

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, Al_2-O_c , expands considerably. The orientation of the long Al_1-O_D 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-

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TABLE 5. Sillimanite, Andalusite, and Kyanite: Anisotropic thermal ellipsoids, axial lengths (Å) and isotropic equivalent temperature factors, B_{eq}^* (Å^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) | 0.68(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) | 0.98(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 | 0.098 | 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 | 0.093 | 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) |

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TABLE 7. Sillimanite, Andalusite, and Kyanite: Bond angles (θ) 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(8) | 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-Al 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 -Al ₂ | 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 -Si | 125.2(1) | 125.1(1) | 125.0(1) | 125.0(1) | 124.9(1) |
| | Al ₂ -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) |
| Si | D-D' | 106.1(2) | 106.2(2) | 106.1(1) | 106.2(1) | 106.4(1) |
| | 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) |
| | Ω_A | $\text{Al}_1^1\text{-Al}_1^1$ | 94.7(2) | 94.5(2) | 94.8(1) | 94.9(1) |
| Ω_B | $\text{Al}_1^1\text{-Al}_1^2$ | 130.7(1) | 130.8(1) | 130.78(6) | 130.82(5) | 130.92(7) |
| | $\text{Al}_1^1\text{-Si}_1^1$ | 98.6(2) | 98.7(2) | 98.8(1) | 98.7(1) | 98.9(1) |
| | $\text{Al}_1^1\text{-Si}_1^1$ | 124.6(1) | 124.8(1) | 124.84(6) | 124.99(6) | 125.15(7) |
| | Ω_C | Si-Al_2^1 | 123.7(2) | 123.8(2) | 123.9(1) | 123.9(1) |
| | Si-Al_2^1 | 130.3(2) | 130.4(2) | 130.1(1) | 130.1(1) | 130.1(1) |
| | $\text{Al}_2^1\text{-Al}_2^1$ | 106.0(2) | 105.9(2) | 106.0(1) | 106.0(1) | 105.9(1) |
| Ω_D | $\text{Al}_1^1\text{-Al}_2^1$ | 121.6(1) | 121.3(1) | 121.27(8) | 121.11(8) | 121.0(1) |
| | $\text{Al}_1^1\text{-Si}_1^1$ | 111.2(1) | 110.9(1) | 110.69(8) | 110.64(8) | 110.38(9) |
| | $\text{Al}_2^1\text{-Si}_1^1$ | 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 |
|-----------------|------|-----------|-----------|-----------|
| A1 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) |
| A1 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) |
| | G-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) |
| A1 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) |
| 0_A | $\text{Al}_4\text{-Al}_4$ | 92.57(7) | 92.58(8) | 92.50(9) |
| | $\text{Al}_4\text{-Si}_2$ | 130.60(9) | 130.7(1) | 130.6(1) |
| | $\text{Al}_4\text{-Si}_2$ | 127.69(9) | 127.6(1) | 127.9(1) |
| 0_B | $\text{Al}_1\text{-Al}_2$ | 94.44(7) | 94.62(8) | 94.6(1) |
| | $\text{Al}_1\text{-Al}_3$ | 95.44(7) | 95.50(8) | 95.49(9) |
| | $\text{Al}_1\text{-Al}_4$ | 101.05(7) | 101.12(8) | 101.1(1) |
| | $\text{Al}_2\text{-Al}_3$ | 164.31(9) | 164.0(1) | 163.9(1) |
| | $\text{Al}_2\text{-Al}_4$ | 96.61(7) | 96.67(8) | 96.89(9) |
| | $\text{Al}_3\text{-Al}_4$ | 93.42(7) | 93.46(8) | 93.47(9) |
| 0_C | $\text{Al}_2\text{-Al}_3$ | 97.26(7) | 97.32(8) | 97.28(9) |
| | $\text{Al}_2\text{-Si}_2$ | 128.81(9) | 129.1(1) | 129.0(1) |
| | $\text{Al}_3\text{-Si}_2$ | 126.83(9) | 126.7(1) | 126.8(1) |
| 0_D | $\text{Al}_2\text{-Al}_4$ | 96.08(7) | 96.12(8) | 96.01(9) |
| | $\text{Al}_2\text{-Si}_1$ | 129.12(9) | 129.3(1) | 129.3(1) |
| | $\text{Al}_4\text{-Si}_1$ | 126.73(9) | 126.8(1) | 127.0(1) |
| 0_E | $\text{Al}_3\text{-Al}_4$ | 94.66(7) | 94.74(8) | 94.81(9) |
| | $\text{Al}_3\text{-Si}_1$ | 131.40(9) | 131.5(1) | 131.5(1) |
| | $\text{Al}_4\text{-Si}_1$ | 124.32(8) | 124.3(1) | 124.4(1) |
| 0_F | $\text{Al}_1\text{-Al}_2$ | 94.51(7) | 94.67(8) | 94.66(9) |
| | $\text{Al}_1\text{-Al}_3$ | 99.43(7) | 99.71(8) | 99.7(1) |
| | $\text{Al}_1\text{-Al}_3$ | 95.71(7) | 95.72(8) | 95.60(9) |
| | $\text{Al}_2\text{-Al}_3$ | 97.57(7) | 97.89(8) | 98.0(1) |
| | $\text{Al}_2\text{-Al}_3$ | 161.30(9) | 160.8(1) | 160.8(1) |
| | $\text{Al}_3\text{-Al}_3$ | 96.15(7) | 96.24(8) | 96.14(9) |

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

John K. Winter

and

Subrata Ghose

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Seattle, Washington 98195

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 |
|--------|-------------|-----------|----------|----------|
| 0_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_1-Si_2 | 128.35(9) | 128.7(1) | 129.0(1) |
| 0_H | Al_1-Al_4 | 96.00(7) | 95.70(8) | 95.65(9) |
| | Al_1-Si_1 | 126.69(9) | 126.6(1) | 126.6(1) |
| | Al_4-Si_1 | 127.13(9) | 127.6(1) | 127.7(1) |
| 0_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) |
| 0_M | Al_1-Al_2 | 95.67(7) | 95.89(8) | 95.86(9) |
| | Al_1-Si_2 | 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 $^0_A-Al_1-^0_B$ angle etc.

LCD MAP - REFINER

CYBER LOADER 1.03-46C

02/28/78 17:30:00

PAGE

1

*** ERROR SUMMARY
 FWA OF THE LOAD
 LWA+1 OF THE LOAD
 TRANSFER ADDRESS -- REFINER

¹¹¹
 74743

112

NE4105// CM BLANK COMMON TRUNCATED BY 207008 WORDS

PROGRAM AND BLOCK ASSIGNMENTS

| BLOCK | ADDRESS | LENGTH | FILE | DATE | PROCESSOR | VER | LEVEL | HARDWARE | COMMENTS | |
|---|--|--|---|--|---|--|---|----------|----------|--|
| REFINE | 111 | 10575 | REFINE | 05/14/76 | RUN | F FB | 74 B | 646X I | | |
| /A/ | 10706 | 1355 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| /C/ | 12263 | 457 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| /D/ | 12742 | 324 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| /E/ | 16206 | 10 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| /F/ | 16216 | 174 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| /G/ | 16412 | 2307 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| /LS/ | 20721 | 334 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| /TAPE/ | 21255 | 6 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| /DEGEN/ | 21263 | 311 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| REFINE | 21574 | 5726 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| BUDAN1 | 27522 | 1147 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| ELVIBI | 30671 | 1312 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| INPUT | 32203 | 241 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| MATRIX | 32444 | 231 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| MODIFY | 32675 | 115 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| RCALC | 33012 | 152 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| RESET | 33164 | 73 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| SFAC | 33257 | 476 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| SYMINV | 33755 | 361 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| WEIGHT | 34336 | 12 | REFINE | 05/14/76 | RUN | F EB | 74 | 646X I | | |
| ASIN COS EXP | 34350 | 136 | SL-RUN2P3 | 02/19/75 | COMPASS | 3° | 74190 | | | |
| SIN COS | 34505 | 55 | SL-RUN2P3 | 02/19/75 | COMPASS | 3° | 74190 | | | |
| SORT | 34563 | 72 | SL-RUN2P3 | 02/19/75 | COMPASS | 3° | 74190 | | | |
| ACGOER | 34655 | 44 | SL-RUN2P3 | 02/19/75 | COMPASS | 3° | 74190 | | | |
| ENDFILE GETBA INPUTB KRAKER OUTPTB S10\$ INPUTC KODER OUTPTC RWINM SYSTEM | 34721 34733 35012 35031 35307 36361 1504 40331 40452 41762 42053 42136 31463 | 17 256 1052 244 57 17 256 244 1504 121 1310 63 1122 1122 31460 | SL-RUN2P3 | 02/19/75 02/19/75 02/19/75 02/19/75 02/19/75 02/19/75 02/19/75 02/19/75 03/17/75 02/19/75 02/19/75 02/19/75 02/19/75 03/17/75 02/19/75 | COMPASS | 3° 3° 3° 3° 3° 3° 3° 3° 3° 3° 3° 3° 3° 3° 3° | 74190 74190 74190 74190 74190 74190 74190 74190 74190 74190 74190 74190 74190 74190 74190 | | | |

