

Thermal expansion and high-temperature crystal chemistry of the Al_2SiO_5 polymorphs

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Abstract

The crystal structures of sillimanite and andalusite have been refined from intensity data collected at 25, 400, 600, 800, and 1000°C. *R* factors following refinement were $0.033 \pm .002$ and $0.029 \pm .002$ for the sillimanite and andalusite data sets respectively. For kyanite 2140, 1773, and 1741 reflections were measured at 25, 400, and 600°C, and the final *R* factors were 0.033, 0.031, and 0.036 respectively.

Unit-cell dimensions of all three polymorphs vary linearly with temperature. Although the unit-cell dimensions determined at room temperature agree within error limits with those of Skinner *et al.* (1961), significant deviations occur between the two data sets at elevated temperatures. All the Al octahedra exhibit considerable expansions with increasing temperature. In contrast, Al- or Si-tetrahedra in all three polymorphs remain relatively constant in size and shape as temperature is increased. Within the five-coordinated Al_2 polyhedron in andalusite the four short bonds remain relatively unchanged, whereas the longest bond, $\text{Al}_2\text{-O}_c$, expands considerably. The orientation of the long $\text{Al}_1\text{-O}_b$ bonds in sillimanite and andalusite, which are more expandable than the other octahedral Al–O bonds, determines the direction of maximum unit-cell expansion. The chains of fully stretched tetrahedra (and Al_2 trigonal bipyramids in andalusite) restrict expansion in the *c* cell direction for these two minerals. The greater number of shared octahedral edges in kyanite, as well as the lack of continuous tetrahedral chains, results in more evenly distributed coefficients of unit-cell expansion.

Polymorphic transitions involve major reconstructive transformations. In addition, the andalusite-sillimanite transition requires diffusive interchange of half the Si and Al_2 atoms. Consequently, although metastable coexistence of two or three polymorphs is commonly observed, coherent replacement textures are rare. The present volume-temperature data agree well with the experimentally-derived thermodynamic properties of the aluminum silicate minerals.

Introduction

Andalusite, kyanite, and sillimanite, the three Al_2SiO_5 polymorphs that commonly occur in metamorphosed pelitic sediments, have been the subject of a great deal of study in the fields of metamorphic and experimental petrology. Due to the small changes in thermodynamic properties associated with the polymorphic phase transitions, metastable coexistence of these phases is common, and the mode of occurrence and relative fields of stability of the polymorphs are not completely clear.

The crystal structures of sillimanite and andalusite were first determined by Taylor (1928, 1929), using estimated intensities from rotation photographs. The

kyanite structure was deduced by inference from the staurolite structure by Naray-Szabo *et al.* (1929). From diffractometer-counter data, the structures of andalusite, sillimanite, and kyanite were refined by Burnham and Buerger (1961) and Burnham (1963a, b) respectively. Refinements of sillimanite and andalusite structures based on neutron diffraction data have been performed by Finger and Prince (1972). Thermal expansions of the three polymorphs were determined by Skinner *et al.* (1961), using the powder-diffraction technique with a heating stage.

We wish to relate the details of the crystal structures of the three polymorphs determined at elevated temperatures to the thermal expansion data, and thereby provide a basis for understanding the behav-

TABLE 5. Sillimanite, Andalusite, and Kyanite: Anisotropic thermal ellipsoids, axial lengths (A) and isotropic equivalent temperature factors, Beq^* (A^2) as a function of temperature.

		25°C	400°C	600°C	800°C	1000°C
Sillimanite						
Al ₁	R ₁	0.049	0.082	0.093	0.106	0.119
	R ₂	0.076	0.102	0.107	0.116	0.124
	R ₃	0.083	0.104	0.114	0.126	0.137
	B	0.40(1)	0.73(2)	0.88(2)	1.07(2)	1.27(2)
Al ₂	R ₁	0.057	0.086	0.098	0.110	0.121
	R ₂	0.084	0.106	0.112	0.120	0.128
	R ₃	0.087	0.108	0.117	0.128	0.142
	B	0.48(2)	0.80(2)	0.94(2)	1.13(2)	1.35(2)
Si	R ₁	0.048	0.079	0.089	0.099	0.108
	R ₂	0.077	0.101	0.107	0.117	0.123
	R ₃	0.087	0.103	0.112	0.122	0.134
	B	0.42(2)	0.71(2)	0.84(2)	1.01(2)	1.18(2)
O _A	R ₁	0.053	0.076	0.087	0.095	0.107
	R ₂	0.092	0.117	0.120	0.135	0.141
	R ₃	0.096	0.127	0.145	0.155	0.170
	B	0.54(3)	0.94(4)	1.13(4)	1.35(5)	1.58(5)
O _B	R ₁	0.055	0.080	0.090	0.097	0.110
	R ₂	0.089	0.113	0.121	0.130	0.132
	R ₃	0.100	0.131	0.141	0.155	0.177
	B	0.55(4)	0.96(4)	1.12(4)	1.33(5)	1.60(5)
O _C	R ₁	0.067	0.098	0.099	0.113	0.119
	R ₂	0.118	0.161	0.177	0.191	0.207
	R ₃	0.123	0.176	0.193	0.215	0.238
	B	0.88(4)	1.75(5)	2.06(6)	2.52(6)	2.98(6)
O _D	R ₁	0.073	0.095	0.105	0.113	0.121
	R ₂	0.086	0.106	0.112	0.122	0.128
	R ₃	0.093	0.130	0.144	0.160	0.173
	B	0.56(2)	0.93(3)	1.17(3)	1.40(3)	1.61(3)
Andalusite						
Al ₁	R ₁	0.060	0.079	0.088	0.096	0.105
	R ₂	0.076	0.103	0.114	0.123	0.131
	R ₃	0.099	0.142	0.164	0.182	0.204
	B	0.50(2)	0.98(2)	1.25(1)	1.51(1)	1.83(2)
Al ₂	R ₁	0.053	0.080	0.091	0.102	0.115
	R ₂	0.066	0.092	0.101	0.111	0.119
	R ₃	0.091	0.109	0.120	0.127	0.138
	B	0.41(2)	0.70(2)	0.87(1)	1.02(1)	1.22(2)

* Isotropic equivalent temperature factors, calculated from anisotropic temperature factors (Hamilton, 1959)

TABLE 5. Continued

		25°C	400°C	600°C	800°C	1000°C
Si	R ₁	0.047	0.078	0.089	0.102	0.112
	R ₂	0.063	0.085	0.094	0.103	0.114
	R ₃	0.087	0.103	0.111	0.118	0.126
	B	0.36(2)	0.63(2)	0.77(1)	0.92(1)	1.09(1)
O _A	R ₁	0.068	0.093	0.105	0.113	0.124
	R ₂	0.073	0.102	0.108	0.119	0.126
	R ₃	0.095	0.119	0.133	0.146	0.161
	B	0.50(5)	0.87(5)	1.07(3)	1.26(3)	1.51(4)
O _B	R ₁	0.055	0.084	0.096	0.104	0.117
	R ₂	0.070	0.094	0.103	0.110	0.121
	R ₃	0.101	0.124	0.139	0.155	0.166
	B	0.48(5)	0.83(5)	1.03(3)	1.24(3)	1.47(4)
O _C	R ₁	0.055	0.085	0.093	0.099	0.110
	R ₂	0.092	0.111	0.120	0.125	0.134
	R ₃	0.116	0.160	0.184	0.201	0.219
	B	0.66(5)	1.19(6)	1.52(3)	1.73(4)	2.05(5)
O _D	R ₁	0.062	0.087	0.096	0.106	0.114
	R ₂	0.072	0.106	0.119	0.129	0.138
	R ₃	0.103	0.137	0.153	0.166	0.182
	B	0.52(3)	0.97(4)	1.23(2)	1.45(2)	1.71(3)
Kyanite						
Al ₁	R ₁	0.047	0.073	0.084		
	R ₂	0.075	0.104	0.123		
	R ₃	0.088	0.111	0.127		
	B	0.41(1)	0.75(1)	1.01(1)		
Al ₂	R ₁	0.055	0.081	0.093		
	R ₂	0.067	0.091	0.107		
	R ₃	0.092	0.113	0.132		
	B	0.42(1)	0.73(1)	0.99(1)		
Al ₃	R ₁	0.052	0.078	0.088		
	R ₂	0.068	0.092	0.109		
	R ₃	0.094	0.117	0.136		
	B	0.42(1)	0.75(1)	1.00(1)		
Al ₄	R ₁	0.050	0.071	0.077		
	R ₂	0.069	0.097	0.116		
	R ₃	0.094	0.116	0.134		
	B	0.43(1)	0.74(1)	0.98(1)		

TABLE 5. Continued

		25°C	400°C	600°C
Si ₁	R ₁	0.040	0.065	0.074
	R ₂	0.062	0.082	0.096
	R ₃	0.087	0.105	0.122
	B	0.35(1)	0.58(1)	0.78(1)
Si ₂	R ₁	0.037	0.063	0.071
	R ₂	0.062	0.081	0.094
	R ₃	0.088	0.106	0.123
	B	0.34(1)	0.57(1)	0.77(1)
O _A	R ₁	0.062	0.087	0.098
	R ₂	0.070	0.091	0.101
	R ₃	0.106	0.132	0.152
	B	0.52(2)	0.88(3)	1.13(3)
O _B	R ₁	0.054	0.079	0.088
	R ₂	0.071	0.095	0.107
	R ₃	0.091	0.112	0.128
	B	0.43(2)	0.73(2)	0.94(3)
O _C	R ₁	0.065	0.083	0.097
	R ₂	0.076	0.103	0.114
	R ₃	0.098	0.128	0.141
	B	0.52(2)	0.89(3)	1.12(3)
O _D	R ₁	0.058	0.080	0.095
	R ₂	0.079	0.110	0.125
	R ₃	0.096	0.121	0.134
	B	0.49(2)	0.87(3)	1.12(3)
O _E	R ₁	0.059	0.075	0.078
	R ₂	0.080	0.111	0.123
	R ₃	0.094	0.119	0.140
	B	0.49(2)	0.85(3)	1.07(3)
O _F	R ₁	0.056	0.078	0.092
	R ₂	0.071	0.093	0.107
	R ₃	0.099	0.113	0.129
	B	0.47(2)	0.73(2)	0.96(3)
O _G	R ₁	0.068	0.096	0.105
	R ₂	0.075	0.106	0.120
	R ₃	0.099	0.118	0.136
	B	0.53(2)	0.90(3)	1.16(3)

TABLE 5. Continued

		25°C	400°C	600°C
O_H	R ₁	0.062	0.090	0.106
	R ₂	0.078	0.097	0.107
	R ₃	0.097	0.127	0.145
	B	0.51(2)	0.88(3)	1.15(3)
O_K	R ₁	0.054	0.078	0.086
	R ₂	0.080	0.111	0.125
	R ₃	0.099	0.120	0.135
	B	0.50(2)	0.87(2)	1.08(3)
O_M	R ₁	0.063	0.093	0.100
	R ₂	0.075	0.103	0.115
	R ₃	0.099	0.116	0.135
	B	0.51(2)	0.85(3)	1.09(3)

TABLE 7. Sillimanite, Andalusite, and Kyanite: Bond angles ($^{\circ}$) as a function of temperature

		25°C	400°C	600°C	800°C	1000°C
Sillimanite						
Al ₁	A-B	99.92(7)	99.93(8)	99.91(8)	99.95(3)	100.11(9)
	A-B'	80.08(7)	80.07(8)	80.09(8)	80.05(8)	79.89(9)
	A-D	88.61(9)	88.6(1)	88.5(1)	88.5(1)	88.5(1)
	A-D'	91.39(9)	91.4(1)	91.5(1)	91.5(1)	91.5(1)
	B-D	90.27(9)	90.3(1)	90.2(1)	90.2(1)	90.5(1)
	B-D'	89.73(9)	89.7(1)	89.8(1)	89.8(1)	89.5(1)
Al ₂	B-C	113.3(1)	113.0(2)	113.2(2)	112.9(2)	112.6(2)
	B-D	105.43(7)	105.55(8)	105.52(8)	105.48(9)	105.55(9)
	C-D	108.13(8)	108.07(9)	108.0(1)	108.1(1)	108.3(1)
	D-D	116.6(1)	116.7(1)	116.7(1)	116.8(1)	116.6(1)
Si	A-C	109.3(2)	109.2(2)	109.2(2)	109.4(2)	109.4(2)
	A-D	107.31(8)	107.31(9)	107.22(9)	107.20(9)	107.1(1)
	C-D	110.60(8)	110.5(1)	110.5(1)	110.4(1)	110.5(1)
	D-D	111.6(1)	111.8(1)	112.0(1)	112.1(1)	112.0(2)
O _A	Al ₁ -Al ₁	98.1(1)	98.0(1)	97.9(1)	97.9(1)	98.1(1)
	Si ¹ -Al ₁ ¹	129.34(6)	129.47(7)	129.48(7)	129.51(7)	129.46(8)
O _B	Al ₁ -Al ₁	101.3(1)	101.4(1)	101.4(1)	101.5(1)	101.6(1)
	Al ₁ ¹ -Al ₂ ¹	129.33(5)	129.29(6)	129.27(6)	129.21(6)	129.18(7)
O _C	Si-Al ₂	171.9(2)	172.0(3)	171.9(3)	172.4(3)	172.5(3)
O _D	Al ₁ -Al ₂	116.93(9)	116.9(1)	117.1(1)	117.0(1)	117.1(1)
	Al ₁ ¹ -Si ²	125.2(1)	125.1(1)	125.0(1)	125.0(1)	124.9(1)
	Al ₂ ¹ -Si	114.18(9)	114.4(1)	114.4(1)	114.5(1)	114.4(1)
Andalusite						
Al ₁	A-A'	85.3(2)	85.4(2)	85.2(1)	85.1(1)	85.3(1)
	A-B	96.7(1)	96.7(1)	96.79(6)	96.79(6)	96.80(7)
	A-B'	178.0(1)	177.9(1)	177.96(8)	177.94(8)	177.7(1)
	A-D	88.6(1)	88.3(1)	88.24(7)	88.04(7)	87.94(7)
	A-D'	90.7(1)	91.0(1)	91.16(8)	91.30(8)	91.4(1)
	B-B'	81.4(2)	81.3(2)	81.2(1)	81.3(1)	81.1(1)
	B-D	89.0(1)	89.3(1)	89.36(7)	89.53(7)	89.79(9)
	B-D'	91.6(1)	91.4(1)	91.26(7)	91.16(7)	90.91(9)
	D-D'	179.2(2)	179.1(2)	179.19(9)	179.09(9)	179.1(1)

TABLE 7. Continued

		25°C	400°C	600°C	800°C	1000°C
Al ₂	A-C	86.7(2)	86.8(2)	86.8(1)	86.78(9)	86.8(1)
	A-C'	160.7(2)	160.9(2)	160.8(1)	160.8(1)	160.9(1)
	A-D	99.1(1)	98.9(1)	98.77(7)	98.72(7)	98.61(9)
	C-C'	74.0(2)	74.2(2)	74.0(1)	74.0(1)	74.1(1)
	C-D	126.1(1)	126.0(1)	126.08(5)	126.07(5)	126.00(6)
	C'-D	92.5(1)	92.6(1)	92.70(7)	92.74(7)	92.79(8)
	D-D'	106.1(2)	106.2(2)	106.1(1)	106.2(1)	106.4(1)
Si	B-C	101.3(2)	101.5(2)	101.7(1)	101.8(1)	101.8(1)
	B-D	111.6(1)	111.3(1)	111.10(1)	111.00(7)	110.83(8)
	C-D	111.4(1)	111.6(1)	111.62(7)	111.69(7)	111.86(8)
	D-D'	109.3(2)	109.3(2)	109.5(1)	109.5(1)	109.5(1)
O _A	Al ₁ ¹ -Al ₁ ¹	94.7(2)	94.5(2)	94.8(1)	94.9(1)	94.7(1)
	Al ₁ ¹ -Al ₂ ¹	130.7(1)	130.8(1)	130.78(6)	130.82(5)	130.92(7)
U _B	Al ₁ ¹ -Al ₁ ¹	98.6(2)	98.7(2)	98.8(1)	98.7(1)	98.9(1)
	Al ₁ ¹ -Si ¹	124.6(1)	124.8(1)	124.84(6)	124.99(6)	125.15(7)
O _C	Si-Al ₂	123.7(2)	123.8(2)	123.9(1)	123.9(1)	124.0(1)
	Si-Al ₂ ²	130.3(2)	130.4(2)	130.1(1)	130.1(1)	130.1(1)
	Al ₂ ² -Al ₂ ²	106.0(2)	105.9(2)	106.0(1)	106.0(1)	105.9(1)
O _D	Al ₁ ¹ -Al ₂	121.6(1)	121.3(1)	121.27(8)	121.11(8)	121.0(1)
	Al ₁ ¹ -Si ²	111.2(1)	110.9(1)	110.69(8)	110.64(8)	110.38(9)
	Al ₂ ² -Si	126.5(2)	127.0(2)	127.26(9)	127.47(9)	127.9(1)
Kyanite						
Al ₁	B-F	87.05(7)	87.16(8)	87.24(9)		
	B-G	89.49(7)	89.39(8)	89.33(9)		
	B-H	79.26(6)	79.19(7)	79.12(9)		
	B-M	85.52(7)	85.31(8)	85.27(9)		
	B-K	172.09(7)	172.10(8)	172.04(9)		
	F-G	80.64(7)	80.47(7)	80.38(9)		
	F-H	88.80(7)	88.86(8)	88.77(9)		
	F-K	85.61(7)	85.53(7)	85.42(9)		
	F-M	172.48(7)	172.39(8)	172.4(1)		
	G-H	164.97(7)	164.77(8)	164.5(1)		
	G-K	92.24(7)	92.34(8)	92.48(9)		
	G-M	98.12(7)	98.27(8)	98.34(9)		
	H-K	97.61(7)	97.66(8)	97.63(9)		
	H-M	90.95(7)	90.87(7)	90.96(9)		
K-M	101.87(7)	102.05(8)	102.12(9)			

TABLE 7. Continued

		25°C	400°C	600°C
Al ₂	F-K	82.58(7)	82.26(7)	82.29(9)
	F-B	104.84(7)	105.21(8)	105.15(9)
	F-C	82.74(7)	82.57(8)	82.51(9)
	F-D	92.37(7)	92.43(8)	92.46(9)
	F-M	173.42(7)	173.36(8)	173.4(1)
	K-B	172.54(7)	172.50(8)	172.51(9)
	K-C	88.76(7)	88.80(8)	88.84(9)
	K-D	96.34(7)	96.47(8)	96.41(9)
	K-M	90.86(6)	90.13(7)	90.12(9)
	B-C	92.94(7)	92.83(8)	92.94(9)
	B-D	82.72(7)	82.68(7)	82.60(9)
	B-M	81.73(6)	81.41(7)	81.45(9)
	C-D	172.44(7)	172.25(9)	172.2(1)
	C-M	96.65(7)	96.78(8)	96.86(9)
	D-M	88.87(7)	88.83(8)	88.82(9)
Al ₃	F-G	82.98(7)	83.05(8)	83.18(9)
	F-C	82.42(7)	82.22(7)	82.17(9)
	F-B	97.78(7)	97.92(7)	97.96(9)
	F-E	173.01(7)	172.82(8)	172.75(9)
	F-F	83.85(7)	83.76(8)	83.86(9)
	C-C	101.21(7)	101.64(8)	101.8(1)
	G-B	171.59(7)	171.29(8)	171.1(1)
	G-E	95.23(7)	95.09(8)	95.02(9)
	G-F	90.01(7)	89.94(8)	89.78(9)
	C-B	87.18(6)	87.06(7)	87.06(9)
	C-E	91.33(7)	91.41(7)	91.36(9)
	C-F	161.03(7)	160.54(8)	160.6(1)
	B-E	84.98(7)	84.97(8)	84.90(9)
	B-F	81.76(6)	81.58(7)	81.63(9)
	E-F	102.93(7)	103.20(8)	103.19(9)
Al ₄	B-H	82.93(7)	83.20(8)	83.33(9)
	B-A	175.73(7)	175.71(8)	175.6(1)
	B-A'	91.29(7)	91.22(7)	90.97(9)
	B-D	84.59(7)	84.54(8)	84.50(9)
	B-E	86.93(7)	86.81(8)	86.79(9)
	H-A	98.89(7)	98.72(8)	98.8(1)
	H-D	102.23(7)	102.81(8)	103.0(1)
	H-E	89.91(7)	89.89(8)	89.9(1)
	A-A'	87.43(7)	87.42(8)	87.50(9)
	H-A'	170.12(7)	170.04(8)	169.9(1)
	A-D	91.24(7)	91.29(8)	91.2(1)
	A-E	96.91(7)	97.00(8)	97.08(9)
	A'-D	85.11(7)	84.78(8)	84.79(9)
	A'-E	81.76(7)	81.54(8)	81.38(9)
	D-E	164.19(7)	163.64(8)	163.4(1)

TABLE 7. Continued

		25°C	400°C	600°C
Si ₁	E-D	109.30(8)	109.30(9)	109.2(1)
	E-H	111.52(8)	111.51(9)	111.5(1)
	E-M	106.89(8)	106.99(9)	107.0(1)
	D-H	107.89(8)	107.98(9)	108.1(1)
	D-M	112.52(8)	112.60(9)	112.6(1)
	H-M	108.76(8)	108.50(9)	108.4(1)
Si ₂	G-A	112.97(8)	112.91(9)	112.8(1)
	G-C	107.97(8)	107.99(9)	108.1(1)
	G-K	108.27(8)	108.10(9)	108.2(1)
	A-C	108.44(8)	108.63(9)	108.5(1)
	A-K	106.68(8)	106.69(9)	106.8(1)
	C-K	112.60(8)	112.61(9)	112.4(1)
O _A	Al ₄ -Al ₄	92.57(7)	92.58(8)	92.50(9)
	Al ₄ -Si ₂	130.60(9)	130.7(1)	130.6(1)
	Al ₄ -Si ₂	127.69(9)	127.6(1)	127.9(1)
O _B	Al ₁ -Al ₂	94.44(7)	94.62(8)	94.6(1)
	Al ₁ -Al ₃	95.44(7)	95.50(8)	95.49(9)
	Al ₁ -Al ₄	101.05(7)	101.12(8)	101.1(1)
	Al ₂ -Al ₃	164.31(9)	164.0(1)	163.9(1)
	Al ₂ -Al ₄	96.61(7)	96.67(8)	96.89(9)
	Al ₃ -Al ₄	93.42(7)	93.46(8)	93.47(9)
O _C	Al ₂ -Al ₃	97.26(7)	97.32(8)	97.28(9)
	Al ₂ -Si ₂	128.81(9)	129.1(1)	129.0(1)
	Al ₃ -Si ₂	126.83(9)	126.7(1)	126.8(1)
O _D	Al ₂ -Al ₄	96.08(7)	96.12(8)	96.01(9)
	Al ₂ -Si ₁	129.12(9)	129.3(1)	129.3(1)
	Al ₄ -Si ₁	126.73(9)	126.8(1)	127.0(1)
O _E	Al ₃ -Al ₄	94.66(7)	94.74(8)	94.81(9)
	Al ₃ -Si ₁	131.40(9)	131.5(1)	131.5(1)
	Al ₄ -Si ₁	124.32(8)	124.3(1)	124.4(1)
O _F	Al ₁ -Al ₂	94.51(7)	94.67(8)	94.66(9)
	Al ₁ -Al ₃	99.43(7)	99.71(8)	99.7(1)
	Al ₁ -Al ₃	95.71(7)	95.72(8)	95.60(9)
	Al ₂ -Al ₃	97.57(7)	97.89(8)	98.0(1)
	Al ₂ -Al ₃	161.30(9)	160.8(1)	160.8(1)
	Al ₃ -Al ₃	96.15(7)	96.24(8)	96.14(9)

The thermal expansion and the high temperature crystal chemistry
of Al_2SiO_5 polymorphs

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and
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Seattle, Washington 98195

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Table 9. Sillimanite, andalusite and kyanite: observed and
calculated structure factors at various temperatures.

Sillimanite 25°C

TABLE 7. Continued

		25°C	400°C	600°C
O_G	Al_1-Al_3	96.35(7)	96.15(8)	96.14(9)
	Al_1-Si_2	126.21(9)	126.2(1)	126.1(1)
	Al_3-Si_2	128.35(9)	128.7(1)	129.0(1)
O_H	Al_1-Al_4	96.00(7)	95.70(8)	95.65(9)
	Al_1-Si_4	126.69(9)	126.6(1)	126.6(1)
	Al_4-Si_1	127.13(9)	127.6(1)	127.7(1)
O_K	Al_1-Al_2	95.14(7)	95.26(8)	95.33(9)
	Al_1-Si_2	126.67(9)	126.8(1)	126.7(1)
	Al_2-Si_2	130.05(9)	130.0(1)	130.1(1)
O_M	Al_1-Al_2	95.67(7)	95.89(8)	95.86(9)
	Al_1-Si_1	125.49(9)	125.6(1)	125.6(1)
	Al_2-Si_1	128.75(9)	128.8(1)	128.8(1)

" Al_1 A-B" indicates the $O_A-Al_1-O_B$ angle etc.

LOAD MAP - REFIN

CYBER IDLE/F 1.3-46C

03/28/78 17.2C.C5.

PAGE

PWA OF THE LOAD 111
LWA+1 OF THE LOAD 74743

TRANSFER ADDRESS --- REFIN 112

***** ERROR SUMMARY

REF4105/// CN BLANK COMMON TRUNCATED BY 207008 WORDS

PROGRAM AND BLOCK ASSIGNMENTS.

BLOCK	ADDRESS	LENGTH	FILE	DATE	PROCESSR	VER	LEVEL	HARDWARE	COMMENTS
REFINE	111	10575	REFINE	05/14/76	RUN	F	EB	74 B	646X I
LA/	10706	1355							
IC/	12263	457							
ID/	12742	3244							
IE/	16206	10							
IF/	16216	174							
IG/	16412	2307							
IJS/	20721	334							
/TAPE/	21255	6							
/OEGEN/	21263	311	REFINE	05/14/76	RUN	F	EB	74 B	646X I
REFINE	21574	5726	REFINE	05/14/76	RUN	F	ER	74 C	646X I
BODAN1	27522	1147	REFINE	05/14/76	RUN	F	ER	74 B	646X I
ELVIB1	30671	1312	REFINE	05/14/76	RUN	F	ER	74 B	646X I
INPUT	32203	241	REFINE	05/14/76	RUN	F	ER	74 B	646X I
MATRIX	32444	231	REFINE	05/14/76	RUN	F	ER	74 B	646X I
KODIFY	32675	115	REFINE	05/14/76	RUN	F	ER	74 B	646X I
RCALC	33012	152	REFINE	05/14/76	RUN	F	ER	74 B	646X I
RESFT	33164	73	REFINE	05/14/76	RUN	F	ER	74 B	646X I
SEAC	33257	476	REFINE	05/14/76	RUN	F	ER	74 B	646X I
SYMINV	33755	361	REFINE	05/14/76	RUN	F	ER	74 B	646X I
WEIGHT	34236	12	REFINE	05/14/76	RUN	F	ER	74 B	646X I
ASTNCS	34350	136	SL-RUN2P3	02/19/75	COMPASS	3		74150	
EXP	34505	55	SL-RUN2P3	02/19/75	COMPASS	3		74150	
SINCS	34563	72	SL-RUN2P3	02/19/75	COMPASS	3		74150	
SOFT	34655	44	SL-RUN2P3	02/19/75	COMPASS	3		74150	
ACGDR	34721	12	SL-RUN2P3	02/19/75	COMPASS	3		74150	
EMOFL	34733	57	SL-RUN2P3	02/19/75	COMPASS	3		74150	
GETBA	35012	17	SL-RUN2P3	02/19/75	COMPASS	3		74150	
INPUTB	35031	256	SL-RUN2P3	02/19/75	COMPASS	3		74150	
KRAKER	35307	1052	SL-RUN2P3	02/19/75	COMPASS	3		74150	
OUTP1B	36361	244	SL-RUN2P3	02/19/75	COMPASS	3		74150	
S105	36625	1504	SL-RUN2P3	02/19/75	COMPASS	3		74150	
INPUTC	40331	121	SL-RUN2P3	03/17/75	COMPASS	3		74150	
KODER	40452	1310	SL-RUN2P3	02/19/75	COMPASS	3		74150	
OUTPTC	41762	71	SL-RUN2P3	02/19/75	COMPASS	3		74150	
REHINM	42053	63	SL-RUN2P3	02/19/75	COMPASS	3		74150	
SYSTEM	42136	1122	SL-RUN2P3	03/04/75	COMPASS	3		74150	
/ /	43260	31463							

LOAD MAP -- REFINE

CYBER LOADER 1.3-460

02/28/70 17.30.09.

