198	0.116
8	11	2	38.175	38.776	38.776	0.0	-0.601	-0.287
7	11	2	43.042	41.983	-41.983	0.0	1.059	0.587
6	11	2	7.789	4.383	4.383	0.0	3.416	0.589
5	11	2	53.114	52.064	52.064	0.0	1.110	0.668
4	11	2	12.576	1.706	1.706	0.0	10.870	2.715 *
3	11	2	60.575	61.425	61.425	0.0	-0.849	-0.506
0	0	0	354.555	372.256	372.256	0.0	-17.792	-2.798 *
2	11	2	4.486	6.561	6.561	0.0	-2.978	-0.274
1	11	2	24.613	24.656	-24.056	0.0	0.622	0.235
0	12	2	12.323	5.564	-5.564	0.0	6.364	1.482
1	12	2	14.256	5.416	9.416	0.0	4.340	1.255
2	12	2	47.136	46.004	-46.004	0.0	1.133	0.427
3	12	2	42.457	46.641	46.641	0.0	1.316	1.039
4	12	2	15.685	8.116	-8.116	0.0	7.572	2.159
5	12	2	21.110	20.696	-20.696	0.0	0.534	0.160
6	12	2	8.938	6.150	-8.750	0.0	0.188	0.033
7	12	2	20.326	13.203	-13.203	0.0	7.133	2.515
9	12	2	35.918	33.964	33.964	0.0	1.954	0.935
10	12	2	15.765	10.571	10.571	0.0	9.195	3.114
3	13	2	13.671	7.959	7.959	0.0	5.673	1.325
1	13	2	25.648	26.021	-26.021	0.0	-0.173	-0.058
0	12	3	5.442	12.775	-12.775	0.0	-7.313	-0.965
2	12	3	10.501	6.267	6.267	0.0	4.235	0.945
3	12	3	12.593	8.933	8.933	0.0	3.65	0.802
0	6	0	355.785	372.256	372.256	0.0	-16.51	-2.564 *
5	12	3	11.045	3.555	3.555	0.0	8.291	1.337
6	12	3	3.729	1.772	1.772	0.0	2.157	0.266
7	12	3	11.612	1.063	1.063	0.0	10.548	2.162 *
12	11	3	1.372	5.266	-5.266	0.0	-7.893	-0.725
11	11	3	13.511	12.888	-12.888	0.0	0.623	0.147
10	11	3	33.941	31.846	-31.846	0.0	2.396	0.923
9	11	3	21.432	18.499	18.499	0.0	2.933	1.029
8	11	3	7.595	2.329	-2.329	0.0	5.265	0.871
7	11	3	7.452	14.303	14.303	0.0	-6.816	-1.053
6	11	3	17.376	13.655	13.655	0.0	3.220	0.930
5	11	3	23.815	22.018	-22.018	0.0	1.798	0.537
4	11	3	14.095	3.175	3.175	0.0	10.922	2.778 *
3	11	3	23.559	21.574	-21.574	0.0	1.934	0.707
2	11	3	36.380	36.295	-36.295	0.0	2.085	1.038
1	11	3	8.450	10.528	10.528	0.0	-1.838	-0.323
0	10	3	12.459	15.121	-19.121	0.0	-6.663	-1.485
1	10	3	14.621	6.661	9.661	0.0	4.960	1.495
2	10	3	13.598	2.174	2.174	0.0	11.425	3.019 *
3	10	3	34.717	31.675	31.675	0.0	2.043	1.761
0	6	0	355.823	372.296	372.296	0.0	-16.473	-2.578 *
4	10	3	40.065	39.617	-39.617	0.0	0.448	0.223
7	10	3	6.222	4.709	4.709	0.0	1.513	0.230
9	10	3	9.556	13.359	13.359	0.0	-3.803	-0.666
11	10	3	20.057	22.393	22.393	0.0	5.654	2.651
13	10	3	7.069	1.542	1.542	0.0	5.527	0.866

CARD 2 OF 4



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

400C ORTHOFERROSILITE 6/26/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
14	10	5	6.076	2.798	0.0	3.288	0.471	
15	10	3	13.329	7.378	0.0	5.650	1.334	
17	9	3	15.323	12.793	0.0	2.529	0.634	
15	9	3	28.057	27.291	0.0	0.766	0.296	
14	9	3	92.867	93.446	0.0	-0.559	-0.305	
13	9	3	55.762	56.155	-56.155	0.0	-0.393	-0.235
12	9	3	9.683	4.986	-4.986	0.0	4.697	0.937
11	9	3	16.155	12.667	-12.667	0.0	3.289	0.919
10	9	3	16.799	13.501	0.0	3.058	0.938	
0	6	0	354.562	372.296	372.296	0.0	-17.314	-2.721 *
9	9	2	14.037	8.674	8.674	0.0	5.163	1.504
8	9	3	13.768	1.515	-1.515	0.0	12.274	3.605 *
7	9	3	-20.847	32.6C5	32.605	0.0	-3.758	-1.679
6	9	3	66.723	67.218	67.218	0.0	-0.495	-0.305
5	9	3	23.347	21.700	-21.700	0.0	1.647	0.732
4	9	3	4.673	1.011	1.011	0.0	3.662	0.561
3	9	3	13.175	15.102	-15.102	0.0	-2.907	-0.516
2	9	3	63.470	65.970	-65.970	0.0	-2.301	-1.515
1	0	3	66.214	66.912	66.912	0.0	1.301	0.899
0	8	3	142.397	145.203	145.203	0.0	-2.256	-0.951
1	8	3	66.923	66.108	66.108	0.0	-1.289	-0.383
2	8	3	14.110	16.680	-16.680	0.0	3.429	1.072
3	8	3	31.365	33.256	33.256	0.0	-1.891	-1.017
4	8	3	26.954	31.283	-31.283	0.0	-3.290	-1.159
5	8	3	31.057	34.155	-34.155	0.0	-3.138	-1.600
6	8	3	d.778	5.195	-5.195	0.0	3.502	0.8C7
7	8	3	64.717	64.733	-64.733	0.0	-0.016	-0.011
8	9	3	66.185	69.906	69.906	0.0	-2.021	-1.304
9	8	3	15.176	11.667	11.667	0.0	4.107	1.278
10	8	3	5.258	2.921	-2.921	0.0	2.337	0.356
0	6	0	356.034	372.256	372.256	0.0	-16.202	-2.545 *
11	9	3	5.633	9.396	9.396	0.0	-3.963	-0.571
12	8	3	56.277	58.136	-58.136	0.0	-1.860	-1.062
13	8	2	46.299	46.069	-46.069	0.0	0.231	0.135
14	8	3	16.588	7.610	-7.610	0.0	9.379	3.100
15	9	3	44.861	43.875	-43.875	0.0	0.986	0.546
16	8	2	27.311	32.8C2	32.802	0.0	-5.491	-1.925
17	8	3	21.359	16.606	16.606	0.0	4.753	1.757
18	8	3	9.625	0.973	-0.973	0.0	8.652	1.722
19	8	3	52.650	48.941	48.941	0.0	3.909	2.375
21	7	3	8.957	4.855	4.855	0.0	4.141	0.718
20	7	3	12.620	11.505	11.505	0.0	1.114	0.248
19	7	3	12.021	5.833	9.833	0.0	2.188	0.464
18	7	3	0.377	5.336	-5.336	0.0	4.000	0.158
17	7	3	13.921	16.426	16.426	0.0	-3.135	-0.711
16	7	3	11.455	2.610	-2.610	0.0	8.885	1.943
15	7	3	9.351	7.624	-7.624	0.0	1.767	0.356
14	7	3	43.350	43.518	-43.518	0.0	-0.168	-0.092
13	7	3	24.293	22.571	22.571	0.0	1.727	0.720
12	7	3	0.201	6.716	-6.716	0.0	2.436	0.524
11	7	3	11.246	5.631	-5.631	0.0	5.615	1.647
0	6	0	355.441	372.296	372.296	0.0	-16.955	-2.647 *
10	7	3	24.857	23.131	-23.131	0.0	1.766	0.833

400C ORTHOFERROSILITE 6/20/73				STRUCTURE FACTORS			PAGE 15	
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
9	7	3	14.621	12.654	12.654	0.0	2.040	0.671
8	7	3	14.621	13.220	13.220	0.0	1.491	0.438
7	7	3	16.433	16.110	-16.110	0.0	0.323	0.108
6	7	3	34.0CJ	33.799	-33.799	0.0	0.211	0.126
5	7	3	7.317	5.683	-9.883	0.0	-2.566	-0.492
4	7	3	20.394	21.101	21.101	0.0	-0.727	-0.310
2	7	3	9.844	6.260	6.260	0.0	3.584	0.399
1	7	3	11.763	16.154	-16.154	0.0	-4.421	-1.155
2	6	3	10.231	20.311	20.311	0.0	-2.080	-0.800
3	6	3	2.229	13.756	13.756	0.0	-11.536	-1.435 *
4	6	3	5.214	3.523	3.523	0.0	1.691	0.303
7	6	3	8.968	5.564	5.564	0.0	3.403	0.323
0	6	3	26.463	26.305	-26.305	0.0	0.158	0.083
6	6	3	13.213	10.742	-10.742	0.0	2.476	0.737
0	6	0	354.333	372.296	372.296	0.0	-17.964	-2.834 *
10	6	1	10.662	8.644	-8.644	0.0	1.818	0.449
12	6	3	5.573	6.182	6.182	0.0	0.389	0.160
13	6	3	8.748	1.461	-1.461	0.0	7.268	1.517
14	6	3	6.777	1.455	-1.455	0.0	5.292	0.977
15	6	3	12.210	1.566	-1.566	0.0	10.645	2.335 *
16	6	3	11.665	2.844	2.844	0.0	8.341	2.177
18	6	3	6.500	5.659	5.659	0.0	2.841	0.531
19	6	3	12.956	1.630	1.630	0.0	11.925	2.936 *
20	6	3	14.728	14.325	14.325	0.0	4.402	1.414
21	6	3	13.467	5.169	9.869	0.0	3.598	0.757
23	5	3	4.527	5.664	5.664	0.0	-0.537	-0.369
22	5	1	7.166	14.024	14.024	0.0	-6.838	-6.754
21	5	3	16.623	13.553	-13.553	0.0	3.370	0.393
1d	5	3	32.419	30.663	-30.663	0.0	1.555	0.781
17	5	3	36.460	37.641	37.641	0.0	-1.351	-0.583
0	6	0	353.570	372.296	372.296	0.0	-18.727	-2.958 *
15	5	3	25.336	25.566	25.566	0.0	-0.569	-0.250
14	5	3	23.653	23.651	23.651	0.0	-5.021	-1.660
13	5	3	17.500	19.342	-18.342	0.0	-0.842	-0.305
12	5	3	8.252	2.642	-2.642	0.0	5.810	1.271
11	5	3	25.365	22.314	-22.314	0.0	3.251	1.822
10	5	3	57.410	57.560	-57.560	0.0	-0.150	-0.167
9	5	3	36.908	36.423	36.423	0.0	0.565	0.367
8	5	3	6.734	5.102	-5.102	0.0	3.632	0.854
7	5	3	5.141	2.617	-2.617	0.0	2.523	0.422
6	5	3	9.377	7.155	-7.155	0.0	2.222	0.524
5	5	3	38.793	40.012	-60.072	0.0	-1.282	-0.833
4	5	3	16.039	12.133	-12.133	0.0	3.906	1.437
3	5	3	50.484	51.158	-51.158	0.0	-1.273	-0.932
2	5	3	79.129	83.531	-83.531	0.0	-4.773	-3.253
1	5	3	33.517	37.046	37.046	0.0	-3.529	-2.152
0	4	3	135.160	147.639	-147.639	0.0	-12.679	-5.821 *
1	4	3	41.429	42.203	-42.203	0.0	-0.771	-0.554
2	4	3	14.709	13.112	-13.112	0.0	2.597	0.893
3	4	3	26.243	26.686	26.686	0.0	-0.463	-0.242
0	6	0	354.676	372.296	372.296	0.0	-17.620	-2.770 *
4	6	2	29.4C3	23.569	-33.569	0.0	4.166	2.277
5	4	3	17.924	18.495	18.495	0.0	-0.571	-0.217

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	4	3	11.889	7.891	0.0	3.998	1.140	
7	4	3	33.396	29.475	29.475	0.0	3.529	2.232
8	4	3	20.029	17.710	-17.710	0.0	2.318	0.927
9	4	3	11.100	16.036	16.036	0.0	-4.936	-1.233
10	4	3	22.762	24.138	24.138	0.0	-1.375	-0.627
11	4	3	7.770	11.475	11.475	0.0	-3.705	-0.757
12	4	3	49.515	49.026	49.026	0.0	0.499	0.343
13	4	3	34.463	34.472	34.472	0.0	-0.289	-0.171
14	4	3	9.342	9.563	9.563	0.0	-0.202	-0.343
15	4	3	18.187	20.574	20.574	0.0	-2.397	-0.842
17	4	3	1.533	1.394	1.394	0.0	0.139	0.015
18	4	3	4.321	5.778	-5.778	0.0	-1.597	-0.208
19	4	3	17.120	13.835	-13.835	0.0	3.285	0.959
20	4	3	48.135	44.616	44.616	0.0	3.519	2.142
22	4	3	13.160	9.599	-9.599	0.0	3.561	0.846
23	4	3	18.523	20.743	-20.743	0.0	-2.223	-0.612
0	6	0	345.460	372.296	372.296	0.0	-19.836	-2.664 *
24	4	3	21.058	21.398	21.398	0.0	-0.340	-0.385
23	3	3	6.484	0.540	-0.540	0.0	5.544	0.022
22	2	3	30.263	37.730	37.730	0.0	-0.532	0.267
21	3	3	66.103	66.871	-66.871	0.0	-0.788	-0.494
23	3	3	3.783	12.383	-12.383	0.0	8.600	1.033
19	3	3	81.425	59.114	-59.114	0.0	1.311	0.392
18	1	1	81.619	62.543	-62.543	0.0	3.924	-0.561
17	3	3	45.228	44.926	44.926	0.0	0.302	0.187
16	3	3	8.602	13.284	-13.284	0.0	-0.682	-0.924
15	3	3	97.851	57.403	-57.403	0.0	0.444	0.314
14	3	3	174.828	173.475	173.475	0.0	1.333	0.475
13	3	3	109.387	109.562	-109.562	0.0	-0.575	-0.362
12	3	3	27.694	26.970	-26.970	0.0	0.634	0.355
11	3	3	37.246	39.235	-39.235	0.0	-1.939	-1.203
10	3	3	14.304	6.084	-6.084	0.0	8.233	3.757
9	3	3	38.277	36.705	36.705	0.0	1.572	1.032
8	3	3	10.462	10.462	10.462	0.0	-0.243	-0.062
7	3	3	82.302	72.108	92.108	0.0	-0.193	0.129
6	3	3	185.395	184.829	184.829	0.0	0.566	0.190
0	6	0	355.020	372.296	372.296	0.0	-17.276	-2.715 *
5	3	3	92.514	92.232	-92.232	0.0	0.342	0.216
4	3	2	29.554	25.782	25.782	0.0	3.812	2.529
3	3	3	54.394	54.798	-54.798	0.0	-0.384	-0.395
2	3	3	171.466	175.533	-175.533	0.0	-6.017	-1.479
1	3	3	161.724	171.221	171.221	0.0	-0.497	-3.668
0	2	3	231.455	252.519	252.519	0.0	-21.034	-0.553 *
1	2	3	102.308	105.268	105.268	0.0	-2.960	1.766
2	2	3	101.779	6.810	6.810	0.0	0.168	1.379
3	2	3	29.042	30.989	30.989	0.0	-1.147	-0.768
4	2	3	25.336	26.115	-26.115	0.0	-0.749	-0.480
5	2	3	45.243	44.738	-44.738	0.0	0.505	0.709
6	2	3	12.767	14.671	-14.671	0.0	-1.954	-0.619
7	2	3	77.677	74.872	-74.872	0.0	2.805	1.954
8	2	3	70.562	68.672	68.672	0.0	1.893	1.361
10	2	3	23.464	15.674	-19.074	0.0	4.391	2.208
11	2	3	17.383	10.777	10.777	0.0	6.606	2.628

STRUCTURE FACTORS								PAGE 17
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	2	3	92.112	55.538	-90.938	0.0	1.175	0.717
13	2	3	63.625	64.677	-64.608	0.0	-0.982	-0.701
14	2	3	5.112	12.789	-12.739	0.0	-7.578	-1.184
0	6	0	355.001	372.256	372.256	0.0	-17.295	-2.718 *
15	2	3	56.144	54.285	-54.285	0.0	1.359	1.303
16	2	3	38.526	37.813	37.813	0.0	0.714	0.439
17	2	3	13.277	17.639	17.639	0.0	-4.662	-1.266
18	2	3	13.303	8.599	8.599	0.0	5.204	1.619
19	2	3	46.446	48.407	49.407	0.0	-1.961	-1.113
20	2	3	81.990	84.469	-84.469	0.0	-2.479	-1.565
21	2	3	19.304	20.492	-20.492	0.0	-2.198	-0.648
22	2	3	3.667	6.221	6.221	0.0	-2.614	-0.258
23	2	3	8.953	5.178	5.178	0.0	3.774	0.766
25	2	3	14.183	8.536	8.936	0.0	5.256	1.273
25	1	3	21.320	14.641	14.641	0.0	6.589	2.447
23	1	3	13.511	9.573	9.573	0.0	12.537	3.233 *
21	1	3	2.702	5.532	-9.032	0.0	-6.333	-0.753
20	1	3	15.266	8.119	8.119	0.0	7.087	2.165
19	1	3	3.958	4.390	4.390	0.0	-0.432	-0.053
19	1	3	23.742	24.558	-24.558	0.0	-0.856	-0.373
17	1	3	41.362	39.169	39.169	0.0	1.393	1.254
0	6	0	355.862	372.256	372.256	0.0	-16.435	-2.572 *
15	1	3	17.573	15.438	15.438	0.0	2.135	0.769
14	1	3	14.563	7.635	-7.635	0.0	6.658	2.325
13	1	3	7.215	2.037	2.037	0.0	5.178	1.187
12	1	3	2.410	4.055	-4.055	0.0	-1.596	-0.203
11	1	3	23.245	15.664	-19.854	0.0	3.351	1.614
10	1	3	57.675	54.199	-54.199	0.0	3.476	2.653
9	1	3	37.310	35.633	35.633	0.0	1.478	0.934
8	1	3	5.656	7.625	7.625	0.0	-1.929	-0.350
7	1	3	17.924	14.598	-14.598	0.0	3.036	1.274
6	1	3	32.433	31.525	-31.505	0.0	0.928	0.654
5	1	3	45.257	43.524	-43.524	0.0	1.733	1.441
3	1	3	46.490	45.362	-45.362	0.0	1.128	0.913
2	1	3	62.962	62.482	-62.482	0.0	0.480	0.357
1	1	3	24.546	28.235	28.235	0.0	-3.689	-2.293
0	0	4	144.387	145.233	-145.023	0.0	-0.636	-0.273
1	0	4	94.183	95.763	-95.763	0.0	-1.579	-0.963
2	0	4	26.419	25.610	25.610	0.0	0.609	0.320
3	0	4	83.370	80.341	80.341	0.0	3.029	2.020
0	6	0	355.269	372.295	372.295	0.0	-17.027	-2.575 *
4	0	4	220.258	213.526	213.526	0.0	6.772	1.861
5	0	4	57.243	56.321	-56.321	0.0	0.927	0.664
6	0	4	15.352	13.085	13.085	0.0	2.267	0.728
7	0	4	61.989	62.692	-62.692	0.0	-0.903	-0.262
8	0	4	166.477	142.567	-162.567	0.0	3.911	1.453
9	0	4	7.595	4.015	-4.015	0.0	2.780	0.597
10	0	4	23.508	21.654	-21.654	0.0	1.354	0.968
11	0	4	67.638	67.891	-67.891	0.0	-0.254	-0.175
12	0	4	135.419	134.244	134.244	0.0	1.175	0.525
13	0	4	45.351	45.113	-45.133	0.0	0.419	0.279
14	0	4	9.084	7.297	7.297	0.0	1.787	0.386
15	0	4	8.719	8.005	-8.005	0.0	0.715	0.143

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
16	0	4	120.872	120.120	-120.120	0.0	C.753	0.364
17	0	4	17.693	19.857	19.857	0.0	-2.207	-0.559
18	0	4	26.914	26.509	-26.509	0.0	0.304	0.127
19	0	4	4.221	6.787	6.787	0.0	-2.567	-0.331
20	0	4	55.453	54.858	54.858	0.0	0.595	0.351
21	0	4	31.540	27.785	-27.785	0.0	3.755	1.794
22	0	4	17.500	0.039	-0.039	0.0	17.461	5.609 *
23	0	4	25.556	26.456	-26.456	0.0	-2.900	-0.314
0	6	0	352.122	372.256	372.256	0.0	-20.175	-3.203 *
23	1	4	10.956	15.087	-15.087	0.0	-4.191	-0.766
22	1	4	39.933	43.532	-43.532	0.0	-3.643	-1.682
21	1	4	17.568	11.431	-11.431	0.0	6.537	1.848
19	1	4	14.957	17.256	-17.256	0.0	-2.339	-0.574
18	1	4	38.629	40.463	-40.463	0.0	-1.834	-0.978
17	1	4	5.371	4.322	-4.322	0.0	1.549	0.245
16	1	4	5.342	6.633	-6.633	0.0	-0.791	-0.125
15	1	4	18.567	21.713	-21.713	0.0	-3.146	-1.945
14	1	4	8.383	12.433	-12.433	0.0	-4.050	-0.772
12	1	4	19.165	21.589	-21.589	0.0	-2.423	-0.863
11	1	4	72.601	73.593	-73.593	0.0	-0.992	-0.678
10	1	4	98.053	95.645	-95.645	0.0	2.247	1.297
9	1	4	34.820	33.295	-33.295	0.0	1.525	1.011
8	1	4	10.981	14.727	-14.727	0.0	-3.346	-0.971
7	1	4	41.165	39.976	-39.976	0.0	1.189	0.854
6	1	4	62.156	60.814	-60.814	0.0	1.382	1.008
5	1	4	42.646	42.245	-42.245	0.0	0.401	0.271
4	1	4	11.553	4.603	-4.603	0.0	6.950	1.911
0	6	0	352.941	372.256	372.256	0.0	-19.355	-3.069 *
3	1	4	6.651	14.450	-14.450	0.0	-5.599	-1.205
2	1	4	65.646	62.836	-62.836	0.0	2.810	2.048
1	1	4	77.292	86.627	-86.627	0.0	-3.515	-2.374
0	2	4	69.853	74.591	-74.591	0.0	-3.738	-2.636
1	2	4	38.116	40.478	-40.478	0.0	-2.362	-1.535
2	2	4	12.751	8.398	-8.398	0.0	4.653	1.397
4	2	4	41.927	42.299	-42.299	0.0	-0.362	-0.242
5	2	4	55.026	57.895	-57.895	0.0	-2.813	-1.976
6	2	4	12.839	3.655	-3.655	0.0	8.984	2.639
7	2	4	26.946	27.455	-27.455	0.0	-C.510	-0.279
8	2	4	54.312	53.225	-53.225	0.0	C.787	0.588
9	2	4	13.248	11.687	-11.687	0.0	1.360	0.423
10	2	4	7.930	10.735	-10.735	0.0	-2.804	-0.573
11	2	4	5.669	2.221	-2.221	0.0	7.248	1.783
12	2	4	40.828	39.468	-39.468	0.0	1.359	0.859
13	2	4	13.613	14.425	-14.425	0.0	-0.912	-0.235
14	2	4	18.458	18.759	-18.759	0.0	-0.105	-0.337
15	2	4	19.575	17.243	-17.243	0.0	2.332	0.961
16	2	4	18.377	21.799	-21.799	0.0	-3.423	-1.074
0	5	0	352.902	372.256	372.256	0.0	-19.394	-3.175 *
17	2	4	11.655	0.559	-0.559	0.0	10.725	2.770 *
19	2	4	5.039	4.008	-4.008	0.0	1.030	0.140
20	2	4	34.703	34.411	-34.411	0.0	0.292	0.141
21	2	4	1.081	7.568	-7.568	0.0	-6.467	-0.606
22	2	4	16.740	13.040	-13.040	0.0	3.700	1.013

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
23	2	4	15.834	7.123	7.123	0.0	8.711	2.347
21	3	4	17.853	7.541	-7.941	0.0	4.912	1.167
20	3	4	12.488	2.212	-2.212	0.0	10.276	2.368 *
19	3	4	9.981	7.698	-7.698	0.0	1.383	0.369
17	3	4	7.526	4.977	4.977	0.0	2.559	0.437
15	3	4	21.221	19.396	-18.396	0.0	2.831	1.153
14	3	4	13.813	5.173	-5.073	0.0	8.744	2.784
12	3	4	5.199	3.274	-3.274	0.0	1.925	0.317
11	3	4	8.821	3.529	-3.529	0.0	4.892	1.060
0	5	0	352.731	372.255	372.256	0.0	-19.565	-3.103 *
9	3	4	15.722	17.386	17.384	0.0	2.338	1.325
7	3	4	20.862	23.489	23.488	0.0	-2.627	-1.174
6	3	4	4.148	4.103	4.103	0.0	0.044	0.007
5	3	4	15.870	13.236	-13.236	0.0	2.562	0.357
3	3	4	6.660	2.977	2.977	0.0	3.683	0.395
2	3	4	16.224	5.543	5.543	0.0	4.281	1.229
1	3	4	16.764	17.351	-17.351	0.0	-0.567	-0.206
0	4	4	40.505	43.976	-43.976	0.0	-3.471	-2.277
3	4	4	3.257	12.982	-12.982	0.0	-6.726	-1.303
4	4	4	6.353	7.353	-7.035	0.0	-0.582	-0.129
5	2	4	39.655	39.726	39.726	0.0	-0.071	-0.351
7	4	4	13.154	7.986	-7.986	0.0	5.398	1.785
9	4	4	30.125	34.743	34.743	0.0	-4.607	-2.367
10	4	4	10.414	5.712	-5.712	0.0	4.701	1.166
0	6	0	354.021	372.256	372.256	0.0	-18.269	-2.384 *
11	4	4	3.242	11.781	-11.781	0.0	-8.539	-1.105
12	4	4	19.692	14.101	14.101	0.0	5.391	2.161
13	4	4	17.588	17.648	17.648	0.0	-0.061	-0.021
14	4	4	17.339	14.511	14.511	0.0	2.829	0.968
15	4	4	35.582	36.325	36.325	0.0	-0.743	-0.419
17	4	4	5.900	12.335	-12.335	0.0	-6.434	-0.910
19	4	4	21.125	21.609	21.609	0.0	-0.485	-0.154
20	4	4	4.892	7.373	7.373	0.0	-2.480	-0.312
21	4	4	26.653	27.753	-27.753	0.0	-1.130	-0.432
22	4	4	14.450	9.128	9.128	0.0	5.362	1.417
21	5	4	25.512	28.681	28.681	0.0	-3.169	-1.117
20	5	4	14.986	1.887	-1.887	0.0	13.100	3.500 *
19	5	4	27.735	28.478	28.478	0.0	-0.743	-0.287
18	5	4	53.556	54.935	-54.935	0.0	-1.380	-0.763
17	5	4	4.892	8.308	-8.308	0.0	-3.415	-0.437
15	5	4	32.301	32.271	32.271	0.0	0.031	0.016
14	5	4	46.325	47.342	47.342	0.0	0.983	0.626
0	6	0	353.951	372.256	372.256	0.0	-18.345	-2.386 *
13	5	4	38.101	37.839	-37.839	0.0	0.263	0.156
12	5	4	20.354	23.920	-23.920	0.0	-3.526	-1.237
11	5	4	67.357	66.995	66.995	0.0	0.362	0.236
10	5	4	119.121	117.875	-117.875	0.0	1.246	0.612
9	5	4	35.556	34.744	-34.744	0.0	0.852	0.524
6	5	4	80.023	81.089	81.089	0.0	-1.056	-0.678
5	5	4	3.223	3.633	-3.633	0.0	-0.405	-0.055
4	5	4	10.983	6.501	-6.501	0.0	4.482	1.189
3	5	4	29.462	20.578	-20.578	0.0	-1.116	-0.646
2	5	4	100.763	103.377	-103.377	0.0	-2.669	-1.535

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STRUCTURE FACTORS

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H	K	L	F(URS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	5	4	44.039	44.616	-44.616	0.0	-2.576	-1.739
0	6	4	70.750	71.870	-71.870	0.0	-1.116	-0.778
1	6	4	39.127	39.566	-39.566	0.0	0.561	0.365
2	6	4	16.656	18.501	-18.501	0.0	-2.235	-0.736
3	6	4	45.081	46.507	-46.507	0.0	-1.428	-1.174
4	6	4	131.615	134.229	-134.229	0.0	-2.604	-1.194
5	6	4	35.289	35.359	-35.359	0.0	-0.111	-0.065
6	6	4	3.417	8.832	-8.832	0.0	-5.465	-0.76
0	6	0	354.256	372.295	-372.295	0.0	-18.040	-2.847 *
7	6	4	20.979	19.444	-19.444	0.0	1.335	0.625
8	6	4	103.356	103.489	-103.489	0.0	-0.133	-0.073
9	6	4	26.816	25.770	-23.970	0.0	2.845	1.409
10	6	4	-11.524	12.614	-12.614	0.0	-1.090	-0.263
11	6	4	32.155	33.125	-33.125	0.0	-0.970	-0.455
12	6	4	82.375	79.367	-79.367	0.0	2.698	1.669
13	6	4	45.551	46.501	-46.501	0.0	-0.913	-0.526
15	6	4	29.292	19.544	-19.544	0.0	0.448	0.150
16	5	4	79.366	78.873	-78.873	0.0	0.493	0.284
17	6	4	17.503	18.559	-18.559	0.0	-1.459	-0.409
18	6	4	19.767	18.385	-18.385	0.0	1.322	0.419
19	6	4	13.891	9.942	-9.942	0.0	3.948	0.910
20	6	4	37.766	38.564	-38.564	0.0	-0.859	-0.381
18	7	4	13.219	6.258	-6.258	0.0	12.961	3.168 *
17	7	4	12.620	9.259	-9.259	0.0	7.181	1.615
16	7	4	8.018	12.594	-12.594	0.0	-4.976	-0.750
15	7	4	35.904	37.082	-37.082	0.0	-1.179	-0.551
14	7	4	22.040	20.595	-20.595	0.0	1.499	0.908
13	7	4	5.564	9.859	-9.859	0.0	-4.235	-0.613
0	6	0	352.959	372.296	-372.296	0.0	-19.331	-3.066 *
12	7	4	2.659	10.019	-10.019	0.0	-7.361	-0.324
11	7	4	40.051	41.002	-41.002	0.0	-0.951	-0.532
10	7	4	22.587	20.975	-20.975	0.0	1.612	0.683
9	7	4	24.429	27.231	-27.231	0.0	-2.801	-1.167
8	7	4	5.873	13.589	-13.589	0.0	-3.716	-0.778
7	7	4	7.872	1.084	-1.084	0.0	6.788	1.277
5	7	4	14.402	13.557	-13.557	0.0	0.945	0.135
3	7	4	21.607	19.297	-19.297	0.0	2.310	1.026
2	7	4	12.722	3.551	-3.551	0.0	9.171	2.683
1	7	4	26.521	26.827	-26.827	0.0	-0.306	-0.141
6	8	4	55.659	56.016	-56.016	0.0	-0.330	-0.225
2	8	4	6.368	3.152	-3.152	0.0	3.216	0.346
3	8	4	4.294	12.238	-12.238	0.0	-7.944	-1.052
4	8	4	38.336	38.234	-38.234	0.0	0.102	0.058
5	8	4	18.326	20.682	-20.682	0.0	-2.356	-0.969
7	8	4	5.661	0.950	-0.950	0.0	4.731	0.738
0	8	0	352.158	372.296	-372.296	0.0	-20.398	-3.190 *
8	8	4	44.773	44.581	-44.581	0.0	-0.208	-0.119
9	8	4	25.457	26.489	-26.489	0.0	-0.992	-0.394
12	8	4	40.329	38.375	-38.375	0.0	1.954	1.010
14	8	4	15.235	10.218	-10.218	0.0	5.016	1.305
15	8	4	9.566	11.113	-11.113	0.0	-1.547	-0.273
16	8	4	24.824	24.665	-24.665	0.0	0.759	0.263
17	3	4	6.543	8.830	-8.830	0.0	-2.287	-0.324

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	48
14	9	4	8.033	5.184	-5.184	0.0	2.849	0.442	
11	9	4	8.602	2.447	-2.447	0.0	5.955	1.312	
10	9	4	6.704	8.669	8.669	0.0	-1.365	-0.197	
9	9	4	13.496	21.361	21.361	0.0	-7.865	-1.656	
8	9	4	9.712	2.864	2.864	0.0	6.849	1.363	
0	6	0	352.350	372.296	372.296	0.0	-19.946	-3.165 *	
5	9	4	6.543	10.821	10.821	0.0	-4.278	-0.644	
4	9	4	9.929	3.153	3.153	0.0	6.679	1.385	
3	9	4	12.473	15.494	15.494	0.0	-3.021	-0.687	
1	9	4	6.859	0.416	-0.416	0.0	9.243	1.977	
0	10	4	10.482	2.235	-2.235	0.0	8.192	1.795	
1	10	4	15.226	15.598	15.598	0.0	9.108	0.027	
3	10	4	23.771	23.260	-23.260	0.0	0.512	0.181	
4	10	4	26.562	26.920	-26.920	0.0	3.043	0.019	
5	10	4	20.057	17.834	17.834	0.0	2.253	0.728	
8	10	4	18.398	20.144	20.144	0.0	-1.255	-0.353	
9	10	4	17.441	9.647	9.647	0.0	7.792	2.360	
10	10	4	12.629	2.865	2.865	0.0	9.756	2.206	
11	10	4	11.714	9.112	9.112	0.0	2.602	0.540	
12	10	4	13.853	9.752	-9.752	0.0	4.051	0.949	
7	11	4	15.849	11.741	11.741	0.0	4.104	1.061	
6	11	4	42.123	43.695	43.695	0.0	-1.562	-0.783	
0	6	0	351.665	372.296	372.296	0.0	-20.631	-3.297 *	
5	11	4	10.940	12.181	-12.181	0.0	-1.242	-0.233	
4	11	4	13.189	6.981	-6.981	0.0	6.309	1.536	
3	11	4	6.969	5.695	-5.695	0.0	3.273	0.572	
2	11	4	57.763	57.261	-57.261	0.0	0.502	0.213	
1	11	4	23.026	24.046	-24.046	0.0	-1.021	-0.323	
0	10	5	19.356	18.439	-18.439	0.0	1.314	0.366	
2	10	5	24.262	27.692	27.692	0.0	0.370	0.145	
3	10	5	10.370	6.237	-6.237	0.0	4.133	0.913	
4	10	5	8.953	8.236	-8.236	0.0	0.719	0.128	
5	10	5	17.661	16.726	-16.726	0.0	0.935	0.252	
10	9	5	42.339	42.911	42.911	0.0	-0.573	-0.277	
4	9	5	39.318	41.657	41.657	0.0	-2.379	-1.054	
8	9	5	37.999	34.764	-34.764	0.0	3.215	1.714	
7	9	5	25.892	30.036	30.036	0.0	-4.144	-1.343	
6	9	5	25.877	28.935	-28.935	0.0	-3.054	-1.054	
5	9	5	45.477	42.624	-42.624	0.0	2.854	1.620	
3	9	5	52.389	51.223	-51.223	0.0	1.163	0.680	
0	6	0	351.437	372.296	372.296	0.0	-20.852	-3.324 *	
2	9	5	30.062	27.565	27.565	0.0	2.096	0.936	
1	9	5	12.181	3.182	-3.182	0.0	9.000	2.000	
0	8	5	13.564	20.932	-20.932	0.0	-7.349	-1.567	
1	8	5	31.979	34.799	34.799	0.0	-3.820	-1.160	
2	8	5	52.614	45.687	-49.887	0.0	3.787	1.823	
3	8	5	43.394	44.325	44.325	0.0	-0.931	-0.524	
4	8	5	52.189	53.039	53.039	0.0	-0.053	-0.490	
5	8	5	32.023	30.829	-30.829	0.0	1.194	0.520	
7	8	5	12.760	14.728	-14.728	0.0	-1.968	-0.415	
8	8	5	35.918	35.224	-35.224	0.0	0.695	0.314	
9	8	5	56.056	57.466	57.466	0.0	-1.410	-0.779	
11	8	5	62.770	61.533	61.533	0.0	1.238	0.750	

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	8	5	37.032	36.893	0.0	0.139	0.067	
13	0	5	14.567	14.568	0.0	0.039	1.326	
15	7	5	14.534	14.402	-14.402	0.0	0.132	0.030
14	7	5	11.056	8.069	-8.069	0.0	2.989	0.618
13	7	5	6.123	2.560	-2.560	0.0	3.203	0.493
12	7	5	21.768	20.183	-20.183	0.0	1.505	0.545
0	6	0	351.939	372.256	372.256	0.0	-29.308	3.224 *
11	7	5	2.561	2.561	2.561	0.0	-1.209	0.435
10	7	5	4.561	11.156	-11.156	0.0	-1.785	0.311
8	7	5	21.257	23.642	-23.642	0.0	-2.585	0.757
7	7	5	11.036	1.391	-1.391	0.0	9.676	1.369
5	7	5	11.916	13.307	-13.307	0.0	-1.388	0.305
4	7	5	23.941	23.628	-23.628	0.0	0.319	0.130
3	7	5	30.955	31.016	-31.016	0.0	-0.062	-0.031
2	7	5	3.934	2.438	-2.438	0.0	1.020	0.135
0	6	5	6.361	6.167	-6.167	0.0	3.184	0.503
0	6	5	19.372	12.720	-12.720	0.0	4.151	1.399
1	6	5	16.444	15.767	-15.767	0.0	0.681	0.222
2	6	5	19.239	18.183	-18.183	0.0	1.056	0.144
4	6	5	11.433	2.433	-2.433	0.0	5.020	2.442
5	6	5	4.909	6.766	-6.766	0.0	-1.156	0.134
6	6	5	11.916	0.347	-0.347	0.0	11.467	2.865 *
6	6	5	5.462	5.457	-5.457	0.0	0.005	0.001
8	6	5	12.225	9.551	-9.551	0.0	2.634	0.238
0	6	0	352.759	372.206	372.206	0.0	-19.546	-3.100 *
4	6	5	14.519	2.319	-2.319	0.0	12.200	3.538 *
10	6	5	3.943	12.012	-12.012	0.0	-8.088	-0.934
14	6	5	16.725	3.488	-3.488	0.0	13.237	3.973 *
15	6	5	17.295	9.016	-9.016	0.0	8.279	2.552
16	6	5	7.974	4.759	-4.759	0.0	3.221	0.525
7	6	5	2.789	6.217	-6.217	0.0	-3.423	-0.363
10	6	5	15.147	12.937	-12.937	0.0	2.241	0.198
17	5	5	11.173	2.214	-2.214	0.0	8.959	1.658
16	5	5	19.993	5.347	-5.347	0.0	5.636	1.143
14	6	5	18.713	19.522	-18.522	0.0	-0.209	-0.040
13	5	5	14.581	19.458	-19.458	0.0	-0.876	-0.266
12	5	5	26.159	27.305	-27.305	0.0	-1.146	-0.633
11	5	5	13.423	9.550	-9.550	0.0	-5.427	-0.269
10	5	5	27.223	26.811	-26.811	0.0	0.412	0.089
9	5	5	29.555	30.565	-30.565	0.0	-2.250	-0.049
0	6	0	351.722	372.296	372.296	0.0	-20.574	-3.278 *
4	5	5	45.085	41.457	-41.457	0.0	2.627	0.658
6	5	5	42.147	42.872	-42.872	0.0	-0.725	-0.458
6	5	5	11.363	17.305	-17.305	0.0	-6.022	-1.321
2	5	5	18.951	24.857	-24.857	0.0	-5.886	-1.997
1	5	5	17.062	18.148	-18.148	0.0	-1.086	-0.532
0	4	5	17.383	14.601	-14.601	0.0	2.582	0.930
1	4	5	9.873	11.436	-11.436	0.0	-1.563	-0.357
2	4	5	46.652	43.537	-43.537	0.0	3.114	2.257
3	4	5	22.669	26.014	-26.014	0.0	-3.324	-1.299
4	4	5	20.540	21.939	-21.939	0.0	-1.399	-0.341
5	4	5	8.208	12.704	-12.704	0.0	-4.457	-0.867
6	4	5	23.494	21.274	-21.274	0.0	2.220	0.955

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STRUCTURE FACTORS

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H	K	L	F(M(S))	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	50
8	4	5	5.929	3.395	3.385	0.0	2.544	0.419	
9	4	5	37.003	35.793	-36.793	0.0	0.210	0.120	
11	4	5	39.860	40.669	-40.869	0.0	-1.309	-0.550	
0	6	3	352.350	372.296	372.256	0.0	-19.946	-3.165 *	
13	4	5	22.572	17.721	-17.721	0.0	4.852	1.923	
14	4	5	15.176	3.763	-3.763	0.0	11.414	3.241 *	
15	4	5	14.345	9.176	-8.176	0.0	5.188	1.259	
16	4	5	16.126	8.156	8.166	0.0	7.989	2.289	
17	4	5	23.976	25.183	-25.183	0.0	-1.207	-0.413	
19	4	5	26.891	25.532	-25.932	0.0	2.959	1.313	
20	3	5	16.450	23.533	23.583	0.0	-5.533	-1.397	
19	3	5	14.256	14.173	-14.173	0.0	0.083	0.019	
18	3	5	46.916	46.235	46.235	0.0	0.681	0.377	
17	3	5	60.339	61.353	61.353	0.0	-1.014	-0.566	
16	3	5	42.734	44.670	-44.670	0.0	-1.936	-1.000	
15	3	5	46.857	47.655	47.855	0.0	-0.998	-0.540	
14	3	5	32.345	30.932	-30.832	0.0	1.514	0.718	
13	3	5	43.101	39.692	-39.692	0.0	3.409	2.003	
12	3	5	56.483	56.448	-58.448	0.0	-1.925	-1.168	
11	3	5	60.649	60.151	-60.151	0.0	0.458	0.311	
10	3	5	95.645	95.744	95.744	0.0	-0.099	-0.056	
9	3	5	78.659	80.443	80.443	0.0	-1.744	-1.070	
8	3	5	53.747	54.233	-54.233	0.0	-0.486	-0.304	
0	6	0	352.150	372.296	372.256	0.0	-24.098	-3.190 *	
7	3	5	63.773	63.457	63.497	0.0	0.276	0.183	
6	3	5	69.646	69.113	-69.113	0.0	0.533	0.354	
5	3	5	85.087	84.916	-84.916	0.0	1.171	0.723	
4	3	5	15.133	11.219	11.219	0.0	3.917	1.269	
3	3	5	104.973	104.299	-104.299	0.0	0.674	0.365	
2	3	5	73.089	75.168	75.168	0.0	-2.379	-1.420	
1	3	5	22.660	22.665	22.865	0.0	-0.205	-0.099	
0	2	5	17.120	12.610	-12.610	0.0	4.510	1.677	
1	2	5	35.595	37.431	37.481	0.0	-1.835	-1.119	
2	2	5	59.883	58.566	-58.566	0.0	0.917	0.648	
3	2	5	SC.779	51.225	51.225	0.0	-0.447	-0.367	
4	2	5	62.432	63.233	63.233	0.0	-0.801	-0.549	
5	2	5	43.834	44.702	-44.702	0.0	-0.368	-0.253	
6	2	5	17.310	18.334	-18.334	0.0	-1.324	-0.349	
7	2	5	16.126	21.345	-21.345	0.0	-5.219	-1.546	
8	2	5	37.603	37.557	-37.597	0.0	-0.394	-0.232	
9	2	5	72.059	70.555	70.555	0.0	1.143	0.737	
11	2	5	77.455	76.913	76.913	0.0	0.542	0.339	
12	2	5	34.673	36.280	36.880	0.0	-2.237	-1.150	
0	6	0	353.703	372.256	372.256	0.0	-18.593	-2.936 *	
13	2	5	6.820	2.503	2.500	0.0	4.329	0.732	
14	2	5	16.272	11.619	11.619	0.0	4.454	1.474	
15	2	5	16.024	13.619	-13.619	0.0	2.405	0.683	
16	2	5	31.262	28.737	-28.737	0.0	2.525	1.190	
17	2	5	36.211	36.569	36.569	0.0	-0.358	-0.170	
18	2	5	17.821	16.519	18.519	0.0	-0.698	-0.186	
19	2	5	18.114	15.339	15.739	0.0	2.374	0.666	
20	2	5	15.060	10.082	10.082	0.0	4.977	1.243	
21	1	5	20.964	14.768	-14.768	0.0	6.196	2.208	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
19	1	5	7.945	9.251	-9.251	0.0	-1.305	-0.205
18	1	5	4.732	2.619	2.619	0.0	2.112	0.279
17	1	5	14.475	12.632	12.632	0.0	1.343	0.455
16	1	5	11.042	5.142	5.142	0.0	5.900	1.234
15	1	5	15.235	12.127	12.127	0.0	3.108	0.351
14	1	5	22.287	16.156	19.754	0.0	2.453	1.317
13	1	5	17.936	15.639	15.939	0.0	1.897	0.518
12	1	5	39.963	37.241	37.261	0.0	2.702	1.631
11	1	5	6.777	11.574	11.574	0.0	-4.758	-0.303
10	1	5	18.947	13.372	13.372	0.0	5.575	2.359
9	0	6	352.956	372.296	372.296	0.0	-15.337	-3.066 *
8	1	5	21.125	10.377	18.377	0.0	2.748	1.190
7	1	5	30.691	30.175	30.775	0.0	-0.084	-0.046
6	1	5	41.165	41.220	41.228	0.0	-1.063	-0.043
4	1	5	17.325	16.738	16.738	0.0	0.587	0.214
2	1	5	18.129	16.521	16.521	0.0	1.607	0.567
1	1	5	14.052	14.067	14.067	0.0	-6.365	-0.314
0	0	6	55.026	53.241	53.261	0.0	1.765	1.200
1	0	6	122.323	120.473	120.478	0.0	1.845	0.878
2	0	6	5.470	4.437	4.437	0.0	2.033	0.536
3	0	6	57.557	56.496	56.498	0.0	3.059	2.058
4	0	6	2.118	5.634	-5.934	0.0	-3.816	-0.340
5	0	6	60.610	60.157	60.157	0.0	0.521	0.331
7	0	6	105.952	104.104	104.104	0.0	1.938	0.972
8	0	6	15.352	13.767	13.767	0.0	1.535	0.544
9	0	6	25.117	26.601	26.601	0.0	-1.565	-0.591
10	0	6	21.651	21.223	21.223	0.0	0.428	0.152
0	0	6	350.751	372.296	372.296	0.0	-21.506	-3.430 *
1	0	6	27.610	25.576	25.576	0.0	2.042	0.889
12	0	6	16.623	18.867	18.867	0.0	-2.244	-0.567
13	0	6	87.128	86.531	86.531	0.0	0.597	0.335
14	0	6	6.425	11.173	-11.173	0.0	2.652	0.321
15	0	6	80.107	79.676	79.676	0.0	0.433	0.242
16	0	6	15.629	8.235	-8.235	0.0	7.395	2.032
17	0	6	29.525	31.747	-31.747	0.0	-2.482	-0.731
16	1	6	21.754	18.455	18.455	0.0	2.758	0.943
15	1	6	22.558	28.656	-28.656	0.0	-6.297	-1.163
14	1	6	22.017	26.515	-26.515	0.0	-4.500	-1.322
13	1	6	60.443	63.817	63.817	0.0	-3.375	-1.304
12	1	6	9.658	18.021	18.021	0.0	-8.323	-1.400
11	1	6	8.768	1.565	1.565	0.0	7.462	1.385
10	1	6	14.592	10.569	-10.569	0.0	4.023	1.076
9	1	6	10.764	0.310	0.310	0.0	10.455	2.223 *
7	1	6	46.534	46.649	-46.649	0.0	-0.115	-0.037
6	1	6	26.024	26.102	-26.102	0.0	-0.078	-0.034
5	1	6	10.651	15.974	15.974	0.0	-5.233	-1.116
0	0	6	351.836	372.296	372.296	0.0	-20.660	-5.240 *
4	1	6	10.580	14.860	-14.860	0.0	-4.219	-0.934
2	1	6	12.620	10.882	10.882	0.0	1.739	0.454
1	1	6	64.333	64.218	-64.218	0.0	-0.285	-0.085
0	2	6	11.144	15.997	15.997	0.0	-4.753	-1.074
1	2	6	14.139	19.182	-19.182	0.0	-5.042	-1.293

STRUCTURE FACTORS								PAGE 25
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	2	6	17.105	21.394	21.054	0.0	-4.789	-1.466
3	2	6	42.133	42.090	-42.050	0.0	0.042	0.125
5	2	6	14.055	17.092	17.092	0.0	-2.997	-0.765
6	2	6	23.643	22.057	-22.057	0.0	1.582	0.652
7	2	6	9.836	1.145	1.145	0.0	7.691	1.455
8	2	6	17.127	10.689	10.689	0.0	6.431	2.106
9	2	6	16.550	17.233	17.233	0.0	-0.783	-0.213
10	2	6	12.868	19.829	19.829	0.0	-6.961	-1.462
11	2	6	34.314	36.515	36.515	0.0	-3.202	-0.996
12	2	6	13.642	3.521	-3.521	0.0	10.121	2.575 *
15	2	6	20.847	15.124	15.124	0.0	5.723	1.364
0	6	0	352.198	372.256	372.256	0.0	-20.093	-3.190 *
16	2	6	6.747	4.456	-4.456	0.0	2.291	0.328
17	2	5	28.277	25.176	-25.176	0.0	3.101	1.285
15	3	5	3.301	9.773	-9.773	0.0	-6.473	-0.720
15	3	6	6.764	0.732	0.732	0.0	5.972	0.459
13	3	6	3.622	1.602	1.602	0.0	2.020	0.236
11	3	6	17.255	4.186	4.186	0.0	13.111	4.465 *
10	3	6	13.628	1.534	1.534	0.0	12.093	3.123 *
9	3	6	9.917	3.260	3.260	0.0	6.657	1.360
7	3	6	6.450	8.003	-8.003	0.0	1.453	0.279
6	3	6	11.180	5.303	-5.303	0.0	5.883	1.326
5	3	6	6.835	5.338	5.338	0.0	1.497	0.243
4	3	6	23.230	20.360	20.360	0.0	2.970	1.300
2	3	6	10.297	4.644	4.644	0.0	5.653	1.281
0	4	6	22.221	24.816	24.816	0.0	-2.595	-0.944
1	4	6	17.105	13.870	13.870	0.0	3.235	1.920
0	6	0	351.655	372.256	372.256	0.0	-20.441	-3.246 *
3	4	5	35.054	33.528	-33.528	0.0	1.526	0.440
6	4	6	13.115	10.055	-10.055	0.0	3.022	0.766
7	4	6	14.504	14.062	-14.062	0.0	0.442	0.110
8	4	6	9.216	12.638	-12.638	0.0	-3.422	-0.613
9	4	6	4.951	12.377	-12.377	0.0	-7.426	-0.933
10	4	6	12.853	7.017	7.017	0.0	5.837	1.437
11	4	6	14.855	12.220	-12.220	0.0	2.635	0.653
12	4	6	13.160	9.738	-9.738	0.0	3.422	0.791
13	4	6	11.582	12.229	-12.229	0.0	-0.667	-0.121
14	5	6	26.185	19.575	19.575	0.0	6.213	2.512
13	5	6	65.675	66.758	-66.758	0.0	-1.083	-0.517
12	5	6	8.456	1.436	-1.436	0.0	7.020	1.158
11	5	6	11.133	19.657	-19.657	0.0	-8.507	-1.482
9	5	6	15.955	9.810	9.810	0.0	6.185	1.749
0	6	0	352.312	372.256	372.256	0.0	-19.984	-3.171 *
8	5	6	17.602	15.818	-15.818	0.0	1.784	0.532
7	5	6	57.527	56.433	56.433	0.0	1.095	0.265
6	5	6	28.174	23.333	23.333	0.0	-0.153	-0.070
5	5	6	47.077	46.116	-46.116	0.0	0.961	0.579
4	5	6	9.318	8.226	-8.226	0.0	1.092	0.195
3	5	6	18.611	12.633	-12.633	0.0	5.928	1.988
2	5	6	15.644	4.870	-4.870	0.0	10.774	3.137 *
1	5	6	78.955	82.174	82.174	0.0	-3.179	-1.858
0	6	6	42.423	47.492	-47.492	0.0	-0.059	-2.196
1	6	6	85.508	E8.216	-88.216	0.0	-2.703	-1.550

400C URTHOFEPPSILITE 6/29/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	6	6	16.258	19.518	19.518	0.0	-3.660	-0.942
3	6	6	20.204	23.924	23.924	0.0	-3.720	-1.078
5	6	6	41.502	44.438	44.438	0.0	-2.936	-1.400
7	6	6	68.730	68.247	68.247	0.0	0.483	0.292
8	6	6	7.551	3.510	3.510	0.0	3.740	0.593
11	6	6	26.068	21.175	21.175	0.0	4.693	1.921
0	6	0	351.950	372.296	372.296	0.0	-20.346	-3.230 *
12	6	6	18.656	17.548	17.548	0.0	1.135	0.313
10	6	6	6.353	9.224	9.224	0.0	-2.871	-0.377
9	7	5	18.742	19.368	19.368	0.0	-0.625	-0.172
7	7	6	23.669	17.648	19.648	0.0	4.021	1.455
6	7	6	23.581	21.436	21.436	0.0	2.175	0.755
4	7	6	13.730	10.295	10.295	0.0	3.525	0.874
3	7	6	17.821	25.283	25.283	0.0	-7.461	-1.725
2	7	6	5.055	1.765	1.765	0.0	7.291	1.367
1	7	6	5.710	17.191	17.191	0.0	-11.370	-1.413 *
1	0	6	14.943	9.616	9.616	0.0	5.326	1.452
1	3	6	16.155	18.099	18.099	0.0	-1.943	-0.471
2	3	5	12.909	4.491	4.491	0.0	8.618	1.966
3	3	6	33.341	35.350	35.350	0.0	-2.009	-0.789
8	6	6	4.664	8.537	8.537	0.0	-4.193	-0.514
6	6	6	19.049	14.337	14.337	0.0	4.712	1.459
0	6	7	6.017	0.291	0.291	0.0	5.416	0.760
1	6	7	8.281	2.535	2.535	0.0	5.776	0.920
0	6	0	352.788	372.296	372.296	0.0	-19.508	-3.054 *
6	9	7	15.849	17.375	17.375	0.0	-1.726	-0.466
4	9	7	9.712	9.394	9.394	0.0	0.318	0.352
2	9	7	23.362	26.587	26.587	0.0	-2.775	0.973
1	9	7	35.843	33.716	33.716	0.0	-0.873	-0.382
3	4	7	10.209	1.636	1.636	0.0	8.574	1.672
1	4	7	24.498	25.136	25.136	0.0	-0.648	-0.231
2	4	7	18.374	16.379	16.379	0.0	2.494	0.726
3	4	7	21.164	2.002	2.002	0.0	6.162	0.966
4	4	7	26.682	25.765	25.765	0.0	0.917	0.352
5	4	7	26.342	25.210	25.210	0.0	-0.889	-0.282
7	4	7	16.798	13.812	13.812	0.0	2.987	0.783
6	4	7	16.309	16.448	16.448	0.0	-0.939	-0.228
9	4	7	17.358	22.671	22.671	0.0	-5.673	-1.348
10	3	7	70.739	70.581	70.581	0.0	-0.242	-0.127
9	3	7	25.565	25.987	25.987	0.0	-0.302	-0.001
9	3	7	12.400	17.335	17.335	0.0	-4.625	-0.901
7	3	7	46.754	42.137	42.137	0.0	3.917	2.300
0	6	0	351.418	372.296	372.296	0.0	-20.878	-3.328 *
6	3	7	52.130	53.201	53.201	0.0	-1.071	-0.574
5	3	7	13.878	48.287	48.287	0.0	0.399	0.205
4	3	7	12.311	2.014	2.014	0.0	10.927	2.615 *
3	3	7	60.500	99.710	99.710	0.0	0.871	0.528
2	3	7	69.523	65.237	65.237	0.0	-4.574	-2.370
1	3	7	12.707	7.746	7.746	0.0	4.961	1.095
0	2	7	20.613	24.174	24.174	0.0	-3.561	-1.052
1	2	7	42.001	42.433	42.433	0.0	-0.432	-0.230
2	2	7	19.780	22.480	22.480	0.0	-2.700	-0.814
4	2	7	53.335	53.189	53.189	0.0	-0.191	-0.083

400C ORTHOEPPOSITITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	2	7	15.717	9.868	-9.868	0.0	5.849	1.555
8	2	7	33.789	36.231	-36.231	0.0	-2.453	-0.956
9	2	7	37.427	37.419	-37.419	0.0	0.008	0.004
10	2	7	12.167	4.108	+4.108	0.0	8.059	1.703
11	2	7	39.664	41.650	-40.660	0.0	-0.975	-0.408
11	1	7	18.533	15.973	15.975	0.0	2.563	0.746
3	6	7	351.694	372.296	372.296	0.0	-20.612	-3.284 *
19	1	7	11.910	9.561	-9.961	0.0	1.957	0.409
9	1	7	20.233	21.596	-21.596	0.0	-1.363	-0.407
8	1	7	17.456	8.666	8.666	0.0	8.791	2.948
7	1	7	0.832	0.675	-0.675	0.0	0.157	0.014
6	1	7	7.478	4.221	-4.221	0.0	3.256	0.513
5	1	7	9.712	9.766	-8.766	0.0	0.946	0.172
4	1	7	15.513	9.195	9.195	0.0	6.568	1.763
3	1	7	7.200	7.027	7.027	0.0	0.173	0.027
2	1	7	12.634	8.820	8.820	0.0	3.814	0.876
1	1	7	31.335	29.653	-29.893	0.0	1.442	0.652