LUG MAP - REFINING

CYBER LOADER 1.3-46C

02128178 17-30498

PAGE 2

*519 CP SECONDS

57300B CM STORAGE USED

2 TABLE MOVES

SILLIMANITE (GRANDY WINE SPRINGS) AT 25 DEGREES C

 STRUCTURE FACTORS
 DELTA F
 DELTA/SIGMA
 EXT. FACTOR
 PAGE 1

| | H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | | | |
|--|---|---|---|---------|---------|---------|---------|---------|----------|--------|
| | 0 | 0 | 2 | 63.835 | 65.656 | -65.655 | -3.53 | -1.771 | -11.693 | 1.0000 |
| | 0 | 0 | 4 | 137.351 | 150.666 | 150.664 | -8.54 | -13.315 | -61.5250 | 1.0000 |
| | 0 | 0 | 6 | 29.212 | 29.752 | -29.750 | -3.03 | -0.540 | -1.7429 | * |
| | 0 | 0 | 8 | 62.107 | 60.597 | 60.593 | -6.83 | 1.510 | 4.1736 | 1.0000 |
| | 0 | 0 | 0 | 12.521 | 12.808 | 12.808 | -0.24 | 2.713 | 12.0101 | 1.0000 |
| | 0 | 2 | 1 | 4.032 | 4.101 | -4.101 | -0.665 | -0.069 | -0.1770 | 1.0000 |
| | 0 | 0 | 2 | 22.863 | 18.668 | -18.661 | -5.22 | 4.195 | 21.6309 | 1.0000 |
| | 0 | 0 | 2 | 6.317 | 6.017 | 6.017 | -0.63 | 3.360 | 2.0410 | 1.0000 |
| | 0 | 0 | 3 | 9.013 | 8.096 | 8.096 | -0.23 | 9.917 | 5.4600 | 1.0000 |
| | 0 | 0 | 4 | 1.100 | *.351 | *.346 | -0.58 | 7.745 | .9534 | 1.0000 |
| | 0 | 0 | 5 | 7.832 | 7.512 | 7.498 | -4.50 | 2.0846 | 1.0000 | * |
| | 0 | 0 | 6 | 4.552 | 4.567 | 4.567 | -0.53 | -0.015 | 0.570 | 1.0000 |
| | 0 | 0 | 7 | 5.570 | 3.860 | 3.860 | -0.19 | 1.710 | 6.6633 | 1.0000 |
| | 0 | 0 | 8 | 21.194 | 20.165 | 20.165 | -1.48 | 1.028 | 4.6998 | 1.0000 |
| | 0 | 0 | 0 | 6.502 | 6.608 | 6.608 | -0.82 | -1.05 | -0.6093 | 1.0000 |
| | 0 | 0 | 1 | 90.031 | 91.758 | 91.756 | -1.77 | -1.727 | -6.4412 | 1.0000 |
| | 0 | 0 | 2 | 10.492 | 10.870 | -10.870 | -0.76 | -0.376 | -2.2980 | 1.0000 |
| | 0 | 0 | 3 | 5.606 | 7.239 | 7.237 | -1.37 | -1.633 | -9.4579 | 1.0000 |
| | 0 | 0 | 4 | 1.679 | *.948 | *.945 | -0.74 | -0.532 | *.8328 | 1.0000 |
| | 0 | 0 | 5 | 46.739 | 48.787 | 48.784 | -0.53 | -2.048 | -6.4386 | 1.0000 |
| | 0 | 0 | 6 | 7.960 | 8.025 | -8.025 | -0.64 | -0.065 | -3.3456 | 1.0000 |
| | 0 | 0 | 7 | 1.410 | *.787 | *.787 | -1.08 | -0.623 | .6187 | 1.0000 |
| | 0 | 0 | 8 | 55.858 | 54.958 | 54.952 | -0.815 | -1.329 | 1.329 | 1.0000 |
| | 0 | 0 | 0 | 8.003 | 8.497 | 8.497 | -0.22 | -4.94 | -1.6106 | 1.0000 |
| | 0 | 0 | 1 | 24.111 | 25.176 | -25.174 | -2.90 | -1.665 | -3.7506 | 1.0000 |
| | 0 | 0 | 2 | 1.109 | 1.037 | -1.037 | -0.23 | -0.072 | .0913 | 1.0000 |
| | 0 | 0 | 3 | 4.553 | 4.862 | 4.862 | -0.757 | -1.329 | -4.4966 | 1.0000 |
| | 0 | 0 | 4 | 8.641 | 8.808 | 8.808 | -0.19 | -0.166 | -1.0906 | 1.0000 |
| | 0 | 0 | 5 | 13.762 | 14.088 | -14.086 | -2.49 | -0.526 | -3.0684 | 1.0000 |
| | 0 | 0 | 6 | 2.375 | 2.097 | -2.097 | -0.20 | -0.65 | -3.7346 | 1.0000 |
| | 0 | 0 | 7 | 1.9439 | 1.9164 | -1.9163 | -0.202 | -0.274 | 1.3799 | 1.0000 |
| | 0 | 0 | 8 | 3.305 | 3.517 | 3.516 | -0.060 | -0.212 | -4.4966 | 1.0000 |
| | 0 | 0 | 9 | 24.657 | 25.586 | 25.585 | -0.83 | -0.926 | -6.4114 | 1.0000 |
| | 0 | 0 | 0 | 6.878 | 7.325 | -7.324 | -0.67 | -0.447 | -3.9263 | 1.0000 |
| | 0 | 0 | 1 | 13.841 | 14.102 | 14.101 | -0.18 | -0.261 | -2.4684 | 1.0000 |
| | 0 | 0 | 2 | 2.113 | *.784 | -1.783 | -0.60 | -0.329 | -1.6818 | 1.0000 |
| | 0 | 0 | 3 | 15.062 | 15.998 | 15.996 | -0.244 | -0.936 | .5437 | 1.0000 |
| | 0 | 0 | 4 | 3.661 | 3.764 | -3.758 | -0.219 | -0.103 | -5.1052 | 1.0000 |
| | 0 | 0 | 5 | 5.316 | 5.120 | 5.119 | -0.09 | -0.196 | -2.7271 | 1.0000 |
| | 0 | 0 | 6 | 33.168 | 33.943 | 33.937 | -0.62 | -0.776 | -1.0412 | 1.0000 |
| | 0 | 0 | 7 | 1.386 | *.743 | -0.737 | -0.93 | -0.643 | -6.497 | 1.0000 |
| | 0 | 0 | 8 | 3.171 | 3.060 | -3.054 | -3.03 | -0.09 | -1.110 | 1.0000 |
| | 0 | 0 | 9 | 12.630 | 12.312 | 12.312 | -0.78 | -0.318 | -1.3797 | 1.0000 |
| | 0 | 0 | 0 | 2.673 | 1.902 | 1.901 | -0.75 | -0.771 | 2.8582 | 1.0000 |
| | 0 | 0 | 1 | 9.521 | 9.766 | 9.766 | -0.69 | -0.245 | -1.4202 | 1.0000 |
| | 0 | 0 | 2 | 1.703 | *.491 | 2.490 | -0.62 | -0.788 | -1.1609 | 1.0000 |
| | 0 | 0 | 3 | 26.132 | 25.028 | 25.028 | -0.71 | -0.104 | 6.6461 | 1.0000 |
| | 0 | 0 | 4 | 4.960 | *.615 | *.615 | -0.27 | -0.345 | 1.0230 | 1.0000 |
| | 0 | 0 | 5 | 62.386 | 64.190 | 64.188 | -1.803 | -4.79 | -1.2127 | 1.0000 |
| | 0 | 0 | 6 | 9.123 | 8.813 | 8.813 | -0.26 | -3.10 | 1.8859 | 1.0000 |
| | 0 | 0 | 7 | 13.623 | 14.082 | 14.082 | -0.66 | -4.459 | -2.5065 | 1.0000 |
| | 0 | 0 | 8 | 4.551 | 5.021 | 5.021 | -0.25 | -0.460 | -1.5189 | 1.0000 |
| | 0 | 0 | 9 | 5.021 | 5.383 | 5.383 | -4.13 | -4.452 | 1.4802 | 1.0000 |