PAGE 2

.519 CP SECONDS

57300R CM STORAGE USED

2 TABLE MOVES

M	K	L	F(DBS)	F(CALC)	A(CALC)	B(CALC)	DELTA T	DELTA/SIGMA	EXT.	FACTPR
0	0	2	63.885	65.656	-65.656	-353	-1.771	-11.6993		1.0000
0	0	4	137.361	150.666	150.666	.854	-13.315	-61.5250		1.0000
0	0	6	29.212	29.752	-29.750	-.303	-.540	-1.7423		1.0000
0	0	8	62.107	60.597	60.593	.683	1.510	4.1735		1.0000
0	0	0	13.521	12.408	12.808	.024	2.713	12.0101		1.0000
0	0	2	4.032	4.101	-4.101	-.065	-.065	-.1770		1.0000
0	0	4	22.863	18.668	-18.661	.522	4.195	21.6309		1.0000
0	0	6	6.377	6.017	6.017	.063	.360	2.0410		1.0000
0	0	8	9.013	8.096	8.096	.023	.917	5.4600		1.0000
0	0	0	1.100	0.351	0.351	-.058	.745	.9534		1.0000
0	0	2	7.832	7.512	7.498	.450	.220	2.0846		1.0000
0	0	4	4.552	4.567	4.567	.053	.015	-.0570		1.0000
0	0	6	5.470	3.860	3.860	.019	1.710	6.6633		1.0000
0	0	8	21.194	20.165	20.165	-.148	1.028	4.6998		1.0000
0	0	0	6.502	6.608	6.608	.052	-.105	-.6093		1.0000
0	0	2	90.031	91.758	91.756	.677	-1.727	-8.4412		1.0000
0	0	4	10.492	10.492	-10.870	-.078	-.376	-2.2980		1.0000
0	0	6	5.606	7.239	7.237	-.137	-1.633	-9.4579		1.0000
0	0	8	1.479	.948	.945	.074	.532	.6326		1.0000
0	0	0	46.739	48.787	48.784	.553	-2.048	-6.4386		1.0000
0	0	2	7.960	8.025	-8.025	-.064	-.065	-.3456		1.0000
0	0	4	1.410	.707	.779	-.108	.623	.6187		1.0000
0	0	6	55.850	54.958	54.952	.815	.900	3.7135		1.0000
0	0	8	8.003	8.497	8.497	-.022	-.484	-2.6106		1.0000
0	0	0	24.111	25.176	-25.174	-.290	-1.065	-3.7506		1.0000
0	0	2	1.109	1.037	-1.037	.023	.072	.0913		1.0000
0	0	4	42.553	43.862	43.862	.757	-1.329	-4.4966		1.0000
0	0	6	8.641	8.808	8.808	-.019	-.166	-1.0906		1.0000
0	0	8	13.462	14.088	-14.086	-.249	-.526	-3.0684		1.0000
0	0	0	1.375	2.057	2.057	.020	.722	-.7348		1.0000
0	0	2	19.439	19.164	19.163	.202	.274	1.3799		1.0000
0	0	4	3.305	3.517	3.516	-.069	-.212	-.6414		1.0000
0	0	6	24.657	25.586	25.585	.253	-.925	-3.9263		1.0000
0	0	8	6.678	7.325	-7.324	.067	-.447	-2.4684		1.0000
0	0	0	13.841	14.102	14.101	.188	-.261	-1.6818		1.0000
0	0	2	2.113	1.764	-1.763	-.060	.329	.5437		1.0000
0	0	4	15.062	15.998	15.996	.244	-.936	-5.1052		1.0000
0	0	6	3.661	3.764	-3.758	-.219	-.103	-.2721		1.0000
0	0	8	5.316	5.120	5.119	.090	.196	.7353		1.0000
0	0	0	33.168	33.943	33.943	.662	-.776	-2.6412		1.0000
0	0	2	1.366	.743	-.737	-.093	.643	.6497		1.0000
0	0	4	3.171	3.060	-3.054	-.203	.110	.2394		1.0000
0	0	6	12.630	12.312	12.312	.078	.318	1.3797		1.0000
0	0	8	2.673	1.902	1.901	-.075	.771	2.8582		1.0000
0	0	0	9.521	9.766	9.766	.069	-.245	-1.4202		1.0000
0	0	2	1.703	2.491	2.490	-.062	-.788	-1.1609		1.0000
0	0	4	26.132	25.028	25.028	.071	1.104	8.6461		1.0000
0	0	6	4.960	.615	.615	.027	4.345	10.2330		1.0000
0	0	8	62.386	64.190	64.188	.479	-1.803	-11.2127		1.0000
0	0	0	9.123	8.813	8.813	-.026	.310	1.8859		1.0000
0	0	2	13.623	14.082	14.082	.066	-.459	-2.5065		1.0000
0	0	4	4.561	5.021	5.021	.025	-.460	-2.1589		1.0000
0	0	6	32.383	31.932	31.929	.413	.452	1.4802		1.0000

H	K	L	F(ORS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	1	7	5.491	5.431	5.431	-.021	.066	.2612	1.0000
1	1	8	5.993	6.160	6.160	.054	-.167	-.6677	1.0000
1	2	0	62.811	62.860	82.958	.465	-.048	-.3502	1.0000
1	2	1	7.890	7.773	-7.773	-.044	.106	.4370	1.0000
1	2	2	66.987	68.057	-68.056	-.456	-1.070	-6.2813	1.0000
1	2	3	2.577	2.352	-2.352	.043	.225	.7606	1.0000
1	2	4	48.823	49.837	49.835	.432	-1.014	-4.2638	1.0000
1	2	5	7.672	8.238	-8.238	-.039	.567	-3.7438	1.0000
1	2	6	40.033	40.710	-40.708	-.593	-.678	-2.7123	1.0000
1	2	7	3.142	2.714	-2.713	.036	.430	1.1538	1.0000
1	2	8	23.517	22.935	22.932	.345	.582	2.4750	1.0000
1	3	0	45.312	46.291	46.287	.642	-.580	-5.8332	1.0000
1	3	1	6.135	5.835	-5.835	-.011	.300	1.6812	1.0000
1	3	2	2.472	3.375	-3.378	-.091	-.607	-2.9970	1.0000
1	3	3	2.210	2.127	-2.127	.011	.004	.2178	1.0000
1	3	4	38.501	39.325	39.321	.596	-.824	-3.2562	1.0000
1	3	5	5.782	6.529	-6.529	-.009	-.747	-4.2665	1.0000
1	3	6	2.834	3.105	-3.104	-.078	-.271	-.7240	1.0000
1	3	7	2.810	3.214	-3.214	.010	-.404	-.5034	1.0000
1	3	8	20.204	20.190	20.184	.477	.014	.0728	1.0000
1	4	0	2.375	1.244	1.189	-.363	1.181	3.2311	1.0000
1	4	1	3.078	2.821	-2.821	-.031	.257	1.0468	1.0000
1	4	2	27.847	28.715	28.717	.357	-.872	-3.7997	1.0000
1	4	3	6.737	7.195	7.194	.030	-.457	-2.4941	1.0000
1	4	4	7.058	6.474	-6.465	-.337	.584	3.9525	1.0000
1	4	5	1.155	1.399	1.399	-.027	-.243	-.2949	1.0000
1	4	6	16.612	16.996	16.994	.307	-.384	-2.2720	1.0000
1	4	7	6.011	5.817	-5.817	.025	.194	.8403	1.0000
1	4	8	3.193	4.362	-4.356	-.269	1.165	-2.6017	1.0000
1	5	0	10.526	9.190	9.188	.190	1.337	7.2980	1.0000
1	5	1	7.021	6.791	6.791	-.022	.230	1.3035	1.0000
1	5	2	68.071	70.455	70.494	.344	-.242	-10.4570	1.0000
1	5	3	1.211	1.300	-1.300	.022	-.089	-.1119	1.0000
1	5	4	9.444	8.200	8.159	.168	.242	1.7442	1.0000
1	5	5	5.110	5.823	5.823	-.018	-.713	-3.2599	1.0000
1	5	6	34.795	36.164	36.163	.797	-1.370	-3.9392	1.0000
1	5	7	3.141	1.546	1.546	.019	1.595	3.7676	1.0000
1	5	8	25.354	25.449	-25.449	-.153	-.095	-.3444	1.0000
1	6	0	2.830	3.022	3.021	.083	-.192	-.5150	1.0000
1	6	1	1.172	1.030	-1.030	.151	-.458	-.5150	1.0000
1	6	2	5.509	5.489	-5.488	-.080	.020	.1096	1.0000
1	6	3	17.762	17.744	-17.743	-.142	.018	.0898	1.0000
1	6	4	1.226	.902	.899	.074	.325	.3711	1.0000
1	6	5	1.332	.529	.513	.130	.803	.8444	1.0000
1	6	6	5.457	4.735	-4.734	-.066	.722	2.7878	1.0000
1	6	7	28.858	30.424	-30.424	-.018	-.156	-5.4258	1.0000
1	7	0	6.477	6.796	6.796	.045	-.319	-1.8982	1.0000
1	7	1	46.639	47.064	47.064	.514	-1.025	-3.6268	1.0000
1	7	2	6.804	7.455	-7.455	-.042	-.651	-3.7213	1.0000
1	7	3	20.424	21.194	-21.194	-.016	-.770	-3.7847	1.0000
1	7	4	3.108	3.534	3.534	.041	-.426	-1.0475	1.0000
1	7	5	27.856	28.952	28.949	.443	-1.094	-3.9716	1.0000
1	7	6	37.498	36.406	36.404	.441	1.092	3.6211	1.0000

H	K	L	F(MGS)	F(CALC)	Δ(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
1	9	1	2.243 *	2.060	2.059	-1.056	.182	.3859		1.0000
1	8	2	13.931	13.862	-13.855	-1.431	.069	.4223		1.0000
1	8	3	2.592	.820	-.819	.054	1.772	4.2325		1.0000
1	8	4	20.355	27.899	27.896	.409	-1.544	-5.8115		1.0000
1	5	5	1.34, *	2.012	2.012	-.050	-.465	-.6911		1.0000
1	8	6	8.601	5.076	-9.068	-.371	-.475	-2.4485		1.0000
1	9	0	37.117	37.117	37.113	.511	.080	.2408		1.0000
1	9	1	1.293 *	.976	-.976	-.022	.316	.3425		1.0000
1	9	2	14.227	14.518	14.518	-.038	-.291	-1.6395		1.0000
1	9	3	2.782	1.241	1.241	.022	1.540	3.4009		1.0000
1	9	4	28.460	26.987	26.983	.475	-.527	-1.9560		1.0000
1	9	5	1.983 *	.207	-.206	-.018	1.777	2.5813		1.0000
1	9	0	26.267	25.599	-25.598	-.193	.668	2.4669		1.0000
1	10	1	6.348	5.931	5.931	-.032	.418	1.7857		1.0000
1	10	2	8.799	9.004	9.002	.191	-.205	-1.1261		1.0000
1	10	3	5.349	5.072	-5.072	.031	.277	1.0084		1.0000
1	10	4	20.797	20.495	-20.494	-.179	.303	1.5694		1.0000
1	10	0	5.432	5.480	5.474	.246	-.048	-.1673		1.0000
1	10	1	4.040	3.900	-3.900	-.031	.140	.5654		1.0000
1	11	2	5.217	5.070	5.066	.185	.147	.5006		1.0000
1	11	0	33.851	32.010	32.010	.096	1.841	11.7933		1.0000
1	11	1	4.847	4.454	4.454	.454	.300	1.0726		1.0000
1	11	2	17.428	17.432	17.431	.089	-.004	-.0170		1.0000
1	11	3	27.150	26.463	26.461	.391	.687	3.0413		1.0000
1	11	4	6.878	6.469	6.469	.072	.409	1.7809		1.0000
1	11	0	88.098	84.688	-84.684	-.508	-.6585	-47.6222		1.0000
1	11	1	7.802	7.312	-7.312	-.027	.570	2.3633		1.0000
1	11	2	5.634	1.505	-1.420	.495	4.125	24.7642		1.0000
1	11	3	6.140	6.285	6.285	.027	-.145	-.7993		1.0000
1	11	4	54.093	54.950	-54.948	-.471	-.857	-3.6245		1.0000
1	11	5	1.127 *	1.575	-1.575	-.024	-.448	-.5585		1.0000
1	11	6	11.918	11.659	11.651	.429	.260	1.6263		1.0000
1	11	7	4.225	3.366	3.366	.022	.895	2.8988		1.0000
1	11	8	24.309	23.354	-23.351	-.376	1.198	4.0773		1.0000
1	11	0	64.999	63.801	63.800	.351	7.6722	7.6722		1.0000
1	11	1	5.440	5.447	5.446	.059	-.007	-.0336		1.0000
1	11	2	12.828	12.514	12.512	.198	.314	1.7035		1.0000
1	11	3	4.391	4.282	-4.282	-.056	.109	.5052		1.0000
1	11	4	38.666	39.646	39.645	.326	-.980	-3.9108		1.0000
1	11	5	3.989	3.325	3.325	.053	.664	2.6215		1.0000
1	11	6	9.790	9.473	9.471	.172	.317	2.2348		1.0000
1	11	7	3.269	2.422	-2.422	-.046	.846	2.01887		1.0000
1	11	8	18.095	17.174	17.172	.262	.921	5.0897		1.0000
1	11	9	65.125	61.620	61.620	-.100	3.505	19.8908		1.0000
1	11	0	15.750	14.567	-14.567	.066	1.183	5.0515		1.0000
1	11	1	7.966	7.207	7.206	.099	.760	4.4293		1.0000
1	11	2	5.564	5.529	5.529	-.063	.035	.1630		1.0000
1	11	3	26.910	29.632	29.631	-.093	-2.721	-9.8758		1.0000
1	11	4	8.213	8.200	-8.200	.059	.013	.0899		1.0000
1	11	5	4.080	3.312	3.310	.085	.768	2.8375		1.0000
1	11	6	1.336 *	.798	-.798	-.052	.538	.5640		1.0000
1	11	7	11.896	11.220	11.220	-.074	.676	4.0826		1.0000
1	11	8	62.166	60.870	60.869	.307	1.296	6.4480		1.0000

SILLIMANITE (FRANDYVINE SPRINGS, AT 25 DEGREES C

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	4	1	4.933	5.073	-5.073	-.054	-.141	-.4908	1.0000
2	4	2	3.197	3.123	3.119	.150	.074	.2534	1.0000
2	4	3	4.176	4.475	4.476	.053	-.295	-1.1694	1.0000
2	4	4	40.609	41.392	41.390	.359	-.783	-2.8930	1.0000
2	4	5	3.554	3.273	-3.273	-.046	.280	.9877	1.0000
2	4	6	3.289	3.794	3.792	.130	-.505	-1.4236	1.0000
2	4	7	2.120	2.620	2.620	.045	-.500	-.7978	1.0000
2	4	8	19.566	18.926	18.926	.288	.642	3.5241	1.0000
2	4	9	52.145	51.624	51.621	.558	.521	2.2810	1.0000
2	5	0	11.644	11.953	-11.953	-.058	-.309	-1.7076	1.0000
2	5	1	76.819	78.629	-78.627	-.545	-1.810	-7.8139	1.0000
2	5	2	14.172	14.971	14.971	.053	-.798	-4.6229	1.0000
2	5	3	38.816	39.855	39.852	.518	-1.035	-3.6014	1.0000
2	5	4	2.944	3.273	-3.273	-.049	.429	-1.1549	1.0000
2	5	5	41.909	43.057	-43.054	-.470	-1.248	-3.6646	1.0000
2	5	6	10.500	10.040	10.040	.044	.461	2.8032	1.0000
2	5	7	25.272	25.038	25.038	.098	.234	.8248	1.0000
2	6	0	2.056	1.667	-1.667	-.006	1.189	3.2133	1.0000
2	6	1	24.870	23.855	23.855	.412	1.015	3.5473	1.0000
2	6	2	1.467	1.441	1.441	.007	.426	.8309	1.0000
2	6	3	16.816	17.258	17.258	.091	-.443	-2.4459	1.0000
2	6	4	1.246	1.065	-1.065	-.004	.181	.2033	1.0000
2	6	5	14.733	15.237	15.232	.375	-.504	-2.9367	1.0000
2	6	6	1.395	.885	-.885	.007	.511	.5124	1.0000
2	6	7	23.387	23.422	-23.422	-.329	-.035	-1.1607	1.0000
2	7	0	1.186	.303	.302	-.015	.884	1.0420	1.0000
2	7	1	34.079	34.371	34.369	.325	-.291	-.9051	1.0000
2	7	2	5.339	5.045	-5.045	.014	.294	1.2957	1.0000
2	7	3	18.743	18.606	-18.606	-.305	.137	.7490	1.0000
2	7	4	3.825	3.800	-3.800	-.013	.025	.0715	1.0000
2	7	5	19.886	20.571	20.571	.279	-.687	-3.1934	1.0000
2	7	6	30.779	29.564	29.562	.263	1.215	3.8480	1.0000
2	7	7	3.407	2.579	-2.579	.058	.828	2.4910	1.0000
2	8	0	9.073	9.057	9.055	.021	.616	1.054	1.0000
2	8	1	1.825	2.205	-2.205	-.054	-.360	-1.054	1.0000
2	8	2	22.331	22.530	22.529	.245	-.195	-.8992	1.0000
2	8	3	2.389	2.018	2.018	.053	.370	.6582	1.0000
2	8	4	5.701	5.667	5.664	.191	.035	.1282	1.0000
2	8	5	26.026	25.265	-25.264	-.243	.766	3.0185	1.0000
2	8	6	10.322	10.335	10.335	.083	-.013	-.0850	1.0000
2	8	7	22.640	22.982	22.982	.241	-.342	-1.5626	1.0000
2	9	0	5.358	5.240	-5.240	-.079	.118	.4484	1.0000
2	9	1	19.687	19.963	19.962	.225	-.277	-1.4523	1.0000
2	9	2	11.566	11.273	11.273	.074	.293	1.8232	1.0000
2	9	3	25.874	25.904	25.902	.351	-.026	-.0949	1.0000
2	9	4	1.394	1.645	-1.645	-.044	-.251	-.2522	1.0000
2	9	5	1.410	1.755	1.752	.100	-.346	-.9434	1.0000
2	9	6	1.422	1.576	1.575	.044	-.154	-.1519	1.0000
2	10	0	20.499	20.593	20.593	.326	-.096	-.4769	1.0000
2	10	1	17.292	16.966	16.954	.458	.332	1.7236	1.0000
2	10	2	1.445	.387	-.381	-.067	1.058	1.0248	1.0000
2	11	0	21.869	21.470	-21.466	-.447	.399	2.0188	1.0000
2	11	1	6.717	6.085	6.085	-.037	.632	3.2777	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	F(CTER)
3	0	3	4.791	4.408	4.408	.036	.282	1.7775	1.0000	1.0000
3	0	5	5.918	5.521	5.521	-.032	.397	2.2221	1.0000	1.0000
3	7	5	5.438	5.139	5.139	.033	.295	1.1928	1.0000	1.0000
3	0	12	12.391	15.658	15.647	.600	-3.267	-18.2941	1.0000	1.0000
3	1	4	4.715	4.908	-4.907	-.037	.193	.5698	1.0000	1.0000
3	1	3	3.213	27.659	37.659	-.045	1.554	7.8201	1.0000	1.0000
3	1	2	4.055	3.257	-3.256	.034	.798	3.3069	1.0000	1.0000
3	1	2	23.910	22.388	22.381	.557	1.530	5.4834	1.0000	1.0000
3	1	5	7.555	7.753	-7.753	-.077	.195	-1.3245	1.0000	1.0000
3	1	6	13.492	13.609	-13.609	-.038	.117	-.6951	1.0000	1.0000
3	1	7	3.378	2.673	-2.672	.069	.705	1.6114	1.0000	1.0000
3	0	12	12.388	12.495	12.487	.446	-.107	-.6783	1.0000	1.0000
3	0	1	29.401	28.614	28.613	.196	.787	4.1078	1.0000	1.0000
3	1	1	6.150	5.976	5.976	.009	.174	.5892	1.0000	1.0000
3	2	1	39.765	40.109	-40.109	-.191	-.244	-1.6533	1.0000	1.0000
3	2	2	10.655	10.707	-10.707	-.009	-.051	-.2760	1.0000	1.0000
3	2	3	18.770	19.604	19.603	.182	-.634	-3.8513	1.0000	1.0000
3	2	5	2.005	1.311	-1.311	.009	.693	1.4092	1.0000	1.0000
3	2	6	19.117	19.352	-19.352	-.165	-.235	-1.1114	1.0000	1.0000
3	2	7	6.458	6.657	-6.657	-.007	-.199	-.8814	1.0000	1.0000
3	2	8	9.557	9.451	9.450	.148	.106	.5731	1.0000	1.0000
3	3	0	34.636	34.342	-34.341	-.300	.294	1.4215	1.0000	1.0000
3	3	1	3.658	3.810	3.810	.009	.152	-.6427	1.0000	1.0000
3	3	2	108.051	110.295	110.292	.829	-2.244	-10.6609	1.0000	1.0000
3	3	3	1.174	2.553	2.553	-.008	-1.379	-1.6445	1.0000	1.0000
3	3	4	23.269	24.340	-24.338	-.278	-1.071	-3.6955	1.0000	1.0000
3	3	5	4.852	5.484	5.484	.008	-.632	-2.7692	1.0000	1.0000
3	3	6	58.287	58.979	58.974	.474	-.691	-2.1647	1.0000	1.0000
3	3	7	3.511	3.539	3.539	-.006	-.028	-.0738	1.0000	1.0000
3	3	8	12.809	11.975	-11.972	-.221	.834	5.4684	1.0000	1.0000
3	4	0	10.817	8.725	8.724	-.146	2.092	11.4140	1.0000	1.0000
3	4	1	7.968	7.939	7.938	.032	.030	.1571	1.0000	1.0000
3	4	2	15.013	15.275	15.275	.145	-.262	-1.4208	1.0000	1.0000
3	4	3	3.104	1.874	-1.873	-.031	1.231	3.6514	1.0000	1.0000
3	4	4	1.835	2.863	2.860	-.136	-1.028	-1.9887	1.0000	1.0000
3	4	5	7.228	7.300	7.299	.029	-.071	-.4250	1.0000	1.0000
3	4	6	8.341	8.230	8.229	.125	.111	.6626	1.0000	1.0000
3	4	7	2.653	1.367	1.366	-.025	1.286	2.5112	1.0000	1.0000
3	5	0	31.916	30.469	30.467	.401	1.447	5.5624	1.0000	1.0000
3	5	1	4.952	4.653	-4.653	.082	.298	1.3273	1.0000	1.0000
3	5	2	2.984	2.332	-2.332	.123	.652	1.8320	1.0000	1.0000
3	5	3	1.575	.079	-.008	-.078	1.498	2.4859	1.0000	1.0000
3	5	4	24.220	24.616	24.613	.373	-.396	-1.7351	1.0000	1.0000
3	5	5	3.491	3.794	3.794	.075	-.302	-.9294	1.0000	1.0000
3	5	6	1.329	.641	-.632	.107	.698	.7245	1.0000	1.0000
3	5	7	3.174	2.290	-2.289	.064	.864	1.9932	1.0000	1.0000
3	6	0	16.965	18.044	-18.044	-.071	-.060	-4.4800	1.0000	1.0000
3	6	1	1.190	1.493	-1.493	-.025	-.304	-.3577	1.0000	1.0000
3	6	2	4.578	4.752	-4.752	.072	-.175	-.7648	1.0000	1.0000
3	6	3	1.194	.981	-.981	.025	.213	.2504	1.0000	1.0000
3	6	4	12.519	12.542	-12.542	-.066	-.023	-.1454	1.0000	1.0000
3	6	5	2.260	2.793	-2.792	-.022	-.512	-.9544	1.0000	1.0000
3	6	6	1.375	2.015	-2.014	.062	-.640	-.6516	1.0000	1.0000

U	V	W	L	F(CBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	6	7	7	1.625 *	1.811	-1.831	.021	-1.066	-.2122	1.0000 *
3	7	0	0	70.172	69.864	69.860	.667	.288	1.0231	1.0000
3	7	1	1	12.867	12.447	-12.446	-.098	.422	2.6267	1.0000
3	7	2	2	5.198	4.751	-4.748	-.163	.447	2.0103	1.0000
3	7	3	3	11.836	12.443	12.443	.095	-.608	-3.8920	1.0000
3	7	4	4	52.150	53.299	53.295	.619	-1.138	-2.4751	1.0000
3	7	5	5	7.534	7.571	-7.571	-.086	.037	-1.0834	1.0000
3	7	6	6	4.194	4.248	-4.245	-.139	-.054	-1.1556	1.0000
3	7	7	7	18.536	18.242	18.241	.186	.294	1.3869	1.0000
3	8	0	0	4.600	4.222	4.222	-.019	.375	1.4627	1.0000
3	8	1	1	1.277 *	1.455	1.445	-.018	-.177	-.1944	1.0000
3	8	2	2	2.895	2.504	-2.504	.018	.211	.4296	1.0000
3	8	3	3	13.719	13.877	13.876	.172	-.157	-.4306	1.0000
3	8	4	4	3.298	3.628	3.628	-.016	.330	-.7556	1.0000
3	8	5	5	23.731	22.897	-22.895	-.198	.834	3.1636	1.0000
3	8	6	6	1.359	.398	-2.897	.014	.961	.9899	1.0000
3	8	7	7	35.191 *	34.776	34.770	.654	.415	1.1685	1.0000
3	9	0	0	1.380 *	.332	.332	-.012	1.048	1.0000	1.0000
3	9	1	1	17.826	17.894	-17.894	-.153	-.066	-.3733	1.0000
3	9	2	2	1.422 *	.525	-.525	.014	.897	.8826	1.0000
3	9	3	3	16.280	15.503	-15.503	-.067	.777	4.0824	1.0000
3	10	0	0	9.393	7.706	7.706	.034	.687	3.4763	1.0000
3	10	1	1	1.432 *	.466	.466	.070	.967	.9449	1.0000
3	10	2	2	7.135	6.812	-6.812	-.032	.322	1.4152	1.0000
3	10	3	3	9.416	8.926	8.924	.181	.490	2.4964	1.0000
3	11	0	0	7.780	6.742	6.741	.089	1.035	4.8255	1.0000
4	0	0	0	79.933	78.355	-78.393	-.243	.885	8.1863	1.0000
4	0	1	1	68.942	67.958	-67.953	.779	.885	4.2026	1.0000
4	0	2	2	45.065	47.148	47.148	-.225	.084	-7.8661	1.0000
4	0	3	3	43.169	42.578	-42.578	.672	.591	1.8382	1.0000
4	0	4	4	23.196	21.153	-21.152	-.179	.424	-1.9639	1.0000
4	0	5	5	23.867	24.300	24.300	.288	-.424	-1.9639	1.0000
4	0	6	6	23.867	2.861	-2.861	.061	.097	.3473	1.0000
4	1	0	0	2.978	21.899	-21.899	-.262	-.365	-1.4142	1.0000
4	1	1	1	1.198	1.329	1.328	-.058	.131	-.1535	1.0000
4	1	2	2	18.903	18.828	18.826	.075	.075	.3374	1.0000
4	1	3	3	1.793	.073	.048	.055	1.629	2.6285	1.0000
4	1	4	4	13.693	13.536	-13.533	-.243	.157	.9093	1.0000
4	1	5	5	1.369	.432	-.429	-.048	.938	.9587	1.0000
4	1	6	6	10.060	9.243	9.240	.213	.818	4.5191	1.0000
4	1	7	7	82.348	80.328	80.327	.477	2.019	10.1036	1.0000
4	2	0	0	1.113 *	1.804	-1.804	.010	-.691	-.8696	1.0000
4	2	1	1	37.309	38.045	38.045	.068	-.736	-3.1602	1.0000
4	2	2	2	1.562 *	1.090	-1.090	-.039	.472	.6960	1.0000
4	2	3	3	52.833	53.369	53.368	.443	-.536	-2.0149	1.0000
4	2	4	4	3.509	2.578	-2.578	.009	.931	2.9595	1.0000
4	2	5	5	17.053	17.328	17.328	.060	-.274	-1.03733	1.0000
4	2	6	6	1.391 *	2.124	-2.124	-.007	-.732	-.7377	1.0000
4	2	7	7	24.323	23.372	-23.370	.355	.951	3.07916	1.0000
4	3	0	0	7.029	5.402	-5.402	.052	1.628	6.3919	1.0000
4	3	1	1	13.026	13.060	-13.059	-.118	-.033	-.1706	1.0000
4	3	2	2	4.850	4.356	4.356	-.049	.494	1.9246	1.0000
4	3	3	3	11.053	11.022	11.022	.114	.031	.1657	1.0000