600C. CRTHOFF POSITIVE 6/28/73

STRUCTURE FACTORS

PAGE 1

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	0	337.746	354.231	354.231	0.0	-16.486	-2.739 *
4	0	0	104.683	185.534	-185.534	0.0	1.149	0.389
6	0	0	22.929	23.772	-23.772	0.0	-0.843	-0.726
8	0	0	99.729	111.772	111.772	0.0	-12.043	-7.622 *
10	0	0	11.219	7.263	7.263	0.0	3.055	1.715
12	0	0	282.560	275.891	-275.891	0.0	6.648	1.381
14	0	0	32.771	30.316	-30.316	0.0	2.455	1.667
16	0	0	159.034	161.075	161.075	0.0	-2.041	-0.792
18	0	0	5.300	6.655	6.655	0.0	-1.355	-0.235
20	0	0	156.039	156.120	-156.120	0.0	-0.081	-0.032
24	0	0	11.659	1.080	-1.080	0.0	10.576	2.501 *
26	0	0	16.022	19.831	19.831	0.0	-3.809	-0.643
28	1	0	29.989	31.923	-31.923	0.0	-1.934	-0.832
24	1	0	15.464	16.713	-16.713	0.0	-1.250	-0.338
22	1	0	31.373	27.993	-27.993	0.0	3.480	2.251
20	1	0	16.654	12.189	-12.189	0.0	4.454	1.657
18	1	0	50.896	52.801	-52.801	0.0	-1.905	-1.343
16	1	0	9.909	3.040	-3.040	0.0	6.768	1.829
14	1	0	127.180	127.646	-127.646	0.0	-0.466	-0.224
12	1	0	2.295	2.135	-2.135	0.0	7.160	2.129
0	6	0	338.146	354.231	-354.231	0.0	-16.085	-2.663 *
10	1	0	46.184	44.800	-44.800	0.0	1.384	1.359
6	1	0	260.418	262.047	-262.047	0.0	-1.429	-0.375
4	1	0	10.690	7.946	-7.946	0.0	2.744	1.448
2	1	0	84.479	86.573	-86.573	0.0	-1.344	-0.034
0	2	0	7.004	11.180	-11.180	0.0	-4.176	-1.766
2	2	0	11.439	3.398	-3.398	0.0	8.041	4.888
4	2	0	165.945	196.800	-196.800	0.0	-3.005	-0.973
6	2	0	16.360	16.354	-16.354	0.0	0.006	0.004
8	2	0	85.107	84.658	-84.658	0.0	0.449	0.323
10	2	0	21.959	23.463	-23.463	0.0	-1.504	-0.948
12	2	0	12.810	11.431	-11.431	0.0	1.380	0.517
16	2	0	70.411	71.316	-71.316	0.0	-0.902	-0.632
20	2	0	14.949	16.251	-16.251	0.0	-1.302	-0.454
22	2	0	14.523	13.326	-13.326	0.0	1.188	0.370
24	2	0	29.533	32.510	-32.510	0.0	-2.977	-1.257
26	3	0	10.468	15.449	-15.449	0.0	-5.391	-1.008
0	6	0	336.508	354.231	-354.231	0.0	-15.723	-2.601 *
22	3	0	14.560	7.314	-7.314	0.0	7.253	2.265
20	3	0	74.033	4.517	-4.517	0.0	2.516	0.488
18	3	0	14.969	11.444	-11.444	0.0	3.505	1.356
14	3	0	42.310	42.388	-42.388	0.0	-0.065	-0.049
10	3	0	7.658	2.889	-2.889	0.0	5.070	1.438
8	3	0	11.145	5.880	-5.880	0.0	5.266	2.269
6	3	0	44.590	43.296	-43.296	0.0	1.295	1.350
4	3	0	14.313	20.465	-20.465	0.0	-1.151	-0.992
2	3	0	42.732	42.392	-42.392	0.0	0.339	0.377
0	4	0	26.324	26.250	-26.250	0.0	0.076	0.077
2	4	0	7.088	9.606	-9.606	0.0	-0.698	-0.283
4	4	0	64.294	67.129	-67.129	0.0	-2.835	-2.482
6	4	0	11.777	3.662	-3.662	0.0	8.115	3.759
8	4	0	61.699	62.673	-62.673	0.0	-0.974	-0.812
10	4	0	32.550	35.318	-35.318	0.0	-2.768	-2.113

600C_ORTHOPRUSOLITE_6/29/73

STRUCTURE FACTORS

PAGE 2

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DETA F	DETA/SIGMA
12	4	0	14.891	14.947	-14.947	0.0	-0.056	-0.021
14	4	0	2.349	3.372	3.372	0.0	-1.022	-0.160
0	6	0	357.803	354.231	354.231	0.0	-16.428	-2.729 *
16	4	0	48.042	49.700	49.700	0.0	-0.866	-0.624
18	4	0	9.967	1.662	1.662	0.0	8.206	2.191
20	4	0	48.680	48.208	48.308	0.0	0.371	0.259
22	4	0	9.074	19.950	-19.950	0.0	-10.875	-2.002 *
24	4	0	25.797	21.339	21.339	0.0	4.458	2.196
22	5	0	23.723	23.343	-23.343	0.0	-0.420	-0.244
20	5	0	18.078	17.835	17.835	0.0	0.244	0.084
18	5	0	60.261	61.673	61.673	0.0	-1.412	-0.925
16	5	0	13.760	8.047	8.047	0.0	5.713	2.036
14	5	0	197.583	197.243	-197.243	0.0	0.340	0.105
12	5	0	17.374	14.643	14.643	0.0	2.920	1.224
10	5	0	11.057	10.595	-10.595	0.0	0.662	0.131
8	5	0	14.450	14.173	-14.173	0.0	0.277	0.100
6	5	0	155.571	156.541	-156.541	0.0	-0.069	-0.391
4	5	0	6.123	9.225	-9.225	0.0	-2.102	-0.551
2	5	0	206.185	212.859	212.859	0.0	-6.674	-2.002
0	6	0	338.013	354.231	354.231	0.0	-16.210	-2.654 *
2	6	0	14.750	13.791	13.791	0.0	0.967	0.397
0	6	0	339.157	354.231	354.231	0.0	-15.075	-2.492 *
4	6	0	86.663	89.165	-89.165	0.0	-2.502	-1.670
6	6	0	7.165	13.381	-13.381	0.0	-6.216	-1.327
8	6	0	125.470	124.634	124.634	0.0	0.835	0.408
10	6	0	2.540	11.697	-11.697	0.0	-0.157	-1.177
12	6	0	125.622	125.892	-125.892	0.0	-0.269	-0.130
14	6	0	21.370	23.638	-23.638	0.0	-0.248	-0.131
16	6	0	71.378	69.931	69.931	0.0	1.446	0.662
18	6	0	12.026	9.654	9.654	0.0	2.372	0.679
20	6	0	122.862	124.716	-124.716	0.0	-1.854	-0.863
24	6	0	7.900	8.646	-8.646	0.0	-0.746	-0.121
22	7	0	18.182	17.212	-17.212	0.0	0.960	0.264
20	7	0	12.599	0.664	-0.664	0.0	11.935	2.149 *
18	7	0	16.213	14.398	14.398	0.0	1.815	0.572
16	7	0	16.962	15.599	-15.599	0.0	1.374	0.495
14	7	0	54.710	56.458	56.458	0.0	-1.748	-1.194
10	7	0	69.148	70.492	-70.492	0.0	-1.344	-0.532
6	7	0	34.641	34.590	34.590	0.0	0.051	0.036
0	6	0	337.917	354.231	354.231	0.0	-16.314	-2.710 *
4	7	0	31.408	31.825	31.825	0.0	-0.217	-0.149
2	7	0	18.005	17.844	17.844	0.0	0.162	0.063
0	8	0	60.795	61.967	61.967	0.0	-1.202	-0.612
2	8	0	16.962	21.734	-21.734	0.0	-4.772	-1.856
4	8	0	86.573	87.214	-87.214	0.0	-0.641	-0.408
6	8	0	12.584	3.478	3.478	0.0	9.107	3.116
8	8	0	29.989	31.628	31.628	0.0	-1.639	-0.891
10	8	0	25.061	22.814	22.814	0.0	2.247	1.253
12	8	0	41.262	42.683	-42.683	0.0	-1.440	-0.568
14	8	0	2.575	1.707	1.707	0.0	2.169	0.311
16	8	0	63.251	63.064	63.064	0.0	0.177	0.115
18	8	0	7.048	1.669	-1.669	0.0	9.379	0.939
20	8	0	9.001	6.968	-6.968	0.0	2.433	0.445

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STRUCTURE_FACTORS

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H	K	I	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
18	9	0	12.217	2.037	2.037	0.0	10.180	2.432 *
14	9	0	19.137	17.395	17.395	0.0	1.742	0.648
12	9	0	9.853	3.523	3.523	0.0	6.330	1.585
0	6	0	338.760	354.231	354.231	0.0	-15.971	-2.643 *
8	9	0	7.679	18.585	-18.585	0.0	-10.905	-2.046 *
6	0	0	21.062	24.009	24.009	0.0	-2.946	-1.261
4	9	0	7.679	7.567	7.567	0.0	0.113	0.023
0	10	0	58.010	59.613	59.613	0.0	-1.602	-1.104
2	10	0	16.062	12.524	12.524	0.0	4.538	1.912
4	10	0	15.767	9.840	9.840	0.0	5.946	2.300
8	10	0	30.342	33.696	-33.696	0.0	-3.343	-1.578
10	10	0	6.269	2.392	-2.392	0.0	3.07	0.677
12	10	0	21.738	20.596	20.596	0.0	1.142	0.471
18	10	0	12.261	6.320	6.320	0.0	5.941	1.482
14	11	0	84.226	83.878	-83.878	0.0	0.348	0.186
8	11	0	12.049	2.264	2.264	0.0	10.585	2.941 *
6	11	0	80.015	76.173	-76.173	0.0	3.843	2.363
0	6	0	338.527	354.231	354.231	0.0	-15.704	-2.598 *
4	11	0	16.903	14.203	14.203	0.0	2.701	0.952
2	11	0	66.802	67.858	67.858	0.0	-1.057	-0.665
0	12	0	21.409	88.594	88.594	0.0	2.815	1.619
8	12	0	26.973	24.418	24.418	0.0	2.555	1.086
10	12	0	7.386	8.195	8.195	0.0	-0.809	-0.132
12	12	0	32.388	32.444	-32.444	0.0	-0.556	-0.248
2	13	0	30.696	30.842	30.842	0.0	-0.146	-0.062
7	13	1	4.757	0.217	-0.217	0.0	4.540	0.597
6	13	1	12.379	8.861	-8.861	0.0	3.519	0.826
3	13	1	15.699	11.810	-11.810	0.0	3.889	1.122
2	13	1	18.579	10.542	10.542	0.0	8.036	3.005
1	13	1	15.890	12.948	12.948	0.0	3.042	0.912
0	6	0	338.009	354.231	354.231	0.0	-16.143	-2.672 *
4	12	1	11.233	6.988	6.988	0.0	4.245	1.029
5	12	1	14.768	14.098	-14.098	0.0	0.690	0.185
6	12	1	2.560	6.309	6.309	0.0	-3.769	-0.417
7	12	1	11.762	0.479	-0.479	0.0	11.283	2.814 *
9	12	1	10.660	4.012	4.012	0.0	6.649	1.496
10	12	1	11.571	3.388	3.388	0.0	8.183	1.941
11	12	1	10.690	7.996	7.996	0.0	2.694	0.573
15	11	1	16.051	15.175	-15.175	0.0	0.876	0.297
14	11	1	22.929	19.596	19.596	0.0	3.334	1.281
13	11	1	9.500	13.615	13.615	0.0	-4.115	-0.751
12	11	1	4.140	3.987	3.987	0.0	0.153	0.020
11	11	1	18.608	17.939	17.939	0.0	0.669	0.211
10	11	1	19.357	15.103	-15.103	0.0	4.255	1.500
9	11	1	13.PLR	11.753	-11.753	0.0	2.065	0.517
0	6	0	338.641	354.231	354.231	0.0	-15.590	-2.579 *
8	11	1	19.622	12.494	12.494	0.0	7.138	2.874
7	11	1	26.591	24.382	-24.382	0.0	2.208	1.001
6	11	1	36.473	32.728	32.728	0.0	3.046	2.251
5	11	1	34.788	32.627	32.627	0.0	2.161	1.233
4	11	1	14.009	10.336	10.336	0.0	3.673	1.021
3	11	1	15.919	12.217	12.217	0.0	3.702	1.241
2	11	1	26.767	23.930	-23.930	0.0	2.828	1.424

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	11	1	19.593	18.342	-18.342	0.0	1.251	0.450
0	10	1	34.538	32.254	32.254	0.0	2.284	1.314
1	10	1	33.919	33.365	-33.365	0.0	0.555	0.319
2	10	1	24.694	26.107	26.107	0.0	-3.413	-1.568
5	10	1	11.062	4.577	-4.577	0.0	6.465	1.799
6	10	1	18.329	17.836	17.836	0.0	0.493	0.184
7	10	1	18.872	15.949	15.949	0.0	2.924	1.124
8	10	1	11.292	15.175	15.175	0.0	-3.883	-1.098
9	10	1	12.144	11.423	-11.423	0.0	0.721	0.190
10	10	1	9.721	2.142	2.142	0.0	7.578	1.697
11	10	1	21.577	17.129	-17.129	0.0	4.448	1.915
0	6	0	338.680	354.231	354.231	0.0	-15.552	-2.572
12	10	1	19.122	21.089	-21.089	0.0	-1.966	-0.605
13	10	1	10.822	5.094	5.094	0.0	5.728	1.252
14	10	1	16.169	19.424	-19.424	0.0	-3.255	-0.849
15	10	1	6.226	3.613	-3.613	0.0	2.612	0.423
17	10	1	8.223	0.228	0.228	0.0	7.995	1.341
18	10	1	12.923	13.323	-13.323	0.0	-0.601	-0.089
20	9	1	9.412	8.142	8.142	0.0	1.270	0.234
19	9	1	20.886	23.189	23.189	0.0	-2.303	-0.716
18	9	1	18.661	22.140	-22.140	0.0	-3.179	-0.929
17	9	1	26.956	26.531	-26.531	0.0	0.427	0.171
16	9	1	13.701	14.174	-14.174	0.0	-0.473	-0.115
14	9	1	26.252	23.273	23.273	0.0	2.979	1.400
12	9	1	53.366	56.095	-56.095	0.0	-2.746	-1.658
11	9	1	68.896	67.551	67.551	0.0	1.344	0.896
10	9	1	63.478	63.334	-63.334	0.0	0.144	0.097
0	9	1	73.678	73.105	-73.105	0.0	0.503	0.235
8	9	1	37.970	36.201	-36.201	0.0	1.764	1.166
0	6	0	337.594	354.231	354.231	0.0	-16.636	-2.769
7	6	0	22.179	21.817	-21.817	0.0	0.362	0.166
6	9	1	28.533	30.422	30.422	0.0	-1.889	-1.403
5	9	1	32.657	32.574	-32.574	0.0	0.123	0.046
3	9	1	38.237	35.470	35.470	0.0	-0.243	-0.154
2	9	1	57.058	58.024	-58.024	0.0	-0.976	-0.117
1	9	1	43.469	43.085	-43.085	0.0	0.385	0.258
0	8	1	25.076	25.142	-25.142	0.0	-0.066	-0.039
1	8	1	8.281	6.515	-6.515	0.0	1.766	0.428
2	8	1	66.564	68.674	-68.674	0.0	-2.110	-1.562
3	8	1	102.922	107.807	-107.807	0.0	4.895	2.794
4	8	1	87.500	86.271	-86.271	0.0	0.630	0.405
5	8	1	61.906	60.186	60.186	0.0	1.732	1.253
6	8	1	13.921	10.306	-10.306	0.0	3.615	1.231
7	8	1	48.074	47.701	47.701	0.0	0.373	0.287
8	8	1	78.450	76.739	76.739	0.0	1.710	1.147
9	8	1	43.572	42.330	-42.330	0.0	1.242	0.916
10	8	1	21.033	19.856	19.856	0.0	1.176	0.530
11	8	1	24.885	27.325	-27.325	0.0	-2.440	-1.160
12	8	1	37.587	38.140	-38.140	0.0	-0.554	-0.348
0	6	0	337.017	354.231	354.231	0.0	-16.314	-2.710
13	8	1	51.797	49.370	49.370	0.0	2.427	1.711
15	8	1	45.018	47.530	47.530	0.0	-2.511	-1.533
16	8	1	41.980	43.278	43.278	0.0	-1.298	-0.733

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(FAC)	R(FAC)	DETA F	DETA/STGMA
17	8	1	30.710	30.384	-30.384	0.0	0.327	0.148
18	8	1	23.517	23.685	23.605	0.0	-0.168	-0.063
19	8	1	14.685	15.255	-15.255	0.0	-0.570	-0.155
20	8	1	18.872	21.067	-21.057	0.0	-2.195	-0.682
21	8	1	17.139	6.442	-6.442	0.0	10.697	3.483 *
19	7	1	22.473	22.932	-22.932	0.0	-0.459	-0.171
18	7	1	11.596	6.681	-6.681	0.0	4.905	1.223
16	7	1	19.313	19.042	19.042	0.0	0.271	0.109
15	7	1	5.624	8.072	-8.072	0.0	-2.448	-0.395
13	7	1	14.568	14.118	14.118	0.0	0.450	0.149
0	6	0	336.794	354.231	354.231	0.0	-15.437	-2.553 *
12	7	1	16.977	18.488	18.488	0.0	-1.511	-0.509
11	7	1	20.386	22.550	-22.550	0.0	-2.164	-0.914
10	7	1	19.387	17.455	17.455	0.0	1.932	0.870
9	7	1	41.055	43.502	43.502	0.0	-1.047	-1.305
8	7	1	30.857	35.116	35.116	0.0	-4.258	-2.494
7	7	1	11.321	5.066	-5.066	0.0	6.255	1.852
6	7	1	8.223	11.007	11.007	0.0	-2.795	-0.620
5	7	1	21.474	22.223	22.223	0.0	-0.748	-0.340
4	7	1	25.916	27.387	27.387	0.0	-1.473	-0.842
3	7	1	27.223	29.957	-29.957	0.0	-2.734	-1.499
2	7	1	15.787	17.878	17.878	0.0	-2.092	-0.765
0	6	1	4.023	0.671	-0.671	0.0	3.352	0.602
1	6	1	0.414	0.959	-0.959	0.0	7.454	2.092
3	6	1	26.753	26.977	26.977	0.0	-0.224	-0.141
4	6	1	7.239	12.104	12.104	0.0	-4.855	-1.092
6	6	1	13.231	8.779	-8.779	0.0	4.452	1.612
7	6	1	12.026	11.245	11.245	0.0	0.742	0.235
0	6	0	336.784	354.231	354.231	0.0	-17.437	-2.901 *
8	6	1	14.708	7.956	-7.956	0.0	6.832	2.514
9	6	1	9.721	13.172	13.172	0.0	-3.451	-0.819
10	6	1	6.559	3.433	-3.433	0.0	6.126	1.598
12	6	1	12.866	5.619	-5.619	0.0	7.245	2.542
13	6	1	15.713	15.618	-15.618	0.0	0.056	0.034
14	6	1	11.821	13.230	-13.230	0.0	-1.409	-0.396
15	6	1	12.834	13.813	-13.813	0.0	-0.979	-0.277
16	6	1	10.558	6.213	-6.213	0.0	4.345	1.212
17	6	1	4.537	0.971	-0.971	0.0	3.566	0.578
18	6	1	6.930	4.583	-4.583	0.0	2.348	0.620
19	6	1	16.230	2.461	-2.461	0.0	11.769	3.779 *
20	6	1	12.496	12.882	-12.882	0.0	-0.385	-0.094
22	6	1	9.236	1.391	-1.391	0.0	7.845	1.509
24	6	1	14.367	3.168	-3.168	0.0	11.179	2.803 *
25	5	1	12.000	16.609	-16.609	0.0	-3.791	-0.807
24	5	1	12.024	4.673	-4.673	0.0	7.353	1.597
0	6	0	337.936	354.231	354.231	0.0	-16.795	-2.707 *
21	5	1	20.180	23.584	23.584	0.0	-3.403	-1.130
20	5	1	15.506	3.686	-3.686	0.0	10.222	3.679 *
19	5	1	6.825	11.962	-11.962	0.0	5.137	-0.647
18	5	1	18.123	18.954	-18.954	0.0	-0.031	-0.311
17	5	1	12.126	14.136	-14.136	0.0	0.950	-0.327
16	5	1	23.444	22.478	22.478	0.0	0.966	0.459
15	5	1	34.037	33.414	-33.414	0.0	0.623	0.396

600C...CRTHDEFROSILITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DFITA F	DELTA/SIGMA	
14	5	1	53.305	51.047	0.0	2.258	14.755		
13	5	1	30.019	30.756	0.0	-0.737	-0.482		
12	5	1	12.100	7.485	7.485	0.0	4.615	1.428	
10	5	1	35.672	35.024	-35.024	0.0	0.647	0.435	
9	5	1	37.484	38.875	-38.875	0.0	-1.391	-0.954	
8	5	1	32.050	31.867	31.867	0.0	0.182	0.128	
7	5	1	64.932	64.831	-64.831	0.0	0.101	0.078	
6	5	1	59.506	59.843	59.843	0.0	-0.337	-0.274	
5	5	1	75.053	75.993	-75.993	0.0	-0.940	-0.701	
4	5	1	28.047	31.362	31.362	0.0	-3.295	-2.262	
3	5	1	42.068	42.916	42.916	0.0	-0.848	-0.777	
0	6	0	337.005	354.231	354.231	0.0	-17.228	-2.865 *	
2	5	1	61.387	65.301	-65.301	0.0	-3.994	-3.327	
1	5	1	14.803	18.652	-18.652	0.0	-3.849	-1.701	
0	4	1	8.149	3.907	-3.907	0.0	4.262	1.740	
1	4	1	47.306	49.515	-49.515	0.0	-2.209	-2.257	
2	4	1	75.604	78.703	-78.703	0.0	-3.100	-2.449	
3	4	1	65.004	47.614	-47.614	0.0	-2.611	-2.602	
4	4	1	46.849	50.015	-50.015	0.0	-3.166	-2.979	
5	4	1	81.269	83.275	-83.275	0.0	-2.006	-1.461	
6	4	1	26.605	29.970	-29.970	0.0	-3.365	-2.288	
7	4	1	32.874	34.371	-34.371	0.0	-1.657	-1.240	
8	4	1	12.555	12.735	-12.735	0.0	-0.180	-0.069	
0	4	1	6.505	7.686	-7.686	0.0	-1.182	-0.263	
10	4	1	10.337	4.037	-4.037	0.0	6.300	1.950	
11	4	1	16.595	11.490	-11.490	0.0	5.104	2.158	
12	4	1	7.297	8.814	-8.814	0.0	-1.516	-0.313	
13	4	1	54.433	11.877	-11.877	0.0	-6.444	-1.100	
14	4	1	28.753	26.255	-26.255	0.0	2.499	1.649	
15	4	1	21.209	15.698	-15.698	0.0	5.512	3.098	
16	4	1	35.581	34.488	-34.488	0.0	1.493	0.965	
17	4	1	30.519	33.364	-33.364	0.0	-2.845	-1.534	
0	6	0	336.224	354.231	354.231	0.0	-18.008	-3.008 *	
18	4	1	27.900	28.566	-28.566	0.0	-0.666	-0.365	
19	4	1	15.713	11.008	-11.008	0.0	4.705	1.677	
21	4	1	16.081	14.491	-14.491	0.0	1.589	0.515	
22	4	1	36.070	34.838	-34.838	0.0	1.232	0.736	
23	4	1	32.506	32.187	-32.187	0.0	0.319	0.146	
24	4	1	18.152	19.767	-19.767	0.0	-1.615	-0.449	
25	4	1	21.562	26.420	-26.420	0.0	-4.658	-1.523	
26	3	1	24.576	22.269	-22.269	0.0	2.307	0.872	
25	3	1	23.209	25.813	-25.813	0.0	-2.604	-0.918	
24	2	1	20.313	27.231	-27.231	0.0	-6.919	-2.056	
23	3	1	32.432	34.270	-34.270	0.0	-1.838	-0.870	
22	3	1	68.390	69.194	-69.194	0.0	-0.804	-0.525	
21	3	1	60.721	60.581	-60.581	0.0	0.140	0.092	
20	3	1	11.483	13.496	-13.496	0.0	-2.013	-0.486	
19	3	1	40.687	43.181	-43.181	0.0	-2.485	-1.518	
18	3	1	64.116	63.679	-63.679	0.0	0.447	0.317	
17	3	1	84.330	85.170	-85.170	0.0	-0.830	-0.540	
16	3	1	24.414	21.034	-21.034	0.0	3.281	-1.965	
0	6	0	337.765	354.231	354.231	0.0	-16.467	-2.736 *	
15	3	1	22.591	22.600	-22.600	0.0	-0.004	-0.004	

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
14	3	1	62.959	62.538	0.0	0.421	0.312		
13	3	1	19.901	23.448	0.0	-3.547	-1.471		
12	3	1	135.083	134.902	-134.902	0.0	0.181	0.083	
11	3	1	204.771	202.550	202.550	0.0	2.221	0.667	
10	3	1	192.417	190.706	-190.706	0.0	1.711	0.552	
9	3	1	165.296	164.287	164.287	0.0	1.009	0.393	
8	3	1	66.431	65.465	-65.465	0.0	1.366	1.136	
7	3	1	77.332	76.170	-76.170	0.0	1.162	0.886	
6	3	1	174.194	171.975	171.975	0.0	2.218	0.802	
5	3	1	166.505	165.813	165.813	0.0	0.602	0.262	
4	3	1	52.876	48.947	48.947	0.0	3.930	3.967	
3	3	1	63.765	68.345	68.345	0.0	-4.600	-4.192	
2	3	1	155.151	165.542	-165.542	0.0	-10.301	-4.250 *	
1	3	1	178.326	192.856	-192.856	0.0	-14.529	-5.146 *	
0	2	1	50.718	54.704	-54.704	0.0	-3.986	-4.214	
1	2	1	13.231	15.164	15.164	0.0	-1.933	-1.125	
2	2	1	130.759	134.681	-134.681	0.0	-3.922	-1.912	
3	2	1	156.070	157.624	-157.624	0.0	-1.554	0.635	
4	2	1	140.467	142.737	-142.737	0.0	-2.070	-0.939	
0	6	0	338.756	354.231	354.231	0.0	-15.476	-2.559 *	
5	2	1	134.223	135.405	-135.405	0.0	-1.182	-0.562	
6	2	1	8.002	14.390	-14.390	0.0	-6.388	-2.430	
7	2	1	103.977	102.316	102.316	0.0	1.661	1.001	
8	2	1	106.542	105.152	-105.152	0.0	1.390	0.815	
9	2	1	61.758	60.942	-60.942	0.0	0.816	0.706	
10	2	1	29.018	26.181	-26.181	0.0	2.837	2.268	
11	2	1	47.646	49.498	-49.498	0.0	-1.852	-1.493	
12	2	1	61.136	60.725	-60.725	0.0	0.410	0.326	
13	2	1	58.765	58.534	-58.534	0.0	0.261	0.205	
14	2	1	2.511	8.500	-8.500	0.0	-5.989	-0.797	
15	2	1	52.507	50.794	-50.794	0.0	1.713	1.273	
16	2	1	67.440	66.714	-66.714	0.0	0.726	0.532	
17	2	1	55.982	55.470	-55.470	0.0	0.512	0.395	
18	2	1	37.675	36.256	-36.256	0.0	1.419	0.944	
19	2	1	16.433	12.097	-12.097	0.0	4.835	2.044	
20	2	1	19.563	17.376	-17.376	0.0	2.188	0.913	
21	2	1	13.554	8.333	-8.333	0.0	5.221	1.566	
22	2	1	38.884	40.170	-40.170	0.0	-1.286	-0.759	
23	2	1	54.000	55.622	-55.622	0.0	-1.622	-1.016	
24	2	1	38.515	40.325	-40.325	0.0	-1.809	-0.937	
0	6	0	338.127	354.231	-354.231	0.0	-16.104	-2.466 *	
25	2	1	41.419	42.221	-42.221	0.0	-1.802	0.986	
26	2	1	24.889	23.862	-23.862	0.0	1.038	0.420	
27	2	1	12.438	5.350	-5.350	0.0	7.088	1.787	
26	1	1	7.797	14.883	-14.883	0.0	-7.086	-1.072	
25	1	1	8.267	10.206	-10.206	0.0	-1.940	-0.354	
22	1	1	8.208	4.321	-4.321	0.0	3.887	0.846	
21	1	1	20.559	15.535	-15.535	0.0	5.625	2.494	
20	1	1	3.083	5.594	-5.594	0.0	-2.511	-0.332	
19	1	1	9.441	7.012	-7.012	0.0	2.429	0.606	
18	1	1	1.165	6.257	-6.257	0.0	-5.112	-0.584	
17	1	1	5.726	7.081	-7.081	0.0	-1.354	-0.253	
16	1	1	32.609	35.654	-35.654	0.0	-3.065	-1.970	

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
15	1	1	30.725	29.424	-29.424	0.0	1.301	0.782
14	1	1	39.498	38.969	38.969	0.0	0.519	0.392
13	1	1	31.980	33.032	33.032	0.0	-1.144	-0.777
12	1	1	10.208	11.627	11.627	0.0	-1.319	-0.389
11	1	1	21.018	16.411	-16.411	0.0	4.607	3.014
0	-6	0	336.201	354.231	354.231	0.0	-17.051	-7.993 *
10	1	1	16.228	21.911	-21.911	0.0	-5.674	-2.632
9	1	1	8.531	2.099	-2.099	0.0	6.432	2.212
8	1	1	48.665	48.357	48.357	0.0	0.308	0.316
7	1	1	55.183	54.195	-54.195	0.0	0.908	0.982
6	1	1	55.494	56.577	56.577	0.0	-1.083	-1.077
5	1	1	87.705	86.569	86.569	0.0	1.215	0.864
4	1	1	58.543	57.352	57.352	0.0	1.191	1.149
3	1	1	8.208	10.358	10.358	0.0	-2.150	-0.941
2	1	1	40.264	40.104	-40.104	0.0	0.180	0.207
1	1	1	14.142	13.514	-13.514	0.0	0.629	0.450
0	0	2	4.464	1.853	1.853	0.0	2.611	0.735
1	0	2	115.368	115.890	115.890	0.0	-0.524	-0.290
2	0	2	170.580	169.085	-169.085	0.0	1.494	0.555
3	0	2	208.774	214.704	214.704	0.0	-5.920	-1.765
4	0	2	39.159	39.491	-39.491	0.0	-0.332	-0.358
5	0	2	248.728	246.318	-246.318	0.0	2.410	0.555
7	0	2	201.660	196.973	-196.973	0.0	4.816	1.679
8	0	2	42.697	42.862	42.862	0.0	-0.175	-0.154
9	0	2	185.087	180.069	180.069	0.0	5.018	1.651
0	6	0	336.775	354.231	354.231	0.0	-17.456	-2.904 *
10	0	2	2.760	7.415	-7.415	0.0	-4.655	-0.656
11	0	2	207.161	204.213	204.213	0.0	2.460	0.875
12	0	2	11.013	8.426	-8.426	0.0	2.587	0.750
13	0	2	71.586	72.788	-72.788	0.0	-1.202	-0.860
15	0	2	83.180	83.646	-83.646	0.0	-0.466	-0.306
16	0	2	21.033	25.122	25.122	0.0	-4.089	-1.717
17	0	2	92.694	94.622	-94.622	0.0	-1.728	-1.038
18	0	2	41.169	41.656	41.656	0.0	-0.488	-0.331
19	0	2	45.328	49.146	49.146	0.0	-3.818	-2.441
21	0	2	33.658	32.609	-32.609	0.0	1.070	0.612
22	0	2	74.606	77.962	-77.962	0.0	-3.356	-1.960
23	0	2	98.977	103.100	-103.100	0.0	-4.123	-2.210
25	0	2	42.186	45.375	-45.375	0.0	-3.189	-1.638
26	0	2	23.055	23.755	23.755	0.0	0.101	0.035
26	1	2	6.067	4.915	4.915	0.0	-0.848	-0.109
25	1	2	22.018	16.064	16.064	0.0	5.954	2.355
24	1	2	23.855	25.237	25.237	0.0	-1.382	-0.531
0	6	0	337.270	354.231	354.231	0.0	-16.962	-2.820 *
23	1	2	41.335	41.604	41.604	0.0	0.331	0.200
22	1	2	19.446	16.930	16.930	0.0	1.516	0.518
21	1	2	16.316	13.963	-13.963	0.0	2.353	0.809
20	1	2	17.947	15.932	-15.932	0.0	2.015	0.753
19	1	2	20.710	16.031	-16.031	0.0	4.670	2.226
18	1	2	7.400	1.768	-1.768	0.0	5.632	1.166
17	1	2	68.420	69.031	69.031	0.0	-0.611	-0.438
16	1	2	53.703	54.500	-54.500	0.0	-0.806	-0.606
15	1	2	15.390	13.382	13.382	0.0	2.008	0.772

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
14	1	2	11.101	6.040	0.0	5.061	1.44P	
13	1	2	10.793	4.536	0.0	6.256	1.775	
12	1	2	116.352	115.090	-115.898	0.0	0.455	0.238
11	1	2	110.336	110.327	-110.327	0.0	0.006	0.005
10	1	2	21.574	21.251	-21.251	0.0	0.722	0.353
9	1	2	78.748	79.662	-79.662	0.0	-0.915	-0.660
8	1	2	62.218	63.316	-63.316	0.0	-1.098	-0.926
7	1	2	43.587	42.812	-42.812	0.0	0.775	0.740
6	1	2	5.066	5.835	-5.835	0.0	-0.769	-0.200
5	1	2	107.423	104.442	-104.442	0.0	2.091	1.752
4	1	2	46.803	41.944	-41.944	0.0	4.949	5.239
0	6	0	336.658	354.231	-354.231	0.0	-17.532	-2.927 *
3	1	2	55.701	58.873	-58.873	0.0	-3.172	-3.107
2	1	2	24.480	23.499	-23.499	0.0	0.489	0.482
1	1	2	60.687	61.790	-61.790	0.0	-0.803	-0.753
0	2	2	5.016	7.822	-7.822	0.0	1.194	0.553
1	2	2	34.403	37.558	-37.558	0.0	-2.755	-2.970
2	2	2	6.828	24.408	-24.408	0.0	4.620	1.601
3	2	2	73.720	71.682	-71.682	0.0	2.046	1.656
4	2	2	11.733	7.948	-7.948	0.0	3.785	1.982
5	2	2	29.242	28.409	-28.409	0.0	0.933	0.457
6	2	2	65.540	61.518	-61.518	0.0	4.022	3.475
7	2	2	56.391	55.205	-55.205	0.0	1.186	0.752
8	2	2	1.165	2.250	-2.250	0.0	-0.386	-0.058
9	2	2	74.591	73.079	-73.079	0.0	1.512	1.129
10	2	2	29.003	31.285	-31.285	0.0	-2.282	-1.410
11	2	2	24.073	19.896	-19.896	0.0	5.077	3.056
12	2	2	8.384	15.989	-15.989	0.0	-7.604	-1.608
13	2	2	39.532	35.938	-35.938	0.0	3.594	2.567
14	2	2	18.004	18.549	-18.549	0.0	-0.455	-0.185
15	2	2	36.260	38.555	-38.555	0.0	-2.265	-1.585
16	2	2	10.925	6.138	-6.138	0.0	4.707	1.423
0	6	0	337.136	354.231	-354.231	0.0	-17.095	-2.863 *
17	2	2	18.709	18.344	-18.344	0.0	0.455	0.190
18	2	2	41.527	43.721	-43.721	0.0	-2.194	-1.371
19	2	2	40.992	43.252	-43.252	0.0	-2.260	-1.446
20	2	2	8.458	0.995	-0.995	0.0	7.463	1.578
21	2	2	18.729	21.059	-21.059	0.0	-2.260	-0.729
22	2	2	15.763	21.729	-21.729	0.0	-5.986	-1.650
23	2	2	11.512	2.196	-2.196	0.0	5.326	2.167
24	3	2	4.508	6.002	-6.002	0.0	-1.494	-0.200
25	3	2	7.165	3.714	-3.714	0.0	3.451	0.637
26	3	2	12.364	5.223	-5.223	0.0	7.141	2.009
10	3	2	8.428	11.882	-11.882	0.0	-3.454	-0.486
18	3	2	11.293	4.662	-4.662	0.0	5.631	1.431
16	3	2	10.469	6.952	-6.952	0.0	3.546	0.598
0	6	0	338.527	354.231	-354.231	0.0	-15.704	-2.598 *
15	3	2	14.274	16.506	-16.506	0.0	-2.232	-0.256
13	3	2	10.910	2.850	-2.850	0.0	8.061	2.439
11	3	2	6.137	7.528	-7.528	0.0	-1.390	-0.272
10	3	2	11.204	3.806	-3.806	0.0	7.398	2.387
9	3	2	21.136	17.140	-17.140	0.0	3.996	2.267
8	3	2	16.771	15.038	-15.038	0.0	1.734	0.776

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	3	2	11.777	6.538	-6.539	0.0	5.238	1.292
6	3	2	4.816	7.211	7.211	0.0	-2.396	-0.523
5	3	2	20.357	19.757	19.757	0.0	0.599	0.385
4	3	2	45.727	42.054	-42.054	0.0	3.673	2.660
3	3	2	38.604	37.310	-37.310	0.0	1.285	1.255
2	3	2	8.149	5.105	-5.105	0.0	3.044	1.074
1	4	2	31.093	32.025	32.025	0.0	-1.732	-1.401
2	4	2	67.618	69.049	69.049	0.0	-1.481	-1.202
3	4	2	36.202	36.930	-36.930	0.0	-0.728	-0.626
4	4	2	5.433	8.114	8.114	0.0	-2.681	-0.593
0	6	0	337.150	354.231	354.231	0.0	-17.076	-2.839 *
5	4	2	5.477	11.135	-11.135	0.0	-5.658	-1.137
6	4	2	32.037	30.448	-30.448	0.0	1.616	1.234
7	4	2	38.913	40.747	-40.747	0.0	-1.834	-1.430
8	4	2	11.263	0.777	-0.777	0.0	10.486	3.552 *
9	4	2	10.749	8.240	-8.240	0.0	2.508	0.739
10	4	2	17.080	16.896	-16.896	0.0	0.184	0.074
11	4	2	18.652	16.251	-16.251	0.0	2.411	0.933
12	4	2	16.463	9.108	-9.108	0.0	11.355	5.187 *
13	4	2	9.295	4.860	-4.860	0.0	4.435	1.198
14	4	2	26.930	20.503	-20.503	0.0	0.227	0.196
16	4	2	7.547	10.759	-10.759	0.0	-2.212	-0.647
17	4	2	19.034	19.793	-19.793	0.0	3.241	1.423
18	4	2	20.166	18.526	-18.526	0.0	1.640	0.672
19	4	2	13.862	9.868	-9.868	0.0	3.995	1.242
20	4	2	15.816	1.365	-1.365	0.0	14.451	5.405 *
21	4	2	13.124	0.232	-0.232	0.0	12.866	3.334 *
22	4	2	16.240	15.716	-15.716	0.0	5.523	1.269
0	6	0	337.936	354.231	354.231	0.0	-16.295	-2.707 *
24	5	2	9.207	3.557	-3.557	0.0	5.650	0.957
23	5	2	36.128	32.552	-32.552	0.0	3.576	1.990
22	5	2	18.987	18.985	-18.985	0.0	0.098	-0.031
21	5	2	28.547	28.285	-28.285	0.0	0.262	0.119
19	5	2	29.077	29.537	-29.537	0.0	-0.461	-0.234
18	5	2	15.772	4.011	-4.011	0.0	11.761	4.654 *
17	5	2	59.254	59.182	-59.182	0.0	0.072	0.047
16	5	2	25.091	24.606	-24.606	0.0	0.484	0.224
15	5	2	40.063	39.492	-39.492	0.0	0.571	0.408
14	5	2	7.724	1.848	-1.848	0.0	5.376	1.126
13	5	2	37.587	38.195	-38.195	0.0	-0.608	-0.393
12	5	2	77.406	78.175	-78.175	0.0	-0.768	-0.532
11	5	2	51.484	91.776	-91.776	0.0	-0.292	-0.100
10	5	2	21.671	23.192	-23.192	0.0	-1.321	-0.587
9	5	2	133.778	133.606	-133.606	0.0	0.133	0.079
8	5	2	81.164	81.159	-81.159	0.0	0.009	0.006
7	5	2	59.150	58.841	-58.841	0.0	0.310	0.223
6	5	2	22.224	20.428	-20.428	0.0	1.795	1.009
0	6	0	338.336	354.231	354.231	0.0	-15.865	-2.630 *
5	5	2	76.571	40.504	-40.504	0.0	3.054	-0.373
4	5	2	12.078	14.242	-14.242	0.0	-1.364	-0.471
3	5	2	129.014	131.374	-131.374	0.0	-2.360	-1.134
2	5	2	12.144	6.309	-6.309	0.0	2.835	1.005
1	5	2	63.997	65.467	-65.467	0.0	-1.471	-1.190

600C. CROTHOPOROSILITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	2	16.742	14.682	0.0	2.059	0.871	
1	6	2	31.001	33.193	33.103	0.0	-1.202	-0.736
2	6	2	121.017	126.726	0.0	-6.908	-2.410	
3	6	2	143.259	148.545	149.545	0.0	-6.287	-2.715
4	6	2	21.121	20.004	-20.004	0.0	1.118	0.543
5	6	2	107.584	105.533	-106.633	0.0	-2.049	-1.140
7	6	2	95.370	98.030	-98.030	0.0	-2.660	-1.596
8	6	2	14.091	14.146	14.146	0.0	0.745	0.267
9	6	2	120.973	120.977	120.977	0.0	-0.004	-0.002
10	6	2	33.124	30.503	30.503	0.0	2.621	1.855
11	6	2	93.779	91.833	91.833	0.0	1.066	1.179
12	6	2	12.702	6.739	-6.739	0.0	3.963	1.297
13	6	2	38.206	37.204	-37.204	0.0	1.002	0.635
14	6	2	14.438	12.331	12.331	0.0	2.207	0.763
0	6	0	340.245	354.231	354.231	0.0	-13.96	-2.301 *
15	6	2	51.029	52.707	-52.707	0.0	-1.678	-1.114
16	6	2	16.110	20.159	20.159	0.0	-4.039	-1.209
17	6	2	47.528	46.558	46.558	0.0	0.970	0.570
18	6	2	15.478	16.127	16.127	0.0	-0.649	-0.198
19	6	2	40.549	38.567	38.567	0.0	1.992	1.245
21	6	2	26.238	25.459	-25.459	0.0	0.735	0.322
22	6	2	48.059	47.876	47.876	0.0	0.193	0.104
23	6	2	58.069	62.261	-62.261	0.0	-4.191	-2.340
22	7	2	13.657	11.372	11.372	0.0	2.285	0.556
21	7	2	7.297	10.169	10.169	0.0	-2.872	-0.455
19	7	2	12.805	2.186	2.186	0.0	10.619	2.903 *
18	7	2	11.336	3.775	-3.775	0.0	7.561	1.826
16	7	2	21.018	19.119	-19.119	0.0	1.859	0.765
13	7	2	20.665	23.980	23.980	0.0	-3.314	-1.274
12	7	2	47.454	44.631	-44.631	0.0	2.823	2.056
0	6	0	339.061	354.231	354.231	0.0	-15.170	-2.508 *
11	7	2	19.034	17.185	-17.185	0.0	1.849	0.749
10	7	2	13.948	6.880	-6.880	0.0	6.968	2.420
9	7	2	17.418	12.399	12.399	0.0	5.019	2.262
8	7	2	65.594	48.022	-48.022	0.0	2.428	-1.750
7	7	2	31.814	32.521	-32.521	0.0	-0.707	-0.471
5	7	2	11.028	15.118	15.118	0.0	-4.090	-1.146
4	7	2	32.756	33.658	-33.658	0.0	0.902	-0.584
3	7	2	20.357	22.105	-22.105	0.0	-1.748	-0.838
2	7	2	14.274	5.716	-5.716	0.0	8.558	3.166
1	7	2	15.258	8.308	-8.308	0.0	6.650	2.458
0	8	2	8.663	2.942	2.942	0.0	5.721	1.381
1	8	2	47.498	48.318	48.318	0.0	-0.819	-0.603
2	8	2	17.726	17.890	17.890	0.0	-0.164	-0.067
3	8	2	30.799	31.901	31.901	0.0	-1.103	-0.630
5	8	2	35.613	34.035	-34.035	0.0	1.578	1.050
6	8	2	16.992	16.847	16.847	0.0	0.144	0.054
7	8	2	50.556	49.124	-49.124	0.0	1.432	1.042
8	8	2	10.939	11.188	11.188	0.0	-0.248	-0.067
0	6	0	337.061	354.231	354.231	0.0	-17.171	-2.856 *
9	8	2	30.799	30.166	30.166	0.0	0.632	0.358
10	8	2	11.013	1.727	-1.727	0.0	9.286	2.679
11	8	2	31.667	32.966	32.966	0.0	-1.299	-0.690

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	8	2	8.751	1.989	-1.889	0.0	6.862	1.584
13	8	2	36.556	35.272	-35.272	0.0	1.283	0.807
14	8	2	6.493	11.119	-11.119	0.0	-4.629	-0.759
15	8	2	24.120	25.293	-25.293	0.0	-1.173	-0.469
16	8	2	7.973	3.254	-3.254	0.0	4.710	0.462
17	9	2	10.117	10.001	-10.001	0.0	0.116	0.024
18	8	2	16.007	15.755	-15.755	0.0	0.252	0.074
19	8	2	28.753	22.330	-22.330	0.0	6.424	2.930
20	8	2	0.837	10.121	-10.121	0.0	-9.286	-0.873
21	8	2	13.172	14.128	-14.128	0.0	-0.956	-0.218
19	9	2	18.490	15.235	-15.235	0.0	3.256	1.119
17	9	2	17.829	8.734	-8.734	0.0	9.096	3.224
16	9	2	13.530	9.884	-9.884	0.0	3.655	0.975
15	9	2	5.374	6.075	-6.075	0.0	-0.701	-0.104
14	9	2	14.991	10.733	-10.733	0.0	4.157	1.204
13	9	2	15.155	8.584	-8.584	0.0	6.571	2.090
0	6	0	339.119	354.231	-354.231	0.0	-15.113	-24.498 *
12	9	2	7.253	6.445	-6.445	0.0	0.809	0.139
11	9	2	14.053	10.821	-10.821	0.0	3.232	1.005
0	0	2	11.791	7.614	-7.614	0.0	4.178	1.129
6	9	2	12.061	4.197	-4.197	0.0	7.845	2.473
3	0	2	10.308	9.014	-9.014	0.0	0.304	0.059
2	0	2	12.731	13.381	-13.381	0.0	-0.650	-0.185
0	10	2	3.304	4.811	-4.811	0.0	-1.507	-0.201
1	10	2	5.080	10.046	-10.046	0.0	-0.957	-0.202
2	10	2	20.738	28.786	-28.786	0.0	-0.048	-0.024
3	10	2	29.621	28.533	-28.533	0.0	1.088	0.582
5	10	2	11.380	14.885	-14.885	0.0	-2.504	-0.874
6	10	2	14.641	16.961	-16.961	0.0	-2.320	-0.696
7	10	2	13.671	8.300	-8.300	0.0	5.371	1.625
0	6	0	338.051	354.231	-354.231	0.0	-16.181	-24.679 *
8	10	2	11.894	12.089	-12.089	0.0	-0.195	-0.047
10	10	2	13.163	2.275	-2.275	0.0	10.868	3.122 *
11	10	2	19.240	20.368	-20.368	0.0	-1.126	-0.366
13	10	2	13.490	12.021	-12.021	0.0	1.456	0.399
15	10	2	18.828	14.589	-14.589	0.0	4.239	1.628
16	10	2	6.769	3.348	-3.348	0.0	3.421	0.534
17	10	2	17.817	18.677	-18.677	0.0	-0.760	-0.234
14	11	2	0.735	8.513	-8.513	0.0	1.222	0.240
13	11	2	15.494	10.763	-10.763	0.0	4.921	1.469
12	11	2	40.505	41.236	-41.236	0.0	-0.731	-0.352
11	11	2	41.021	41.704	-41.704	0.0	-0.773	-0.397
10	11	2	15.082	9.725	-9.725	0.0	5.327	1.433
9	11	2	61.730	60.523	-60.523	0.0	0.717	0.426
8	11	2	36.477	33.878	-33.878	0.0	2.898	1.525
7	11	2	29.224	31.440	-31.440	0.0	-2.216	-0.947
5	11	2	42.437	41.052	-41.052	0.0	0.484	0.286
0	6	0	339.710	354.231	-354.231	0.0	-14.521	-24.291 *
4	11	2	7.430	1.031	-1.031	0.0	6.397	1.117
3	11	2	45.609	47.560	-47.560	0.0	-1.921	-1.039
2	11	2	9.997	9.680	-9.680	0.0	-0.723	-0.146
1	11	2	22.429	19.572	-19.572	0.0	2.876	1.143
0	12	2	7.518	3.775	-3.775	0.0	3.743	0.639

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DETA F	DETA/SIGMA
1	12	2	3.817	3.792	0.0	0.026	0.003	
2	12	2	40.608	39.092	-39.092	0.0	1.516	0.843
3	12	2	37.661	38.131	38.131	0.0	-0.471	-0.237
4	12	2	2.458	8.731	-8.731	0.0	-6.073	-0.677
5	12	2	24.650	17.909	-17.909	0.0	6.741	2.957
7	12	2	16.139	9.693	-9.693	0.0	6.447	1.950
9	12	2	27.106	25.714	25.714	0.0	1.392	0.553
10	12	2	9.177	7.430	7.430	0.0	1.740	0.312
2	13	2	14.259	5.536	-5.536	0.0	8.723	2.404
1	13	2	24.635	19.150	-19.150	0.0	5.485	2.220
0	12	3	16.595	14.374	-14.374	0.0	2.221	0.617
1	12	3	11.644	6.722	-6.722	0.0	4.523	1.132
0	6	0	338.317	354.231	354.231	0.0	-15.914	-2.634 *
3	12	3	13.099	5.205	5.295	0.0	7.804	1.975
5	12	3	10.558	3.918	3.918	0.0	6.630	1.395
12	11	3	16.610	4.825	-4.825	0.0	11.785	3.875 *
11	11	3	3.524	10.431	-10.431	0.0	-6.908	-0.769
10	11	3	28.989	30.459	-30.459	0.0	-1.471	-0.581
9	11	3	17.447	13.663	13.663	0.0	3.764	1.170
7	11	3	15.566	10.352	10.392	0.0	5.174	1.455
6	11	3	4.801	14.286	14.286	0.0	-9.485	-1.169
5	11	3	11.233	17.927	-17.927	0.0	-6.693	-1.348
4	11	3	12.247	4.029	4.029	0.0	8.217	2.135
3	11	3	19.769	16.755	-16.755	0.0	3.014	1.121
2	11	3	33.860	33.084	-33.084	0.0	0.777	0.371
1	11	3	10.014	8.318	8.318	0.0	1.697	0.348
0	10	3	20.239	15.404	-15.404	0.0	4.835	1.947
1	10	3	4.500	7.160	7.160	0.0	-2.652	-0.367
0	6	0	338.508	354.231	354.231	0.0	-15.723	-2.601 *
2	10	3	8.531	2.947	2.947	0.0	5.584	1.156
3	10	3	25.179	25.984	25.984	0.0	-0.805	-0.332
4	10	3	36.158	36.943	-36.943	0.0	-0.785	-0.407
7	10	3	5.154	5.221	-5.221	0.0	-0.057	-0.010
8	10	3	0.221	2.564	-2.564	0.0	6.658	1.378
9	10	3	11.380	11.595	11.595	0.0	-0.215	-0.049
11	10	3	12.364	16.390	-16.390	0.0	-4.026	-0.838
12	10	3	8.957	2.499	-2.499	0.0	6.458	1.242
14	10	3	13.892	2.549	2.549	0.0	11.342	3.028 *
15	10	3	13.334	5.226	-5.226	0.0	8.107	1.978
17	9	3	11.454	9.078	9.078	0.0	2.375	0.504
15	9	3	16.477	10.733	10.733	0.0	-2.256	-0.602
14	9	3	85.451	84.937	84.937	0.0	0.515	0.297
13	9	3	44.959	41.736	-41.736	0.0	3.223	1.986
0	6	0	330.405	354.231	354.231	0.0	-14.827	-2.442 *
11	9	3	6.270	8.586	-8.586	0.0	-2.316	-0.358
10	9	3	4.405	14.456	14.456	0.0	-10.051	-1.270 *
8	9	3	10.455	1.625	-1.625	0.0	8.830	2.140
7	9	3	21.489	23.766	23.766	0.0	-2.278	-0.824
6	9	3	62.900	62.064	62.064	0.0	0.835	0.542
5	9	3	18.696	16.963	-16.963	0.0	1.733	0.655
4	9	3	3.661	1.289	1.289	0.0	2.352	0.322
3	9	3	8.169	7.637	-7.637	0.0	0.513	0.104
2	9	3	60.780	61.131	-61.131	0.0	-0.351	-0.240

600C_ERTHOFFERROSILITE_6/28/73					STRUCTURE FACTORS		PAGE 14		
H	K	L	F(HKL)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DFIT/A/SIGMA	68
1	9	3	54.666	53.510	53.510	0.0	1.156	0.797	
0	8	3	136.450	139.254	139.254	0.0	-2.804	-1.241	
1	8	3	52.093	51.854	51.854	0.0	0.230	0.176	
2	8	3	10.499	9.388	-9.388	0.0	1.111	0.290	
3	8	3	24.517	23.819	23.819	0.0	0.698	0.354	
4	8	3	27.576	27.746	-27.746	0.0	-0.170	-0.090	
5	8	3	26.870	26.691	26.691	0.0	0.179	0.090	
7	8	3	52.270	50.847	-50.847	0.0	1.423	0.943	
8	8	2	65.154	64.553	64.553	0.0	0.602	0.409	
0	6	0	340.551	354.231	354.231	0.0	-13.683	-2.250 *	
9	8	3	10.073	6.581	6.581	0.0	3.492	0.655	
11	8	3	15.660	6.799	-6.799	0.0	9.061	3.281	
12	8	3	52.255	51.669	-51.669	0.0	0.587	0.367	
13	8	3	33.831	34.626	-34.626	0.0	-0.795	-0.397	
14	8	3	8.296	5.568	-5.568	0.0	2.728	0.503	
15	8	3	34.494	32.583	-32.583	0.0	1.910	1.006	
16	8	3	30.431	28.141	28.141	0.0	2.289	1.152	
18	8	3	4.566	2.091	-2.091	0.0	2.476	0.320	
19	8	3	35.628	34.705	34.705	0.0	0.922	0.429	
21	7	3	11.982	2.744	2.744	0.0	9.230	1.184	
19	7	3	5.506	9.071	-9.071	0.0	-3.565	-0.490	
14	7	3	42.628	43.627	-43.627	0.0	-0.909	-0.616	
13	7	3	18.285	19.308	19.308	0.0	-1.023	-0.338	
0	6	0	340.112	354.231	354.231	0.0	-14.120	-2.323 *	
12	7	3	3.318	5.586	-5.586	0.0	-2.268	-0.302	
11	7	3	0.001	3.657	-3.657	0.0	5.344	1.238	
10	7	3	22.580	21.838	-21.838	0.0	1.150	0.518	
9	7	3	14.479	10.102	10.102	0.0	4.377	1.713	
8	7	3	16.830	11.919	11.919	0.0	4.910	1.978	
7	7	3	10.631	15.006	-15.006	0.0	-4.375	-1.028	
6	7	3	31.667	32.883	-32.883	0.0	-1.216	-0.604	
5	7	3	10.763	8.502	-8.502	0.0	2.261	0.611	
4	7	3	8.369	14.488	-14.488	0.0	-6.119	-1.243	
3	7	3	4.302	6.470	-6.470	0.0	-2.168	-0.334	
2	7	3	6.675	6.872	-6.872	0.0	-0.396	-0.081	
1	7	3	12.746	14.856	-14.856	0.0	-2.109	-0.659	
0	6	3	10.381	2.422	2.422	0.0	7.960	2.212	
1	6	3	8.135	1.808	1.808	0.0	6.326	1.465	
2	6	3	9.559	15.441	15.441	0.0	-5.882	-1.396	
5	6	3	6.013	8.945	8.945	0.0	-2.132	-0.436	
7	6	3	5.506	5.815	5.815	0.0	-0.309	-0.055	
0	6	0	330.908	354.231	354.231	0.0	-15.323	-2.534 *	
8	6	3	24.468	29.135	-29.135	0.0	-4.648	-2.136	
9	6	3	3.904	11.097	-11.097	0.0	-7.103	-1.073	
10	6	3	6.593	5.313	-5.313	0.0	1.280	0.247	
11	6	3	6.960	1.215	-1.215	0.0	5.745	1.168	
17	6	3	11.879	0.915	0.915	0.0	10.964	2.657 *	
18	6	3	8.359	5.605	5.605	0.0	2.704	0.528	
20	6	3	21.386	14.318	14.318	0.0	7.068	2.914	
21	5	3	5.902	10.218	10.218	0.0	-4.315	-0.605	
23	5	3	7.209	4.678	4.678	0.0	2.732	0.420	
22	5	3	15.787	14.191	14.191	0.0	1.596	0.421	
21	5	3	8.883	9.504	-9.504	0.0	-0.421	-0.110	