SILLIMANITE (GRANDYINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS

PAGE 2

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|---|--------|---------|---------|---------|---------|-------------|-------------|
| 1 | 1 | 7 | 5.491 | 5.431 | -0.021 | 0.060 | 0.2612 | 1.0000 | |
| 1 | 1 | 8 | 5.993 | 6.160 | +0.054 | -0.167 | -0.6677 | 1.0000 | |
| 1 | 2 | 0 | 6.811 | 6.860 | -0.058 | +0.465 | -0.3502 | 1.0000 | |
| 1 | 2 | 1 | 7.690 | 7.773 | -0.073 | +0.044 | +0.4370 | 1.0000 | |
| 1 | 2 | 2 | 8.987 | 8.056 | -0.087 | -0.456 | +1.070 | -0.2813 | 1.0000 |
| 1 | 2 | 3 | 2.577 | 2.352 | -0.235 | +0.043 | +0.225 | -0.7606 | 1.0000 |
| 1 | 2 | 4 | 4.8823 | 4.9835 | +0.432 | -0.432 | +1.014 | -0.42638 | 1.0000 |
| 1 | 2 | 5 | 7.672 | 8.236 | -0.088 | +0.039 | +0.567 | -0.37438 | 1.0000 |
| 1 | 2 | 6 | 4.0033 | 4.0710 | -0.393 | -0.393 | -0.678 | -0.678 | 1.0000 |
| 1 | 2 | 7 | 3.142 | 2.714 | -0.217 | +0.036 | +0.430 | +0.1538 | 1.0000 |
| 1 | 2 | 8 | 2.935 | 2.935 | +0.345 | +0.582 | +0.4750 | +0.4750 | 1.0000 |
| 1 | 3 | 0 | 4.5312 | 4.6291 | +0.642 | -0.980 | +0.980 | -0.58332 | 1.0000 |
| 1 | 3 | 1 | 6.135 | 6.835 | -0.085 | +0.011 | +0.300 | 1.06612 | 1.0000 |
| 1 | 3 | 2 | 2.6472 | 3.379 | -0.3378 | +0.091 | +0.907 | -0.29970 | 1.0000 |
| 1 | 3 | 3 | 2.2110 | * | -0.2127 | +0.011 | +0.084 | +0.2178 | 1.0000 |
| 1 | 3 | 4 | 3.8450 | 3.9325 | +0.596 | +0.824 | +0.824 | -0.32562 | 1.0000 |
| 1 | 3 | 5 | 5.6782 | 6.529 | -0.065 | +0.009 | +0.747 | -0.42665 | 1.0000 |
| 1 | 3 | 6 | 2.834 | 3.105 | -0.3104 | +0.078 | +0.271 | +0.7240 | 1.0000 |
| 1 | 3 | 7 | 2.810 | 3.214 | -0.3214 | +0.010 | +0.404 | +0.9034 | 1.0000 |
| 1 | 3 | 8 | 2.0204 | 2.0190 | +0.0184 | +0.477 | +0.14 | +0.0728 | 1.0000 |
| 1 | 3 | 9 | 2.375 | 2.424 | +0.424 | +0.363 | +1.131 | +0.2311 | 1.0000 |
| 1 | 4 | 0 | 3.078 | 2.821 | -0.2821 | +0.031 | +0.257 | +0.7997 | 1.0000 |
| 1 | 4 | 1 | 2.847 | 2.8719 | -0.3104 | +0.357 | +0.872 | -0.37997 | 1.0000 |
| 1 | 4 | 2 | 6.737 | 7.195 | -0.2127 | +0.010 | +0.404 | +0.9034 | 1.0000 |
| 1 | 4 | 3 | 2.0190 | 2.0184 | +0.0184 | +0.477 | +0.14 | +0.0728 | 1.0000 |
| 1 | 4 | 4 | 7.058 | 6.474 | -0.6465 | +0.337 | +0.584 | +0.59525 | 1.0000 |
| 1 | 4 | 5 | 1.155 | 1.399 | +1.399 | +0.373 | +0.243 | +0.2949 | 1.0000 |
| 1 | 4 | 6 | 16.612 | 16.996 | -0.2821 | +0.027 | +0.307 | +0.384 | 1.0000 |
| 1 | 4 | 7 | 6.011 | 5.817 | -0.194 | +0.025 | +0.194 | +0.8403 | 1.0000 |
| 1 | 4 | 8 | 3.193 | 4.362 | -0.4354 | +0.269 | +1.165 | -0.26017 | 1.0000 |
| 1 | 4 | 9 | 7.058 | 6.474 | -0.6465 | +0.337 | +0.584 | +0.59525 | 1.0000 |
| 1 | 5 | 0 | 10.528 | 9.190 | -0.180 | +0.180 | +1.337 | +0.230 | 1.0000 |
| 1 | 5 | 1 | 7.021 | 6.791 | -0.022 | +0.022 | +1.019 | +0.4570 | 1.0000 |
| 1 | 5 | 2 | 68.071 | 70.495 | -2.424 | -2.424 | +0.1119 | +0.1119 | 1.0000 |
| 1 | 5 | 3 | 1.211 | * | +0.022 | +0.022 | +0.089 | +0.089 | 1.0000 |
| 1 | 5 | 4 | 9.444 | 8.200 | +0.168 | +0.243 | +1.7442 | +1.7442 | 1.0000 |
| 1 | 5 | 5 | 5.110 | 5.823 | -0.018 | +0.018 | +3.2599 | +3.2599 | 1.0000 |
| 1 | 5 | 6 | 34.795 | 36.164 | -0.297 | -0.297 | +3.9392 | +3.9392 | 1.0000 |
| 1 | 5 | 7 | 3.141 | 1.300 | +0.019 | +0.019 | +1.595 | +1.595 | 1.0000 |
| 1 | 5 | 8 | 25.354 | -2.5449 | -0.153 | -0.153 | +3.7676 | +3.7676 | 1.0000 |
| 1 | 6 | 0 | 2.830 | 3.022 | +0.083 | +0.192 | +0.5150 | +0.5150 | 1.0000 |
| 1 | 6 | 1 | 1.172 | * | +0.022 | +0.022 | +0.5466 | +0.5466 | 1.0000 |
| 1 | 6 | 2 | 1.630 | -5.489 | -1.623 | +1.51 | +0.458 | +0.458 | 1.0000 |
| 1 | 6 | 3 | 5.509 | -5.488 | -0.080 | +0.080 | +0.020 | +0.020 | 1.0000 |
| 1 | 6 | 4 | 17.762 | 17.744 | -17.743 | +1.42 | +0.018 | +0.018 | 1.0000 |
| 1 | 6 | 5 | 1.226 | * | +0.902 | +0.74 | +0.325 | +0.325 | 1.0000 |
| 1 | 6 | 6 | 1.332 | * | +0.529 | +0.513 | +0.130 | +0.130 | 1.0000 |
| 1 | 6 | 7 | 5.457 | 4.735 | -4.734 | +0.066 | +0.722 | +0.722 | 1.0000 |
| 1 | 7 | 0 | 26.858 | 30.424 | -30.424 | +0.018 | +1.566 | +5.4258 | 1.0000 |
| 1 | 7 | 1 | 6.477 | 6.796 | +0.45 | +0.319 | +1.8082 | +1.8082 | 1.0000 |
| 1 | 7 | 2 | 4.639 | 4.664 | +0.514 | +1.025 | +3.6268 | +3.6268 | 1.0000 |
| 1 | 7 | 3 | 6.804 | 7.455 | -0.042 | +0.651 | +3.7213 | +3.7213 | 1.0000 |
| 1 | 7 | 4 | 20.424 | 21.194 | -0.016 | +0.770 | +3.7847 | +3.7847 | 1.0000 |
| 1 | 7 | 5 | 3.108 | 3.534 | +0.041 | +0.426 | +1.0475 | +1.0475 | 1.0000 |
| 1 | 7 | 6 | 27.858 | 28.952 | +0.443 | +1.094 | +3.9716 | +3.9716 | 1.0000 |
| 1 | 7 | 7 | 37.498 | 36.406 | +0.441 | +1.6211 | +3.6211 | +3.6211 | 1.0000 |