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS

M	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
4	3	4	3.243	2.600	-2.599	.048	.643	2.0597	1.0000	
4	5	4	7.907	8.031	-2.030	-.104	-.124	-.7751	1.0000	
4	6	6	3.091	1.643	1.642	-.042	1.444	2.6790	1.0000	
4	7	7	6.254	5.914	5.913	.095	.340	1.3886	1.0000	
4	3	3	59.097	59.422	59.418	.609	-.335	-1.4222	1.0000	
4	4	0	1.220	.542	-.541	-.032	.679	.7785	1.0000	**
4	1	2	36.365	38.181	-38.181	-.075	-1.816	-6.9174	1.0000	**
4	2	3	4.604	4.963	4.963	.031	-.355	-1.1614	1.0000	
4	3	4	44.453	45.107	45.104	.565	-.654	-2.2300	1.0000	
4	4	5	3.174	2.151	2.151	-.029	1.023	2.1394	1.0000	
4	5	6	19.156	19.047	-19.047	-.063	.109	.5340	1.0000	
4	6	7	4.980	5.188	5.188	.027	-.209	-.6808	1.0000	
4	7	0	32.141	31.340	-31.338	-.311	.601	2.9258	1.0000	**
4	5	0	1.478	.325	-.321	.051	1.153	1.5937	1.0000	**
4	5	1	28.693	28.965	28.963	.309	-.572	-.9515	1.0000	**
4	5	2	1.507	.190	-.184	-.048	1.216	1.8824	1.0000	**
4	5	3	24.320	23.708	-23.706	-.289	.612	2.4024	1.0000	**
4	4	4	1.277	.385	.382	.046	.892	.9785	1.0000	**
4	5	5	17.383	17.526	17.524	.266	-.143	-.7333	1.0000	**
4	6	6	1.417	.526	-.524	-.039	.891	.8614	1.0000	**
4	7	0	17.629	18.110	18.109	-.193	-.481	-2.4939	1.0000	**
4	6	1	4.469	4.730	-4.730	.032	-.261	-1.0778	1.0000	**
4	6	2	44.885	43.412	43.407	.691	1.472	5.0819	1.0000	**
4	6	3	2.253	.485	-.485	-.030	1.767	3.6099	1.0000	**
4	6	4	11.164	11.543	11.542	-.178	-.375	-2.5672	1.0000	**
4	6	5	6.886	6.503	-6.503	.030	.382	1.8523	1.0000	**
4	6	6	25.831	26.233	26.226	.595	-.402	-1.7267	1.0000	**
4	6	7	17.024	16.508	-16.507	.198	2.8118	2.8118	1.0000	**
4	7	1	1.530	1.557	-1.557	.067	-.027	-.0370	1.0000	**
4	7	2	14.589	14.361	-14.359	-.190	.226	1.4179	1.0000	**
4	7	3	1.420	1.239	1.238	-.064	.181	.2226	1.0000	**
4	7	4	12.451	12.820	12.818	.184	-.369	-2.3116	1.0000	**
4	7	5	1.380	.557	-.554	.060	.823	.8358	1.0000	**
4	7	6	9.172	9.034	-9.032	-.164	.135	.7233	1.0000	**
4	8	0	27.707	28.214	28.213	.268	-.506	-2.0787	1.0000	**
4	8	1	5.332	4.861	-4.860	.016	.472	1.9656	1.0000	**
4	8	2	1.340	1.098	1.076	.210	.242	.2526	1.0000	**
4	8	3	8.440	8.379	8.379	-.014	.023	.1258	1.0000	**
4	8	4	22.167	22.177	22.176	.249	-.010	-.0494	1.0000	**
4	8	5	1.418	.239	.239	.015	1.179	1.1643	1.0000	**
4	9	0	11.787	11.284	-11.283	.128	.503	1.6316	1.0000	**
4	9	1	11.481	11.218	-11.218	-.0107	.262	1.6316	1.0000	**
4	9	2	12.123	11.339	-11.338	-.121	.784	4.4812	1.0000	**
4	9	3	10.247	10.063	10.063	.104	.184	1.0814	1.0000	**
4	9	4	9.396	9.064	9.063	.119	.332	1.7780	1.0000	**
4	9	5	54.932	54.974	54.974	.590	.953	2.4341	1.0000	**
4	10	1	3.200	2.488	-2.487	-.060	.712	1.5361	1.0000	**
4	10	2	10.363	10.099	-10.098	-.140	.264	1.4790	1.0000	**
4	10	3	1.450	1.104	-1.102	.060	.346	.3340	1.0000	**
5	0	1	5.130	5.202	5.202	-.086	-.072	-.3004	1.0000	**
5	0	3	8.463	8.574	8.573	.084	-.111	-.5763	1.0000	**
5	0	5	2.886	2.466	-2.464	-.076	.420	1.0698	1.0000	**
5	0	7	5.393	5.187	-5.187	.070	.205	.7151	1.0000	**

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	1	0	13.240	11.738	11.735	.292	1.507	7.7229	1.0000
5	1	1	8.395	8.460	8.459	.089	-.065	-.3032	1.0000
5	1	2	36.817	36.918	36.917	.248	-.101	-.4022	1.0000
5	1	3	12.084	12.546	-12.546	-.065	-.2976	-2.2976	1.0000
5	1	4	12.530	11.625	11.622	.272	.905	5.5062	1.0000
5	1	5	1.246	2.048	2.047	.080	-.802	-.9005	1.0000
5	1	6	20.782	15.976	15.975	.214	.806	3.6268	1.0000
5	1	7	9.166	8.759	-8.799	-.071	.367	1.9903	1.0000
5	2	0	67.259	67.966	-67.964	-.554	-.708	-3.1168	1.0000
5	2	1	15.782	15.767	15.767	.050	.015	.0670	1.0000
5	2	2	72.060	73.793	73.791	.545	-1.733	-7.1485	1.0000
5	2	3	7.174	7.601	-7.601	-.047	-.428	-2.2747	1.0000
5	2	4	49.198	49.667	-49.664	-.514	-.469	-1.6378	1.0000
5	2	5	12.156	12.371	12.371	.046	-.215	-1.2573	1.0000
5	2	6	41.919	41.413	41.411	.469	.506	1.44695	1.0000
5	2	7	2.065	1.521	-1.521	-.039	.543	.7775	1.0000
5	3	0	23.057	22.632	22.631	.238	.425	1.4731	1.0000
5	3	1	4.701	4.642	4.642	.018	.056	.2166	1.0000
5	3	2	42.520	43.062	43.061	.293	-.542	-2.0645	1.0000
5	3	3	1.185	4.457	.457	-.017	.728	.8594	1.0000
5	3	4	17.446	17.146	17.144	.221	.300	1.4424	1.0000
5	3	5	5.724	5.809	5.809	.017	-.085	-.3945	1.0000
5	3	6	23.653	23.681	23.480	.253	.172	.7620	1.0000
5	3	7	2.631	2.358	2.358	-.014	.274	.4861	1.0000
5	4	0	10.286	8.118	8.106	.434	2.169	10.7235	1.0000
5	4	1	10.192	10.955	10.955	.033	-.764	-4.1926	1.0000
5	4	2	27.376	26.161	-26.158	-.423	1.215	4.2117	1.0000
5	4	3	12.359	12.359	-12.359	-.031	-.352	-2.1268	1.0000
5	4	4	9.146	8.935	8.935	.403	.202	1.3156	1.0000
5	4	5	4.481	4.390	4.390	.030	.091	.3164	1.0000
5	4	6	15.525	15.789	-15.785	-.364	-.264	-1.5058	1.0000
5	4	7	8.954	8.563	-8.563	-.025	.291	1.4755	1.0000
5	5	0	12.413	11.005	11.002	.255	1.407	8.1504	1.0000
5	5	1	9.960	9.620	-9.619	-.097	.340	2.0389	1.0000
5	5	2	16.073	15.269	15.267	.258	.803	4.4697	1.0000
5	5	3	5.745	5.660	5.679	.095	.065	.3122	1.0000
5	5	4	10.694	9.430	9.427	.237	1.264	8.6911	1.0000
5	5	5	8.402	8.501	-8.500	-.086	-.098	-.5403	1.0000
5	5	6	9.552	9.351	9.349	.223	.200	1.1008	1.0000
5	5	7	21.033	20.820	20.819	.186	.213	.8837	1.0000
5	6	0	2.474	2.953	2.953	-.093	-.479	-1.0201	1.0000
5	6	1	2.510	.359	-.311	-.178	2.151	4.6873	1.0000
5	6	2	1.644	.176	-.150	.090	1.468	2.0937	1.0000
5	6	3	15.858	15.639	15.638	.173	.219	1.1560	1.0000
5	6	4	2.168	2.641	2.640	.052	-.474	-.7376	1.0000
5	6	5	2.091	.634	-.615	-.154	1.457	2.0952	1.0000
5	6	6	27.776	28.268	28.267	.279	-.492	-1.4492	1.0000
5	7	0	1.610	2.624	2.623	.057	-.1014	-1.4492	1.0000
5	7	1	25.256	25.077	25.076	.210	.179	1.3809	1.0000
5	7	2	1.352	.803	-.801	-.053	.549	.7195	1.0000
5	7	3	21.531	21.807	21.805	.259	-.276	-1.3745	1.0000
5	7	4	2.846	3.009	3.009	.052	-.162	-.3179	1.0000
5	7	5	36.577	35.976	-35.972	-.522	.601	1.7348	1.0000

H	K	L	F(UBS)	F(CALC)	A(CALC)	P(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	5	1	1.377 *	2.719	2.716	.006	-1.342	-1.2849	1.0000 *
5	6	2	17.360	17.477	17.469	.018	-.017	-.6081	1.0000
5	8	3	3.087	2.980	-2.080	-.062	1.007	2.7259	1.0000
5	8	4	28.306	28.175	-28.171	-.035	.131	.6606	1.0000
5	8	5	1.444 *	1.210	1.209	.009	.234	.2265	1.0000 *
5	9	0	2.028 *	1.454	1.437	.017	.575	.7952	1.0000 *
5	9	1	2.447 *	2.000	2.007	.044	.435	.7294	1.0000 *
5	9	2	10.658	10.731	10.728	.041	-.072	.4284	1.0000
5	9	3	1.798 *	2.084	-2.083	-.041	-.266	-.3369	1.0000 *
5	10	0	25.360	24.638	24.637	.232	.722	2.9787	1.0000
5	10	1	3.245	2.936	-2.936	.025	.309	.6288	1.0000
5	10	2	9.583	9.752	-9.749	-.222	-.165	-.8056	1.0000
5	10	3	9.177	8.706	8.703	.732	-.529	-2.1618	1.0000
5	0	2	30.945	31.160	-31.159	-.189	-.214	-.7771	1.0000
5	0	4	65.503	65.198	65.195	.680	.304	1.0240	1.0000
5	0	6	18.798	17.869	-17.868	-.162	.925	4.4356	1.0000
5	0	6	45.064	42.351	42.350	.319	.672	2.6322	1.0000
5	1	0	12.919	13.187	-13.187	-.031	-.268	-1.2992	1.0000
5	1	1	1.869 *	1.784	.719	-.312	1.085	1.9029	1.0000 *
5	1	2	9.318	9.638	9.637	.031	.320	-2.0328	1.0000
5	1	3	30.534	30.244	30.243	.296	-.290	.9175	1.0000
5	1	4	8.518	8.124	-8.124	-.027	.394	2.3655	1.0000
5	1	5	1.407 *	2.136	-2.121	-.269	-.731	-.7272	1.0000 *
5	1	7	4.074	3.944	3.944	.027	.130	.3966	1.0000
5	2	0	23.079	23.621	23.621	.081	-.542	-1.8233	1.0000
5	2	1	7.566	8.035	-8.034	-.127	-.376	-1.7465	1.0000
5	2	2	26.680	25.976	25.972	.446	.504	1.7267	1.0000
5	2	3	7.330	7.378	7.377	.123	-.040	-.2407	1.0000
5	2	4	17.053	16.365	16.365	.075	.488	3.6842	1.0000
5	2	5	5.846	5.830	-5.826	-.113	.018	.0783	1.0000
5	2	6	16.467	16.290	16.285	.385	.177	.9381	1.0000
5	2	7	5.270	4.545	4.544	.102	.724	2.4116	1.0000
5	2	7	26.767	27.183	-27.183	.071	-.416	-1.4404	1.0000
5	3	0	3.747	3.780	3.780	.045	-.034	-.1171	1.0000
5	3	1	7.003	6.734	-6.734	-.067	.269	1.6145	1.0000
5	3	3	1.244 *	.540	-.538	-.042	.704	.7920	1.0000
5	3	4	17.790	18.116	-18.116	.065	-.326	-1.7221	1.0000
5	3	5	4.800	4.712	4.712	.041	.088	.3065	1.0000
5	3	6	3.966	2.988	-2.988	-.057	.978	2.6680	1.0000
5	3	7	1.463 *	1.268	1.267	-.034	.195	.1867	1.0000
5	4	0	2.679	1.544	1.542	-.036	1.135	2.8908	1.0000
5	4	1	9.344	9.062	9.062	.121	.281	1.6762	1.0000
5	4	2	41.549	41.247	41.247	.548	.302	1.0288	1.0000
5	4	3	8.441	8.182	-8.182	-.116	.259	1.6358	1.0000
5	4	4	1.290 *	.610	.617	-.033	.672	.7292	1.0000
5	4	5	6.637	6.504	6.503	.109	.133	.5973	1.0000
5	4	6	26.235	25.487	25.483	.472	.748	3.1941	1.0000
5	5	0	22.787	22.932	-22.929	-.351	-.146	-.6185	1.0000
5	5	1	2.046 *	2.711	-2.711	.013	-.665	-1.1794	1.0000
5	5	2	40.607	41.597	41.595	.345	-.990	-3.1817	1.0000
5	5	3	1.269 *	1.381	-1.381	-.012	-.092	-.0959	1.0000
5	5	4	18.867	18.377	-18.377	-.325	.491	2.5004	1.0000
5	5	5	3.782	4.274	-4.274	.013	-.492	-1.2717	1.0000

H	K	L	F(CRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	5	6	25.010	25.360	25.358	.300	.650	2.7083	1.0000
6	6	0	44.330	44.480	44.475	.656	-.150	-.4708	1.0000
6	6	1	3.830	3.498	3.498	.011	.333	1.0541	1.0000
6	6	2	5.500	5.340	5.338	-.152	.166	.7135	1.0000
6	6	3	2.544	2.924	2.924	-.009	-.380	-.7384	1.0000
6	6	4	34.257	34.561	34.555	.609	-.304	-.8431	1.0000
6	6	5	3.255	2.795	2.795	.010	.948	.9948	1.0000
6	6	6	13.718	12.487	12.485	.200	1.232	6.6328	1.0000
6	6	7	9.229	9.229	9.229	-.052	-.000	-.0016	1.0000
6	6	8	20.554	20.364	20.363	-.191	.189	.9481	1.0000
6	6	9	12.095	11.853	11.853	.051	.242	1.3895	1.0000
6	6	0	9.813	10.068	10.066	.186	-.254	-.1.4157	1.0000
6	6	1	3.446	3.171	3.170	-.046	.275	.6097	1.0000
6	6	2	11.171	11.120	11.118	.192	.051	.2873	1.0000
6	6	3	3.583	3.833	3.831	-.125	-.249	-.5975	1.0000
6	6	4	16.632	16.628	16.625	.275	.005	.0244	1.0000
6	6	5	1.470	3.472	3.470	.121	-.2.002	-.1.9068	1.0000
6	6	6	9.067	8.608	8.606	.179	.460	2.2857	1.0000
6	6	7	17.876	17.287	17.287	.171	.589	2.8625	1.0000
6	6	8	8.510	7.933	7.933	.013	.577	2.8366	1.0000
6	6	9	16.094	15.236	15.235	-.160	.858	4.9351	1.0000
6	6	0	4.772	3.904	3.904	-.012	.868	2.5745	1.0000
6	6	1	16.975	17.220	17.220	.166	-.245	-.1.2482	1.0000
6	6	2	18.275	18.630	18.630	-.158	-.355	-.1.6981	1.0000
6	6	3	8.632	8.490	8.489	.149	.142	.7651	1.0000
6	6	4	12.624	13.023	13.023	-.046	-.399	-.2.3084	1.0000
6	6	5	1.212	.042	.014	.040	1.170	1.3514	1.0000
6	6	6	36.964	36.314	36.310	.567	.650	2.1881	1.0000
6	6	7	2.920	3.567	3.567	-.038	-.667	-.1.6398	1.0000
6	6	8	9.066	9.202	9.202	-.043	-.136	-.8541	1.0000
6	6	9	4.367	3.514	3.514	.036	.853	2.6141	1.0000
6	6	0	22.014	21.698	21.693	.489	.316	1.4769	1.0000
6	6	1	11.279	11.132	11.131	.125	.147	.8609	1.0000
6	6	2	1.238	2.426	2.425	-.069	-.1.188	-.1.3429	1.0000
6	6	3	3.388	3.149	3.147	-.121	.239	.6865	1.0000
6	6	4	2.394	1.946	1.945	.068	.447	.9205	1.0000
6	6	5	8.812	8.527	8.526	.116	.285	1.7188	1.0000
6	6	6	4.322	3.625	3.625	-.051	.497	1.4801	1.0000
6	6	7	55.235	2.351	55.170	.811	.059	.2036	1.0000
6	6	8	2.525	2.666	2.666	-.015	-.141	-.3098	1.0000
6	6	9	22.348	22.448	22.446	-.283	-.100	-.4210	1.0000
6	6	0	1.283	.647	-.847	.015	.436	.4761	1.0000
6	6	1	42.795	43.258	43.252	.753	-.463	-.1.3832	1.0000
6	6	2	4.060	4.108	4.108	-.013	-.048	-.1.1322	1.0000
6	6	3	14.744	14.111	14.109	-.243	.632	3.9905	1.0000
6	6	4	14.916	14.915	14.915	-.106	.001	.0057	1.0000
6	6	5	1.280	.955	-.950	-.102	.324	.3546	1.0000
6	6	6	1.851	2.331	2.331	.108	-.480	-.7614	1.0000
6	6	7	1.316	1.569	1.566	.099	-.253	-.2690	1.0000
6	6	8	11.366	11.343	11.343	-.098	.023	.1491	1.0000
6	6	9	3.707	3.148	3.147	-.090	.559	1.4112	1.0000
6	6	0	2.010	1.802	1.800	.093	.208	.2706	1.0000

H	K	L	F(ORS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT	FACTOR
7	5	0	4.4006	4.150	4.148	.126	.254	.8923		1.0000
7	5	1	5.576	5.661	5.661	-.032	-.085	-.3647		1.0000
7	5	2	45.623	46.266	46.266	.372	-.645	-1.9693		1.0000
7	5	3	3.372	2.656	-2.656	.032	.716	1.7797		1.0000
7	5	4	3.348	2.914	2.912	.117	.434	.9832		1.0000
7	5	5	5.666	5.388	5.388	-.028	.277	.9816		1.0000
7	6	0	6.165	6.138	6.138	-.022	.027	.1171		1.0000
7	6	1	15.085	15.249	15.249	.148	-.164	-.9176		1.0000
7	6	2	8.236	8.425	8.425	.028	-.189	-.9827		1.0000
7	6	3	11.590	11.688	-11.688	-.141	-.098	-.5679		1.0000
7	6	4	5.218	4.683	4.683	-.021	.535	1.7395		1.0000
7	6	5	12.459	12.265	12.264	.133	.194	1.1868		1.0000
7	7	0	29.597	29.817	-29.816	-.165	-.219	-.5833		1.0000
7	7	1	8.810	8.887	8.887	.065	-.077	-.4016		1.0000
7	7	2	41.135	41.974	41.969	.634	-.839	-2.2739		1.0000
7	7	3	6.932	8.962	-8.962	-.061	-.030	-.1509		1.0000
7	7	4	24.966	23.999	-23.998	-.153	.968	3.9337		1.0000
7	7	5	3.803	.362	-.340	.123	3.441	8.5842		1.0000
7	8	0	1.470	2.513	2.513	-.026	-1.043	-.9932		1.0000
7	8	1	15.059	12.725	-12.725	-.113	.330	1.9903		1.0000
7	8	2	1.487	2.970	-2.970	.026	-1.483	-1.3968		1.0000
7	8	3	36.960	35.360	35.354	.634	1.500	3.7632		1.0000
7	8	4	1.495	.319	.317	-.031	1.176	1.1014		1.0000
7	8	5	46.675	67.849	67.848	.483	-1.175	-3.9735		1.0000
8	0	0	3.432	4.516	4.516	.040	-1.084	-2.9473		1.0000
8	0	1	51.062	51.467	51.467	.449	-.406	-1.1796		1.0000
8	0	2	4.617	1.936	1.935	.035	2.681	7.5831		1.0000
8	0	3	26.401	26.245	-26.242	-.440	.152	4.722		1.0000
8	0	4	11.339	11.359	-11.359	-.070	-.020	-.4722		1.0000
8	1	1	23.875	24.149	24.145	.433	-.274	-1.1202		1.0000
8	1	2	9.764	10.057	10.057	.069	-.294	-1.7867		1.0000
8	1	3	20.769	20.626	-20.622	-.408	.144	.7096		1.0000
8	1	4	8.141	7.730	-7.730	-.061	.411	1.9860		1.0000
8	1	5	15.550	15.060	15.056	.373	.490	2.8959		1.0000
8	2	0	9.872	8.368	8.366	.178	1.604	10.1205		1.0000
8	2	1	7.540	7.537	7.536	.115	.004	.0209		1.0000
8	2	2	4.060	3.654	3.638	.335	.406	1.3259		1.0000
8	2	3	4.974	5.078	-5.077	-.110	-.104	-1.3774		1.0000
8	2	4	6.662	6.925	6.923	.166	-.264	-.3772		1.0000
8	2	5	6.435	6.327	6.327	.103	.107	.4155		1.0000
8	3	0	2.551	2.555	2.538	.289	-.004	-.0061		1.0000
8	3	1	5.630	5.603	-5.603	-.080	.027	.1211		1.0000
8	3	2	2.496	1.563	-1.555	.140	.935	1.9425		1.0000
8	3	3	4.833	4.781	-4.781	.082	.052	.1870		1.0000
8	3	4	2.019	.985	.976	-.133	.052	1.5360		1.0000
8	3	5	4.901	4.429	4.428	-.074	.472	1.5051		1.0000
8	4	0	1.455	.588	-.574	.126	.867	.9350		1.0000
8	4	1	16.009	16.097	16.096	.099	-.088	-.4693		1.0000
8	4	2	6.869	6.908	-6.907	-.079	-.039	-.1926		1.0000
8	4	3	37.967	38.337	38.334	.401	-.370	-1.0714		1.0000
8	4	4	3.434	3.516	3.515	.077	-.082	-.1911		1.0000
8	4	5	12.458	12.154	12.153	.092	.304	1.7859		1.0000
8	4	6	6.909	6.811	-6.811	-.070	-.097	.3979		1.0000

H	K	L	F(0KLS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
6	5	0	26.232	36.929	36.926	.484	-.698	-1.9730	1.0000
6	5	1	11.095	10.617	-10.617	-.066	.478	3.0842	1.0000
6	5	2	34.245	33.964	-33.961	-.469	.280	.7601	1.0000
6	5	3	9.919	9.644	9.644	.064	.275	1.5589	1.0000
6	5	4	29.452	29.442	29.443	.449	.009	.0334	1.0000
6	6	0	15.152	15.194	15.188	.428	-.042	-.1960	1.0000
6	6	1	2.914	*.251	*.245	-.051	.472	5.2865	1.0000
6	6	2	3.657	3.184	3.184	.057	.472	1.1510	1.0000
6	6	3	2.980	2.866	2.866	.050	.114	.2204	1.0000
6	6	4	1.787	1.869	1.869	.398	-.102	-.5955	1.0000
6	6	5	16.897	17.025	-17.022	-.291	-.128	-.6037	1.0000
6	7	0	5.936	5.795	-5.794	-.073	.141	.5104	1.0000
6	7	1	14.929	15.433	15.430	.293	-.503	-2.9361	1.0000
6	7	2	3.906	5.131	5.131	.072	-.1225	-2.6776	1.0000
6	7	3	13.816	13.299	13.299	.239	.518	2.8647	1.0000
6	7	4	7.020	7.201	7.200	.109	-.181	-.7156	1.0000
6	8	0	3.355	3.377	3.377	-.024	-.022	-.0563	1.0000
6	8	1	1.440	*.076	*.072	.024	1.364	1.3638	1.0000
6	8	2	4.765	5.038	5.036	-.020	-.273	-.7862	1.0000
6	8	3	25.236	25.555	25.551	.408	-.319	-1.2427	1.0000
6	8	4	9.298	9.523	-9.521	-.170	-.225	-1.3482	1.0000
6	8	5	12.304	12.380	12.380	.104	-.076	-.4567	1.0000
6	8	6	11.339	11.429	11.428	.164	-.090	-.5590	1.0000
6	8	7	19.681	20.089	20.085	.379	-.408	-2.0660	1.0000
6	8	8	5.202	4.513	-4.510	-.152	.690	2.1920	1.0000
6	8	9	35.406	36.080	36.077	.436	-.674	-1.9572	1.0000
6	9	0	4.531	4.044	4.044	-.002	-.486	1.5695	1.0000
6	9	1	30.816	40.001	-39.999	-.428	-.146	-2.3292	1.0000
6	9	2	5.712	6.076	-6.076	.003	-.364	-1.3216	1.0000
6	9	3	29.012	28.811	28.808	.404	.201	.7098	1.0000
6	9	4	1.471	*.345	*.345	-.000	1.127	1.0728	1.0000
6	9	5	3.196	5.745	-5.745	-.022	.451	1.8598	1.0000
6	9	6	2.716	2.546	-2.546	-.021	.172	.3289	1.0000
6	9	7	29.057	29.761	29.756	.518	-.704	-2.5995	1.0000
6	9	8	1.444	*.160	*.158	.021	1.284	1.2453	1.0000
6	9	9	4.745	4.664	-4.664	-.020	.081	.2343	1.0000
6	9	0	3.620	3.437	-3.437	-.329	.183	.4521	1.0000
6	9	1	4.833	5.350	5.350	.033	-.517	-1.6241	1.0000
6	9	2	13.893	14.117	14.113	.328	-.224	-1.2776	1.0000
6	9	3	3.082	2.443	-2.443	-.030	.639	1.2827	1.0000
6	9	4	4.254	2.461	-2.442	-.305	1.793	4.16216	1.0000
6	9	5	23.702	23.766	23.764	.326	-.064	-.2683	1.0000
6	9	6	9.417	9.466	9.464	.180	-.045	-.2619	1.0000
6	9	7	15.603	15.672	15.672	.160	-.069	-.3972	1.0000
6	9	8	6.626	6.605	-6.602	-.172	.022	.0849	1.0000
6	9	9	14.319	13.784	-13.783	-.151	.535	2.9009	1.0000
6	9	0	1.474	1.499	1.499	-.007	-.025	-.0240	1.0000
6	9	1	1.489	*.781	*.765	.156	.708	.6657	1.0000
6	9	2	15.797	15.556	15.550	.419	.242	1.2469	1.0000
6	9	3	25.373	25.788	-25.786	-.281	-.415	-1.4931	1.0000
6	9	4	52.030	53.398	53.393	.771	-.415	-3.7562	1.0000
6	9	5	21.965	21.102	-21.100	-.260	.863	4.3420	1.0000
6	9	6	10.829	10.898	-10.898	-.043	-.069	-.4069	1.0000