STRUCTURE FACTORS						PAGE 15			
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DETA F	DETA/SIGMA	69
20	5	3	1.067	2.044	2.044	0.0	-0.076	-0.095	
19	5	3	11.556	2.310	2.310	0.0	9.239	2.253	
0	6	0	339.386	354.231	354.231	0.0	-14.866	-2.445 *	
18	5	3	29.003	27.913	27.913	0.0	1.090	0.404	
17	5	3	29.165	32.201	32.201	0.0	-3.116	-1.513	
16	5	3	13.701	8.112	8.112	0.0	5.585	1.745	
15	5	3	23.003	20.785	20.785	0.0	2.218	1.085	
14	5	3	24.900	27.514	27.514	0.0	-0.614	-0.309	
13	5	3	13.995	14.018	14.018	0.0	-0.023	-0.007	
12	5	3	8.737	0.609	0.609	0.0	8.127	1.915	
11	5	3	22.559	21.253	21.253	0.0	1.706	0.359	
10	5	3	61.017	60.199	60.199	0.0	0.810	0.606	
9	5	3	23.576	28.332	28.332	0.0	-4.756	-2.231	
5	5	3	37.052	37.006	37.006	0.0	0.036	0.024	
4	5	3	5.021	7.940	7.940	0.0	-2.918	-0.471	
3	5	3	39.532	41.297	41.297	0.0	-1.764	-1.197	
2	5	3	83.031	86.472	86.472	0.0	-2.442	-2.304	
1	5	3	28.753	33.089	33.089	0.0	-4.335	-2.320	
0	4	3	134.530	147.403	147.403	0.0	-12.873	-5.906 *	
1	4	3	34.502	36.569	36.569	0.0	-1.987	-1.405	
0	0	0	338.013	354.231	354.231	0.0	-16.219	-2.694 *	
2	4	3	10.073	8.648	8.648	0.0	1.425	0.391	
3	4	3	18.211	20.720	20.720	0.0	-2.518	-1.026	
4	4	3	33.019	34.675	34.675	0.0	-0.556	-0.367	
5	4	3	6.784	14.214	14.214	0.0	-7.430	-1.454	
6	4	3	11.258	5.770	5.770	0.0	5.478	1.622	
7	4	3	23.106	24.782	24.782	0.0	-1.676	0.803	
8	4	3	19.666	20.932	20.932	0.0	-1.266	0.522	
9	4	3	11.336	15.431	15.431	0.0	-4.095	-1.133	
10	4	3	21.020	19.918	19.918	0.0	2.012	1.069	
11	4	3	8.355	11.724	11.724	0.0	-3.369	-0.783	
12	4	3	47.631	48.110	48.110	0.0	-0.479	-0.349	
13	4	3	31.770	31.406	31.406	0.0	0.364	0.213	
14	4	3	11.057	7.518	7.518	0.0	3.539	0.964	
15	4	3	13.745	18.184	18.184	0.0	-4.439	-1.256	
16	4	3	9.486	2.320	2.320	0.0	7.266	1.724	
18	4	3	10.851	3.239	3.239	0.0	7.612	1.934	
19	4	3	11.586	11.645	11.645	0.0	-0.059	-0.014	
20	4	3	42.112	42.813	42.813	0.0	-0.701	-0.393	
21	4	3	11.351	7.771	7.771	0.0	3.580	0.779	
0	6	0	339.023	354.231	354.231	0.0	-15.208	-2.514 *	
22	4	3	12.731	0.054	0.054	0.0	3.673	0.839	
23	4	3	15.082	16.196	16.196	0.0	-1.114	-0.286	
24	4	3	17.330	19.200	19.200	0.0	-1.071	-0.511	
23	3	2	14.788	3.553	3.553	0.0	11.235	3.071 *	
22	3	3	36.423	35.795	35.795	0.0	0.628	0.364	
21	3	3	51.649	52.667	52.667	0.0	-1.017	-0.538	
19	3	3	37.764	38.323	38.323	0.0	-0.560	-0.311	
18	3	3	76.408	76.059	76.059	0.0	0.349	0.221	
17	3	3	36.791	34.908	34.908	0.0	1.884	1.184	
16	3	3	14.714	12.795	12.795	0.0	1.920	0.628	
15	3	3	44.738	43.008	43.008	0.0	1.731	1.185	
14	3	3	172.425	171.096	171.096	0.0	1.329	0.470	

STRUCTURE FACTORS								PAGE 16
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
13	3	3	89.521	89.639	-90.630	0.0	-0.117	-0.072
12	2	3	22.856	19.591	-19.591	0.0	3.264	1.657
11	3	3	30.607	30.793	-30.793	0.0	-0.186	-0.118
10	3	3	11.204	6.792	-6.792	0.0	4.412	1.216
9	3	3	30.386	31.978	-31.978	0.0	-1.592	-0.933
8	2	3	2.091	0.416	-0.416	0.0	-6.375	-0.403
0	6	0	339.851	354.231	-354.231	0.0	-15.380	-2.543 *
7	3	3	69.207	69.660	-69.660	0.0	-0.363	-0.263
6	2	3	189.874	189.775	-189.775	0.0	0.099	0.032
5	3	3	79.434	78.698	-78.698	0.0	0.736	0.514
4	3	3	17.578	21.921	-21.921	0.0	-2.343	-1.070
3	3	3	40.933	42.294	-42.294	0.0	-1.372	-1.038
2	3	3	178.120	182.492	-182.492	0.0	-4.382	-1.923
1	3	3	140.222	146.541	-146.541	0.0	-6.058	-2.693
0	2	3	234.156	259.722	-259.722	0.0	-25.566	-6.653 *
1	2	3	87.680	90.609	-90.609	0.0	-2.929	-1.998
2	2	3	4.302	4.689	-4.689	0.0	-0.387	-0.074
3	2	3	27.209	27.928	-27.928	0.0	-0.720	-0.470
4	2	3	26.723	26.990	-26.990	0.0	-0.267	-0.173
5	2	3	36.747	36.064	-36.064	0.0	0.217	-0.150
6	2	3	10.508	9.440	-9.440	0.0	0.468	0.251
7	2	3	65.933	63.017	-63.017	0.0	2.686	2.081
8	2	3	73.401	71.441	-71.441	0.0	1.050	1.416
9	2	3	11.223	0.232	-0.232	0.0	11.001	3.285 *
10	2	3	17.592	16.700	-16.700	0.0	1.232	0.485
11	2	3	11.615	7.601	-7.601	0.0	4.014	1.168
12	2	3	50.544	90.300	-90.300	0.0	0.644	0.406
0	6	0	339.908	354.231	-354.231	0.0	-15.123	-2.601 *
13	2	3	55.642	55.991	-55.991	0.0	-0.344	-0.262
14	2	3	12.760	9.694	-9.694	0.0	4.064	1.445
15	2	3	4.037	46.039	-46.039	0.0	-0.002	-0.002
16	2	3	31.225	35.816	-35.816	0.0	-4.591	-2.204
17	2	3	16.301	11.778	-11.778	0.0	4.523	1.664
19	2	3	35.687	37.049	-37.049	0.0	-2.153	-1.204
20	2	3	81.194	80.339	-80.339	0.0	0.856	0.521
21	2	3	10.470	16.107	-16.107	0.0	-5.727	-1.171
23	2	3	11.835	5.034	-5.034	0.0	6.012	1.565
24	2	3	14.494	10.078	-10.078	0.0	4.416	1.134
25	1	3	15.260	10.327	-10.327	0.0	2.933	0.756
24	1	3	14.171	10.469	-10.469	0.0	3.702	0.951
23	1	3	14.068	0.380	-0.380	0.0	13.688	4.087 *
22	1	3	13.157	7.536	-7.536	0.0	5.621	1.450
21	1	3	8.560	6.817	-6.817	0.0	1.744	0.344
20	1	3	15.082	3.558	-3.558	0.0	11.524	3.845 *
19	1	3	7.694	8.225	-8.225	0.0	-0.331	-0.103
0	6	0	339.165	354.231	-354.231	0.0	-16.066	-2.659 *
18	1	3	23.973	23.003	-23.003	0.0	0.910	0.455
17	1	3	31.667	32.349	-32.349	0.0	-0.682	-0.396
16	1	3	6.093	6.215	-6.215	0.0	-0.122	-0.022
15	1	3	17.261	9.849	-9.849	0.0	7.393	3.145
14	1	3	12.937	10.017	-10.017	0.0	2.920	0.951
13	1	3	7.136	2.532	-2.532	0.0	4.604	1.028
11	1	3	19.181	17.310	-17.310	0.0	1.871	0.806

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	7/
10	1	3	57.847	56.425	-56.425	0.0	1.423	1.080	
9	1	3	29.230	29.420	29.420	0.0	-0.182	-0.110	
8	1	3	8.046	8.328	8.328	0.0	-0.281	-0.066	
7	1	2	16.169	15.128	-15.128	0.0	1.041	0.416	
6	1	3	30.195	29.864	-29.864	0.0	0.331	0.232	
5	1	2	42.098	40.217	-40.217	0.0	1.480	1.634	
3	1	3	32.874	35.103	-35.103	0.0	-2.226	-1.761	
2	1	3	65.688	65.347	-65.347	0.0	0.241	0.280	
1	1	3	15.695	23.480	-23.480	0.0	-3.714	-2.093	
0	0	4	132.567	131.624	-131.624	0.0	0.963	0.439	
1	0	4	75.931	75.968	-75.968	0.0	-0.037	-0.026	
0	6	0	337.689	354.231	-354.231	0.0	-1.652	-2.749 *	
2	0	4	40.770	41.365	-41.365	0.0	-0.595	-0.434	
3	0	4	93.224	92.942	-92.942	0.0	0.281	0.174	
4	0	4	205.307	198.971	-198.971	0.0	6.336	1.893	
5	0	4	71.652	71.558	-71.558	0.0	-0.106	-0.076	
6	0	4	7.797	10.973	-10.973	0.0	-3.177	-0.644	
7	0	4	69.713	70.414	-70.414	0.0	-0.701	-0.407	
8	0	4	151.388	151.029	-151.029	0.0	0.358	0.145	
9	0	4	9.663	12.107	-12.107	0.0	-3.443	-0.803	
10	0	4	26.458	27.985	-27.985	0.0	3.473	1.984	
11	0	4	51.014	50.719	-50.719	0.0	0.295	0.222	
12	0	4	121.263	119.754	-119.754	0.0	1.508	0.745	
13	0	4	50.984	50.256	-50.256	0.0	0.729	0.503	
14	0	4	9.632	7.601	-7.601	0.0	2.031	0.482	
15	0	4	22.856	18.641	-18.641	0.0	4.214	2.033	
16	0	4	104.007	104.548	-104.548	0.0	-0.560	-2.289	
17	0	4	26.002	29.717	-29.717	0.0	-2.715	-1.14	
18	0	4	24.120	22.610	-23.610	0.0	0.510	0.221	
19	0	4	8.544	8.104	-8.104	0.0	1.440	0.303	
20	0	4	44.945	45.005	-45.005	0.0	-0.060	-0.026	
21	0	4	12.570	15.622	-15.622	0.0	-3.063	-0.622	
0	6	0	340.245	354.231	-354.231	0.0	-13.966	-2.301 *	
22	0	4	11.762	6.899	-6.899	0.0	4.863	1.086	
23	0	4	25.047	26.584	-26.584	0.0	-1.538	-0.231	
23	1	4	16.801	8.473	-8.473	0.0	8.328	2.625	
22	1	4	38.442	35.272	-35.272	0.0	3.170	1.421	
21	1	4	15.978	11.952	-11.952	0.0	4.026	1.176	
20	1	4	9.295	3.231	-3.231	0.0	6.064	1.225	
19	1	4	17.300	17.144	-17.144	0.0	0.156	0.047	
18	1	4	36.187	35.905	-35.905	0.0	0.282	0.162	
17	1	4	6.402	5.664	-5.664	0.0	0.738	0.125	
16	1	4	13.245	10.334	-10.334	0.0	2.911	0.901	
15	1	4	15.713	15.847	-15.847	0.0	-0.134	-0.042	
14	1	4	17.888	13.237	-13.237	0.0	4.651	1.942	
13	1	4	6.501	1.472	-1.472	0.0	5.029	1.024	
12	1	4	24.135	24.738	-24.738	0.0	-0.603	-0.277	
11	1	4	74.919	74.799	-74.799	0.0	0.119	0.081	
10	1	4	89.731	86.956	-86.956	0.0	2.775	1.532	
9	1	4	35.878	37.659	-37.659	0.0	-1.781	-1.130	
8	1	4	19.225	20.882	-20.882	0.0	-1.657	-0.683	
7	1	4	33.227	33.335	-33.335	0.0	-0.108	-0.059	
6	1	4	53.749	53.294	-53.294	0.0	0.455	0.394	

STRUCTURE FACTORS							PAGE 1A		
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTAF/SIGMA	72
0	6	0	336.566	354.231	354.231	0.0	-17.666	-2.949 *	
5	1	4	34.214	35.577	35.577	0.0	-1.363	-0.865	
4	1	4	9.588	7.974	7.974	0.0	1.615	0.403	
2	1	4	62.440	61.847	61.847	0.0	0.592	0.449	
1	1	4	76.915	81.459	81.459	0.0	-4.545	-3.211	
0	2	4	67.069	72.017	72.017	0.0	-5.948	-3.622	
1	2	4	41.021	46.320	46.320	0.0	-4.399	-3.013	
2	2	4	12.276	10.418	10.418	0.0	1.858	0.572	
3	2	4	10.225	5.125	5.125	0.0	5.110	1.333	
4	2	4	39.591	38.422	38.422	0.0	1.169	0.785	
5	2	4	49.714	49.860	49.860	0.0	-0.147	-0.112	
6	2	4	7.474	6.719	6.719	0.0	0.755	0.153	
7	2	4	22.547	21.872	21.872	0.0	0.675	0.338	
8	2	4	27.424	45.394	45.394	0.0	2.031	1.545	
9	2	4	16.198	15.270	15.270	0.0	0.925	0.361	
10	2	4	9.721	11.096	11.096	0.0	-1.375	-0.347	
11	2	4	14.685	8.142	8.142	0.0	6.543	2.434	
12	2	4	37.307	36.654	36.654	0.0	0.613	0.380	
13	2	4	17.555	18.457	18.457	0.0	-0.892	-0.330	
14	2	4	17.491	18.677	18.677	0.0	-1.186	-0.436	
0	6	0	338.146	354.231	354.231	0.0	-16.685	-2.463 *	
15	2	4	7.767	11.090	11.090	0.0	-3.323	-0.625	
16	2	4	22.488	19.525	19.525	0.0	2.963	1.344	
18	2	4	5.330	0.011	0.011	0.0	5.310	0.900	
20	2	4	27.450	26.863	26.863	0.0	0.787	0.347	
21	2	4	7.679	8.246	8.246	0.0	-0.566	-0.003	
23	2	4	7.063	6.753	6.753	0.0	0.306	0.048	
22	3	4	3.832	3.330	3.330	0.0	0.502	0.059	
21	3	4	10.984	6.342	6.342	0.0	4.642	0.958	
20	3	4	10.249	24.408	24.408	0.0	7.841	1.674	
19	3	4	7.635	7.820	7.820	0.0	-0.185	-0.033	
17	3	4	8.648	4.932	4.932	0.0	3.716	0.758	
15	3	4	21.004	15.359	15.359	0.0	5.644	2.526	
14	3	4	11.101	4.089	4.089	0.0	7.012	1.033	
13	3	4	7.018	11.077	11.077	0.0	-4.059	-0.764	
0	6	0	337.117	354.231	354.231	0.0	-17.114	-2.846 *	
9	3	4	20.122	14.861	14.861	0.0	5.260	2.521	
7	3	4	21.033	22.909	22.909	0.0	-1.876	-0.905	
6	3	4	4.082	0.426	0.426	0.0	3.656	0.587	
4	3	4	4.977	0.164	0.164	0.0	4.814	0.822	
3	3	4	12.629	2.296	2.296	0.0	10.332	3.303 *	
2	3	4	4.816	7.546	7.546	0.0	-2.730	-0.443	
1	3	4	11.777	16.621	16.621	0.0	-4.844	-1.341	
0	4	4	34.273	38.319	38.319	0.0	-4.047	-2.544	
1	4	4	9.794	4.370	4.370	0.0	5.624	1.415	
2	4	4	7.591	10.371	10.371	0.0	-2.780	-0.609	
3	4	4	9.809	11.819	11.819	0.0	-2.010	-0.516	
4	4	4	4.684	10.123	10.123	0.0	-5.440	-0.910	
5	4	4	34.685	33.067	33.067	0.0	1.618	1.121	
7	4	4	15.302	9.146	9.146	0.0	6.156	2.524	
8	4	4	11.053	1.271	1.271	0.0	10.682	3.306 *	
0	6	0	337.117	354.231	354.231	0.0	-17.114	-2.846 *	
9	4	4	31.711	30.692	30.692	0.0	1.019	0.613	

STRUCTURE FACTORS								PAGE 19
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DFIT/A/SIGMA
10	4	4	9.911	8.795	-8.795	0.0	1.116	0.270
12	4	4	17.403	11.193	11.193	0.0	6.210	2.443
13	4	4	17.648	16.246	16.246	0.0	1.472	0.515
15	4	4	28.709	29.059	29.059	0.0	-0.350	-0.161
19	4	4	20.857	20.753	20.753	0.0	0.103	0.034
20	4	4	7.151	4.828	4.828	0.0	2.323	0.270
21	4	4	17.579	24.284	-24.284	0.0	-6.705	-1.709
22	4	4	15.963	10.708	10.708	0.0	5.255	1.542
21	5	4	20.136	26.115	26.115	0.0	-5.078	-1.621
14	5	4	31.579	28.774	28.774	0.0	2.804	1.361
15	5	4	40.160	46.005	-46.005	0.0	0.135	0.070
17	5	4	7.738	11.512	-11.512	0.0	-3.774	-0.666
16	5	4	11.409	3.150	-3.150	0.0	8.260	2.023
0	6	0	337.679	354.231	354.231	0.0	-16.352	-2.716 *
5	6	4	17.374	24.864	24.864	0.0	-7.470	-2.163
15	5	6	39.429	39.060	39.060	0.0	0.361	0.225
14	5	4	30.372	31.091	-31.091	0.0	-0.719	-0.352
13	5	4	27.635	27.983	-27.983	0.0	-0.348	-0.167
12	5	4	69.074	67.810	67.810	0.0	1.264	0.834
11	5	4	105.274	104.601	-104.601	0.0	0.673	0.366
10	5	4	39.421	41.057	-41.057	0.0	-1.437	-0.911
8	5	4	14.474	14.074	-14.074	0.0	0.200	0.063
5	5	4	70.723	70.591	70.591	0.0	-0.268	-0.186
4	5	4	4.904	5.684	-5.684	0.0	-0.780	-0.135
3	5	4	20.004	19.185	-19.185	0.0	0.819	0.382
2	5	4	88.452	92.435	-92.435	0.0	-3.403	-2.174
1	5	4	45.860	47.288	-47.288	0.0	-1.428	-1.030
0	6	4	62.618	63.210	-63.210	0.0	-0.592	-0.420
1	6	4	27.400	26.385	-26.385	0.0	1.515	0.831
2	6	4	29.783	27.054	-27.054	0.0	2.729	1.801
3	6	4	51.546	54.087	-54.087	0.0	-2.541	-1.949
4	6	4	116.175	118.166	118.166	0.0	0.009	0.004
0	6	0	336.984	354.231	354.231	0.0	-17.247	-2.869 *
5	6	4	38.515	41.382	-41.382	0.0	-2.867	-1.721
6	6	4	10.425	9.178	9.178	0.0	1.248	0.318
7	6	4	25.738	22.956	-22.956	0.0	2.782	-1.513
8	6	4	88.460	88.460	-88.460	0.0	-0.914	-0.556
9	6	4	3.465	12.825	-12.825	0.0	-9.360	-1.260
10	6	4	13.025	12.704	-12.704	0.0	0.321	0.087
11	6	4	20.063	22.098	-22.098	0.0	-2.035	-0.689
12	6	4	69.272	67.105	67.105	0.0	1.166	0.748
13	6	4	45.550	48.286	-48.286	0.0	-2.737	-1.545
14	6	4	13.818	2.925	-2.925	0.0	10.893	3.281 *
15	6	4	26.002	24.389	-24.389	0.0	1.614	0.694
16	6	4	66.282	66.163	-66.163	0.0	0.119	0.073
17	6	4	24.164	23.501	-23.501	0.0	0.664	0.255
18	6	4	21.106	16.741	-16.741	0.0	4.366	1.661
20	6	4	29.283	28.804	28.804	0.0	0.479	0.231
18	7	4	4.992	0.606	0.606	0.0	4.386	0.573
16	7	4	16.389	12.020	12.020	0.0	4.369	1.214
15	7	4	35.731	33.864	-33.864	0.0	1.867	1.047
0	6	0	336.737	354.231	354.231	0.0	-17.494	-2.911 *
14	7	4	12.305	16.298	16.298	0.0	-3.992	-0.834

STRUCTURE FACTORS								PAGE 20
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	7	4	11.821	11.274	0.0	0.0	0.547	0.126
11	7	4	32.742	35.990	-35.990	0.0	-3.249	-1.532
10	7	4	22.444	17.681	17.681	0.0	4.753	2.113
9	7	4	24.223	25.773	25.773	0.0	-1.550	-0.613
8	7	4	7.283	15.029	15.029	0.0	-7.746	-1.339
7	7	4	11.454	-0.234	0.234	0.0	11.220	3.068 *
5	7	4	6.475	13.993	13.993	0.0	-7.518	-1.306
3	7	4	13.951	15.937	15.937	0.0	-1.986	-0.585
2	7	4	11.101	-2.105	-2.105	0.0	8.986	2.440
1	7	4	23.282	22.993	22.993	0.0	0.289	0.141
0	8	4	50.910	50.572	-50.572	0.0	0.339	0.216
1	8	4	8.575	5.079	5.079	0.0	3.496	0.746
2	8	4	10.146	3.657	-3.657	0.0	6.490	1.578
3	8	4	13.745	13.785	13.785	0.0	-0.040	-0.011
4	8	4	35.508	35.082	35.082	0.0	0.826	0.501
5	8	4	14.303	15.595	15.595	0.0	-1.282	-0.375
0	6	0	337.632	354.231	354.231	0.0	-16.600	-2.758 *
7	8	4	6.108	3.915	-3.915	0.0	2.153	0.366
8	8	4	30.871	37.282	-37.282	0.0	2.589	1.527
9	8	4	27.841	27.895	27.895	0.0	-0.054	-0.026
10	8	4	13.804	6.972	-6.972	0.0	6.452	1.971
11	8	4	8.830	1.124	-1.124	0.0	7.715	1.510
12	8	4	33.257	33.007	33.007	0.0	0.250	0.120
16	8	4	18.990	21.435	-21.435	0.0	-2.445	-0.705
15	9	4	4.963	1.338	-1.338	0.0	3.625	0.472
13	9	4	8.751	5.082	-5.082	0.0	3.669	0.654
10	9	4	10.631	10.848	10.848	0.0	-0.217	-0.044
9	9	4	13.378	17.248	17.248	0.0	-3.870	-0.902
0	6	0	337.727	354.231	354.231	0.0	-16.505	-2.742 *
7	9	4	6.813	2.815	-2.815	0.0	3.998	0.612
6	9	4	10.749	5.303	-5.303	0.0	5.446	1.204
4	9	4	5.785	3.159	-3.159	0.0	2.626	0.405
2	9	4	11.101	10.583	-10.583	0.0	0.518	0.119
0	10	4	16.712	1.807	-1.807	0.0	14.905	5.068 *
1	10	4	2.966	14.430	14.430	0.0	-11.465	-1.249 *
3	10	4	23.650	20.716	-20.716	0.0	2.934	1.217
4	10	4	25.414	24.660	-24.660	0.0	0.754	0.322
5	10	4	16.345	16.878	16.878	0.0	-0.533	-0.149
8	10	4	21.180	16.481	-16.481	0.0	4.699	1.903
9	10	4	10.675	3.762	-3.762	0.0	6.913	1.499
11	10	4	18.138	6.024	-6.024	0.0	12.114	4.081 *
12	10	4	11.307	8.522	-8.522	0.0	2.784	0.612
0	6	0	337.536	354.231	354.231	0.0	-16.695	-2.775 *
7	11	4	12.041	7.114	-7.114	0.0	4.927	1.096
6	11	4	31.726	31.703	31.703	0.0	0.023	0.010
5	11	4	10.690	6.859	-6.859	0.0	3.831	0.741
3	11	4	15.866	0.143	-0.143	0.0	15.703	4.793 *
2	11	4	44.487	43.604	-43.604	0.0	0.883	0.483
1	11	4	23.297	23.010	-23.010	0.0	0.287	0.102
0	10	5	17.300	14.087	-14.087	0.0	3.213	1.056
1	10	5	3.010	5.192	-5.192	0.0	-2.182	-0.244
2	10	5	28.959	25.148	-25.148	0.0	3.811	1.799
3	10	5	8.766	7.349	-7.349	0.0	1.417	0.269

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H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA
5	10	5	14.171	13.453	-13.453	0.0	0.718	0.167
6	10	5	16.974	6.290	0.290	0.0	0.784	2.717
10	9	5	26.164	27.316	27.316	0.0	-1.152	-0.433
9	9	5	37.970	38.162	28.102	0.0	-0.212	-0.046
8	9	5	34.435	32.910	-32.910	0.0	1.525	0.724
7	9	5	26.797	23.959	23.959	0.0	2.838	1.434
6	9	5	9.695	16.981	-16.981	0.0	5.996	-1.196
0	6	0	336.756	354.231	354.231	0.0	-17.475	-2.917 *
5	0	5	36.759	36.339	-36.339	0.0	-1.580	-0.740
3	9	5	45.948	45.512	-45.512	0.0	0.436	0.246
2	9	5	17.800	16.729	16.729	0.0	1.070	0.315
1	9	5	2.702	0.254	-0.254	0.0	2.447	0.280
0	8	5	5.691	12.604	-12.604	0.0	-6.814	-0.921
1	8	5	23.326	26.953	26.953	0.0	-3.626	-1.239
2	8	5	48.104	48.822	-48.822	0.0	-0.718	-0.446
3	8	5	39.146	43.602	43.602	0.0	-4.543	-2.218
4	8	5	34.803	36.819	36.819	0.0	-0.016	-0.008
5	8	5	29.327	30.896	-30.896	0.0	-1.559	-0.656
6	8	5	8.325	4.923	-4.923	0.0	3.403	0.608
7	8	5	8.164	16.233	-16.233	0.0	-8.069	-1.287
8	8	5	20.489	22.357	-22.357	0.0	-1.868	-0.988
9	8	5	51.457	52.072	52.072	0.0	-0.615	-0.359
11	8	5	53.482	51.649	51.649	0.0	1.833	1.137
12	8	5	22.408	22.987	22.987	0.0	-0.498	-0.162
13	8	5	13.580	9.640	-9.640	0.0	4.340	1.076
0	6	0	336.566	354.231	354.231	0.0	-17.666	-2.949 *
12	7	5	23.135	20.343	20.343	0.0	2.192	1.092
11	7	5	3.906	2.505	2.505	0.0	1.401	0.178
10	7	5	12.594	9.261	-9.261	0.0	3.324	0.797
8	7	5	26.061	23.399	23.399	0.0	2.662	1.153
7	7	5	11.777	1.280	1.280	0.0	10.497	2.738 *
6	7	5	1.777	5.025	-5.025	0.0	-3.248	-0.347
5	7	5	14.362	10.408	10.408	0.0	3.953	1.121
4	7	5	23.311	22.395	22.395	0.0	0.917	0.416
3	7	5	27.150	28.980	28.980	0.0	-1.830	-0.824
1	7	5	11.791	4.738	-4.738	0.0	7.053	1.785
1	6	5	7.342	11.381	-11.381	0.0	-4.039	-0.743
2	6	5	8.927	15.516	15.516	0.0	-6.588	-1.297
3	6	5	14.053	15.956	-15.956	0.0	-1.902	-0.531
4	6	5	12.496	1.732	-1.732	0.0	10.764	3.173 *
5	6	5	4.743	1.262	-1.262	0.0	3.481	0.511
0	6	0	336.737	354.231	354.231	0.0	-17.494	-2.920 *
8	6	5	7.900	4.591	-4.591	0.0	3.309	0.609
10	6	5	14.303	11.423	-11.423	0.0	2.880	0.800
15	6	5	8.120	6.269	6.269	0.0	1.851	0.302
18	5	5	15.669	8.730	8.730	0.0	6.940	2.072
17	5	5	4.287	1.376	-1.376	0.0	2.911	0.371
16	5	5	0.177	6.547	6.547	0.0	2.630	0.487
15	5	5	11.468	3.965	3.965	0.0	7.503	1.617
14	5	5	7.342	13.410	-13.410	0.0	-6.069	-0.961
13	5	5	23.767	20.525	-20.525	0.0	3.243	1.313
12	5	5	24.223	27.324	27.324	0.0	-3.100	-1.122
11	5	5	13.055	15.294	-15.294	0.0	-2.240	-0.555

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/STOMA	
0	6	0	337.727	354.231	354.231	0.0	-16.505	-7.742	*
10	6	5	12.408	17.647	17.647	0.0	-5.239	-1.201	
9	5	5	26.164	26.968	26.968	0.0	-0.804	-0.357	
7	5	5	34.842	38.847	37.847	0.0	-0.006	-0.003	
6	5	5	32.241	32.153	32.153	0.0	0.088	0.049	
5	5	5	17.205	19.084	19.084	0.0	-2.599	-0.854	
4	5	5	5.726	5.149	5.149	0.0	0.577	0.097	
2	5	5	16.242	17.855	17.855	0.0	-1.612	-0.528	
1	5	5	22.606	21.665	21.665	0.0	0.961	0.424	
0	4	5	11.465	13.817	13.817	0.0	-1.952	-0.504	
2	4	5	41.744	41.602	41.602	0.0	0.142	0.094	
3	4	5	30.813	29.307	29.297	0.0	1.426	0.829	
4	4	5	17.506	15.536	15.536	0.0	1.970	0.749	
5	4	5	14.568	13.652	13.652	0.0	0.915	0.282	
6	4	5	21.445	21.736	21.736	0.0	-0.292	-0.117	
7	4	5	5.705	5.234	5.234	0.0	0.551	0.093	
9	4	5	32.497	32.751	32.751	0.0	-0.093	-0.050	
0	6	0	337.536	354.231	354.231	0.0	-16.265	-2.707	*
10	4	5	5.800	3.165	3.165	0.0	2.635	0.430	
11	4	5	39.494	36.666	36.666	0.0	3.048	1.970	
13	4	5	19.725	12.666	12.666	0.0	7.079	2.646	
14	4	5	11.586	5.592	5.592	0.0	5.994	1.369	
16	4	5	4.574	4.800	4.800	0.0	4.774	0.929	
17	4	5	22.324	24.317	24.317	0.0	-2.093	-0.723	
18	4	5	23.106	23.895	23.895	0.0	5.112	2.296	
19	4	5	11.498	3.565	3.565	0.0	7.933	1.789	
20	3	5	16.607	20.467	20.467	0.0	-0.860	-0.259	
19	3	5	16.887	17.671	17.671	0.0	-1.216	0.394	
18	3	5	24.494	30.334	30.334	0.0	-1.650	-0.619	
17	3	5	57.551	56.602	56.602	0.0	0.969	0.558	
16	3	5	39.576	42.143	42.143	0.0	-2.567	-1.319	
15	3	5	43.056	41.665	41.665	0.0	1.091	0.592	
14	3	5	21.485	20.197	20.197	0.0	1.489	0.631	
13	3	5	35.569	33.364	33.364	0.0	2.205	1.248	
12	3	5	55.538	55.402	55.402	0.0	0.136	0.089	
11	3	5	65.302	65.203	65.203	0.0	0.100	0.065	
0	6	0	337.822	354.231	354.231	0.0	-16.410	-2.726	*
10	3	5	61.173	65.938	65.938	0.0	1.235	0.792	
9	3	5	62.881	63.007	63.007	0.0	-0.126	-0.080	
8	3	5	54.861	54.188	54.188	0.0	0.773	0.513	
7	3	5	62.143	63.677	63.677	0.0	-1.533	-1.055	
6	3	5	46.030	47.392	47.392	0.0	0.637	0.427	
5	3	5	65.182	85.122	85.122	0.0	-0.060	0.038	
4	3	5	12.614	10.323	10.323	0.0	2.291	0.690	
3	3	5	101.822	101.843	101.843	0.0	-0.021	-0.012	
2	3	5	53.586	54.345	54.345	0.0	-0.768	-0.580	
1	3	5	28.562	25.916	25.916	0.0	2.645	1.605	
0	2	5	5.485	6.031	6.031	0.0	0.852	0.201	
1	2	5	33.124	34.572	34.572	0.0	-1.448	-0.910	
2	2	5	56.721	59.216	59.216	0.0	-0.495	-0.355	
3	2	5	56.030	56.598	56.598	0.0	-2.568	-1.772	
4	2	5	45.874	45.522	45.522	0.0	0.352	0.246	
5	2	5	46.450	46.718	46.718	0.0	-0.268	-0.178	

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(FCALC)	B(FCALC)	DELTA F	DELTA/SIGMA
6	2	5	16.477	17.862	-17.862	0.0	-1.385	-0.423
7	2	5	22.238	21.471	-21.471	0.0	0.767	0.337
8	2	5	28.797	27.511	-27.511	0.0	1.286	0.705
9	2	5	68.613	67.671	-67.671	0.0	0.943	0.629
0	6	0	339.203	354.231	-354.231	0.0	-16.028	-2.653 *
11	2	5	70.723	70.274	-70.274	0.0	0.449	0.296
12	2	5	25.032	25.450	-25.450	0.0	-0.419	-0.190
14	2	5	17.697	11.608	-11.608	0.0	6.089	2.181
15	2	5	13.554	13.780	-13.780	0.0	-0.226	-0.055
16	2	5	11.527	18.471	-18.471	0.0	-7.044	-1.356
17	2	5	30.864	37.175	-37.175	0.0	1.709	0.913
18	2	5	19.431	18.446	-18.446	0.0	0.985	0.322
19	2	5	15.331	14.373	-14.373	0.0	0.958	0.241
20	2	5	11.600	6.467	-6.467	0.0	5.124	1.117
21	1	5	16.933	13.617	-13.617	0.0	3.316	0.929
19	1	5	11.762	7.057	-7.057	0.0	4.705	1.017
17	1	5	5.932	10.112	-10.112	0.0	-4.100	-0.610
16	1	5	6.560	7.050	-7.050	0.0	-0.090	-0.016
15	1	5	15.082	8.453	-8.453	0.0	6.629	2.079
14	1	5	13.319	13.052	-13.052	0.0	0.267	0.070
13	1	5	4.275	16.094	-16.094	0.0	-12.619	-1.625 *
0	6	0	337.022	354.231	-354.231	0.0	-17.209	-2.862 *
12	1	5	39.709	37.288	-37.288	0.0	2.421	1.610
11	1	5	6.725	8.038	-8.038	0.0	-1.313	-0.226
10	1	5	11.130	7.418	-7.418	0.0	3.712	0.965
9	1	5	5.800	12.373	-12.373	0.0	-6.573	-1.071
8	1	5	21.944	17.422	-17.422	0.0	4.522	2.197
7	1	5	29.827	30.229	-30.229	0.0	-0.402	-0.212
6	1	5	30.372	29.054	-29.054	0.0	1.317	0.772
6	1	5	16.242	16.129	-16.129	0.0	0.113	0.040
3	1	5	11.997	13.486	-13.486	0.0	-1.489	-0.441
2	1	5	12.482	13.081	-13.081	0.0	-0.599	-0.181
1	1	5	20.768	14.857	-14.857	0.0	5.911	3.001
0	6	0	81.000	79.986	-79.986	0.0	1.014	0.635
1	0	6	103.329	101.097	-101.097	0.0	2.232	1.214
2	0	6	13.521	5.173	-5.173	0.0	8.748	2.683
3	0	6	51.590	50.107	-50.107	0.0	1.493	1.045
4	0	6	5.256	6.667	-6.667	0.0	-1.410	-0.213
5	0	6	48.990	48.664	-48.664	0.0	0.326	0.204
6	0	6	4.498	0.276	-0.276	0.0	4.622	0.672
7	0	6	90.390	89.596	-89.596	0.0	0.794	0.461
0	6	0	337.708	354.231	-354.231	0.0	-16.524	-2.745 *
8	0	6	27.498	29.339	-29.339	0.0	-1.851	-0.801
9	0	6	19.343	20.665	-20.665	0.0	-1.322	-0.437
10	0	6	20.548	18.796	-18.796	0.0	1.751	0.630
11	0	6	20.445	16.785	-16.785	0.0	3.660	1.287
12	0	6	30.357	30.728	-30.728	0.0	-0.371	-0.161
13	0	6	70.188	74.799	-74.799	0.0	-4.611	-2.629
15	0	6	67.098	67.231	-67.231	0.0	-0.133	-0.075
16	0	6	15.581	16.460	-16.460	0.0	-0.879	-0.223
17	0	6	14.700	20.509	-20.509	0.0	-5.809	-1.243
17	1	6	5.624	5.405	-5.405	0.0	0.218	0.030
16	1	6	16.874	17.081	-17.081	0.0	-0.207	-0.057

600C_CRTHOFERROSILITE_6/26/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DFLT A F	DELTA/SIGMA
15	1	6	24.675	22.707	-22.707	0.0	1.972	0.790
14	1	6	36.515	34.502	-34.502	0.0	2.112	1.120
13	1	6	59.349	53.016	-53.016	0.0	0.134	0.205
11	1	6	12.061	0.101	-0.101	0.0	11.940	2.842 *
10	1	6	8.017	11.239	-11.239	0.0	-3.372	0.768
8	1	6	5.274	0.734	-0.734	0.0	2.540	0.328
0	6	0	337.364	354.231	-354.231	0.0	-16.885	-2.807 *
7	1	6	42.746	41.607	-41.607	0.0	1.135	0.129
6	1	6	32.089	32.913	-32.913	0.0	-0.024	-0.012
5	1	6	12.070	11.326	-11.326	0.0	0.744	0.197
4	1	6	12.100	12.520	-12.520	0.0	-0.420	-0.107
2	1	6	9.280	16.368	-16.368	0.0	-7.088	-1.821
1	1	6	55.805	56.010	-56.010	0.0	-0.206	-0.135
0	2	6	10.650	9.705	-9.705	0.0	0.958	0.238
1	2	6	16.212	14.694	-14.694	0.0	1.576	0.364
2	2	6	16.624	17.341	-17.341	0.0	-0.717	-0.235
3	2	6	35.478	35.431	-35.431	0.0	0.447	0.251
4	2	6	1.321	11.984	-11.984	0.0	-10.863	-1.936 *
5	2	6	24.672	13.517	-13.517	0.0	-10.845	-1.241 *
9	2	6	15.434	15.803	-15.803	0.0	-0.368	-0.103
10	2	6	18.593	16.276	-16.276	0.0	2.317	0.784
11	2	6	32.493	31.748	-31.748	0.0	0.743	0.341
0	6	0	336.547	354.231	-354.231	0.0	-17.675	-2.953 *
15	2	6	18.108	9.721	-9.721	0.0	8.288	2.744
16	2	6	14.156	9.432	-9.432	0.0	4.724	1.182
17	2	6	18.975	18.835	-18.835	0.0	0.141	0.041
16	3	6	8.061	8.424	-8.424	0.0	-0.273	-0.062
14	3	6	8.458	24.705	-24.705	0.0	5.752	1.025
12	3	6	11.568	7.567	-7.567	0.0	4.401	1.055
11	3	6	17.873	5.506	-5.506	0.0	12.368	4.339 *
7	3	6	0.675	7.791	-7.791	0.0	-7.115	-0.884
6	3	6	7.562	6.535	-6.535	0.0	1.026	0.187
5	3	6	10.572	5.822	-5.822	0.0	4.750	1.108
4	3	6	16.462	15.223	-15.223	0.0	1.766	0.602
3	3	6	7.297	4.081	-4.081	0.0	3.217	0.581
2	3	6	7.253	2.946	-2.946	0.0	4.308	0.204
0	6	0	337.936	354.231	-354.231	0.0	-16.295	-2.707 *
1	3	6	15.258	24.692	-24.692	0.0	12.566	4.432 *
28	974	25.216	25.216	25.216	0.0	3.758	2.094	
0	4	6	28.974	25.216	-25.216	0.0	3.758	2.094
1	4	6	14.553	14.695	-14.695	0.0	-0.143	-0.041
2	4	6	2.349	6.406	-6.406	0.0	-4.057	-0.476
3	4	6	26.723	29.662	-29.662	0.0	-2.942	-1.227
7	4	6	12.848	11.639	-11.639	0.0	2.209	0.570
8	4	6	13.818	11.086	-11.086	0.0	2.732	0.732
9	4	6	5.785	11.063	-11.063	0.0	-5.278	-0.741
11	4	6	7.247	7.916	-7.916	0.0	-0.369	-0.061
12	4	6	13.833	8.692	-8.692	0.0	5.141	1.311
13	4	6	5.418	12.674	-12.674	0.0	-7.256	-0.965
14	5	6	37.366	30.112	-30.112	0.0	7.256	4.827
13	5	6	51.309	52.833	-52.833	0.0	-1.524	-0.799
12	5	6	7.929	0.108	-0.108	0.0	7.821	1.312
0	6	0	336.338	354.231	-354.231	0.0	-17.894	-2.988 *
11	5	6	13.716	15.555	-15.555	0.0	-1.840	-0.400

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
10	5	6	6.666	5.802	5.802	0.0	0.864	0.135	
9	5	6	18.872	7.228	7.228	0.0	11.644	4.717 *	
8	5	6	17.403	13.448	13.448	0.0	3.955	1.264	
7	5	6	48.857	47.323	47.323	0.0	1.534	1.008	
6	5	6	38.515	37.247	37.247	0.0	1.268	0.672	
5	5	6	34.592	37.545	37.545	0.0	-2.953	-1.369	
3	5	6	3.083	7.417	7.417	0.0	-4.333	-0.489	
2	5	6	13.936	15.250	15.250	0.0	-1.314	-0.310	
1	5	6	67.024	70.160	70.160	0.0	-3.136	-1.956	
0	6	6	55.509	62.160	62.160	0.0	-6.651	-3.842	
1	6	6	68.712	71.107	71.107	0.0	-2.804	-1.740	
2	6	6	14.318	18.280	18.280	0.0	-3.963	-0.977	
3	6	6	19.887	18.599	18.599	0.0	1.287	0.409	
5	6	6	33.404	34.937	34.937	0.0	-1.533	-0.667	
7	6	6	59.254	56.526	56.526	0.0	2.728	1.674	
8	6	6	12.509	14.634	14.634	0.0	-2.035	-0.437	
0	6	0	338.013	354.231	354.231	0.0	-16.219	-2.694 *	
9	6	6	8.428	2.737	2.737	0.0	5.691	1.020	
11	6	6	12.673	15.375	15.375	0.0	-2.702	-0.599	
12	6	6	24.003	24.822	24.822	0.0	-0.820	-0.275	
10	7	6	11.615	11.860	11.860	0.0	-0.253	-0.049	
9	7	6	12.702	14.976	14.976	0.0	-2.274	-0.485	
8	7	6	3.362	4.205	4.205	0.0	-0.842	-0.097	
7	7	6	15.155	17.733	17.733	0.0	-2.578	-0.616	
6	7	6	17.065	20.850	20.850	0.0	-3.785	-0.980	
4	7	6	15.317	9.626	9.626	0.0	5.691	1.575	
3	7	6	16.125	22.114	22.114	0.0	-5.980	-1.527	
1	7	6	19.064	14.291	14.291	0.0	4.773	1.616	
1	8	6	12.496	12.962	12.962	0.0	-0.466	-0.096	
2	8	6	16.918	1.421	1.421	0.0	15.497	5.247 *	
3	8	6	34.405	30.100	30.100	0.0	4.306	2.134	
4	8	6	20.078	13.618	13.618	0.0	6.459	2.123	
5	8	6	15.126	11.145	11.145	0.0	3.981	1.080	
0	6	0	336.584	354.231	354.231	0.0	-17.247	-2.869 *	
7	9	6	18.799	10.408	10.408	0.0	8.391	2.943	
0	6	7	10.293	3.079	3.079	0.0	7.214	1.302	
2	6	7	11.865	1.152	-1.152	0.0	10.713	2.507 *	
6	5	7	21.151	17.408	-17.408	0.0	3.743	1.254	
5	5	7	10.616	7.061	-7.061	0.0	3.556	0.714	
4	5	7	7.029	3.850	3.850	0.0	4.079	0.673	
2	5	7	20.239	19.950	19.950	0.0	0.289	0.085	
1	5	7	22.312	25.222	-25.222	0.0	-2.910	-0.905	
1	4	7	24.664	23.745	23.745	0.0	0.919	0.344	
2	4	7	7.723	8.219	8.219	0.0	-0.496	-0.080	
3	4	7	19.034	5.871	-5.871	0.0	13.163	5.060 *	
4	4	7	25.164	23.735	-23.735	0.0	1.430	0.528	
5	4	7	20.023	25.547	25.547	0.0	-5.514	-1.590	
7	4	7	18.623	13.554	13.554	0.0	5.069	1.635	
0	6	0	336.072	354.231	354.231	0.0	-16.160	-3.034 *	
8	4	7	14.788	16.673	16.673	0.0	-1.886	-0.440	
9	4	7	19.019	18.254	18.254	0.0	0.765	0.215	
10	3	7	67.009	66.029	66.029	0.0	0.980	0.550	
9	3	7	8.781	10.116	-10.116	0.0	-1.335	-0.228	

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(FCALC)	R(CALC)	DELTA F	DELTA/SIGMA
8	3	7	12.878	8.619	-8.619	0.0	4.239	0.976
7	3	7	22.371	28.350	-28.350	0.0	-5.988	-0.763
6	3	7	46.878	48.576	-48.576	0.0	-1.657	-0.891
5	3	7	33.757	35.681	-35.681	0.0	-1.924	-0.949
3	3	7	42.157	41.651	-41.651	0.0	0.505	0.258
2	3	7	65.404	64.154	-64.154	0.0	-0.750	-0.456
1	3	7	23.577	19.010	-19.010	0.0	4.507	1.916
0	2	7	20.621	22.379	-22.379	0.0	-1.752	-0.583
1	2	7	34.994	35.108	-35.108	0.0	-0.115	-0.059
3	2	7	11.204	3.257	-3.257	0.0	7.944	1.718
4	2	7	51.295	50.910	-50.910	0.0	0.385	0.230
5	2	7	16.233	15.943	-15.943	0.0	0.250	0.208
6	2	7	9.687	1.612	-1.612	0.0	8.255	1.692
7	2	7	10.388	2.693	-2.693	0.0	7.615	1.552
0	6	0	336.737	354.231	-354.231	0.0	-17.494	-2.420 *
8	2	7	36.158	36.032	-36.032	0.0	0.126	0.064
9	2	7	30.740	27.365	-27.365	0.0	3.375	1.470
10	2	7	4.498	2.713	-2.713	0.0	4.275	0.752
11	2	7	51.002	32.972	-32.972	0.0	1.069	-0.458
12	1	7	15.400	3.630	-3.630	0.0	11.910	3.363 *
11	1	7	6.460	13.119	-13.119	0.0	-6.650	-0.902
9	1	7	22.224	18.701	-18.701	0.0	3.523	1.362
8	1	7	4.311	3.809	-3.809	0.0	0.552	0.070
4	1	7	5.444	3.616	-3.616	0.0	2.228	0.326
2	1	7	14.377	8.126	-8.126	0.0	6.250	1.695
1	1	7	22.444	23.457	-23.457	0.0	-1.012	-0.352

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STRUCTURE FACTORS

PAGE 1

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H	K	I	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	0	326.428	334.474	0.0	-7.786	-1.298 *	
4	0	0	185.667	182.549	0.0	2.118	0.712	
6	0	0	17.044	16.756	0.0	0.288	0.235	
8	0	0	101.065	106.110	0.0	-7.046	-4.373	
10	0	0	10.650	4.812	0.0	5.746	2.364	
12	0	0	274.258	262.548	0.0	11.710	2.456 *	
14	0	0	21.443	20.962	0.0	0.986	0.481	
16	0	0	147.090	149.582	0.0	-1.692	-0.698	
18	0	0	1.516	3.038	0.0	-1.522	-0.144	
20	0	0	143.469	142.107	0.0	1.302	0.576	
22	0	0	5.831	4.847	0.0	0.982	0.164	
24	1	0	22.361	24.525	-24.939	0.0	-2.577	-0.767
24	1	0	7.580	13.404	0.0	-5.424	-0.832	
22	1	0	73.762	22.325	22.325	0.0	1.438	0.594
20	1	0	8.511	0.226	0.0	-0.716	-0.150	
18	1	0	46.557	40.062	-40.082	0.0	-1.125	-0.807
16	1	0	2.105	3.288	0.0	-1.182	-0.153	
14	1	0	124.532	125.266	125.266	0.0	-0.733	-0.357
12	1	0	10.204	1.289	-1.289	0.0	8.915	2.855
0	6	0	327.445	334.474	334.474	0.0	-6.529	-1.082 *
10	1	0	48.796	47.993	47.993	0.0	0.803	0.773
6	1	0	261.447	250.932	250.932	0.0	1.534	0.342
4	1	0	14.108	7.454	7.454	0.0	6.654	4.805
2	1	0	85.813	86.842	86.842	0.0	-1.029	-0.776
0	2	0	10.726	10.373	10.373	0.0	0.553	0.348
2	2	0	6.037	2.796	2.796	0.0	3.241	1.117
4	2	0	195.543	192.416	190.116	0.0	-2.173	-0.684
6	2	0	10.705	11.485	11.485	0.0	-0.780	-0.392
8	2	0	82.122	82.885	82.885	0.0	-0.262	-0.192
10	2	0	17.114	10.414	10.414	0.0	-1.799	-0.961
12	2	0	7.391	9.512	9.512	0.0	-2.121	-0.298
14	2	0	6.773	1.821	-1.821	0.0	4.952	1.038
16	2	0	67.248	66.848	66.848	0.0	0.399	0.291
18	2	0	8.725	7.084	7.084	0.0	1.441	0.332
20	2	0	27.465	24.254	20.254	0.0	-1.759	-0.731
22	2	0	11.930	3.597	3.597	0.0	7.852	1.884
24	3	0	8.605	13.860	13.860	0.0	-5.054	-0.839
0	4	0	327.396	334.474	334.474	0.0	-7.088	-1.180 *
24	3	0	14.697	4.197	-4.197	0.0	10.510	2.572 *
20	3	0	3.671	3.245	3.245	0.0	0.716	0.103
18	3	0	6.217	9.010	9.010	0.0	-0.702	-0.177
14	3	0	46.171	44.455	44.455	0.0	1.716	1.331
12	3	0	0.972	0.042	-0.042	0.0	0.929	0.117
10	3	0	12.733	6.399	-6.399	0.0	6.338	2.640
8	3	0	11.780	6.861	-6.861	0.0	4.919	2.272
6	3	0	43.223	41.126	-41.126	0.0	2.097	2.284
4	3	0	15.551	15.363	15.363	0.0	0.189	0.139
2	3	0	48.173	49.556	-48.559	0.0	-0.386	-0.414
0	4	0	25.919	25.675	25.675	0.0	1.244	1.278
2	4	0	8.584	7.755	-7.755	0.0	0.829	0.366
4	4	0	50.522	63.444	-63.444	0.0	-2.921	-2.651
6	4	0	102.734	4.828	-4.828	0.0	5.806	2.491
8	4	0	64.934	64.039	-64.039	0.0	0.096	0.732

8000 CRITICALITY 6/28/72

STRUCTURE FACTORS

PAGE 2

H	K	I	F(HK)	F(CALC)	A(CALC)	B(CALC)	D(FIT) F	DELTA/SIGMA
10	4	0	26.182	29.406	-26.406	0.0	-2.224	-1.436
12	4	0	15.006	15.210	-15.210	0.0	-0.204	-0.074
14	4	0	12.060	2.629	0.0	5.631	3.364	
0	6	0	326.148	334.474	334.474	0.0	-7.026	-1.304 *
14	4	0	45.327	44.418	44.418	0.0	-1.092	-0.752
20	4	0	45.445	47.300	47.300	0.0	-1.535	-1.015
22	4	0	13.415	13.404	-13.404	0.0	-0.179	-1.267
24	4	0	19.000	21.616	21.519	0.0	-2.519	-0.750
26	4	0	10.793	5.830	5.830	0.0	4.963	1.043
22	5	0	21.432	17.262	17.282	0.0	4.150	1.618
20	5	0	14.889	14.019	14.019	0.0	0.860	0.278
18	5	0	51.393	50.865	50.865	0.0	0.528	0.367
16	5	0	5.207	5.096	5.096	0.0	-0.450	-0.079
14	5	0	185.683	183.673	-183.673	0.0	1.811	0.589
12	5	0	4.705	7.647	7.647	0.0	-3.142	-0.301
10	5	0	15.102	16.351	-16.351	0.0	-0.589	0.231
8	5	0	11.029	12.124	-12.124	0.0	-1.095	-0.356
6	5	0	145.172	145.448	-145.448	0.0	-0.776	-0.311
2	6	0	200.735	204.406	204.406	0.0	-3.471	-1.115
0	6	0	325.781	334.474	334.474	0.0	-8.583	-1.437 *
-2	6	0	11.653	9.644	9.644	0.0	1.989	0.593
0	6	0	327.027	334.474	334.474	0.0	-7.447	-1.240 *
4	6	0	70.467	62.861	-62.861	0.0	-2.974	-2.934
6	6	0	5.271	8.615	-8.615	0.0	-3.244	-0.407
8	6	0	119.515	119.327	119.327	0.0	0.548	-0.276
10	6	0	12.310	8.402	-8.402	0.0	3.908	1.190
12	6	0	112.704	112.378	-112.378	0.0	0.526	-0.275
14	6	0	19.588	17.920	-17.920	0.0	2.968	1.591
16	6	0	60.671	60.088	60.088	0.0	0.583	0.407
18	6	0	3.666	4.497	4.497	0.0	-2.231	-0.167
20	6	0	107.202	110.280	-110.280	0.0	-1.078	-0.334
22	6	0	1.400	1.250	1.250	0.0	4.261	0.17
24	6	0	16.175	16.121	-16.121	0.0	2.053	0.445
26	6	0	15.578	15.986	-15.986	0.0	2.542	0.329
22	7	0	11.307	14.015	14.015	0.0	-2.618	-0.593
18	7	0	11.430	10.250	-10.250	0.0	1.609	0.444
16	7	0	11.139	10.250	-10.250	0.0	-1.009	-0.730
14	7	0	5.574	6.6324	6.6324	0.0	-2.054	-2.472
12	7	0	11.471	3.022	-3.022	0.0	8.449	-2.472
10	7	0	22.546	65.933	65.933	0.0	-1.287	-0.928
6	7	0	50.078	51.603	51.603	0.0	-1.525	-0.922
0	6	0	326.647	334.474	334.474	0.0	-7.507	-1.450 *
-4	7	0	14.417	21.248	21.248	0.0	-2.631	-1.059
2	7	0	17.669	14.767	14.767	0.0	2.272	0.907
0	8	0	55.584	62.184	62.184	0.0	-2.600	-1.658
2	8	0	11.382	12.950	-12.950	0.0	-1.568	-0.453
4	8	0	62.386	62.788	-62.788	0.0	-0.407	-0.278
6	8	0	8.582	3.637	3.637	0.0	5.345	1.401
8	8	0	20.811	26.405	26.405	0.0	-0.335	-0.190
10	8	0	15.766	12.372	12.372	0.0	3.194	1.123
12	8	0	40.726	40.513	-40.513	0.0	0.222	0.147
14	8	0	10.322	2.609	2.609	0.0	7.513	1.903
16	8	0	56.578	57.519	57.519	0.0	-0.941	-0.603
18	8	0	9.394	1.532	-1.532	0.0	7.862	1.663

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
20	8	0	6.970	3.343	-3.343	0.0	3.636	0.577
22	8	0	7.156	3.604	-3.604	0.0	3.551	0.536
18	9	0	10.400	0.043	-0.043	0.0	10.647	2.317 *
16	9	0	23.187	18.060	18.060	0.0	5.127	2.398
12	9	0	13.293	4.894	4.894	0.0	8.289	2.558
10	9	0	12.767	11.272	-11.272	0.0	1.495	0.449
0	6	0	328.165	334.474	334.474	0.0	-6.306	-1.045 *
8	6	0	15.080	13.251	-13.251	0.0	1.829	0.606
6	6	0	24.706	27.132	27.132	0.0	-2.425	-1.118
7	9	0	6.520	4.504	-4.504	0.0	2.416	0.497
0	10	0	56.678	56.275	-56.275	0.0	0.304	0.215
4	10	0	10.652	10.158	-10.158	0.0	0.600	0.008
8	10	0	25.400	29.281	-29.281	0.0	-3.881	-1.634
10	10	0	11.382	0.110	0.110	0.0	11.273	2.921 *
12	10	0	16.701	17.695	17.695	0.0	-0.984	-0.290
16	10	0	3.607	1.619	1.619	0.0	1.989	0.238
18	10	0	11.368	3.427	3.427	0.0	7.941	1.659
14	11	0	68.916	67.697	-67.697	0.0	1.119	0.651
10	11	0	9.493	10.364	-10.364	0.0	-0.882	-0.169
8	11	0	17.747	1.440	-1.440	0.0	16.308	6.065 *
6	11	0	69.474	65.907	-65.907	0.0	3.567	2.340
0	6	0	326.210	334.474	334.474	0.0	-6.264	-1.378 *
2	11	0	54.334	53.071	-53.071	0.0	1.262	0.794
0	12	0	80.082	74.945	-74.945	0.0	5.133	3.051
2	12	0	15.493	3.960	-3.960	0.0	11.532	3.692 *
4	12	0	7.677	5.319	-5.319	0.0	2.559	0.458
0	12	0	20.371	20.252	-20.252	0.0	0.119	0.039
12	12	0	24.203	26.635	-26.635	0.0	-2.432	-0.790
4	13	0	2.494	0.241	-0.241	0.0	2.453	0.274
2	12	0	26.211	25.514	-25.514	0.0	0.697	0.268
7	13	1	10.431	0.922	-0.922	0.0	9.709	2.140
6	13	1	17.059	4.938	-4.938	0.0	12.161	3.856 *
5	13	1	10.248	0.649	-0.649	0.0	9.300	1.913
4	13	1	11.568	6.794	-6.794	0.0	4.866	1.035
3	13	1	2.086	8.736	-8.736	0.0	-5.850	-0.642
1	13	1	9.777	12.507	-12.507	0.0	-2.730	-0.518
0	5	0	325.632	334.474	334.474	0.0	-6.442	-1.447 *
0	12	1	10.490	8.347	-8.347	0.0	2.344	0.517
2	12	1	12.119	3.048	-3.048	0.0	6.071	2.307
4	12	1	14.726	8.977	-8.977	0.0	5.746	1.719
9	12	1	15.551	14.596	-14.596	0.0	0.955	0.266
6	12	1	8.235	5.719	-5.719	0.0	3.116	0.608
7	12	1	15.227	3.419	-3.419	0.0	11.808	3.929 *
8	12	1	7.318	2.641	-2.641	0.0	4.677	0.786
11	12	1	7.697	7.144	-7.144	0.0	-0.048	-0.008
12	12	1	0.351	4.045	-4.045	0.0	-3.294	-0.291
15	11	1	14.108	14.784	-14.784	0.0	-0.677	-0.165
14	11	1	16.178	14.205	-14.205	0.0	1.972	0.567
13	11	1	11.829	13.829	-13.829	0.0	-1.990	-0.441
12	11	1	9.889	3.323	-3.323	0.0	2.566	0.306
11	11	1	16.686	17.026	-17.026	0.0	-0.340	-0.046
10	11	1	16.551	13.238	-13.238	0.0	3.612	1.162
9	11	1	13.121	8.746	-8.746	0.0	4.375	1.188