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS

PAGE 3

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR | |
|---|---|----|----------|---------|---------|---------|---------|-------------|--------------|--------|
| 1 | 9 | 1 | 2.0243 * | 2.060 | 2.059 | -0.056 | 0.183 | 3.3659 | 1.0000 * * * | |
| 1 | 8 | 2 | 1.5931 | 1.3862 | -13.655 | -0.431 | 0.069 | 4.4223 | 1.0000 | |
| 1 | 8 | 3 | 2.592 | 0.820 | -0.819 | -0.541 | 1.772 | 6.2325 | 1.0000 | |
| 1 | 8 | 4 | 2.6355 | 2.7899 | 27.896 | -0.409 | -1.544 | -5.8815 | 1.0000 | |
| 1 | 8 | 5 | 1.341 * | 2.012 | 2.012 | -0.500 | -0.222 | -6.911 | 1.0000 * * * | |
| 1 | 8 | 6 | 8.601 | 9.076 | -9.068 | -0.371 | -0.475 | -2.485 | 1.0000 | |
| 1 | 8 | 7 | 37.197 | 37.117 | 37.113 | -0.511 | -0.527 | -1.9560 | 1.0000 | |
| 1 | 9 | 0 | 1.963 * | 0.976 | -0.976 | -0.022 | 0.316 | 3.4225 | 1.0000 * * * | |
| 1 | 9 | 1 | 1.293 * | 1.4518 | 14.518 | -0.038 | -0.291 | -1.6395 | 1.0000 | |
| 1 | 9 | 2 | 1.6227 | 1.241 | 1.241 | -0.022 | 1.540 | 3.4009 | 1.0000 | |
| 1 | 9 | 3 | 2.762 | 2.8987 | 28.983 | -0.475 | -1.9560 | 1.0000 | 1.0000 | |
| 1 | 9 | 4 | 2.8460 | -0.207 | -0.206 | -0.018 | 1.777 | 2.5613 | 1.0000 * * * | |
| 1 | 9 | 5 | 1.963 * | 2.5599 | -25.598 | -0.193 | 0.668 | 2.4669 | 1.0000 | |
| 1 | 0 | 0 | 2.367 | 5.931 | 5.931 | -0.032 | -0.416 | 1.7657 | 1.0000 | |
| 1 | 0 | 1 | 6.348 | 9.004 | 9.002 | -0.191 | -0.205 | -1.1261 | 1.0000 | |
| 1 | 0 | 2 | 8.799 | -0.066 | -0.066 | -0.031 | 0.277 | 1.0084 | 1.0000 | |
| 1 | 0 | 3 | 5.349 | 5.072 | -5.072 | -0.072 | 0.277 | 1.5694 | 1.0000 | |
| 1 | 0 | 4 | 20.797 | 20.495 | -20.494 | -0.179 | 0.303 | 1.7265 | 1.0000 | |
| 1 | 0 | 5 | 5.432 | 5.480 | 5.474 | -0.246 | -0.300 | -1.1673 | 1.0000 | |
| 1 | 1 | 0 | 4.040 | 3.900 | -3.900 | -0.031 | -0.140 | -0.1261 | 1.0000 | |
| 1 | 1 | 1 | 11.0 | -0.066 | -0.066 | -0.185 | -0.147 | 0.5066 | 1.0000 | |
| 1 | 1 | 2 | 5.217 | 5.070 | -5.070 | -0.072 | 1.841 | 1.0413 | 1.0000 | |
| 1 | 1 | 3 | 33.851 | 32.010 | 32.010 | -0.096 | -0.409 | 1.7809 | 1.0000 | |
| 1 | 1 | 4 | 20.797 | 20.495 | -20.494 | -0.179 | 0.303 | 1.7265 | 1.0000 | |
| 1 | 1 | 5 | 4.487 | 4.547 | 4.545 | -0.454 | -0.048 | -0.0170 | 1.0000 | |
| 1 | 0 | 0 | 17.428 | 17.432 | 17.431 | -0.089 | -0.0404 | -0.0404 | 1.0000 | |
| 2 | 0 | 1 | 27.150 | 26.463 | 26.461 | -0.91 | -0.687 | 3.0413 | 1.0000 | |
| 2 | 0 | 2 | 6.878 | 6.469 | -6.469 | -0.072 | -0.409 | 1.7809 | 1.0000 | |
| 2 | 0 | 3 | 6.806 | 9.4686 | -9.4686 | -0.508 | -0.505 | -4.7622 | 1.0000 | |
| 2 | 0 | 4 | 7.312 | -7.312 | -7.312 | -0.027 | 2.2633 | 1.0000 | 1.0000 | |
| 2 | 1 | 1 | 1.634 | 1.505 | -1.620 | -0.499 | 4.7642 | 1.0000 | 1.0000 | |
| 2 | 1 | 2 | 6.140 | 6.285 | 6.285 | -0.027 | -0.145 | -7.993 | 1.0000 | 1.0000 |
| 2 | 1 | 3 | 5.403 | 5.950 | -5.948 | -0.471 | -0.657 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 1 | 4 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | * * * |
| 2 | 1 | 5 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 1 | 6 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 1 | 7 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 1 | 8 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 1 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 2 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 3 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 4 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 5 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 6 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 7 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 8 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 9 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 10 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 11 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 12 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 13 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 14 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 15 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 16 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 17 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 18 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 19 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 20 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 21 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 22 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 23 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 24 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 25 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 26 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 27 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 28 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 29 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 30 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 31 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 32 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 33 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 34 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 35 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 36 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 37 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 38 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 39 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 40 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 41 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 42 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 43 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 44 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 45 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 46 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 47 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 48 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 49 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 50 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 51 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 52 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 53 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 54 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 55 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 56 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 57 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 58 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 59 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 60 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 61 | 11.916 | 11.659 | 11.651 | -0.429 | -0.260 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 62 | 6.34 | 1.659 | -1.659 | -0.429 | -0.129 | 4.7642 | 1.0000 | 1.0000 |
| 2 | 2 | 63 | 4.225 | 3.366 | -3.366 | -0.022 | -0.860 | -7.993 | 1.0000 | 1.0000 |
| 2 | 2 | 64 | 6.140 | 6.285 | -6.285 | -0.027 | -0.145 | -3.6245 | 1.0000 | 1.0000 |
| 2 | 2 | 65 | 2.903 | 2.354 | -2.351 | -0.376 | -0.955 | 4.0773 | 1.0000 | 1.0000 |
| 2 | 2 | 66 | 5.4950 | 1.575 | -1.575 | -0.024 | 0.448 | -5.565 | 1.0000 | 1.0000 |
| 2 | 2 | 67 | 6.878 | 6.300 | -6.300 | -0.508 | -0.505 | 2.2633 | 1.0000 | 1.0000 |
| 2 | 2 | 68 | 1.127 * | 1.575 | -1.575 | -0.024 | 0.448 | 4.7642 | 1.0000 | 1.0 |