H	K	L	F(NBS)	F(CALC)	A(CALC)	D(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
10	1	1	2.562 *	2.110	2.107	.105	.452	.7906		1.0000 *
10	1	2	11.063	10.872	-10.872	.043	.191	1.1367		1.0000
10	1	3	1.474 *	1.234	-1.230	-.100	.240	.2276		1.0000 **
10	1	4	8.763	8.424	-8.424	-.039	.340	1.5951		1.0000
10	1	4	21.338	22.065	22.061	.463	-.728	-3.0010		1.0000
10	2	1	3.357	3.350	3.349	.088	.007	.0165		1.0000
10	2	2	8.023	8.359	8.359	.037	-.337	-1.5984		1.0000
10	2	3	2.595 *	3.158	-3.157	-.084	-.564	-.9182		1.0000 **
10	3	0	14.772	14.695	14.695	-.020	.077	.4230		1.0000
10	3	1	16.874	10.879	-16.878	-.184	-.005	-.0284		1.0000
10	3	2	4.723	4.191	4.191	.024	.532	1.5516		1.0000
10	3	3	13.626	13.525	13.524	.179	.103	.6522		1.0000
10	4	0	34.859	36.284	36.279	.592	-1.425	-3.5555		1.0000
10	4	1	6.172	5.951	-5.951	-.092	.221	.8046		1.0000
10	4	2	8.379	7.994	-7.993	-.101	.365	1.7986		1.0000
10	4	3	2.519 *	.092	-.073	-.059	2.426	3.8411		1.0000 **
10	5	0	4.248	3.609	-3.608	.042	.634	1.6790		1.0000
10	5	1	3.755	3.047	-3.040	-.205	.806	1.6571		1.0000
11	0	1	12.232	13.037	13.030	.439	-.430	-4.3952		1.0000
11	1	0	5.604	5.599	5.599	.063	.005	.0169		1.0000
11	1	1	10.324	10.754	10.754	.052	-.430	-2.2458		1.0000
11	2	0	21.211	21.874	-21.871	-.342	-.662	-2.8720		1.0000
11	2	1	9.415	9.215	9.214	.091	.200	.5953		1.0000

SILLIMANITE (BRADYVINE SPRINGS, AT 25 DEGREES C

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS

WEIGHTED R	NUMERATOR	DENOMINATOR	NUMBER	R
13353.63	7158729.14		659	.053
UNWEIGHTED R	403.97	9822.30	659	.041

RANGES OF F(OBS)

3759.33	920855.41	480	.064
1544.22	1142885.87	105	.037
541.15	1048900.95	45	.023
967.42	1422697.21	17	.026
279.34	963608.21	6	.017
2383.39	993524.77	4	.049
113.66	263468.62	1	.021
3785.32	402787.91	1	.097

RANGES OF (SIN(THETA)/LAMBDA)**2

5196.26	2232349.90	38	.048
4769.11	1813287.99	56	.051
977.10	792739.78	67	.035
367.79	672276.37	54	.024
509.94	407748.14	90	.035
352.70	443261.08	98	.028
468.56	447939.16	113	.032
692.37	349125.92	113	.045

UNREJECTED REFLECTIONS

WEIGHTED R	UNWEIGHTED R	7103.74	6349655.55	537	.032
	299.52		9398.36	537	.032

RANGES OF F(OBS)

3542.44	919946.82	360	.062
1544.22	1142885.87	105	.037
541.15	1048900.95	45	.022
967.42	1422697.21	17	.026
279.34	963608.21	6	.017
115.51	588147.67	3	.014
113.66	263468.62	1	.021
		0	.000

RANGES OF (SIN(THETA)/LAMBDA)**2

2928.39	1826972.81	37	.040
979.65	1410459.18	50	.026
961.87	7922698.64	56	.035
361.03	672106.16	67	.023
460.92	407595.89	71	.034
339.83	443159.19	84	.028
417.60	447745.15	89	.031
653.65	348918.55	83	.043

SUM FCAL 9748.97
 STANDARD DEV OF UNIT WEIGHT OBS 3.80

17.30.50. 03/28/78 XLLGGYP TRR68Zv2 40 PH

XLLGGYP /// END OF LIST ///
XLLGGYP /// END OF LIST ///

The thermal expansion and the high temperature crystal chemistry
of Al_2SiO_5 polymorphs

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and
Subrata Ghose

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Table 1.¹⁰
Sillimanite, andalusite and kyanite: observed and
calculated structure factors at various temperatures.

Sillimanite 400°C

LOAD MAP - REFINE

CYBER LOADCP 1.2-46C

03/18/78 14.46.17.

PAGE 1

FAA OF THE LOAD 111
LFA+1 OF THE LOAD 74743

TRANSFER ADDRESS -- REFINE 112

***** REPORT SUMMARY

REAGI6/// CM FLAGR CORPDR TRUNCATED BY 20700R WORDS

PROGRAM AND BLOCK ASSIGNMENTS *

BLOCK	ADDRESS	LENGTH	FILE	DATE	PROGSSR	VER	LEVEL	HARDWARE	COMMENTS
REFINE	111	10971	REFINE				74 F	646X I	
FA/	10706	1355	REFINE	05/14/76	RUN	F	74 F	646X I	
FC/	12263	457	REFINE	05/14/76	RUN	F	74 F	646X I	
FD/	12742	3244	REFINE	05/14/76	RUN	F	74 F	646X I	
FE/	16206	10	REFINE	05/14/76	RUN	F	74 F	646X I	
FF/	16216	174	REFINE	05/14/76	RUN	F	74 F	646X I	
FG/	16412	2307	REFINE	05/14/76	RUN	F	74 F	646X I	
FLS/	20721	334	REFINE	05/14/76	RUN	F	74 F	646X I	
FTAPE/	21255	4	REFINE	05/14/76	RUN	F	74 F	646X I	
/DEGEN/	21263	311	REFINE	05/14/76	RUN	F	74 F	646X I	
RI LINE	21574	5724	REFINE	05/14/76	RUN	F	74 F	646X I	
SDDAMI	27522	1147	REFINE	05/14/76	RUN	F	74 F	646X I	
FLVIAL	30671	1312	REFINE	05/14/76	RUN	F	74 F	646X I	
INPUT	32203	241	REFINE	05/14/76	RUN	F	74 F	646X I	
MATRIX	32444	231	REFINE	05/14/76	RUN	F	74 F	646X I	
MODIFY	32675	115	REFINE	05/14/76	RUN	F	74 F	646X I	
RCALC	35012	152	REFINE	05/14/76	RUN	F	74 F	646X I	
RESET	33164	73	REFINE	05/14/76	RUN	F	74 F	646X I	
SFAC	33257	476	REFINE	05/14/76	RUN	F	74 F	646X I	
SYMINV	33255	361	REFINE	05/14/76	RUN	F	74 F	646X I	
WEIGHT	34336	12	REFINE	05/14/76	RUN	F	74 F	646X I	
ASINCO5	34350	136	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
EXP	34504	55	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
SINCO5	34563	72	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
SORT	34655	44	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
ACGOER	34721	12	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
ENDFIL	34733	57	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
GETRA	35012	17	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
INPUTB	35031	256	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
KRAKER	35307	1052	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
OUTPTB	36361	244	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
SIOS	36625	1504	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
INPUIC	40331	121	SL-RUN2P3	03/17/75	COMPASS	3*	74150		
KODEP	40452	1310	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
OUTPTC	41762	71	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
REMINH	42053	63	SL-RUN2P3	02/19/75	COMPASS	3*	74150		
SYSTEM	42136	1122	SL-RUN2P3	03/04/75	COMPASS	3*	74150		
//	43260	31463							

A	B	L	F(EFS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	0	2	62.764	64.659	-64.658	-.351	-1.895	-12.8106	1.0000
0	0	4	133.513	145.697	147.695	.632	-12.164	-57.6150	1.0000
0	0	6	27.106	26.542	-26.541	-.293	.663	1.8680	1.0000
0	0	8	5.144	53.272	53.268	.615	1.675	9.5361	1.0000
0	0	10	15.161	13.185	13.185	.027	1.566	8.6816	1.0000
0	0	12	4.607	4.347	-4.347	-.665	.266	.6149	1.0000
0	0	14	22.034	15.035	-15.035	.512	3.798	19.0207	1.0000
0	0	16	6.544	6.293	6.293	.063	.201	1.8422	1.0000
0	0	18	F.272	F.279	F.279	.026	.573	5.3772	1.0000
0	0	20	F.272	F.279	F.279	.026	.573	1.2860	1.0000
0	0	22	F.272	F.279	F.279	.026	.573	2.6702	1.0000
0	0	24	F.272	F.279	F.279	.026	.573	.7682	1.0000
0	0	26	F.272	F.279	F.279	.026	.573	-1.3161	1.0000
0	0	28	F.272	F.279	F.279	.026	.573	8.6724	1.0000
0	0	30	F.272	F.279	F.279	.026	.573	-.1985	1.0000
0	0	32	F.272	F.279	F.279	.026	.573	-9.6356	1.0000
0	0	34	F.272	F.279	F.279	.026	.573	-4.0908	1.0000
0	0	36	F.272	F.279	F.279	.026	.573	-9.1251	1.0000
0	0	38	F.272	F.279	F.279	.026	.573	2.0761	1.0000
0	0	40	F.272	F.279	F.279	.026	.573	-3.6411	1.0000
0	0	42	F.272	F.279	F.279	.026	.573	-1.8102	1.0000
0	0	44	F.272	F.279	F.279	.026	.573	1.1459	1.0000
0	0	46	F.272	F.279	F.279	.026	.573	1.7318	1.0000
0	0	48	F.272	F.279	F.279	.026	.573	.3533	1.0000
0	0	50	F.272	F.279	F.279	.026	.573	-4.3125	1.0000
0	0	52	F.272	F.279	F.279	.026	.573	.4935	1.0000
0	0	54	F.272	F.279	F.279	.026	.573	-5.3695	1.0000
0	0	56	F.272	F.279	F.279	.026	.573	.3875	1.0000
0	0	58	F.272	F.279	F.279	.026	.573	-6.2170	1.0000
0	0	60	F.272	F.279	F.279	.026	.573	-6.6846	1.0000
0	0	62	F.272	F.279	F.279	.026	.573	-6.6285	1.0000
0	0	64	F.272	F.279	F.279	.026	.573	-3.0406	1.0000
0	0	66	F.272	F.279	F.279	.026	.573	-2.7780	1.0000
0	0	68	F.272	F.279	F.279	.026	.573	-2.2914	1.0000
0	0	70	F.272	F.279	F.279	.026	.573	.1083	1.0000
0	0	72	F.272	F.279	F.279	.026	.573	-4.6329	1.0000
0	0	74	F.272	F.279	F.279	.026	.573	-1.0520	1.0000
0	0	76	F.272	F.279	F.279	.026	.573	-.7661	1.0000
0	0	78	F.272	F.279	F.279	.026	.573	-4.0030	1.0000
0	0	80	F.272	F.279	F.279	.026	.573	.2417	1.0000
0	0	82	F.272	F.279	F.279	.026	.573	23.2175	1.0000
0	0	84	F.272	F.279	F.279	.026	.573	3.7451	1.0000
0	0	86	F.272	F.279	F.279	.026	.573	-.0411	1.0000
0	0	88	F.272	F.279	F.279	.026	.573	-1.3408	1.0000
0	0	90	F.272	F.279	F.279	.026	.573	.0864	1.0000
0	0	92	F.272	F.279	F.279	.026	.573	12.6766	1.0000
0	0	94	F.272	F.279	F.279	.026	.573	5.9871	1.0000
0	0	96	F.272	F.279	F.279	.026	.573	-5.0933	1.0000
0	0	98	F.272	F.279	F.279	.026	.573	.2907	1.0000
0	0	100	F.272	F.279	F.279	.026	.573	-2.9880	1.0000
0	0	102	F.272	F.279	F.279	.026	.573	-.6692	1.0000
0	0	104	F.272	F.279	F.279	.026	.573	3.0162	1.0000

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	FXI	FACTOR
1	1	7	4.566	4.813	4.813	-.023	-.246	-.9359	1.0000	
1	1	8	6.340	6.274	6.273	.050	.066	.2842	1.0000	
1	2	6	10.857	12.439	12.438	.463	-1.582	-11.7003	1.0000	
1	2	1	8.253	7.932	-7.932	-.044	1.2894	1.2894	1.0000	
1	2	2	16.057	16.196	-16.195	-.471	-4.4543	-4.4543	1.0000	
1	2	3	1.242	2.007	-2.007	.043	-1.2632	-1.2632	1.0000	
1	2	4	46.917	48.160	48.159	.418	-5.3521	-5.3521	1.0000	
1	2	5	7.426	8.102	-8.101	-.036	-3.4886	-3.4886	1.0000	
1	2	6	37.741	37.628	-37.636	-.367	-4.297	-4.297	1.0000	
1	2	7	2.167	2.199	-2.199	.035	-4.022	-4.022	1.0000	
1	2	8	20.571	20.331	20.326	.307	1.1450	1.1450	1.0000	
1	3	0	46.149	47.111	47.106	.634	-.642	-5.4618	1.0000	
1	3	1	5.543	5.673	-5.673	-.010	-4.660	-4.660	1.0000	
1	3	2	2.943	3.699	-3.698	-.090	-3.256	-3.256	1.0000	
1	3	3	2.783	2.257	-2.257	.010	1.7764	1.7764	1.0000	
1	3	4	27.838	29.284	29.280	.474	-1.447	-5.7558	1.0000	
1	3	5	5.617	6.131	-6.131	-.008	-5.14	-2.5730	1.0000	
1	3	6	3.678	3.557	-3.556	-.071	1.123	4.503	1.0000	
1	3	7	2.933	3.085	-3.089	.006	-1.56	-0.3799	1.0000	
1	3	8	19.448	19.168	19.163	.425	4.280	1.4669	1.0000	
1	4	0	2.119	.949	.982	-.350	1.171	3.1655	1.0000	
1	4	1	3.510	3.125	-3.125	-.031	1.8172	1.8172	1.0000	
1	4	2	26.579	27.178	27.176	.342	-.259	-2.4599	1.0000	
1	4	3	6.978	7.240	7.240	.030	-.267	-1.4355	1.0000	
1	4	4	6.657	6.366	-6.366	-.216	4.901	3.2180	1.0000	
1	4	5	2.777	.950	.950	-.027	1.677	5.2590	1.0000	
1	4	6	14.974	15.343	15.340	.279	-3.65	-2.1125	1.0000	
1	4	7	4.850	5.550	5.549	.026	-.295	-2.5433	1.0000	
1	4	8	4.934	4.097	-4.097	-.233	3.1600	3.1600	1.0000	
1	5	0	10.970	10.049	10.047	.179	.821	4.6070	1.0000	
1	5	1	6.601	6.449	6.449	-.024	1.112	1.692	1.0000	
1	5	2	63.085	65.305	65.304	.323	-.215	-9.7492	1.0000	
1	5	3	2.155	1.130	-1.130	.024	1.625	2.3780	1.0000	
1	5	4	9.155	9.067	9.066	.163	.687	1.091	1.0000	
1	5	5	4.093	5.178	5.178	-.021	-1.685	-4.1904	1.0000	
1	5	6	30.310	31.105	31.104	.266	-.795	-2.3488	1.0000	
1	5	7	2.836	1.607	1.607	.021	1.229	2.7201	1.0000	
1	6	0	24.291	24.284	-24.284	-.082	.007	6.241	1.0000	
1	6	1	3.575	2.845	2.844	.082	7.30	2.5171	1.0000	
1	6	2	1.153	.819	-.805	.150	.334	4.059	1.0000	
1	6	3	5.007	5.041	-5.041	-.079	-.634	-0.1770	1.0000	
1	6	4	16.440	16.485	-16.484	-.138	-.645	-1.2586	1.0000	
1	6	5	1.537	1.006	1.003	.073	.531	1.7806	1.0000	
1	6	6	1.307	.911	.902	.122	.396	4.245	1.0000	
1	6	7	3.947	4.171	-4.171	-.063	-.324	-.9134	1.0000	
1	7	0	26.523	27.728	-27.728	-.026	-1.205	-4.1713	1.0000	
1	7	1	6.459	6.712	6.712	.044	-.253	-1.5315	1.0000	
1	7	2	42.660	43.839	43.836	.462	-.975	-3.5151	1.0000	
1	7	3	6.817	7.158	-7.158	-.041	-2.0091	-2.0091	1.0000	
1	7	4	17.637	18.320	-18.320	-.022	-.684	-3.2507	1.0000	
1	7	5	4.413	3.423	3.422	.040	.591	3.6019	1.0000	
1	7	6	24.452	24.850	24.847	.394	-.398	-1.7921	1.0000	
1	8	0	33.916	33.895	33.893	.405	.020	1.0672	1.0000	

H	K	L	F(PBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	0	1	1.746 *	1.291	-1.290	-.052	.474	.7956	1.0000 *
1	0	2	13.260	13.503	-13.497	-.394	.357	2.0071	1.0000
1	0	3	1.225 *	.316	-.312	.050	.505	1.0395	1.0000 *
1	0	4	23.726	25.327	25.324	.366	-1.1591	-6.4202	1.0000 *
1	0	5	1.344 *	1.224	1.224	-.045	.115	.1744	1.0000 *
1	0	6	7.674	8.440	-8.440	-.321	-.406	-3.5410	1.0000
1	0	7	34.314	33.581	33.578	.453	.733	2.2410	1.0000
1	0	8	1.249 *	.559	-.559	-.016	.710	.7931	1.0000 *
1	0	9	12.237	12.110	12.110	-.034	.127	.127	1.0000
1	0	10	2.043 *	.715	.714	.015	1.325	.8334	1.0000 *
1	0	11	25.521	25.773	25.780	.410	-1.157	-4.6849	1.0000 *
1	0	12	2.033 *	.025	.026	-.012	2.004	3.0474	1.0000 *
1	0	13	21.574	21.506	-21.506	-.140	.047	.2960	1.0000 *
1	0	14	4.780	4.493	4.493	-.034	.296	.5908	1.0000
1	0	15	6.707	7.035	7.032	.157	-.328	-1.4711	1.0000
1	0	16	4.112	3.562	-3.562	.033	.545	1.6214	1.0000
1	0	17	16.707	16.707	-16.706	-.145	.090	.5202	1.0000
1	0	18	5.772	5.341	5.336	.215	.432	1.5890	1.0000
1	0	19	3.454	3.251	-3.251	-.034	.233	.4522	1.0000
1	0	20	3.845	3.108	3.105	-.143	.732	1.9078	1.0000
1	0	21	33.945	22.070	32.070	.098	1.875	12.2905	1.0000
1	0	22	45.274	44.755	44.753	.445	.519	3.0747	1.0000
1	0	23	16.519	16.317	16.387	.090	.132	.4347	1.0000
1	0	24	26.296	25.797	25.794	.365	.495	.4347	1.0000
1	0	25	9.592	5.176	5.175	.049	.517	1.5811	1.0000
1	0	26	37.597	93.934	-93.933	-.504	-4.238	-46.1739	1.0000 *
1	0	27	7.296	7.088	-7.088	-.027	.208	.4198	1.0000
1	0	28	5.117	1.298	-1.202	.491	3.515	19.7878	1.0000
1	0	29	6.107	6.082	6.082	.028	.025	.1420	1.0000
1	0	30	52.156	53.161	-53.179	-.455	-1.025	-4.4357	1.0000
1	0	31	1.127 *	1.282	-1.282	-.024	-.155	-.1925	1.0000 *
1	0	32	11.418	11.056	11.049	.400	.363	2.2742	1.0000
1	0	33	4.004	3.074	3.074	.024	.933	3.1298	1.0000
1	0	34	22.079	20.937	-20.935	-.334	1.142	4.8429	1.0000
1	0	35	62.592	61.803	61.802	.345	.785	5.1731	1.0000
1	0	36	5.118	5.262	5.262	.056	-.144	-.6936	1.0000
1	0	37	13.138	13.102	13.101	.197	.036	.2018	1.0000
1	0	38	4.448	4.121	-4.121	-.054	.337	1.6286	1.0000
1	0	39	36.684	36.946	36.945	.313	-.262	-1.0531	1.0000
1	0	40	2.913	3.121	3.121	.049	-.208	-.6542	1.0000
1	0	41	10.209	9.987	9.986	.162	.222	1.5468	1.0000
1	0	42	3.136	2.248	-2.247	-.042	.885	2.2845	1.0000
1	0	43	14.312	14.406	14.404	.233	.407	2.2845	1.0000
1	0	44	63.894	60.029	60.029	-.105	3.866	22.4500	1.0000
1	0	45	14.748	13.988	-13.988	.067	.760	4.4412	1.0000
1	0	46	8.412	8.011	8.010	.103	.401	2.4436	1.0000
1	0	47	5.062	4.795	4.795	-.064	.287	1.4280	1.0000
1	0	48	25.377	27.776	27.778	-.094	-2.140	-8.4028	1.0000
1	0	49	7.085	7.109	-7.108	.061	-.024	-.1559	1.0000
1	0	50	3.996	3.820	3.819	.083	.176	.6478	1.0000
1	0	51	1.919 *	1.433	-1.432	-.053	.487	.7451	1.0000 *
1	0	52	10.191	9.439	9.439	-.069	.752	4.4906	1.0000
1	0	53	60.188	58.565	58.564	.375	1.623	8.2612	1.0000

H	K	L	F(DRS)	F(CALC)	A(CALC)	S(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTR
2	4	1	4.494	4.944	-4.994	-.052	-.300	-1.4200		1.0000
2	4	2	4.104	4.560	4.357	.146	-.256	-.4613		1.0000
2	4	3	4.794	4.337	4.337	.051	.257	1.1941		1.0000
2	4	4	37.657	36.303	36.306	.339	-.450	-2.1446		1.0000
2	4	5	3.469	3.126	-3.126	-.045	.283	.4522		1.0000
2	4	6	5.037	4.743	4.743	.121	.274	1.1933		1.0000
2	4	7	1.906	2.401	2.401	.040	-.496	-.7272		1.0000
2	4	8	16.020	15.727	15.727	.253	.292	1.6382		1.0000
2	4	9	40.150	49.901	49.901	.540	.245	1.1092		1.0000
2	4	10	11.709	11.466	-11.466	-.053	.227	1.2490		1.0000
2	4	11	74.644	76.444	-76.442	-.526	-.1796	-7.7310		1.0000
2	4	12	13.727	14.274	14.274	.052	-.546	-3.2616		1.0000
2	4	13	26.426	27.297	27.294	.498	-.871	-3.0774		1.0000
2	4	14	2.482	2.741	-2.760	-.046	.121	.3333		1.0000
2	4	15	27.207	29.516	-29.516	-.428	-.211	-6.7793		1.0000
2	4	16	9.439	6.822	6.822	.041	.617	3.6930		1.0000
2	4	17	23.456	22.734	22.733	.094	.723	2.4426		1.0000
2	4	18	1.438	1.772	-1.772	-.095	-.331	-.4420		1.0000
2	4	19	23.084	22.752	22.746	.354	.332	1.1751		1.0000
2	4	20	1.166	1.489	1.489	.006	-.322	-.5874		1.0000
2	4	21	14.942	14.942	14.942	.006	-.234	-1.7043		1.0000
2	4	22	2.876	1.084	-1.084	-.004	1.484	5.2190		1.0000
2	4	23	13.457	14.355	14.352	.315	-.469	-4.0298		1.0000
2	4	24	1.972	.835	.835	.005	.537	.4477		1.0000
2	4	25	20.058	19.468	-19.466	-.298	.589	2.6647		1.0000
2	4	26	1.179	.015	-.003	-.019	1.160	1.3787		1.0000
2	4	27	30.711	31.013	31.011	.292	-.201	-1.0227		1.0000
2	4	28	3.091	4.399	-4.399	.019	-.408	-1.4087		1.0000
2	4	29	14.978	15.120	-15.118	-.249	-.143	-.8813		1.0000
2	4	30	2.530	3.638	-3.638	-.017	-1.105	-2.1951		1.0000
2	4	31	17.284	17.728	17.726	.239	-.444	-2.2723		1.0000
2	4	32	27.775	26.404	26.403	.237	1.370	4.3282		1.0000
2	4	33	2.130	1.973	1.972	.052	.157	.3040		1.0000
2	4	34	9.201	9.107	9.104	.199	.094	.4476		1.0000
2	4	35	1.921	1.736	-1.735	-.048	.185	.3149		1.0000
2	4	36	19.973	19.348	15.347	.215	-.376	-1.6905		1.0000
2	4	37	1.355	1.525	1.524	.047	-.167	-.1720		1.0000
2	4	38	6.030	5.808	5.805	.164	.222	.6982		1.0000
2	4	39	24.324	23.349	-23.348	-.231	.975	3.9423		1.0000
2	4	40	9.544	9.672	9.672	.082	-.075	-.4894		1.0000
2	4	41	19.786	19.621	19.620	.226	.165	.7544		1.0000
2	4	42	4.612	5.028	-5.027	-.076	-.416	-1.4169		1.0000
2	4	43	17.770	18.015	-18.014	-.208	-.245	-1.4049		1.0000
2	4	44	9.934	10.082	10.082	.072	-.148	-.8385		1.0000
2	4	45	2.108	21.581	21.579	.302	.527	2.2792		1.0000
2	4	46	1.392	1.962	-1.962	-.040	-.570	-.2725		1.0000
2	4	47	1.402	1.743	1.741	.094	-.341	-.3409		1.0000
2	4	48	2.371	1.859	1.859	.039	.512	.6691		1.0000
2	4	49	16.369	16.553	16.550	.273	-.184	-1.1028		1.0000
2	4	50	15.714	15.502	15.497	.369	.212	1.1664		1.0000
2	4	51	1.448	.253	-.247	-.055	1.195	1.1557		1.0000
2	4	52	18.089	17.844	-17.840	-.378	.245	1.3091		1.0000
2	4	53	6.293	5.862	5.862	-.033	.432	2.1841		1.0000