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DETA F	DETA/SIGMA
0	4	0	327.625	334.474	334.474	0.0	-6.448	-1.136 *
7	11	1	22.051	22.617	-22.617	0.0	1.234	0.516
6	11	1	27.203	27.785	27.785	0.0	-0.482	-0.211
5	11	1	29.429	27.664	27.664	0.0	1.764	0.842
4	11	1	10.037	11.398	11.398	0.0	-0.560	-0.134
3	11	1	20.396	11.531	11.531	0.0	8.254	4.086
2	11	1	21.550	21.107	-21.107	0.0	0.443	0.184
1	11	1	15.659	16.719	-16.719	0.0	-4.020	-1.161
0	10	1	30.521	26.917	26.917	0.0	3.605	2.141
1	10	1	33.258	28.932	-28.932	0.0	4.366	2.687
2	10	1	26.699	27.528	27.528	0.0	-0.930	-0.430
3	10	1	13.145	8.446	8.446	0.0	4.719	1.490
4	10	1	19.531	17.188	17.188	0.0	2.342	0.975
5	10	1	16.774	16.645	16.645	0.0	0.129	0.046
6	10	1	12.399	12.217	12.217	0.0	0.182	0.048
7	10	1	2.806	10.265	-10.265	0.0	-7.379	-0.890
8	10	1	10.026	0.177	0.177	0.0	10.749	2.744 *
9	10	1	16.436	13.945	13.945	0.0	2.490	0.751
10	10	1	326.449	334.474	334.474	0.0	-8.025	-1.338 *
11	10	1	18.351	16.401	-16.401	0.0	1.050	0.665
12	10	1	17.625	11.654	-11.654	0.0	0.371	0.114
13	10	1	11.736	5.248	-5.248	0.0	6.488	1.430
14	10	1	17.406	12.284	-12.284	0.0	5.522	1.837
15	10	1	14.815	7.775	7.775	0.0	7.040	1.999
16	10	1	12.434	16.802	16.802	0.0	-7.168	-1.419
17	10	1	18.970	16.876	-16.876	0.0	2.095	0.637
18	10	1	16.268	22.518	-22.518	0.0	-3.150	-0.967
19	10	1	21.742	14.905	-14.905	0.0	6.837	2.972
20	10	1	19.590	15.498	-15.498	0.0	4.102	1.546
21	10	1	53.368	52.190	-52.190	0.0	1.178	0.793
22	10	1	58.869	58.798	58.798	0.0	0.071	0.044
23	10	1	55.255	54.654	-54.654	0.0	0.601	0.421
24	10	1	65.000	65.211	-65.211	0.0	-0.202	-0.137
25	10	1	31.791	35.195	-35.195	0.0	-3.404	-1.815
26	10	1	326.270	334.474	334.474	0.0	-8.204	-1.368 *
27	10	1	18.558	19.853	-19.853	0.0	-1.355	-0.567
28	10	1	24.455	25.442	25.442	0.0	-0.957	-0.464
29	10	1	26.403	23.252	23.252	0.0	-1.849	-0.942
30	10	1	8.319	5.986	-5.986	0.0	2.335	0.541
31	10	1	33.579	33.502	33.502	0.0	0.077	0.048
32	10	1	40.410	48.613	-48.613	0.0	-0.203	-0.149
33	10	1	36.593	38.196	-38.196	0.0	-1.203	-0.746
34	10	1	18.425	18.593	18.593	0.0	-0.168	-0.065
35	10	1	8.315	8.262	-8.262	0.0	-2.947	-0.545
36	10	1	64.487	66.907	-66.907	0.0	-2.420	-1.803
37	10	1	95.254	97.608	-97.608	0.0	-2.354	-1.400
38	10	1	72.615	75.160	-75.160	0.0	-2.546	-1.772
39	10	1	57.486	55.709	55.709	0.0	1.777	1.312
40	10	1	11.468	10.744	-10.744	0.0	0.904	0.268
41	10	1	37.732	41.890	41.890	0.0	-4.158	-2.628
42	10	1	61.033	61.907	61.907	0.0	-0.074	-0.054
43	10	1	41.731	37.891	-37.891	0.0	3.540	2.544
44	10	1	17.511	16.799	16.799	0.0	0.712	0.279

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
11	6	1	23.554	24.932	0.0	-0.978	-0.448	
12	8	1	30.676	31.916	-0.016	0.0	-1.040	-0.568
0	6	0	326.613	334.474	0.0	-0.861	-1.494	*
13	8	1	42.312	43.031	0.0	2.250	1.524	
15	8	1	41.644	41.411	0.0	0.213	0.136	
16	8	1	30.441	34.877	0.0	-0.436	-1.161	
17	6	1	21.747	26.587	-0.057	0.0	0.761	0.320
18	8	1	25.496	21.078	0.0	4.210	2.000	
19	6	1	17.791	10.008	-10.008	0.0	-2.417	-0.624
20	8	1	16.951	12.480	-12.480	0.0	4.472	1.331
22	8	1	27.598	25.088	-25.088	0.0	2.511	1.031
23	7	1	4.902	0.144	0.144	0.0	4.810	0.612
21	7	1	6.287	5.051	-5.051	0.0	-2.236	0.187
20	7	1	4.029	0.306	-0.306	0.0	4.523	0.628
19	7	1	15.663	20.306	-20.306	0.0	-0.362	-0.124
16	7	1	18.607	17.872	0.0	-4.266	-1.177	
15	7	1	14.038	6.730	-6.730	0.0	9.307	3.529
16	7	1	16.696	0.659	0.659	0.0	9.428	2.389
0	6	0	326.498	334.474	0.0	-7.706	-1.290	*
12	7	1	23.740	20.269	0.0	3.470	1.734	
11	7	1	19.457	20.176	-20.176	0.0	-0.710	-0.301
10	7	1	16.038	16.449	0.0	-0.431	-1.245	
0	7	1	37.010	30.837	0.0	-1.027	-1.372	
9	7	1	33.505	34.491	0.0	-0.976	-0.601	
1	7	1	5.168	4.061	0.0	0.0	0.200	
6	7	1	12.449	8.736	0.0	5.914	1.302	
5	7	1	20.436	18.092	18.092	0.0	1.725	0.022
4	7	1	24.720	26.419	0.0	-1.687	-0.853	
3	7	1	23.511	27.438	-27.438	0.0	-5.617	-1.751
2	7	1	14.505	15.639	0.0	-1.133	-0.381	
1	6	1	10.675	6.950	0.0	4.025	1.598	
2	6	1	8.930	6.778	0.0	2.159	0.611	
3	6	1	21.197	25.179	25.179	0.0	-4.222	-1.904
4	6	1	15.314	16.751	16.751	0.0	-0.760	-0.340
5	6	1	13.062	0.036	-4.936	0.0	5.026	3.330
8	6	1	14.093	9.302	-0.902	0.0	5.761	1.642
0	6	1	7.539	13.607	0.0	-6.260	-1.308	
11	6	1	6.630	1.227	1.227	0.0	8.712	2.606
12	6	1	8.481	1.975	-1.975	0.0	6.506	1.655
13	6	1	13.016	17.248	-17.248	0.0	-5.332	-1.083
14	6	1	11.589	11.611	-11.611	0.0	-0.022	-0.006
15	6	1	7.156	12.500	-12.500	0.0	-5.453	-1.183
16	6	1	7.152	7.469	-7.469	0.0	-0.107	-0.022
18	6	1	6.476	5.260	5.260	0.0	-0.764	-0.115
19	6	1	6.468	2.074	-2.074	0.0	7.354	1.668
21	6	1	1.399	3.117	-3.117	0.0	-1.213	-0.132
22	6	1	7.244	2.333	2.333	0.0	4.911	0.864
23	6	1	11.423	0.508	-0.508	0.0	10.415	2.605
24	6	1	0.108	5.076	-5.076	0.0	1.112	0.160
25	5	1	0.733	13.096	-13.096	0.0	-3.353	-0.598
0	6	0	326.728	334.474	0.0	-7.746	-1.281	*
23	5	1	17.202	5.600	-5.600	0.0	11.212	3.823
21	5	1	15.669	19.215	19.215	0.0	-3.516	-1.047

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STRUCTURE FACTORS

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H	K	L	F(000)	F(CFC)	$\Delta(FAL)$	B(CALC)	DELTA F	DELTA/SIGMA
10	5	1	-13.448	12.425	0.0	1.123	0.322	
10	5	1	8.349	17.109	-17.109	0.0	-8.761	-1.690
17	5	1	11.147	19.742	-19.742	0.0	0.384	0.102
16	5	1	15.051	18.861	-18.861	0.0	-3.811	-1.129
15	5	1	33.015	33.998	-33.998	0.0	-0.193	-0.118
14	5	1	44.319	42.768	-42.768	0.0	1.551	0.114
13	5	1	29.651	30.053	-30.053	0.0	-0.462	-0.272
11	5	1	9.561	8.812	-8.812	0.0	0.729	0.176
10	5	1	32.382	32.523	-32.523	0.0	-0.241	-0.159
9	5	1	36.497	35.700	-35.700	0.0	0.997	0.710
8	5	1	27.288	30.058	-30.058	0.0	-2.769	-1.564
7	5	1	65.770	66.158	-66.158	0.0	-0.388	-0.302
6	5	1	58.916	58.025	-58.025	0.0	0.889	0.733
5	5	1	74.402	74.259	-74.259	0.0	0.242	0.104
4	5	1	33.401	34.110	-34.110	0.0	-0.708	-0.564
0	5	0	327.027	334.674	-334.674	0.0	-7.447	-1.240 *
3	5	1	42.512	43.347	-43.347	0.0	-0.835	-0.742
2	5	1	56.682	59.934	-59.934	0.0	-3.151	-2.825
1	5	1	20.943	24.457	-24.457	0.0	-3.614	-2.095
0	4	1	9.718	1.481	-1.481	0.0	8.237	4.237
1	4	1	44.467	45.733	-45.733	0.0	-1.266	-1.315
2	4	1	77.565	90.760	-90.760	0.0	-3.216	-2.492
3	4	1	49.078	50.913	-50.913	0.0	-1.835	-1.819
4	4	1	45.693	49.054	-49.054	0.0	-3.061	-2.050
5	4	1	77.070	76.257	-76.257	0.0	-1.207	-0.925
6	4	1	26.148	30.747	-30.747	0.0	-1.590	-1.259
7	4	1	28.750	30.280	-30.280	0.0	-1.530	-1.152
8	4	1	15.678	14.582	-14.582	0.0	4.696	2.870
0	4	1	10.189	9.856	-9.856	0.0	0.293	0.089
11	4	1	13.115	10.876	-10.876	0.0	2.539	0.849
12	4	1	11.623	8.327	-8.327	0.0	3.205	0.984
13	4	1	11.515	11.320	-11.320	0.0	0.195	0.056
14	4	1	23.217	23.969	-23.969	0.0	-0.753	-0.393
15	4	1	15.360	16.518	-16.518	0.0	-1.158	0.389
16	4	1	27.023	28.732	-28.732	0.0	-1.709	0.871
0	6	0	324.042	314.674	-314.674	0.0	-10.431	-1.750 *
17	4	1	32.121	31.359	-31.359	0.0	-1.762	1.104
18	4	1	26.610	26.287	-26.287	0.0	0.322	0.161
19	4	1	7.553	10.582	-10.582	0.0	-3.029	-0.591
21	4	1	14.620	14.940	-14.940	0.0	-13.329	-1.353 *
22	4	1	31.594	33.589	-33.589	0.0	-2.003	-0.990
23	4	1	26.346	29.405	-29.405	0.0	-3.061	-1.172
24	4	1	18.907	17.836	-17.836	0.0	1.061	0.333
25	4	1	16.407	33.930	-33.930	0.0	-7.023	-1.758
26	4	1	21.663	17.065	-17.065	0.0	4.890	1.098
26	3	1	19.064	16.592	-16.592	0.0	2.052	0.624
25	2	1	22.685	19.016	-19.016	0.0	2.870	1.030
24	3	1	25.987	21.880	-21.880	0.0	4.007	1.899
23	3	1	30.380	31.863	-31.863	0.0	-1.475	-0.657
22	3	1	53.003	54.883	-54.883	0.0	-0.780	-0.611
21	3	1	51.704	52.470	-52.470	0.0	-0.765	-0.510
20	3	1	17.894	15.493	-15.493	0.0	2.801	0.947
10	3	1	40.984	40.288	-40.288	0.0	0.596	0.391

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
10	3	1	53.650	53.664	0.0	-0.014	-0.009	
17	3	1	75.670	75.886	0.0	-0.215	-0.147	
0	6	0	324.698	324.474	0.0	-9.776	-1.446 *	
16	3	1	22.184	25.168	0.0	-2.983	-1.307	
15	3	1	21.064	23.425	0.0	-2.362	-0.989	
14	3	1	54.562	54.480	0.0	0.053	0.039	
13	3	1	17.231	16.256	0.0	-2.025	-0.743	
12	3	1	130.307	133.004	0.0	-2.698	-1.260	
11	3	1	201.717	196.821	0.0	4.086	1.471	
10	3	1	176.136	174.846	0.0	1.290	0.650	
9	3	1	165.048	163.716	0.0	1.332	0.499	
8	3	1	67.015	64.685	0.0	-0.870	-0.702	
7	2	1	82.553	81.513	-0.113	0.0	1.446	1.061
6	3	1	157.713	151.240	156.260	0.0	1.473	0.583
5	3	1	166.664	163.824	163.824	0.0	0.841	0.310
4	2	1	55.612	50.896	50.896	0.0	4.716	4.734
3	3	1	74.621	79.423	79.423	0.0	-4.801	-3.208
2	3	1	148.615	157.160	-157.160	0.0	-2.545	-3.615
1	3	1	175.292	148.553	148.553	0.0	-13.258	-4.712 *
0	2	1	45.208	47.556	47.556	0.0	-2.346	-2.641
1	2	1	9.305	10.036	10.036	0.0	-0.730	-0.326
2	2	1	135.055	139.104	-139.104	0.0	-4.009	-1.878
3	2	1	158.285	150.373	-159.373	0.0	-1.088	-0.433
0	0	0	326.330	334.474	334.474	0.0	-0.144	-1.358 *
4	2	1	136.971	132.774	134.774	0.0	0.157	0.092
5	2	1	133.150	133.100	133.100	0.0	0.050	0.024
6	2	1	142.152	134.667	-134.667	0.0	0.406	0.329
7	2	1	101.909	96.650	96.650	0.0	2.160	1.327
8	2	1	96.008	97.261	97.261	0.0	0.827	0.519
9	2	1	66.083	63.415	-63.415	0.0	2.669	2.207
10	2	1	26.757	24.775	24.775	0.0	1.982	1.510
11	2	1	47.417	40.055	-40.055	0.0	-0.430	-0.332
12	2	1	55.205	55.681	-55.681	0.0	-0.397	-0.318
13	2	1	55.456	57.169	57.169	0.0	-1.513	-1.157
14	2	1	6.920	7.026	7.026	0.0	-0.106	-0.021
15	2	1	49.567	47.643	47.643	0.0	1.926	1.441
16	2	1	58.066	56.962	56.962	0.0	1.107	0.863
17	2	1	53.880	52.672	-52.672	0.0	1.214	0.871
18	2	1	36.293	32.901	-32.901	0.0	2.397	2.250
19	2	1	8.275	8.457	-8.457	0.0	-0.192	-0.041
20	2	1	15.330	12.833	-12.833	0.0	2.467	0.865
22	2	1	46.869	41.156	41.156	0.0	-0.207	-0.165
23	2	1	46.693	50.103	50.103	0.0	-5.413	-1.960
0	6	0	324.281	334.474	334.474	0.0	-10.183	-1.717
24	2	1	33.570	33.033	32.593	0.0	-0.006	-0.003
25	2	1	38.960	39.092	-39.092	0.0	-0.131	-0.067
26	2	1	26.866	23.943	23.943	0.0	2.903	1.347
24	1	1	6.919	6.056	-6.056	0.0	-0.137	-0.020
23	1	1	7.715	12.661	-12.661	0.0	6.054	1.111
22	1	1	8.084	4.890	-4.890	0.0	3.183	0.667
21	1	1	13.533	12.669	12.669	0.0	0.864	0.255
20	1	1	8.525	3.421	-3.421	0.0	5.102	1.183
18	1	1	8.452	4.730	-4.730	0.0	3.721	0.874

8000 CATHODELESS TITRIF 6/28/73

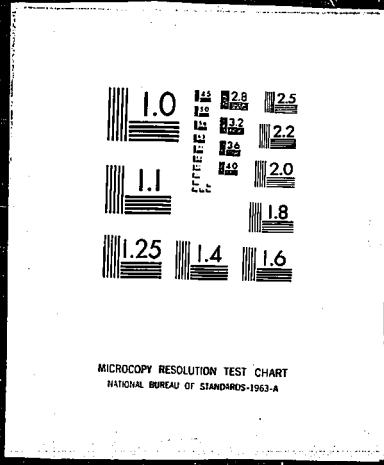
STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(FAC)	B(CALC)	DETA F	DETAZ/TIGMA
17	1	1	34.534	4.367	0.0	-0.933	-0.129	
14	1	1	31.776	33.499	0.0	-1.723	-1.166	
15	1	1	30.059	28.618	0.0	1.430	0.873	
16	1	1	34.170	35.262	0.0	-1.092	-0.724	
13	1	1	29.104	31.389	0.0	-2.285	-1.370	
12	1	1	16.471	15.190	0.0	1.481	0.648	
9	0	0	325.016	334.474	0.0	-0.458	-1.586 *	
11	1	1	17.767	13.630	-12.430	4.317	2.093	
10	1	1	13.224	17.256	-17.256	-4.033	-1.711	
8	1	1	47.817	47.486	0.0	0.331	0.338	
7	1	1	55.463	54.249	-54.249	0.514	0.501	
6	1	1	52.692	52.681	0.0	0.300	0.306	
5	1	1	85.376	84.909	0.0	0.467	0.361	
4	1	1	59.571	59.684	0.0	0.287	0.272	
3	1	1	7.598	11.457	11.457	-4.059	1.523	
2	1	1	37.659	36.048	0.0	1.610	1.910	
1	1	1	13.556	17.154	-17.154	1.802	1.652	
0	0	2	19.531	20.357	20.357	-0.827	0.692	
2	0	2	107.553	107.468	107.468	0.05	0.032	
2	0	2	163.549	161.231	-161.231	2.610	0.999	
3	0	2	210.574	217.782	217.782	-6.809	-1.964	
6	0	2	65.233	65.514	65.514	-0.281	-0.251	
5	0	2	240.590	237.041	-237.041	3.549	0.875	
6	0	2	6.390	1.651	1.651	4.739	1.560	
7	0	2	152.678	168.360	-168.360	4.628	1.470	
8	0	2	59.122	59.347	59.347	-0.224	0.191	
0	0	0	323.493	334.474	334.474	-10.491	-1.768 *	
0	0	0	175.640	173.621	173.621	1.819	0.639	
11	0	2	186.747	183.882	183.882	2.865	0.936	
12	0	2	21.373	24.000	-24.000	2.627	-1.149	
13	0	2	73.019	73.232	-73.232	0.313	-0.227	
14	0	2	5.100	3.239	3.239	1.870	0.321	
15	0	2	75.071	74.678	-74.678	0.393	0.267	
16	0	2	28.399	32.023	32.023	2.624	-1.481	
17	0	2	85.723	85.561	85.561	0.162	0.100	
18	0	2	36.760	38.418	38.418	-1.558	-0.924	
19	0	2	37.640	38.128	38.128	-0.608	-0.384	
21	0	2	22.823	22.825	-22.825	0.008	0.003	
22	0	2	71.922	75.227	75.227	-3.405	-2.147	
23	0	2	84.563	88.500	-88.500	3.936	-2.235	
24	0	2	9.276	14.520	14.520	-5.243	-0.937	
25	0	2	30.250	43.406	43.406	-5.156	-2.437	
26	0	2	25.473	23.660	23.660	1.813	0.749	
0	0	0	223.004	334.474	334.474	-10.570	-1.782 *	
24	1	2	19.914	21.207	21.207	-1.373	-0.439	
23	1	2	36.283	36.975	36.975	0.692	0.366	
22	1	2	12.222	17.692	17.692	-5.770	-1.337	
21	1	2	12.529	13.979	-13.979	-1.050	-0.283	
20	1	2	14.864	14.216	14.216	0.628	0.196	
19	1	2	15.917	15.820	-15.820	-0.003	-0.001	
12	1	2	5.168	5.413	-5.413	0.245	-0.041	
17	1	2	60.373	61.723	61.723	-1.350	-0.964	
16	1	2	92.803	93.727	93.727	-0.924	-0.707	

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POOC ORTHOPERSOLITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SEGMA
15	1	2	10.236	6.530	6.530	0.0	3.704	1.006
14	1	2	3.451	3.256	3.256	0.0	0.326	0.059
12	1	2	110.562	111.569	-111.569	0.0	-1.006	-0.343
11	1	2	110.564	109.347	-109.347	0.0	1.307	0.718
10	1	2	29.281	30.115	-30.115	0.0	-0.834	0.538
9	1	2	80.683	80.708	-80.708	0.0	0.275	0.195
4	1	2	50.021	60.240	-60.240	0.0	-2.218	1.011
7	1	2	44.526	43.275	-43.275	0.0	1.252	1.207
6	1	2	19.206	15.808	-15.808	0.0	3.309	2.620
5	1	2	103.224	101.292	-101.292	0.0	1.932	1.175
0	6	0	325.453	334.474	-334.474	0.0	-9.021	-1.511 *
4	1	2	47.906	43.730	-43.730	0.0	4.176	4.332
3	1	2	53.465	54.615	-54.615	0.0	-0.951	0.955
2	1	2	27.323	26.967	-26.967	0.0	0.366	0.400
1	1	2	60.701	60.628	-60.628	0.0	0.073	0.069
0	2	2	11.250	8.437	-8.437	0.0	2.813	1.565
1	2	2	34.766	37.417	-37.417	0.0	-2.671	-2.963
2	2	2	6.567	5.035	-5.035	0.0	1.532	0.818
3	2	2	66.265	67.995	-67.995	0.0	1.270	1.075
4	2	2	3.961	1.147	-1.147	0.0	2.814	0.654
5	2	2	27.097	26.115	-26.115	0.0	0.981	0.831
6	2	2	62.876	59.767	-59.767	0.0	3.108	2.708
7	2	2	92.817	92.132	-92.132	0.0	0.685	0.444
8	2	2	16.347	16.726	-16.726	0.0	-0.379	-0.195
9	2	2	73.932	74.130	-74.130	0.0	-0.187	-0.146
10	2	2	30.920	31.495	-31.495	0.0	-0.524	-0.395
11	2	2	20.046	18.083	-18.083	0.0	1.963	0.925
12	2	2	12.201	17.675	-17.675	0.0	-5.398	-1.595
13	2	2	34.923	34.718	-34.718	0.0	0.206	0.141
14	2	2	13.651	14.907	-14.907	0.0	-1.256	-0.391
15	2	2	27.097	30.043	-30.043	0.0	-2.047	-1.175
0	6	0	326.220	334.474	-334.474	0.0	-8.244	-1.375 *
17	2	2	14.682	16.815	-16.815	0.0	-2.132	0.717
18	2	2	40.795	40.746	-40.746	0.0	0.026	0.032
19	2	2	39.315	38.611	-38.611	0.0	0.705	0.496
21	2	2	20.710	20.660	-20.660	0.0	0.050	0.019
22	2	2	21.578	21.594	-21.594	0.0	-0.006	-0.002
25	2	2	10.823	6.003	-6.003	0.0	3.910	0.642
26	2	2	17.062	8.597	-8.597	0.0	8.072	2.513
26	3	2	6.110	1.835	-1.835	0.0	4.275	0.628
25	3	2	12.414	6.907	-6.907	0.0	5.507	1.350
26	3	2	19.619	6.058	-6.058	0.0	13.561	5.542 *
16	3	2	11.103	11.339	-11.339	0.0	-0.236	-0.080
0	6	0	324.476	334.474	-334.474	0.0	-8.498	-1.593 *
17	3	2	6.876	5.589	-5.589	0.0	0.887	0.177
16	3	2	4.024	6.650	-6.650	0.0	-2.614	-0.406
15	3	2	17.172	18.081	-18.081	0.0	-0.908	-0.376
13	3	2	13.017	4.254	-4.254	0.0	8.764	2.960
11	3	2	4.607	5.111	-5.112	0.0	-0.415	-0.070
0	3	2	18.337	16.033	-16.033	0.0	1.403	0.652
8	3	2	20.356	16.810	-16.810	0.0	3.537	2.050
6	3	2	4.950	3.651	-3.651	0.0	0.898	0.200
5	3	2	18.638	15.961	-15.961	0.0	2.876	1.628

800C CRYSTALLOGRAPHIC SITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(CALC)	F(CALC)	A(CALC)	B(CALC)	DF(T4 F)	DELTA/SIGMA
4	3	2	44.907	42.558	-47.550	0.0	2.33n	2.223
3	3	2	38.102	39.954	-39.954	0.0	-1.141	-1.029
2	3	2	6.594	7.729	-7.729	0.0	-0.435	-0.293
1	3	2	4.214	2.232	2.332	0.0	1.982	0.499
1	4	2	26.528	31.922	31.922	0.0	-2.304	-2.446
2	4	2	68.084	69.054	69.054	0.0	-1.070	-1.508
0	5	0	324.619	334.474	334.474	0.0	-6.855	-1.659 *
3	6	2	37.496	37.440	-37.440	0.0	0.056	0.050
4	4	2	8.466	0.034	0.034	0.0	-0.569	-0.171
6	4	2	28.251	28.647	28.647	0.0	-0.296	-0.163
7	4	2	33.324	37.084	-37.084	0.0	1.240	1.035
8	4	2	8.967	0.471	0.471	0.0	0.496	2.364
6	4	2	7.777	8.768	-8.768	0.0	-0.890	-0.203
10	2	2	18.183	17.316	-17.316	0.0	0.873	0.377
11	2	2	14.255	13.434	13.434	0.0	0.821	0.272
12	4	2	12.475	6.906	-6.906	0.0	5.860	1.940
13	4	2	5.727	5.305	-5.305	0.0	0.422	0.083
14	4	2	21.742	19.067	-19.067	0.0	2.675	1.395
15	2	2	6.125	0.697	0.697	0.0	5.428	1.072
16	4	2	8.746	7.160	-7.160	0.0	1.666	0.379
17	4	2	12.970	15.014	-15.014	0.0	-2.144	-0.625
18	6	2	1.758	16.661	-16.661	0.0	-0.903	-0.300
19	4	2	3.651	8.366	-8.366	0.0	-4.715	-0.644
20	4	2	6.314	1.476	1.476	0.0	4.860	0.845
22	4	2	18.704	15.364	-15.364	0.0	3.430	1.130
0	6	0	325.215	334.474	334.474	0.0	-9.250	-1.552 *
23	4	2	14.250	6.463	-6.463	0.0	7.836	2.128
24	4	2	2.630	2.378	-2.378	0.0	0.552	0.062
25	4	2	6.169	10.573	-10.573	0.0	-4.404	-0.622
24	4	2	6.174	1.706	-1.706	0.0	4.449	0.664
23	5	2	28.883	26.956	-26.956	0.0	1.896	0.898
22	5	2	17.674	17.455	-17.455	0.0	0.169	0.048
21	5	2	19.373	23.064	-23.064	0.0	-3.740	-1.153
20	5	2	8.067	11.947	-11.947	0.0	-2.990	-0.593
19	5	2	23.354	24.384	-24.384	0.0	-0.990	-0.402
17	5	2	49.018	50.612	-50.612	0.0	-1.506	-1.033
16	5	2	20.725	21.875	-21.875	0.0	-1.151	-0.431
15	5	2	28.085	31.440	-31.440	0.0	-3.364	-1.540
14	5	2	12.178	6.605	-6.605	0.0	5.492	1.662
13	5	2	27.097	29.006	-29.006	0.0	-1.910	-1.019
12	5	2	6.459	73.096	-73.096	0.0	-3.637	-2.561
11	5	2	87.004	87.378	-87.378	0.0	-0.374	-0.241
10	5	2	33.785	33.247	33.247	0.0	0.538	0.350
0	5	2	125.351	123.722	-123.722	0.0	1.620	0.786
8	5	2	30.232	80.026	80.026	0.0	0.206	0.138
0	6	0	324.201	334.474	334.474	0.0	-10.272	-1.731 *
7	2	52.373	52.392	-52.392	0.0	-0.019	0.015	
6	5	2	24.279	23.586	-22.586	0.0	0.690	0.390
5	5	2	73.463	73.528	-73.528	0.0	-0.060	-0.044
4	5	2	7.863	17.230	17.230	0.0	-9.368	-2.128
3	5	2	117.245	120.620	120.620	0.0	-3.375	-1.757
2	5	2	16.701	27.317	27.317	0.0	-5.617	-2.324
1	5	2	55.048	61.309	-61.309	0.0	-2.261	-1.787

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STRUCTURE FACTORS

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H	K	L	F(PBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	2	8.084	11.819	11.819	0.0	-2.735	-0.937
1	6	2	26.049	27.466	27.466	0.0	-1.417	-0.821
2	6	2	115.308	120.957	120.957	0.0	-4.649	-2.493
3	6	2	137.028	142.786	142.786	0.0	-5.757	-2.581
4	6	2	35.012	33.997	33.997	0.0	1.015	0.694
5	6	2	100.457	101.844	101.844	0.0	-1.387	-0.808
7	6	2	76.763	88.520	88.520	0.0	-1.759	-1.121
8	6	2	27.653	27.384	27.384	0.0	0.509	0.300
9	6	2	108.406	109.862	109.862	0.0	-1.256	-0.674
10	6	2	25.252	27.674	27.674	0.0	-2.622	-1.346
11	6	2	78.745	77.731	77.731	0.0	1.014	0.683
12	6	2	15.870	12.983	12.983	0.0	4.886	3.361
0	6	0	324.303	334.474	334.474	0.0	-10.471	-1.765 *
13	6	2	39.383	34.646	34.646	0.0	3.737	2.659
14	6	2	10.234	12.390	12.390	0.0	-2.156	-0.519
15	6	2	47.417	45.480	45.480	0.0	1.918	1.362
16	6	2	20.553	19.712	19.712	0.0	0.821	0.330
17	6	2	41.180	40.137	40.137	0.0	1.032	0.629
18	6	2	18.071	14.316	14.316	0.0	3.755	1.324
19	6	2	27.510	29.069	29.069	0.0	-1.559	-0.636
20	6	2	9.321	2.958	2.958	0.0	6.363	1.372
21	6	2	7.490	17.775	17.775	0.0	-10.235	-1.513 *
22	6	2	44.749	43.713	43.713	0.0	1.035	0.564
23	6	2	50.393	51.558	51.558	0.0	-1.174	-0.694
17	7	2	16.204	9.090	9.090	0.0	7.714	2.726
16	7	2	16.701	17.201	17.201	0.0	-0.500	-0.183
14	7	2	13.062	6.322	6.322	0.0	6.740	2.061
0	6	0	326.509	334.474	334.474	0.0	-7.955	-1.328 *
13	7	2	21.945	22.763	22.763	0.0	-0.918	-0.388
12	7	2	43.075	40.862	40.862	0.0	2.233	1.508
11	7	2	10.189	16.396	16.396	0.0	-6.195	-1.394
10	7	2	8.559	6.073	6.073	0.0	2.526	0.576
9	7	2	12.531	16.036	16.036	0.0	-3.505	-1.034
8	7	2	41.499	45.968	45.968	0.0	-4.359	-2.944
7	7	2	29.458	28.799	28.799	0.0	0.459	0.392
5	7	2	16.067	15.587	15.587	0.0	0.480	0.192
4	7	2	33.150	33.693	33.693	0.0	-0.563	-0.357
3	7	2	20.818	21.186	21.186	0.0	-0.468	-0.304
2	7	2	16.848	6.631	6.631	0.0	10.217	4.592 *
1	7	2	11.176	6.528	6.528	0.0	4.648	1.321
0	8	2	16.200	9.583	9.583	0.0	6.617	2.824
1	8	2	43.667	46.437	46.437	0.0	-2.770	-1.289
2	8	2	15.108	17.068	17.068	0.0	-2.951	-0.338
3	8	2	28.720	28.309	28.309	0.0	0.322	0.194
4	8	2	8.378	6.729	6.729	0.0	1.649	0.301
5	8	2	32.175	31.259	31.259	0.0	0.916	0.530
6	8	2	11.721	15.196	15.196	0.0	-3.475	-0.936
0	8	0	325.434	334.474	334.474	0.0	-0.040	-1.515 *
7	8	2	46.572	45.266	45.266	0.0	1.305	0.957
8	8	2	8.864	13.193	13.193	0.0	-4.329	-0.924
9	8	2	30.817	31.001	31.001	0.0	-0.185	-0.104
10	8	2	2.282	3.448	3.448	0.0	-1.166	-0.147
11	8	2	30.040	30.144	30.144	0.0	-0.095	-0.050

RGC01 PTHOLEFESTOSILITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OFF)	F(C/LC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	8	2	11.627	5.026	-5.926	0.0	6.002	1.650
13	9	2	29.281	31.476	-31.426	0.0	-2.145	-1.061
14	8	2	14.967	9.476	-9.445	0.0	5.301	1.826
15	4	2	19.472	17.048	-17.048	0.0	2.424	0.899
16	8	2	5.419	0.354	-0.354	0.0	5.945	0.875
17	9	2	5.727	10.159	10.159	0.0	-6.431	-0.542
18	8	2	5.021	14.446	-14.446	0.0	-6.425	-1.250
19	8	2	17.408	19.015	19.015	0.0	-1.607	-0.468
20	6	2	8.761	2.295	-2.295	0.0	-0.534	-0.995
21	8	2	6.483	14.186	-14.186	0.0	-6.733	-0.820
19	9	2	9.768	12.496	-12.496	0.0	-2.749	-0.517
18	9	2	6.851	2.735	-2.735	0.0	7.116	1.492
17	9	2	14.191	8.125	-8.125	0.0	6.056	1.383
16	9	2	6.547	10.482	-10.482	0.0	-5.535	-0.767
15	9	2	6.743	8.578	-8.578	0.0	-1.835	-0.302
0	6	0	320.110	334.474	334.474	0.0	-8.364	-11.395 *
14	9	2	15.610	4.658	-4.658	0.0	10.953	3.379 *
13	9	2	16.229	4.823	-4.823	0.0	11.406	3.870 *
12	9	2	12.017	6.540	-6.540	0.0	6.478	1.817
11	9	2	6.569	11.999	-11.999	0.0	-2.930	-0.461
9	5	2	6.346	6.786	-6.786	0.0	-0.460	-0.077
8	0	2	6.037	2.754	-2.754	0.0	3.253	0.581
6	9	2	13.445	0.073	0.073	0.0	13.372	4.631 *
5	9	2	13.342	11.094	-13.094	0.0	0.246	0.078
3	9	2	8.960	12.619	-12.619	0.0	-3.770	-0.856
2	9	2	12.738	9.623	-9.623	0.0	3.114	0.961
1	9	2	11.000	7.201	-7.201	0.0	3.709	1.079
0	10	2	7.568	3.220	-3.220	0.0	6.346	0.887
2	10	2	25.672	25.519	-25.519	0.0	0.353	0.163
3	10	2	22.926	24.491	-24.491	0.0	-1.555	-0.624
4	10	2	12.458	8.684	-8.684	0.0	3.774	1.109
5	10	2	11.613	13.555	-13.555	0.0	-1.942	-0.479
0	6	0	324.429	334.474	334.474	0.0	-10.034	-1.690 *
6	10	2	11.586	15.840	-15.840	0.0	-4.251	-1.009
8	10	2	10.351	8.245	-8.245	0.0	2.006	0.459
0	10	2	3.999	10.038	-10.038	0.0	-6.048	-0.901
10	10	2	8.462	3.422	-3.422	0.0	5.030	1.005
11	10	2	17.246	16.493	-16.493	0.0	-1.247	-0.397
12	10	2	5.245	2.473	-2.473	0.0	2.871	0.420
13	10	2	15.640	7.762	-7.762	0.0	7.878	2.546
14	10	2	9.748	6.593	-6.593	0.0	3.156	0.612
15	10	2	6.284	11.095	-11.095	0.0	-6.811	-0.835
16	10	2	7.185	5.005	-5.005	0.0	2.191	0.352
17	10	2	17.762	15.616	-15.616	0.0	-2.145	0.622
13	11	2	15.095	6.446	-6.446	0.0	8.619	2.500
12	11	2	34.584	35.403	35.403	0.0	-1.019	-0.496
11	11	2	38.546	34.566	-34.566	0.0	3.200	2.054
10	11	2	14.859	15.044	15.044	0.0	-0.185	-0.049
9	11	2	47.476	47.480	-47.480	0.0	-0.004	-0.002
8	11	2	25.783	30.031	30.031	0.0	-4.248	-1.568
7	11	2	21.734	21.897	-21.897	0.0	0.037	0.013
0	6	0	324.539	334.474	334.474	0.0	-9.935	-1.673 *
6	11	2	13.253	2.989	-2.989	0.0	10.264	2.832 *

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	11	2	35.860	32.648	0.0	3.197	1.663	
4	11	2	10.779	2.507	0.0	8.271	1.984	
3	11	2	35.226	38.204	0.0	1.022	0.576	
1	11	2	7.701	16.404	-16.04	0.0	-8.703	-1.481
0	12	2	11.780	4.271	-4.271	0.0	7.509	1.834
-1	12	2	9.439	1.025	1.025	0.0	8.014	1.934
2	12	2	33.453	23.117	-33.117	0.0	0.836	0.256
3	12	2	28.828	30.584	30.884	0.0	-2.046	-0.540
4	12	2	6.302	10.193	-10.193	0.0	-3.552	-0.553
5	12	2	17.791	16.019	-16.019	0.0	1.773	0.554
6	12	2	11.795	8.866	-8.866	0.0	2.929	0.688
7	12	2	10.351	7.342	-7.342	0.0	3.010	0.619
8	12	2	17.526	10.263	-10.263	0.0	-1.726	-0.466
10	12	2	11.471	5.304	-5.304	0.0	6.167	1.333
11	12	2	21.152	16.849	-16.849	0.0	4.303	1.640
4	13	2	19.118	11.651	-11.651	0.0	7.427	2.624
3	13	2	11.883	3.887	-3.887	0.0	7.896	1.675
0	6	0	325.652	334.474	334.474	0.0	-0.822	-1.478 *
2	13	2	2.683	2.222	-2.222	0.0	0.456	0.046
1	13	2	18.027	13.490	-13.490	0.0	4.337	1.429
0	12	3	15.597	14.967	-14.967	0.0	0.540	0.144
1	12	3	10.638	5.215	-5.215	0.0	5.553	1.225
3	12	3	1.970	2.454	-2.454	0.0	-0.554	-0.060
4	12	3	6.481	3.733	-3.733	0.0	4.748	0.862
11	11	3	17.821	6.960	-6.960	0.0	10.861	3.666 *
10	11	3	28.115	28.771	-28.771	0.0	-0.657	-0.256
8	11	3	17.526	11.159	-11.159	0.0	6.327	2.116
7	11	3	9.527	9.428	-9.428	0.0	0.090	0.020
6	11	3	16.480	13.424	-13.424	0.0	3.046	0.935
5	11	2	10.638	12.513	-12.513	0.0	-1.705	-0.349
3	11	3	15.163	11.329	-11.329	0.0	3.854	1.076
0	6	0	324.201	334.474	334.474	0.0	-10.272	-1.731 *
2	11	3	34.565	31.362	-31.362	0.0	3.206	1.619
11	11	3	11.854	5.862	-5.862	0.0	5.952	1.453
0	10	3	15.095	14.237	-14.237	0.0	0.858	0.251
1	10	3	8.511	6.631	-6.631	0.0	3.880	0.775
2	10	3	9.712	2.334	-2.334	0.0	6.896	1.516
3	10	3	20.504	19.446	-19.446	0.0	1.010	0.396
4	10	3	30.797	35.927	-35.927	0.0	2.871	1.688
8	10	2	14.181	2.947	-2.947	0.0	11.234	3.359 *
10	10	3	17.600	0.339	-0.339	0.0	17.261	4.655 *
11	10	3	5.201	10.149	-10.149	0.0	-4.348	-0.569
12	10	3	6.321	2.226	-2.226	0.0	4.105	0.618
13	10	3	4.156	0.336	-0.336	0.0	3.060	0.486
17	9	3	14.255	7.056	-7.056	0.0	7.199	1.830
16	9	3	5.801	1.425	-1.425	0.0	4.376	0.630
0	6	0	325.812	334.474	334.474	0.0	-8.662	-1.451 *
15	9	3	11.441	10.724	-10.724	0.0	0.718	0.149
14	9	3	76.475	77.018	-77.018	0.0	-0.343	-0.196
13	9	3	28.839	29.558	-29.558	0.0	-0.720	-0.204
17	9	3	8.290	8.050	-8.050	0.0	0.249	0.047
10	9	3	18.057	15.250	-15.250	0.0	2.806	0.952
9	9	3	9.085	1.468	-1.468	0.0	7.617	1.621

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STRUCTURE FACTORS

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H	K	I	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	0	3	8.260	1.160	-1.100	0.0	7.100	1.378
7	0	3	18.175	16.553	16.693	0.0	1.522	0.530
6	0	3	60.477	55.587	55.587	0.0	1.950	1.269
5	0	3	15.213	12.596	-12.486	0.0	2.227	0.741
2	0	3	53.501	55.076	-55.076	0.0	-1.575	-1.000
1	0	3	40.706	41.549	41.549	0.0	-0.643	-0.529
0	4	2	130.757	132.994	132.994	0.0	-2.227	-1.015
1	0	3	34.214	36.283	36.283	0.0	-2.069	-1.157
2	0	3	4.453	6.160	-6.160	0.0	-1.507	-0.233
3	0	3	11.324	14.848	14.848	0.0	-3.524	-0.896
4	0	3	25.172	24.776	-24.776	0.0	0.993	0.538
0	6	0	325.354	334.474	334.474	0.0	-9.120	-1.520 *
5	0	3	15.055	20.636	-20.636	0.0	-5.542	-1.679
7	0	3	30.034	40.403	-40.403	0.0	-1.368	-0.833
6	0	3	60.075	60.175	60.175	0.0	-0.100	-0.067
10	0	3	8.084	1.073	1.073	0.0	6.110	1.273
12	0	3	47.728	46.307	-46.307	0.0	1.421	0.939
13	0	3	22.317	24.083	-24.083	0.0	-1.766	-0.658
15	0	3	21.160	21.761	-21.761	0.0	0.099	0.035
16	0	3	24.100	24.274	24.274	0.0	-0.084	-0.033
17	0	3	13.621	5.193	5.193	0.0	8.428	2.354
19	0	3	22.602	24.626	24.626	0.0	-1.737	-0.598
21	0	2	10.121	3.147	3.147	0.0	6.983	1.391
19	0	3	15.061	7.261	7.261	0.0	8.600	2.702
0	6	0	324.420	334.474	334.474	0.0	-10.054	-1.653 * -40
15	7	3	8.509	4.815	-4.815	0.0	5.764	0.765
14	7	3	43.282	41.102	-41.102	0.0	2.180	1.443
13	7	3	12.826	15.944	15.944	0.0	-3.118	-0.624
12	7	3	9.777	4.537	-4.537	0.0	5.240	1.227
10	7	2	22.109	20.855	-20.855	0.0	1.344	0.577
7	7	2	15.920	12.544	-12.544	0.0	2.976	1.181
6	7	3	31.456	32.417	-32.417	0.0	-0.921	-0.520
4	7	3	10.101	10.303	10.303	0.0	-0.202	-0.052
2	7	2	11.780	7.187	7.187	0.0	4.593	1.471
1	7	3	20.459	15.950	-15.950	0.0	4.506	2.353
1	4	2	4.064	0.236	0.236	0.0	3.828	0.602
2	6	3	6.247	9.689	9.689	0.0	-0.442	-0.111
0	5	0	324.400	334.474	334.474	0.0	-10.074	-1.697 * --
5	6	3	0.457	12.655	12.655	0.0	-2.958	-0.828
7	6	3	7.229	9.131	9.131	0.0	-1.902	-0.419
8	6	3	28.023	28.047	-28.047	0.0	0.777	0.470
9	6	3	8.452	8.952	-8.952	0.0	-0.500	-0.113
14	6	3	15.154	3.078	-3.078	0.0	12.076	4.553 *
15	6	3	7.377	1.130	1.130	0.0	6.247	1.268
16	6	3	11.357	4.314	4.314	0.0	7.053	1.676
15	6	3	4.226	0.728	-0.728	0.0	3.496	0.460
20	6	3	1.090	12.741	12.741	0.0	-11.651	-1.081 *
23	6	3	6.443	3.523	3.523	0.0	2.960	0.448
0	6	0	324.477	334.474	334.474	0.0	-9.597	-1.610 *
22	5	3	20.223	13.492	13.492	0.0	6.731	2.504
20	5	3	11.204	4.740	4.740	0.0	7.054	1.669
18	5	3	29.311	27.826	-27.826	0.0	1.485	0.751
17	5	3	22.007	23.165	23.165	0.0	-1.156	-0.454

BUOC CATHODEPROSOLITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
15	5	3	8.473	14.126	14.126	0.0	-5.453	-1.029
14	5	3	24.205	24.051	24.051	0.0	-0.157	-0.347
11	5	3	16.651	18.680	18.680	0.0	-2.129	-0.599
10	5	3	61.682	62.126	62.126	0.0	-0.144	-0.104
9	5	3	23.541	21.239	21.239	0.0	2.302	1.369
8	5	3	10.617	4.073	4.073	0.0	4.543	2.019
6	5	3	11.191	0.602	0.602	0.0	10.599	2.956 *
5	5	3	30.035	31.318	31.318	0.0	-0.383	-0.243
4	5	3	14.753	5.531	5.531	0.0	9.172	3.311
3	5	3	31.068	27.337	27.337	0.0	4.731	2.526
0	6	0	325.473	334.474	334.474	0.0	-9.001	-1.508 *
2	5	3	84.095	80.985	80.985	0.0	-4.090	-2.663
1	5	3	29.753	28.534	28.534	0.0	1.220	0.772
0	4	3	133.643	145.584	145.584	0.0	-11.661	-5.343 *
1	4	3	27.451	29.809	29.809	0.0	-2.359	-1.416
2	4	3	8.290	4.509	4.509	0.0	3.791	0.940
3	4	3	14.888	14.238	14.238	0.0	0.651	0.238
4	4	3	34.052	35.310	35.310	0.0	-1.258	-0.835
5	4	3	12.178	11.221	11.221	0.0	0.957	0.293
7	4	3	17.000	18.426	18.426	0.0	-0.546	-0.217
8	4	3	28.425	23.275	23.275	0.0	5.150	3.143
9	4	3	11.572	10.792	10.792	0.0	1.170	0.348
10	4	3	15.006	15.069	15.069	0.0	-0.062	-0.024
11	4	3	13.017	9.683	9.683	0.0	3.335	1.073
12	4	3	42.157	45.506	45.506	0.0	-3.439	-2.233
13	4	3	30.093	25.652	25.652	0.0	4.441	2.811
14	4	3	8.614	5.496	5.496	0.0	3.117	0.761
15	4	3	9.036	16.560	16.560	0.0	-7.724	-1.502
16	4	3	5.521	3.250	3.250	0.0	2.271	0.378
17	4	3	5.536	3.374	3.374	0.0	2.162	0.362
0	6	0	325.175	334.474	334.474	0.0	-1.559	-0.559 *
20	4	3	40.839	41.685	41.685	0.0	-0.846	-0.436
21	4	3	9.703	5.840	5.840	0.0	3.844	0.800
22	4	3	4.873	7.617	7.617	0.0	-2.743	-0.359
23	4	3	17.379	12.896	12.896	0.0	4.492	1.401
24	4	3	10.656	21.356	21.356	0.0	-1.400	-0.699
23	3	1	1.614	5.587	5.587	0.0	-3.933	-0.371
22	3	3	40.551	28.802	28.802	0.0	1.769	0.705
21	3	3	38.472	40.619	40.619	0.0	-2.146	-1.142
20	3	3	5.399	5.291	5.291	0.0	0.698	0.015
19	3	3	26.536	27.220	27.220	0.0	-0.685	-0.316
18	3	3	60.677	69.913	69.913	0.0	-1.336	-0.931
17	3	3	27.523	26.325	26.325	0.0	1.398	0.473
16	3	3	11.353	12.056	12.056	0.0	-0.703	-0.185
15	3	3	27.111	29.362	29.362	0.0	-2.250	-1.010
14	3	3	170.006	171.394	171.394	0.0	-0.478	-0.172
13	3	3	66.695	66.441	66.441	0.0	0.254	0.011
12	3	3	17.673	14.327	14.327	0.0	2.846	1.230
0	6	0	326.449	334.474	334.474	0.0	-8.025	-1.535 *
11	3	3	21.706	21.413	21.413	0.0	0.373	0.181
10	3	3	10.837	5.729	5.729	0.0	5.108	1.355
9	3	3	24.618	24.638	24.638	0.0	-0.020	-0.010
8	3	3	1.207	4.898	4.898	0.0	-3.670	-0.440

ROSC CATHODEFESTITE 6/29/73							STRUCTURE FACTORS		PAGE 16
H	K	L	F(OBS)	F(CALC)	A(FAC)	B(FAC)	DELTA F	DELTA/SIGMA	
7	3	3	53.109	54.175	54.175	0.0	-0.986	-0.737	
6	2	2	101.118	100.129	100.129	0.0	1.690	0.537	
5	3	3	65.009	65.161	65.161	0.0	-0.132	-0.102	
4	3	3	18.351	17.925	17.925	0.0	0.421	0.167	
3	2	3	24.726	29.443	28.443	0.0	-6.017	-2.179	
2	3	3	186.536	191.063	191.063	0.0	-5.507	-1.321	
1	3	3	111.291	117.734	117.734	0.0	-6.453	-2.564	
0	2	3	242.112	264.742	264.742	0.0	-22.830	-8.648 *	
1	2	3	65.414	71.655	71.655	0.0	-2.241	-1.785	
3	2	3	25.075	23.618	23.618	0.0	1.457	0.959	
4	2	3	29.473	29.479	29.479	0.0	-0.007	-0.005	
5	2	3	27.256	28.181	28.181	0.0	-0.922	-0.584	
6	2	3	4.505	6.244	6.244	0.0	-1.710	-0.108	
7	2	3	53.764	51.013	51.013	0.0	2.251	1.026	
8	2	3	75.206	73.925	73.925	0.0	1.231	0.900	
0	0	0	323.824	336.474	336.474	0.0	-10.645	-1.705 *	
10	2	3	15.507	12.417	12.417	0.0	3.090	1.140	
11	2	3	56.816	1.692	1.692	0.0	3.823	0.693	
12	2	3	87.803	87.514	87.514	0.0	0.283	0.181	
13	2	3	42.053	43.952	43.952	0.0	-1.799	-1.115	
14	2	3	8.805	7.075	7.075	0.0	1.730	0.400	
15	2	3	37.215	36.244	36.244	0.0	0.966	0.680	
16	2	3	32.010	34.910	34.910	0.0	-2.100	-1.236	
17	2	3	13.621	55.652	55.652	0.0	7.959	2.672	
18	2	3	12.031	1.926	1.926	0.0	10.105	5.949 *	
19	2	3	26.016	29.397	29.397	0.0	-3.361	-1.574	
20	2	3	76.030	76.006	76.006	0.0	-0.775	-0.479	
21	2	3	15.931	11.585	11.585	0.0	4.246	1.328	
24	2	3	17.939	15.051	15.051	0.0	2.887	0.951	
25	2	3	6.007	4.452	4.452	0.0	1.356	0.196	
25	1	2	5.219	8.227	8.227	0.0	-2.409	-0.350	
23	1	3	9.453	0.310	0.310	0.0	9.134	1.837	
0	6	0	323.130	336.474	336.474	0.0	-11.345	-1.921 *	
22	1	3	8.878	6.862	6.862	0.0	-5.969	-0.569	
21	1	3	12.193	4.180	4.180	0.0	8.013	2.084	
10	1	3	9.010	8.586	8.586	0.0	1.324	0.311	
18	1	3	24.220	22.547	22.547	0.0	1.672	0.904	
17	1	3	20.327	24.965	24.965	0.0	-3.738	-1.433	
16	1	3	4.270	4.763	4.763	0.0	-0.493	-0.078	
15	1	3	13.901	6.546	6.546	0.0	7.356	2.642	
14	1	3	16.097	11.604	11.604	0.0	4.493	1.871	
13	1	3	2.253	4.183	4.183	0.0	-1.931	-0.244	
11	1	3	14.137	13.560	13.560	0.0	0.560	0.153	
10	1	3	60.499	50.372	50.372	0.0	2.597	1.959	
8	1	3	20.386	22.777	22.777	0.0	-2.591	-1.156	
7	1	3	11.441	7.300	7.300	0.0	4.142	1.326	
6	1	3	19.254	15.715	15.715	0.0	3.638	1.928	
5	1	3	27.392	26.724	26.724	0.0	0.668	0.427	
4	1	3	26.105	35.667	35.667	0.0	0.320	0.204	
3	1	3	74.205	74.560	74.560	0.0	-0.376	-0.241	
0	6	0	323.646	336.474	336.474	0.0	-10.341	-1.026 *	
2	1	3	65.392	67.669	67.669	0.0	-1.087	-0.877	
1	1	3	13.942	17.867	17.867	0.0	-4.025	-1.666	

R002 FRTHOEFERFOSILITE 6/20/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	0	4	110.413	110.425	0.0	0.988	0.502	
1	0	4	51.393	53.461	-53.461	0.0	-2.066	-1.465
2	0	4	60.150	61.266	61.266	0.0	-1.117	-0.843
3	0	4	110.088	108.721	108.721	0.0	1.358	0.745
4	0	4	186.268	190.276	190.276	0.0	6.012	1.965
5	0	4	85.079	86.365	-86.365	0.0	-0.386	-0.247
6	0	4	9.173	7.915	7.915	0.0	1.250	0.292
7	0	4	78.775	76.898	-76.898	0.0	-1.123	-0.771
8	0	4	135.495	133.636	-133.636	0.0	1.849	0.826
9	0	4	28.144	30.703	30.703	0.0	-2.550	-1.421
10	0	4	32.692	30.392	-30.392	0.0	2.300	1.693
11	0	4	29.370	31.675	-31.675	0.0	-2.306	-1.324
12	0	4	103.635	102.491	102.491	0.0	1.154	0.643
13	0	4	57.222	54.092	-54.092	0.0	2.329	1.709
15	0	4	27.649	25.227	-25.227	0.0	2.622	1.377
16	0	4	89.085	88.811	-88.811	0.0	0.275	0.163
17	0	4	33.372	35.693	35.693	0.0	-2.311	-1.142
0	6	0	326.380	334.474	334.474	0.0	-10.094	-1.707 *
18	0	4	19.516	17.299	-17.299	0.0	2.217	0.775
19	0	4	4.550	10.875	10.875	0.0	-6.325	-0.841
20	0	6	31.171	34.032	34.032	0.0	-2.961	-1.203
21	0	4	10.926	9.449	9.449	0.0	1.477	0.324
22	0	4	16.678	12.451	-12.451	0.0	4.426	1.267
23	0	4	33.062	30.510	-30.510	0.0	2.551	1.360
23	1	4	18.425	3.602	-3.602	0.0	14.823	5.496 *
22	1	4	29.517	27.420	-27.420	0.0	2.097	0.973
21	1	4	8.304	12.558	-12.558	0.0	-2.763	-0.726
19	1	4	9.972	15.145	-15.145	0.0	-14.198	-1.337 *
18	1	4	28.506	27.756	-27.756	0.0	1.230	0.571
17	1	4	6.994	8.591	8.591	0.0	-1.587	-0.274
16	1	4	11.279	12.008	12.008	0.0	-0.729	-0.185
15	1	4	9.554	10.802	-10.802	0.0	-0.659	-0.195
14	1	4	15.262	13.495	-13.495	0.0	1.757	0.611
12	1	4	28.454	28.291	28.291	0.0	0.164	0.082
11	1	4	73.618	76.110	-76.110	0.0	-2.492	-1.716
10	1	4	80.307	78.429	-78.429	0.0	1.978	1.250
0	6	0	323.527	334.474	334.474	0.0	-10.547	-1.845 *
9	1	4	44.156	43.133	43.133	0.0	1.023	0.768
8	1	4	30.757	28.094	28.094	0.0	2.663	1.655
7	1	4	28.440	26.259	-26.259	0.0	2.181	1.285
6	1	4	44.201	44.179	-44.179	0.0	0.022	0.016
5	1	4	25.105	26.327	26.327	0.0	-1.222	-0.614
4	1	4	15.183	15.438	15.438	0.0	-0.255	-0.099
3	1	4	5.055	2.624	-2.624	0.0	2.440	0.427
2	1	4	50.554	55.166	55.166	0.0	0.389	0.297
1	1	4	75.570	74.350	74.350	0.0	-2.350	-1.654
0	2	4	64.427	67.759	-67.759	0.0	-3.332	-2.482
1	2	4	49.686	53.787	53.787	0.0	-4.101	-3.004
2	2	4	17.231	16.715	-16.715	0.0	0.516	0.206
3	2	4	11.101	8.766	8.766	0.0	2.425	0.677
4	2	4	32.014	33.390	33.390	0.0	-0.466	-0.277
5	2	4	30.448	38.880	38.880	0.0	0.568	0.413
6	2	4	14.314	9.639	-9.639	0.0	4.675	1.556