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS

PAGE 4

| 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 | -0.54 | -1.141 | -6.908 | 1.0000 | |
| 2 | 4 | 2 | 3.197 | 3.123 | 3.119 | 0.150 | -0.2534 | 1.0000 | | |
| 2 | 4 | 3 | 4.176 | 4.475 | 4.474 | 0.053 | -1.1694 | 1.0000 | | |
| 2 | 4 | 4 | 4.0609 | 4.1390 | 4.1390 | 0.359 | -0.299 | 1.0000 | | |
| 2 | 4 | 5 | 3.554 | 3.273 | -3.273 | -0.049 | -0.783 | -2.8930 | 1.0000 | |
| 2 | 4 | 6 | 3.289 | 3.794 | 3.792 | 0.130 | -0.280 | 0.9677 | 1.0000 | |
| 2 | 4 | 7 | 2.120 | 2.620 | 2.620 | 0.045 | -0.505 | -1.4236 | 1.0000 | |
| 2 | 4 | 8 | 19.568 | 18.926 | 18.923 | 0.285 | -0.546 | -7.978 | 1.0000 | |
| 2 | 5 | 0 | 52.145 | 51.621 | 51.621 | 0.558 | -0.642 | 3.5241 | 1.0000 | |
| 2 | 5 | 1 | 11.644 | 11.953 | -11.953 | -0.53 | -0.521 | 2.2610 | 1.0000 | |
| 2 | 5 | 2 | 76.819 | 78.629 | -78.627 | -1.010 | -0.209 | -1.7076 | 1.0000 | |
| 2 | 5 | 3 | 14.172 | 14.971 | 14.971 | 0.053 | -0.798 | -4.6229 | 1.0000 | |
| 2 | 5 | 4 | 38.816 | 39.855 | 39.852 | 0.118 | -1.039 | -3.6014 | 1.0000 | |
| 2 | 5 | 5 | 2.944 | 3.273 | -3.273 | -0.049 | -0.429 | -1.1549 | 1.0000 | |
| 2 | 6 | 6 | 41.809 | 43.057 | -43.054 | -0.470 | -1.248 | -3.6646 | 1.0000 | |
| 2 | 6 | 7 | 10.500 | 10.040 | 10.040 | 0.944 | -0.461 | 2.8032 | 1.0000 | |
| 2 | 6 | 8 | 25.272 | 25.038 | 25.038 | 0.098 | -0.234 | 0.6248 | 1.0000 | |
| 2 | 6 | 9 | 2.056 | 1.667 | -1.667 | -0.005 | 1.189 | 1.189 | 1.0000 | |
| 2 | 6 | 10 | 24.873 | 23.855 | 23.852 | 0.412 | -0.105 | 1.0115 | 1.0000 | |
| 2 | 6 | 11 | 1.967 | 1.441 | 1.441 | 0.007 | -0.426 | 0.8309 | 1.0000 | |
| 2 | 6 | 12 | 16.816 | 17.258 | 17.258 | 0.091 | -0.443 | -2.4459 | 1.0000 | |
| 2 | 6 | 13 | 1.246 | 1.065 | -1.065 | -0.004 | 0.181 | 0.2033 | 1.0000 | |
| 2 | 6 | 14 | 14.733 | 15.237 | 15.232 | 0.375 | -0.504 | -2.9367 | 1.0000 | |
| 2 | 6 | 15 | 1.395 | 0.885 | 0.885 | 0.007 | -0.511 | 0.5124 | 1.0000 | |
| 2 | 6 | 16 | 23.387 | 23.422 | -23.420 | -0.329 | -0.035 | -1.1607 | 1.0000 | |
| 2 | 7 | 1 | 1.186 | * 3.03 | * 3.02 | -0.015 | -0.884 | 1.0420 | 1.0000 | |
| 2 | 7 | 2 | 34.079 | 34.371 | 34.369 | 0.325 | -0.291 | 0.291 | 1.0000 | |
| 2 | 7 | 3 | 5.339 | 5.045 | -5.045 | -0.014 | -0.294 | 0.9851 | 1.0000 | |
| 2 | 7 | 4 | 18.743 | 18.606 | -18.603 | -0.305 | -0.137 | 1.3967 | 1.0000 | |
| 2 | 7 | 5 | 3.825 | 3.800 | -3.800 | -0.013 | -0.025 | 0.7115 | 1.0000 | |
| 2 | 7 | 6 | 19.886 | 20.573 | 20.571 | 0.279 | -0.687 | -3.1934 | 1.0000 | |
| 2 | 7 | 7 | 30.779 | 29.564 | 29.562 | 0.263 | 1.215 | 3.8480 | 1.0000 | |
| 2 | 7 | 8 | 3.407 | 2.579 | 2.579 | 0.053 | 0.828 | 2.4910 | 1.0000 | |
| 2 | 7 | 9 | 9.073 | 9.057 | 9.055 | 0.221 | -0.016 | 0.1054 | 1.0000 | |
| 2 | 7 | 10 | 1.825 | 2.205 | -2.205 | -0.054 | -0.286 | -0.6047 | 1.0000 | |
| 2 | 7 | 11 | 22.331 | 22.530 | 22.529 | 0.245 | -0.199 | -0.8992 | 1.0000 | |
| 2 | 7 | 12 | 2.389 | * 2.018 | 2.018 | 0.053 | 0.370 | 0.6582 | 1.0000 | |
| 2 | 8 | 1 | 5.701 | 5.667 | 5.664 | 0.191 | -0.035 | 0.1282 | 1.0000 | |
| 2 | 8 | 2 | 26.026 | 25.265 | -25.264 | -0.243 | -0.760 | 3.0185 | 1.0000 | |
| 2 | 8 | 3 | 10.322 | 10.335 | 10.335 | 0.083 | -0.013 | 0.0850 | 1.0000 | |
| 2 | 8 | 4 | 25.878 | 25.904 | 25.902 | 0.351 | -0.241 | -1.5626 | 1.0000 | |
| 2 | 8 | 5 | 22.640 | 22.982 | 22.981 | 0.241 | -0.342 | -0.2522 | 1.0000 | |
| 2 | 8 | 6 | 5.358 | 5.240 | -5.240 | -0.079 | -0.118 | 0.4484 | 1.0000 | |
| 2 | 8 | 7 | 19.687 | 19.963 | -19.962 | -0.225 | -0.277 | -1.4523 | 1.0000 | |
| 2 | 8 | 8 | 11.565 | 11.273 | 11.272 | -0.074 | -0.293 | 1.8232 | 1.0000 | |
| 2 | 8 | 9 | 10 | 1.394 | 1.645 | -1.645 | -0.044 | -0.026 | -0.9449 | 1.0000 |
| 2 | 8 | 10 | 1.410 | * | 1.755 | 1.752 | -0.100 | -0.251 | -1.5626 | 1.0000 |
| 2 | 8 | 11 | 1.422 | * | 1.576 | 1.575 | -0.044 | -0.251 | -0.2522 | 1.0000 |
| 2 | 8 | 12 | 20.499 | 20.595 | 20.593 | 0.326 | -0.096 | -0.4769 | 1.0000 | |
| 2 | 8 | 13 | 17.292 | 16.960 | 16.954 | 0.458 | -0.332 | 1.7236 | 1.0000 | |
| 2 | 8 | 14 | 1.445 | * | 3.367 | 3.381 | -0.067 | 1.0246 | 1.0246 | 1.0000 |
| 2 | 8 | 15 | 21.470 | 21.470 | 21.470 | -0.447 | -0.399 | 2.0188 | 1.0000 | |
| 2 | 8 | 16 | 6.717 | 6.085 | 6.085 | -0.037 | -0.632 | 3.2777 | 1.0000 | |