SILLIMANITE (EPHRAIM) WINE SPOILINGS AT 400 DEGREES C

STRUCTURE FACTORS

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	0	3	4.832	4.718	4.718	.026	.121	.5143	1.0000
3	0	3	4.940	5.135	5.135	-.026	-.195	-.9324	1.0000
3	0	7	5.464	5.073	5.073	.025	.391	1.5FR3	1.0000
3	0	6	12.898	15.764	15.753	.593	-2.867	-16.7406	1.0000
3	1	1	4.590	4.529	-4.526	-.095	.061	.2825	1.0000
3	1	1	34.470	36.711	36.711	-.045	1.758	9.0042	1.0000
3	1	2	3.140	3.132	-3.131	.082	.007	.0256	1.0000
3	1	4	27.129	22.535	22.533	.536	1.590	5.7806	1.0000
3	1	4	7.154	7.352	-7.352	-.075	-.198	-1.3086	1.0000
3	1	6	12.129	11.859	11.858	-.024	.271	1.5511	1.0000
3	1	7	12.901	2.134	-2.137	.067	-.237	-.3567	1.0000
3	1	7	12.291	12.282	12.282	.297	.003	.0155	1.0000
3	1	8	29.200	28.645	28.644	.198	.551	2.9263	1.0000
3	2	1	5.160	5.296	5.296	.006	-.126	-.4481	1.0000
3	2	1	31.710	28.690	-38.690	-.192	.020	.0991	1.0000
3	2	2	9.967	9.787	-9.787	-.007	.180	.5431	1.0000
3	2	4	18.142	19.105	19.105	.178	-.964	-.4.4609	1.0000
3	2	4	2.973	1.820	-1.820	.008	1.153	3.4776	1.0000
3	2	6	17.573	17.684	-17.685	-.156	-.112	-.6161	1.0000
3	2	7	6.193	5.498	-5.498	-.003	.495	3.0926	1.0000
3	3	8	8.684	8.453	-8.452	.131	.232	1.2072	1.0000
3	3	8	33.963	33.968	-33.966	-.291	-.005	-.0223	1.0000
3	3	8	5.046	4.250	-4.250	.008	.796	3.5376	1.0000
3	3	1	103.858	106.247	106.244	.801	-2.385	-11.5477	1.0000
3	3	2	2.087	1.511	-1.511	-.007	.176	.3737	1.0000
3	3	3	21.949	22.730	-22.728	-.262	-.780	-3.7712	1.0000
3	3	3	4.710	5.204	5.204	.007	-.494	-2.1814	1.0000
3	3	3	52.848	53.307	53.303	.455	-.445	-1.4332	1.0000
3	3	3	2.964	2.974	-2.974	-.005	.010	.0218	1.0000
3	3	3	10.450	9.771	-9.769	-.150	.675	3.5688	1.0000
3	3	3	9.589	6.857	-6.895	-.142	2.693	13.7970	1.0000
3	3	4	7.375	7.217	-7.217	.028	.156	.7057	1.0000
3	3	4	14.729	14.708	14.708	.139	.021	.0917	1.0000
3	3	4	1.729	1.144	-1.143	-.026	.585	.8965	1.0000
3	3	4	1.785	1.753	-1.749	-.128	.032	.0613	1.0000
3	3	4	6.631	6.340	-6.340	.025	.291	1.6872	1.0000
3	3	4	7.761	7.430	-7.429	.113	.331	1.6850	1.0000
3	3	4	2.419	1.853	-1.853	-.018	.566	1.0378	1.0000
3	3	5	30.635	30.685	28.682	.374	2.150	8.4197	1.0000
3	3	5	3.819	3.701	-3.700	.081	.116	.4223	1.0000
3	3	5	2.703	1.236	-1.230	.124	1.467	3.8579	1.0000
3	3	5	1.138	.516	-.510	-.077	.623	.7654	1.0000
3	3	5	22.983	22.964	-22.961	.339	.015	.0838	1.0000
3	3	5	3.478	2.747	-2.746	.073	.732	2.2854	1.0000
3	3	5	1.317	.266	-.266	.103	1.032	1.0968	1.0000
3	3	5	4.085	2.424	-2.424	-.063	1.661	4.7739	1.0000
3	3	6	17.514	17.682	-17.682	-.075	-.166	-.7463	1.0000
3	3	6	2.405	1.308	-1.308	-.020	1.097	2.6582	1.0000
3	3	6	2.691	2.964	-2.963	.075	-.272	-.7395	1.0000
3	3	6	1.194	.910	-.910	.020	.283	.3324	1.0000
3	3	6	12.063	11.895	-11.895	-.068	.168	1.1474	1.0000
3	3	6	2.662	2.537	-2.537	-.015	.125	.2823	1.0000
3	3	6	1.356	.990	-.988	.061	.366	.2775	1.0000

M	N	L	F(FRS)	F(CALC)	A(FCALC)	P(CALC)	DELTA F	DELTA/SIGMA	EXT.	ELECTOR
3	7	7	1.412 *	1.460	-1.460	.018	-.066	-.0672	1.0000	**
3	7	0	45.596	65.177	45.174	.622	.420	1.5278	1.0000	
3	7	1	11.712	11.619	-11.618	-.004	.007	.0260	1.0000	
3	7	2	5.356	5.723	-5.721	-.158	-.267	-1.7255	1.0000	
3	7	3	11.076	11.241	11.241	.090	-.145	-1.1167	1.0000	
3	7	4	47.521	48.611	48.606	.562	-1.080	-3.2506	1.0000	
3	7	5	7.630	6.968	-6.987	-.061	.643	3.3714	1.0000	
3	7	6	4.290	4.676	-4.675	-.126	-.387	-1.1466	1.0000	
3	7	7	14.761	16.536	16.535	.172	.228	1.1096	1.0000	
3	7	8	3.750	3.462	3.462	.015	.287	1.1096	1.0000	
3	7	9	1.254	.787	.787	-.165	.497	.9292	1.0000	**
3	7	10	1.312 *	1.981	-1.981	.018	-.665	-.7138	1.0000	**
3	7	11	12.108	12.295	12.294	.155	-.197	-1.1284	1.0000	
3	7	12	2.295	2.818	2.818	.018	-.665	-.7138	1.0000	**
3	7	13	19.334	19.974	-19.973	-.012	.487	1.1163	1.0000	
3	7	14	1.382 *	.422	-4.462	.009	.871	.9143	1.0000	**
3	7	15	29.219	29.427	29.421	.640	-.208	-.6162	1.0000	
3	7	16	1.372 *	.574	.574	-.007	.790	.8140	1.0000	**
3	7	17	14.141	14.200	-14.199	-.154	-.050	-.5608	1.0000	**
3	7	18	1.421 *	.463	-4.463	.008	.658	.9438	1.0000	**
3	7	19	13.750	12.962	-12.963	-.053	.787	4.5100	1.0000	
3	7	20	5.920	5.773	5.773	.024	.147	.5732	1.0000	
3	7	21	2.932	.099	-.083	-.021	.690	5.0504	1.0000	
3	7	22	4.899	4.909	-4.909	-.021	.400	1.7517	1.0000	
3	7	23	7.439	7.947	7.945	.136	.407	-1.7804	1.0000	
3	7	24	6.822	5.659	5.659	.064	.663	2.6677	1.0000	
3	7	25	74.238	76.605	-76.604	-.242	1.543	8.3052	1.0000	
3	7	26	44.201	47.405	47.401	.741	.796	3.6692	1.0000	
3	7	27	43.949	45.240	-45.240	-.217	-.1251	-4.8558	1.0000	
3	7	28	41.202	40.241	40.237	.622	.960	2.0000	1.0000	
3	7	29	20.105	18.827	-18.827	-.156	1.278	5.7825	1.0000	
3	7	30	22.046	22.902	22.901	.977	.043	.1963	1.0000	
3	7	31	3.317	2.611	-2.610	.059	.706	2.4837	1.0000	
3	7	32	21.743	21.941	-21.940	-.269	.442	1.7860	1.0000	
3	7	33	1.149 *	1.012	1.012	-.054	.176	.2072	1.0000	**
3	7	34	17.625	17.422	17.421	.250	.203	1.3111	1.0000	**
3	7	35	1.544 *	.614	-12.404	.053	.520	1.3784	1.0000	**
3	7	36	12.725	12.406	-12.404	-.220	.315	1.9453	1.0000	**
3	7	37	1.366 *	.821	-.820	-.042	.547	.5596	1.0000	**
3	7	38	5.464	7.960	7.976	.194	.484	2.4187	1.0000	
3	7	39	77.795	76.973	76.972	.461	.622	4.2066	1.0000	
3	7	40	2.312	1.720	-1.720	.013	.592	1.5808	1.0000	
3	7	41	36.983	37.267	37.267	.069	-.284	-1.2489	1.0000	
3	7	42	1.424 *	1.227	-1.227	-.013	.197	.2689	1.0000	**
3	7	43	49.324	49.550	49.548	.418	.374	1.4324	1.0000	**
3	7	44	1.951 *	2.197	-2.196	.014	-.345	-.5975	1.0000	**
3	7	45	16.793	16.690	16.690	.058	.103	.5204	1.0000	**
3	7	46	2.825	2.201	-2.201	-.013	.624	1.3046	1.0000	**
3	7	47	20.976	19.788	19.788	.310	1.189	5.4711	1.0000	
3	7	48	6.057	4.513	-4.513	.051	1.573	6.7072	1.0000	
3	7	49	12.197	11.873	-11.873	-.112	.324	1.6306	1.0000	
3	7	50	5.350	4.388	4.388	-.049	.962	4.1019	1.0000	
3	7	51	9.412	9.921	9.921	.108	-.505	-2.5031	1.0000	

H	K	L	F(DRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	FXI	FACTORS
4	3	4	3.941	2.060	-2.059	.046	1.871	7.3988	1.0000	
4	3	5	6.159	6.777	-6.777	-.096	-.116	-.6500	1.0000	
4	3	6	2.552	1.520	1.520	-.039	1.031	2.1585	1.0000	*
4	3	7	5.042	4.907	4.907	.057	.135	.4754	1.0000	
4	4	0	56.509	56.715	56.715	.591	-.119	-.5146	1.0000	
4	4	1	1.953	1.219	-1.218	-.034	.744	1.3974	1.0000	**
4	4	2	35.478	36.214	-36.214	-.080	-.727	-2.5415	1.0000	
4	4	3	4.619	5.311	5.311	.033	-.652	-3.1204	1.0000	
4	4	4	41.650	41.584	41.581	.535	.066	.2297	1.0000	
4	4	5	2.323	1.507	1.506	-.030	.717	1.7141	1.0000	*
4	4	6	16.785	16.583	-16.583	-.043	.202	.6678	1.0000	**
4	4	7	5.964	4.957	4.957	.028	1.007	4.0520	1.0000	
4	5	0	30.560	30.033	-30.032	-.028	.520	1.0807	1.0000	
4	5	1	1.462	.675	.674	.049	.766	1.0853	1.0000	**
4	5	2	27.003	26.545	26.563	.256	.432	1.5702	1.0000	**
4	5	3	1.364	1.000	-.999	-.045	.964	1.5901	1.0000	**
4	5	4	22.064	22.081	-22.079	-.263	.583	2.1099	1.0000	
4	5	5	1.459	1.236	1.235	.043	.423	.6155	1.0000	**
4	5	6	15.369	15.349	15.347	.235	.021	.1152	1.0000	**
4	5	7	1.666	1.082	-1.081	-.034	.585	.6673	1.0000	**
4	6	0	15.777	16.117	16.116	-.181	-.340	-1.7085	1.0000	
4	6	1	4.614	4.902	-4.902	.027	-.226	-1.4233	1.0000	
4	6	2	43.030	41.697	41.692	.638	1.335	4.6899	1.0000	
4	6	3	1.225	.087	-.084	-.024	1.138	1.3007	1.0000	**
4	6	4	9.704	9.451	9.686	-.162	.013	.0647	1.0000	
4	6	5	6.575	6.115	-6.115	.023	.461	2.1504	1.0000	
4	6	6	24.144	24.530	24.524	.522	-.386	-1.6783	1.0000	
4	6	7	15.709	15.135	15.134	.177	.571	3.0886	1.0000	
4	7	0	2.665	.545	-.541	.061	2.120	5.0959	1.0000	
4	7	1	12.569	12.233	-12.233	-.170	.337	1.9422	1.0000	
4	7	2	1.260	.279	.273	-.057	.481	1.0910	1.0000	**
4	7	3	11.744	11.338	11.337	.160	.407	2.6450	1.0000	**
4	7	4	1.382	.367	.363	.055	1.015	1.0286	1.0000	**
4	7	5	7.590	7.233	-7.231	-.139	.357	1.6360	1.0000	
4	7	6	23.152	22.905	22.908	.225	.989	1.0920	1.0000	
4	8	0	3.927	4.089	-4.089	.023	-.163	-.5196	1.0000	
4	8	1	2.754	1.905	1.899	.198	.844	1.6736	1.0000	
4	8	2	6.570	7.051	7.051	-.021	-.491	-2.1921	1.0000	
4	8	3	17.079	17.237	17.236	.204	-.159	-.4079	1.0000	
4	8	4	1.411	.551	.550	.022	.660	.8539	1.0000	*
4	8	5	9.888	9.534	9.533	.114	.355	2.0334	1.0000	**
4	9	0	9.392	9.372	-9.372	-.095	.020	.1124	1.0000	
4	9	1	10.729	10.423	-10.422	-.108	.306	1.7013	1.0000	
4	9	2	8.376	8.366	8.365	.093	-.010	-.0508	1.0000	
4	9	3	7.986	7.376	7.375	.102	.510	2.4244	1.0000	
4	9	4	30.812	29.970	29.966	.512	.842	3.6608	1.0000	
4	10	0	3.542	2.783	-2.782	-.055	.759	1.7799	1.0000	
4	10	1	8.018	8.358	-8.357	-.132	-.341	-1.6211	1.0000	*
4	10	2	1.436	.307	-.302	.054	1.130	1.1010	1.0000	**
5	0	1	3.844	4.217	4.216	-.084	-.274	-1.2785	1.0000	
5	0	3	7.540	6.862	-6.862	.083	.678	3.7598	1.0000	
5	0	5	3.332	3.021	-3.020	-.073	.310	.5012	1.0000	
5	0	7	3.735	3.283	-3.282	.070	.452	1.1300	1.0000	

U	V	W	X	Y	Z	F(00S)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	ENT	FACTORS
5	5	5	5	5	5	14.667	-13.027	13.024	.287	1.635	7.4466	1.0000	
5	5	5	5	5	5	8.116	7.875	7.875	.082	.240	1.1122	1.0000	
5	5	5	5	5	5	34.034	34.294	34.293	.233	-.260	-1.0466	1.0000	
5	5	5	5	5	5	11.447	11.711	-11.711	-.078	-.264	-1.4729	1.0000	
5	5	5	5	5	5	13.355	12.491	12.488	.260	.466	6.2034	1.0000	
5	5	5	5	5	5	2.177	1.533	1.631	.070	.545	1.0589	1.0000	*
5	5	5	5	5	5	17.634	17.252	17.251	.192	.383	1.0931	1.0000	
5	5	5	5	5	5	8.109	7.674	-7.674	-.060	.434	2.1606	1.0000	
5	5	5	5	5	5	44.926	66.052	-66.050	-.535	-1.124	-5.0474	1.0000	
5	5	5	5	5	5	14.718	14.569	14.569	.049	.145	6.402	1.0000	
5	5	5	5	5	5	6.686	70.416	70.414	.522	-1.227	-5.1791	1.0000	
5	5	5	5	5	5	46.452	46.788	-46.785	-.025	-.072	-.4358	1.0000	
5	5	5	5	5	5	10.576	10.737	10.737	.045	-.396	-1.2011	1.0000	
5	5	5	5	5	5	38.455	27.211	37.208	.425	-.161	-.9087	1.0000	
5	5	5	5	5	5	1.603	.922	-.921	-.035	.481	3.6617	1.0000	*
5	5	5	5	5	5	21.029	21.125	21.123	.220	.503	1.7758	1.0000	*
5	5	5	5	5	5	4.635	4.463	4.463	.016	.173	.6726	1.0000	
5	5	5	5	5	5	39.970	39.986	39.985	.284	-.284	-1.1070	1.0000	
5	5	5	5	5	5	1.362	.476	.476	-.015	.487	1.2257	1.0000	*
5	5	5	5	5	5	15.453	15.955	15.954	.200	-.502	-2.6501	1.0000	*
5	5	5	5	5	5	4.493	5.284	5.284	.014	-.791	-2.6497	1.0000	
5	5	5	5	5	5	20.253	20.332	20.330	.233	-.075	-.3934	1.0000	
5	5	5	5	5	5	4.173	2.187	2.187	-.011	1.586	5.7852	1.0000	
5	5	5	5	5	5	8.620	7.200	7.166	.405	1.420	6.5020	1.0000	
5	5	5	5	5	5	9.572	10.248	10.248	.034	-.675	-3.7208	1.0000	
5	5	5	5	5	5	24.592	23.429	-23.425	-.393	1.164	4.0121	1.0000	
5	5	5	5	5	5	10.582	10.959	-10.956	-.031	-.377	-2.2637	1.0000	
5	5	5	5	5	5	8.214	8.079	8.071	.365	.135	.6827	1.0000	
5	5	5	5	5	5	4.440	3.984	3.984	.033	.456	1.4043	1.0000	
5	5	5	5	5	5	13.482	13.637	-13.632	-.320	-.135	-.8935	1.0000	
5	5	5	5	5	5	7.360	6.809	-6.809	-.025	.551	2.5241	1.0000	
5	5	5	5	5	5	12.571	11.088	11.086	-.056	1.482	8.7847	1.0000	
5	5	5	5	5	5	8.577	8.318	-8.317	-.056	.259	1.6006	1.0000	
5	5	5	5	5	5	15.019	14.526	14.524	.242	.499	2.7367	1.0000	
5	5	5	5	5	5	5.615	4.627	4.626	.082	.586	4.7256	1.0000	
5	5	5	5	5	5	10.304	9.452	9.450	.212	.852	5.2308	1.0000	
5	5	5	5	5	5	7.168	7.276	-7.276	-.073	-.108	-.5301	1.0000	
5	5	5	5	5	5	8.194	8.275	8.272	.209	-.080	-.4043	1.0000	
5	5	5	5	5	5	19.307	18.626	18.625	.181	.681	2.8330	1.0000	*
5	5	5	5	5	5	1.248	1.972	1.970	-.091	-.724	-.8119	1.0000	*
5	5	5	5	5	5	2.001	.760	-.760	-.178	1.222	2.1751	1.0000	*
5	5	5	5	5	5	1.270	.512	.504	.089	.758	.8357	1.0000	*
5	5	5	5	5	5	14.193	13.705	13.704	.163	.488	2.7237	1.0000	*
5	5	5	5	5	5	1.389	1.331	1.328	-.078	.058	.0587	1.0000	*
5	5	5	5	5	5	2.124	.948	-.937	-.141	1.176	1.7131	1.0000	*
5	5	5	5	5	5	25.398	25.770	25.769	.259	-.372	-1.5715	1.0000	*
5	5	5	5	5	5	2.884	2.951	2.950	.050	-.066	-.01639	1.0000	*
5	5	5	5	5	5	21.459	21.256	21.256	.179	.242	1.1714	1.0000	*
5	5	5	5	5	5	1.329	1.173	-1.172	-.046	.156	.1640	1.0000	*
5	5	5	5	5	5	19.230	19.530	19.529	.235	-.300	-1.4749	1.0000	*
5	5	5	5	5	5	3.463	2.986	2.985	.043	.478	1.1356	1.0000	*
5	5	5	5	5	5	33.489	32.758	-32.755	-.467	.731	2.1441	1.0000	*

W	K	L	F(COFS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
5	6	1	1.357 *	2.323	2.322	.059	-.566	-.5974		1.0000 * **
5	6	2	16.151	16.763	16.757	.459	-.613	-3.1742		1.0000
5	6	3	3.028	2.079	-2.078	-.054	.545	2.0530		1.0000
5	6	4	25.050	24.962	-2.422	-.422	.3727	.3727		1.0000
5	6	5	2.354 *	1.055	1.054	.002	1.335	2.1252		1.0000 * **
5	6	6	2.176 *	1.548	1.537	.184	.626	.5510		1.0000 * **
5	6	7	2.205 *	2.278	2.278	.034	-.073	-.1108		1.0000 * **
5	6	8	9.1357	9.052	9.079	.205	.275	1.4683		1.0000
5	6	9	2.671 *	2.256	-2.286	-.031	.384	.6911		1.0000 * **
5	6	10	2.405 *	1.500	1.493	.168	1.104	1.6464		1.0000 * **
5	6	11	19.877	19.424	19.423	.185	.453	2.0330		1.0000
5	6	12	1.955 *	2.371	-2.370	.039	-.406	-.5201		1.0000 * **
5	6	13	7.100	7.437	-7.434	-.177	-.537	-1.4708		1.0000
5	6	14	12.767	13.603	13.601	.692	-.836	-3.5462		1.0000
5	6	15	29.741	29.306	-29.307	-.173	-.367	-1.3291		1.0000
5	6	16	60.111	59.601	59.598	.626	.510	1.7567		1.0000
5	6	17	16.082	15.318	-15.317	-.139	.765	4.2151		1.0000
5	6	18	40.729	39.982	39.981	.308	.747	2.8639		1.0000
5	6	19	11.259	11.464	-11.464	-.026	-.205	-.9974		1.0000
5	6	20	1.201 *	.754	-.692	-.300	.447	.5209		1.0000 * **
5	6	21	8.006	8.083	8.083	.027	-.077	-.4804		1.0000
5	6	22	27.767	27.864	27.862	.278	-.097	-.3039		1.0000
5	6	23	6.367	6.228	-6.228	-.019	.135	.6624		1.0000
5	6	24	1.412 *	2.619	-2.608	-.244	-1.207	-1.1968		1.0000 * **
5	6	25	1.455 *	2.612	2.612	.021	-1.157	-1.1138		1.0000 * **
5	6	26	22.587	23.267	23.267	.090	-.679	-2.3241		1.0000
5	6	27	8.103	8.133	-8.133	-.119	-.030	-.1673		1.0000
5	6	28	25.319	24.592	24.588	.416	.728	2.5083		1.0000
5	6	29	7.076	7.341	7.340	.114	-.263	-1.5793		1.0000
5	6	30	15.687	15.423	15.422	.073	.265	1.3800		1.0000
5	6	31	4.674	5.663	-5.662	-.104	-.986	-3.4481		1.0000
5	6	32	14.773	15.014	15.010	.341	-.241	-1.2487		1.0000
5	6	33	4.450	4.264	4.263	.091	.166	.4659		1.0000
5	6	34	23.659	23.036	-23.936	-.073	-.276	-.9533		1.0000
5	6	35	2.891	3.823	3.823	.037	-.932	-2.5841		1.0000
5	6	36	7.348	6.910	-6.909	-.070	.439	2.7707		1.0000
5	6	37	1.242 *	.704	-.703	-.032	.536	.6067		1.0000 * **
5	6	38	15.149	15.435	-15.435	.066	-.286	-1.4657		1.0000
5	6	39	4.607	4.631	4.631	.032	-.024	-.0821		1.0000
5	6	40	3.790	3.129	-3.128	-.057	.662	1.7191		1.0000
5	6	41	1.463 *	.870	.870	.020	.593	.5676		1.0000 * **
5	6	42	1.208 *	.949	.948	-.034	.259	.2998		1.0000 * **
5	6	43	7.997	7.746	7.745	.113	.250	1.4283		1.0000
5	6	44	38.109	37.693	37.690	.506	.414	1.4283		1.0000
5	6	45	7.323	7.022	-7.021	-.107	.301	1.7147		1.0000
5	6	46	1.958 *	.115	.112	-.029	1.842	3.0366		1.0000 * **
5	6	47	5.557	5.515	5.515	.099	.042	.1587		1.0000
5	6	48	22.386	22.469	22.465	.415	-.082	-.3406		1.0000
5	6	49	21.099	21.391	-21.386	-.333	-.292	-1.2437		1.0000
5	6	50	1.252 *	1.825	-1.825	.013	-.574	-.6422		1.0000 * **
5	6	51	37.478	38.131	38.130	.327	-.653	-2.1315		1.0000
5	6	52	1.287 *	1.788	-1.788	-.010	-.501	-.5446		1.0000 * **
5	6	53	16.637	16.626	-16.623	-.300	.011	.0604		1.0000

H	K	L	F (Obs)	F (Calc)	A (Calc)	B (Calc)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
5	5	1	2.207 *	2.967	-2.967	.013	-.760	-1.1979	1.0000	**
5	5	6	71.450	22.097	22.096	.266	-.247	-1.1384	1.0000	**
5	6	6	39.950	40.257	40.253	.599	-.307	-.9913	1.0000	**
6	6	1	2.401	2.656	2.656	.010	.745	2.1356	1.0000	**
6	6	2	3.094	3.750	-3.748	-.134	-.668	-1.4699	1.0000	**
6	6	3	1.652	2.257	-2.257	-.009	-.425	-.6125	1.0000	**
6	6	4	30.436	30.340	30.336	.593	.698	.5930	1.0000	**
6	6	5	2.624	2.135	2.135	.010	.385	.6770	1.0000	**
6	7	0	11.412	10.455	10.454	.171	.522	5.2908	1.0000	**
6	7	1	7.759	7.159	-7.159	-.038	.560	2.5704	1.0000	**
6	7	2	19.426	18.144	-18.143	-.164	.282	1.3952	1.0000	**
6	7	3	9.261	9.391	9.391	.038	-.130	-.7349	1.0000	**
6	7	4	4.391	8.070	8.065	.155	.320	1.6308	1.0000	**
6	7	5	2.961 *	1.712	-1.712	-.029	1.245	2.4281	1.0000	**
6	7	6	9.396	8.658	-8.657	.171	.735	4.1191	1.0000	**
6	8	1	4.042	3.647	-3.645	-.112	.291	1.0964	1.0000	**
6	8	2	14.228	14.231	14.229	.282	-.003	-.0186	1.0000	**
6	8	3	2.994 *	3.321	3.320	.108	-.327	-.4556	1.0000	**
6	8	4	7.124	6.422	-6.420	.155	.703	2.5809	1.0000	**
6	8	5	15.604	15.897	15.896	.160	-.293	-1.4454	1.0000	**
6	8	6	6.766	6.352	-6.352	.004	.414	1.6966	1.0000	**
6	9	1	14.001	13.026	-13.025	-.152	.576	5.7429	1.0000	**
6	9	2	2.765	2.998	2.998	-.002	-.233	-.4091	1.0000	**
6	9	3	15.024	15.189	15.188	.150	-.165	-.9391	1.0000	**
6	9	4	15.922	16.084	-16.083	-.140	-.462	-.8660	1.0000	**
6	9	5	7.035	6.872	-6.871	.132	.163	.7753	1.0000	**
7	7	0	11.549	12.257	12.257	-.047	-.798	-3.5783	1.0000	**
7	7	1	1.205 *	1.264	.260	.041	.542	1.6937	1.0000	**
7	7	2	34.217	33.329	33.325	.530	.888	3.0128	1.0000	**
7	7	3	3.253	2.693	-2.693	-.040	.560	1.5828	1.0000	**
7	7	4	8.278	8.562	8.562	-.041	-.285	-1.6773	1.0000	**
7	7	5	3.155	3.199	3.199	.038	-.654	-1.1010	1.0000	**
7	7	6	19.262	18.859	-18.859	.434	.403	2.0616	1.0000	**
7	7	7	9.032	9.210	9.209	.107	-.177	-1.1211	1.0000	**
7	7	8	1.914	1.666	-1.666	-.062	.246	.4474	1.0000	**
7	7	9	2.792	2.764	-2.762	-.103	.028	.0675	1.0000	**
7	7	0	2.303 *	2.535	2.534	.062	-.237	-.4621	1.0000	**
7	7	1	7.158	6.919	-6.919	.097	.928	1.2660	1.0000	**
7	7	2	3.261	2.792	-2.792	-.051	.465	1.0906	1.0000	**
7	7	3	3.818	2.073	-2.072	-.085	1.745	4.4015	1.0000	**
7	7	4	11.848	52.142	52.136	.751	-.293	-1.0404	1.0000	**
7	7	5	2.500	2.060	-2.060	-.012	.740	1.8182	1.0000	**
7	7	6	20.431	20.948	-20.946	-.262	-.517	-2.1191	1.0000	**
7	7	7	1.715 *	.786	-.786	.012	.925	1.3533	1.0000	**
7	7	8	39.965	39.965	39.965	.679	-.442	-1.3098	1.0000	**
7	7	9	2.806 *	3.164	-3.164	-.010	-.355	-.6990	1.0000	**
7	7	0	12.755	12.565	-12.563	-.211	.190	.9985	1.0000	**
7	7	1	12.238	12.440	-12.439	-.093	-.202	-1.1428	1.0000	**
7	7	2	1.279 *	1.575	-1.572	-.089	-.296	-.3234	1.0000	**
7	7	3	2.657 *	2.173	2.171	.093	.484	1.0823	1.0000	**
7	7	4	2.053 *	.566	-.566	.087	1.487	2.4941	1.0000	**
7	7	5	9.093	9.142	-9.142	-.084	-.045	-.2822	1.0000	**
7	7	6	2.524 *	3.446	-3.445	-.074	-.922	-1.5897	1.0000	**