800C CATHODEFOSSTITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	2	4	13.297	13.444	0.0	-0.147	-0.046	
8	2	4	39.533	38.370	-38.370	0.0	1.453	1.041
9	2	4	16.978	16.714	16.714	0.0	0.164	0.062
0	4	0	324.457	334.474	334.474	0.0	-9.417	-1.413 *
11	2	4	13.047	12.050	12.050	0.0	0.998	0.318
12	2	4	32.043	32.781	32.781	0.0	0.162	0.091
13	2	4	22.751	23.036	23.036	0.0	-0.085	-0.019
14	2	4	20.415	18.031	18.031	0.0	1.484	0.458
15	2	4	4.902	6.468	6.468	0.0	-1.565	-0.268
16	2	4	13.533	15.384	-15.384	0.0	-1.851	-0.503
18	2	4	11.827	11.262	11.262	0.0	10.665	2.839 *
20	2	4	26.424	21.238	21.238	0.0	5.397	2.518
21	2	4	11.332	9.840	-9.840	0.0	1.099	0.468
22	3	4	7.612	3.236	-3.236	0.0	4.376	0.727
21	3	4	11.562	5.224	-5.224	0.0	6.719	1.505
20	3	4	2.621	3.914	-3.914	0.0	-1.293	-0.146
19	3	4	8.731	8.652	-8.652	0.0	0.080	0.015
17	3	4	9.615	3.675	-3.675	0.0	5.900	1.211
0	7	0	324.474	334.474	334.474	0.0	-9.477	-1.623 *
15	3	4	13.301	12.793	-12.793	0.0	1.110	0.324
14	3	4	7.465	3.796	-3.796	0.0	3.669	0.733
13	3	4	13.268	6.710	-6.710	0.0	3.549	1.137
12	3	4	9.998	0.663	0.663	0.0	0.355	2.353
11	3	4	3.560	2.102	-2.102	0.0	1.356	0.373
0	3	4	14.325	13.391	13.391	0.0	0.835	0.271
7	3	4	21.226	23.227	23.227	0.0	-2.001	-0.569
6	3	4	12.355	4.420	-4.420	0.0	7.035	2.748
4	3	4	12.561	5.635	-5.635	0.0	5.026	1.871
3	3	4	5.330	2.463	2.463	0.0	2.967	0.493
2	3	4	14.196	6.050	-6.050	0.0	6.146	2.077
1	2	4	7.053	14.866	-14.866	0.0	7.793	-1.512
0	4	4	29.144	30.022	-30.022	0.0	-1.877	-1.026
2	4	4	8.530	0.000	-0.000	0.0	-0.152	-0.036
3	4	4	13.283	11.154	-11.154	0.0	2.128	0.588
4	4	4	10.381	7.000	-7.000	0.0	0.581	0.163
0	6	0	324.618	334.474	334.474	0.0	-9.855	-1.659 *
5	4	4	28.455	27.426	27.426	0.0	1.024	0.627
6	4	4	13.238	12.385	-12.385	0.0	0.853	0.285
7	4	4	11.854	5.997	-5.997	0.0	2.946	0.346
6	4	4	6.181	3.034	-3.034	0.0	3.147	0.420
9	4	4	27.620	27.022	27.022	0.0	0.606	0.320
10	4	4	15.635	12.693	-12.693	0.0	3.441	1.250
11	4	4	7.436	6.880	-6.880	0.0	2.057	0.445
12	4	4	9.061	9.935	9.935	0.0	3.106	0.703
13	4	4	19.280	15.446	15.446	0.0	3.034	1.626
14	4	4	16.530	15.717	15.717	0.0	0.822	0.242
15	4	4	25.046	24.859	24.859	0.0	0.087	0.038
17	4	4	10.543	6.389	-6.389	0.0	4.256	0.849
18	4	4	6.773	6.261	-6.261	0.0	1.512	0.242
19	4	4	15.655	16.112	16.112	0.0	-3.457	-0.931
21	4	4	16.250	21.547	-21.547	0.0	-5.208	-1.435
21	5	4	24.928	25.959	25.959	0.0	-1.032	-0.414
20	5	4	9.512	1.569	1.569	0.0	7.943	1.554

800C ORTHOPEROVOSILITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	0	323.785	334.474	334.474	0.0	-10.689	-1.802 *
19	5	4	29.753	29.071	29.071	0.0	0.682	0.208
18	5	4	35.523	36.557	36.557	0.0	-1.265	-0.606
17	5	4	10.115	14.254	14.254	0.0	-4.139	-0.824
16	5	4	12.045	8.330	8.330	0.0	3.715	0.876
15	5	4	19.101	16.907	16.907	0.0	1.194	0.422
14	5	4	30.728	30.773	30.773	0.0	-0.045	-0.023
13	5	4	23.477	24.405	24.405	0.0	-0.938	-0.350
12	5	4	33.520	36.025	36.025	0.0	-2.505	-1.285
11	5	4	69.115	66.478	66.478	0.0	2.637	1.720
10	5	4	83.603	88.356	88.356	0.0	-0.246	0.147
9	5	4	46.472	48.562	48.562	0.0	-1.991	-1.255
8	5	4	16.468	16.739	16.739	0.0	0.059	0.021
7	5	4	11.734	10.057	10.057	0.0	1.679	0.439
6	5	4	59.937	60.305	60.305	0.0	-0.468	-0.339
4	5	4	11.353	1.327	1.327	0.0	10.026	2.747 *
3	5	4	8.908	4.939	4.939	0.0	3.962	0.987
2	5	4	77.785	79.858	79.858	0.0	-2.063	-1.403
1	5	4	46.048	49.276	49.276	0.0	-3.209	-2.303
0	6	4	55.478	55.540	55.540	0.0	-0.070	-0.054
0	6	0	325.003	334.474	334.474	0.0	-19.471	-1.765 *
1	6	4	14.962	14.165	14.165	0.0	0.797	0.260
2	6	4	33.387	33.436	33.436	0.0	-0.050	-0.029
3	6	4	61.445	61.076	61.076	0.0	0.370	0.273
4	6	4	103.493	101.027	101.027	0.0	2.556	1.356
5	6	4	45.169	45.341	45.341	0.0	-0.192	-0.132
7	6	4	24.677	25.620	25.620	0.0	-0.944	-0.421
8	6	4	73.663	72.727	72.727	0.0	0.936	0.631
10	6	4	19.250	11.923	11.923	0.0	7.728	3.236
12	6	4	59.122	56.308	56.308	0.0	2.814	1.997
13	6	4	47.224	48.251	48.251	0.0	-1.027	-0.647
15	6	4	25.450	26.975	26.975	0.0	-1.325	-0.507
16	6	4	50.354	53.322	53.322	0.0	-2.968	-1.587
17	6	4	19.737	24.516	24.516	0.0	-4.779	-1.385
18	6	4	18.396	16.270	16.270	0.0	2.126	0.699
20	6	4	9.438	18.866	18.866	0.0	-9.428	-1.462
0	6	0	325.672	334.474	334.474	0.0	-8.202	-1.574 *
19	7	4	8.834	10.121	10.121	0.0	-1.297	-0.215
16	7	4	22.096	14.167	14.167	0.0	7.929	3.073
15	7	4	28.764	29.134	29.134	0.0	-0.340	-0.141
14	7	4	8.157	12.984	12.984	0.0	-4.826	-0.792
13	7	4	19.133	13.682	13.682	0.0	5.451	2.032
12	7	4	6.792	16.761	16.761	0.0	-6.960	-1.352
11	7	4	20.802	29.492	29.492	0.0	6.610	0.428
10	7	4	16.457	16.108	16.108	0.0	0.549	0.196
9	7	4	25.975	23.697	23.697	0.0	2.278	1.087
8	7	4	18.263	17.287	17.287	0.0	0.976	0.366
6	7	4	7.695	10.852	10.852	0.0	-2.857	-0.559
5	7	4	6.169	13.994	13.994	0.0	-7.825	-1.369
3	7	4	16.318	11.351	11.351	0.0	4.967	1.973
1	7	4	8.967	14.827	14.827	0.0	-5.860	-1.224
0	8	4	42.853	43.993	43.993	0.0	-1.140	-0.797
0	6	0	322.002	334.474	334.474	0.0	-12.472	-2.123 *

ROUC CATHODE/CONCRETE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(ORG)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA		
1	P	4	14.409	10.960	10.960	0.0	3.649	1.141		
2	S	4	7.524	3.420	-3.420	0.0	4.104	0.766		
3	R	4	0.070	11.578	11.508	0.0	-2.538	-0.527		
4	P	4	29.827	30.726	30.726	0.0	-0.899	-0.454		
6	S	4	8.363	9.599	-9.599	0.0	-1.236	-0.255		
7	R	4	0.120	9.436	-9.436	0.0	-0.307	-0.052		
8	S	4	31.370	31.915	-31.915	0.0	-0.537	-0.273		
9	R	4	20.636	24.800	24.800	0.0	-4.164	-1.351		
10	R	4	14.661	8.029	-8.029	0.0	6.432	1.923		
11	S	4	8.407	2.235	2.235	0.0	6.172	1.198		
12	R	4	26.462	27.322	27.322	0.0	-0.860	-0.343		
14	S	4	13.297	9.177	-9.177	0.0	4.121	0.988		
15	S	4	10.690	3.553	3.553	0.0	7.137	1.468		
16	P	4	25.344	17.025	-17.025	0.0	9.319	5.053		
17	S	4	7.259	0.307	-0.307	0.0	6.862	1.047		
0	S	0	322.576	334.474	334.474	0.0	-11.898	-2.017	*	
12	S	6	7.427	4.637	-4.637	0.0	2.990	0.493		
10	S	4	12.675	11.265	11.255	0.0	1.414	0.346		
6	S	4	9.746	12.558	12.558	0.0	-4.212	-0.732		
8	S	4	9.512	2.168	2.168	0.0	7.364	1.475		
7	S	4	4.092	4.084	4.084	0.0	-0.035	-0.005		
5	P	4	10.086	7.544	7.544	0.0	2.542	0.572		
4	S	4	4.859	2.016	2.016	0.0	2.863	0.414		
3	S	4	7.818	9.620	-9.620	0.0	-1.802	-0.315		
2	S	4	10.307	11.762	11.762	0.0	-1.454	-0.328		
0	T	4	15.272	1.066	-1.066	0.0	14.206	4.591	*	
1	T	10	15.802	13.031	11.031	0.0	4.771	1.372		
2	T	10	9.365	8.641	-8.641	0.0	0.724	0.145		
3	T	10	17.762	16.792	-16.792	0.0	0.970	0.326		
4	T	10	16.407	20.450	-20.450	0.0	-3.563	-0.977		
5	T	10	19.059	17.367	17.367	0.0	1.192	0.397		
6	T	10	12.885	4.586	-4.586	0.0	8.269	2.103		
7	T	10	2.753	6.345	6.345	0.0	-3.592	-0.407		
0	S	0	322.725	334.474	334.474	0.0	-10.740	-1.812	*	
4	T	10	2.473	3.716	3.716	0.0	-1.243	-0.137		
10	T	10	13.194	0.163	-0.163	0.0	13.032	3.326	*	
11	T	10	10.322	3.957	3.857	0.0	6.465	1.359		
8	T	11	4	10.720	8.520	-8.520	0.0	2.200	0.446	
7	T	11	4	14.019	2.536	2.536	0.0	11.484	3.131	*
6	T	11	4	20.282	21.770	21.770	0.0	-2.1487	-0.448	
4	T	11	4	7.421	4.175	-4.175	0.0	3.246	0.543	
2	T	11	4	35.012	32.436	-32.436	0.0	2.576	1.245	
1	T	11	4	15.831	23.610	-23.610	0.0	-7.779	-1.908	
0	T	10	5	6.802	5.195	-5.195	0.0	1.617	0.257	
1	T	10	5	10.455	8.575	8.575	0.0	1.879	0.382	
2	T	10	5	25.193	23.421	23.421	0.0	1.772	0.686	
4	T	10	5	10.572	3.697	3.697	0.0	6.475	1.415	
5	T	10	5	9.742	8.532	-8.532	0.0	1.230	0.246	
6	T	10	5	11.103	8.248	8.248	0.0	2.855	0.586	
0	S	0	322.655	334.474	334.474	0.0	-11.819	-2.003	*	
11	S	5	26.875	23.319	-23.319	0.0	3.556	1.385		
10	S	5	16.072	13.106	13.106	0.0	2.976	0.808		
0	S	5	32.264	33.738	33.738	0.0	-1.474	-0.605		

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
R	0	5	29.635	30.691	-30.691	0.0	-1.055	-0.639
7	0	5	18.057	18.051	18.051	0.0	0.065	0.001
6	0	5	10.223	9.610	-9.610	0.0	1.213	0.240
5	0	5	27.452	29.977	-29.977	0.0	-2.025	-0.758
4	0	5	9.085	9.437	-9.437	0.0	0.458	0.090
3	0	5	39.182	38.784	-38.784	0.0	0.309	0.206
2	0	5	9.201	7.485	-7.485	0.0	1.806	0.323
1	0	5	13.386	3.468	3.468	0.0	9.918	2.704
0	0	5	12.296	6.183	-6.183	0.0	6.112	1.531
1	0	5	20.489	10.873	-10.873	0.0	0.516	0.216
2	0	5	46.453	44.195	-44.195	0.0	2.258	1.348
3	0	5	35.781	42.345	-42.345	0.0	-6.564	-2.941
4	0	5	20.223	17.211	-17.211	0.0	3.012	1.043
5	0	5	24.706	30.119	-30.119	0.0	-5.611	-1.553
7	0	5	16.156	17.113	-17.113	0.0	-0.059	-0.274
8	0	5	4.815	8.793	-8.793	0.0	-3.978	-0.530
0	0	5	322.932	334.474	-334.474	0.0	-11.542	-1.955 *
0	0	5	49.834	46.565	-46.565	0.0	3.269	2.181
10	0	5	2.856	4.575	-4.575	0.0	-1.718	-0.197
11	0	5	41.727	43.669	-43.669	0.0	-1.941	-0.937
13	0	5	10.852	7.517	-7.517	0.0	3.335	0.730
15	0	5	5.315	11.959	-11.959	0.0	-6.644	-0.946
14	0	5	13.990	4.713	-4.713	0.0	9.277	2.358
13	0	5	5.989	1.990	-1.990	0.0	3.900	0.562
12	0	5	15.537	18.680	-18.680	0.0	-3.144	-0.762
10	0	5	11.059	6.800	-6.800	0.0	4.250	0.919
9	0	5	11.878	10.196	-10.196	0.0	1.702	0.417
8	0	5	22.612	21.377	-21.377	0.0	1.235	0.434
6	0	5	11.544	2.474	-2.474	0.0	9.071	2.248
5	0	5	5.551	9.822	-9.822	0.0	-4.271	-0.649
4	0	5	20.179	18.997	-18.997	0.0	1.182	0.466
3	0	5	21.002	26.245	-26.245	0.0	-5.152	-1.839
0	0	5	321.966	334.474	-334.474	0.0	-12.610	-2.147 *
0	0	5	4.461	1.260	-1.260	0.0	3.202	0.473
1	0	5	12.064	10.436	-10.436	0.0	2.508	0.692
2	0	5	12.502	13.089	-13.089	0.0	-0.587	-0.167
3	0	5	7.377	15.017	-15.017	0.0	-7.641	-1.329
4	0	5	11.471	2.469	-2.469	0.0	9.003	2.406
9	0	5	14.653	8.538	-8.538	0.0	6.115	1.774
12	0	5	9.128	3.842	-3.842	0.0	5.287	1.064
18	0	5	4.167	5.368	-5.368	0.0	-1.201	-0.169
0	0	5	323.904	334.474	-334.474	0.0	-10.570	-1.702 *
14	0	5	10.425	7.445	-7.445	0.0	3.060	0.632
13	0	5	20.421	21.458	-21.458	0.0	-0.037	-0.274
12	0	5	27.569	25.933	-25.933	0.0	1.736	0.834
11	0	5	20.872	14.885	-14.885	0.0	5.987	2.586
10	0	5	13.872	9.819	-9.819	0.0	4.053	1.251
0	0	5	20.758	22.384	-22.384	0.0	-1.506	-0.552
7	0	5	37.570	37.964	-37.964	0.0	-0.375	-0.217
6	0	5	12.561	17.068	-17.068	0.0	-4.507	-1.129
5	0	5	24.559	23.353	-23.353	0.0	1.206	0.572
3	0	5	13.857	11.358	-11.358	0.0	2.599	0.821
2	0	5	7.215	12.095	-12.095	0.0	-4.880	-0.926

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	5	5	18.752	21.760	0.9	-2.017	-0.738	
0	4	5	4.792	1.620	-10.290	0.0	-0.498	-0.116
1	5	5	17.073	4.014	-6.966	0.0	6.109	1.700
2	4	5	34.694	41.470	41.470	0.0	-2.786	-1.734
3	4	5	22.087	32.773	-32.773	0.0	-0.006	-0.307
0	6	0	320.876	335.474	335.474	0.0	-13.598	-2.319 *
4	4	5	19.705	19.861	-19.661	0.0	2.044	0.524
6	4	5	17.043	20.448	20.448	0.0	-2.600	-0.017
7	4	5	12.338	5.580	-5.580	0.0	5.758	1.602
8	4	5	10.337	2.624	2.624	0.0	7.713	1.864
0	4	5	27.628	27.647	-27.647	0.0	0.200	0.144
10	4	5	7.057	3.058	3.058	0.0	4.009	0.734
11	4	5	31.036	29.176	-29.176	0.0	1.962	0.993
12	4	5	12.444	2.406	-2.406	0.0	10.058	2.856 *
13	4	5	9.571	9.107	-9.107	0.0	0.464	0.087
14	4	5	6.034	5.845	-5.845	0.0	2.746	0.515
16	4	5	7.215	1.214	-1.214	0.0	6.001	0.989
17	4	5	22.302	21.600	-21.600	0.0	0.702	0.263
18	4	5	23.522	21.701	-21.701	0.0	2.253	0.821
19	4	5	2.412	1.015	-1.015	0.0	1.497	0.199
20	3	5	19.570	18.269	-18.269	0.0	0.702	0.231
10	3	5	13.204	17.146	-17.146	0.0	-3.442	-0.777
18	3	5	6.018	14.012	-14.012	0.0	-5.193	-0.900
17	2	5	52.483	51.164	-51.164	0.0	1.699	1.100
0	5	0	323.768	334.474	-334.474	0.0	-11.106	-1.880 *
16	3	5	35.448	39.786	-39.786	0.0	-3.138	-1.454
15	2	5	21.643	32.572	-32.572	0.0	-6.930	-1.796
13	3	5	30.521	25.144	-25.144	0.0	5.377	2.823
12	3	5	54.021	52.500	-52.500	0.0	1.431	0.973
11	3	5	70.454	69.612	-69.612	0.0	1.221	0.817
10	3	5	39.034	37.285	-37.285	0.0	1.750	1.105
9	3	5	41.120	45.088	-45.088	0.0	-0.052	0.032
9	3	5	51.457	52.189	-52.189	0.0	-1.292	-0.621
7	3	5	60.550	61.958	-61.958	0.0	-1.108	-0.783
6	3	5	26.270	24.607	-24.607	0.0	1.663	0.881
5	3	5	62.502	63.144	-63.144	0.0	-0.552	-0.350
3	3	5	49.265	65.782	-65.782	0.0	-0.515	-0.302
2	2	5	29.443	30.461	-30.461	0.0	-1.018	-0.556
1	3	5	25.365	30.956	-30.956	0.0	-1.557	-0.844
1	2	5	21.126	29.358	-29.358	0.0	-2.232	-1.240
2	2	5	49.216	58.220	-58.220	0.0	0.992	0.724
3	2	5	58.597	62.373	-62.373	0.0	-3.016	-2.757
0	2	0	323.150	336.474	-336.474	0.0	-11.323	-1.917 *
4	2	5	24.779	25.809	-25.809	0.0	-1.030	-0.710
5	2	5	46.122	48.256	-48.256	0.0	0.466	0.614
6	2	5	12.761	16.467	-16.467	0.0	-3.660	-0.980
7	2	5	10.611	22.534	-22.534	0.0	-2.723	-1.015
8	2	5	11.500	14.958	-14.958	0.0	2.532	0.905
9	2	5	65.024	63.934	-63.934	0.0	1.083	0.753
11	2	5	62.116	62.037	-62.037	0.0	0.079	0.053
12	2	5	14.225	14.154	-14.154	0.0	0.071	0.021
13	2	5	7.252	6.561	-6.561	0.0	0.672	0.138
14	2	5	10.911	10.293	-10.293	0.0	0.618	0.141

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
15	2	5	24.483	15.020	-15.620	0.0	-6.138	-1.132
16	2	5	14.428	9.313	-8.308	0.0	6.250	1.700
17	2	5	34.465	33.213	33.213	0.0	1.253	0.619
18	2	5	20.605	16.955	16.955	0.0	3.736	1.321
19	1	5	14.316	4.703	-4.703	0.0	9.611	2.707
0	6	0	323.150	334.474	334.474	0.0	-11.323	-1.917
17	1	5	13.106	9.082	-9.082	0.0	4.024	1.040
15	1	5	8.157	4.204	-6.204	0.0	3.953	0.804
14	1	5	15.507	8.244	-8.244	0.0	7.263	2.314
13	1	5	15.505	10.505	-10.505	0.0	2.600	-0.771
12	1	5	36.497	35.510	25.510	0.0	1.180	0.699
0	6	0	2.105	10.432	10.432	0.0	-8.327	-0.994
8	1	5	21.439	17.553	17.553	0.0	4.086	1.048
7	1	5	31.380	29.923	29.923	0.0	1.367	0.791
6	1	5	10.450	17.835	-16.535	0.0	-6.036	-1.304
4	1	5	12.975	14.715	14.715	0.0	-0.740	-0.240
3	1	5	8.496	10.977	10.977	0.0	-2.482	-0.556
2	1	5	16.686	8.663	8.663	0.0	7.223	3.193
1	1	5	12.960	13.820	13.820	0.0	0.132	0.062
0	0	6	104.518	102.509	-102.509	0.0	2.009	1.081
1	0	6	81.900	80.076	-80.076	0.0	1.004	1.122
0	6	0	323.091	334.474	334.474	0.0	-11.303	-1.926
2	0	6	10.248	6.778	6.778	0.0	3.471	0.049
3	0	6	43.401	44.002	-44.002	0.0	-0.691	-0.466
4	0	6	19.050	18.685	18.685	0.0	0.376	0.177
5	0	6	36.165	35.100	35.100	0.0	1.065	0.600
6	0	6	5.227	1.140	-1.140	0.0	4.087	0.640
7	0	6	68.443	70.073	70.073	0.0	-1.631	-1.001
8	0	6	44.601	44.723	-44.723	0.0	-0.122	-0.074
0	0	6	0.232	14.264	-14.264	0.0	-5.032	-0.957
10	0	6	11.730	14.638	14.638	0.0	-2.902	-0.663
11	0	6	11.324	9.821	-8.821	0.0	1.503	0.332
12	0	6	41.240	40.911	-40.911	0.0	0.358	0.103
13	0	6	59.331	57.371	57.371	0.0	1.060	1.176
15	0	6	52.477	55.116	55.116	0.0	-2.640	-1.532
16	0	6	19.840	23.122	-23.122	0.0	-2.282	-0.966
17	0	6	22.184	10.666	-10.666	0.0	11.181	4.773
15	1	6	14.034	16.166	-16.166	0.0	-2.132	-0.481
14	1	6	44.082	44.412	-44.412	0.0	-0.230	-0.125
0	6	0	322.982	334.474	334.474	0.0	-10.601	-1.768
13	1	6	41.047	39.572	39.572	0.0	1.474	0.823
12	1	6	12.110	12.108	12.108	0.0	0.011	0.003
11	1	6	7.980	2.123	-2.123	0.0	5.840	1.076
10	1	6	16.612	13.408	-13.408	0.0	3.125	0.751
9	1	6	12.966	4.949	-4.949	0.0	7.986	2.073
8	1	6	51.256	0.256	0.256	0.0	5.001	0.678
7	1	6	34.258	35.052	-35.052	0.0	-0.793	-0.401
6	1	6	37.033	36.310	-36.310	0.0	0.612	0.353
5	1	6	11.650	8.662	8.662	0.0	3.236	0.838
4	1	6	11.382	11.704	-11.704	0.0	0.009	0.021
3	1	6	6.450	4.494	4.494	0.0	2.455	0.432
2	1	6	26.778	23.557	23.557	0.0	3.472	1.840
1	1	6	42.201	42.944	-42.944	0.0	-0.743	-0.452

BUC FTHMFFESTLITE 6/20/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	2	6	5.369	3.054	3.054	0.0	2.334	0.372
1	2	6	6.022	6.028	-6.019	0.0	-2.706	-0.456
2	2	6	11.735	12.540	12.540	0.0	-0.022	-0.205
3	2	6	30.55	27.882	-27.882	0.0	2.667	1.468
4	2	6	27.067	20.457	20.457	0.0	6.410	3.241
5	2	6	16.137	6.471	6.471	0.0	4.466	1.341
6	2	6	2.744	13.910	-13.910	0.0	-11.514	-1.293 *
0	6	0	323.765	334.474	334.474	0.0	-10.709	-1.805 *
9	2	6	13.205	12.538	12.538	0.0	0.671	0.167
10	2	6	11.751	11.441	-11.441	0.0	0.310	0.073
11	2	6	30.506	24.083	-24.083	0.0	6.423	3.534
12	2	6	12.104	5.683	5.683	0.0	6.421	1.508
16	2	6	4.417	15.444	-15.444	0.0	-11.027	-1.293 *
17	2	6	17.423	12.705	12.705	0.0	4.719	1.374
15	2	6	16.622	6.569	6.569	0.0	13.654	3.767 *
14	3	6	14.830	6.618	-6.618	0.0	14.211	3.953 *
11	3	6	17.517	6.282	6.282	0.0	6.235	1.485
10	3	6	10.967	7.890	2.898	0.0	7.969	1.786
9	3	6	5.746	4.491	4.491	0.0	4.055	0.815
0	6	0	323.643	334.474	334.474	0.0	-10.531	-1.775 *
7	2	6	9.540	7.163	-7.163	0.0	2.377	0.267
6	3	6	10.425	7.487	-7.487	0.0	2.938	0.654
1	3	6	15.330	6.246	-6.246	0.0	0.056	3.262
0	6	0	26.578	27.818	27.818	0.0	-0.210	-0.053
1	4	6	12.207	12.417	12.417	0.0	-0.210	-0.053
2	4	6	9.792	7.270	-7.270	0.0	2.513	0.558
3	4	6	26.754	26.675	-26.675	0.0	0.795	0.130
4	4	6	11.627	9.352	9.352	0.0	2.626	0.613
5	4	6	11.000	10.462	-10.462	0.0	0.538	0.121
6	4	6	5.345	4.738	4.738	0.0	0.507	0.072
7	4	6	17.880	12.190	12.190	0.0	5.650	1.902
8	4	6	12.739	7.486	7.486	0.0	5.252	1.340
9	4	6	11.547	6.392	-6.392	0.0	2.973	0.575
10	4	6	6.512	6.544	6.544	0.0	4.568	0.946
11	4	6	6.123	5.606	-5.606	0.0	-1.483	-0.186
12	4	6	15.005	6.456	6.456	0.0	6.553	1.853
0	4	0	323.428	334.474	334.474	0.0	-11.046	-1.863 *
13	4	6	17.231	10.036	-10.036	0.0	7.195	2.170
14	5	6	11.441	1.978	1.978	0.0	5.944	2.104
15	5	6	37.204	37.526	37.526	0.0	-0.323	-0.151
13	5	6	42.731	40.700	-40.700	0.0	1.933	1.010
12	5	6	6.669	1.587	-1.587	0.0	4.680	0.571
10	5	6	17.408	2.111	2.111	0.0	14.877	5.051 *
9	5	6	9.719	3.063	3.063	0.0	6.655	1.329
8	5	6	14.888	11.221	-11.221	0.0	3.627	0.958
7	5	6	30.605	35.068	35.068	0.0	3.537	2.026
6	5	6	44.363	45.959	45.959	0.0	-1.235	-0.672
5	5	6	20.735	28.033	-28.033	0.0	0.702	0.323
4	5	6	6.113	4.267	-4.267	0.0	3.426	0.712
2	5	6	21.244	23.740	-23.740	0.0	-2.396	-0.821
1	5	6	54.809	57.883	57.883	0.0	-3.074	-1.880
0	6	6	72.650	75.469	-75.469	0.0	-2.509	-1.510
1	6	6	49.508	51.571	-51.571	0.0	-2.063	-1.168

POOC CPTHDEFFCOST/LITE 6/28/73

STRUCTURE FACTORS

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(cS)

H	K	L	F(LOR)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
2	6	6	9.645	15.410	15.410	0.0	-5.345	-1.056
0	6	0	322.022	334.474	334.474	0.0	-12.452	-2.120 *
2	6	6	9.733	13.502	13.502	0.0	-3.769	-0.715
4	6	6	12.252	5.483	5.483	0.0	6.769	1.618
5	6	6	30.403	26.877	26.877	0.0	3.526	1.670
7	6	6	44.406	46.022	46.022	0.0	-1.614	-0.356
8	6	6	20.091	20.841	20.841	0.0	-0.750	-0.227
9	5	6	8.746	0.509	0.509	0.0	8.239	1.488
10	6	6	10.690	2.734	2.734	0.0	7.755	1.583
11	6	6	9.511	9.590	9.590	0.0	-1.079	-0.189
12	6	6	26.578	30.395	30.395	0.0	-3.616	-1.169
13	6	6	38.896	36.352	36.352	0.0	2.533	1.370
10	7	6	12.738	16.297	16.297	0.0	-3.549	-0.753
9	7	6	15.493	12.675	12.675	0.0	2.418	0.733
7	7	6	17.968	13.011	13.011	0.0	4.957	1.495
6	7	6	22.111	20.695	20.695	0.0	1.415	0.508
2	7	6	14.476	16.167	16.167	0.0	-1.691	-0.416
0	6	0	323.249	334.474	334.474	0.0	-11.225	-1.000 *
1	7	6	6.022	1.644	1.644	0.0	-6.622	-0.925
0	8	7	10.055	0.549	0.549	0.0	10.386	2.246 *
2	8	6	10.366	0.814	0.814	0.0	9.552	1.954
2	8	6	24.424	24.062	24.062	0.0	0.763	0.286
4	8	6	23.541	20.000	20.000	0.0	3.541	1.312
7	8	6	5.153	8.554	8.554	0.0	-3.401	-0.445
7	5	7	7.509	5.362	5.362	0.0	2.147	0.339
6	5	7	16.553	10.020	10.020	0.0	-1.466	-0.365
2	5	7	20.105	18.244	18.244	0.0	1.861	0.584
1	5	7	12.738	14.488	14.488	0.0	-1.751	-0.316
0	6	0	322.512	334.474	334.474	0.0	-11.562	-1.959 *
0	4	7	8.555	2.685	2.685	0.0	5.869	1.052
1	4	7	26.742	22.401	22.401	0.0	4.251	2.001
2	4	7	6.037	1.019	1.019	0.0	5.018	0.719
3	6	7	5.624	8.743	8.743	0.0	-4.119	-0.583
4	6	7	18.086	21.243	21.243	0.0	-3.127	-0.816
5	4	7	21.491	23.446	23.446	0.0	-1.957	-0.593
6	4	7	8.428	0.575	0.575	0.0	8.053	1.432
7	4	7	15.774	11.503	11.503	0.0	4.283	1.114
8	4	7	10.057	14.422	14.422	0.0	-4.345	-0.774
11	3	7	35.456	35.055	35.055	0.0	0.491	0.177
10	3	7	60.373	56.031	56.031	0.0	1.342	0.730
8	3	7	13.568	2.208	2.208	0.0	11.340	2.809 *
7	3	7	11.162	14.944	14.944	0.0	-3.783	-0.713
6	3	7	41.520	42.680	42.680	0.0	-1.160	-0.593
5	3	7	20.769	21.081	21.081	0.0	-0.312	-0.103
3	3	7	14.314	22.263	22.263	0.0	-8.249	-1.728
2	3	7	58.894	59.510	59.510	0.0	-0.626	-0.360
0	6	0	323.448	334.474	334.474	0.0	-11.026	-1.860 *
1	3	7	24.662	25.003	25.003	0.0	-1.241	-0.434
0	2	7	23.620	21.584	21.584	0.0	1.416	0.787
1	2	7	27.023	27.477	27.477	0.0	0.461	0.202
2	2	7	3.769	1.676	1.676	0.0	2.123	0.263
3	2	7	11.682	12.970	12.970	0.0	-1.289	-0.264
4	2	7	44.689	46.360	46.360	0.0	-1.671	-0.274

2000 FETHOFFFOSILITE 6/28/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(FCALC)	B(FCALC)	DELTA F	DELTA/SIGMA
5	2	7	22.037	21.225	-21.225	0.0	0.812	0.273
6	2	7	11.309	1.311	1.311	0.0	9.997	2.197
7	2	7	6.406	8.410	-8.410	0.0	-1.416	-0.210
8	2	7	29.251	32.735	-32.735	0.0	-3.484	-1.311
9	2	7	14.701	14.830	-14.830	0.0	1.870	0.520
10	2	7	14.093	6.105	-6.105	0.0	13.068	2.768 *
11	2	7	26.713	23.272	-23.272	0.0	3.441	1.364
12	1	7	12.266	2.527	-2.527	0.0	9.740	2.254
13	1	7	16.406	10.922	-10.922	0.0	5.484	1.513
14	1	7	6.243	7.405	-7.405	0.0	-1.163	-0.168
9	1	7	7.377	16.896	-16.896	0.0	-9.519	-1.396
8	1	7	0.674	0.396	-0.396	0.0	0.278	1.765
7	1	7	5.215	2.661	-2.661	0.0	2.354	0.335
0	6	0	222.576	334.474	-334.474	0.0	-11.898	-2.017 *
5	1	7	12.266	11.883	-11.883	0.0	0.383	0.085
4	1	7	10.793	0.243	-0.243	0.0	10.550	2.267 *
3	1	7	13.227	0.658	-0.658	0.0	12.669	3.20 *
2	1	7	10.431	7.562	-7.562	0.0	3.069	0.617
1	1	7	18.495	15.352	-15.352	0.0	3.633	1.245

STRUCTURE FACTORS							PAGE 1	
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
4	0	0	180.442	161.517	-181.617	0.0	-0.648	-0.224
6	0	0	15.211	13.415	-13.415	0.0	1.796	1.227
8	0	0	ac.27	112.108	112.108	0.0	-12.451	-7.453 *
10	0	0	10.771	2.761	4.761	0.0	5.010	25.566
12	0	0	263.556	255.836	-255.826	0.0	8.124	1.784
14	0	0	17.015	16.631	-16.631	0.0	0.384	0.146
16	0	0	130.011	140.044	-140.044	0.0	-2.033	-0.894
20	0	0	125.115	136.702	-136.702	0.0	-1.508	-0.700
24	0	0	18.665	10.085	-10.085	0.0	8.380	3.020
26	0	0	17.675	10.249	-10.249	0.0	7.446	25.330
28	1	0	23.748	24.106	-24.106	0.0	-0.358	-0.124
24	1	0	7.094	11.460	-11.460	0.0	-4.366	-0.689
22	1	0	251.704	24.090	-24.090	0.0	1.603	0.853
20	1	0	19.679	8.101	-8.101	0.0	1.978	0.511
18	1	0	45.105	45.108	-45.108	0.0	0.559	0.755
14	1	0	123.460	123.022	-123.022	0.0	-0.482	-0.737
12	1	0	6.814	2.620	-2.620	0.0	7.194	2.222
0	6	0	310.646	325.713	-325.713	0.0	-15.068	-2.683 *
10	1	0	49.427	49.123	-49.123	0.0	0.304	0.287
8	1	0	5.572	2.493	-2.493	0.0	3.088	0.995
6	1	0	256.236	259.627	-259.627	0.0	-3.201	-0.778
4	1	0	c.486	5.261	-5.261	0.0	-4.527	2.268
2	1	0	85.583	47.908	-87.908	0.0	-2.325	-1.747
0	2	0	7.404	9.600	-9.600	0.0	-2.196	-0.971
2	2	0	11.233	2.392	-2.392	0.0	8.851	5.031
4	2	0	194.060	199.343	-199.363	0.0	-4.283	-1.360
6	2	0	10.804	13.619	-13.619	0.0	-2.815	-1.421
8	2	0	81.776	80.705	-80.705	0.0	1.071	0.798
10	2	0	7.567	14.821	-14.821	0.0	-7.225	-1.924
12	2	0	10.470	8.867	-8.867	0.0	1.612	0.485
14	2	0	61.694	62.397	-62.397	0.0	-0.703	-0.505
18	2	0	12.727	9.467	-9.467	0.0	2.950	0.891
20	2	0	6.267	6.399	-6.399	0.0	-0.133	0.030
22	2	0	4.522	7.286	-7.286	0.0	-2.763	-0.406
24	2	0	24.709	27.031	-27.031	0.0	-2.232	-0.837
26	2	0	12.400	12.924	-12.924	0.0	11.506	2.759 *
0	6	0	313.165	325.713	-325.713	0.0	-12.547	-2.209 *
24	3	0	6.206	1.726	-1.726	0.0	4.569	0.596
14	3	0	44.334	44.614	-44.614	0.0	-0.276	0.195
12	3	0	6.110	3.133	-3.133	0.0	2.985	0.635
10	3	0	14.338	8.047	-8.047	0.0	6.292	2.781
8	3	0	12.460	6.510	-6.510	0.0	5.950	2.834
6	3	0	422.896	405.582	-405.583	0.0	2.312	2.631
4	3	0	11.601	11.612	-11.612	0.0	0.079	0.045
2	2	0	50.057	49.684	-49.684	0.0	0.413	0.427
0	2	0	27.776	26.364	-26.364	0.0	1.412	1.513
4	4	0	58.445	61.073	-61.073	0.0	-2.428	-3.280
6	4	0	8.469	3.133	-3.133	0.0	5.336	1.805
8	4	0	65.575	65.821	-65.822	0.0	0.154	0.123
10	4	0	21.232	24.526	-24.526	0.0	-3.204	-1.795
0	6	0	311.172	325.713	-325.713	0.0	-14.541	-2.587 *
16	2	0	30.973	39.779	-39.779	0.0	-0.806	0.537
18	4	0	2.857	1.216	-1.216	0.0	1.651	0.222

Final cyl d.p

900 FMT DIFFERENTIALITE 7/03/79

STRUCTURE FACTORS

PAGE 2

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H	K	L	F(OFC)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
20	4	0	46.493	46.551	46.551	0.0	-3.068	-1.064
22	4	0	8.471	11.308	-11.308	0.0	-2.336	-0.458
24	4	0	18.404	19.804	19.804	0.0	-0.910	-0.267
22	5	0	21.054	18.242	-18.242	0.0	2.812	1.151
20	5	0	5.734	9.398	9.398	0.0	-3.663	-0.579
14	5	0	44.323	45.419	45.419	0.0	-1.096	-0.603
16	5	0	10.390	5.750	5.750	0.0	4.640	1.236
14	5	0	178.227	178.079	-178.079	0.0	0.198	0.050
10	5	0	16.258	17.194	-17.194	0.0	1.064	0.473
8	5	0	6.400	8.503	-8.503	0.0	0.857	0.247
6	5	0	139.454	142.103	-142.103	0.0	-2.649	-1.180
4	5	0	5.765	3.673	-3.673	0.0	1.692	0.409
2	5	0	107.647	201.680	201.680	0.0	-4.023	-1.249
0	6	0	311.014	325.713	325.713	0.0	-13.759	-2.443 *
0	6	0	312.403	325.713	325.713	0.0	-13.310	-2.355 *
4	6	0	76.1697	78.959	-78.959	0.0	-2.262	-1.633
6	6	0	5.220	6.944	-6.944	0.0	-1.624	-0.305
8	6	0	116.054	116.438	116.438	0.0	-0.304	-0.199
12	6	0	105.194	103.851	-103.851	0.0	1.333	0.738
16	6	0	56.423	54.089	-54.089	0.0	0.734	0.502
18	6	0	3.466	3.779	3.779	0.0	0.166	0.023
20	6	0	101.053	104.118	-104.118	0.0	-2.225	-1.168
24	6	0	12.327	15.575	-15.575	0.0	-3.248	-0.702
22	7	0	11.667	13.438	-13.438	0.0	-1.791	-0.382
20	7	0	12.648	11.031	-11.031	0.0	11.917	3.136 *
14	7	0	10.272	15.060	15.060	0.0	-4.788	-1.045
16	7	0	9.357	9.114	-9.114	0.0	0.241	0.054
14	7	0	55.723	55.617	55.617	0.0	0.116	0.084
10	7	0	62.247	63.767	63.767	0.0	-1.520	-1.069
6	7	0	27.495	28.631	28.631	0.0	-1.136	-0.619
0	6	0	313.676	325.713	325.713	0.0	-12.037	-2.118 *
4	7	0	11.765	18.266	18.266	0.0	-6.501	-1.745
2	7	0	13.428	13.974	13.974	0.0	-0.364	0.116
0	8	0	60.842	63.277	63.277	0.0	-2.435	-1.751
2	9	0	18.198	10.088	-10.088	0.0	7.210	3.361
4	8	0	75.393	79.155	-79.155	0.0	0.238	0.158
0	8	0	26.724	24.122	24.122	0.0	2.603	1.440
10	9	0	5.459	10.621	10.621	0.0	-1.162	0.269
12	6	0	35.427	40.014	-40.014	0.0	-0.387	0.244
14	8	0	7.330	0.903	0.903	0.0	6.427	1.228
16	8	0	54.554	53.301	53.301	0.0	1.253	0.785
22	8	0	1.256	3.664	-3.664	0.0	-2.408	-0.231
16	9	0	5.764	47.347	47.347	0.0	-1.417	0.212
14	9	0	10.627	16.832	16.832	0.0	-6.205	1.231
12	9	0	8.471	2.905	2.905	0.0	6.066	1.299
10	9	0	12.061	117.966	-117.966	0.0	0.095	0.026
0	6	0	313.576	325.713	325.713	0.0	-12.135	-2.135 *
6	9	0	27.747	28.410	28.410	0.0	-0.663	-0.350
6	9	0	8.587	32.973	-32.973	0.0	4.613	1.084
2	9	0	11.613	3.501	-3.501	0.0	8.412	2.598
0	10	0	52.452	53.665	-53.665	0.0	-1.213	-0.406
4	10	0	17.222	10.126	-10.126	0.0	7.096	2.925
6	10	0	12.830	0.090	0.090	0.0	12.740	3.934 *

900 ORTHOFEPROSILITE 7/03/73

STRUCTURE FACTORS

PAGE 3

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
8	10	0	23.092	27.609	-27.609	0.0	-4.527	-1.778
12	10	0	19.774	17.978	17.078	0.0	2.496	0.902
14	10	0	6.739	0.513	-0.513	0.0	6.226	1.008
18	10	0	9.297	2.447	2.447	0.0	6.790	1.235
14	11	0	63.235	60.072	-60.072	0.0	3.163	1.921
12	11	0	12.298	2.116	-2.116	0.0	10.182	2.551 *
10	11	0	12.623	12.017	-12.017	0.0	0.505	0.143
9	11	0	10.390	0.141	-0.141	0.0	10.250	2.208 *
6	11	0	61.275	60.411	-60.411	0.0	0.864	0.525
0	6	0	312.012	325.713	-325.713	0.0	-13.701	-2.425 *
4	11	0	15.211	6.157	-6.157	0.0	9.053	2.972
2	11	0	48.489	47.564	-47.564	0.0	0.925	0.592
0	12	0	70.539	67.950	-67.950	0.0	1.089	0.636
2	12	0	7.666	3.261	-3.261	0.0	4.705	0.925
4	12	0	5.025	6.880	-6.880	0.0	-1.855	-0.254
6	12	0	8.223	2.644	-2.644	0.0	6.179	1.139
9	12	0	13.643	16.296	-16.296	0.0	-2.653	-0.592
12	12	0	22.475	22.925	-22.925	0.0	-0.450	-0.143
8	13	0	13.421	0.495	-0.495	0.0	12.936	-3.006 *
4	13	0	14.752	0.429	-0.429	0.0	14.323	4.057 *
2	13	0	25.703	23.871	-23.871	0.0	1.832	0.695
6	13	1	14.456	4.198	-4.198	0.0	10.258	2.742 *
4	13	1	13.732	6.397	-6.397	0.0	7.334	1.879
3	13	1	15.551	0.447	-0.447	0.0	7.104	2.135
1	13	1	12.342	10.952	-10.952	0.0	1.350	0.324
0	6	0	311.760	325.713	-325.713	0.0	-14.013	-2.482 *
0	12	1	10.789	6.786	-6.786	0.0	4.003	0.841
3	12	1	7.922	9.935	-9.935	0.0	1.987	0.354
4	12	1	5.202	7.970	-7.970	0.0	-2.768	-0.401
5	12	1	7.670	13.875	-13.875	0.0	-6.205	-0.978
8	12	1	8.498	3.215	-3.215	0.0	5.283	0.976
9	12	1	5.616	3.020	-3.020	0.0	2.596	0.358
10	12	1	14.249	2.728	-2.728	0.0	11.522	3.233 *
12	12	1	13.628	3.174	-3.174	0.0	10.454	2.874 *
15	11	1	13.658	12.602	-12.602	0.0	1.056	0.246
13	11	1	20.003	13.897	-13.897	0.0	6.116	2.199
12	11	1	7.641	17.798	-17.798	0.0	5.843	1.001
11	11	1	16.911	15.535	-15.535	0.0	1.377	0.394
10	11	1	15.137	11.141	-11.141	0.0	3.995	1.054
0	6	0	310.860	325.713	-325.713	0.0	-14.853	-2.644 *
8	11	1	18.642	11.507	-11.507	0.0	7.135	2.621
7	11	1	20.248	20.799	-20.799	0.0	-0.500	-0.165
6	11	1	23.230	24.607	-24.607	0.0	-1.377	-0.520
5	11	1	30.621	26.157	-26.157	0.0	4.465	2.372
3	11	1	14.956	10.730	-10.730	0.0	4.126	1.268
2	11	1	20.211	18.309	-18.309	0.0	1.902	0.703
1	11	1	19.367	19.024	-19.024	0.0	0.343	0.125
0	10	1	28.695	24.571	-24.571	0.0	4.124	2.420
1	10	1	26.413	26.724	-26.724	0.0	-0.310	-0.138
2	10	1	23.289	26.308	-26.308	0.0	-3.099	-1.333
3	10	1	5.793	7.287	-7.287	0.0	-1.494	-0.247
4	10	1	7.290	0.064	-0.064	0.0	7.326	1.445
5	10	1	9.636	2.118	-2.118	0.0	7.519	1.754

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	10	1	16.032	16.076	16.076	0.0	-6.044	-1.445
7	10	1	16.483	17.064	17.064	0.0	-0.561	-0.199
8	10	1	15.630	12.097	12.097	0.0	3.542	1.151
9	10	1	6.724	6.309	6.392	0.0	-2.674	-0.452
10	10	1	10.627	1.183	1.183	0.0	9.444	2.269
11	10	1	10.996	12.692	-12.692	0.0	-1.695	-0.371
0	4	0	312.286	325.713	325.713	0.0	-13.427	-2.376
12	10	1	13.510	13.387	-13.387	0.0	0.123	0.031
14	10	1	15.630	15.078	-15.078	0.0	1.552	0.445
15	10	1	13.865	6.615	-6.615	0.0	9.250	2.434
17	10	1	5.187	0.240	0.240	0.0	4.947	0.694
18	10	1	12.046	11.325	-11.325	0.0	0.721	0.154
20	9	1	11.455	6.254	6.254	0.0	5.200	1.079
19	9	1	17.270	18.231	18.231	0.0	-0.861	-0.235
18	9	1	17.178	14.030	-14.030	0.0	2.347	0.687
17	9	1	18.000	21.099	-21.099	0.0	-3.019	-0.095
16	9	1	7.730	15.294	-15.294	0.0	-7.564	-1.210
15	9	1	8.203	0.660	-0.660	0.0	7.542	1.413
14	9	1	8.321	11.400	-11.400	0.0	-3.079	-0.530
12	9	1	47.313	49.861	-49.861	0.0	-2.548	-0.630
11	9	1	57.121	49.200	49.200	0.0	1.921	1.207
10	9	1	49.159	49.986	-49.986	0.0	-0.027	-0.529
9	9	1	60.408	60.032	-60.032	0.0	0.376	0.294
8	9	1	32.765	34.795	-34.795	0.0	-1.030	-0.584
0	6	0	110.353	325.713	325.713	0.0	-15.360	-2.736
7	6	0	11.440	18.798	-18.798	0.0	-7.299	-1.770
6	6	0	22.647	23.989	-23.989	0.0	-0.322	-0.150
5	6	0	29.445	27.528	27.528	0.0	1.937	1.127
4	6	0	11.810	4.624	-4.624	0.0	7.185	2.150
3	6	0	31.011	31.806	-31.806	0.0	0.105	0.054
2	6	0	42.020	42.531	-42.531	0.0	0.410	0.287
1	6	0	33.690	35.293	-35.293	0.0	-1.603	-0.960
0	6	0	17.533	18.321	-18.321	0.0	-0.788	-0.313
1	8	1	52.719	75.590	-75.590	0.0	-12.871	-0.353
2	8	1	63.564	66.417	-66.417	0.0	-2.853	-2.094
3	8	1	90.696	92.461	-92.461	0.0	-1.775	-1.104
4	8	1	69.003	69.349	-69.349	0.0	-0.345	-0.250
5	8	1	55.091	53.809	53.809	0.0	1.282	0.944
6	8	1	13.066	0.908	-0.908	0.0	3.159	1.027
7	8	1	37.815	38.735	38.735	0.0	-0.920	-0.607
6	8	1	56.495	54.172	54.172	0.0	0.323	0.235
9	8	1	40.370	39.158	-39.158	0.0	2.211	1.519
10	8	1	41.776	135.882	135.882	0.0	-10.306	-1.367
11	8	1	22.312	24.591	-24.591	0.0	-2.279	-0.944
12	8	1	31.318	30.002	-30.002	0.0	1.316	0.779
0	6	0	310.529	325.713	325.713	0.0	-15.185	-2.704
13	8	1	41.350	40.150	40.150	0.0	1.200	0.816
14	8	1	6.163	0.436	0.436	0.0	5.677	0.990
15	8	1	35.441	37.566	37.566	0.0	-2.125	-1.146
16	8	1	31.220	31.807	31.807	0.0	-0.578	-0.296
17	8	1	30.458	26.335	-26.335	0.0	4.123	2.061
18	8	1	21.981	19.713	19.713	0.0	4.168	1.666
20	8	1	19.086	10.066	-10.066	0.0	9.020	3.332

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
21	8	1	11.765	4.007	-4.097	0.0	7.669	1.746
22	8	1	25.125	24.912	24.912	0.0	0.213	0.080
23	7	1	14.323	14.236	1.236	0.0	13.087	3.687 *
22	7	1	9.616	9.740	-9.740	0.0	-1.124	-0.291
21	7	1	5.512	5.000	-5.000	0.0	0.011	0.002
19	7	1	9.676	18.415	-18.415	0.0	-8.439	-1.555
19	7	1	11.432	7.951	7.951	0.0	3.681	0.896
17	7	1	9.651	6.656	6.656	0.0	2.995	0.541
16	7	1	17.077	16.002	16.002	0.0	1.074	0.405
15	7	1	3.724	4.950	-4.950	0.0	-1.226	-0.170
0	6	0	311.563	325.713	325.713	0.0	-14.150	-2.516 *
13	7	1	10.078	11.329	11.329	0.0	-0.450	-0.110
12	7	1	24.652	20.720	20.720	0.0	3.339	1.776
11	7	1	21.953	20.090	-20.090	0.0	1.764	0.851
10	7	1	19.574	18.903	18.903	0.0	0.671	0.290
9	7	1	36.316	38.772	38.772	0.0	-2.456	-1.655
8	7	1	31.526	34.211	34.211	0.0	-2.685	-1.700
7	7	1	9.563	4.692	-4.692	0.0	3.951	0.395
6	7	1	11.252	5.782	5.782	0.0	5.510	1.586
5	7	1	16.852	17.150	17.150	0.0	-0.208	-0.108
4	7	1	29.450	26.988	26.988	0.0	1.662	1.029
3	7	1	26.076	27.709	-27.709	0.0	-0.733	-0.419
2	7	1	10.442	14.051	14.051	0.0	-3.410	-0.912
1	7	1	9.454	3.867	3.867	0.0	4.586	1.052
1	6	1	8.912	7.575	7.575	0.0	1.337	0.390
2	6	1	5.251	6.844	6.844	0.0	-1.553	-0.306
3	6	1	21.483	25.150	25.150	0.0	-3.267	-1.623
4	6	1	17.149	15.544	15.544	0.0	1.604	0.753
5	6	1	11.056	5.613	-5.613	0.0	5.443	1.696
6	6	1	6.207	9.398	9.398	0.0	-3.191	-0.531
0	6	0	311.016	325.713	325.713	0.0	-14.697	-2.615 *
8	6	1	12.475	8.686	-8.686	0.0	3.799	1.150
0	5	1	14.427	13.262	13.262	0.0	1.164	0.382
10	6	1	6.976	0.410	0.410	0.0	6.566	1.914
11	6	1	1.133	5.030	5.030	0.0	-3.942	-0.481
12	6	1	5.926	1.250	-1.250	0.0	4.677	0.936
13	6	1	10.766	14.403	-14.403	0.0	-3.717	-0.949
14	6	1	10.760	9.761	-9.761	0.0	0.999	0.263
15	6	1	20.240	15.242	-15.242	0.0	4.998	2.362
16	6	1	11.706	7.233	-7.233	0.0	4.474	1.256
17	6	1	5.912	2.979	2.979	0.0	3.115	0.538
18	6	1	3.281	3.035	3.035	0.0	0.245	0.032
20	6	1	13.170	10.177	10.177	0.0	2.993	0.785
21	6	1	13.347	3.216	-3.216	0.0	10.131	2.741 *
24	6	1	13.495	4.704	-4.704	0.0	8.792	2.244
25	5	1	8.572	11.263	-11.263	0.0	-2.691	-0.427
0	6	0	312.110	325.713	325.713	0.0	-13.603	-2.408 *
21	5	1	17.977	17.399	17.399	0.0	0.578	0.191
18	5	1	7.478	13.672	-13.672	0.0	-6.194	-1.112
17	5	1	16.616	11.615	-11.615	0.0	5.001	1.966
16	5	1	21.898	18.869	18.869	0.0	3.029	1.452
15	5	1	35.337	33.465	-33.465	0.0	1.872	1.314
14	5	1	37.593	37.469	37.469	0.0	0.124	0.078

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
13	5	1	30.436	30.093	0.0	0.643	0.345	
11	5	1	12.978	12.664	0.0	3.334	1.049	
10	5	1	34.061	30.405	-31.495	0.0	3.556	2.613
9	5	1	32.395	32.258	-35.268	0.0	-2.983	-1.859
8	5	1	30.266	30.636	30.636	0.0	-0.371	-0.258
7	5	1	63.609	64.125	-64.135	0.0	-0.526	-0.409
6	5	1	56.643	57.647	-57.647	0.0	-1.004	-0.910
5	5	1	76.380	75.285	75.285	0.0	-0.705	-0.676
4	5	1	32.163	34.160	34.160	0.0	-1.697	-1.496
0	6	0	312.953	325.712	325.712	0.0	-12.860	-2.273
3	5	1	41.083	42.073	42.073	0.0	-1.700	-1.628
2	5	1	51.911	56.710	-56.710	0.0	-5.809	-2.155
1	3	1	26.754	27.271	-27.271	0.0	-0.517	-0.375
1	4	1	42.673	43.886	-43.886	0.0	-1.223	-1.286
2	4	1	78.052	83.617	81.417	0.0	-3.365	-2.597
3	4	1	69.531	62.410	52.410	0.0	-2.578	-2.473
4	4	1	45.780	47.436	27.436	0.0	-1.656	-1.637
5	4	1	73.463	76.055	-76.055	0.0	-2.592	-2.029
6	4	1	28.602	31.009	31.009	0.0	-2.107	-1.562
7	4	1	29.502	28.933	-28.933	0.0	-0.431	-0.346
2	4	1	17.291	15.156	-15.156	0.0	2.065	1.022
10	4	1	8.543	8.284	-8.284	0.0	5.258	1.358
11	4	1	11.410	9.875	9.875	0.0	1.536	0.446
12	4	1	9.247	9.244	9.244	0.0	-0.677	-0.148
13	4	1	12.371	10.995	-10.995	0.0	1.677	0.436
14	4	1	19.330	21.228	-21.228	0.0	-1.891	-0.765
15	4	1	19.116	16.950	-16.950	0.0	2.157	0.402
16	4	1	26.749	25.406	-25.406	0.0	1.363	0.730
0	5	0	311.758	325.713	325.713	0.0	-13.955	-2.471
17	4	1	31.659	30.740	30.740	0.0	0.219	0.530
18	4	1	26.764	26.936	-26.936	0.0	0.219	0.113
20	4	1	9.120	4.448	-4.448	0.0	3.680	0.761
21	4	1	14.066	13.460	13.460	0.0	1.484	0.469
22	4	1	29.460	32.217	-32.217	0.0	-3.618	-1.628
23	4	1	26.467	26.947	-26.947	0.0	-0.400	-0.162
24	4	1	17.797	17.520	-17.520	0.0	-2.723	-0.660
25	4	1	20.773	22.472	-22.472	0.0	-1.699	-0.549
26	4	1	21.460	14.503	-16.503	0.0	5.365	1.908
26	4	1	20.151	16.597	-15.597	0.0	4.555	1.570
25	3	1	12.120	17.460	-17.460	0.0	-5.370	-1.068
24	3	1	14.453	17.776	17.776	0.0	-1.323	-0.392
23	3	1	31.714	31.333	-31.333	0.0	3.381	1.853
22	3	1	47.150	47.358	47.358	0.0	0.282	0.169
21	3	1	47.239	46.401	46.401	0.0	0.747	0.449
20	3	1	10.083	11.722	11.722	0.0	-1.642	-0.361
19	3	1	41.632	41.805	41.805	0.0	-0.173	-0.120
18	3	1	46.919	50.648	-50.648	0.0	-0.730	-0.480
17	3	1	70.714	72.561	-72.561	0.0	-1.847	-1.268
0	6	0	310.275	325.713	325.713	0.0	-15.438	-2.750
16	3	1	25.930	26.858	-26.858	0.0	-0.919	-0.492
15	3	1	27.035	24.907	-24.907	0.0	2.128	1.197
14	3	1	47.700	49.958	49.958	0.0	-2.158	-1.526
13	3	1	21.597	21.174	21.174	0.0	0.812	0.387