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS PAGE 5

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA SIGMA | EXT. FACTOR | |
|---|---|----|---------|---------|---------|---------|---------|-------------|-------------|--------|
| 3 | 0 | 3 | 4.791 | 4.408 | 4.408 | .036 | .363 | 1.7775 | 1.0000 | |
| 3 | 0 | 5 | 5.918 | 5.521 | 5.521 | -.032 | .397 | 2.2221 | 1.0000 | |
| 3 | 1 | 5 | 5.438 | 5.139 | 5.139 | -.033 | .299 | 1.1928 | 1.0000 | |
| 3 | 0 | 7 | 12.391 | 15.658 | 15.647 | -.030 | -3.267 | -1.82941 | 1.0000 | |
| 3 | 1 | 1 | 4.715 | 4.908 | 4.907 | -.087 | -.193 | -.5696 | 1.0000 | |
| 3 | 1 | 2 | 3.213 | 3.659 | 3.659 | -.045 | 1.554 | 7.8201 | 1.0000 | |
| 3 | 1 | 3 | 4.055 | 3.257 | 3.256 | -.084 | .798 | 3.3069 | 1.0000 | |
| 3 | 1 | 4 | 23.918 | 22.388 | 22.381 | -.557 | 1.530 | 5.4834 | 1.0000 | |
| 3 | 1 | 5 | 7.555 | 7.753 | 7.753 | -.077 | -.195 | -1.3245 | 1.0000 | |
| 3 | 1 | 6 | 13.492 | 13.609 | 13.609 | -.038 | -.117 | -.6951 | 1.0000 | |
| 3 | 1 | 7 | 3.378 | 2.673 | 2.672 | -.059 | .705 | 1.6114 | 1.0000 | |
| 3 | 1 | 8 | 12.386 | 12.495 | 12.487 | -.446 | -.107 | -.6783 | 1.0000 | |
| 3 | 2 | 0 | 29.401 | 28.613 | 28.613 | -.195 | .787 | 4.1075 | 1.0000 | |
| 3 | 2 | 1 | 6.150 | 5.976 | 5.976 | -.009 | .174 | 1.9492 | 1.0000 | |
| 3 | 2 | 2 | 39.765 | 40.109 | 40.109 | -.191 | -.344 | -1.6533 | 1.0000 | |
| 3 | 2 | 3 | 10.655 | 10.707 | 10.707 | -.009 | -.051 | -.2760 | 1.0000 | |
| 3 | 2 | 4 | 18.770 | 19.604 | 19.603 | -.162 | -.834 | -.8513 | 1.0000 | |
| 3 | 2 | 5 | 2.005 | * | 1.311 | -.009 | .693 | 1.4092 | 1.0000 | |
| 3 | 2 | 6 | 19.117 | 19.352 | 19.352 | -.165 | -.235 | -1.1114 | 1.0000 | |
| 3 | 2 | 7 | 6.458 | 6.657 | 6.657 | -.007 | .199 | -.8814 | 1.0000 | |
| 3 | 2 | 8 | 9.557 | 9.451 | 9.450 | -.145 | -.5731 | 1.0000 | * | |
| 3 | 3 | 0 | 34.636 | 34.342 | 34.341 | -.300 | .294 | 1.4215 | 1.0000 | |
| 3 | 3 | 1 | 3.650 | 3.810 | 3.810 | -.009 | -.152 | -.5427 | 1.0000 | |
| 3 | 3 | 2 | 106.051 | 110.295 | 110.292 | -.008 | -.244 | -10.6609 | 1.0000 | |
| 3 | 3 | 3 | 1.174 | * | 2.653 | -.629 | -.244 | 1.0000 | * | |
| 3 | 3 | 4 | 23.269 | 24.340 | 24.338 | -.276 | -.1376 | -1.6445 | 1.0000 | |
| 3 | 3 | 5 | 4.852 | 5.484 | 5.484 | -.008 | -.071 | -.6955 | 1.0000 | |
| 3 | 3 | 6 | 5.827 | 5.974 | 5.974 | -.714 | -.632 | -.7692 | 1.0000 | |
| 3 | 3 | 7 | 3.511 | 3.539 | 3.539 | -.006 | -.691 | -.21647 | 1.0000 | |
| 3 | 3 | 8 | 12.809 | 11.975 | 11.973 | -.221 | -.028 | -.0738 | 1.0000 | |
| 3 | 3 | 9 | 10.817 | 8.725 | 8.725 | -.146 | -.092 | 5.4684 | 1.0000 | |
| 3 | 3 | 10 | 7.968 | 7.939 | 7.938 | -.032 | -.036 | 1.4140 | 1.0000 | |
| 3 | 3 | 11 | 15.013 | 15.275 | 15.275 | -.145 | -.262 | 1.571 | 1.0000 | |
| 3 | 3 | 12 | 3.104 | 1.874 | 1.873 | -.031 | -.021 | -.026 | 1.0000 | |
| 3 | 3 | 13 | 1.835 | * | 2.863 | -.136 | -.071 | -.4250 | 1.0000 | |
| 3 | 3 | 14 | 7.228 | 7.300 | 7.299 | -.029 | -.111 | -.6626 | 1.0000 | |
| 3 | 3 | 15 | 8.341 | 8.230 | 8.229 | -.125 | -.286 | 2.5112 | 1.0000 | |
| 3 | 3 | 16 | 2.653 | * | 1.367 | -.025 | 1.231 | 3.6514 | 1.0000 | |
| 3 | 3 | 17 | 31.916 | 30.469 | 30.467 | -.401 | -.136 | 1.9837 | 1.0000 | |
| 3 | 3 | 18 | 4.952 | 4.653 | 4.653 | -.062 | -.026 | 1.3273 | 1.0000 | |
| 3 | 3 | 19 | 2.984 | 2.332 | 2.328 | -.123 | -.028 | 1.8320 | 1.0000 | |
| 3 | 3 | 20 | 1.575 | * | 0.079 | -.008 | -.078 | 1.4946 | 1.0000 | |
| 3 | 3 | 21 | 16.985 | 18.044 | 18.044 | -.079 | -.071 | 2.4859 | 1.0000 | |
| 3 | 3 | 22 | 24.620 | 24.616 | 24.613 | -.373 | -.396 | -1.7351 | 1.0000 | |
| 3 | 3 | 23 | 3.491 | 3.794 | 3.794 | -.075 | -.303 | -.9294 | 1.0000 | |
| 3 | 3 | 24 | 1.329 | * | 6.641 | -.632 | -.075 | .7648 | 1.0000 | |
| 3 | 3 | 25 | 3.174 | 2.290 | 2.289 | -.025 | -.078 | -.745 | 1.0000 | |
| 3 | 3 | 26 | 16.985 | 18.044 | 18.044 | -.064 | -.071 | -.981 | 1.0000 | |
| 3 | 3 | 27 | 24.620 | 24.616 | 24.613 | -.373 | -.396 | -.066 | 1.0000 | |
| 3 | 3 | 28 | 1.190 | * | 1.493 | -.493 | -.025 | -.014 | 1.519 | 1.0000 |
| 3 | 3 | 29 | 4.578 | 4.752 | 4.752 | -.072 | -.175 | -.7648 | 1.0000 | |
| 3 | 3 | 30 | 1.194 | * | 9.981 | -.981 | -.025 | -.213 | -.2504 | 1.0000 |
| 3 | 3 | 31 | 12.519 | 12.542 | 12.542 | -.066 | -.071 | -.9544 | 1.0000 | |
| 3 | 3 | 32 | 2.280 | * | 2.793 | -.022 | -.304 | -.512 | -.6516 | 1.0000 |
| 3 | 3 | 33 | 1.375 | * | 2.015 | -.014 | -.025 | -.014 | -.6516 | 1.0000 |