H	R	L	F(CRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTRS
7	4	7	3.1226	1.987	1.985	.076	1.439	3.1941	1.0000
7	4	0	4.4997	4.432	4.431	.122	.465	1.6052	1.0000
7	5	1	4.9956	4.955	4.956	-.036	-.069	-.2652	1.0000
7	4	2	10.9957	99.830	39.829	.925	.127	.3952	1.0000
7	5	3	1.052	2.435	-2.435	.036	-.683	-1.0423	1.0000
7	5	4	3.299	3.322	3.330	.111	-.032	-.0743	1.0000
7	5	5	4.476	4.075	4.075	-.023	.401	1.1369	1.0000
7	6	6	5.622	5.461	5.461	-.014	.161	.6616	1.0000
7	6	1	12.237	12.324	12.324	.129	-.098	-.5495	1.0000
7	6	2	6.150	6.123	6.123	.017	.057	.2408	1.0000
7	6	3	8.599	8.939	-8.938	-.129	-.240	-1.7820	1.0000
7	6	4	3.831	4.072	4.072	-.013	-.241	-.4104	1.0000
7	6	5	9.925	9.467	9.466	.113	.439	2.3730	1.0000
7	7	0	25.892	25.865	-25.898	-.157	.093	.3464	1.0000
7	7	1	8.596	8.633	8.633	.041	-.077	-.4614	1.0000
7	7	2	26.603	37.075	37.071	.561	-.672	-1.8354	1.0000
7	7	3	8.591	8.195	-8.194	-.057	.306	2.0137	1.0000
7	7	4	20.492	20.050	-20.045	-.141	.432	1.8382	1.0000
7	7	5	1.462	.288	-.4271	.098	1.174	1.1324	1.0000
7	7	6	1.447	1.161	1.161	-.024	.266	.2570	1.0000
7	7	7	10.207	10.181	-10.181	-.091	.026	.1431	1.0000
7	8	3	1.463	1.532	-1.532	.025	-.069	-.0459	1.0000
7	8	4	30.029	29.082	29.1083	.528	.962	3.2726	1.0000
7	8	5	2.533	1.126	1.126	-.019	1.407	2.2473	1.0000
8	0	0	9.739	61.358	61.356	.454	-1.615	-5.5597	1.0000
8	0	2	3.672	2.926	2.926	.026	.746	2.2900	1.0000
8	0	4	45.167	45.191	45.190	.410	-.004	-.0119	1.0000
8	0	6	5.087	1.395	1.395	.025	1.492	3.3273	1.0000
8	1	0	23.316	23.285	-23.281	-.005	.033	.1378	1.0000
8	1	1	9.117	9.351	-9.351	-.064	-.235	-1.4011	1.0000
8	1	2	21.652	21.982	21.979	.390	-.296	-1.4198	1.0000
8	1	3	8.456	8.213	8.213	.049	.242	1.4282	1.0000
8	1	4	16.181	17.916	-17.912	-.360	.265	1.2673	1.0000
8	1	5	5.736	5.755	-5.756	-.054	.178	.6654	1.0000
8	1	6	13.047	13.010	13.006	.318	.037	.2015	1.0000
8	2	0	10.333	8.080	8.079	.162	2.253	13.3546	1.0000
8	2	1	6.594	6.186	6.185	.097	.410	2.1525	1.0000
8	2	2	4.665	4.685	4.675	.304	-.020	-.0752	1.0000
8	2	3	3.294	4.036	-4.035	-.091	-.752	-1.8651	1.0000
8	2	4	5.889	6.357	6.355	.148	-.446	-1.8168	1.0000
8	2	5	5.079	5.025	5.024	.082	.054	.1735	1.0000
8	2	6	4.006	3.235	3.225	.249	.772	1.9992	1.0000
8	3	0	4.492	4.722	4.721	-.076	-.230	-.6292	1.0000
8	3	1	1.285	.483	-.463	.129	.802	4.7730	1.0000
8	3	2	5.108	4.841	-4.840	.076	.267	1.0443	1.0000
8	3	3	1.619	.121	-.016	-.120	1.408	1.8356	1.0000
8	3	4	4.313	3.580	3.579	-.068	.732	2.1429	1.0000
8	3	5	1.449	.658	.647	.115	.792	.7653	1.0000
8	4	0	12.705	12.778	12.778	.076	-.073	-.3953	1.0000
8	4	1	5.918	6.173	-6.173	-.066	-.255	-1.1046	1.0000
8	4	2	34.357	34.730	34.728	.369	-.373	-1.0932	1.0000
8	4	3	1.418	3.132	3.131	.063	-1.714	-1.6928	1.0000
8	4	4	9.903	9.376	9.376	.070	.527	3.0420	1.0000

H	K	L	F(CALC)	F(CALC)	L(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	4	5	5.894	5.648	-5.647	-.056	.237	.6462	1.0000
4	5	0	23.168	23.786	33.783	.427	-.618	-1.7516	1.0000
4	1	1	9.128	9.043	-9.043	-.085	-.011	-.0875	1.0000
4	2	2	30.301	30.000	-20.997	-.413	.201	1.1686	1.0000
4	3	3	4.150	4.086	4.086	.058	.064	.3146	1.0000
4	4	4	29.877	26.118	26.115	.386	-.141	-.6090	1.0000
4	5	0	13.754	13.604	13.598	.278	.140	.7471	1.0000
4	6	1	1.423	.104	-.096	-.030	1.315	1.2981	1.0000
4	7	2	2.103	2.487	2.487	.064	-.387	-.5495	1.0000
4	8	3	1.440	2.584	2.584	.038	-1.014	-1.0385	1.0000
4	9	4	10.227	10.225	10.279	.342	-.058	-.3198	1.0000
4	0	4	13.911	14.265	-14.267	-.245	-.058	-.3198	1.0000
4	1	0	4.028	4.026	-4.925	-.067	.012	.0370	1.0000
4	2	1	11.491	11.665	11.667	.243	-.188	-1.1401	1.0000
4	3	2	4.153	4.338	4.337	.067	-.188	-.5090	1.0000
4	4	3	12.491	12.139	12.137	.079	.352	1.4516	1.0000
4	5	0	4.761	4.699	4.899	.079	-.136	-.4025	1.0000
4	6	1	1.347	2.651	2.651	-.013	-1.302	-1.3543	1.0000
4	7	2	1.604	.224	.224	.015	1.380	1.5754	1.0000
4	8	3	4.386	.224	.224	-.006	.625	1.6845	1.0000
4	9	4	21.332	3.713	3.713	.340	-.657	-3.0567	1.0000
4	0	0	8.058	8.132	-8.130	-.149	-.074	-.4001	1.0000
4	1	1	11.141	11.398	11.398	.098	-.257	-1.6243	1.0000
4	2	2	9.677	9.667	9.666	.142	.010	.0577	1.0000
4	3	3	16.889	16.945	16.942	.326	-.226	-1.3505	1.0000
4	4	4	4.354	3.756	-3.755	-.125	.585	1.5943	1.0000
4	5	0	32.660	32.906	32.904	.306	-.247	-.7236	1.0000
4	6	1	2.586	2.734	2.734	-.003	-.178	-.3406	1.0000
4	7	2	35.477	35.566	-25.564	-.354	-.449	-.2541	1.0000
4	8	3	3.507	3.917	3.917	.097	-.449	-1.0569	1.0000
4	9	4	25.540	25.499	25.499	.357	.081	.3448	1.0000
4	0	4	1.476	.217	-.217	-.001	1.259	1.1942	1.0000
4	1	0	5.647	4.298	-4.298	-.011	1.545	6.2653	1.0000
4	2	1	1.399	1.562	-1.562	-.017	-.162	-.1630	1.0000
4	3	2	26.050	26.476	26.473	.447	-.427	-1.5925	1.0000
4	4	3	1.436	.656	-.656	.017	.780	.7602	1.0000
4	5	4	4.525	3.306	-3.306	-.009	1.219	3.5530	1.0000
4	6	0	4.797	3.551	-3.530	-.258	1.246	4.0993	1.0000
4	7	1	3.745	3.315	3.315	.022	.430	1.0689	1.0000
4	8	2	11.390	11.757	11.754	.284	-.268	-2.0662	1.0000
4	9	3	1.463	1.000	-1.000	-.017	.452	.4359	1.0000
4	0	4	3.150	2.567	-2.554	-.260	.533	1.1644	1.0000
4	1	0	19.379	19.832	19.930	.281	-.453	-2.0729	1.0000
4	2	1	8.376	8.664	8.662	.153	-.268	-1.4076	1.0000
4	3	2	12.582	12.796	12.795	.137	-.213	-1.1761	1.0000
4	4	3	5.261	6.060	-6.066	-.145	-.206	-.7320	1.0000
4	5	0	12.662	11.914	-11.913	-.144	.748	4.2960	1.0000
4	6	1	3.506	1.019	1.019	.004	2.487	5.6781	1.0000
4	7	2	2.307	1.800	1.794	.145	.507	.7472	1.0000
4	8	0	14.095	13.717	13.713	.344	.377	2.1211	1.0000
4	9	0	22.792	22.507	-22.506	-.245	.285	1.2562	1.0000
4	0	2	45.784	46.940	46.935	.668	-.115	-3.2075	1.0000
4	1	4	18.700	17.879	-17.878	-.220	.621	4.3037	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
10	1	0	9.084	8.904	-1.904	-.047	.180	.4732	1.0000
10	1	1	3.457	2.457	-2.456	.087	1.200	2.6591	1.0000
10	1	1	2.517	2.417	-2.456	.047	1.200	2.6591	1.0000
10	1	0	9.084	8.904	-1.904	-.047	.180	.4732	1.0000
10	1	1	3.417	2.417	-2.456	.047	1.200	2.6591	1.0000
10	1	1	7.618	7.811	-7.811	.046	.133	.1999	1.0000
10	1	2	2.510	1.422	-1.620	-.079	1.228	2.2945	1.0000
10	1	4	7.014	4.700	-4.700	-.042	.314	1.2716	1.0000
10	1	0	17.555	16.274	-1.269	.099	.419	-1.8948	1.0000
10	2	1	2.279	2.249	3.248	.081	-.371	-.7053	1.0000
10	2	2	7.372	7.372	7.372	.035	-.111	-.4814	1.0000
10	2	3	4.492	3.049	-3.068	-.077	1.422	4.0774	1.0000
10	2	0	16.772	11.136	-11.136	-.025	-.264	-2.0046	1.0000
10	2	1	12.227	13.172	-13.171	-.150	-.344	-1.8080	1.0000
10	2	2	4.122	3.216	-3.316	.024	.606	2.1202	1.0000
10	2	3	10.391	10.399	10.398	.145	-.007	-.0409	1.0000
10	2	0	30.035	31.407	31.403	.410	-1.322	-4.7268	1.0000
10	4	1	5.941	5.257	-5.356	-.092	.594	2.1670	1.0000
10	4	2	6.311	6.375	-6.375	-.091	.065	-.2381	1.0000
10	5	0	2.562	.546	-.545	.060	2.014	3.2816	1.0000
10	5	1	2.503	2.033	-2.033	.035	.470	.7417	1.0000
10	0	1	3.356	3.710	-3.706	-.172	-.322	-.6934	1.0000
11	1	1	11.934	11.467	-11.461	.350	-.493	-2.3441	1.0000
11	1	1	4.844	4.515	-4.515	.062	.208	1.1550	1.0000
11	1	2	8.721	8.563	8.563	.037	-.242	-1.1552	1.0000
11	2	0	17.951	17.924	-17.922	-.282	.027	.2396	1.0000
11	2	1	6.059	6.887	6.857	.077	-.798	-2.8420	1.0000

**

SILICONITE (BRANDYVINE SPINNS, AT 400 DEGREES C

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS

WEIGHTED P	NUMERATOR	DEPINOMINATOR	NUMER	R
13043.96	6769665.02		663	.044
UNWEIGHTED R	414.25	9046.41	663	.046

RANGES OF F (OBS)

3998.73	660028.97	500	.066
1516.45	1031711.35	66	.038
469.75	636724.79	39	.022
1010.45	1257597.26	16	.028
359.22	1115416.66	7	.017
2290.45	883196.64	3	.051
133.35	252093.75	1	.023
3319.49	393595.98	1	.091

RANGES OF (SIN(THETA)/LAMBDA)**2

4911.98	2270501.37	38	.046
4349.56	1758178.94	56	.050
756.98	752074.36	67	.032
512.05	192085.10	66	.029
455.24	346936.45	66	.027
478.87	396333.17	66	.035
376.81	379558.88	117	.022
1170.48	264996.74	112	.066

UNREJECTED REFLECTIONS

WEIGHTED R	UNWEIGHTED R	NUMER	R
7325.73	301.06	524	.035

RANGES OF F(OBS)

3767.14	657764.02	363	.046
1516.55	1031711.35	66	.038
465.75	636724.79	39	.022
1010.45	1287897.28	16	.028
339.22	1115416.66	7	.017
93.27	463447.70	2	.014
133.35	252093.75	1	.023
*C0	*C0	0	.000

RANGES OF (SIN(THETA)/LAMBDA)**2

2704.79	1659694.20	36	.038
1026.34	1359544.01	51	.027
737.34	751979.63	54	.031
490.58	591957.76	60	.029
451.94	346748.58	60	.036
447.45	396148.94	77	.034
358.51	379264.21	86	.031
1108.74	264718.23	83	.065

SUM FCAL 8931.90
 STANDARD DEV OF UNIT WEIGHT OBS 3.91

The thermal expansion and the high temperature crystal chemistry
of Al_2SiO_5 polymorphs

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and

Subrata Ghose

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Table #. ¹⁰ Sillimanite, andalusite and kyanite: observed and
calculated structure factors at various temperatures.

Sillimanite 600°C

LOAD MAP - REFINE

CYSED LOADEP 1.3-460

02/19/78 16.46.01

PAGE

FWA OF THE LOAD 111
LWALD OF THE LOAD 74743

TRANSFER ADDRESS -- REFINE 112

***** FEED SUMMARY

MP4105777 ON BLANK COMMON TRUNCATED BY 207000 WORDS

PROGRAM AND BLOCK ASSIGNMENTS

BLOCK	ADDRESS	LENGTH	FILE	DATE	PROCESSOR	VER	LEVEL	HARDWARE	COMMENTS
REFINE	111	10575	REFINE	05/14/76	RUN	F	74 B	646X I	
AA/	10704	1351	REFINE	05/14/76	RUN	C	74 B	646X I	
AC/	12262	457	REFINE	05/14/76	RUN	F	74 F	646X I	
AD/	12742	3244	REFINE	05/14/76	RUN	F	74 R	646X I	
AE/	16206	10	REFINE	05/14/76	RUN	F	74 R	646X I	
AF/	16216	174	REFINE	05/14/76	RUN	F	74 R	646X I	
AG/	14412	2307	REFINE	05/14/76	RUN	F	74 R	646X I	
AH/	20721	334	REFINE	05/14/76	RUN	F	74 R	646X I	
AI/	21253	1	REFINE	05/14/76	RUN	F	74 R	646X I	
AJ/	21273	311	REFINE	05/14/76	RUN	F	74 R	646X I	
AK/	21276	5726	REFINE	05/14/76	RUN	C	74 B	646X I	
AL/	27522	1147	REFINE	05/14/76	RUN	F	74 F	646X I	
AM/	30671	1312	REFINE	05/14/76	RUN	F	74 F	646X I	
AN/	32203	241	REFINE	05/14/76	RUN	F	74 F	646X I	
AO/	32444	231	REFINE	05/14/76	RUN	F	74 F	646X I	
AP/	32675	115	REFINE	05/14/76	RUN	F	74 F	646X I	
AQ/	33012	152	REFINE	05/14/76	RUN	F	74 F	646X I	
AR/	33164	73	REFINE	05/14/76	RUN	F	74 F	646X I	
AS/	33257	476	REFINE	05/14/76	RUN	F	74 F	646X I	
AT/	33755	361	REFINE	05/14/76	RUN	F	74 F	646X I	
AU/	34936	12	REFINE	05/14/76	RUN	F	74 F	646X I	
AV/	34950	136	REFINE	02/19/75	COMPASS	3	74150		
AW/	34505	55	REFINE	02/19/75	COMPASS	3	74150		
AX/	34563	72	REFINE	02/19/75	COMPASS	3	74150		
AY/	34655	44	REFINE	02/19/75	COMPASS	3	74150		
AZ/	34721	12	REFINE	02/19/75	COMPASS	3	74150		
BA/	34733	57	REFINE	02/19/75	COMPASS	3	74150		
BB/	35012	17	REFINE	02/19/75	COMPASS	3	74150		
BC/	35031	256	REFINE	02/19/75	COMPASS	3	74150		
BD/	35307	1052	REFINE	02/19/75	COMPASS	3	74150		
BE/	36361	244	REFINE	02/19/75	COMPASS	3	74150		
BF/	36625	1504	REFINE	02/19/75	COMPASS	3	74150		
BG/	40331	121	REFINE	03/17/75	COMPASS	3	74150		
BH/	40452	1310	REFINE	02/19/75	COMPASS	3	74150		
BI/	41762	71	REFINE	02/19/75	COMPASS	3	74150		
BJ/	42053	63	REFINE	02/19/75	COMPASS	3	74150		
BK/	42136	1122	REFINE	03/04/75	COMPASS	3	74150		
BL/	43260	31463	REFINE	03/04/75	COMPASS	3	74150		

H	K	L	F (OBS)	F (CALC)	A (CALC)	R (CALC)	DELTA F	DELTA/SIGMA	EXT.	FACTOR
0	0	2	63.018	64.325	-64.324	-0.350	-1.307	-9.0549		1.0000
0	0	4	132.414	143.860	-143.858	0.223	-11.444	-55.4853		1.0000
0	0	6	26.344	25.632	-25.630	0.278	0.412	1.3745	*	1.0000
0	0	8	41.315	50.650	-50.626	0.590	0.485	1.3929		1.0000
0	0	10	15.490	13.241	13.241	0.029	2.244	10.3365		1.0000
0	0	12	4.719	4.311	-4.311	-0.065	0.407	1.0210		1.0000
0	0	14	23.005	18.752	-18.745	0.507	4.223	23.0045		1.0000
0	0	16	6.270	6.072	6.071	0.063	1.946	1.0000		1.0000
0	0	18	7.542	6.539	6.539	0.027	0.704	3.7935		1.0000
0	0	20	1.074	1.207	-1.201	-0.059	0.778	1.0131		1.0000
0	0	22	8.576	8.015	8.005	0.407	0.581	4.2080	**	1.0000
0	0	24	4.322	4.522	4.522	0.054	-0.101	-0.7314		1.0000
0	0	26	9.063	2.142	2.142	0.021	1.723	5.2016		1.0000
0	0	28	21.330	19.565	19.565	-0.153	1.765	8.4537		1.0000
0	0	30	6.364	6.630	6.629	0.091	-0.265	-1.5897		1.0000
0	0	32	8.629	19.780	19.777	0.657	-1.373	-7.0651		1.0000
0	0	34	4.172	10.359	-10.359	-0.077	0.730	-4.2189		1.0000
0	0	36	2.363	5.801	5.799	-0.134	-1.629	-7.4488		1.0000
0	0	38	43.044	1.222	1.224	0.072	1.337	3.9280		1.0000
0	0	40	7.046	45.230	45.227	0.527	-2.185	-7.1807		1.0000
0	0	42	1.822	6.979	-6.978	-0.042	0.061	0.3565		1.0000
0	0	44	6.014	0.335	-0.322	-0.095	1.484	2.6926	**	1.0000
0	0	46	7.411	49.563	49.558	0.751	0.579	2.4954	**	1.0000
0	0	48	22.505	7.338	7.338	-0.021	0.072	0.4200		1.0000
0	0	50	1.083	23.704	-23.703	0.264	-1.200	-4.3624		1.0000
0	0	52	36.086	0.707	0.707	0.020	0.376	0.4867	**	1.0000
0	0	54	10.996	37.862	37.856	0.672	-1.776	-6.1539	**	1.0000
0	0	56	2.606	7.246	7.246	-0.015	0.021	0.1566		1.0000
0	0	58	18.968	11.744	-11.742	-0.210	-0.747	-5.1795		1.0000
0	0	60	5.840	1.725	1.725	0.014	0.681	1.6212	**	1.0000
0	0	62	1.425	16.506	16.505	0.194	0.462	1.5890	**	1.0000
0	0	64	21.876	2.270	2.269	-0.067	0.845	-1.1865	**	1.0000
0	0	66	4.129	5.361	-5.361	0.225	-0.635	-2.8041	**	1.0000
0	0	68	12.765	12.899	12.899	0.065	-1.292	-4.6716		1.0000
0	0	70	2.870	2.137	-2.136	-0.174	-0.138	-0.9248		1.0000
0	0	72	12.960	13.555	13.554	0.059	0.733	1.7625		1.0000
0	0	74	5.840	6.362	-6.359	-0.192	-0.595	-4.0009		1.0000
0	0	76	4.087	4.596	4.595	0.085	-0.501	-2.1924		1.0000
0	0	78	27.669	28.481	28.476	0.541	-0.813	-1.5542		1.0000
0	0	80	1.343	1.121	-1.118	-0.080	0.221	-3.1759	**	1.0000
0	0	82	6.977	5.225	5.222	-0.171	1.752	8.0512	**	1.0000
0	0	84	12.625	12.107	12.107	0.077	0.518	2.3560		1.0000
0	0	86	2.408	1.668	1.666	-0.074	0.740	2.4500		1.0000
0	0	88	9.175	9.239	9.239	0.069	-0.064	-0.4086		1.0000
0	0	90	1.249	1.796	1.795	-0.060	-0.547	-0.6131	**	1.0000
0	0	92	25.479	24.008	24.008	0.067	1.471	11.6640	**	1.0000
0	0	94	4.635	0.846	0.846	0.029	3.785	6.1904		1.0000
0	0	96	62.253	62.849	62.848	0.475	-0.597	-3.9200		1.0000
0	0	98	8.424	8.313	8.313	-0.028	0.111	0.6546		1.0000
0	0	100	13.107	14.234	14.234	0.061	-1.127	-6.2896		1.0000
0	0	102	4.328	4.959	4.959	0.026	-0.632	-2.9644		1.0000
0	0	104	29.023	28.244	28.242	0.381	-0.775	2.6485		1.0000

H	K	L	F(DRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGN/	FAI	FACTOR
1	1	7	4.666	4.487	4.487	-.024	.178	.7220	1.0000	
1	1	6	6.350	6.238	6.238	.046	.112	.5091	1.0000	
1	0	0	11.800	12.211	12.211	.461	-1.003	-7.6022	1.0000	
1	2	1	7.818	7.818	-7.818	-.044	-.287	-1.1729	1.0000	
1	2	2	15.462	15.522	-15.522	-.048	-.120	-.7863	1.0000	
1	2	3	2.342	1.862	-1.862	.042	.481	1.5864	1.0000	
1	2	4	4.672	4.750	-4.750	.412	-.839	-3.7016	1.0000	
1	2	5	7.150	7.855	-7.855	-.038	-.696	-4.3204	1.0000	
1	2	6	36.120	36.709	-36.709	-.358	-.581	-1.9656	1.0000	
1	2	7	1.255	1.987	-1.987	.034	-.732	-.8170	1.0000	
1	2	8	20.064	19.499	19.499	.295	.565	2.6140	1.0000	
1	2	0	46.565	47.069	47.069	.630	-.509	-3.1729	1.0000	
1	2	1	5.478	5.554	-5.554	-.011	-.078	-.2948	1.0000	
1	2	2	3.434	3.606	-3.606	-.090	-.179	-.8604	1.0000	
1	2	3	2.845	2.155	-2.155	.010	.693	2.4507	1.0000	
1	2	4	38.217	39.031	39.031	.584	-.814	-3.3902	1.0000	
1	2	5	5.676	6.003	-6.003	-.008	-.328	-1.5902	1.0000	
1	2	6	3.428	3.836	-3.836	.007	-.208	-.7337	1.0000	
1	2	7	2.598	2.839	-2.839	.007	-.241	-.5297	1.0000	
1	2	8	18.717	18.569	18.569	.405	.148	.7923	1.0000	
1	3	0	2.125	.770	-.689	-.344	1.355	3.6306	1.0000	
1	3	1	3.046	2.872	-2.872	-.030	.174	.6634	1.0000	
1	3	2	25.849	26.555	26.555	.334	-.686	-3.1031	1.0000	
1	3	3	6.142	6.972	6.972	.029	-.790	-3.8092	1.0000	
1	3	4	6.505	6.288	-6.288	.308	.237	1.5947	1.0000	
1	3	5	1.359	.866	-.866	-.027	.494	.7389	1.0000	
1	3	6	14.457	14.775	14.775	.268	-.318	-1.4423	1.0000	
1	3	7	5.506	5.329	-5.329	.025	.176	.7516	1.0000	
1	3	8	3.927	3.898	-3.898	-.220	.030	-.0665	1.0000	
1	4	0	10.990	10.054	10.054	.179	.936	4.7429	1.0000	
1	4	1	6.739	6.400	6.400	-.023	.339	1.7986	1.0000	
1	4	2	61.902	63.281	63.281	.314	-.137	-6.2109	1.0000	
1	4	3	2.129	1.011	-1.011	.024	1.119	2.6112	1.0000	
1	4	4	9.645	9.189	9.189	.161	.486	3.0642	1.0000	
1	4	5	4.520	4.977	4.977	-.021	-.457	-2.0148	1.0000	
1	4	6	28.233	29.311	29.311	.252	-.107	-4.5520	1.0000	
1	4	7	2.311	1.666	-1.666	.022	.645	1.1897	1.0000	
1	4	8	23.992	23.662	-23.662	-.153	-.571	-2.0667	1.0000	
1	5	1	3.170	2.850	2.850	.050	.320	.9996	1.0000	
1	5	2	1.144	.293	-.293	.149	.849	1.0400	1.0000	
1	5	3	5.090	5.023	-5.023	-.076	.066	.3602	1.0000	
1	5	4	15.753	16.159	16.159	-.137	.066	-.2.3670	1.0000	
1	5	5	1.187	.920	-.920	.070	.267	.3155	1.0000	
1	5	6	1.279	1.125	1.125	.119	.155	.1691	1.0000	
1	5	7	2.808	4.001	-4.001	-.061	-.119	-.2.5326	1.0000	
1	5	8	25.847	26.576	26.576	-.027	-.729	-2.5963	1.0000	
1	6	1	6.207	6.379	6.379	.043	-.172	-1.0547	1.0000	
1	6	2	41.241	42.312	42.312	.446	-.1.071	-3.9435	1.0000	
1	6	3	6.912	6.966	-6.966	-.041	-.053	-.3378	1.0000	
1	6	4	16.886	17.267	-17.267	-.023	-.981	-2.1231	1.0000	
1	6	5	3.594	3.137	3.137	.039	.456	1.4011	1.0000	
1	6	6	22.445	23.279	23.279	.374	-.834	-3.7564	1.0000	
1	6	7	31.711	32.201	32.201	.386	-.490	-1.6544	1.0000	