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	3	1	129.502	130.539	-130.539	0.0	-0.637	-0.299
11	3	1	196.117	192.505	192.505	0.0	3.612	1.121
10	2	1	167.313	165.792	-165.792	0.0	1.521	0.559
9	2	1	164.466	162.690	-162.690	0.0	1.776	0.655
8	3	1	76.429	76.628	-76.628	0.0	-0.200	-0.156
7	2	1	87.868	85.173	-85.173	0.0	2.695	1.054
6	3	1	148.246	147.001	-147.001	0.0	1.545	0.651
5	3	1	153.400	162.379	162.379	0.0	1.220	0.467
4	3	1	84.223	82.458	82.458	0.0	2.365	2.331
3	3	1	80.167	95.304	85.305	0.0	-5.157	-3.931
2	3	1	142.047	151.574	-151.574	0.0	-9.528	-4.236
1	3	1	171.330	196.516	-186.516	0.0	-15.185	-5.525 *
0	2	1	41.320	43.875	43.975	0.0	-2.555	-2.866
2	2	1	136.448	141.225	-141.225	0.0	-4.577	-2.118
3	2	1	158.158	160.278	-160.278	0.0	-2.119	-0.866
0	6	0	312.071	325.713	325.713	0.0	-13.642	-2.415 *
4	2	1	131.055	131.116	-131.116	0.0	-0.061	-0.029
5	2	1	130.277	133.265	133.265	0.0	-2.288	-1.104
6	2	1	111.662	133.785	-133.785	0.0	-2.123	-1.157
7	2	1	99.488	98.806	98.806	0.0	0.692	0.426
8	2	1	93.089	92.891	92.891	0.0	0.208	0.135
9	2	1	69.143	65.872	-65.872	0.0	2.771	2.236
10	2	1	19.663	21.400	21.400	0.0	-1.737	-0.896
11	2	1	47.760	48.605	-48.605	0.0	-0.846	-0.702
12	2	1	51.1602	53.965	-53.965	0.0	-2.363	-1.865
13	2	1	55.668	56.633	56.633	0.0	-0.944	-0.736
15	2	1	48.006	47.569	47.569	0.0	1.337	0.987
16	2	1	52.154	52.810	-52.810	0.0	-0.656	-0.489
17	2	1	56.509	53.283	-53.283	0.0	3.226	2.573
18	2	1	35.530	33.146	-33.146	0.0	2.304	1.575
19	2	1	3.829	8.162	-8.162	0.0	-4.334	-0.633
20	2	1	10.405	12.144	-12.144	0.0	-1.738	-0.416
21	2	1	155.713	6.553	-6.553	0.0	8.760	2.976
22	2	1	37.046	40.842	-40.842	0.0	-2.893	-1.547
23	2	1	46.301	46.354	-46.354	0.0	-0.052	-0.035
0	6	0	313.206	325.713	325.713	0.0	-12.507	-2.202 *
24	2	1	31.229	32.297	-32.297	0.0	-1.068	-0.518
25	2	1	37.446	36.792	-36.792	0.0	0.653	0.343
26	2	1	23.260	22.679	-22.679	0.0	0.580	0.217
27	1	1	13.229	1.052	-1.052	0.0	11.277	2.804 *
26	1	1	10.956	7.877	-7.877	0.0	3.120	0.662
25	1	1	14.500	6.148	-6.148	0.0	8.752	2.415
24	1	1	14.856	52.368	-52.368	0.0	9.488	2.990
21	1	1	5.246	9.454	9.454	0.0	-4.208	-0.638
20	1	1	9.292	1.460	-1.460	0.0	7.822	1.083
19	1	1	14.757	52.362	-52.362	0.0	9.435	3.709
17	1	1	8.232	2.665	-2.665	0.0	5.567	1.331
16	1	1	25.851	31.758	31.758	0.0	-5.907	-2.977
15	1	1	24.325	28.379	-28.379	0.0	-4.054	-1.850
14	1	1	33.112	31.672	31.672	0.0	1.440	0.652
13	1	1	28.547	30.350	30.350	0.0	-1.804	-1.059
12	1	1	18.243	17.870	-17.870	0.0	0.373	0.177
0	6	0	312.714	325.713	325.713	0.0	-12.997	-2.298 *

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STRUCTURE FACTORS

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H	K	L	F(OFC)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/STGMA
11	1	1	19.494	12.519	-12.519	0.0	7.035	2.900
10	1	1	10.272	15.637	-15.637	0.0	-5.365	-1.890
9	1	1	3.928	0.241	0.241	0.0	3.586	0.740
8	1	1	48.057	47.891	47.891	0.0	0.167	0.167
7	1	1	54.450	54.438	-54.438	0.0	-0.188	-0.186
6	1	1	51.110	50.925	-50.925	0.0	0.195	0.191
5	1	1	83.655	93.306	-93.306	0.0	-9.039	0.029
4	1	1	61.350	60.370	-60.370	0.0	0.980	0.923
2	1	1	34.640	33.677	-33.677	0.0	0.963	1.118
1	1	1	20.019	19.592	-19.592	0.0	0.425	0.405
0	0	2	31.822	32.410	-32.410	0.0	-0.588	-0.630
1	0	2	102.159	102.562	-102.562	0.0	-0.373	-0.231
2	0	2	158.159	156.229	-156.229	0.0	1.930	0.765
3	0	2	212.738	215.781	-215.781	0.0	-6.043	-1.723
6	0	2	80.378	79.907	-79.907	0.0	0.482	0.367
5	0	2	233.747	230.216	-230.216	0.0	3.531	0.902
7	0	2	198.855	194.470	-194.470	0.0	4.485	1.456
8	0	2	66.273	70.583	-70.583	0.0	-1.309	-1.339
0	6	0	311.211	325.713	-325.713	0.0	-14.502	-2.480
9	0	2	158.657	164.328	-164.328	0.0	4.429	1.615
10	0	2	13.022	4.042	-4.042	0.0	8.980	3.337
11	0	2	174.472	173.346	-173.346	0.0	1.126	0.397
12	0	2	37.291	38.135	-38.135	0.0	-0.854	-0.606
13	0	2	74.891	75.795	-75.795	0.0	-0.904	-0.639
14	0	2	8.305	4.139	-4.139	0.0	4.255	0.976
15	0	2	72.651	73.443	-73.443	0.0	-0.791	-0.554
16	0	2	23.053	33.435	-33.435	0.0	-0.302	-0.236
17	0	2	62.250	94.565	-94.565	0.0	-2.306	-1.469
18	0	2	38.670	37.847	-37.847	0.0	1.022	0.710
19	0	2	32.267	33.300	-33.300	0.0	-1.034	-0.576
20	0	2	6.429	92.686	-92.686	0.0	-0.458	-0.193
21	0	2	19.012	17.482	-17.482	0.0	1.530	0.530
22	0	2	65.273	70.972	-70.972	0.0	-1.499	-1.089
23	0	2	76.170	79.620	-79.620	0.0	-3.457	-2.015
24	0	2	10.472	20.758	-20.758	0.0	-10.279	-1.864 *
25	0	2	36.301	40.102	-40.102	0.0	-3.800	-1.674
26	0	2	67.099	212.462	-212.462	0.0	-12.373	-1.902 *
26	1	2	10.464	0.652	-0.652	0.0	9.813	2.183
25	1	2	14.204	10.304	-10.304	0.0	3.900	1.093
0	6	0	312.716	325.713	-325.713	0.0	-12.997	-2.298
24	1	2	19.515	19.038	-19.038	0.0	0.477	0.145
23	1	2	28.435	33.873	-33.873	0.0	-5.238	-2.117
22	1	2	15.492	16.934	-16.934	0.0	0.765	0.213
21	1	2	4.049	14.239	-14.239	0.0	-10.190	-1.331 *
20	1	2	9.118	11.211	-11.211	0.0	-1.693	-0.366
19	1	2	16.838	17.813	-17.813	0.0	-0.975	-0.2373
18	1	2	10.685	10.497	-10.497	0.0	0.189	0.051
17	1	2	57.808	58.105	-58.105	0.0	-0.297	-0.216
16	1	2	53.093	54.604	-54.604	0.0	-1.251	-1.226
15	1	2	10.442	3.050	3.050	0.0	6.792	2.033
14	1	2	5.306	3.550	-3.550	0.0	1.755	0.287
13	1	2	6.395	9.999	-9.999	0.0	-3.614	-0.2689
12	1	2	110.287	108.332	-108.332	0.0	1.954	1.061

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STRUCTURE FACTORS

PAGE 9

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
11	1	2	105.495	107.057	-107.057	0.0	-1.862	-1.049
10	1	2	36.262	35.439	-35.439	0.0	0.204	0.582
10	1	2	01.308	01.553	-01.553	0.0	-0.245	-0.174
8	1	2	55.568	57.800	-57.800	0.0	-2.231	-1.917
7	1	2	45.721	42.972	-42.972	0.0	2.749	2.678
6	1	2	23.771	23.027	-23.027	0.0	-0.256	-0.201
5	1	2	100.373	97.441	-97.441	0.0	-3.32	1.914
0	6	0	311.614	325.713	-325.713	0.0	-13.709	-2.443 *
4	1	2	50.648	45.862	-45.862	0.0	4.786	4.868
3	1	2	50.202	50.782	-50.782	0.0	-0.500	-0.609
2	1	2	20.813	20.406	-20.406	0.0	-0.623	-0.667
1	1	2	58.426	60.291	-60.291	0.0	-1.455	-1.800
0	2	2	11.090	11.023	-11.023	0.0	-0.028	-0.015
1	2	2	32.553	35.856	-35.856	0.0	-3.263	-2.443
2	2	2	12.741	17.433	-17.433	0.0	5.308	3.264
3	2	2	66.739	65.377	-65.377	0.0	1.362	1.996
4	2	2	8.350	8.204	-8.204	0.0	0.146	0.094
5	2	2	26.561	26.772	-26.772	0.0	0.190	0.182
6	2	2	62.951	60.056	-60.056	0.0	2.895	2.512
7	2	2	52.599	50.210	-50.210	0.0	2.380	1.552
8	2	2	25.404	23.111	-23.111	0.0	2.205	1.550
9	2	2	74.771	75.157	-75.157	0.0	-1.14	1.246
10	2	2	32.619	32.620	-32.620	0.0	0.100	0.070
11	2	2	18.169	18.191	-18.191	0.0	-0.022	-0.009
12	2	2	172.622	155.539	-155.539	0.0	2.082	0.864
13	2	2	33.002	29.405	-29.405	0.0	3.677	2.361
14	2	2	14.501	13.246	-13.246	0.0	1.335	0.403
15	2	2	26.117	26.684	-26.684	0.0	-0.567	-0.314
0	6	0	310.918	325.713	-325.713	0.0	-14.795	-2.633 *
17	2	2	18.963	16.057	-16.057	0.0	2.011	1.338
18	2	2	98.039	98.025	-98.025	0.0	-0.787	-0.510
19	2	2	34.604	31.231	-31.231	0.0	-0.546	-0.320
20	2	2	10.331	6.376	-6.376	0.0	3.055	0.932
21	2	2	14.326	21.058	-21.058	0.0	-6.760	-1.550
22	2	2	21.543	21.768	-21.768	0.0	-0.166	-0.060
23	2	2	14.747	14.671	-14.671	0.0	11.096	3.365 *
26	2	2	12.524	8.758	-8.758	0.0	3.736	0.042
26	3	2	14.471	0.530	-0.530	0.0	13.941	3.811 *
23	3	2	9.459	3.033	-3.033	0.0	6.428	1.317
22	3	2	9.385	4.352	-4.352	0.0	5.007	1.007
21	3	2	6.784	1.985	-1.985	0.0	4.199	0.786
20	3	2	4.227	2.872	-2.872	0.0	1.354	0.193
19	3	2	3.103	0.055	-0.055	0.0	-5.951	-0.747
0	6	0	311.719	325.713	-325.713	0.0	-13.94	-2.479 *
16	3	2	4.182	7.061	-7.061	0.0	-2.878	-0.442
15	3	2	19.368	17.423	-17.423	0.0	1.883	0.891
13	3	2	5.838	6.246	-6.246	0.0	-0.408	-0.072
9	3	2	1.000	17.552	-17.552	0.0	-0.352	-0.236
4	3	2	19.317	16.760	-16.760	0.0	1.556	0.716
7	3	2	11.189	7.370	-7.370	0.0	3.815	1.359
5	3	2	17.178	19.015	-19.015	0.0	1.262	0.700
4	3	2	45.364	42.956	-42.956	0.0	2.407	2.217
3	3	2	38.023	39.826	-39.826	0.0	-1.803	-1.641

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STRUCTURE FACTORS

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H	K	I	F(ORM)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	2	2	3.251	5.014	5.014	0.0	-1.762	-0.379
1	4	2	31.770	32.476	32.476	0.0	-0.698	-0.581
2	4	2	69.378	69.222	69.222	0.0	0.116	0.093
0	6	0	311.036	325.713	325.713	0.0	-14.677	-2.611 *
3	4	2	37.682	37.658	37.658	0.0	-0.177	-0.157
4	4	2	4.521	10.719	10.719	0.0	-5.798	-1.192
5	6	2	10.109	6.279	6.279	0.0	3.830	1.226
6	4	2	28.097	28.213	28.213	0.0	-0.126	-0.081
7	4	2	32.726	33.052	33.052	0.0	-1.226	-0.826
9	4	2	11.100	1.684	1.684	0.0	9.416	2.990
10	4	2	14.323	17.398	17.398	0.0	-3.075	-0.995
11	4	2	13.410	12.250	12.250	0.0	1.260	0.384
14	6	2	15.107	18.290	18.290	0.0	-3.182	-1.076
17	4	2	6.468	14.783	14.783	0.0	-8.295	-1.379
18	4	2	15.499	14.955	14.955	0.0	0.744	0.236
19	4	2	9.326	6.345	6.345	0.0	2.981	0.670
22	4	2	21.232	14.756	14.756	0.0	6.475	2.574
0	6	0	310.743	325.713	325.713	0.0	-14.970	-2.665 *
24	6	2	15.936	2.516	2.516	0.0	-0.580	-1.061
25	4	2	16.261	10.905	10.805	0.0	5.456	1.662
24	5	2	9.794	0.548	0.548	0.0	9.251	1.937
23	5	2	16.841	23.725	23.725	0.0	-3.884	-1.136
22	5	2	15.211	16.782	16.782	0.0	-1.571	-0.430
21	5	2	19.042	21.048	21.048	0.0	-2.006	-0.631
20	5	2	5.572	9.178	9.178	0.0	-3.606	-0.526
19	5	2	27.910	24.207	24.207	0.0	3.703	1.953
10	5	2	12.309	0.652	0.652	0.0	2.937	0.807
17	5	2	44.025	45.631	45.631	0.0	-1.805	-1.124
16	5	2	23.778	22.331	22.331	0.0	1.447	0.643
15	5	2	26.191	30.631	30.631	0.0	-4.440	-2.157
14	5	2	7.411	7.480	7.480	0.0	0.122	0.025
13	6	2	25.865	25.490	25.490	0.0	0.175	0.090
12	5	2	66.656	68.371	68.371	0.0	-1.676	-1.190
11	5	2	87.020	87.132	87.132	0.0	-0.111	-0.071
10	5	2	39.464	40.353	40.353	0.0	-0.889	-0.605
9	5	2	120.407	119.628	119.628	0.0	0.770	0.391
8	5	2	78.706	78.352	78.352	0.0	0.543	0.368
0	6	0	310.606	325.713	325.713	0.0	-15.107	-2.690 *
7	5	2	45.676	47.790	47.790	0.0	-2.114	-1.528
6	5	2	26.473	25.875	25.875	0.0	0.598	0.348
5	5	2	69.228	68.733	68.733	0.0	0.496	0.371
4	5	2	13.052	17.822	17.822	0.0	-4.770	-1.566
3	5	2	111.055	113.814	113.814	0.0	-2.729	-1.493
2	5	2	25.554	27.506	27.506	0.0	-1.952	-1.136
1	5	2	58.435	61.597	61.597	0.0	-3.162	-2.490
0	6	2	155.402	131.378	131.378	0.0	2.025	0.765
1	6	2	18.557	21.612	21.612	0.0	-2.955	-1.203
2	6	2	112.545	118.039	118.039	0.0	-5.495	-2.930
3	4	2	131.648	137.875	137.876	0.0	-6.228	-2.873
4	6	2	42.022	41.981	41.981	0.0	0.112	0.085
5	6	2	97.325	97.034	97.034	0.0	-0.609	-0.364
6	6	2	117.484	24.488	24.488	0.0	82.96	2.535
7	6	2	83.120	84.839	84.839	0.0	-1.719	-1.127

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	2	31.240	32.042	0.0	-0.694	-0.406	
9	6	2	102.066	102.087	0.0	-0.920	-0.524	
10	6	2	75.554	75.023	0.0	0.632	0.499	
11	6	2	71.375	69.591	0.0	1.704	1.225	
12	6	2	12.682	17.040	-17.080	0.0	-5.198	-1.423
0	6	0	305.411	325.713	325.713	0.0	-16.042	-2.471 *
13	6	2	36.272	33.295	-33.285	0.0	2.987	1.350
14	6	2	4.847	11.734	11.734	0.0	-4.896	-1.081
15	6	2	42.765	42.707	-42.707	0.0	0.158	0.107
16	6	2	19.012	21.295	21.295	0.0	-2.203	-0.711
6	6	2	36.643	38.420	38.420	0.0	-1.777	-0.021
14	6	2	16.764	13.365	13.365	0.0	3.306	1.089
10	6	2	24.446	26.035	24.035	0.0	-9.059	-1.003
21	6	2	16.011	14.026	-14.026	0.0	1.005	0.633
72	6	2	3N.910	40.652	40.652	0.0	-1.842	-0.683
25	5	2	46.614	44.089	-44.089	0.0	1.020	1.029
22	7	2	10.251	5.756	5.756	0.0	5.596	1.447
20	7	2	10.257	0.720	0.720	0.0	9.567	2.020
18	7	2	10.071	24.042	-24.042	0.0	16.379	7.051 *
17	7	2	4.301	7.407	7.407	0.0	-3.306	-0.440
16	7	2	13.428	17.481	-17.481	0.0	-3.053	-0.110
14	7	2	7.257	6.876	-6.876	0.0	0.380	0.073
0	6	0	311.231	325.713	325.713	0.0	-14.402	-24.976 *
13	7	2	19.116	21.151	21.151	0.0	-2.035	-0.749
12	7	2	40.220	38.403	-38.403	0.0	1.878	1.132
11	7	2	14.097	15.859	-15.859	0.0	-1.772	-0.555
10	7	2	12.948	0.240	-0.240	0.0	4.708	1.486
6	7	2	16.793	15.845	15.845	0.0	0.046	0.356
8	7	2	43.504	42.690	-42.690	0.0	-0.094	-0.074
7	7	2	27.110	27.832	-27.832	0.0	-0.782	-0.410
6	7	2	4.656	5.072	-5.072	0.0	-0.977	-0.174
5	7	2	18.971	17.372	17.372	0.0	-0.402	-0.160
4	7	2	30.858	32.467	-32.467	0.0	-1.608	-0.944
3	7	2	17.052	20.173	-20.173	0.0	-2.241	-0.876
2	7	2	10.376	5.953	-5.953	0.0	4.443	1.206
1	7	2	3.117	5.440	-5.440	0.0	-2.322	-0.311
0	8	2	14.501	13.777	13.777	0.0	-0.774	0.251
1	8	2	42.013	43.307	-43.307	0.0	-0.677	-0.347
2	8	2	17.607	16.624	16.624	0.0	0.983	0.398
3	8	2	26.707	26.304	26.304	0.0	0.405	0.233
4	8	2	9.696	9.915	-9.915	0.0	-0.233	-0.034
5	8	2	30.755	29.316	-29.316	0.0	1.438	0.859
6	9	2	14.559	14.540	14.540	0.0	-0.223	-0.007
0	6	0	311.472	325.713	325.713	0.0	-13.740	-24.433 *
7	9	2	40.089	43.245	-43.245	0.0	-2.356	-1.458
8	8	2	16.005	16.453	-16.453	0.0	-0.433	0.012
9	8	2	25.880	27.406	27.406	0.0	-2.074	1.111
10	8	2	14.486	2.091	-2.091	0.0	12.395	4.506 *
11	8	2	25.732	26.700	26.700	0.0	-0.032	0.017
12	8	2	12.519	7.727	-7.727	0.0	4.822	1.279
13	8	2	27.717	28.818	-28.818	0.0	0.899	0.433
14	8	2	14.015	9.529	-8.529	0.0	6.386	1.019
15	8	2	14.619	15.945	-15.945	0.0	-1.326	-0.360

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA
16	8	2	8.431	1.055	0.0	7.577	1.408	
17	8	7	12.440	8.763	0.0	3.697	0.846	
18	8	2	11.573	12.684	-12.694	0.0	-1.111	-0.229
19	7	2	13.938	17.158	17.158	0.0	-3.220	-0.743
20	8	2	11.691	10.734	-10.734	0.0	0.958	0.211
21	8	2	10.293	11.867	-11.867	0.0	-1.284	-0.247
19	9	2	3.089	10.357	-10.357	0.0	-7.388	-0.811
17	9	2	16.335	18.446	-18.446	0.0	5.388	1.591
14	9	2	15.377	18.306	-18.306	0.0	3.571	0.940
15	9	2	10.923	6.766	-6.766	0.0	4.157	0.976
0	6	0	310.411	325.713	325.713	0.0	-15.302	-2.725 *
11	6	2	11.041	10.459	-10.459	0.0	0.182	0.042
10	6	2	10.523	1.200	-1.200	0.0	9.324	2.398
9	6	2	10.273	7.050	-7.050	0.0	3.222	0.804
8	6	2	7.257	2.291	-2.291	0.0	4.965	0.857
7	6	2	7.403	6.382	-6.382	0.0	1.421	0.285
4	6	2	6.823	3.991	-3.991	0.0	4.832	1.131
3	9	2	11.884	11.899	-11.899	0.0	-0.015	-0.004
2	6	2	2.276	10.290	-10.290	0.0	-8.014	-0.999
1	6	2	15.211	8.778	-8.778	0.0	6.433	2.544
0	10	2	11.218	3.275	-3.275	0.0	7.944	2.091
2	10	2	25.473	23.328	-23.328	0.0	2.344	1.147
3	10	2	27.865	22.305	-22.305	0.0	5.560	3.128
4	10	2	15.318	9.110	-9.110	0.0	4.208	1.293
5	10	2	13.170	14.228	-14.228	0.0	-1.058	-0.289
0	6	0	311.407	325.713	325.713	0.0	-14.306	-2.544 *
6	10	2	12.497	15.559	-15.559	0.0	-2.863	-0.747
7	10	2	14.478	5.810	-5.810	0.0	8.865	2.802
8	10	2	6.385	7.216	-7.216	0.0	2.169	0.457
9	10	2	10.345	7.876	-7.876	0.0	2.865	0.634
10	10	2	14.353	4.025	-4.025	0.0	10.328	3.248 *
11	10	2	14.244	17.127	-17.127	0.0	-2.863	-0.712
13	10	2	12.596	7.181	-7.181	0.0	5.718	1.487
12	10	2	12.215	6.932	-6.932	0.0	5.883	1.401
15	10	2	1.951	10.378	-10.378	0.0	-8.427	-0.856
16	10	2	12.519	5.161	-5.161	0.0	7.358	1.722
17	10	2	13.024	15.735	-15.735	0.0	-1.411	-0.412
14	11	2	11.765	3.977	-3.977	0.0	7.788	1.792
12	11	2	31.377	32.649	-32.649	0.0	-1.271	-0.533
11	11	2	35.574	33.480	-33.480	0.0	2.094	1.045
10	11	2	13.466	15.059	-15.059	0.0	-2.494	-0.600
9	11	2	43.550	41.908	-41.908	0.0	1.641	0.869
8	11	2	30.769	28.253	-28.253	0.0	2.546	1.184
7	11	2	22.447	18.675	-18.675	0.0	3.993	1.606
0	6	0	317.638	325.713	325.713	0.0	-13.075	-2.312 *
6	11	2	10.021	37.756	-37.756	0.0	6.265	1.316
5	11	2	27.258	28.460	-28.460	0.0	-1.202	-0.501
3	11	2	34.572	32.236	-32.236	0.0	2.685	1.448
2	11	2	13.185	10.266	-10.266	0.0	2.919	0.748
1	11	2	20.447	15.136	-15.136	0.0	5.312	2.094
0	12	2	7.587	4.002	-4.002	0.0	3.594	0.630
2	12	2	31.866	30.621	-30.621	0.0	1.246	0.592
3	12	2	29.613	26.647	-26.647	0.0	2.967	1.300

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DFLT8 F	DELTA/SIGMA	119
4	12	2	9.322	10.493	-10.493	0.0	-1.270	-0.5225	
5	12	2	16.596	15.253	-15.253	0.0	1.703	0.490	
6	12	2	10.804	9.216	-8.216	0.0	2.588	0.527	
0	12	2	7.155	6.049	-6.049	0.0	1.297	0.195	
9	12	2	22.445	16.371	-16.371	0.0	6.075	2.372	
10	12	2	6.503	4.126	-4.126	0.0	2.376	0.330	
11	12	2	6.380	12.613	-12.613	0.0	-5.233	-0.225	
4	13	2	14.427	10.419	-10.419	0.0	4.007	0.968	
3	13	2	15.322	12.943	-12.943	0.0	12.420	2.735 *	
0	13	2	308.135	325.713	-325.713	0.0	-17.579	-0.164 *	
1	13	2	9.451	10.934	-10.934	0.0	-1.203	-0.228	
0	12	3	9.577	14.283	-14.283	0.0	-2.607	-0.528	
3	12	3	9.104	23.623	-23.623	0.0	6.421	1.305	
6	12	3	6.372	0.247	-0.247	0.0	6.585	1.113	
7	12	3	12.150	1.912	-1.912	0.0	10.238	2.402 *	
11	11	3	10.152	4.156	-4.156	0.0	6.826	1.445	
10	11	3	20.724	24.656	-24.656	0.0	2.058	0.485	
9	11	3	17.237	8.180	-8.180	0.0	9.057	2.916	
6	11	3	7.523	12.252	-12.252	0.0	-5.420	-0.842	
5	11	3	13.273	8.193	-8.193	0.0	4.081	1.111	
4	11	3	2.616	1.803	-1.803	0.0	0.812	0.092	
0	6	0	311.775	325.713	-325.713	0.0	-13.838	-2.450 *	
2	11	3	28.013	30.495	-30.495	0.0	-1.682	-0.684	
1	11	3	11.507	3.945	-3.945	0.0	8.042	1.929	
0	10	3	12.726	12.784	-12.784	0.0	-0.058	-0.007	
1	10	3	8.093	3.279	-3.279	0.0	4.820	0.951	
2	10	3	2.409	0.902	-0.902	0.0	1.507	0.180	
3	10	3	14.368	16.750	-16.750	0.0	-2.391	0.620	
4	10	3	35.241	34.892	-34.892	0.0	0.950	0.508	
6	10	3	9.501	1.263	-1.263	0.0	4.339	0.630	
7	10	3	3.325	2.472	-2.472	0.0	-0.146	-0.018	
8	10	3	13.540	2.830	-2.830	0.0	10.609	2.995 *	
0	10	3	23.335	7.210	-7.210	0.0	-4.935	-0.537	
11	10	3	8.454	7.567	-7.567	0.0	0.887	0.148	
12	10	3	4.250	2.870	-2.870	0.0	1.881	0.249	
0	6	0	306.301	325.713	-325.713	0.0	-16.412	-2.939 *	
14	9	3	73.673	71.719	-71.719	0.0	1.894	1.115	
13	9	3	25.436	23.199	-23.199	0.0	2.237	0.938	
10	9	3	16.124	15.780	-15.780	0.0	2.345	0.800	
8	9	3	12.120	0.500	-0.500	0.0	11.620	3.070 *	
7	9	3	14.041	12.080	-12.080	0.0	2.761	0.845	
6	9	3	57.435	55.680	-55.680	0.0	1.755	1.164	
9	9	3	2.320	10.432	-10.432	0.0	-8.112	-0.429	
4	9	3	7.936	1.836	-1.836	0.0	6.100	1.207	
3	9	3	14.900	1.762	-1.762	0.0	13.138	4.700 *	
2	9	3	51.498	22.560	-22.560	0.0	-1.062	-0.706	
1	9	3	33.779	34.319	-34.319	0.0	-0.540	-0.303	
0	8	3	129.700	130.724	-130.724	0.0	-1.024	-0.470	
1	8	3	27.050	28.885	-28.885	0.0	-1.835	-0.885	
2	8	3	10.567	4.818	-4.818	0.0	6.149	1.800	
3	8	3	20.003	11.908	-11.908	0.0	8.895	4.485	
4	8	3	22.653	23.008	-23.008	0.0	-0.355	-0.161	
0	6	0	310.646	325.713	-325.713	0.0	-15.068	-2.683 *	

SOO DETHIOPROSTIMATE 7/03/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	8	2	20.803	17.059	0.0	3.704	1.814	
6	8	3	14.249	0.964	-0.964	0.0	13.285	6.704 *
7	8	2	34.477	34.370	-34.320	0.0	0.157	0.094
8	6	3	55.420	56.982	0.0	-0.563	-0.381	
10	8	3	5.660	0.418	0.418	0.0	5.243	0.845
12	9	3	43.015	42.734	-42.734	0.0	0.281	0.173
13	7	3	21.232	19.947	-19.847	0.0	1.385	0.538
15	9	3	15.151	16.766	-15.746	0.0	-1.594	-0.407
16	8	2	17.651	22.442	22.442	0.0	-4.791	-1.322
17	6	3	11.395	4.338	4.338	0.0	7.057	1.540
19	9	3	20.462	19.349	19.349	0.0	1.113	0.368
21	7	3	11.425	2.177	2.177	0.0	9.248	1.925
16	7	3	14.087	5.764	5.764	0.0	8.323	2.190
15	7	2	7.789	4.069	-4.069	0.0	3.720	0.618
0	4	0	310.639	325.713	325.713	0.0	-14.775	-2.629 *
16	7	3	41.499	39.828	-39.828	0.0	1.671	1.103
13	7	3	18.701	14.134	14.134	0.0	4.567	1.705
12	7	3	11.870	3.619	-3.619	0.0	8.279	2.187
11	7	3	1.951	0.505	0.505	0.0	1.446	0.170
10	7	2	23.093	20.061	-20.061	0.0	2.947	1.363
0	7	3	10.593	6.604	6.604	0.0	3.979	1.051
2	7	3	6.666	8.085	8.085	0.0	-1.581	0.376
7	7	3	10.696	11.104	-11.104	0.0	-0.418	-0.111
6	7	3	32.282	33.938	-33.838	0.0	-1.557	-0.875
5	7	3	10.316	7.213	-7.213	0.0	3.103	0.930
4	7	3	10.612	8.926	8.926	0.0	1.686	0.458
3	7	3	7.262	7.278	-7.278	0.0	-0.036	-0.008
7	7	3	0.740	5.492	5.492	0.0	-4.247	1.114
1	7	3	6.798	13.557	-13.557	0.0	-6.759	-1.281
0	6	3	3.000	6.084	-6.084	0.0	-2.094	-0.308
2	6	3	8.180	7.974	7.974	0.0	0.314	0.064
3	6	3	5.690	11.663	11.663	0.0	-5.973	-1.078
0	4	0	310.651	325.713	325.713	0.0	-15.262	-2.718 *
4	6	3	7.715	9.679	9.679	0.0	-1.964	-0.423
5	6	3	12.550	11.791	11.791	0.0	1.068	0.356
6	6	3	0.163	2.489	-2.489	0.0	-2.326	-0.248
7	6	3	11.705	7.627	7.627	0.0	4.168	1.355
8	6	3	27.301	27.803	-27.803	0.0	-0.412	-0.232
0	5	3	9.947	4.677	-4.677	0.0	5.470	1.445
10	6	3	10.376	0.542	-0.542	0.0	9.834	2.715
12	6	3	11.507	6.997	6.997	0.0	4.990	1.395
13	6	3	2.453	0.439	0.439	0.0	2.014	0.245
14	6	3	3.206	6.809	-6.809	0.0	-1.514	-0.193
18	6	3	15.137	0.372	0.372	0.0	14.765	4.870 *
20	6	3	16.098	12.748	12.748	0.0	3.350	0.960
0	6	0	312.169	325.713	325.713	0.0	-13.545	-2.397 *
21	6	3	13.638	5.011	-5.011	0.0	8.987	2.283
20	5	3	9.267	2.022	2.022	0.0	7.245	1.454
19	6	3	6.133	5.245	5.245	0.0	0.889	0.138
18	6	3	28.200	26.919	-26.919	0.0	1.361	0.604
17	6	3	20.166	20.291	20.291	0.0	-0.124	-0.048
16	6	3	10.882	6.909	-6.909	0.0	6.073	1.499
15	5	3	11.070	8.579	8.579	0.0	2.491	0.613

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/STGMA
16	5	2	23.348	23.124	0.0	0.224	0.101	
13	6	3	11.543	9.250	-0.250	0.0	2.293	0.621
11	5	2	15.004	15.813	-15.813	0.0	-0.809	-0.271
10	5	3	62.726	63.132	-63.132	0.0	-0.466	-0.335
9	6	2	12.342	14.672	14.672	0.0	-2.331	-0.674
6	5	3	8.232	8.642	2.642	0.0	5.590	1.171
5	5	3	25.007	27.205	-27.205	0.0	-2.198	-1.100
4	5	2	7.267	4.744	-4.744	0.0	2.823	0.584
3	6	2	19.027	18.578	-18.578	0.0	0.449	0.180
0	6	0	307.824	325.713	325.713	0.0	-17.891	-3.222 *
2	6	2	83.558	88.740	-88.740	0.0	-6.210	-0.671
1	6	3	20.936	26.140	26.140	0.0	-5.204	-2.284
0	4	3	133.068	143.680	-143.680	0.0	-10.613	-4.926 *
1	4	2	25.202	24.025	-24.025	0.0	1.278	0.750
2	4	3	10.662	9.598	-9.598	0.0	1.043	1.825
3	4	3	13.583	11.027	-11.027	0.0	2.456	1.068
4	4	3	35.307	37.550	-37.550	0.0	-0.243	-0.170
5	6	3	12.902	14.522	14.522	0.0	-5.480	1.708
6	4	3	14.116	11.520	-11.520	0.0	12.566	4.436 *
7	4	2	10.124	12.521	12.521	0.0	-3.407	-0.847
8	4	3	24.703	25.411	-25.411	0.0	-1.378	-0.455
9	4	3	11.750	8.526	-8.526	0.0	3.225	0.963
10	4	2	8.380	11.948	11.948	0.0	-3.568	-0.815
11	4	3	13.318	8.065	-8.065	0.0	5.253	1.850
12	4	2	42.651	43.076	43.076	0.0	-0.225	-0.164
13	4	3	21.513	22.093	22.093	0.0	-0.570	-0.241
14	6	2	19.625	17.172	-17.172	0.0	11.493	4.722 *
15	4	3	16.541	14.644	-14.644	0.0	2.297	0.839
16	4	3	6.104	3.995	-3.995	0.0	2.108	0.368
17	4	3	7.651	4.512	-4.512	0.0	3.439	0.684
0	6	0	308.485	325.713	325.713	0.0	-17.229	-3.100 *
20	4	3	40.368	42.253	42.253	0.0	-1.854	-0.203
21	4	3	3.384	4.344	4.344	0.0	-0.960	-0.114
23	4	3	11.528	9.808	-9.808	0.0	2.118	0.458
24	4	3	24.451	19.685	-19.685	0.0	4.966	1.973
25	3	2	11.440	7.517	-7.517	0.0	3.923	0.899
22	3	3	33.527	30.156	-30.156	0.0	3.371	1.079
21	3	3	32.630	34.030	-34.030	0.0	-1.209	-0.585
20	3	2	11.043	4.585	-4.585	0.0	7.357	1.971
16	3	3	16.204	20.047	-20.047	0.0	-0.842	-0.293
18	3	3	66.510	65.558	-65.558	0.0	1.361	0.899
17	3	3	21.765	21.198	-21.198	0.0	0.566	0.245
16	3	3	8.646	9.914	-9.914	0.0	-1.268	-0.266
15	2	3	23.570	23.156	-23.156	0.0	0.414	0.182
14	3	3	172.042	165.505	165.505	0.0	2.537	0.891
13	3	3	53.830	54.012	-54.012	0.0	-0.174	-0.127
12	3	3	13.318	9.404	-9.404	0.0	3.913	1.310
0	2	0	310.107	325.713	325.713	0.0	-15.516	-2.774 *
11	2	3	16.616	15.523	-15.523	0.0	1.092	0.410
10	2	3	11.322	5.474	-5.474	0.0	5.647	1.552
9	3	3	21.765	22.089	-22.089	0.0	-1.225	-0.559
8	2	3	6.118	4.636	-4.636	0.0	1.483	0.282
7	3	3	43.505	42.236	-42.236	0.0	1.269	0.928

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	3	3	163.100	191.646	191.646	0.0	-1.454	0.457
5	3	3	55.275	55.744	-55.744	0.0	-0.369	-0.298
4	3	2	13.564	15.717	15.717	0.0	-2.148	-0.737
3	3	3	15.032	21.499	-21.499	0.0	-5.668	-21.153
2	3	3	186.717	195.990	-195.990	0.0	-9.273	-3.033
1	3	3	53.504	97.824	97.824	0.0	-3.920	-2.481
0	2	3	241.161	267.616	-267.616	0.0	-26.455	-6.489 *
1	2	3	56.405	58.789	58.789	0.0	-2.385	-1.997
3	2	3	21.251	22.000	22.000	0.0	-0.746	-0.620
2	2	3	31.218	30.658	-30.658	0.0	0.660	0.494
5	2	3	18.775	20.664	-20.664	0.0	-1.888	-0.851
7	2	3	45.910	43.119	-43.119	0.0	2.692	2.262
8	2	3	78.715	77.475	-77.475	0.0	1.240	0.849
0	0	0	309.544	325.713	-325.713	0.0	-15.769	-2.821 *
9	2	3	5.082	1.976	-1.976	0.0	3.906	0.724
10	2	3	10.109	10.803	-10.803	0.0	-0.694	-0.169
12	2	3	86.113	85.445	-85.445	0.0	0.698	0.448
13	2	3	37.207	37.336	-37.336	0.0	-0.130	-0.086
15	2	3	34.744	30.960	-30.960	0.0	3.783	2.429
16	2	3	32.160	33.287	-33.287	0.0	-0.427	-0.255
17	2	3	10.169	2.559	-2.559	0.0	7.609	1.913
18	2	2	4.345	0.693	-0.693	0.0	3.652	0.522
19	2	3	22.653	22.939	-22.939	0.0	-0.287	-0.109
20	2	3	74.756	77.008	-77.008	0.0	-2.252	-1.400
21	2	3	14.220	8.189	-8.189	0.0	6.031	1.750
22	2	3	8.038	5.757	-5.757	0.0	3.081	0.559
23	2	3	8.676	3.080	-3.080	0.0	5.595	1.020
24	2	3	10.763	13.274	-13.274	0.0	-2.410	-0.443
25	1	3	8.720	5.549	-5.549	0.0	3.171	0.556
24	1	3	7.611	6.457	-6.457	0.0	1.155	0.180
23	1	3	5.109	0.594	-0.594	0.0	4.815	0.665
0	6	0	309.574	325.713	-325.713	0.0	-16.139	-2.888 *
20	1	3	11.550	2.535	-2.535	0.0	9.023	2.252
13	1	3	19.782	20.911	-20.911	0.0	-11.130	-0.422
17	1	3	24.474	21.222	-21.222	0.0	3.252	1.615
14	1	3	16.736	13.836	-13.836	0.0	2.098	1.209
12	1	3	5.641	32.270	-32.270	0.0	22.564	0.496
11	1	3	14.612	11.672	-11.672	0.0	3.947	0.972
10	1	3	60.273	59.566	-59.566	0.0	0.708	0.532
0	1	3	14.702	16.699	-16.699	0.0	-12.918	-0.648
7	1	3	12.031	14.037	-14.037	0.0	-2.806	-0.904
6	1	3	25.530	25.837	-25.837	0.0	0.103	0.066
5	1	2	32.202	33.121	-33.121	0.0	-0.240	-0.609
3	1	3	15.551	18.246	-18.246	0.0	-2.695	-1.248
0	6	0	310.132	325.713	-325.713	0.0	-15.574	-2.785 *
1	1	3	68.203	68.767	-68.767	0.0	-0.484	-0.389
1	1	3	13.523	13.316	-13.316	0.0	4.318	-1.908
0	0	4	105.857	106.191	-106.191	0.0	3.666	1.991
1	0	4	38.617	38.084	-38.084	0.0	0.534	0.374
2	0	4	72.892	73.616	-73.616	0.0	-0.724	-0.518
3	0	4	119.372	116.366	-116.366	0.0	3.005	1.520
4	0	4	171.994	163.282	-163.282	0.0	3.712	1.318
5	0	4	94.405	93.201	-93.201	0.0	1.204	0.727

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STRUCTURE FACTORS

PAGE 17

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	0	4	11.498	9.438	0.0	3.460	0.892	
7	0	4	92.099	94.511	-84.511	0.0	-1.602	-1.050
8	0	4	124.252	123.508	-123.508	0.0	0.756	0.366
9	0	4	38.498	41.567	41.567	0.0	-3.069	-2.007
10	0	4	31.451	32.495	-32.495	0.0	-1.044	-0.634
11	0	4	13.569	19.172	-19.172	0.0	-5.603	-1.662
12	0	4	91.308	92.162	-92.162	0.0	-0.854	-0.516
13	0	4	59.401	57.994	-57.994	0.0	1.487	1.059
14	0	4	6.872	5.731	5.731	0.0	0.141	0.027
15	0	4	28.250	29.357	-29.357	0.0	-1.107	-0.515
16	0	4	80.162	78.513	-78.513	0.0	1.640	1.022
17	0	4	37.400	40.141	40.141	0.0	-2.251	-1.233
0	6	0	309.885	325.713	325.713	0.0	-15.828	-2.831
18	0	4	19.737	20.241	-20.241	0.0	-0.504	-0.190
19	0	4	13.717	12.742	12.742	0.0	0.975	0.262
20	0	4	27.635	30.408	30.408	0.0	-2.572	-1.092
21	0	4	9.149	3.703	3.703	0.0	5.446	0.993
22	0	4	7.685	14.146	-14.146	0.0	-5.461	-0.952
23	0	4	29.836	26.328	-26.328	0.0	3.508	0.197
23	1	4	8.453	0.540	-0.540	0.0	8.003	1.417
22	1	4	15.160	23.391	-23.391	0.0	-4.231	-1.187
21	1	4	11.011	10.390	-10.390	0.0	0.421	0.085
20	1	4	9.163	2.130	-2.130	0.0	7.034	1.404
19	1	4	21.735	17.289	-17.289	0.0	4.446	1.736
18	1	4	27.855	26.638	-26.638	0.0	0.926	0.440
17	1	4	10.257	10.360	10.360	0.0	-0.103	-0.023
16	1	4	6.444	9.874	-9.874	0.0	-3.430	-0.561
15	1	4	6.887	6.919	-6.919	0.0	-0.032	0.006
14	1	4	10.652	12.182	-12.182	0.0	-1.229	-0.295
13	1	4	8.528	1.062	-1.062	0.0	7.465	1.689
12	1	4	35.601	33.214	-33.214	0.0	2.697	1.811
11	1	4	72.206	73.761	-73.761	0.0	-1.454	-0.909
10	1	4	72.441	71.107	71.107	0.0	1.334	0.935
0	6	0	311.153	325.713	325.713	0.0	-14.560	-2.590
9	1	4	45.379	44.845	44.845	0.0	0.524	0.382
8	1	4	34.744	35.501	-35.501	0.0	-1.157	-0.722
7	1	4	20.536	16.900	-16.900	0.0	0.636	0.264
6	1	4	35.421	37.933	-37.933	0.0	-1.112	-0.607
5	1	4	16.468	20.823	-20.823	0.0	-4.355	-1.526
4	1	4	18.302	15.438	-15.438	0.0	1.136	-0.660
3	1	4	2.823	10.156	-10.156	0.0	-7.333	-0.990
2	1	4	55.121	56.651	-56.651	0.0	-1.530	-1.152
1	1	4	72.471	76.566	-76.566	0.0	-4.055	-2.931
0	2	4	61.111	66.426	-66.426	0.0	-5.315	-3.863
1	2	4	53.033	55.523	-55.523	0.0	-2.490	-1.876
2	2	4	25.425	21.905	-21.905	0.0	4.019	2.381
3	2	4	16.202	12.707	12.707	0.0	3.494	1.358
4	2	4	28.632	29.526	29.526	0.0	-0.595	-0.321
5	2	4	32.679	32.457	32.457	0.0	0.522	0.332
6	2	4	15.018	10.539	-10.539	0.0	4.480	1.594
7	2	4	12.445	9.118	9.118	0.0	3.327	1.037
8	2	4	35.130	33.682	-33.682	0.0	1.418	0.966
9	2	4	17.261	18.166	18.166	0.0	-0.864	-0.326

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(FCALC)	B(FCALC)	DELTA F	DELTA/SIGMA
10	2	6	10.069	-6.091	0.0	4.758	1.381	
0	6	0	311.563	325.713	325.713	0.0	-14.150	-2.516 *
11	2	4	11.721	14.160	14.160	0.0	-2.438	-0.652
12	2	6	21.248	30.293	30.293	0.0	-8.555	0.526
13	2	6	26.280	24.065	24.065	0.0	2.215	1.177
14	2	6	21.217	20.252	20.252	0.0	0.945	0.410
16	2	6	18.406	13.710	13.710	0.0	4.608	1.734
20	2	6	17.163	17.163	17.163	0.0	-3.815	-0.900
21	2	6	5.198	5.093	5.093	0.0	-1.215	-0.201
22	2	6	15.590	16.577	16.577	0.0	-1.973	1.566
23	3	4	1.567	4.260	4.260	0.0	-2.693	-0.256
22	3	4	2.291	4.286	4.286	0.0	-1.995	-0.207
17	3	4	9.503	9.008	9.008	0.0	1.605	0.604
17	3	4	4.774	5.003	5.003	0.0	-0.229	-0.031
0	6	0	310.172	325.713	325.713	0.0	-14.531	-7.658 *
15	2	4	11.721	10.672	10.672	0.0	1.049	0.270
19	2	4	7.922	8.650	8.650	0.0	-0.728	-0.193
11	3	4	11.130	3.538	3.538	0.0	7.592	2.223
11	3	4	12.712	14.523	14.523	0.0	-1.812	-0.550
7	2	4	16.098	22.613	22.613	0.0	-6.515	-2.294
5	3	4	13.364	13.196	13.196	0.0	0.166	0.051
2	3	4	9.762	0.266	0.266	0.0	9.716	2.434
2	3	4	6.178	5.176	5.176	0.0	1.001	0.186
0	2	4	26.369	27.507	27.507	0.0	-1.109	-0.576
1	4	4	3.771	7.255	7.255	0.0	-3.972	-0.569
0	5	0	309.466	325.713	325.713	0.0	-16.217	-2.903 *
4	4	4	7.712	9.876	9.876	0.0	-2.664	-0.558
5	4	2	24.020	26.006	26.006	0.0	-1.976	-1.027
6	4	4	5.350	14.216	14.216	0.0	-8.666	-1.453
7	4	4	13.233	10.508	10.508	0.0	2.025	0.901
9	4	2	23.940	24.047	24.047	0.0	-0.106	-0.092
10	4	4	8.040	14.688	14.688	0.0	-6.648	-1.291
11	4	4	15.107	7.481	7.481	0.0	7.626	2.381
12	4	4	11.526	5.734	5.734	0.0	5.764	1.640
12	4	4	6.680	12.373	12.373	0.0	-5.693	-0.998
14	4	4	12.756	12.671	12.671	0.0	0.085	0.023
15	4	4	21.173	23.323	23.323	0.0	-2.150	-0.785
19	4	4	13.765	0.004	0.004	0.0	5.561	1.485
16	4	4	3.133	18.446	18.446	0.0	-15.313	-1.627 *
22	4	2	17.456	13.660	13.660	0.0	3.760	1.115
21	5	6	20.091	23.505	23.505	0.0	-2.614	-0.785
0	6	0	310.529	325.713	325.713	0.0	-15.185	-2.704 *
20	5	4	13.540	0.034	0.034	0.0	13.505	3.668 *
16	5	4	23.576	28.509	28.509	0.0	-0.067	0.029
18	5	4	30.760	33.212	33.212	0.0	-2.472	-1.017
17	5	2	17.059	15.707	15.707	0.0	1.353	0.416
16	5	4	0.784	10.652	10.652	0.0	-0.860	-0.168
15	5	4	3.365	11.334	11.334	0.0	-2.939	-0.571
14	5	4	25.540	26.280	26.280	0.0	-0.741	-0.323
13	5	4	19.204	20.592	20.592	0.0	-1.388	-0.457
12	5	4	38.825	39.513	39.513	0.0	-0.688	-0.403
11	5	4	66.295	65.512	65.512	0.0	0.883	0.572
10	5	4	80.057	80.168	80.168	0.0	-0.111	-0.070

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	5	4	501.470	501.474	0.0	-0.004	-0.003	
0	5	6	14.889	20.261	-20.261	0.0	-5.273	-1.571
0	5	4	16.497	13.940	-13.940	0.0	2.558	0.350
1	5	4	53.182	54.254	54.254	0.0	-1.072	-0.157
6	5	4	7.025	17.347	17.347	0.0	-10.312	-1.691 *
5	5	4	12.002	0.462	0.462	0.0	11.540	3.620 *
3	5	4	7.197	3.025	-3.025	0.0	4.172	0.953
2	5	4	71.029	73.086	-73.086	0.0	-2.057	-1.437
1	5	4	47.268	48.257	-48.257	0.0	-0.069	-0.730
0	6	0	309.451	325.713	325.713	0.0	-16.022	-2.667
0	6	4	47.447	48.707	-48.707	0.0	-1.260	-0.866
1	6	4	8.513	8.801	-8.801	0.0	1.712	0.370
2	6	4	36.965	37.428	37.428	0.0	-0.463	-0.364
3	6	4	64.477	64.457	64.457	0.0	0.320	0.225
4	6	4	90.980	91.620	91.620	0.0	-0.631	-0.578
5	6	4	46.896	47.071	-47.071	0.0	0.174	-0.120
6	6	4	10.789	11.534	11.534	0.0	-0.744	-0.199
7	6	4	25.554	26.691	-26.691	0.0	-1.136	-0.512
8	6	4	65.151	63.323	-63.323	0.0	1.828	0.558
9	6	4	16.852	19.688	19.688	0.0	7.164	2.476
10	6	4	48.565	49.069	49.069	0.0	-0.103	-0.065
11	6	4	42.747	46.899	46.899	0.0	-4.151	-2.270
12	6	4	31.437	28.340	-28.340	0.0	3.096	1.503
13	6	4	50.000	46.834	-46.834	0.0	3.174	1.937
14	6	4	25.466	26.488	26.488	0.0	-1.022	-0.393
15	6	4	13.421	17.815	-17.815	0.0	-4.393	-0.948
16	6	4	0.444	3.886	-3.886	0.0	4.198	0.706
17	6	0	309.574	325.713	325.713	0.0	-16.139	-2.888 *
20	6	4	17.178	15.570	15.570	0.0	1.608	0.449
19	7	4	7.966	9.113	-9.113	0.0	-1.147	-0.176
18	7	4	2.438	0.479	0.479	0.0	1.459	0.195
16	7	4	19.915	19.747	19.747	0.0	5.169	1.810
15	7	4	29.465	26.007	-26.007	0.0	2.459	1.632
14	7	4	0.025	12.592	12.592	0.0	-4.567	-0.745
13	7	4	12.135	13.961	13.961	0.0	-1.826	-0.400
12	7	4	19.782	17.963	17.963	0.0	1.818	0.686
11	7	4	26.236	26.633	-26.633	0.0	-0.398	-0.171
10	7	4	18.021	15.302	15.302	0.0	2.719	0.972
9	7	4	24.261	21.776	21.776	0.0	2.505	1.106
8	7	4	22.031	18.489	18.489	0.0	3.543	1.564
7	7	4	7.730	1.731	-1.731	0.0	5.598	1.166
6	7	4	16.571	10.970	10.970	0.0	5.502	2.116
5	7	4	11.765	12.486	12.486	0.0	-0.721	-0.198
3	7	4	11.266	9.355	9.355	0.0	2.011	0.506
2	7	4	12.623	1.169	-1.169	0.0	11.554	3.654 *
1	7	4	14.205	11.533	11.533	0.0	2.672	0.860
0	6	0	310.353	325.713	325.713	0.0	-15.360	-2.736 *
0	6	4	39.939	36.930	-36.930	0.0	0.109	0.067
1	8	4	18.731	13.178	13.178	0.0	5.553	2.133
2	8	4	7.330	3.424	-3.424	0.0	3.906	0.751
3	8	4	14.856	14.555	14.555	0.0	0.301	0.088
4	8	4	23.067	25.580	25.580	0.0	-2.513	-0.948
5	8	4	6.843	1.214	1.214	0.0	5.629	0.976

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	8	4	13.490	8.495	-8.495	0.0	5.104	1.576
7	8	4	18.021	13.034	-13.094	0.0	4.927	1.735
8	8	4	30.169	20.119	-20.119	0.0	2.042	1.029
9	8	4	21.069	25.304	25.394	0.0	-4.325	-1.536
10	8	4	16.926	9.855	-9.855	0.0	7.071	2.452
11	8	4	12.450	4.772	4.772	0.0	7.718	1.845
12	8	4	25.007	23.961	23.961	0.0	-1.046	0.348
13	8	4	14.471	10.736	-10.736	0.0	3.736	0.995
15	8	4	13.800	0.658	0.658	0.0	13.222	3.695 *
16	8	4	13.609	13.144	-13.144	0.0	0.765	0.180
0	6	0	308.523	325.713	325.713	0.0	-17.190	-3.093 *
12	0	4	7.695	6.491	-6.491	0.0	1.195	0.200
11	0	4	10.093	5.971	-5.971	0.0	4.922	1.044
10	0	4	21.143	9.491	-9.491	0.0	11.652	4.801 *
9	0	4	13.208	12.979	-12.979	0.0	0.309	0.078
8	0	4	8.291	1.948	1.948	0.0	6.343	1.144
4	0	4	9.710	5.669	5.669	0.0	4.041	0.852
4	0	4	8.040	3.545	3.545	0.0	4.495	0.815
3	0	4	8.716	11.153	-11.153	0.0	-2.537	-0.488
2	0	4	14.757	8.810	8.810	0.0	5.957	1.782
1	0	4	11.573	5.949	5.949	0.0	5.624	1.312
0	10	4	7.523	0.482	-0.482	0.0	7.041	1.212
1	10	4	7.301	9.644	-9.644	0.0	-2.343	-0.387
2	10	4	12.623	0.945	-0.945	0.0	2.678	0.622
3	10	4	17.755	16.628	-16.628	0.0	2.926	0.912
4	10	4	9.119	17.877	-17.877	0.0	-8.758	-1.435
5	10	4	12.404	17.344	-17.344	0.0	-4.441	-0.956
6	10	2	18.497	5.373	-5.373	0.0	13.626	5.262 *
0	6	0	309.320	325.713	325.713	0.0	-16.353	-2.928 *
7	10	4	12.540	5.505	5.505	0.0	7.044	1.609 *
8	11	4	18.302	10.655	-10.655	0.0	7.647	2.450
7	11	4	9.623	1.793	1.793	0.0	7.740	1.471
6	11	4	10.346	18.154	-18.154	0.0	-7.808	-1.390
2	11	2	22.271	27.373	-27.373	0.0	-5.001	-1.529
1	11	4	21.824	21.672	-21.672	0.0	0.151	0.050
0	10	4	6.030	1.659	-1.659	0.0	4.371	0.643
2	10	5	24.592	21.307	21.307	0.0	3.285	1.282
4	10	5	3.458	3.284	3.284	0.0	0.174	0.021
5	10	5	13.654	6.460	-6.460	0.0	7.494	2.027
0	6	0	301.853	325.713	325.713	0.0	-16.820	-3.024 *
6	10	5	10.878	8.268	8.268	0.0	2.611	0.533
11	0	5	22.845	23.650	-23.650	0.0	-0.805	-0.258
10	0	5	16.793	6.875	6.875	0.0	11.918	3.874 *
9	0	5	28.961	31.533	-31.533	0.0	-2.571	-0.980
8	0	5	25.608	28.806	-28.806	0.0	-3.118	-1.091
7	0	5	17.773	15.136	15.136	0.0	2.737	0.812
5	0	5	27.613	26.088	-26.088	0.0	1.525	0.648
4	0	5	6.577	0.247	-0.247	0.0	-1.670	-0.244
3	0	5	34.758	33.822	-33.822	0.0	0.936	0.460
1	8	5	18.021	14.781	14.781	0.0	3.240	1.090
2	8	5	39.642	41.256	-41.256	0.0	-1.614	-0.782
3	8	5	40.310	40.058	40.058	0.0	0.252	0.141
4	8	5	11.026	8.541	8.541	0.0	2.405	0.530