SILLIMANITE (GRANDYMIKE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS

PAGE 6

| M | K | L | F(CBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|----|---|---------|---------|---------|---------|---------|-------------|-------------|
| 3 | 6 | 7 | 1.625 * | 1.611 | -1.831 | .021 | -1.186 | -2.212 | 1.0000 * ** |
| 3 | 7 | 0 | 70.172 | 69.884 | 69.880 | .667 | .288 | 1.0231 | 1.0000 |
| 3 | 7 | 1 | 12.869 | 12.447 | -12.446 | -.098 | .422 | 2.0103 | 1.0000 |
| 3 | 7 | 2 | 5.196 | 4.751 | -4.746 | -.163 | .4447 | -3.8920 | 1.0000 |
| 3 | 7 | 3 | 11.836 | 12.443 | 12.443 | .095 | .606 | -3.4751 | 1.0000 |
| 3 | 7 | 4 | 52.150 | 53.299 | 53.295 | .619 | 1.138 | -1.1834 | 1.0000 |
| 3 | 7 | 5 | 7.534 | 7.571 | -7.571 | -.086 | .037 | 1.1556 | 1.0000 |
| 3 | 7 | 6 | 4.194 | 4.248 | -4.245 | -.139 | .054 | 1.3969 | 1.0000 |
| 3 | 7 | 7 | 18.536 | 18.242 | 18.241 | -.186 | .379 | 1.4627 | 1.0000 |
| 3 | 8 | 0 | 4.600 | 4.222 | 4.222 | -.019 | .379 | 1.1944 | 1.0000 |
| 3 | 8 | 1 | 1.277 | 1.453 | 1.443 | -.177 | .177 | 1.0000 | ** ** |
| 3 | 8 | 2 | 2.895 | 2.684 | -2.684 | -.018 | .211 | .4896 | 1.0000 |
| 3 | 8 | 3 | 13.719 | 13.877 | 13.876 | .172 | .157 | 1.3036 | 1.0000 |
| 3 | 8 | 4 | 3.296 | 3.620 | 3.620 | -.016 | .330 | 1.7556 | 1.0000 |
| 3 | 8 | 5 | 23.731 | 28.897 | -2.896 | -.198 | .634 | 1.0000 | ** ** |
| 3 | 8 | 6 | 1.359 | .398 | -.397 | -.014 | .961 | .9899 | 1.0000 |
| 3 | 8 | 7 | 35.191 | 34.776 | 34.770 | .654 | .415 | 1.1685 | 1.0000 |
| 3 | 9 | 2 | 1.380 | * .332 | -.332 | -.012 | .048 | 1.0639 | 1.0000 |
| 3 | 9 | 3 | 17.926 | 17.894 | -17.893 | -.163 | .068 | 1.3733 | 1.0000 |
| 3 | 9 | 4 | 1.422 | * .525 | -.525 | -.014 | .897 | .8836 | 1.0000 |
| 3 | 9 | 5 | 16.20 | 15.503 | -15.503 | -.067 | .777 | 1.0804 | 1.0000 |
| 3 | 9 | 6 | 9.393 | 7.706 | 7.706 | .034 | .687 | 1.4763 | 1.0000 |
| 3 | 9 | 7 | 1.432 | * .466 | -.466 | .070 | .967 | 1.9449 | 1.0000 |
| 3 | 9 | 8 | 7.013 | 6.812 | -6.812 | -.032 | .322 | 1.4192 | 1.0000 |
| 3 | 9 | 9 | 9.416 | 8.926 | 8.924 | .181 | .490 | 1.4964 | 1.0000 |
| 3 | 10 | 0 | 7.780 | 6.742 | 6.741 | .089 | .035 | 1.035 | 1.0000 |
| 3 | 10 | 1 | 79.933 | 78.355 | -78.353 | -.243 | 1.539 | 1.6863 | 1.0000 |
| 3 | 10 | 2 | 6.932 | 6.795 | 6.795 | .779 | .885 | 1.2026 | 1.0000 |
| 3 | 10 | 3 | 45.065 | 47.148 | 47.148 | -.084 | .284 | 1.8661 | 1.0000 |
| 3 | 10 | 4 | 43.159 | 42.578 | 42.572 | -.672 | .591 | 1.8382 | 1.0000 |
| 3 | 10 | 5 | 7.916 | 21.153 | -21.152 | -.179 | .043 | 4.5255 | 1.0000 |
| 3 | 10 | 6 | 23.867 | 24.302 | 24.300 | .288 | .434 | 1.9570 | 1.0000 |
| 3 | 10 | 7 | 2.978 | 2.881 | -2.881 | .061 | .097 | 1.3673 | 1.0000 |
| 3 | 11 | 1 | 21.534 | 21.699 | -21.697 | -.282 | .235 | 1.6142 | 1.0000 |
| 3 | 11 | 2 | 1.198 | * 1.329 | 1.328 | -.058 | .131 | 1.1535 | 1.0000 |
| 3 | 11 | 3 | 18.903 | 18.828 | 18.826 | .267 | .075 | 3.374 | 1.0000 |
| 3 | 11 | 4 | 1.702 | * .073 | -.073 | .055 | .626 | 2.6286 | 1.0000 |
| 3 | 11 | 5 | 13.693 | 13.536 | -13.534 | -.243 | .157 | .9093 | 1.0000 |
| 3 | 11 | 6 | 1.369 | * .432 | -.432 | -.048 | .938 | .9587 | 1.0000 |
| 3 | 11 | 7 | 10.060 | 9.243 | 9.240 | .213 | .818 | 4.5191 | 1.0000 |
| 3 | 11 | 8 | 82.348 | 80.326 | 80.327 | .477 | .019 | 1.0136 | 1.0000 |
| 3 | 11 | 9 | 1.113 | * 1.804 | -1.804 | .010 | .691 | 1.8696 | 1.0000 |
| 3 | 12 | 0 | 37.309 | 38.045 | 38.045 | .068 | .736 | 1.1602 | 1.0000 |
| 3 | 12 | 1 | 1.562 | 1.090 | -1.090 | -.039 | .472 | .6950 | 1.0000 |
| 3 | 12 | 2 | 52.839 | 53.369 | 53.368 | .443 | .536 | 2.0149 | 1.0000 |
| 3 | 12 | 3 | 3.509 | 2.578 | -2.578 | .009 | .931 | 2.9595 | 1.0000 |
| 3 | 12 | 4 | 17.053 | 17.328 | 17.328 | .060 | .274 | 1.3733 | 1.0000 |
| 3 | 12 | 5 | 1.391 | * 2.124 | -2.124 | -.007 | .732 | .7377 | 1.0000 |
| 3 | 12 | 6 | 24.323 | 23.372 | 23.370 | .355 | .951 | 3.7916 | 1.0000 |
| 3 | 12 | 7 | 7.029 | 5.402 | -5.402 | .052 | 1.628 | 6.3919 | 1.0000 |
| 3 | 13 | 0 | 13.026 | 13.060 | -13.059 | -.118 | .033 | 1.1706 | 1.0000 |
| 3 | 13 | 1 | 4.850 | 4.356 | -4.356 | -.049 | .494 | 1.9246 | 1.0000 |
| 3 | 13 | 2 | 11.053 | 11.022 | 11.022 | .114 | .031 | .1557 | 1.0000 |