H	K	L	F(00S)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA	FXT	FACTPR
1	1	1	2.170 *	1.105	1.104	-.051	1.065	2.2604	1.0000	**
1	1	2	14.119	12.980	-12.974	-.375	1.135	6.6275	1.0000	
1	1	3	1.213 *	.055	-.026	.048	1.156	1.3366	1.0000	**
1	1	4	22.919	23.656	23.853	.345	-.936	-3.6591	1.0000	**
1	1	5	2.032 *	1.110	1.110	-.043	1.5318	1.0000	1.0000	**
1	1	6	7.480	7.999	-7.993	-.300	-.319	-1.6337	1.0000	**
1	1	7	32.626 *	31.558	31.555	.424	1.068	3.3599	1.0000	**
1	1	8	1.636 *	.688	-.688	-.016	.947	1.3939	1.0000	**
1	1	9	11.177	11.305	11.305	-.029	-.128	-.6182	1.0000	**
1	1	9	1.648 *	.974	.974	.016	.674	.6442	1.0000	**
1	1	9	23.621 *	24.101	24.096	.350	-.481	-2.2221	1.0000	**
1	1	9	2.241 *	.105	.104	-.012	2.188	3.6014	1.0000	**
1	1	9	20.065	19.635	-19.634	-.144	.634	1.0337	1.0000	**
1	1	10	4.100	3.960	3.959	-.091	.140	.4366	1.0000	**
1	1	10	6.263	6.277	6.275	.140	.000	.0285	1.0000	**
1	1	10	2.212 *	3.252	-3.252	.032	-1.7245	-1.5205	1.0000	**
1	1	10	14.516	15.083	-15.083	-.129	-.265	-1.5905	1.0000	**
1	1	11	5.207	5.172	5.169	.202	.024	.1199	1.0000	**
1	1	11	2.668 *	3.048	-3.047	-.031	-.375	-.7070	1.0000	**
1	1	11	2.694 *	2.653	2.651	.126	.641	.0772	1.0000	**
2	0	0	34.423	32.276	32.276	.100	2.147	14.5384	1.0000	**
2	0	2	45.504	44.656	44.654	.441	.648	5.1503	1.0000	**
2	0	4	15.920	15.927	15.927	.090	-.007	-.0334	1.0000	**
2	0	6	26.660	25.445	25.443	.354	1.214	3.9902	1.0000	**
2	0	6	5.506	4.606	4.605	.066	.900	2.5160	1.0000	**
2	0	0	90.400	93.432	-93.431	-.502	-3.032	-22.9687	1.0000	**
2	1	0	7.859	7.145	-7.144	-.628	.714	3.6598	1.0000	**
2	1	2	4.934	1.357	-1.266	.488	3.577	18.2411	1.0000	**
2	1	3	6.172	5.792	5.792	.027	.375	2.6641	1.0000	**
2	1	4	51.339	52.427	-52.425	-.449	-1.088	-4.6013	1.0000	**
2	1	5	1.102 *	1.226	-1.226	-.025	-.126	-.1574	1.0000	**
2	1	6	11.386	10.810	10.803	.390	.577	3.7353	1.0000	**
2	1	7	2.647	2.700	2.700	.024	-.052	-.1200	1.0000	**
2	1	8	20.233	20.087	-20.085	-.321	.747	3.7206	1.0000	**
2	2	0	62.235	61.102	61.101	.343	1.133	7.6133	1.0000	**
2	2	1	4.915	5.116	5.116	.058	-.201	-.5541	1.0000	**
2	2	2	13.720	13.224	13.222	.196	.496	2.9329	1.0000	**
2	2	3	4.440	4.012	-4.012	-.037	.428	2.0187	1.0000	**
2	2	4	35.896	35.858	35.856	.307	.359	.1599	1.0000	**
2	2	5	2.950	3.042	3.041	.048	-.052	-.3090	1.0000	**
2	2	6	10.046	10.070	10.068	.158	-.023	-.1482	1.0000	**
2	2	7	3.242	2.188	-2.188	-.041	1.054	2.6854	1.0000	**
2	2	8	13.854	13.373	13.371	.222	.481	2.8844	1.0000	**
2	2	9	63.072	59.335	59.335	-.107	2.737	22.1008	1.0000	**
2	3	1	14.574	13.573	-13.573	.083	1.001	6.0430	1.0000	**
2	3	2	8.762	8.146	8.146	.104	.616	3.5713	1.0000	**
2	3	3	5.040	4.697	4.697	-.084	.342	1.6621	1.0000	**
2	3	4	24.690	27.038	27.038	-.095	-.2148	-8.0410	1.0000	**
2	3	5	6.511	6.443	-6.443	.061	.068	.4253	1.0000	**
2	3	6	3.912	3.848	3.847	.083	.064	.2362	1.0000	**
2	3	7	1.504 *	1.479	-1.478	-.054	.025	.0313	1.0000	**
2	3	8	0.987	0.823	0.823	-.058	1.164	7.2210	1.0000	**
2	4	0	59.441	57.696	57.694	.369	1.746	9.1105	1.0000	**

H	K	L	F(RES)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	4	1	4.573	4.788	-4.788	-.051	-.215	-.9076	1.0000
2	4	2	4.454	4.704	4.701	.144	-.250	-1.1250	1.0000
2	4	3	4.150	4.147	4.147	.049	.000	.0376	1.0000
2	4	4	38.197	37.075	37.074	.330	-.278	-1.0824	1.0000
2	4	5	38.299	28.961	-7.561	-.043	.286	1.1461	1.0000
2	4	6	4.987	4.961	4.961	.116	-.345	-1.5063	1.0000
2	4	7	1.320	2.250	2.250	.039	-.530	-2.0950	1.0000
2	4	8	14.969	14.564	14.564	.298	.408	2.4622	1.0000
2	4	9	69.292	48.900	48.897	.530	.952	1.6085	1.0000
2	4	10	11.359	11.259	-11.259	-.052	.195	.6333	1.0000
2	4	11	73.439	75.108	-75.100	-.518	-1.663	-7.3048	1.0000
2	4	12	13.200	13.572	13.572	.051	-.346	-2.1932	1.0000
2	4	13	38.409	28.202	-28.202	.474	-.800	-2.6095	1.0000
2	4	14	2.419	2.925	-2.925	-.045	-.516	-1.8211	1.0000
2	4	15	36.767	37.935	-37.935	-.412	-1.171	-3.5452	1.0000
2	4	16	8.196	8.054	8.054	.040	.102	.5432	1.0000
2	4	17	22.990	22.047	22.047	.009	.543	3.4725	1.0000
2	4	18	2.055	1.567	-1.567	-.004	.492	1.6086	1.0000
2	4	19	22.456	21.930	21.927	.571	.526	2.6362	1.0000
2	4	20	1.134	1.919	1.919	.005	-.185	-.8275	1.0000
2	4	21	14.139	14.157	14.157	.003	-.016	-.1107	1.0000
2	4	22	1.210	.944	-1.944	-.003	.265	.3069	1.0000
2	4	23	13.624	13.766	13.763	.296	-.142	-.6063	1.0000
2	4	24	1.344	.729	-.729	.005	.615	.6410	1.0000
2	4	25	18.308	17.914	-17.912	-.283	.396	1.7824	1.0000
2	4	26	1.663	1.274	-1.273	-.018	1.385	2.4306	1.0000
2	4	27	29.398	29.367	29.385	.278	.031	.0383	1.0000
2	4	28	4.163	4.150	-4.150	.018	-.027	-.1058	1.0000
2	4	29	13.952	13.987	-13.987	-.293	-.015	-.0954	1.0000
2	4	30	7.691	3.170	-3.170	-.017	-.480	-1.0690	1.0000
2	4	31	16.731	16.480	16.479	.220	.240	1.4424	1.0000
2	4	32	25.594	25.250	25.249	.225	.345	1.1081	1.0000
2	4	33	2.835	1.847	-1.846	.049	.988	2.6642	1.0000
2	4	34	8.748	8.662	8.660	.190	.135	.9127	1.0000
2	4	35	1.735	1.625	-1.625	-.046	.117	-.1752	1.0000
2	4	36	17.601	18.172	18.171	.202	-.571	-2.9125	1.0000
2	4	37	2.737	1.417	-1.416	.043	1.320	2.8703	1.0000
2	4	38	5.654	5.655	5.655	.153	-.001	-.0031	1.0000
2	4	39	22.886	22.332	-22.331	-.223	.553	2.2730	1.0000
2	4	40	9.122	9.012	-9.012	.077	.105	.7090	1.0000
2	4	41	17.680	16.228	16.227	.217	-.548	-2.6266	1.0000
2	4	42	4.881	4.813	-4.812	-.074	.668	.2535	1.0000
2	4	43	16.572	17.029	-17.028	-.199	-.458	-2.3467	1.0000
2	4	44	9.194	9.196	9.195	.068	-.002	-.0090	1.0000
2	4	45	20.342	19.879	19.877	.279	.665	2.6243	1.0000
2	4	46	2.049	1.864	-1.864	-.037	.185	-.2846	1.0000
2	4	47	2.225	1.609	-1.607	.078	.616	1.0471	1.0000
2	4	48	1.367	1.771	1.771	.026	-.404	-1.4136	1.0000
2	4	49	14.661	15.005	15.003	.250	.344	-2.0629	1.0000
2	4	50	14.926	14.492	14.497	.353	.424	2.1755	1.0000
2	4	51	1.461	.518	-.516	-.052	.948	.9813	1.0000
2	4	52	16.572	16.154	-16.150	-.343	.378	2.1626	1.0000
2	4	53	6.034	5.764	-5.764	-.031	.270	1.3303	1.0000

SILLIMANITE (SILICON) SPRINGS, VT 600 DEGREES C

STRUCTURE FACTORS

SCALE 1

H	K	L	F(OBS)	F(CALC)	Δ(C%)(C)	Δ(C%)(C)	Δ(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	0	3	5.252	4.553	4.553	0.020	.698	3.1409	1.0000	*
3	0	5	4.676	4.840	4.560	-.024	-.164	-.5684	1.0000	*
3	0	7	4.271	4.736	4.736	.021	-.467	-1.4525	1.0000	*
3	1	0	13.054	15.863	15.863	.569	-2.810	-12.0416	1.0000	*
3	1	1	5.463	4.452	-4.452	-.085	.010	.7452	1.0000	*
3	1	1	87.991	26.151	36.151	-.045	1.825	9.7124	1.0000	*
3	1	1	2.895	2.856	-2.856	.082	.729	2.6752	1.0000	*
3	1	1	23.043	22.545	22.545	.527	1.054	4.0434	1.0000	*
3	1	1	7.045	7.045	-7.045	.075	-.001	-.0067	1.0000	*
3	1	1	10.025	11.028	11.028	-.025	-.090	-.3709	1.0000	*
3	1	1	2.689	1.517	-1.517	.966	.872	1.6336	1.0000	*
3	1	1	12.197	12.041	12.041	.379	.176	1.6379	1.0000	*
3	1	1	26.154	26.695	26.695	.198	.469	2.5374	1.0000	*
3	2	0	2.126	4.947	4.947	.007	.179	.8510	1.0000	*
3	2	2	21.291	36.202	36.202	-.192	.076	.3889	1.0000	*
3	2	2	8.521	9.334	9.334	-.006	.187	.6714	1.0000	*
3	2	4	18.391	16.962	16.962	.177	-.571	-2.7239	1.0000	*
3	2	4	1.170	2.018	2.018	.005	-.247	-.4815	1.0000	*
3	2	4	17.230	17.234	-17.234	-.002	-.002	-.0166	1.0000	*
3	2	6	4.657	5.046	5.046	-.003	.156	-.5957	1.0000	*
3	2	6	6.373	8.147	8.147	.326	.427	1.4033	1.0000	*
3	2	6	33.779	33.484	-33.484	-.285	.295	1.4292	1.0000	*
3	2	6	4.439	4.247	4.247	.009	.197	.8551	1.0000	*
3	2	6	102.740	104.301	104.301	.788	-.156	-7.4764	1.0000	*
3	2	6	2.144	1.649	1.649	-.007	.465	-1.1094	1.0000	*
3	2	6	21.514	21.550	-21.550	-.255	-.615	-3.0499	1.0000	*
3	2	6	5.200	5.061	5.061	.007	.139	.6854	1.0000	*
3	2	6	50.851	51.066	51.066	.632	-.236	-.7710	1.0000	*
3	2	6	2.759	2.601	2.601	-.004	.137	.2971	1.0000	*
3	2	6	9.597	9.012	9.012	-.191	.587	3.4233	1.0000	*
3	2	6	8.140	5.956	5.956	-.140	.218	10.1425	1.0000	*
3	2	6	7.010	6.959	6.959	.027	.052	.2560	1.0000	*
3	2	6	14.711	14.487	14.487	.136	.222	1.2627	1.0000	*
3	2	6	2.345	.931	-.931	-.024	1.455	3.5556	1.0000	*
3	2	6	1.125	1.285	1.285	-.125	-.160	-.1985	1.0000	*
3	2	6	5.767	5.891	5.891	.022	-.104	-.5449	1.0000	*
3	2	6	6.936	7.165	7.165	.109	-.230	-1.2359	1.0000	*
3	2	6	2.796	1.945	1.945	-.016	.850	1.48764	1.0000	*
3	2	6	29.676	27.760	27.760	.341	1.616	7.4523	1.0000	*
3	2	6	3.673	3.428	3.428	.079	.244	.6574	1.0000	*
3	2	6	1.173	.799	-.799	.125	.380	.4510	1.0000	*
3	2	6	1.119	.672	-.668	-.075	.447	.5594	1.0000	*
3	2	6	21.525	22.163	22.163	.324	-.646	-2.9468	1.0000	*
3	2	6	2.337	2.410	2.410	.071	-.073	-.1644	1.0000	*
3	2	6	1.291	.352	-.337	.100	.935	1.6181	1.0000	*
3	2	6	3.049	2.474	-2.474	.061	.576	1.2893	1.0000	*
3	2	6	17.6240	17.675	-17.675	-.077	-.435	-1.9675	1.0000	*
3	2	6	1.166	1.075	1.075	-.018	.091	.1091	1.0000	*
3	2	6	1.614	2.077	2.077	.075	-.463	-.8066	1.0000	*
3	2	6	1.818	1.157	-1.157	.017	.661	1.2405	1.0000	*
3	2	6	11.923	11.779	-11.779	-.069	.244	.9259	1.0000	*
3	2	6	2.562	2.498	-2.498	-.013	.143	.4634	1.0000	*
3	2	6	1.320	.589	-.586	.060	.731	.7756	1.0000	*

H	K	L	F(INS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	FVT	FACTOR
3	6	7	1.651 *	1.506	-1.506	.012	.146	.1825	1.0000	* **
3	7	0	03.173	62.586	62.586	.598	.566	2.1760	1.0000	
3	7	1	11.301	10.870	-10.870	-.090	.430	2.8080	1.0000	
3	7	2	6.227	5.776	-5.776	-.153	.471	2.6666	1.0000	
3	7	3	10.353	10.601	10.600	.087	-.246	-1.7665	1.0000	
3	7	4	45.728	46.348	46.348	.536	-.622	-1.6744	1.0000	
3	7	5	6.572	6.437	-6.437	-.077	.135	1.4770	1.0000	
3	7	6	4.394	4.699	4.699	-.121	-.205	-.9517	1.0000	
3	8	0	18.666	15.459	-15.459	-.165	.705	1.0799	1.0000	
3	8	1	2.998	3.338	3.338	-.015	-.293	-.9420	1.0000	
3	8	2	2.998	3.334	3.334	-.160	1.764	3.7715	1.0000	
3	8	3	2.646	1.726	-1.726	-.015	.520	2.0771	1.0000	
3	8	4	11.930	11.430	-11.429	-.012	-.046	-.3064	1.0000	
3	8	5	3.125	2.713	-2.712	-.159	.412	.9587	1.0000	
3	8	6	17.707	17.257	-17.257	-.029	1.137	1.2167	1.0000	
3	9	0	1.309	1.172	-1.172	-.029	-.346	-1.63780	1.0000	
3	9	1	26.974	27.321	27.315	.528	1.116	1.1712	1.0000	
3	9	2	1.334	1.218	-.117	-.007	1.184	1.1252	1.0000	
3	9	3	13.002	12.818	-12.817	-.042	.986	.9942	1.0000	
3	9	4	1.389	.403	-.402	-.007	.630	3.5348	1.0000	
3	10	0	12.475	11.846	-11.846	-.027	.036	.1351	1.0000	
3	10	1	5.180	5.142	5.142	.021	.036	.1351	1.0000	
3	10	2	2.856	.219	-.219	-.035	.635	5.5873	1.0000	
3	10	3	5.348	4.531	-4.531	-.019	.817	3.0308	1.0000	
3	11	0	7.624	7.056	-7.056	-.119	.568	2.6244	1.0000	
3	11	1	4.939	5.332	5.332	.076	-.394	-1.2942	1.0000	
4	0	0	77.865	75.944	-75.943	-.241	1.777	9.6006	1.0000	
4	0	1	67.463	67.043	-67.038	-.425	1.441	2.1963	1.0000	
4	0	2	42.998	44.666	44.666	.175	-.668	-6.6351	1.0000	
4	0	3	39.622	39.377	39.372	-.003	.245	.7887	1.0000	
4	0	4	19.868	18.258	-18.258	-.151	1.605	8.3761	1.0000	
4	0	5	22.617	22.357	22.355	-.021	.260	1.2157	1.0000	
4	1	1	1.313	2.667	-2.667	-.057	1.354	-2.0350	1.0000	
4	1	2	21.126	21.104	-21.103	-.024	.022	.0596	1.0000	
4	1	3	1.169	.917	-.915	-.053	.252	.3021	1.0000	
4	1	4	17.005	16.884	-16.882	-.050	.121	.4489	1.0000	
4	1	5	2.353	.642	-.640	-.050	3.9241	3.9240	1.0000	
4	1	6	12.367	11.972	-11.970	-.211	.397	2.5020	1.0000	
4	1	7	1.337	.958	-.958	-.041	.378	.3964	1.0000	
4	1	8	8.069	7.556	-7.554	-.041	.513	2.5728	1.0000	
4	2	0	77.878	75.661	-75.660	-.054	11.6346	11.6346	1.0000	
4	2	1	2.094	1.704	-1.704	-.015	.391	.9240	1.0000	
4	2	2	36.775	36.764	36.764	.068	.010	.0460	1.0000	
4	2	3	2.631	1.107	-1.107	-.015	1.524	3.5933	1.0000	
4	2	4	48.013	48.000	47.999	-.015	.013	.0508	1.0000	
4	2	5	2.428	1.815	-1.815	-.015	.613	1.4578	1.0000	
4	2	6	16.544	16.282	-16.282	-.015	.262	1.3813	1.0000	
4	2	7	3.358	2.178	-2.178	-.015	1.180	3.0172	1.0000	
4	2	8	19.393	18.444	-18.444	-.292	.947	4.8541	1.0000	
4	3	0	5.436	3.999	-3.999	-.049	5.7138	5.7138	1.0000	
4	3	1	11.827	11.703	-11.703	-.109	1.436	.6308	1.0000	
4	3	2	5.297	4.184	-4.184	-.048	1.113	5.1691	1.0000	
4	3	3	9.308	9.603	9.603	.105	-.296	-1.4902	1.0000	

H	K	L	F(CALC)	F(OBS)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	FXT. FACTOR
4	3	4	1.814	2.050	-1.914	.044	1.144	3.2472	1.0000
4	3	5	6.522	6.457	-6.522	-.093	-.065	-.3452	1.0000
4	3	6	1.431	1.742	1.411	-.039	.331	.5024	1.0000
4	3	7	4.553	4.946	4.553	.083	.393	1.4118	1.0000
4	4	4	5.771	5.046	5.771	.592	1.2221	1.2221	1.0000
4	4	5	1.794	2.167	-1.794	-.085	.373	.7891	1.0000
4	4	6	35.562	34.546	-35.562	-.062	-1.016	-4.0432	1.0000
4	4	7	5.354	5.043	5.354	.084	-.291	-1.4737	1.0000
4	4	8	40.353	39.738	40.353	.521	.616	2.1772	1.0000
4	4	9	1.981	1.860	.981	-.031	.675	1.0011	1.0000
4	4	0	15.836	14.205	-15.836	-.064	.367	2.2020	1.0000
4	4	1	4.588	5.079	4.588	.030	.491	1.7636	1.0000
4	4	2	29.120	29.404	-29.120	-.282	.694	2.4149	1.0000
4	4	3	.611	1.364	.609	.047	.757	1.0102	1.0000
4	4	4	25.100	25.389	25.159	.274	.225	.8287	1.0000
4	4	5	1.045	2.326	-1.046	-.044	1.275	3.0747	1.0000
4	4	6	21.238	21.435	-21.236	-.252	.197	.8575	1.0000
4	4	7	1.264	1.243	1.263	.041	-.020	-.0227	1.0000
4	4	8	14.371	14.161	14.349	.220	-.216	-1.8264	1.0000
4	4	9	1.375	1.375	-1.211	-.033	.167	.1698	1.0000
4	4	0	15.074	15.074	15.537	-.174	-.464	-2.3927	1.0000
4	4	1	3.782	3.782	-4.732	.026	-.950	-3.5126	1.0000
4	4	2	42.156	42.156	40.403	.613	1.749	6.3310	1.0000
4	4	3	1.472	1.472	.172	-.023	1.298	1.8251	1.0000
4	4	4	8.772	8.772	9.026	-.155	-.254	-1.7198	1.0000
4	4	5	5.165	5.165	-5.587	.022	-.422	-1.4575	1.0000
4	4	6	23.021	23.021	23.381	.491	-.360	-1.5751	1.0000
4	4	7	14.593	14.593	14.599	.165	-.018	-.0845	1.0000
4	4	8	1.219	1.219	-1.449	.057	.766	.8801	1.0000
4	4	9	11.446	11.446	-11.507	-.160	-.061	-.3787	1.0000
4	4	0	1.993	1.993	.096	-.054	1.883	3.4024	1.0000
4	4	1	10.250	10.250	10.772	.148	-.522	-3.2179	1.0000
4	4	2	1.376	1.376	.484	.051	.993	1.0000	1.0000
4	4	3	6.646	6.646	-6.647	-.129	-.175	-.7702	1.0000
4	4	4	21.012	21.012	20.904	.207	.108	.4355	1.0000
4	4	5	3.939	3.939	-3.741	.023	.198	.6617	1.0000
4	4	6	2.625	2.625	2.200	.193	.425	.9407	1.0000
4	4	7	6.260	6.260	6.319	-.022	-.035	-.2772	1.0000
4	4	8	15.560	15.560	15.490	.186	.355	.8555	1.0000
4	4	9	1.376	1.376	.488	.023	.888	.9037	1.0000
4	4	0	8.814	9.473	8.866	.105	.607	3.6654	1.0000
4	4	1	8.814	8.814	-8.464	-.089	.350	2.0027	1.0000
4	4	2	10.567	10.567	-10.191	-.102	.375	2.3282	1.0000
4	4	3	7.541	7.541	7.483	.085	.058	.2925	1.0000
4	4	4	7.393	7.393	6.757	.094	.636	3.0807	1.0000
4	4	5	29.058	29.058	28.102	.475	.957	3.5514	1.0000
4	4	6	3.086	3.086	-2.598	-.052	.489	1.0023	1.0000
4	4	7	7.379	7.379	-7.691	-.125	-.513	-1.4528	1.0000
4	4	8	2.355	2.355	-.147	.051	2.200	3.6474	1.0000
4	4	9	3.924	3.924	4.012	-.085	-.089	-.5028	1.0000
4	4	0	6.782	6.782	-6.226	.083	.515	3.1978	1.0000
4	4	1	3.008	3.008	-3.245	-.074	-.738	-.6611	1.0000
4	4	2	2.762	2.762	-2.483	.069	.278	.5609	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT.	FACETP
5	1	0	14.869	13.364	13.361	.285	1.505	7.0996		1.0000
5	1	1	7.921	7.603	7.603	.078	.318	1.4863		1.0000
5	1	2	32.922	33.244	33.244	.225	-.292	-1.1950		1.0000
5	1	3	11.150	11.251	-11.250	-.074	-.101	-.47120		1.0000
5	1	4	13.613	12.645	12.646	.255	.964	5.3791		1.0000
5	1	5	1.692	1.545	1.544	.066	.147	.2354		1.0000
5	1	6	16.276	16.167	16.166	.192	.105	.6059		1.0000
5	1	7	7.681	7.158	-7.157	-.055	.523	2.6666		1.0000
5	2	0	64.258	65.059	-65.057	-.525	-.800	-3.6794		1.0000
5	2	1	13.994	14.158	14.158	.049	-.164	-.6574		1.0000
5	2	2	67.571	66.926	68.924	.511	-1.355	-5.8634		1.0000
5	2	3	6.176	6.651	-6.680	-.045	-.504	-2.7785		1.0000
5	2	4	45.309	45.589	-45.587	-.044	-.280	-1.0282		1.0000
5	2	5	10.068	9.930	9.930	.044	.137	.8764		1.0000
5	2	6	35.691	35.731	35.729	.408	-.050	-.1504		1.0000
5	2	7	1.375	.912	-.911	-.035	.467	.4742		1.0000
5	3	0	20.242	20.305	20.304	.211	-.063	-.2203		1.0000
5	3	1	3.832	4.378	4.378	.015	-.546	-1.6646		1.0000
5	3	2	36.595	38.754	38.753	.280	-.159	-.6307		1.0000
5	3	3	1.150	.452	.452	-.014	.698	.8491		1.0000
5	3	4	15.192	15.346	15.345	.150	-.154	-.8470		1.0000
5	3	5	4.632	5.040	5.040	.113	-.428	-1.7043		1.0000
5	3	6	19.110	19.155	19.154	.224	-.045	-.2306		1.0000
5	3	7	2.858	2.047	2.047	-.010	.611	1.6928		1.0000
5	4	0	8.111	6.588	6.577	.391	1.522	9.6346		1.0000
5	4	1	9.219	9.756	9.756	.034	-.537	-2.8720		1.0000
5	4	2	23.479	22.333	-22.330	-.380	1.145	4.0501		1.0000
5	4	3	9.857	10.350	-10.350	-.032	-.493	-2.9363		1.0000
5	4	4	7.345	7.550	7.542	.350	-.205	-1.3295		1.0000
5	4	5	4.191	3.685	3.685	.032	.506	1.7895		1.0000
5	4	6	13.244	12.917	-12.913	-.304	.327	2.0026		1.0000
5	4	7	6.646	6.235	-6.235	-.027	.412	1.7642		1.0000
5	5	0	11.944	10.926	10.924	.325	1.018	5.2439		1.0000
5	5	1	7.971	7.898	-7.898	-.080	.072	.4867		1.0000
5	5	2	14.091	14.278	14.278	.235	.613	3.5105		1.0000
5	5	3	4.367	4.264	4.263	.077	.102	.4096		1.0000
5	5	4	10.045	9.267	9.265	.201	.778	4.8597		1.0000
5	5	5	6.875	6.908	-6.908	-.067	-.033	-.1639		1.0000
5	5	6	7.957	7.771	7.768	.189	.187	.9849		1.0000
5	6	0	18.154	17.624	17.623	.177	.531	2.7051		1.0000
5	6	1	1.551	1.567	1.565	-.098	-.016	-.0239		1.0000
5	6	2	1.638	.963	-.947	-.171	.675	1.0136		1.0000
5	6	3	2.505	.754	.749	.085	1.751	4.0344		1.0000
5	6	4	13.031	12.958	12.957	.158	.074	.4026		1.0000
5	6	5	2.586	.895	.892	-.077	1.691	3.3106		1.0000
5	6	6	1.391	1.094	-1.085	-.137	.298	.2996		1.0000
5	7	0	24.386	24.839	24.838	.045	.003	.0140		1.0000
5	7	1	3.047	2.833	2.833	.045	.211	.5609		1.0000
5	7	2	19.807	19.807	19.806	.165	.071	.3458		1.0000
5	7	3	2.037	.968	-.967	-.042	1.069	1.8203		1.0000
5	7	4	17.832	18.360	18.379	.224	-.498	-2.7121		1.0000
5	7	5	2.277	2.868	2.868	.039	-.591	-.9823		1.0000
5	8	0	31.905	31.117	-31.114	-.440	.787	2.3282		1.0000