900 DENTAL PROSTHETIC SITE 7/03/73

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/A SIGMA
5	8	5	28.151	30.186	-30.186	0.0	+1.995	-0.837
7	9	5	17.311	18.042	-18.042	0.0	-0.731	-0.226
0	6	0	21.153	325.713	325.713	0.0	-1.580	-2.594 *
6	8	5	49.117	42.024	42.024	0.0	-1.107	-0.644
10	0	5	10.404	3.040	3.040	0.0	7.764	1.661
11	8	5	36.731	36.159	36.159	0.0	1.572	0.847
12	7	5	12.392	7.543	7.543	0.0	5.848	1.403
13	8	5	11.026	8.391	-8.391	0.0	2.945	0.574
16	7	5	13.636	4.231	4.231	0.0	9.205	2.239
15	7	5	6.606	11.563	-11.563	0.0	-4.957	-0.714
14	7	5	11.056	3.151	-3.151	0.0	7.904	1.666
13	7	5	10.745	1.362	-1.362	0.0	9.393	1.028
12	7	5	21.809	17.773	17.773	0.0	4.036	1.435
11	7	5	14.782	9.184	9.184	0.0	5.598	1.532
10	7	5	8.616	2.429	-2.429	0.0	6.187	1.192
6	7	5	8.868	9.964	-9.964	0.0	-1.096	-0.200
8	7	5	20.285	20.449	20.449	0.0	-0.164	-0.055
6	7	5	7.330	1.399	-1.399	0.0	5.991	1.059
5	7	5	15.832	6.567	-6.567	0.0	9.264	3.196
4	7	5	20.107	17.370	17.370	0.0	2.137	0.785
3	7	5	21.557	23.702	23.702	0.0	-2.145	-0.776
0	6	0	310.587	325.713	325.713	0.0	-15.126	-26.693 *
1	7	5	6.325	1.923	-1.923	0.0	4.402	0.745
1	6	5	6.622	9.008	-9.008	0.0	0.614	0.133
2	6	5	14.930	13.015	13.015	0.0	1.915	0.611
3	6	5	9.607	14.668	-14.668	0.0	-5.061	-1.025
4	6	5	14.752	1.619	1.619	0.0	13.133	4.246 *
9	6	5	12.652	6.780	-6.780	0.0	5.872	1.539
10	6	5	16.542	8.710	-8.710	0.0	7.831	2.497
11	6	5	7.670	3.762	-3.762	0.0	3.928	0.656
15	5	5	10.272	3.070	-3.070	0.0	7.202	1.463
16	6	5	4.360	1.521	-1.521	0.0	2.839	0.359
17	6	5	7.803	8.604	-8.604	0.0	-0.801	-0.126
0	6	0	310.158	325.713	325.713	0.0	-15.555	-26.781 *
17	5	5	3.251	1.793	-1.793	0.0	1.459	0.165
15	5	5	11.765	8.618	-8.618	0.0	3.147	0.696
13	5	5	22.431	22.183	-22.183	0.0	0.247	0.048
12	5	5	23.057	24.188	24.188	0.0	-1.092	-0.394
11	5	5	19.308	13.801	-13.801	0.0	5.507	2.164
10	5	5	13.199	5.319	-5.319	0.0	7.081	2.184
9	5	5	22.209	21.426	21.426	0.0	0.783	0.315
8	5	5	8.070	5.606	-5.606	0.0	2.444	0.462
7	5	5	38.617	34.320	35.320	0.0	3.297	2.075
6	5	5	12.874	9.738	-9.738	0.0	3.137	0.880
5	5	5	25.273	24.312	-24.312	0.0	0.662	0.461
4	5	5	11.233	6.572	-6.572	0.0	4.661	1.236
3	5	5	20.181	11.920	-11.920	0.0	8.261	3.511
2	5	5	9.400	5.569	-5.569	0.0	3.801	0.905
1	5	5	23.659	22.613	22.613	0.0	1.046	0.404
0	4	5	7.759	8.493	-8.493	0.0	-0.734	-0.153
1	4	5	12.505	3.416	-3.416	0.0	9.088	2.955
0	6	0	309.983	325.713	325.713	0.0	-15.730	-26.813 *
2	4	5	34.002	40.211	40.211	0.0	-6.209	-3.220

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STRUCTURE FACTORS

PAGE 22

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
3	4	5	-20.459	32.997	-32.997	0.0	-3.358	-1.626
5	4	5	13.463	15.074	15.074	0.0	-1.431	-0.412
6	4	5	13.498	19.841	19.841	0.0	-5.844	-1.526
7	4	5	10.331	5.386	5.386	0.0	4.945	1.212
9	4	5	26.724	23.661	-23.661	0.0	2.763	1.296
10	4	5	0.623	3.712	3.712	0.0	5.821	1.367
11	4	5	24.456	26.120	-26.120	0.0	-1.661	-0.710
15	4	5	7.419	1.925	1.925	0.0	5.496	0.907
16	4	5	11.573	0.601	-0.601	0.0	10.972	2.348 *
17	4	5	6.043	20.495	-20.495	0.0	-13.652	1.836 *
18	4	5	23.694	19.686	-19.686	0.0	3.958	1.469
19	4	5	5.498	0.413	0.413	0.0	5.085	0.698
20	3	5	16.197	15.205	-15.205	0.0	0.982	0.275
19	3	5	13.347	19.235	-18.235	0.0	-4.888	-1.109
0	4	0	311.641	325.713	325.713	0.0	-14.072	-2.493 *
19	2	5	6.059	6.857	-6.857	0.0	-1.759	-0.228
17	3	5	44.501	47.159	47.159	0.0	-2.658	-1.375
16	3	5	37.311	37.941	-37.941	0.0	-0.631	-0.317
15	2	5	30.495	28.469	28.469	0.0	1.227	0.591
13	3	5	26.265	23.031	-23.031	0.0	3.235	1.560
12	3	5	50.932	48.611	-48.611	0.0	2.321	1.403
11	3	5	71.375	69.415	-69.415	0.0	1.460	0.953
10	3	5	18.716	18.089	-18.089	0.0	0.627	0.224
c	2	5	96.950	86.316	-86.316	0.0	0.674	0.409
3	3	5	51.662	52.266	-52.266	0.0	-0.605	-0.354
7	3	6	59.078	59.485	-59.485	0.0	-0.408	-0.287
6	3	6	10.923	11.861	-11.861	0.0	-0.938	-0.228
5	3	5	70.203	80.326	-80.326	0.0	-2.123	-1.368
4	3	5	12.061	7.766	7.766	0.0	4.295	1.196
3	3	5	91.629	90.251	-90.251	0.0	1.179	0.713
2	3	5	16.026	16.556	-16.556	0.0	-0.532	-0.193
1	3	5	30.562	32.940	-32.940	0.0	-2.378	-1.263
0	2	5	8.084	1.060	-1.060	0.0	7.024	1.622
1	2	5	25.056	25.986	-25.986	0.0	-0.032	-0.018
0	6	0	308.695	325.713	325.713	0.0	-17.229	-3.100 *
2	2	5	58.749	56.564	-56.564	0.0	2.185	1.556
3	2	5	62.014	63.714	-63.714	0.0	-1.616	-1.149
5	2	5	40.412	47.647	-47.647	0.0	1.766	1.235
6	2	5	12.978	16.233	-16.233	0.0	-3.255	-0.888
7	2	5	25.184	23.478	-23.478	0.0	1.707	0.893
c	2	5	56.525	59.048	-59.048	0.0	-0.523	-0.350
10	2	5	9.370	5.624	-5.624	0.0	3.746	0.871
11	2	5	56.196	57.604	-57.604	0.0	-1.408	-0.916
12	2	5	2.512	6.341	-6.341	0.0	-3.825	-0.459
13	2	5	8.666	10.866	-10.866	0.0	-2.220	-0.447
14	2	5	13.451	10.900	-10.900	0.0	2.551	0.644
15	2	5	13.126	17.131	-17.131	0.0	-4.006	-0.957
17	2	5	32.667	32.866	-32.866	0.0	-0.199	-0.094
18	2	5	21.572	15.954	-15.954	0.0	5.618	2.109
19	2	5	13.480	0.994	9.994	0.0	3.487	0.851
0	4	0	309.418	325.713	325.713	0.0	-16.295	-2.917 *
21	1	5	9.163	9.037	-9.037	0.0	0.127	0.023
20	1	5	8.463	6.339	6.339	0.0	2.145	0.369

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
19	1	5	97.104	32.385	-32.385	0.0	5.719	-1.054
17	1	5	7.212	7.998	-7.998	0.0	-0.786	-0.125
16	1	5	11.499	8.640	8.640	0.0	2.059	0.649
14	1	5	12.401	4.270	-4.270	0.0	0.131	2.157
13	1	5	20.077	18.245	-18.245	0.0	1.033	0.716
12	1	5	32.815	33.865	33.865	0.0	-1.050	-0.562
11	1	5	5.749	2.696	-2.696	0.0	3.053	0.513
10	1	5	5.675	2.814	-2.814	0.0	2.861	0.405
9	1	5	11.024	8.643	8.643	0.0	3.102	0.578
8	1	5	17.917	16.571	-16.571	0.0	1.346	0.503
7	1	5	31.214	30.396	30.396	0.0	0.018	0.484
6	1	5	13.421	11.035	-11.035	0.0	1.886	0.521
5	1	5	8.217	10.571	-10.571	0.0	-2.353	-0.505
4	1	5	16.349	14.546	14.546	0.0	1.803	0.645
3	1	5	10.656	9.144	9.144	0.0	1.513	0.403
2	1	5	8.454	6.934	-6.934	0.0	1.519	0.366
0	6	0	310.177	325.713	325.713	0.0	-15.536	-2.778 *
1	1	5	14.634	12.423	12.423	0.0	2.211	0.787
0	0	6	118.103	113.427	-113.427	0.0	4.756	2.317
1	0	6	64.492	65.103	-65.103	0.0	-0.611	-0.388
2	0	6	13.451	5.330	5.330	0.0	8.121	2.441
3	0	6	37.370	40.749	-40.749	0.0	-3.379	-1.913
4	0	6	25.229	25.242	25.242	0.0	-0.014	-0.007
5	0	6	24.133	24.172	24.172	0.0	-0.039	-0.016
6	0	6	6.562	3.187	-3.187	0.0	3.375	0.604
7	0	6	58.122	58.912	58.912	0.0	-0.790	-0.495
8	0	6	51.423	52.919	-52.919	0.0	-1.496	-0.938
9	0	6	15.063	11.087	-11.087	0.0	3.976	1.211
10	0	6	16.926	12.528	12.528	0.0	4.399	1.451
11	0	6	16.483	8.459	-8.459	0.0	8.023	2.620
12	0	6	43.570	43.121	43.121	0.0	0.458	0.239
13	0	6	48.310	48.970	48.970	0.0	-0.660	-0.360
15	0	6	46.256	46.295	46.295	0.0	-0.039	-0.021
16	0	6	20.368	24.746	-24.746	0.0	-4.357	-1.280
17	0	6	12.978	3.882	-3.882	0.0	9.094	2.158
17	1	6	4.077	3.869	3.869	0.0	1.008	0.126
0	6	0	308.368	325.713	325.713	0.0	-17.345	-3.121 *
16	1	6	0.451	11.723	11.723	0.0	-2.072	-0.371
15	1	6	11.307	12.670	-12.670	0.0	-1.363	-0.272
14	1	6	47.953	47.734	-47.734	0.0	0.219	0.127
13	1	6	29.139	31.379	31.379	0.0	-2.240	-0.900
12	1	6	8.483	7.843	7.843	0.0	0.640	0.123
9	1	6	12.076	6.644	-6.644	0.0	5.432	1.381
7	1	6	29.806	29.472	-29.472	0.0	0.335	0.157
6	1	6	41.766	38.859	-38.859	0.0	2.907	1.672
5	1	6	172.043	67.767	67.767	0.0	11.076	4.328 *
4	1	6	6.281	9.646	-9.646	0.0	-3.365	-0.565
3	1	6	8.439	3.955	3.955	0.0	4.484	0.939
2	1	6	25.392	27.264	27.264	0.0	-1.873	-0.790
1	1	6	33.423	33.460	-33.460	0.0	-0.067	-0.037
0	2	6	8.471	1.278	-1.278	0.0	7.693	1.684
1	2	6	6.724	7.098	-7.098	0.0	-0.373	-0.065
2	2	6	9.193	11.821	11.821	0.0	-2.628	-0.537

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
3	2	6	70.214	23.446	-23.446	0.0	-3.132	-1.157
0	6	0	309.107	325.713	325.713	0.0	-16.606	-2.974 *
4	2	6	28.665	24.116	24.116	0.0	4.549	2.344
6	2	6	9.740	11.058	-11.058	0.0	-1.319	-0.273
8	2	6	7.463	3.694	3.694	0.0	3.770	0.673
10	2	6	3.916	9.994	-9.994	0.0	-6.078	-0.752
11	2	6	18.775	19.232	-19.232	0.0	-0.557	-0.170
12	2	6	8.779	9.943	-9.943	0.0	-0.164	-0.030
14	2	6	12.342	16.710	-16.710	0.0	-4.368	-0.846
17	2	6	13.056	11.233	-11.233	0.0	1.833	0.599
15	3	6	4.803	5.084	-5.084	0.0	-0.280	-0.036
15	3	6	9.991	0.427	0.427	0.0	9.565	1.859
12	3	6	1.345	4.781	-4.781	0.0	-3.437	-0.331
11	3	6	4.759	6.569	-6.569	0.0	-1.810	-0.247
0	6	0	310.236	325.713	325.713	0.0	-15.477	-2.767 *
10	3	6	7.153	3.542	-3.542	0.0	3.611	0.602
9	3	6	12.978	4.195	-4.195	0.0	8.783	2.367
6	3	6	14.308	10.584	-10.584	0.0	3.724	1.086
5	3	6	17.474	2.451	-2.451	0.0	15.022	6.045 *
4	3	6	14.604	10.768	-10.768	0.0	3.837	1.190
2	3	6	13.025	2.381	-2.381	0.0	11.144	3.555 *
1	3	6	13.185	6.177	-6.177	0.0	7.007	2.017
0	4	6	30.947	29.950	29.950	0.0	0.997	0.542
3	4	6	21.0%2	24.075	-24.075	0.0	-2.133	-0.810
4	4	6	9.2%1	11.761	-11.761	0.0	-2.400	-0.456
7	4	6	6.015	10.441	-10.441	0.0	-4.426	-0.649
4	4	6	15.166	7.214	-7.214	0.0	7.953	2.411
0	6	0	310.139	325.713	325.713	0.0	-15.574	-2.785 *
11	4	6	20.501	4.174	-4.174	0.3	16.407	7.200 *
13	4	6	10.130	7.428	-7.428	0.0	2.711	0.511
15	4	6	2.498	0.828	-0.828	0.0	1.670	0.176
14	4	6	40.255	38.900	38.900	0.0	1.395	0.712
13	5	6	32.712	32.410	-32.410	0.0	0.302	0.127
12	5	6	3.665	0.710	-0.710	0.0	3.455	0.407
11	5	6	11.054	10.459	-10.459	0.0	1.356	0.327
10	5	6	5.379	3.668	-3.668	0.0	1.711	0.233
9	5	6	12.257	4.432	-4.432	0.0	7.924	1.970
8	5	6	14.307	9.838	-9.838	0.0	4.555	1.233
7	5	6	28.704	27.233	-27.233	0.0	1.550	0.737
6	5	6	50.038	50.137	-50.137	0.0	-0.059	-0.060
5	5	6	21.232	23.180	-23.180	0.0	-1.948	-0.636
2	5	6	24.355	26.333	-26.333	0.0	-1.978	-0.791
0	6	0	310.214	325.713	325.713	0.0	-15.399	-2.743 *
1	6	0	46.792	48.636	-48.636	0.0	-1.844	-1.087
0	6	0	79.861	81.573	-81.573	0.0	-1.712	-0.962
1	6	0	37.457	40.122	-40.122	0.0	-2.425	-1.228
2	6	6	14.501	12.579	-12.579	0.0	1.522	0.500
3	6	6	18.958	12.211	-12.211	0.0	6.287	2.225
4	6	6	4.020	7.709	-7.709	0.0	-3.690	-0.458
5	6	6	19.249	20.965	-20.965	0.0	-1.716	-0.515
6	6	6	3.429	4.654	-4.654	0.0	-1.525	-0.182
7	6	6	42.182	38.167	-38.167	0.0	4.015	2.456
8	6	6	25.066	23.736	-23.736	0.0	1.329	0.483

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
10	6	6	9.710	2.513	-2.513	0.0	7.197	1.375
11	6	6	12.357	6.797	-6.797	0.0	5.550	1.221
12	6	6	35.056	31.721	31.721	0.0	4.126	2.161
13	6	6	20.117	20.534	20.534	0.0	1.582	0.650
10	7	6	14.463	17.450	-17.450	0.0	-2.787	-0.628
9	7	6	15.052	9.285	9.285	0.0	5.800	1.177
7	7	6	15.468	9.032	-9.032	0.0	3.726	0.893
0	6	0	210.197	325.713	325.713	0.0	-15.517	-2.444 *
6	7	6	17.743	20.357	-20.357	0.0	-2.617	-0.711
5	7	6	13.495	5.256	-5.256	0.0	8.240	2.079
3	7	6	6.680	13.277	-13.277	0.0	-6.598	-0.940
1	7	6	8.802	10.016	-10.016	0.0	-1.217	-0.204
0	8	6	15.425	3.375	-3.375	0.0	12.250	3.565 *
1	8	6	14.749	7.446	-7.446	0.0	6.404	1.070
3	8	4	20.169	10.266	-10.266	0.0	1.403	0.447
4	8	6	22.238	22.339	-22.339	0.0	-0.101	-0.032
5	9	6	11.721	4.036	-4.036	0.0	7.687	1.727
6	8	6	7.050	2.417	-2.417	0.0	4.633	0.711
7	8	6	10.552	7.039	-7.039	0.0	3.913	0.781
0	6	7	6.020	5.421	-5.421	0.0	0.600	0.084
2	6	7	15.657	1.927	-1.927	0.0	13.810	4.165 *
7	5	7	12.458	4.951	-4.951	0.0	5.627	1.295
6	5	7	22.845	17.483	-17.483	0.0	5.362	2.011
0	5	0	300.262	325.713	325.713	0.0	-16.431	-2.946 *
5	8	7	15.954	11.520	-11.520	0.0	4.474	1.310
3	5	7	12.238	0.487	-0.487	0.0	11.782	2.711 *
2	6	7	10.478	16.481	-16.481	0.0	5.181	1.044
1	2	7	19.145	10.531	-10.531	0.0	5.045	0.111
2	4	7	12.455	6.968	-6.968	0.0	5.847	1.307
4	4	7	21.513	19.459	-19.459	0.0	1.954	0.599
5	4	7	16.454	21.878	-21.878	0.0	-5.447	-1.299
6	4	7	14.740	1.090	-1.090	0.0	12.571	3.513 *
7	4	7	16.497	10.988	-10.988	0.0	5.610	1.614
8	4	7	16.882	12.741	-12.741	0.0	4.141	1.235
9	4	7	7.294	9.154	-9.154	0.0	-0.868	-0.128
11	3	7	25.040	36.720	-36.720	0.0	-1.688	-0.725
10	3	7	53.028	53.047	-53.047	0.0	0.880	0.476
9	3	7	10.050	10.536	-10.536	0.0	-0.486	-0.087
7	3	7	8.183	7.280	-7.280	0.0	0.863	0.138
0	5	0	307.624	325.713	325.713	0.0	-17.889	-3.222 *
6	3	7	37.698	37.517	-37.517	0.0	0.291	0.145
5	2	7	17.444	12.710	-12.710	0.0	4.734	1.416
7	3	7	26.503	2.717	-2.717	0.0	6.787	1.327
3	3	7	14.974	12.587	-12.587	0.0	2.417	0.612
2	3	7	51.155	55.719	-55.719	0.0	-4.554	-2.412
1	3	7	31.066	2.094	-2.094	0.0	1.972	0.450
0	2	7	20.051	19.291	-19.291	0.0	1.659	0.641
1	2	7	21.044	20.646	-20.646	0.0	0.428	0.151
3	2	7	144.456	162.295	-162.295	0.0	-1.839	-0.447
4	2	7	43.356	42.971	-42.971	0.0	0.386	0.214
5	2	7	21.306	25.130	-25.130	0.0	-1.024	-0.565
7	2	7	71.759	10.350	-10.350	0.0	-2.591	-0.421
8	2	7	27.628	29.396	-29.396	0.0	-1.768	-0.686

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STRUCTURE FACTORS

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H	K	I	F(PRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
9	2	7	1.271	0.072	0.0	-7.001	-0.722	
10	2	7	12.097	1.277	0.0	11.820	2.788 *	
11	2	7	14.294	16.867	-16.867	0.0	-2.573	-0.545
12	2	7	22.223	24.363	24.363	0.0	-2.140	-0.710
12	1	7	14.294	0.076	-0.076	0.0	1.827	3.561 *
0	6	0	309.503	325.713	325.713	0.0	-14.220	-2.885 *
10	1	7	17.455	6.078	6.078	0.0	11.373	4.054 *
6	1	7	11.061	4.238	-4.228	0.0	6.813	1.445
7	1	7	6.784	3.207	3.207	0.0	3.567	0.554
4	1	7	15.308	4.937	-4.937	0.0	10.451	2.944 *
5	1	7	10.867	11.407	-11.987	0.0	-1.020	-0.213
4	1	7	14.062	2.119	-2.119	0.0	11.923	3.264 *
2	1	7	4.095	7.452	7.452	0.0	-2.957	-0.392
1	1	7	17.917	12.230	-12.239	0.0	5.679	1.979

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STRUCTURE FACTORS

PAGE 1

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
0	6	0	298.303	310.230	0.0	-12.027	-2.249 *	
4	0	0	174.407	170.944	-170.944	0.0	-5.047	-1.001
6	0	0	56.261	10.508	-10.508	0.0	-1.327	-0.573
8	0	0	90.765	111.509	111.509	0.0	-12.745	-0.054 *
10	0	0	11.838	6.992	6.992	0.0	4.846	2.232
12	0	0	253.714	250.550	-270.550	0.0	3.165	0.728
14	0	0	18.035	13.389	-13.389	0.0	4.646	2.030
16	0	0	131.728	132.056	132.056	0.0	-1.229	-0.566
20	0	0	127.058	127.377	-127.377	0.0	-0.319	-0.149
20	1	0	52.469	1.445	-1.445	0.0	4.054	0.680
18	1	0	42.158	41.426	-41.426	0.0	0.732	0.508
16	1	0	5.472	2.475	-2.475	0.0	6.207	1.474
14	1	0	120.268	120.260	-120.260	0.0	0.128	0.064
12	1	0	7.788	2.307	-2.307	0.0	5.680	1.438
10	1	0	50.246	40.151	-40.151	0.0	1.195	0.154
8	1	0	5.739	5.548	-5.548	0.0	4.191	2.194
6	1	0	248.894	257.450	257.450	0.0	-8.555	-2.024
4	1	0	11.852	6.296	6.296	0.0	5.556	3.367
2	1	0	93.631	96.922	-96.922	0.0	-2.951	-2.297
0	2	0	2.662	5.165	-9.165	0.0	-6.503	-1.582
0	6	0	208.662	310.330	310.330	0.0	-11.678	-2.194 *
2	2	0	6.048	1.762	1.762	0.0	4.257	1.474
4	2	0	102.050	198.828	-198.828	0.0	-6.770	-2.175
6	2	0	10.578	9.481	-9.481	0.0	0.597	0.313
8	2	0	76.865	80.115	-80.115	0.0	-0.270	-0.190
12	2	0	10.585	9.824	-9.824	0.0	1.121	0.357
14	2	0	4.881	4.990	-4.990	0.0	-0.099	-0.017
16	2	0	61.015	60.935	-60.935	0.0	0.080	0.360
18	2	0	11.707	7.899	7.899	0.0	3.808	1.175
20	2	0	10.695	8.763	-8.763	0.0	1.662	0.404
20	3	0	4.601	2.521	2.521	0.0	2.031	0.327
18	3	0	5.310	7.993	7.993	0.0	-2.682	-0.467
16	3	0	43.458	43.763	-43.763	0.0	-0.296	-0.207
10	2	0	2.518	1.044	-1.044	0.0	-6.526	-1.009
8	3	0	10.198	6.136	-6.136	0.0	4.052	1.656
6	3	0	42.261	40.241	-40.241	0.0	2.120	2.276
2	3	0	0.073	10.543	10.543	0.0	-1.470	-0.564
2	3	0	52.082	51.846	-51.846	0.0	0.236	0.245
0	6	0	208.585	310.330	310.330	0.0	-11.744	-2.195 *
0	2	0	24.023	24.511	24.511	0.0	0.422	0.383
4	4	0	56.669	58.285	-58.285	0.0	-1.626	-1.566
6	4	0	8.089	3.330	-3.330	0.0	4.759	1.522
8	4	0	64.654	64.024	-64.024	0.0	0.2670	0.544
10	4	0	20.360	21.949	21.949	0.0	-1.089	-0.601
12	4	0	11.117	14.302	-14.302	0.0	-2.985	-0.818
16	4	0	37.74	37.395	-37.395	0.0	0.080	0.051
20	4	0	4.6074	45.063	45.063	0.0	1.011	0.680
18	5	0	40.050	40.203	40.203	0.0	0.767	0.446
16	5	0	6.613	3.800	3.800	0.0	2.004	0.537
14	5	0	171.047	169.468	-169.468	0.0	1.599	0.566
12	5	0	11.548	6.213	6.213	0.0	5.336	1.536
10	5	0	20.889	17.695	-17.695	0.0	3.2190	1.631
8	5	0	6.642	8.464	-8.464	0.0	-1.823	-0.408

Final cycle

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STRUCTURE FACTORS

PAGE 2

H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA
6	5	0	133.748	134.783	-134.783	0.0	-1.035	-0.479
2	5	0	190.015	190.036	-190.036	0.0	-7.122	-2.288
0	6	0	297.320	310.330	-310.330	0.0	-12.930	-2.430 *
0	6	0	297.889	310.330	-310.330	0.0	-12.441	-2.335 *
2	6	0	9.406	7.043	-7.043	0.0	2.363	0.680
4	6	0	70.361	74.015	-74.015	0.0	-3.654	-2.701
8	6	0	111.944	111.973	-111.973	0.0	-0.029	-0.016
10	6	0	9.302	5.179	-5.179	0.0	4.212	1.007
12	6	0	97.422	65.584	-65.584	0.0	1.438	0.853
14	6	0	141.063	111.032	-111.032	0.0	3.861	1.481
16	6	0	52.009	48.319	-48.319	0.0	3.690	2.580
16	7	0	0.752	8.792	-8.792	0.0	-8.030	-0.928
14	7	0	52.925	52.296	-52.296	0.0	0.633	0.443
12	7	0	7.756	3.024	-3.024	0.0	4.732	1.009
10	7	0	61.572	61.505	-61.505	0.0	0.067	0.049
8	7	0	12.263	3.939	-3.939	0.0	8.306	2.758
6	7	0	23.063	24.768	-24.768	0.0	-1.705	-0.817
4	7	0	14.342	15.676	-15.676	0.0	-1.334	-0.452
2	7	0	18.122	13.553	-13.553	0.0	4.569	1.996
0	8	0	60.125	61.435	-61.435	0.0	-1.240	-0.931
2	8	0	6.466	11.035	-11.035	0.0	-2.471	-0.625
4	8	0	72.567	74.601	-74.601	0.0	-2.383	-1.549
0	6	0	296.272	310.330	-310.330	0.0	-14.057	-2.456 *
8	8	0	22.561	21.271	-21.271	0.0	1.271	0.569
12	8	0	38.129	30.256	-30.256	0.0	-1.729	-0.549
8	9	0	5.441	11.122	-11.122	0.0	-5.682	-0.299
6	9	0	20.183	28.070	-28.070	0.0	-1.092	0.622
4	9	0	0.521	37.531	-37.531	0.0	-3.010	-0.073
0	10	0	50.609	52.320	-52.320	0.0	-1.711	-1.117
2	10	0	10.202	2.074	-2.074	0.0	7.326	1.834
4	10	0	14.574	6.717	-6.717	0.0	4.857	1.597
6	10	0	8.267	1.317	-1.317	0.0	7.930	1.790
0	10	1	26.485	23.236	-23.236	0.0	3.251	1.751
1	10	1	27.703	24.270	-24.270	0.0	3.452	1.766
2	10	1	21.498	25.779	-25.779	0.0	-4.282	-1.623
4	10	1	16.080	0.140	-0.140	0.0	15.940	6.437 *
0	6	0	297.704	310.330	-310.330	0.0	-12.783	-2.411 *
6	10	1	13.109	15.756	-15.756	0.0	-2.658	-0.687
11	9	1	53.382	50.517	-50.517	0.0	2.865	1.923
10	9	1	62.514	63.772	-63.772	0.0	-0.858	-0.504
9	6	1	54.171	53.389	-53.389	0.0	0.781	0.514
8	9	1	35.440	33.091	-33.091	0.0	2.349	1.526
7	9	1	13.245	16.465	-16.465	0.0	-3.020	-0.358
6	9	1	19.774	19.687	-19.687	0.0	0.086	0.035
5	9	1	23.048	24.227	-24.227	0.0	-1.178	0.561
4	9	1	6.917	52.131	-52.131	0.0	1.786	0.386
3	0	1	32.419	29.060	-29.060	0.0	3.359	2.162
2	0	1	38.478	36.762	-36.762	0.0	1.715	1.168
1	0	1	334.882	32.627	-32.627	0.0	1.056	0.421
0	0	1	19.774	17.253	-17.253	0.0	2.521	1.279
1	8	1	12.980	5.830	-5.830	0.0	7.050	2.590
2	8	1	60.327	63.481	-63.481	0.0	-3.156	-2.394
3	8	1	84.497	86.109	-86.109	0.0	-1.112	-0.729

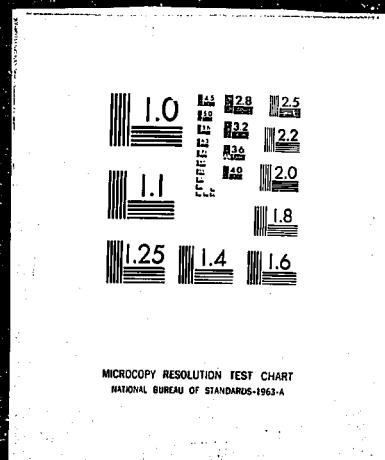
SPO ORTHOFEOSITE JTFC 7/03/72

STRUCTURE FACTORS

PAGE 3

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/F(GR)
4	8	1	63.154	62.447	-62.447	0.0	0.707	0.524
5	8	1	51.864	51.739	51.739	0.0	0.124	0.051
6	8	1	13.401	9.649	-9.649	0.0	3.753	1.271
7	8	1	36.065	37.814	37.814	0.0	-1.750	-1.117
0	6	0	297.851	310.330	310.330	0.0	-12.479	-2.343 *
9	8	1	49.363	45.433	45.433	0.0	2.930	2.093
6	6	1	36.798	36.119	-36.118	0.0	0.470	0.291
10	8	1	8.972	13.706	13.706	0.0	-4.734	-1.025
11	8	1	21.512	22.935	-22.935	0.0	-1.423	-0.696
12	8	1	28.747	26.420	-26.420	0.0	2.327	1.158
13	8	1	37.562	34.783	34.783	0.0	2.778	1.662
14	7	1	4.283	2.413	2.413	0.0	1.870	0.292
13	7	1	16.594	16.915	16.915	0.0	-1.431	-0.764
12	7	1	24.889	19.419	19.419	0.0	5.471	2.795
11	7	1	16.991	20.729	-20.729	0.0	-0.297	-0.340
10	7	1	15.817	15.209	15.209	0.0	0.608	0.230
9	7	1	34.990	35.729	35.729	0.0	-0.740	-0.499
8	7	1	30.735	32.109	-32.109	0.0	-1.453	-0.919
6	7	1	9.522	2.484	2.484	0.0	7.034	1.829
5	7	1	16.597	15.489	15.489	0.0	1.093	0.421
4	7	1	22.237	24.536	24.536	0.0	-2.300	-1.058
3	7	1	22.425	25.612	-25.612	0.0	-3.187	-1.619
2	7	1	12.735	11.649	11.649	0.0	1.087	0.340
0	6	0	297.682	310.330	310.330	0.0	-12.648	-2.375 *
1	7	1	10.768	5.661	5.661	0.0	4.907	1.443
1	6	1	9.565	6.944	6.944	0.0	2.422	0.774
2	6	1	8.659	6.295	6.295	0.0	2.364	0.717
3	6	1	24.875	24.837	24.837	0.0	0.436	0.023
4	6	1	4.109	14.875	14.875	0.0	-10.766	-1.751 *
5	6	1	11.664	8.744	8.744	0.0	2.920	0.943
6	6	1	10.130	6.155	6.155	0.0	3.974	1.103
7	6	1	9.559	13.891	13.891	0.0	-3.852	-0.953
10	6	1	9.140	1.320	1.320	0.0	7.840	1.970
12	6	1	6.251	2.082	2.082	0.0	3.360	0.650
13	6	1	4.563	13.226	-13.226	0.0	-8.363	-1.341
14	6	1	9.927	9.615	-9.615	0.0	0.312	0.076
15	6	1	132.599	132.120	-132.120	0.0	0.470	0.141
16	6	1	9.768	7.460	-7.460	0.0	2.208	0.578
17	6	1	11.664	5.339	5.339	0.0	6.325	1.720
18	6	1	9.527	13.539	-13.539	0.0	-3.612	-0.802
0	6	0	297.531	310.330	310.330	0.0	-12.758	-2.404 *
16	5	1	18.464	18.224	18.224	0.0	0.260	0.106
15	5	1	32.826	32.001	-32.001	0.0	0.825	0.521
14	5	1	37.634	35.542	35.542	0.0	2.092	1.484
13	5	1	29.458	28.170	28.170	0.0	1.288	0.796
12	5	1	17.210	10.308	-10.308	0.0	6.502	2.924
11	5	1	5.697	13.392	13.392	0.0	-7.706	-1.318
10	5	1	30.966	27.417	-27.417	0.0	3.449	2.242
9	5	1	23.426	33.600	-33.600	0.0	-0.164	-0.119
8	5	1	30.069	30.626	30.626	0.0	-0.550	-0.363
7	5	1	63.579	62.519	-62.519	0.0	1.050	0.841
6	5	1	56.567	57.053	57.053	0.0	-0.486	-0.405
5	5	1	73.068	72.906	72.906	0.0	0.162	0.125

CARD
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STRUCTURE FACTORS

PAGE 4

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
4	5	1	31.960	34.636	34.636	0.0	-2.696	-1.897
3	5	1	40.026	42.212	42.212	0.0	-1.477	-1.376
2	5	1	40.660	51.511	51.511	0.0	-1.951	-1.763
5	6	1	30.405	30.746	30.746	0.0	0.186	0.153
1	6	1	39.830	41.345	41.345	0.0	-1.515	-1.620
2	6	1	76.746	91.673	91.673	0.0	-4.907	-3.824
0	6	0	297.795	310.330	310.330	0.0	-12.535	2.354
3	4	1	50.060	52.180	52.180	0.0	-2.150	-2.105
4	4	1	41.450	46.290	46.290	0.0	-4.831	-4.887
5	4	1	68.310	71.344	71.344	0.0	-3.025	-2.512
6	4	1	28.690	31.467	31.467	0.0	-2.778	-2.104
7	4	1	24.337	24.562	24.562	0.0	-0.166	0.119
8	4	1	14.212	15.024	15.024	0.0	0.489	0.228
9	4	1	10.188	11.402	11.402	0.0	-1.414	0.423
10	4	1	24.416	0.975	0.975	0.0	1.441	0.204
11	4	1	9.145	6.677	6.677	0.0	2.274	0.565
12	4	1	16.405	9.116	9.116	0.0	7.371	3.030
13	4	1	14.400	11.221	11.221	0.0	3.180	1.192
14	4	1	21.728	22.057	22.057	0.0	-0.280	-0.194
15	4	1	17.224	15.160	15.160	0.0	2.064	0.762
16	4	1	25.019	22.584	22.584	0.0	0.435	0.192
17	4	1	20.160	26.562	26.562	0.0	-0.958	0.555
18	4	1	27.529	25.246	25.246	0.0	2.223	1.301
19	4	1	5.723	9.059	9.059	0.0	-5.324	-0.133
20	4	1	15.720	10.244	10.244	0.0	5.416	1.352
10	5	1	38.707	38.955	38.955	0.0	-0.158	-0.103
18	5	1	47.498	49.631	49.631	0.0	-1.653	-1.332
0	6	0	207.912	310.330	310.330	0.0	-12.817	-2.408
17	6	1	65.985	66.214	66.214	0.0	-0.230	-0.232
16	3	1	29.647	27.968	27.968	0.0	1.679	1.052
15	3	1	26.238	25.005	25.005	0.0	1.233	0.654
14	3	1	45.700	47.512	47.512	0.0	-2.311	-1.706
13	3	1	14.046	19.656	19.656	0.0	-1.190	0.526
12	3	1	126.601	127.170	127.170	0.0	-0.569	-0.275
11	3	1	190.801	187.651	187.651	0.0	3.150	1.007
10	3	1	158.051	154.597	154.597	0.0	3.454	1.345
9	3	1	164.748	160.779	160.779	0.0	3.869	1.453
8	2	1	70.097	70.433	70.433	0.0	-0.336	-0.266
7	2	1	84.140	87.660	87.660	0.0	0.180	0.122
6	2	1	140.521	137.630	137.630	0.0	2.891	1.294
5	2	1	162.381	160.193	160.193	0.0	2.188	0.858
4	3	1	56.304	53.018	53.018	0.0	3.286	3.212
3	3	1	94.361	90.054	90.054	0.0	-5.693	-6.180
2	2	1	137.883	147.872	147.872	0.0	-10.289	-4.716
1	3	1	157.763	182.607	182.607	0.0	-14.644	-5.448
0	2	1	37.940	40.125	40.125	0.0	-2.186	-2.506
1	2	1	76.148	57.873	57.873	0.0	1.386	0.539
2	2	1	137.705	142.456	142.456	0.0	-4.570	-2.085
0	6	0	294.903	210.730	210.730	0.0	-15.426	-26.931
3	2	1	160.732	161.978	161.978	0.0	-1.246	-0.487
4	2	1	125.170	127.617	127.617	0.0	-2.446	-1.237
5	2	1	127.609	131.823	131.823	0.0	-1.914	-0.928
6	2	1	12.721	13.942	13.942	0.0	-1.222	-0.703

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STRUCTURE FACTORS

PAGE 5

H	K	L	F(ORS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	
7	2	1	96.318	97.525	0.0	-1.207	-0.779		
8	2	1	85.479	88.653	0.0	-1.774	-1.234		
0	2	1	70.714	68.650	0.0	2.065	1.352		
10	2	1	21.628	20.692	0.0	0.936	0.557		
11	2	1	46.147	46.561	0.0	-0.414	-0.338		
12	2	1	49.421	51.520	0.0	-1.689	-1.339		
13	2	1	54.024	54.958	0.0	-0.833	-0.456		
15	2	1	46.759	45.534	0.0	1.176	0.858		
16	2	1	49.352	48.871	0.0	-0.480	-0.370		
17	2	1	50.482	49.876	0.0	0.806	0.600		
18	2	1	33.363	31.597	0.0	1.766	1.126		
20	2	1	16.370	10.521	0.0	5.849	2.137		
21	1	1	4.091	6.753	8.753	0.0	-3.863	-0.596	
0	6	0	297.042	310.330	310.330	0.0	-13.287	-2.498	*
19	1	1	4.643	4.757	-4.757	0.0	-0.214	-0.034	
17	1	1	4.471	2.641	-2.641	0.0	1.830	0.311	
16	1	1	25.677	31.282	31.282	0.0	-5.305	-2.751	
15	1	1	31.185	27.321	-27.321	0.0	3.865	2.420	
14	1	1	28.256	29.267	29.267	0.0	-0.912	-0.524	
13	1	1	31.171	31.500	31.500	0.0	-0.329	-0.213	
12	1	1	19.064	17.029	17.029	0.0	2.035	0.956	
11	1	1	15.544	10.998	-10.998	0.0	4.546	1.987	
8	1	1	47.721	48.795	48.795	0.0	-1.074	-1.099	
7	1	1	53.474	54.362	-54.362	0.0	-0.498	-0.494	
6	1	1	47.750	49.127	49.127	0.0	-1.377	-1.476	
5	1	1	80.426	82.509	82.509	0.0	-1.683	-1.280	
4	1	1	61.777	60.598	60.598	0.0	1.179	1.103	
3	1	1	12.492	11.753	11.753	0.0	0.939	0.564	
2	1	1	34.104	32.039	-32.039	0.0	2.065	2.494	
1	1	1	21.585	20.704	-20.704	0.0	0.881	0.921	
0	0	2	39.103	38.804	38.804	0.0	0.299	0.332	
0	6	0	295.422	310.330	310.330	0.0	-13.907	-2.627	*
1	0	2	95.611	96.179	96.179	0.0	-0.368	-0.242	
2	0	2	152.789	151.778	-151.778	0.0	1.011	0.416	
3	0	2	214.604	219.784	219.784	0.0	-5.180	-1.458	
4	0	2	93.444	91.825	-91.825	0.0	1.619	1.077	
5	0	2	225.725	221.589	-221.589	0.0	4.136	1.095	
7	0	2	182.470	180.277	-180.277	0.0	2.393	0.805	
8	0	2	76.796	75.993	75.993	0.0	0.803	0.568	
9	0	2	160.716	161.655	161.655	0.0	-0.939	-0.362	
10	0	2	11.548	7.959	-7.959	0.0	3.590	1.192	
11	0	2	161.541	161.624	161.624	0.0	0.318	0.120	
12	0	2	43.295	43.051	-43.051	0.0	0.344	0.254	
13	0	2	73.274	75.440	-75.440	0.0	-2.166	-1.549	
15	0	2	68.936	68.361	-68.361	0.0	0.575	0.421	
16	0	2	38.503	38.589	38.589	0.0	-0.296	-0.196	
17	0	2	76.398	78.073	78.073	0.0	-1.675	-1.114	
18	0	2	34.263	34.802	34.802	0.0	-0.538	-0.319	
19	0	2	31.055	30.678	30.678	0.0	0.377	0.213	
20	0	2	11.302	11.239	-11.239	0.0	0.063	0.016	
0	6	0	294.304	310.330	310.330	0.0	-16.025	-3.048	*
20	1	2	9.464	6.886	9.886	0.0	-0.422	-0.087	
19	1	2	18.108	17.564	-17.564	0.0	0.543	0.208	

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
18	1	2	4.300	11.327	-11.327	0.0	-5.018	-0.876
17	1	2	54.550	53.362	53.362	0.0	1.189	0.366
16	1	2	52.222	53.524	-53.524	0.0	-1.296	-0.935
15	1	2	10.434	2.657	2.657	0.0	7.777	2.248
13	1	2	12.272	12.390	12.390	0.0	-0.118	-0.034
12	1	2	105.722	104.677	-104.677	0.0	1.045	0.591
11	1	2	105.977	104.679	-104.679	0.0	1.298	0.733
10	1	2	40.082	39.271	-39.271	0.0	0.821	0.649
9	1	2	90.276	79.827	79.827	0.0	0.432	0.322
8	1	2	55.222	56.237	-56.237	0.0	-1.015	-0.926
7	1	2	45.060	43.532	43.532	0.0	1.538	1.508
6	1	2	25.846	24.721	24.721	0.0	1.126	0.598
5	1	2	66.020	92.711	-92.711	0.0	3.309	2.135
4	1	2	50.536	47.570	47.570	0.0	2.966	3.034
3	1	2	55.222	52.262	-52.262	0.0	3.071	3.008
1	1	2	56.158	58.095	58.095	0.0	-1.937	-1.893
0	6	0	295.372	310.330	310.330	0.0	-14.958	-2.840
0	6	0	13.926	13.716	13.716	0.0	-2.790	-1.428
1	2	2	32.652	34.710	-34.710	0.0	-2.058	-2.215
2	2	2	7.032	8.265	-8.265	0.0	-1.232	-0.428
3	2	2	62.441	63.103	63.103	0.0	-0.461	-0.414
4	2	2	11.143	10.483	-10.483	0.0	0.659	0.302
5	2	2	23.034	24.557	-24.557	0.0	-1.523	-1.095
6	2	2	60.820	58.550	58.550	0.0	2.290	2.031
7	2	2	95.000	89.692	-89.692	0.0	-6.682	-0.460
8	2	2	30.576	29.754	29.754	0.0	0.822	0.636
9	2	2	71.097	70.625	70.625	0.0	0.471	0.360
10	2	2	31.156	32.346	32.346	0.0	-1.190	-0.820
11	2	2	17.774	17.910	17.910	0.0	-0.136	-0.057
12	2	2	17.586	17.326	-17.326	0.0	0.261	0.105
13	2	2	30.486	28.900	-28.900	0.0	1.965	1.188
14	2	2	11.461	9.794	-9.794	0.0	1.668	0.455
15	2	2	11.722	24.026	-24.026	0.0	-12.304	-3.025
16	2	2	8.017	12.204	-12.204	0.0	6.813	1.569
17	2	2	15.732	14.634	-14.634	0.0	1.099	0.391
18	2	2	36.222	37.445	-37.445	0.0	-1.220	-0.743
19	2	2	21.350	34.713	-34.713	0.0	-2.782	-1.441
0	6	0	296.817	310.330	310.330	0.0	-13.513	-2.550
20	2	2	10.651	8.308	-8.308	0.0	2.343	0.568
10	2	2	19.565	8.681	-8.681	0.0	10.904	4.856
18	3	2	5.180	2.764	-2.764	0.0	2.416	0.388
17	3	2	7.134	4.397	-4.397	0.0	2.737	0.540
16	3	2	11.497	7.083	7.083	0.0	4.914	1.496
15	3	2	20.568	16.934	16.934	0.0	3.434	1.693
4	3	2	15.617	16.795	16.795	0.0	-1.178	-0.465
8	3	2	18.023	18.015	-18.015	0.0	0.918	0.663
7	3	2	7.293	3.616	-3.616	0.0	3.677	0.945
6	3	2	7.336	1.945	1.945	0.0	5.352	1.641
5	3	2	16.181	15.893	15.893	0.0	0.208	0.146
4	3	2	45.870	43.735	-43.735	0.0	2.135	2.124
3	3	2	40.484	40.621	-40.621	0.0	-0.137	-0.134
2	3	2	55.412	92.655	-92.655	0.0	-4.243	-1.082
0	6	0	294.735	310.330	310.330	0.0	-15.595	-2.964

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	4	2	28.450	31.742	0.0	-2.791	-2.138	
2	4	2	57.819	70.475	0.0	-2.656	-2.153	
3	4	2	36.554	37.508	0.0	-0.964	-0.951	
5	4	2	13.387	0.714	-0.714	0.0	12.673	5.370
6	4	2	25.504	25.513	0.0	0.391	0.243	
7	4	2	30.372	31.880	0.0	-1.507	-1.018	
9	4	2	8.219	2.605	0.0	5.614	1.421	
10	4	2	14.710	9.554	-0.554	0.0	5.164	1.960
11	4	2	21.440	17.670	-18.670	0.0	2.790	1.309
11'	4	2	17.354	12.742	-12.742	0.0	4.613	1.830
12	4	2	10.202	5.068	-5.068	0.0	5.134	1.349
13	4	2	3.762	6.194	-6.194	0.0	-2.422	-0.390
14	4	2	21.440	19.901	-15.901	0.0	5.539	2.583
15	4	2	11.956	14.342	-4.362	0.0	7.534	2.283
17	4	2	17.427	15.033	-15.033	0.0	2.794	0.923
18	4	2	6.489	13.951	-13.951	0.0	-6.962	-1.221
17	5	2	39.045	40.924	-40.924	0.0	-1.879	-1.077
0	6	0	295.507	310.330	310.330	0.0	-14.733	-2.786 *
16	5	2	23.759	21.394	21.394	0.0	2.365	1.053
15	5	2	24.208	26.952	-26.952	0.0	-2.746	-1.254
14	5	2	0.302	0.760	-0.760	0.0	-0.369	-0.084
13	5	2	22.759	21.314	-21.314	0.0	1.644	0.683
12	5	2	61.791	64.409	-64.409	0.0	-2.616	-1.000
11	5	2	83.221	93.702	-93.702	0.0	-0.481	-0.313
10	5	2	41.455	41.474	-41.474	0.0	-0.015	-0.010
9	5	2	112.697	114.676	-114.676	0.0	-1.979	-1.062
8	5	2	77.061	75.504	-75.504	0.0	1.477	1.022
7	5	2	42.798	42.520	-42.520	0.0	0.278	0.207
6	5	2	30.256	30.035	-30.035	0.0	0.222	0.143
5	5	2	53.799	65.392	-65.392	0.0	-1.503	-1.249
4	5	2	15.165	18.395	-18.395	0.0	0.770	0.385
3	5	2	104.373	107.055	-107.055	0.0	-2.682	-1.543
2	5	2	31.698	31.605	-31.605	0.0	0.393	0.274
1	5	2	55.529	55.824	-55.824	0.0	-4.295	-2.378
0	6	2	15.457	13.836	-13.836	0.0	1.622	0.615
1	6	2	19.426	16.492	-16.492	0.0	2.944	1.411
2	6	2	108.679	113.734	-113.734	0.0	-5.054	-2.780
3	6	2	127.210	131.711	-131.711	0.0	-4.501	-2.157
0	6	0	204.248	310.330	310.330	0.0	-16.082	-3.070 *
4	6	2	45.361	45.367	-45.367	0.0	-0.006	-0.005
5	6	2	91.287	91.792	-91.792	0.0	-0.505	-0.315
6	6	2	11.910	3.053	-3.053	0.0	8.857	2.502
7	6	2	78.315	78.477	-78.477	0.0	-0.162	-0.112
8	6	2	31.272	33.748	-33.748	0.0	-2.475	-1.343
9	6	2	95.409	96.759	-96.759	0.0	-1.350	-0.816
10	6	2	22.324	22.642	-22.642	0.0	0.319	-0.161
11	6	2	60.829	60.716	-60.716	0.0	0.123	0.089
12	6	2	16.876	20.013	-20.013	0.0	-3.137	-1.062
13	6	2	32.056	30.988	-30.988	0.0	1.168	0.682
14	6	2	17.094	13.135	-13.135	0.0	3.956	1.544
15	6	2	39.570	38.807	-38.807	0.0	-0.227	-0.134
16	6	2	22.382	21.705	-21.705	0.0	0.677	0.285
14	7	2	10.709	8.202	-8.202	0.0	2.507	0.639

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
13	7	2	-20.208	20.380	-20.380	0.0	-0.172	-0.071
12	7	2	38.768	35.327	-35.327	0.0	3.661	2.233
11	7	2	12.566	15.054	-15.054	0.0	-1.088	-0.339
10	7	2	16.267	7.902	-7.902	0.0	1.344	0.313
9	7	2	18.562	15.405	-15.405	0.0	3.138	1.380
8	7	2	37.011	42.250	-42.250	0.0	-4.350	-2.823
0	6	0	294.098	310.330	-310.330	0.0	-16.231	-3.099
7	7	2	28.602	25.873	-25.873	0.0	2.729	1.650
5	7	2	19.468	19.475	-19.475	0.0	-0.357	-0.178
4	7	2	28.723	31.375	-31.375	0.0	-2.663	-1.491
3	7	2	16.239	20.690	-20.690	0.0	-4.451	-1.552
2	7	2	10.086	5.370	-5.370	0.0	4.716	1.308
1	7	2	10.332	6.116	-6.116	0.0	4.216	1.067
0	6	2	13.570	16.784	-16.784	0.0	-2.106	0.996
1	6	2	41.736	40.613	-40.613	0.0	0.892	0.639
2	6	2	16.394	17.120	-17.120	0.0	-0.806	-0.221
3	6	2	22.672	22.080	-22.080	0.0	-0.208	-0.097
4	6	2	7.408	8.256	-8.256	0.0	-0.867	-0.169
5	6	2	29.098	28.004	-28.004	0.0	1.005	0.572
6	6	2	12.185	13.349	-13.349	0.0	-1.144	0.325
7	6	2	41.052	40.513	-40.513	0.0	0.539	0.367
8	6	2	19.035	16.730	-16.730	0.0	2.377	1.013
9	6	2	29.125	27.698	-27.698	0.0	1.427	0.793
10	6	2	10.926	9.681	-9.681	0.0	1.265	1.138
11	6	2	29.618	26.954	-26.954	0.0	2.664	1.517
12	6	2	5.325	9.220	-9.220	0.0	-2.895	-0.438
0	5	0	204.520	310.330	-310.330	0.0	-15.901	-3.004 *
4	5	2	8.556	5.676	-5.676	0.0	3.180	0.676
9	5	2	9.406	2.511	-2.511	0.0	6.895	1.666
7	5	2	6.479	9.009	-9.009	0.0	-2.031	-0.400
3	5	2	12.177	12.177	-12.177	0.0	2.727	-0.604
2	5	2	10.860	7.503	-7.503	0.0	3.365	0.887
1	5	2	2.182	8.401	-8.401	0.0	5.218	-0.703
0	10	2	8.960	11.123	-11.123	0.0	-8.766	-2.041
1	10	2	4.360	5.379	-5.379	0.0	-0.980	-0.147
2	10	2	22.239	21.464	-21.464	0.0	0.874	0.361
4	9	3	5.364	8.173	-8.173	0.0	-2.805	-0.442
4	9	3	4.100	3.445	-3.445	0.0	0.415	0.338
2	9	3	47.163	46.161	-46.161	0.0	0.291	0.624
1	9	3	28.462	27.932	-27.932	0.0	1.010	0.571
0	9	3	123.377	124.477	-124.477	0.0	-1.100	-0.629
1	8	3	29.623	32.145	-32.145	0.0	-1.890	0.605
2	8	3	2.623	3.158	-3.158	0.0	6.665	1.578
0	6	0	267.813	310.330	-310.330	0.0	-16.512	-3.154 *
3	6	0	2.898	7.475	-7.475	0.0	2.423	0.571
4	6	3	183.55	202.430	-202.430	0.0	-1.964	-0.718
5	6	3	7.525	12.465	-12.465	0.0	-4.940	-0.403
6	6	3	28.462	28.568	-28.568	0.0	0.324	0.168
8	6	3	52.788	52.151	-52.151	0.0	0.837	0.551
0	5	3	12.272	3.045	-3.045	0.0	9.327	2.505
11	7	3	7.423	0.401	-0.401	0.0	7.023	1.359
10	7	3	22.425	19.426	-19.426	0.0	2.997	1.302
9	7	3	13.271	7.587	-7.587	0.0	5.684	1.809

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STRUCTURE FACTORS

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H	K	I	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
8	7	3	9.536	6.408	0.0	3.128	0.733	
6	7	3	33.189	32.377	-32.377	0.0	0.811	0.478
5	7	3	10.824	9.905	-9.905	0.0	4.920	1.376
4	7	3	6.002	6.629	6.629	0.0	1.373	0.312
2	7	3	12.069	7.104	7.104	0.0	4.965	1.595
1	7	3	12.229	13.515	-13.515	0.0	-1.287	-0.383
0	6	3	10.839	9.904	-9.904	0.0	4.935	1.322
0	6	0	294.042	310.330	310.330	0.0	-16.287	-3.119 *
1	6	3	4.703	3.628	-3.628	0.0	1.073	0.178
2	6	3	13.343	13.392	13.392	0.0	5.951	2.097
3	6	3	6.700	6.960	6.960	0.0	-2.261	-0.457
4	5	3	6.856	10.003	10.003	0.0	-1.147	-0.280
5	6	2	2.970	11.000	11.000	0.0	-8.201	-1.178
6	6	3	5.604	2.379	-2.379	0.0	3.525	0.658
7	6	3	6.280	7.998	7.998	0.0	-1.718	-0.446
8	6	3	24.078	24.078	24.078	0.0	-1.189	-0.577
14	6	3	8.697	4.645	-4.645	0.0	4.052	0.936
15	5	3	11.406	9.925	-9.925	0.0	4.681	1.239
14	5	3	25.832	21.223	-21.223	0.0	4.505	2.321
12	5	3	10.449	2.672	-2.672	0.0	8.297	2.293
11	5	3	6.266	13.658	-13.658	0.0	-7.433	-1.267
10	5	3	60.430	62.455	-62.455	0.0	-1.616	-1.152
0	6	0	293.444	310.330	310.330	0.0	-16.885	-3.227 *
5	5	3	10.492	12.817	12.817	0.0	-2.325	-0.620
6	5	3	4.182	3.126	-3.126	0.0	1.426	0.156
5	5	3	26.324	27.218	-27.218	0.0	-2.893	-1.468
3	5	3	15.037	12.105	-12.105	0.0	2.932	0.993
2	5	3	82.718	47.092	-47.092	0.0	-4.374	-2.009
1	5	3	19.004	22.216	22.216	0.0	-2.312	-0.973
0	4	3	128.158	139.320	-139.320	0.0	-10.682	-5.103 *
1	4	3	21.164	21.798	-21.798	0.0	-0.634	-0.317
3	4	3	11.490	7.425	-7.425	0.0	4.065	1.271
4	4	3	37.329	36.974	-36.974	0.0	0.381	0.262
5	2	3	14.632	6.170	-6.170	0.0	8.462	3.776
6	4	2	11.679	0.653	-0.653	0.0	11.025	3.297 *
8	4	3	27.978	26.348	-26.348	0.0	1.630	0.237
9	4	3	8.494	7.474	-7.474	0.0	1.020	0.222
0	6	0	202.446	310.330	310.330	0.0	-17.483	-3.557 *
11	4	3	14.299	8.784	-8.784	0.0	5.515	1.886
12	4	3	39.488	40.203	40.203	0.0	-0.315	-0.198
13	4	3	22.440	19.942	-19.942	0.0	2.497	1.098
15	4	3	4.124	1.560	-1.560	0.0	-9.456	-1.266
16	4	3	11.331	7.752	-7.752	0.0	5.579	1.427
17	4	3	1.707	2.007	-2.007	0.0	-1.200	-0.124
17	3	3	18.644	18.666	18.666	0.0	1.977	0.696
16	3	3	9.044	17.981	-17.981	0.0	1.063	0.230
15	3	3	6.407	16.158	16.158	0.0	-4.661	-1.933
14	3	3	167.741	164.425	-164.425	0.0	3.316	1.102
13	3	3	45.011	45.810	-45.810	0.0	-0.790	-0.566
12	3	3	14.038	8.421	-8.421	0.0	5.617	1.963
10	3	3	7.047	4.770	-4.770	0.0	2.277	0.423
9	3	3	181.191	217.035	-217.035	0.0	-2.341	-1.094
8	3	3	3.907	0.168	-0.168	0.0	3.739	0.570

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
7	2	5	-36.060	34.285	34.285	0.0	-0.225	-0.147
6	3	2	192.059	186.396	186.396	0.0	3.703	1.170
5	3	3	69.261	48.674	48.674	0.0	0.408	0.333
0	6	0	292.137	310.330	310.330	0.0	-18.192	-37.467 *
4	2	2	13.170	11.026	11.026	0.0	2.143	0.715
3	3	3	4.572	13.289	13.289	0.0	-8.717	-1.466
2	2	2	120.412	193.529	193.529	0.0	-73.127	-1.000
1	3	3	75.319	83.764	83.764	0.0	-6.444	-3.136
0	2	2	251.256	266.098	266.098	0.0	-16.861	-3.022 *
1	2	2	48.115	50.541	50.541	0.0	-2.426	-2.107
3	2	3	20.672	19.113	19.113	0.0	1.559	0.861
2	3	3	31.853	30.503	30.503	0.0	1.350	1.000
5	2	3	14.038	15.494	15.494	0.0	-1.455	-0.503
6	2	3	7.001	3.051	3.051	0.0	4.850	1.176
7	2	2	42.172	38.007	38.007	0.0	4.165	3.045
8	2	2	79.729	76.531	76.531	0.0	1.598	1.293
9	2	3	8.572	3.079	3.079	0.0	5.893	1.366
10	2	3	6.468	7.150	7.150	0.0	-0.680	-0.125
11	2	3	-7.018	0.423	0.423	0.0	6.395	1.255
12	2	3	82.584	83.480	83.480	0.0	-0.696	-0.322
13	2	3	30.387	31.866	31.866	0.0	-1.479	-0.894
15	2	3	29.415	26.824	26.824	0.0	2.591	1.450
0	6	0	291.634	310.330	310.330	0.0	-18.696	-3.609 *
16	2	3	28.109	31.321	31.321	0.0	-3.212	-1.496
18	2	2	19.387	0.516	0.516	0.0	18.880	6.969 *
18	1	2	16.456	20.670	20.670	0.0	-4.214	-1.159
17	1	3	19.093	17.563	17.563	0.0	1.550	0.408
16	1	2	4.403	47.282	47.282	0.0	0.623	0.598
14	1	2	13.256	13.315	13.315	0.0	-0.058	-0.018
11	1	3	12.639	9.532	9.532	0.0	3.377	0.988
10	1	2	62.049	59.267	59.267	0.0	3.662	2.746
9	1	3	18.470	16.726	16.726	0.0	1.745	0.735
7	1	3	16.513	15.521	15.521	0.0	3.992	1.968
6	1	2	24.632	25.449	25.449	0.0	-0.667	-0.383
9	1	3	30.082	30.770	30.770	0.0	-0.608	-0.489
3	1	3	8.451	10.872	10.872	0.0	-2.421	-0.694
2	1	2	67.570	67.509	67.509	0.0	-0.539	-0.272
0	6	0	290.406	310.330	310.330	0.0	-19.926	-3.868 *
0	0	4	95.484	92.774	92.774	0.0	0.710	0.433
1	0	4	29.312	29.087	29.087	0.0	-0.775	-0.231
2	0	4	79.050	79.302	79.302	0.0	-1.252	-0.849
3	0	4	120.634	121.230	121.230	0.0	-0.296	-0.148
4	0	4	158.083	155.052	155.052	0.0	3.031	1.173
5	0	6	58.212	58.748	58.748	0.0	-0.536	-0.318
7	0	4	93.008	82.167	82.167	0.0	0.941	0.618
8	0	4	112.380	117.837	117.837	0.0	-0.457	-0.239
9	0	4	47.469	47.918	47.918	0.0	-0.450	-0.318
10	0	4	32.665	34.493	34.493	0.0	-1.793	-1.077
11	0	6	105.607	122.406	122.406	0.0	-1.799	-0.662
12	0	4	90.471	81.700	81.700	0.0	-1.229	-0.792
13	0	4	57.342	56.482	56.482	0.0	0.860	0.588
15	0	4	32.650	32.088	32.088	0.0	0.662	0.263
16	0	4	69.509	68.951	68.951	0.0	0.558	0.348

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA
16	1	4	67145	11.593	11.593	0.0	-2.447	-0.483
15	1	4	84856	5.304	-5.304	0.0	3.552	0.728
0	6	0	290.682	310.330	310.330	0.0	-10.347	-1.720 *
14	1	4	16.150	13.104	-13.104	0.0	6.554	3.792
12	1	4	35.396	32.631	-32.631	0.0	2.765	1.694
11	1	4	69.553	72.650	-72.659	0.0	-3.106	-2.072
10	1	4	65.770	64.467	-64.467	0.0	1.312	0.422
9	1	4	45.856	46.489	-46.489	0.0	-0.633	-0.444
8	1	4	38.470	37.794	-37.794	0.0	1.076	0.725
7	1	4	21.74	19.331	-19.331	0.0	3.413	1.570
6	1	4	35.353	33.381	-33.381	0.0	1.072	1.257
5	1	4	17.968	18.006	-18.006	0.0	-0.058	-0.023
4	1	4	24.614	21.655	-21.655	0.0	3.159	1.664
3	1	4	20.892	14.470	-14.470	0.0	6.332	3.035
2	1	4	56.600	54.718	-54.718	0.0	1.952	1.552
1	1	4	71.500	73.869	-73.869	0.0	-2.361	-1.707
0	2	4	59.039	63.449	-63.449	0.0	-4.410	-3.276
1	2	4	54.375	57.200	-57.200	0.0	-2.825	-2.080
2	2	4	26.325	23.333	-23.333	0.0	2.092	1.587
3	2	4	10.492	11.170	-11.170	0.0	-0.687	-0.472
4	2	4	26.695	26.201	-26.201	0.0	0.704	0.362
5	2	4	29.007	26.429	-26.429	0.0	2.638	1.541
0	6	0	200.463	310.330	310.330	0.0	-19.987	-3.460 *
6	2	4	76.727	12.024	-12.024	0.0	4.297	-0.823
8	2	4	27.470	26.503	-26.503	0.0	1.476	0.795
9	2	4	15.204	16.644	-16.644	0.0	-3.360	-1.090
10	2	4	15.573	7.167	-7.167	0.0	8.406	3.225
11	2	4	16.688	154.015	-154.015	0.0	0.873	0.304
12	2	4	30.030	26.114	-26.114	0.0	3.925	2.018
13	2	4	22.585	24.393	-24.393	0.0	-1.798	-0.756
14	2	4	20.208	21.458	-21.458	0.0	-1.250	-0.496
15	2	4	4.401	2.320	-2.320	0.0	2.562	0.374
16	2	4	20.324	14.228	-14.228	0.0	6.056	2.460
15	3	4	10.172	9.854	-9.854	0.0	0.319	0.067
13	3	4	12.272	0.881	-0.881	0.0	2.391	0.621
12	3	4	9.710	0.389	-0.389	0.0	9.320	2.139
11	3	6	07.868	3.780	-3.780	0.0	2.920	-0.308
9	3	4	8.827	11.103	-11.103	0.0	-2.276	-0.485
7	3	4	20.223	20.016	-20.016	0.0	-0.207	0.098
0	6	0	291.224	310.330	310.330	0.0	-19.105	-3.691 *
5	3	4	14.125	11.939	-11.939	0.0	2.156	0.680
4	3	4	13.676	8.916	-8.916	0.0	4.761	1.448
2	3	4	10.101	6.280	-6.280	0.0	3.811	0.937
1	3	4	9.507	11.094	-11.094	0.0	-1.587	-0.356
0	4	4	20.295	21.827	-21.827	0.0	-1.532	-0.618
2	4	4	10.072	8.702	-8.702	0.0	1.370	0.340
3	4	4	11.838	12.105	-12.105	0.0	-0.268	-0.074
4	4	4	10.014	11.060	-11.060	0.0	-1.047	-0.262
5	6	4	20.179	22.993	-22.993	0.0	-2.814	-1.156
6	4	4	14.704	14.131	-14.131	0.0	0.574	0.186
7	4	4	10.651	10.213	-10.213	0.0	0.438	0.113
9	4	4	25.494	22.479	-22.479	0.0	3.005	1.535
10	4	4	14.227	15.782	-15.782	0.0	-1.555	-0.473

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P	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/STGMA
11	4	4	-7.015	-4.668	0.0	3.247	0.648	
13	4	4	4.050	11.394	0.0	-2.336	-0.472	
0	6	0	294.068	310.330	310.330	0.0	-21.261	-4.151 *
14	4	4	11.765	13.718	13.718	0.0	-1.952	-0.2445
13	5	4	22.324	17.503	-17.503	0.0	4.821	1.838
12	5	4	42.216	40.931	-40.931	0.0	1.285	0.736
11	5	4	65.031	64.590	-64.590	0.0	0.441	0.278
10	5	4	71.273	70.815	-70.815	0.0	0.458	0.294
9	5	4	40.835	51.833	-51.833	0.0	-1.997	-1.356
8	5	4	20.614	20.003	-20.003	0.0	0.611	0.235
7	5	4	24.252	16.484	-16.484	0.0	7.768	4.186
6	5	4	45.564	49.032	-49.032	0.0	-3.438	-2.185
5	5	4	17.123	19.388	-19.388	0.0	-2.265	-0.806
4	5	4	9.753	2.214	-2.214	0.0	7.530	1.880
3	5	4	11.519	8.648	-8.648	0.0	2.871	0.806
2	5	4	61.630	64.249	-64.249	0.0	-2.618	-1.862
1	5	4	43.773	48.445	-48.445	0.0	-4.672	-3.146
0	6	4	41.271	43.327	-43.327	0.0	-2.086	-1.315
2	6	4	60.135	38.054	-38.054	0.0	1.2P1	0.855
3	6	4	63.447	63.443	-63.443	0.0	0.005	0.003
4	6	4	81.273	80.421	-80.421	0.0	0.952	0.608
5	6	4	47.478	47.046	-47.046	0.0	0.052	0.034
0	6	0	288.567	310.330	310.330	0.0	-21.762	-4.253 *
6	6	4	8.248	12.291	-12.291	0.0	-4.042	-0.772
7	6	4	24.175	25.258	-25.258	0.0	-1.079	-0.435
8	6	4	54.916	53.037	-53.037	0.0	1.679	1.237
2	6	4	7.930	8.439	-8.439	0.0	-1.509	-0.781
10	6	4	4.442	6.536	-6.536	0.0	-5.093	-0.680
8	7	4	22.570	20.270	-20.270	0.0	2.300	0.992
7	7	4	11.114	2.732	-2.732	0.0	8.282	1.963
6	7	4	7.073	9.262	-9.262	0.0	-1.288	-0.240
5	7	4	13.676	11.390	-11.390	0.0	2.227	0.658
3	7	4	3.158	8.972	-8.972	0.0	-5.775	-0.720
2	7	4	11.201	11.669	-11.669	0.0	9.632	2.520
1	7	4	5.547	0.035	-0.035	0.0	-3.088	-0.495
0	8	4	39.146	36.712	-36.712	0.0	2.435	1.431
1	8	4	232.454	127.263	-127.263	0.0	11.191	4.949 *
2	9	4	7.510	5.646	-5.646	0.0	1.864	0.324
3	8	4	14.762	13.690	-13.690	0.0	1.064	0.293
0	6	5	9.565	3.559	-3.559	0.0	6.007	1.261
1	6	5	13.546	7.913	-7.913	0.0	5.633	1.502
0	6	0	298.289	310.330	310.330	0.0	-22.041	-4.309 *
3	6	5	16.008	11.840	-11.840	0.0	4.159	1.276
7	6	5	34.354	32.507	-32.507	0.0	1.887	1.023
5	5	5	22.527	23.769	-23.769	0.0	-1.243	-0.466
3	5	5	13.404	0.654	-0.654	0.0	3.534	0.957
2	5	5	3.198	4.774	-4.774	0.0	-1.576	-0.204
1	5	5	22.923	21.304	-21.304	0.0	1.628	0.725
0	4	5	51.455	7.055	-7.055	0.0	-1.600	-0.266
1	4	5	13.667	1.106	-1.106	0.0	12.541	3.833 *
2	4	5	41.1P3	38.815	-38.815	0.0	2.367	1.627
3	4	5	272.210	32.822	-32.822	0.0	5.613	-2.749
5	4	5	18.919	16.789	-16.789	0.0	2.130	0.799

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	4	5	21.483	19.495	-19.695	0.0	1.989	0.703
9	4	5	27.535	21.349	-21.349	0.0	6.586	3.414
11	3	5	69.627	66.148	-66.148	0.0	0.479	0.257
0	6	0	295.554	310.330	-310.330	0.0	-21.765	-4.193 *
10	3	5	7.771	7.907	-7.907	0.0	-0.136	-0.025
9	3	5	43.152	83.492	-83.492	0.0	-0.359	-0.221
8	3	5	50.576	50.593	-50.593	0.0	-0.112	-0.050
7	3	5	53.148	53.592	-53.592	0.0	-0.443	-0.301
5	3	5	74.124	74.210	-74.210	0.0	-0.092	-0.053
4	3	5	11.186	55.777	-55.777	0.0	5.409	1.364
3	3	5	52.215	83.855	-83.855	0.0	-1.640	-1.037
2	3	5	14.450	7.704	-7.704	0.0	7.157	2.323
1	3	5	32.652	31.611	-31.611	0.0	1.041	0.560
0	2	5	18.680	5.100	-5.100	0.0	5.570	1.460
1	2	5	10.223	22.327	-22.327	0.0	-3.104	-1.190
2	2	5	57.196	55.088	-55.088	0.0	1.108	0.405
3	2	5	62.876	63.677	-63.677	0.0	-0.001	-0.054
5	2	5	40.004	47.254	-47.254	0.0	1.750	1.212
6	2	5	11.268	15.963	-15.963	0.0	-4.672	-1.069
7	2	5	22.324	22.409	-22.409	0.0	-0.085	-0.034
9	2	5	56.129	54.723	-54.723	0.0	1.406	0.916
0	6	0	295.556	310.330	-310.330	0.0	-22.374	-4.376 *
11	2	5	50.623	51.974	-51.974	0.0	-1.351	-0.005
12	2	5	10.767	1.520	-1.520	0.0	0.247	2.003
12	1	5	36.156	33.717	-33.717	0.0	2.842	1.427
10	1	5	10.636	1.453	-1.453	0.0	8.713	2.009
9	1	5	12.663	6.220	-6.220	0.0	6.443	1.750
8	1	5	19.595	16.585	-16.585	0.0	2.000	1.119
7	1	5	24.589	28.360	-28.360	0.0	3.229	1.766
6	1	5	13.445	5.822	-5.822	0.0	7.622	2.361
4	1	5	17.745	13.956	-13.956	0.0	3.786	1.478
2	1	5	13.170	4.772	-4.772	0.0	8.497	2.636
1	1	5	15.037	11.142	-11.142	0.0	3.095	1.387
0	0	6	122.582	116.120	-116.120	0.0	6.062	3.251
1	0	6	56.280	52.939	-52.939	0.0	3.350	2.113
3	0	6	35.048	34.188	-34.188	0.0	0.459	0.459
4	0	6	23.730	24.966	-24.966	0.0	-1.237	-0.464
0	6	0	292.809	310.330	-310.330	0.0	-27.551	-5.521 *
5	0	6	19.976	15.509	-15.509	0.0	4.667	1.511
3	1	6	13.836	3.372	-3.372	0.0	10.464	2.969 *
2	1	6	27.659	26.957	-26.957	0.0	0.703	0.311
1	1	6	26.818	28.868	-28.868	0.0	-2.000	-0.862
0	2	6	9.435	0.066	-0.066	0.0	8.364	1.757
2	2	6	3.678	7.287	-7.287	0.0	-3.409	-0.441
3	2	6	20.425	18.400	-18.400	0.0	0.025	0.682
20	5	0	92.938	96.287	-94.287	0.0	-1.358	-0.732 *
24	0	0	0.117	10.402	-10.402	0.0	-1.205	-0.219
26	0	0	16.065	7.688	-7.688	0.0	8.377	2.229
26	1	0	23.483	21.262	-21.262	0.0	2.221	0.706
24	2	0	19.122	25.235	-25.235	0.0	-6.113	-1.625
26	2	0	12.706	3.022	-3.022	0.0	9.694	2.052
24	3	0	8.711	12.376	-12.376	0.0	-3.664	-0.560
22	4	0	6.692	10.118	-10.118	0.0	-4.026	-0.589

PRO OF THIOFERROSILITE 7/03/73

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
26	4	0	15.452	19.342	-18.342	0.0	-3.450	-0.833
22	5	0	18.673	14.821	-14.821	0.0	3.852	1.209
20	6	0	0.124	0.427	-0.427	0.0	-3.162	-1.690 *
22	6	0	5.484	2.859	-2.859	0.0	2.625	0.346
24	6	0	16.098	15.146	-15.146	0.0	0.461	0.200
22	7	0	11.661	11.776	-11.776	0.0	-0.315	-0.063
20	7	0	0.319	0.005	-0.005	0.0	5.317	1.773
18	7	0	21.164	15.655	-15.655	0.0	5.509	2.236
20	6	0	0.912	0.427	-0.427	0.0	-3.476	-1.917 *
16	9	0	46.541	48.871	-48.871	0.0	-2.330	-1.279
20	8	0	1.447	0.318	-0.318	0.0	1.120	0.107
22	8	0	13.807	0.781	-0.781	0.0	13.025	2.763 *
20	9	0	15.110	3.215	-3.215	0.0	11.855	2.738 *
16	9	0	11.360	0.550	-0.550	0.0	10.810	2.326 *
14	6	0	18.281	14.650	-14.650	0.0	3.631	1.124
10	10	0	8.726	0.687	-0.687	0.0	8.039	1.513
12	10	0	18.267	16.485	-16.485	0.0	1.781	0.562
14	11	0	51.907	50.759	-50.759	0.0	1.148	0.579
12	11	0	6.290	0.010	-0.010	0.0	6.261	0.903
10	11	0	10.289	12.176	-12.176	0.0	-1.887	-0.340
8	11	0	1.735	0.362	-0.362	0.0	1.374	0.133
6	11	0	54.726	53.692	-53.692	0.0	1.043	0.632
20	6	0	92.551	94.287	-94.287	0.0	-1.736	-0.949 *
0	12	0	64.048	61.145	-61.145	0.0	2.904	1.664
6	12	0	15.157	2.789	-2.789	0.0	12.408	2.258 *
8	12	0	18.135	12.060	-12.060	0.0	2.278	0.541
10	12	0	6.456	2.444	-2.444	0.0	4.010	0.544
12	12	0	24.966	19.207	-19.207	0.0	5.639	1.809
6	13	0	5.426	2.584	-2.584	0.0	2.842	0.345
2	13	0	20.744	20.900	-20.900	0.0	-0.156	-0.016
6	13	1	17.253	3.476	-3.476	0.0	14.486	4.348 *
5	13	1	10.289	0.025	-0.025	0.0	10.264	1.981 *
4	13	1	11.534	4.690	-4.690	0.0	6.844	1.274
2	13	1	11.375	5.699	-5.699	0.0	5.676	1.108
0	12	1	6.020	5.752	-5.752	0.0	1.078	0.157
1	12	1	12.026	2.382	-2.382	0.0	9.644	2.115
20	6	0	93.248	92.287	-92.287	0.0	-0.709	-0.237 *
3	12	1	12.605	6.230	-6.230	0.0	6.375	1.444
4	12	1	15.621	6.751	-6.751	0.0	9.169	2.563
5	12	1	81.190	12.323	-12.323	0.0	24.133	-0.626
6	12	1	0.001	4.266	-4.266	0.0	4.735	0.828
7	12	1	8.769	2.425	-2.425	0.0	6.344	1.024
9	12	1	9.212	3.125	-3.125	0.0	6.108	1.060
11	12	1	12.619	4.603	-4.603	0.0	8.016	1.605
15	11	1	12.214	11.101	-11.101	0.0	1.113	0.220
14	11	1	16.430	13.053	-13.053	0.0	3.477	0.915
13	11	1	14.284	10.472	-10.472	0.0	3.812	0.872
12	11	1	17.138	3.050	-3.050	0.0	16.058	4.166 *
11	11	1	17.283	14.486	-14.486	0.0	2.868	0.772
10	11	1	11.042	8.497	-8.497	0.0	2.154	0.416
7	11	1	23.556	18.905	-18.905	0.0	4.650	1.763
20	6	0	91.667	94.287	-94.287	0.0	-2.620	-1.313 *
6	11	1	22.562	21.265	-21.265	0.0	1.697	0.600

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	11	1	24.513	23.725	22.725	0.0	-1.788	-0.652
4	11	1	16.226	11.081	11.081	0.0	5.245	1.502
3	11	1	10.781	10.396	10.396	0.0	0.395	0.093
2	11	1	17.108	16.744	-16.744	0.0	0.364	0.111
10	10	1	4.091	1.509	1.509	0.0	3.382	0.456
11	10	1	13.561	11.264	-11.264	0.0	1.506	0.303
12	10	1	7.177	10.710	-10.710	0.0	-3.542	-0.534
13	10	1	12.417	10.175	-10.175	0.0	2.238	0.443
19	9	1	18.919	15.147	15.147	0.0	3.771	1.029
18	9	1	13.740	14.016	-14.016	0.0	-0.271	-0.061
17	9	1	15.703	17.440	-17.440	0.0	-1.737	-0.346
16	9	1	8.538	14.059	-14.059	0.0	-6.321	-0.973
15	9	1	15.294	0.710	-0.710	0.0	14.564	4.023 *
20	8	0	92.298	64.297	-64.297	0.0	-1.068	-1.098 *
14	9	1	19.226	0.556	0.556	0.0	6.680	1.716
13	9	1	6.446	6.318	-6.318	0.0	0.627	0.101
16	8	1	24.342	28.414	-28.414	0.0	-3.872	-1.428
17	8	1	26.020	25.247	-25.247	0.0	2.774	1.093
19	8	1	20.425	25.528	-25.528	0.0	-2.597	-0.834
20	9	1	10.911	1.700	-1.700	0.0	3.212	0.598
21	8	1	18.426	4.607	-4.607	0.0	14.419	4.446 *
22	7	1	75.078	21.552	-21.552	0.0	3.466	1.221
23	7	1	7.105	1.057	-1.057	0.0	5.168	0.724
22	7	1	5.381	0.056	-0.056	0.0	-1.674	-0.222
21	7	1	7.455	5.584	-5.584	0.0	2.071	0.322
20	7	1	15.356	0.181	-0.181	0.0	15.175	4.175 *
19	7	1	17.441	15.163	-15.163	0.0	2.279	0.645
18	7	1	4.413	6.291	-6.291	0.0	-1.878	-0.260
20	6	1	14.661	4.597	-4.597	0.0	6.964	1.829
22	6	1	5.002	2.250	-2.250	0.0	3.553	0.489
23	6	1	10.607	1.030	-1.030	0.0	9.569	1.749
20	6	0	91.689	94.287	-94.287	0.0	-2.569	-1.421 *
24	6	1	7.297	4.054	-4.054	0.0	3.643	0.505
25	4	1	15.506	9.711	-9.711	0.0	6.195	1.506
24	5	1	11.317	3.543	-3.543	0.0	7.774	1.424
23	5	1	9.522	5.739	-5.739	0.0	3.783	0.668
21	5	1	17.963	16.053	-16.053	0.0	1.910	0.549
21	4	1	16.226	11.611	-11.611	0.0	4.715	1.345
22	4	1	29.849	31.673	-31.673	0.0	-2.824	-1.173
23	4	1	24.918	23.398	-23.398	0.0	1.531	0.535
24	4	1	16.746	15.684	-15.684	0.0	1.043	0.266
25	4	1	24.875	20.460	-20.460	0.0	4.415	1.378
26	4	1	9.998	14.370	-14.370	0.0	-4.472	-0.685
26	3	1	17.615	11.896	-11.896	0.0	5.720	1.473
23	3	1	26.530	30.686	-30.686	0.0	-2.157	-0.821
22	3	1	37.227	38.755	-38.755	0.0	-1.528	-0.735
22	2	1	34.583	38.335	-38.335	0.0	-3.752	-1.757
23	2	1	43.089	42.406	-42.406	0.0	0.683	0.341
20	2	0	90.501	24.287	-24.287	0.0	-3.306	-1.609 *
24	2	1	17.731	27.637	-27.637	0.0	-10.106	-2.295 *
25	2	1	32.884	34.017	-34.017	0.0	-1.133	-0.476
26	2	1	21.049	20.532	-20.532	0.0	0.516	0.154
26	1	1	12.142	5.726	-5.726	0.0	6.416	1.266

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STRUCTURE FACTORS

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N	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
25	1	1	4.128	7.360	-7.040	0.0	-2.921	-0.336
24	1	1	20.291	3.873	-3.873	0.0	16.407	6.326 *
22	1	1	11.085	0.000	0.009	0.0	10.986	2.364 *
22	0	2	61.206	65.757	65.707	0.0	-4.502	-2.605
23	0	2	57.746	72.937	-72.937	0.0	-5.181	-2.946
24	0	2	16.456	18.727	18.727	0.0	-2.270	-0.542
25	0	2	33.076	37.070	37.070	0.0	-4.889	-1.853
26	0	2	25.620	19.029	19.029	0.0	6.600	2.322
24	1	2	12.978	16.568	16.568	0.0	-4.500	-0.873
23	1	2	20.341	31.286	31.286	0.0	-2.945	-1.173
22	1	2	5.631	13.147	13.147	0.0	-6.216	-0.904
22	2	2	23.440	20.687	-20.687	0.0	2.753	1.021
20	6	0	90.203	94.287	94.287	0.0	-4.085	-2.200 *
23	2	2	4.264	2.488	2.488	0.0	1.896	0.237
26	2	2	14.603	8.356	-8.356	0.0	6.240	1.366
26	3	2	13.155	0.403	0.403	0.0	12.752	2.645 *
24	3	2	3.878	5.573	5.573	0.0	-1.605	-0.190
22	3	2	12.619	1.753	1.753	0.0	10.826	2.564 *
21	4	2	14.245	0.372	0.372	0.0	14.473	3.874 *
22	4	2	11.679	14.089	-14.089	0.0	-2.411	-0.463
25	4	2	7.699	9.781	9.781	0.0	-2.092	-0.294
24	6	2	10.680	0.522	-0.522	0.0	10.157	1.813 *
23	5	2	23.106	20.989	-20.989	0.0	2.217	0.735
22	5	2	10.709	14.191	-14.191	0.0	-3.482	-0.620
21	5	2	17.268	20.702	20.702	0.0	-3.434	-0.865
20	6	0	90.207	94.287	-94.287	0.0	-3.091	-2.094 *
20	5	2	5.730	8.056	-8.056	0.0	2.326	0.316
16	5	2	19.716	19.526	19.526	0.0	0.209	-0.060
13	6	2	18.050	11.502	11.502	0.0	6.547	2.132
15	6	2	19.687	21.600	21.600	0.0	-1.914	-0.562
21	6	2	19.245	11.554	-11.554	0.0	12.308	0.231
22	6	2	33.755	35.933	35.933	0.0	-2.177	-0.920
23	5	2	41.615	39.797	-39.797	0.0	2.656	1.268
21	7	2	9.203	4.886	4.886	0.0	4.317	0.735
20	7	2	4.601	0.220	0.220	0.0	4.381	0.530
15	7	2	12.619	2.099	-2.099	0.0	10.522	2.399 *
17	7	2	11.693	5.711	5.711	0.0	5.982	1.329
15	8	2	17.007	12.540	-12.540	0.0	4.467	1.280
17	8	2	8.429	8.068	8.068	0.0	0.831	0.139
16	9	2	19.247	11.295	-11.295	0.0	8.652	3.070
20	9	2	9.609	10.318	-10.318	0.0	-0.500	0.117
20	6	0	91.733	94.287	-94.287	0.0	-2.554	-0.408 *
16	9	2	9.710	9.865	-9.865	0.0	0.155	-0.025
17	9	2	13.752	9.175	9.175	0.0	4.617	1.009
16	6	2	11.751	0.066	-0.064	0.0	2.207	0.558
12	6	2	5.504	6.712	-6.712	0.0	-0.206	0.116
9	10	2	9.768	6.706	-6.706	0.0	3.142	0.581
11	10	2	18.180	15.153	-15.153	0.0	3.027	0.897
12	10	2	15.255	0.207	0.207	0.0	15.248	4.108 *
13	10	2	13.256	5.374	5.374	0.0	7.842	1.809
15	10	2	9.203	8.490	8.490	0.0	0.713	0.118
16	10	2	13.242	4.210	-4.210	0.0	9.032	1.968
14	11	2	13.865	3.751	-3.751	0.0	10.114	2.329 *

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
20	6	0	20.546	24.207	-24.207	0.0	-4.441	-2.374
13	11	2	3.710	1.559	1.559	0.0	2.160	0.240
12	11	2	22.558	28.800	28.000	0.0	5.393	1.419
11	11	2	32.415	29.427	29.427	0.0	2.992	1.257
10	11	2	8.665	17.210	17.210	0.0	-6.745	-0.983
9	11	2	34.612	35.314	35.314	0.0	-0.762	-0.310
8	11	2	22.3P2	24.229	24.229	0.0	-1.446	-0.557
7	11	2	5.708	13.023	13.023	0.0	-1.035	-1.034
5	11	2	17.524	24.622	24.622	0.0	-7.398	-1.709
3	11	2	25.194	28.400	28.400	0.0	-3.466	-0.229
2	11	2	18.461	10.305	10.305	0.0	8.555	2.734
1	11	2	13.050	13.339	13.339	0.0	0.511	0.116
0	12	2	11.005	2.798	2.798	0.0	8.011	1.577
1	12	2	14.617	2.471	2.471	0.0	12.147	2.913 *
2	12	2	23.574	26.033	26.033	0.0	-2.434	-0.740
3	12	2	21.730	21.625	21.625	0.0	-0.105	0.032
4	12	2	12.127	10.040	10.040	0.0	2.098	0.460
5	12	2	20.554	13.399	13.399	0.0	6.425	2.134
6	12	2	8.456	7.812	7.812	0.0	1.044	0.167
20	6	0	11.391	0.427	0.427	0.0	-1.096	-1.550 *
9	12	2	19.447	15.249	15.249	0.0	6.698	1.918
4	13	2	9.026	7.810	7.810	0.0	2.016	0.328
1	13	2	6.728	8.035	8.035	0.0	-2.206	-0.287
0	12	3	13.256	13.037	13.037	0.0	0.219	0.046
1	12	3	12.551	4.666	4.666	0.0	7.425	1.690
2	12	3	11.505	2.144	2.144	0.0	9.361	1.786
4	12	3	17.369	3.203	3.203	0.0	14.166	3.960 *
6	12	3	13.300	0.259	0.259	0.0	13.004	2.307 *
12	11	3	8.147	1.832	1.832	0.0	6.315	0.940
11	11	3	14.516	2.901	2.901	0.0	11.615	2.665 *
10	11	3	27.007	24.358	24.358	0.0	2.609	0.895
20	6	0	91.451	94.227	94.227	0.0	-2.837	-1.564 *
4	11	3	8.017	5.713	5.713	0.0	2.304	0.347
6	11	3	6.772	11.440	11.440	0.0	-4.676	-0.602
4	11	3	12.605	1.463	1.463	0.0	11.142	2.507
3	11	3	10.130	5.650	5.650	0.0	4.480	0.641
2	11	3	28.762	26.408	26.408	0.0	2.354	0.922
1	11	3	10.029	3.792	3.792	0.0	6.236	1.131
0	10	3	16.210	11.714	11.714	0.0	4.497	1.333
1	10	3	11.129	2.446	2.446	0.0	8.683	1.851
2	10	3	12.272	0.747	0.747	0.0	11.525	2.020 *
3	10	3	15.197	12.402	12.402	0.0	2.795	0.664
4	10	3	33.610	33.119	33.119	0.0	0.491	0.235
6	10	3	8.610	0.348	0.348	0.0	7.762	1.372
7	10	3	11.215	1.462	1.462	0.0	9.753	1.276
6	10	3	8.726	6.543	6.543	0.0	2.182	0.370
10	10	3	12.706	1.493	1.493	0.0	11.213	2.413 *
20	5	0	28.585	94.287	94.287	0.0	-5.302	-2.813 *
12	10	3	12.546	3.569	3.569	0.0	8.876	1.923
17	9	3	5.697	3.596	3.596	0.0	2.091	0.267
16	9	3	9.015	2.426	2.426	0.0	6.589	1.007
14	9	3	66.175	64.483	64.483	0.0	1.692	0.961
13	9	3	23.585	17.448	17.448	0.0	6.137	2.392

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STRUCTURE FACTORS

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H	K	L	F(DPS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	0	3	0.710	1.046	-1.846	0.0	7.964	1.457
10	0	3	7.207	15.750	15.750	0.0	-8.451	-1.232
9	0	3	3.444	0.478	0.378	0.0	3.066	0.359
12	0	3	34.292	34.629	-30.629	0.0	-5.336	-2.268
13	0	3	16.698	14.577	-14.577	0.0	2.111	0.579
15	0	3	19.151	13.223	-13.223	0.0	6.928	1.429
14	0	3	21.170	19.931	-19.931	0.0	1.268	0.408
17	0	3	13.112	1.279	-1.279	0.0	11.833	2.538 *
20	0	0	91.525	94.287	-94.287	0.0	-2.762	-1.511 *
12	0	3	15.779	14.212	-14.212	0.0	1.767	0.403
21	7	3	5.402	1.856	-1.856	0.0	3.046	0.494
10	7	3	11.841	3.225	-3.225	0.0	8.763	1.810
17	7	3	12.040	6.370	-6.370	0.0	5.670	1.205
16	5	3	16.256	4.712	-4.712	0.0	12.042	1.797 *
17	6	2	16.550	2.014	-2.014	0.0	12.936	1.545 *
18	6	3	0.493	1.420	-1.420	0.0	7.673	1.363
20	6	3	10.874	11.032	-11.032	0.0	-0.208	-0.010
21	6	3	14.125	5.994	-5.994	0.0	8.141	1.814
22	6	3	14.690	3.565	-3.565	0.0	11.105	2.635 *
22	5	3	11.780	11.445	-11.445	0.0	0.335	0.061
21	5	3	10.290	5.171	-5.171	0.0	5.219	0.909
20	5	3	8.074	16.179	-16.179	0.0	4.956	0.762
20	6	0	23.860	94.287	-94.287	0.0	-0.437	-0.233 *
18	6	3	24.330	26.170	-26.170	0.0	-1.031	-0.644
10	4	2	0.798	14.453	-14.453	0.0	3.345	0.581
20	4	3	38.070	39.102	-39.102	0.0	-1.021	-0.500
24	4	3	11.476	18.787	-18.787	0.0	-7.311	-1.177
23	3	3	15.139	72.458	-72.458	0.0	7.681	17.623
22	3	3	27.761	26.634	-26.634	0.0	1.127	0.420
21	3	3	30.040	28.886	-28.886	0.0	1.182	0.506
20	3	3	16.575	0.8216	-0.8216	0.0	16.660	4.753 *
20	3	3	61.775	71.095	-71.095	0.0	-4.220	-2.499
23	2	3	9.232	3.070	-3.070	0.0	6.153	1.012
24	2	3	9.944	13.143	-13.143	0.0	5.510	0.755
20	6	0	93.265	94.287	-94.287	0.0	-1.022	-0.560 *
11	1	3	7.742	0.025	-0.025	0.0	7.717	1.120
22	1	3	12.517	5.567	-5.567	0.0	7.009	1.345
21	1	3	13.576	2.812	-2.812	0.0	10.864	2.413 *
15	0	4	13.251	10.364	-10.364	0.0	6.513	-1.410
10	0	4	19.397	10.723	-10.723	0.0	7.674	2.397
20	0	4	26.412	27.333	-27.333	0.0	-0.921	-0.351
22	0	4	15.549	14.305	-14.305	0.0	2.564	0.629
22	0	0	27.790	27.552	-27.552	0.0	0.162	-0.056
23	1	4	12.653	1.394	-1.394	0.0	11.269	2.205 *
22	1	1	11.427	17.789	-17.789	0.0	0.362	-0.084
22	1	4	8.364	15.717	-15.717	0.0	7.353	-1.162
19	1	4	10.758	24.120	-24.120	0.0	-4.360	-1.267
19	2	4	11.128	2.111	-2.111	0.0	9.017	1.876
14	2	4	14.710	6.557	-6.557	0.0	8.161	2.013
20	2	4	16.053	14.919	-14.919	0.0	-0.866	-0.196
20	6	0	91.595	94.287	-94.287	0.0	2.732	-1.493 *
21	2	4	14.594	9.478	-9.478	0.0	5.016	1.228
16	4	4	13.503	5.447	-5.447	0.0	8.056	2.038

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
17	4	4	13.054	6.807	-6.807	0.0	6.247	1.410
19	4	4	16.804	16.240	16.240	0.0	0.555	0.135
20	4	4	11.387	3.551	3.551	0.0	8.416	1.674
21	4	4	7.386	17.540	-17.540	0.0	-9.653	-1.371
22	4	4	10.011	12.891	12.891	0.0	-1.980	-0.330
21	5	4	20.901	21.806	21.806	0.0	-0.916	-0.229
20	5	4	17.108	0.259	0.259	0.0	16.850	4.475
19	4	4	19.428	26.530	26.530	0.0	-7.593	-1.811
20	6	0	61.500	44.287	-44.287	0.0	-2.608	-1.442 *
18	5	4	26.281	28.659	-28.659	0.0	-2.378	-0.820
17	5	4	15.776	16.776	-16.776	0.0	-1.001	-0.260
15	5	4	14.036	9.962	9.962	0.0	4.974	1.286
13	6	4	41.852	43.082	-43.082	0.0	-2.030	-1.175
14	6	4	9.927	2.375	2.375	0.0	7.552	1.437
15	6	4	23.193	26.472	-26.472	0.0	-3.278	-0.988
16	6	4	41.663	40.486	-40.486	0.0	1.177	0.608
17	6	4	24.237	25.622	-25.622	0.0	-1.385	-0.475
19	6	4	54.166	44.228	-44.228	0.0	0.938	0.111
20	6	4	19.397	12.899	12.899	0.0	6.498	1.816
19	7	4	13.575	9.428	-9.428	0.0	5.147	1.084
17	7	4	6.700	4.053	4.053	0.0	2.647	0.370
16	7	4	11.454	15.009	-15.009	0.0	-3.935	-0.733
15	7	4	21.443	23.320	-23.320	0.0	-1.687	-0.508
14	7	4	12.793	10.375	10.375	0.0	2.418	0.525
13	7	4	13.720	15.174	-15.174	0.0	-1.454	-0.345
12	7	4	19.426	17.561	17.561	0.0	1.865	0.585
20	6	0	89.405	94.267	-94.267	0.0	-4.783	-2.619 *
11	7	4	25.927	23.332	-23.332	0.0	2.195	0.658
8	8	4	26.630	23.037	-23.037	0.0	3.592	1.416
9	8	4	15.458	23.659	-23.659	0.0	-8.071	-1.846
11	8	4	16.601	3.089	3.089	0.0	13.512	3.703 *
12	8	4	24.860	20.590	-20.590	0.0	4.270	1.473
13	8	4	14.970	0.184	-0.184	0.0	5.795	1.371
14	8	4	11.447	8.887	8.887	0.0	2.560	0.504
16	8	4	13.532	13.316	-13.316	0.0	0.216	0.045
17	9	4	9.277	1.733	1.733	0.0	7.644	1.246
15	9	4	11.071	1.558	1.558	0.0	0.512	1.711
13	9	4	6.305	3.443	-3.443	0.0	4.843	0.729
11	9	4	11.422	6.869	-6.869	0.0	4.554	0.895
10	9	4	3.502	10.115	-10.115	0.0	-6.613	-0.707
9	9	4	17.832	9.085	9.085	0.0	7.948	2.296
8	9	4	13.387	1.049	1.049	0.0	12.337	2.749 *
7	9	4	0.623	1.253	-1.253	0.0	8.370	1.518
20	6	0	90.449	94.287	-94.287	0.0	-3.639	-2.008 *
6	9	4	16.167	7.005	-7.005	0.0	8.361	2.338
4	9	4	44.500	2.513	-2.513	0.0	1.987	0.245
3	9	4	7.423	9.323	-9.323	0.0	-1.899	-0.271
1	9	4	5.281	7.264	7.264	0.0	-1.983	-0.267
0	10	4	34.429	0.896	-0.896	0.0	2.534	0.290
1	10	4	16.659	10.078	10.078	0.0	6.592	1.796
3	10	4	14.791	15.257	-15.257	0.0	-0.466	-0.103
4	10	4	15.666	15.513	-15.513	0.0	0.132	0.032
5	10	4	14.400	16.714	16.714	0.0	-2.313	-0.506

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(FCALC)	B(FCALC)	DELTA F	DELTA/SIGMA
6	10	4	10.130	9.814	-2.814	0.0	6.316	1.164
7	10	4	4.657	6.195	6.196	0.0	-1.527	-0.190
0	10	4	12.052	0.154	0.154	0.0	3.799	0.758
10	10	4	12.653	0.605	-0.605	0.0	12.058	2.2509 *
12	10	4	11.983	6.288	-6.288	0.0	5.694	1.032
20	6	0	0.132	9.4287	-9.4287	0.0	-2.926	-1.593 *
7	11	6	5.368	1.224	1.224	0.0	4.144	0.511
6	11	6	21.720	13.943	13.943	0.0	7.787	2.571
2	11	6	16.269	21.155	-21.155	0.0	-4.987	-1.068
1	11	6	15.602	29.333	-20.333	0.0	-4.731	-1.002
1	10	5	6.483	10.453	10.453	0.0	-3.970	-0.512
2	10	5	10.035	10.996	10.996	0.0	0.038	0.010
3	10	5	13.213	0.047	-5.047	0.0	8.166	1.684
6	10	5	10.622	7.474	7.474	0.0	3.148	0.527
11	0	5	27.601	22.092	-22.092	0.0	5.509	1.880
10	0	5	15.153	1.672	1.672	0.0	13.174	3.023 *
9	0	5	30.024	27.729	27.729	0.0	2.295	0.846
9	0	5	17.520	25.591	-25.591	0.0	-8.463	-1.837
7	0	5	17.021	10.721	-10.721	0.0	6.800	1.726
20	6	0	90.752	94.287	-94.287	0.0	-3.535	-1.950 *
5	0	5	22.121	20.063	-20.063	0.0	2.058	0.612
4	0	5	6.760	8.539	-8.539	0.0	0.231	0.036
3	0	5	32.635	29.672	-29.672	0.0	2.863	1.210
1	0	5	12.026	5.133	5.133	0.0	6.893	1.376
1	0	5	13.647	10.058	10.058	0.0	3.589	0.821
2	0	5	38.772	13.914	-33.914	0.0	0.058	0.028
3	0	5	36.632	37.823	37.823	0.0	-1.172	-0.552
4	0	5	1.577	3.750	3.750	0.0	-2.413	-0.234
5	0	5	27.529	27.378	-27.378	0.0	0.151	0.056
7	0	5	11.215	17.648	-17.648	0.0	-6.432	-1.157
6	0	5	40.863	36.955	-36.955	0.0	3.907	2.132
10	0	5	7.296	2.820	2.820	0.0	4.386	0.631
11	0	5	30.770	32.011	32.011	0.0	-1.232	-0.469
12	0	5	5.357	1.516	1.516	0.0	3.882	0.474
14	0	5	20.121	9.013	9.013	0.0	11.108	3.378 *
20	6	0	0.043	9.4287	-9.4287	0.0	-6.166	-2.250 *
16	7	5	11.765	3.480	3.480	0.0	8.275	1.520
12	7	5	17.000	18.098	18.098	0.0	-0.208	-0.055
11	7	5	4.732	9.177	9.177	0.0	-4.445	-0.523
10	7	5	8.760	3.705	-3.705	0.0	5.036	0.840
0	7	5	12.171	10.034	-10.034	0.0	2.137	0.429
9	7	5	22.670	19.864	19.864	0.0	2.706	0.924
4	7	5	10.636	15.998	15.998	0.0	-5.172	-0.893
3	7	5	22.306	23.136	23.136	0.0	-0.760	-0.267
2	7	5	3.632	1.055	1.055	0.0	2.577	0.304
0	6	5	26.398	0.835	-0.835	0.0	16.562	5.979 *
20	6	0	0.243	9.4287	-9.4287	0.0	-1.304	-0.781 *
13	5	5	15.056	1.559	-1.559	0.0	13.507	3.392 *
15	6	5	9.064	1.126	1.126	0.0	7.918	1.227
16	6	5	6.512	2.657	2.657	0.0	3.854	0.504
17	6	5	6.759	7.314	-7.314	0.0	-0.556	-0.072
16	5	5	14.603	5.121	5.121	0.0	9.482	2.133
15	5	5	13.430	10.565	10.565	0.0	2.865	0.601

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
14	5	6	11.706	-0.548	-0.548	0.0	11.058	2.240 *
13	5	5	18.745	21.500	-21.500	0.0	-2.755	-0.734
12	5	5	23.251	23.699	23.688	0.0	-0.436	-0.156
11	5	5	6.002	12.250	-12.250	0.0	-6.243	-0.678
12	4	5	13.937	0.136	0.136	0.0	13.801	3.666 *
17	4	5	22.460	19.692	-19.692	0.0	3.168	1.056
18	4	5	27.166	18.227	-18.227	0.0	8.939	3.525
20	6	0	78.941	94.207	-94.207	0.0	-5.367	-2.229 *
10	3	5	19.239	16.127	-16.127	0.0	3.211	0.846
17	3	5	41.794	43.046	-43.046	0.0	-1.050	-0.512
16	3	5	31.780	37.335	-37.339	0.0	-5.559	-2.226
15	3	5	31.548	24.639	24.639	0.0	6.910	3.352
14	3	5	7.494	0.052	0.052	0.0	7.631	1.212
13	3	5	21.135	17.034	-17.034	0.0	4.101	1.367
14	2	5	13.580	10.676	-10.676	0.0	3.306	0.784
15	2	5	20.483	17.539	-17.539	0.0	2.944	0.541
16	2	5	5.745	0.452	-0.452	0.0	4.793	0.647
17	2	5	26.578	30.656	-30.656	0.0	-3.678	-1.268
18	2	5	18.151	14.662	-14.662	0.0	3.480	0.827
19	2	5	13.401	8.021	-8.021	0.0	5.380	1.126
20	2	5	19.556	1.447	-1.447	0.0	18.109	5.342 *
21	2	5	14.791	0.862	-0.862	0.0	4.930	1.088
21	1	5	14.777	8.858	-8.858	0.0	5.919	1.302
19	1	5	7.455	1.741	-1.741	0.0	5.913	0.849
20	6	0	91.169	94.287	-94.287	0.0	-3.110	1.720 *
17	1	5	8.240	6.519	-6.519	0.0	1.720	0.265
16	1	5	9.911	7.112	-7.112	0.0	2.699	0.473
9	0	6	17.694	8.056	-8.056	0.0	8.998	2.644
10	0	6	12.499	8.886	-8.886	0.0	2.604	0.557
12	0	6	43.351	43.743	-43.743	0.0	-0.392	-0.196
13	0	6	40.761	39.530	-39.530	0.0	1.730	0.571
15	0	6	38.163	38.688	-38.688	0.0	-0.545	-0.242
16	0	6	21.163	23.871	-23.871	0.0	-2.678	-0.714
17	0	6	12.576	0.616	-0.616	0.0	11.960	2.347 *
18	0	6	9.305	2.055	-2.055	0.0	7.210	1.122
16	1	6	7.307	10.753	-10.753	0.0	-3.445	-0.462
15	1	6	14.502	10.423	-10.423	0.0	3.678	0.799
14	1	6	47.368	47.662	-47.662	0.0	0.336	0.175
13	1	6	22.472	26.570	-26.570	0.0	-3.998	-1.164
20	6	0	92.849	94.287	-94.287	0.0	-1.435	0.786 *
11	1	6	1.360	4.482	-4.482	0.0	-3.122	-0.296
10	1	6	23.773	14.774	-14.774	0.0	8.999	3.673
9	1	6	14.415	5.571	-5.571	0.0	8.844	2.174
8	2	6	6.658	4.131	-4.131	0.0	2.757	0.435
10	2	6	18.975	6.683	-6.683	0.0	12.193	3.915 *
11	2	6	15.264	17.572	-17.572	0.0	-2.288	-0.539
12	2	6	9.319	9.339	-9.339	0.0	-0.010	-0.003
13	2	6	15.095	4.861	-4.861	0.0	10.254	2.450 *
14	2	6	15.564	1.971	-1.971	0.0	13.573	3.408 *
15	2	6	16.529	1.167	-1.167	0.0	15.362	3.829 *
16	2	6	13.763	17.434	-17.434	0.0	-3.671	-0.697
17	2	6	13.705	6.838	-6.838	0.0	6.807	1.407
14	3	6	10.526	0.224	0.224	0.0	10.702	1.901 *

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PROG. OUTLINE FOR CASTITE 7/03/72

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	3	6	-19.265	2.526	-2.026	0.0	16.370	4.768 *
10	3	6	13.734	3.717	2.717	0.0	10.017	2.365 *
20	6	0	88.778	64.297	-64.297	0.0	-5.510	-2.043 *
8	3	6	11.603	5.138	5.128	0.0	6.555	1.406
7	3	6	7.090	5.496	-5.496	0.0	1.594	0.250
6	3	6	16.963	10.235	-10.235	0.0	5.720	1.054
3	4	6	20.223	20.055	-20.055	0.0	-0.732	-0.233
4	4	6	12.866	11.759	11.759	0.0	1.106	0.244
6	4	6	11.172	4.313	-4.313	0.0	6.859	1.398
7	4	6	11.375	0.412	0.412	0.0	1.063	0.404
8	4	6	17.354	6.636	6.636	0.0	10.718	3.109 *
9	4	6	2.348	5.800	-5.800	0.0	2.458	0.417
12	4	6	12.162	0.047	-0.047	0.0	3.094	0.590
12	4	6	6.456	8.315	-8.315	0.0	-1.659	-0.216
15	4	6	16.473	0.707	-0.707	0.0	13.765	3.077 *
16	4	6	0.436	2.257	-2.257	0.0	6.180	0.888
14	5	6	40.048	39.003	39.003	0.0	1.045	0.473
13	5	6	30.262	27.049	-27.049	0.0	3.193	1.279
20	5	0	80.762	64.287	-64.287	0.0	-4.545	-2.666 *
12	5	6	4.104	1.564	-1.564	0.0	2.632	0.282
11	5	6	20.136	6.425	-6.425	0.0	13.711	4.114 *
10	5	6	12.764	3.079	-3.079	0.0	8.785	1.073
9	5	6	15.501	1.680	-1.680	0.0	13.820	3.306 *
7	5	6	18.424	23.250	-23.250	0.0	-3.824	-0.989
5	5	6	46.002	50.432	-50.432	0.0	-4.631	-2.188
5	5	6	19.464	20.099	-20.099	0.0	-1.445	-0.467
2	5	6	24.716	27.363	-27.363	0.0	-2.648	-0.961
1	5	6	32.401	40.727	-40.727	0.0	-0.746	-0.610
0	5	6	75.675	80.236	-80.236	0.0	-4.560	-2.691
1	6	6	29.052	31.625	-31.625	0.0	-2.573	-0.990
2	6	6	13.762	12.929	-12.929	0.0	0.733	0.157
3	6	6	16.394	9.230	-9.230	0.0	8.168	2.212
4	6	6	9.702	6.911	-6.911	0.0	3.871	0.662
5	6	6	27.062	14.876	-14.876	0.0	12.907	3.930 *
7	6	6	31.214	31.014	-31.014	0.0	-0.700	-0.273
20	6	0	91.852	44.287	-44.287	0.0	-2.435	-1.343 *
8	6	6	23.746	23.753	-23.753	0.0	-0.008	-0.001
10	6	6	9.073	2.122	-2.122	0.0	6.952	1.044
12	6	6	28.270	31.035	-31.035	0.0	-2.665	-0.854
13	6	6	14.350	22.279	-22.279	0.0	12.520	-0.600
11	7	6	14.024	1.733	-1.733	0.0	12.291	2.604 *
10	7	6	17.427	17.017	-17.017	0.0	-0.490	-0.111
9	7	6	16.355	8.198	-8.198	0.0	8.158	1.975
7	7	6	13.601	8.106	-8.106	0.0	5.301	1.146
6	7	6	17.557	20.395	-20.395	0.0	-2.837	-0.669
7	7	6	11.952	5.522	-5.522	0.0	6.330	1.264
2	7	6	10.604	6.609	-6.609	0.0	4.098	0.837
2	7	6	4.040	0.119	0.119	0.0	4.830	0.566
20	6	0	90.262	0.4287	-0.4287	0.0	-4.025	-2.203 *
3	8	6	20.005	15.242	-15.242	0.0	4.763	1.320
4	8	6	18.586	21.572	-21.572	0.0	-2.986	-0.716
5	8	6	142.560	17.956	-17.956	0.0	12.603	2.672 *
7	8	6	5.991	7.429	-7.429	0.0	-1.439	-0.174

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STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
3	6	7	16.008	14.483	-17.483	0.0	14.525	3.455 *
4	6	7	12.923	7.492	-7.482	0.0	5.441	1.065
7	5	7	15.066	8.226	8.226	0.0	6.841	1.509
6	5	7	15.493	13.707	-13.707	0.0	2.287	0.7493
2	5	7	13.285	14.628	14.628	0.0	-1.343	-0.260
1	5	7	15.361	5.965	-5.965	0.0	5.376	2.202
0	4	7	10.150	2.662	-2.662	0.0	7.516	1.332
1	4	7	6.763	18.893	18.893	0.0	-12.140	-1.493 *
2	4	7	8.894	8.675	-8.675	0.0	0.239	0.036
20	6	0	20.365	9.4297	-9.4297	0.0	3.021	-2.146 *
4	4	7	20.701	16.702	-16.702	0.0	3.799	1.102
5	4	7	17.934	20.183	20.183	0.0	-2.249	-0.516
6	4	7	7.450	3.339	-3.339	0.0	4.619	0.678
7	4	7	14.630	8.278	8.278	0.0	8.353	2.045
8	4	7	8.465	12.838	10.838	0.0	-2.437	-0.331
11	3	7	31.301	37.233	-37.233	0.0	-5.032	-1.703
10	3	7	42.390	44.765	44.765	0.0	-2.374	-0.965
9	3	7	14.162	15.699	15.699	0.0	-1.531	-0.291
0	3	7	10.636	6.935	-6.935	0.0	5.301	0.968
7	3	7	12.460	4.878	-4.878	0.0	7.582	1.443
6	3	7	21.469	31.913	-31.913	0.0	-10.344	-2.479 *
5	2	7	15.703	10.363	-10.363	0.0	5.341	1.272
4	3	7	9.180	2.302	2.302	0.0	6.987	1.125
2	3	7	44.953	47.965	47.965	0.0	-3.012	-1.407
1	2	7	26.151	25.713	-25.713	0.0	-3.562	-1.198
0	2	7	11.650	14.894	-16.995	0.0	-5.335	-1.015
20	6	0	21.183	6.337	-6.297	0.0	-3.104	-1.684 *
1	2	7	18.923	10.611	-18.611	0.0	0.322	0.092
2	2	7	10.796	7.840	7.840	0.0	2.956	0.521
3	2	7	10.115	21.243	21.243	0.0	-11.128	-1.739 *
4	2	7	35.040	38.256	38.256	0.0	-3.209	-1.2315
5	2	7	23.251	24.374	-24.374	0.0	-1.123	-0.347
6	2	7	4.486	2.626	2.626	0.0	1.859	0.207
7	2	7	2.497	0.475	-0.475	0.0	-6.987	-0.640
8	2	7	12.084	25.760	-25.760	0.0	-13.676	-2.192 *
10	2	7	6.700	2.223	-2.223	0.0	4.477	0.560
11	2	7	13.451	13.509	-13.509	0.0	0.442	0.088
12	2	7	23.237	21.555	21.555	0.0	1.682	0.510
12	1	7	5.200	1.434	1.434	0.0	3.775	0.426
11	1	7	7.727	8.751	8.751	0.0	-1.024	-0.139
9	1	7	16.225	14.530	-14.530	0.0	1.695	0.396
8	1	7	6.053	5.054	-5.054	0.0	1.009	0.132
7	1	7	18.209	5.567	5.597	0.0	12.612	3.659 *
6	1	7	10.274	3.191	-3.191	0.0	7.083	1.265
5	1	7	11.693	11.650	-11.650	0.0	0.034	0.006
20	6	0	90.283	94.287	-94.287	0.0	-4.05	-2.202 *
3	1	7	11.658	1.125	-1.125	0.0	10.843	2.184 *
1	1	7	12.359	9.561	-9.561	0.0	2.818	0.563