SILLIMANITE (BANDYVINE SPRINGS, AT 600 DEGREES C

STRUCTURE FACTORS

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
6	5	5	2.944 *	2.435	-2.434	.015	.410	.6630	1.0000
6	5	6	20.707	20.620	20.618	.252	.087	.5603	1.0000
6	6	0	37.479	36.346	36.342	.557	.467	-1.5220	1.0000
6	6	1	1.525 *	2.019	2.016	.009	-.193	-.2089	1.0000
6	6	2	2.411 *	3.110	-3.107	-.124	-.698	-1.4376	1.0000
6	6	3	2.209 *	1.735	-1.735	-.008	.475	.6609	1.0000
6	6	4	27.774	26.515	26.511	.499	-.741	-2.8794	1.0000
6	6	5	1.376 *	1.720	1.720	.009	-.363	-.2483	1.0000
6	6	6	10.428	9.740	9.739	.157	.688	3.8155	1.0000
6	7	0	7.167	6.886	-6.886	-.034	.279	1.4489	1.0000
6	7	1	17.554	17.270	-17.269	-.153	.284	1.4133	1.0000
6	7	2	9.011	8.577	8.577	.092	.434	2.5007	1.0000
6	7	3	7.699	7.427	7.426	.141	.272	1.3548	1.0000
6	7	4	1.408	1.597	-1.597	-.026	.285	-4.2873	1.0000
6	7	5	8.122	7.857	-7.856	.161	.265	1.3726	1.0000
6	7	6	4.195	3.727	-3.725	-.104	.468	1.3876	1.0000
6	7	7	12.997	12.998	12.996	.213	-.001	-.0049	1.0000
6	7	8	4.179	3.367	3.365	.100	.812	2.3389	1.0000
6	8	3	8.519	5.655	5.655	.145	-.176	-.6304	1.0000
6	8	4	15.350	15.102	15.102	.152	.248	1.2916	1.0000
6	8	5	5.897	5.986	-5.986	-.001	-.089	-.3358	1.0000
6	8	6	13.145	12.260	-12.259	-.147	.885	5.4495	1.0000
6	8	7	3.106	2.930	2.930	.001	.175	.3717	1.0000
6	8	8	14.216	14.432	14.431	.142	-.214	-1.2312	1.0000
6	9	0	15.376	15.159	-15.159	-.133	.180	.9803	1.0000
6	9	1	6.625	6.253	6.251	.122	.372	1.7476	1.0000
6	9	2	10.863	11.762	11.762	-.047	-.598	-5.4582	1.0000
6	9	3	1.184	1.623	1.623	.043	.661	.6632	1.0000
6	9	4	32.809	32.151	32.147	.512	.296	2.2968	1.0000
6	9	5	2.732	2.063	2.063	-.042	.689	1.6544	1.0000
6	9	6	7.997	8.168	8.168	-.041	-.171	-1.0407	1.0000
6	9	7	3.465	3.115	3.115	.039	.350	.9216	1.0000
6	9	8	17.966	17.765	17.760	.411	.101	.5164	1.0000
6	0	0	8.502	8.197	8.196	.098	.405	2.3820	1.0000
6	0	1	1.205	1.676	1.675	-.059	-.471	-.5479	1.0000
6	0	2	2.617	2.443	-2.441	-.095	.175	.4131	1.0000
6	0	3	2.711	2.332	2.331	.058	.375	.9295	1.0000
6	0	4	6.079	6.150	6.150	.023	-.071	-.3323	1.0000
6	0	5	3.901	2.457	2.456	-.049	1.445	4.2721	1.0000
6	0	6	2.927	1.856	-1.854	-.077	1.072	2.2109	1.0000
6	0	7	50.223	50.359	50.354	.723	-.136	-.4919	1.0000
6	0	8	2.409 *	1.552	-1.552	-.012	.857	1.9044	1.0000
6	0	9	20.416	20.177	-20.176	-.252	.238	1.0166	1.0000
6	1	2	1.718 *	.902	-.901	.011	.816	1.2336	1.0000
6	1	3	37.513	38.251	38.246	.647	-.738	-2.2737	1.0000
6	1	4	2.723	2.707	-2.707	-.009	.016	.0327	1.0000
6	1	5	12.266	12.017	-12.016	-.200	.246	1.5742	1.0000
6	1	6	11.583	11.597	-11.597	-.088	-.015	-.0771	1.0000
6	1	7	1.252 *	1.422	-1.419	-.083	-.169	-.1891	1.0000
6	1	8	1.257 *	2.101	2.101	.086	-.844	-.0397	1.0000
6	1	9	1.284 *	.638	-.633	.080	.646	.7039	1.0000
6	1	0	8.596	8.425	-8.425	-.079	.171	.9801	1.0000
6	1	1	3.595	3.372	-3.372	-.069	.223	.5690	1.0000

H	K	L	F(CRS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	WT. FACTOR
7	4	6	1.619 *	1.441	1.450	.069	.143	.1832	1.0000
7	5	0	5.069	4.495	4.497	.120	.571	2.3883	1.0000
7	5	1	4.210	4.744	4.744	-.038	-.526	-1.1442	1.0000
7	5	2	34.992	37.278	37.277	.304	-.896	-.8949	1.0000
7	5	3	2.236	2.337	-2.337	.037	.899	2.3057	1.0000
7	5	4	3.443	3.407	3.405	.108	.025	.0856	1.0000
7	5	5	3.934	3.612	3.613	-.034	.220	.5767	1.0000
7	5	6	4.535	4.987	4.987	-.012	-.452	-1.5554	1.0000
7	6	1	11.155	11.296	11.296	.119	-.141	-.5004	1.0000
7	6	2	4.842	5.245	5.245	.012	-.402	-1.4304	1.0000
7	6	3	7.799	8.020	-8.020	-.111	-.221	-1.1264	1.0000
7	6	4	3.790	3.729	3.729	-.011	.060	.1601	1.0000
7	6	5	8.457	8.521	8.521	.102	-.065	-.3234	1.0000
7	6	6	24.741	24.224	-24.223	-.151	.517	1.4866	1.0000
7	7	1	8.577	8.258	8.258	.059	.275	1.5201	1.0000
7	7	2	33.618	34.801	34.797	.526	-.163	-3.2490	1.0000
7	7	3	7.805	7.798	-7.798	-.095	.007	.0357	1.0000
7	7	4	19.021	18.536	-18.535	.134	.485	2.2082	1.0000
7	7	5	1.426 *	.594	-.588	.085	.832	.8175	1.0000
7	7	6	1.423 *	.837	.837	-.022	.586	.5765	1.0000
7	7	7	8.343	8.957	-8.957	-.092	-.114	-.5827	1.0000
7	7	8	2.451 *	1.317	-1.316	.022	1.134	1.5019	1.0000
7	7	9	27.168	26.239	26.234	.479	.925	3.2326	1.0000
7	8	0	1.948	1.157	1.157	-.016	.791	1.0239	1.0000
7	8	1	57.298	58.627	58.625	.439	-1.325	-4.6566	1.0000
7	8	2	3.501	2.350	2.349	.020	1.232	3.8341	1.0000
7	8	3	42.885	42.701	42.699	.293	.185	.5551	1.0000
7	8	4	3.534	1.087	1.087	.018	2.447	5.8671	1.0000
7	8	5	22.445	22.077	-22.074	-.351	.366	1.5827	1.0000
7	8	6	9.035	8.891	-8.891	-.063	.144	.9539	1.0000
7	8	7	20.854	20.980	20.976	.370	-.125	-.6315	1.0000
7	8	8	7.334	7.625	7.625	.062	-.291	-1.5844	1.0000
7	8	9	17.125	16.878	-16.875	-.341	.247	1.1900	1.0000
7	8	10	5.918	5.307	-5.307	-.053	.611	2.4083	1.0000
7	8	11	11.875	12.182	12.178	.297	-.307	-1.8295	1.0000
7	8	12	10.282	7.806	7.806	.154	2.474	14.9288	1.0000
7	8	13	5.510	5.576	5.576	.087	-.066	-.3038	1.0000
7	8	14	5.551	4.896	4.898	.250	.654	2.9609	1.0000
7	8	15	3.418	3.648	-3.647	-.082	-.232	-.6276	1.0000
7	8	16	5.538	6.006	6.004	.139	-.468	-1.8040	1.0000
7	8	17	4.279	4.394	4.394	.073	-.115	-.3320	1.0000
7	8	18	3.405	3.312	3.304	.232	.093	.2115	1.0000
7	8	19	3.343	4.260	4.259	-.074	-.916	-2.5317	1.0000
7	8	20	1.471 *	.135	-.052	.124	1.336	1.7107	1.0000
7	8	21	4.601	4.789	-4.788	.072	-.188	-.6932	1.0000
7	8	22	1.341 *	.517	-.503	-.117	.825	.8608	1.0000
7	8	23	4.098	3.187	3.187	-.666	.910	2.6824	1.0000
7	8	24	2.571 *	.999	.993	.109	1.572	2.6010	1.0000
7	8	25	11.276	11.534	11.534	.066	-.258	-1.5946	1.0000
7	8	26	5.539	5.537	-5.537	-.059	.002	.0099	1.0000
7	8	27	32.862	33.071	33.069	.353	-.209	-.6239	1.0000
7	8	28	2.571 *	2.840	2.840	.056	-.265	-.5110	1.0000
7	8	29	8.144	8.280	8.280	.060	-.135	-.6788	1.0000

F	K	L	F(OBS)	F(CALC)	A(CALC)	(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	4	5	4.118	4.884	-4.684	-.049	-.766	-2.0721	1.0000
2	5	0	31.712	32.070	32.066	.358	-.358	-1.0447	1.0000
3	5	1	7.992	8.338	-8.335	-.055	-.345	-1.8463	1.0000
4	5	2	28.644	28.202	-28.199	-.388	.442	1.7508	1.0000
5	5	3	7.413	7.318	7.317	.095	.095	.4546	1.0000
6	5	4	24.557	24.508	24.505	.357	.056	.2148	1.0000
7	6	0	12.966	12.999	12.995	.355	-.034	-.1967	1.0000
8	6	1	2.100	.241	-.239	-.035	1.859	2.8427	1.0000
9	6	2	1.674	2.097	2.096	.038	-.423	-.4994	1.0000
10	6	3	3.637	2.283	2.283	.034	1.324	3.2810	1.0000
11	6	4	5.635	9.711	9.706	.318	-.077	-.4230	1.0000
12	7	0	13.145	13.104	-13.102	-.225	.041	.2276	1.0000
13	7	1	5.246	4.877	-4.677	-.063	.565	1.9407	1.0000
14	7	2	9.219	10.044	10.041	.219	-.623	-4.3595	1.0000
15	7	3	2.650	4.091	4.090	.002	-1.441	-2.4815	1.0000
16	8	0	11.501	11.668	11.666	.198	-.164	-.9059	1.0000
17	8	1	4.045	3.923	3.922	.068	.122	.6221	1.0000
18	8	2	1.453	2.404	2.404	-.006	-.951	-1.1145	1.0000
19	8	3	1.381	.039	.038	.007	1.342	1.3606	1.0000
20	0	5	2.313	3.178	3.178	-.001	-.864	-1.3384	1.0000
21	1	0	19.777	20.584	20.581	.328	-.807	-3.7306	1.0000
22	1	1	7.121	7.587	-7.586	-.139	-.467	-2.3925	1.0000
23	1	2	10.673	10.811	10.810	.094	-.198	-.7932	1.0000
24	1	3	8.769	8.967	8.966	.132	-.198	-1.0861	1.0000
25	1	4	15.333	15.731	15.728	.303	-.293	-2.2045	1.0000
26	1	5	3.923	3.518	-3.516	-.119	.405	1.0323	1.0000
27	2	0	30.765	31.169	31.166	.377	-.403	-1.1930	1.0000
28	2	1	2.155	2.172	2.172	-.006	-.017	-.0282	1.0000
29	2	2	32.851	33.575	-33.573	-.366	-.724	-2.0654	1.0000
30	2	3	2.740	3.216	3.216	.068	-.476	-.9278	1.0000
31	2	4	24.079	23.922	23.920	.356	.157	.4894	1.0000
32	2	5	1.436	.476	-.476	-.004	.963	.9383	1.0000
33	3	0	4.262	3.693	-3.693	-.007	.576	1.7731	1.0000
34	3	1	2.663	1.213	-1.213	-.016	1.445	2.9020	1.0000
35	3	2	24.778	24.883	24.880	.415	-.105	-.4004	1.0000
36	3	3	1.570	.801	-.801	.016	.765	.6580	1.0000
37	3	4	2.903	2.824	-2.824	-.006	.084	.1644	1.0000
38	4	0	3.102	3.635	-3.625	-.270	-.533	-1.1644	1.0000
39	4	1	3.348	2.033	2.033	.016	.515	1.2254	1.0000
40	4	2	10.957	10.933	10.929	.263	.025	.1567	1.0000
41	4	3	1.418	.809	-.908	-.013	.610	.4021	1.0000
42	4	4	2.803	2.609	-2.597	-.242	.195	.3657	1.0000
43	5	0	17.751	18.192	18.190	.261	-.441	-2.0357	1.0000
44	5	1	8.247	8.469	8.468	.141	-.222	-1.1120	1.0000
45	5	2	11.265	11.658	11.657	.127	-.393	-2.1940	1.0000
46	5	3	5.935	5.928	-5.926	-.133	.007	.0262	1.0000
47	5	4	12.233	11.326	-11.325	-.140	.507	5.6293	1.0000
48	6	0	1.438	1.358	1.358	.008	.088	.6781	1.0000
49	6	1	2.147	2.013	2.008	.136	.135	.1945	1.0000
50	7	0	12.919	12.722	12.718	.310	.198	1.1477	1.0000
51	7	1	4.257	4.032	-4.031	-.099	.224	.6122	1.0000
52	7	2	20.621	20.901	-20.900	-.229	-.260	-1.0205	1.0000
53	0	2	42.561	43.820	43.816	.623	-1.259	-3.5463	1.0000

H	K	L	F(DMS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
10	0	4	17.132	16.493	-16.492	-.204	.635	3.4130	1.0000
10	1	0	8.284	8.243	-8.243	-.048	.041	.2164	1.0000
10	1	1	1.720	2.114	2.113	.072	-.394	-.4712	1.0000
10	1	2	7.328	6.797	-6.797	-.036	.531	2.4812	1.0000
10	1	3	2.713	1.509	-1.509	-.072	1.204	2.2065	1.0000
10	1	4	6.946	6.136	-6.136	-.042	.813	3.4822	1.0000
10	2	0	16.076	16.817	16.813	.370	-.741	-3.7139	1.0000
10	2	1	4.207	3.024	3.023	.050	1.183	3.4263	1.0000
10	2	2	7.015	6.852	-6.852	.034	.163	.7135	1.0000
10	2	3	3.382	2.884	-2.883	-.076	.498	1.1273	1.0000
10	2	4	9.746	9.807	9.807	-.027	-.060	-.3410	1.0000
10	3	0	11.247	11.914	-11.913	-.134	-.667	-3.5703	1.0000
10	3	1	3.795	3.011	3.011	.026	.784	1.9598	1.0000
10	3	2	9.016	9.343	9.342	.129	-.227	-1.6760	1.0000
10	3	3	27.946	29.125	29.121	.472	-1.179	-6.2532	1.0000
10	4	0	5.807	5.344	-5.344	-.079	.462	1.6801	1.0000
10	4	1	6.405	5.688	-5.687	-.065	.718	2.6417	1.0000
10	4	2	1.454	.676	-.673	.059	.776	.7490	1.0000
10	5	0	2.929	1.838	-1.837	.038	1.091	2.5947	1.0000
10	5	1	4.344	3.716	-3.712	-.160	.629	-1.7426	1.0000
11	0	0	9.956	10.831	10.825	.353	-.875	-4.7599	1.0000
11	1	1	2.802	3.855	3.855	.051	1.053	-1.8987	1.0000
11	1	2	7.686	8.034	8.034	.021	-.349	-1.5624	1.0000
11	2	0	16.152	16.214	-16.212	-.257	-.062	-.2165	1.0000
11	2	1	5.440	6.046	6.045	.071	-.606	-2.0505	1.0000

SILLIMANITE (BRANDYWINE SPONGS, AT 600 DEGREES C

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS

WEIGHTED P	NUMERATOR	DENOMINATOR	NUMBER	P
10290.26	6837009.55		661	.039
UNWEIGHTED R	392.22	6673.66	661	.045

RANGES OF F(OBS)

3271.40	649969.78	505	.062
1423.07	947286.35	93	.039
660.36	1020445.83	37	.025
839.56	1233409.19	14	.026
377.91	1159596.69	7	.018
578.84	952097.52	3	.025
60.48	262176.52	1	.015
3078.61	412022.68	1	.086

RANGES OF (SIN(THETA)/LAMBDA)**2

3134.37	2412865.09	29	.036
3971.44	1810921.26	55	.047
688.64	748692.98	67	.030
485.53	575794.10	67	.029
587.98	326726.53	67	.042
349.08	379722.52	104	.030
410.06	342917.40	110	.035
662.98	239369.67	112	.052

UNREJECTED REFLECTIONS

WEIGHTED P	NUMERATOR	DENOMINATOR	NUMBER	P
6983.09	6422122.52		509	.039
UNWEIGHTED R	275.85	8261.04	509	.033

RANGES OF F(OBS)

2942.85	848106.43	354	.059
1423.07	947286.35	93	.039
660.36	1020445.83	37	.025
839.56	1233409.19	14	.026
377.91	1159596.69	7	.018
578.84	952097.52	3	.025
60.48	262176.52	1	.015
.00	.00	0	.000

RANGES OF (SIN(THETA)/LAMBDA)**2

3121.19	2412862.65	35	.036
885.89	1398823.26	49	.025
663.72	748597.44	55	.030
429.47	575566.22	66	.027
528.43	326504.62	66	.040
318.53	379423.41	82	.029
363.55	342532.84	80	.033
572.31	238848.07	73	.049

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STANDARD DEV OF UNIT WEIGHT OBS 3.86

The thermal expansion and the high-temperature crystal chemistry
of Al_2SiO_5 polymorphs

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Table I
Sillimanite, andalusite and kyanite: observed and
calculated structure factors at various temperatures.

Sillimanite 800°C

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	0	2	52.536	63.711	-63.710	-.346	-1.175	-8.4851	1.0000
0	0	4	130.200	140.702	140.700	.808	-10.502	-53.0573	1.0000
0	0	4	24.387	23.851	-23.850	-.265	.536	1.8632	1.0000
0	0	8	48.033	46.654	46.650	.546	1.379	4.1399	1.0000
0	0	2	15.565	13.221	13.221	.030	2.343	11.4636	1.0000
0	0	2	4.5310	4.536	-4.535	-.065	-.225	-.5396	1.0000
0	0	2	22.575	16.624	-16.617	.502	3.951	22.1377	1.0000
0	0	3	6.311	6.168	6.168	.062	.143	.8383	1.0000
0	0	4	7.318	6.341	6.341	.028	.977	5.8275	1.0000
0	0	5	1.045	.056	.010	-.056	.986	1.3245	1.0000
0	0	6	8.202	8.015	8.005	.388	.187	1.3517	1.0000
0	0	6	4.461	4.121	4.121	.049	.340	1.3952	1.0000
0	0	7	2.491	1.696	1.696	.021	.795	1.6293	1.0000
0	0	8	21.220	19.142	19.142	-.153	2.076	10.4979	1.0000
0	0	1	6.211	6.217	6.217	.081	-.006	-.0395	1.0000
0	0	2	87.435	88.736	88.734	.647	-1.301	-6.9526	1.0000
0	0	3	9.898	10.109	-10.109	-.076	-.211	-1.2189	1.0000
0	0	4	4.127	5.457	5.456	-.133	-1.330	-6.4706	1.0000
0	0	5	1.078	1.055	1.055	.070	.023	.0302	1.0000
0	0	6	41.029	43.162	43.159	.499	-2.133	-7.3030	1.0000
0	0	7	6.702	6.633	-6.633	-.056	.069	.3641	1.0000
0	0	8	1.283	.286	-.272	-.047	.997	1.0885	1.0000
0	0	4	48.261	47.537	47.532	.727	.723	3.2471	1.0000
0	0	1	6.726	6.928	6.928	-.020	-.202	-1.1201	1.0000
0	0	2	21.560	23.051	-23.050	-.255	-1.491	-5.5812	1.0000
0	0	3	1.056	.264	-.263	.020	.772	1.0235	1.0000
0	0	4	34.718	35.680	35.675	.639	-.962	-3.5308	1.0000
0	0	5	6.839	6.863	6.863	-.014	-.024	-.1513	1.0000
0	0	6	10.556	11.047	-11.045	.195	-.491	-3.2152	1.0000
0	0	7	2.677	1.918	1.918	.014	.759	1.6910	1.0000
0	0	8	18.666	17.741	17.740	.186	.924	4.1476	1.0000
0	0	1	1.925	1.836	1.835	-.066	.089	.1822	1.0000
0	0	2	20.605	21.389	21.388	.207	-.784	-3.5360	1.0000
0	0	3	4.307	4.805	-4.805	.064	-.498	-2.0929	1.0000
0	0	4	11.928	12.179	12.178	.164	-.251	-1.6676	1.0000
0	0	5	2.516	2.247	-2.247	-.055	.266	.5770	1.0000
0	0	6	12.298	12.513	12.512	.161	-.215	-1.5675	1.0000
0	0	8	6.648	6.704	-6.701	-.182	-.056	-.2796	1.0000
0	0	10	4.550	4.397	4.396	.081	.153	.5490	1.0000
0	0	2	25.948	26.254	26.249	.497	-.305	-1.2280	1.0000
0	0	3	2.320	1.053	-1.051	.074	1.267	2.4299	1.0000
0	0	4	7.474	5.455	-5.453	.159	2.019	10.6645	1.0000
0	0	1	12.630	12.073	12.072	.077	.558	2.6712	1.0000
0	0	3	2.613	2.009	2.008	-.072	.604	2.1814	1.0000
0	0	5	8.755	8.831	8.831	.066	-.077	-.4991	1.0000
0	0	7	2.918	2.128	2.128	-.055	.790	2.1609	1.0000
0	0	1	25.231	23.758	23.758	.066	1.473	12.3796	1.0000
0	0	1	5.263	1.091	1.091	.029	4.172	8.2068	1.0000
0	0	2	61.614	62.322	62.320	.473	-.708	-4.8159	1.0000
0	0	3	8.338	8.265	8.265	-.027	.073	.4563	1.0000
0	0	4	13.019	14.066	14.065	.060	-.447	-2.1741	1.0000
0	0	5	4.585	5.054	5.053	.025	-.469	-2.4895	1.0000
0	0	5	26.454	26.934	26.932	.366	-.480	-1.6436	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	1	7	4.407	4.331	4.331	-0.021	0.076	0.3091	1.0000
1	1	8	6.122	5.868	5.868	0.043	0.294	1.1564	1.0000
1	1	0	81.321	81.924	81.922	0.459	-0.603	-4.7550	1.0000
1	2	1	7.872	7.968	-7.988	-0.044	-0.116	-0.5190	1.0000
1	2	2	84.441	84.504	-84.502	-0.444	-0.062	-0.4007	1.0000
1	2	3	0.981	1.768	-1.767	0.042	-0.786	-1.1221	1.0000
1	2	4	45.400	46.372	46.370	0.403	-0.572	-4.4479	1.0000
1	2	5	7.415	7.818	-7.818	-0.037	-0.504	-3.0336	1.0000
1	2	6	34.532	34.772	-34.770	-0.342	-0.240	-0.5523	1.0000
1	2	7	1.220	1.865	-1.865	0.032	-0.645	-0.7402	1.0000
1	2	8	18.643	17.835	17.833	0.272	0.806	4.5812	1.0000
1	3	0	46.497	47.174	47.170	0.625	-0.677	-4.4413	1.0000
1	3	1	5.140	5.269	-5.269	-0.100	-0.129	-0.6693	1.0000
1	3	2	2.522	3.684	-3.683	-0.089	-1.161	-4.0362	1.0000
1	3	3	2.695	2.404	-2.404	0.100	0.291	1.0246	1.0000
1	3	4	37.369	38.531	38.528	0.549	-1.162	-5.0220	1.0000
1	3	5	5.105	5.678	-5.678	-0.007	-0.573	-3.2473	1.0000
1	3	6	4.156	3.837	-3.837	-0.067	0.316	1.3379	1.0000
1	3	7	3.049	2.880	-2.880	0.008	0.169	0.4662	1.0000
1	3	8	17.234	17.456	17.452	0.373	-0.223	-1.2092	1.0000
1	4	0	1.857	0.652	0.558	-0.338	1.765	2.8345	1.0000
1	4	1	2.898	3.048	-3.048	-0.029	-1.151	-0.5422	1.0000
1	4	2	25.162	25.917	25.914	0.327	0.755	-3.5421	1.0000
1	4	3	6.811	6.969	6.969	0.029	-0.158	-0.8279	1.0000
1	4	4	6.466	6.211	-6.204	-0.296	0.258	1.5509	1.0000
1	4	5	2.513	0.882	0.882	-0.025	1.650	4.7847	1.0000
1	4	6	13.956	13.976	13.973	0.252	-0.019	-0.1184	1.0000
1	4	7	5.200	4.954	4.954	0.023	0.237	1.0184	1.0000
1	4	8	4.775	3.743	10.061	-0.200	1.032	3.7722	1.0000
1	5	0	10.499	10.063	10.063	0.176	0.416	2.1267	1.0000
1	5	1	6.969	6.508	6.508	-0.024	0.461	2.6992	1.0000
1	5	2	59.178	60.846	60.845	0.303	-1.668	-7.8301	1.0000
1	5	3	1.105	1.061	-1.061	0.024	0.044	0.0560	1.0000
1	5	4	9.053	9.238	9.236	0.156	-0.184	-1.3011	1.0000
1	5	5	4.826	4.948	4.948	-0.020	-0.122	-0.6100	1.0000
1	5	6	26.232	26.887	26.886	0.235	-0.655	-2.6307	1.0000
1	5	7	2.656	1.555	1.555	0.021	1.102	2.4905	1.0000
1	6	0	23.040	23.322	-23.322	-0.151	-0.283	-1.0932	1.0000
1	6	1	3.413	2.678	2.677	0.079	0.735	2.6432	1.0000
1	6	2	1.104	0.150	0.033	0.146	0.955	1.2105	1.0000
1	6	3	4.445	4.745	-4.745	-0.074	-0.300	-1.4994	1.0000
1	6	4	15.080	15.410	-15.410	-0.132	-0.130	-0.7932	1.0000
1	6	5	2.038	0.881	0.878	0.067	1.157	2.4202	1.0000
1	6	6	1.596	1.182	1.176	0.112	0.415	0.5880	1.0000
1	6	7	4.197	3.677	-3.677	-0.056	0.519	1.7088	1.0000
1	7	0	24.422	25.281	-25.281	-0.030	-0.859	-3.1898	1.0000
1	7	1	6.200	6.495	6.495	0.043	0.295	-1.8687	1.0000
1	7	2	39.017	40.213	40.211	0.446	-1.196	-4.5317	1.0000
1	7	3	6.635	6.806	-6.806	-0.039	-0.172	-1.0862	1.0000
1	7	4	15.368	15.954	-15.954	-0.025	-0.586	-3.6885	1.0000
1	7	5	3.169	3.088	3.088	0.358	0.081	0.2339	1.0000
1	7	6	20.282	21.211	21.208	0.345	-0.929	-4.82325	1.0000
1	7	7	4.064	4.118	-4.118	-0.028	-0.054	-0.1655	1.0000