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS

PAGE 7

| q | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|---|--------|---------|---------|---------|---------|-------------|-------------|
| 4 | 3 | 4 | 3.243 | 2.600 | -2.0599 | .048 | .643 | 2.0597 | 1.0000 |
| 4 | 5 | 7 | 7.907 | 8.031 | -6.030 | -.048 | 1.04 | -.7751 | 1.0000 |
| 4 | 6 | 3 | 3.091 | 1.643 | 1.642 | -.042 | 1.446 | 3.6790 | 1.0000 |
| 4 | 7 | 6 | 6.254 | 5.914 | 5.913 | -.045 | 1.340 | 1.3886 | 1.0000 |
| 4 | 0 | 5 | 5.9087 | 5.9422 | 5.9418 | -.045 | 1.422 | 1.4222 | 1.0000 |
| 4 | 1 | 2 | 1.220 | 1.542 | 1.541 | -.032 | 1.679 | .7785 | 1.0000 |
| 4 | 2 | 3 | 36.365 | 38.181 | -38.181 | -.075 | 1.616 | 6.9174 | 1.0000 |
| 4 | 3 | 4 | 4.604 | 4.963 | 4.963 | -.027 | 1.6146 | 1.6146 | 1.0000 |
| 4 | 4 | 5 | 44.453 | 45.107 | 45.104 | -.027 | 1.654 | 2.2300 | 1.0000 |
| 4 | 5 | 6 | 3.174 | 2.151 | 2.151 | -.023 | 1.023 | 2.8940 | 1.0000 |
| 4 | 6 | 7 | 19.156 | 19.047 | -19.047 | -.063 | 1.03 | .5340 | 1.0000 |
| 4 | 7 | 0 | 4.980 | 5.188 | 5.188 | -.027 | 1.209 | 6.6808 | 1.0000 |
| 4 | 0 | 1 | 32.141 | 31.338 | -31.338 | -.031 | 1.601 | 2.9458 | 1.0000 |
| 4 | 1 | 2 | 1.478 | *.325 | -.321 | -.051 | 1.153 | 1.5937 | 1.0000 |
| 4 | 2 | 3 | 28.693 | 28.965 | 28.963 | -.309 | 1.272 | 9.5115 | 1.0000 |
| 4 | 3 | 4 | 1.507 | *.190 | -.184 | -.048 | 1.316 | 1.8334 | 1.0000 |
| 4 | 4 | 5 | 24.320 | 23.708 | -23.706 | -.0289 | 1.612 | 6.6024 | 1.0000 |
| 4 | 5 | 6 | 1.277 | *.365 | -.362 | -.046 | 1.892 | .9765 | 1.0000 |
| 4 | 6 | 7 | 17.383 | 17.526 | 17.524 | -.266 | 1.143 | 7.333 | 1.0000 |
| 4 | 7 | 0 | 1.474 | *.526 | -.524 | -.039 | 1.814 | .8614 | 1.0000 |
| 4 | 0 | 1 | 17.629 | 18.110 | 18.109 | -.103 | 1.481 | 4.9339 | 1.0000 |
| 4 | 1 | 2 | 4.669 | 4.730 | 4.730 | -.032 | 1.778 | 1.7778 | 1.0000 |
| 4 | 2 | 3 | 4.469 | 4.3412 | 4.3407 | -.691 | 1.472 | 5.0819 | 1.0000 |
| 4 | 3 | 4 | 4.885 | *.485 | -.485 | -.030 | 1.767 | 6.099 | 1.0000 |
| 4 | 4 | 5 | 11.164 | 11.543 | 11.542 | -.176 | 1.379 | 2.6712 | 1.0000 |
| 4 | 5 | 6 | 6.886 | 6.503 | -6.503 | -.030 | 1.8523 | 1.8523 | 1.0000 |
| 4 | 6 | 7 | 25.831 | 26.233 | 26.226 | -.595 | 1.402 | 1.7267 | 1.0000 |
| 4 | 7 | 0 | 17.024 | 16.508 | 16.507 | -.198 | 1.515 | 2.6118 | 1.0000 |
| 4 | 0 | 1 | 1.530 | 1.557 | 1.557 | -.067 | 1.027 | 3.6099 | 1.0000 |
| 4 | 1 | 2 | 14.589 | 14.361 | -14.359 | -.190 | 1.479 | 2.5672 | 1.0000 |
| 4 | 2 | 3 | 1.420 | *.239 | 1.236 | -.064 | 1.81 | 2.226 | 1.0000 |
| 4 | 3 | 4 | 12.451 | 12.820 | 12.818 | -.184 | 1.369 | 2.3116 | 1.0000 |
| 4 | 4 | 5 | 1.360 | *.557 | -.554 | -.060 | 1.823 | .8358 | 1.0000 |
| 4 | 5 | 6 | ?1.72 | *.034 | -.032 | -.164 | 1.139 | .7233 | 1.0000 |
| 4 | 6 | 7 | 27.707 | 28.214 | 28.213 | -.268 | 1.506 | 2.0787 | 1.0000 |
| 4 | 7 | 0 | 5.332 | 4.861 | -4.860 | -.016 | 1.472 | 1.9656 | 1.0000 |
| 4 | 0 | 1 | 1.340 | 1.098 | 1.076 | -.242 | 1.2526 | 1.0000 | 1.0000 |
| 4 | 1 | 2 | 8.401 | 8.379 | 8.379 | -.014 | 1.1258 | 1.0000 | 1.0000 |
| 4 | 2 | 3 | 22.167 | 22.177 | 22.176 | -.249 | 1.010 | .0494 | 1.0000 |
| 4 | 3 | 4 | 1.418 | *.239 | 1.239 | -.015 | 1.179 | 1.1643 | 1.0000 |
| 4 | 4 | 5 | 11.787 | 11.284 | 11.283 | -.128 | 1.503 | 2.6759 | 1.0000 |
| 4 | 5 | 0 | 11.481 | 11.218 | -11.218 | -.107 | 1.262 | 1.6316 | 1.0000 |
| 4 | 0 | 1 | 12.123 | 11.339 | -11.338 | -.121 | 1.784 | 4.812 | 1.0000 |
| 4 | 1 | 2 | 10.247 | 10.063 | 10.063 | -.104 | 1.184 | 1.0814 | 1.0000 |
| 4 | 2 | 3 | 9.396 | 9.064 | 9.063 | -.119 | 1.332 | 1.7780 | 1.0000 |
| 4 | 3 | 4 | 5.130 | 5.202 | 5.202 | -.086 | 1.072 | 3.0064 | 1.0000 |
| 4 | 4 | 5 | 8.463 | 8.574 | -8.573 | -.084 | 1.111 | 5.763 | 1.0000 |
| 4 | 5 | 6 | 2.886 | 2.466 | -2.464 | -.070 | 1.420 | 1.0698 | 1.0000 |
| 4 | 6 | 7 | ?3.93 | 5.187 | -5.187 | -.205 | 1.7151 | 1.0000 | 1.0000 |

SILLIVANITE (BRANDYWINE SPRINGS, AT) 25 DEGREES C

STRUCTURE FACTORS

PAGE 8

| H | K | L | F(OBS) | F(CALC) | A(CALC)* | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|----|--------|---------|---------|----------|---------|---------|-------------|-------------|
| 5 | 1 | 0 | 13.245 | 11.736 | 11.735 | *292 | 1.507 | 7.7229 | 1.0000 |
| 5 | 1 | 1 | 8.395 | 8.459 | 8.459 | *089 | -0.065 | -0.3032 | 1.0000 |
| 5 | 2 | 36.817 | 36.918 | 36.917 | *248 | -1.01 | -4.022 | 1.0000 | |
| 5 | 3 | 12.084 | 12.546 | 12.546 | -12.546 | -0.65 | -4.62 | -2.2976 | 1.0000 |
| 5 | 4 | 12.530 | 11.625 | 11.622 | -1.622 | -2.72 | *905 | 5.5862 | 1.0000 |
| 5 | 5 | 1.246 | 2.048 | 2.047 | *080 | -0.802 | -0.905 | 1.0000 | |
| 5 | 6 | 20.782 | 19.976 | 19.975 | *214 | -0.606 | 3.6268 | 1.0000 | |
| 5 | 7 | 9.166 | 8.799 | 8.799 | -0.71 | 1.9903 | 1.0000 | | |
| 5 | 8 | 6.725 | 6.966 | 6.966 | -0.706 | -1.1668 | 1.0000 | | |
| 5 | 9 | 15.782 | 15.767 | 15.767 | *050 | -0.670 | 1.0000 | | |
| 5 | 10 | 72.060 | 73.793 | 73.791 | *545 | -1.733 | -2.1485 | 1.0000 | |
| 5 | 11 | 7.174 | 7.601 | 7.601 | -0.47 | -0.426 | -2.2747 | 1.0000 | |
| 5 | 12 | 49.198 | 49.667 | 49.667 | -0.514 | -0.469 | -1.6376 | 1.0000 | |
| 5 | 13 | 12.156 | 12.371 | 12.371 | *046 | -0.215 | -1.2873 | 1.0000 | |
| 5 | 14 | 41.919 | 41.413 | 41.411 | *0469 | *506 | 1.4695 | 1.0000 | |
| 5 | 15 | 2.065 | 1.521 | -1.521 | -0.39 | *543 | 7.775 | 1.0000 | |
| 5 | 16 | 23.057 | 22.632 | 22.631 | *238 | *425 | 1.4731 | 1.0000 | |
| 5 | 17 | 5.724 | 5.809 | 5.809 | *017 | -0.685 | *3945 | 1.0000 | |
| 5 | 18 | 4.701 | 4.642 | 4.642 | *018 | *056 | *2166 | 1.0000 | |
| 5 | 19 | 42.520 | 43.062 | 43.061 | *0293 | -0.542 | -2.0645 | 1.0000 | |
| 5 | 20 | 2.631 | 1.85 | *457 | -0.17 | *8594 | 1.0000 | | |
| 5 | 21 | 17.446 | 17.146 | 17.144 | *221 | *300 | 1.4424 | 1.0000 | |
| 5 | 22 | 5.724 | 5.809 | 5.809 | *017 | -0.685 | *3945 | 1.0000 | |
| 5 | 23 | 23.653 | 23.481 | 23.480 | *253 | *172 | *7620 | 1.0000 | |
| 5 | 24 | 2.631 | 2.358 | -0.014 | *274 | *274 | *4861 | 1.0000 | |
| 5 | 25 | 10.286 | 8.118 | 8.118 | *434 | 2.169 | 10.7235 | 1.0000 | |
| 5 | 26 | 10.192 | 10.955 | 10.955 | *033 | -0.764 | -4.1926 | 1.0000 | |
| 5 | 27 | 27.576 | -6.161 | -6.161 | -0.423 | *1.215 | *4.2117 | 1.0000 | |
| 5 | 28 | 12.359 | -12.359 | -0.031 | -0.352 | -2.1268 | 1.0000 | | |
| 5 | 29 | 9.146 | 8.946 | 8.935 | *403 | *202 | 1.3156 | 1.0000 | |
| 5 | 30 | 4.481 | 4.390 | 4.390 | *030 | *030 | *3164 | 1.0000 | |
| 5 | 31 | 15.525 | 15.789 | 15.785 | -3.64 | *0264 | -1.5058 | 1.0000 | |
| 5 | 32 | 8.854 | 8.563 | -8.563 | -0.25 | *291 | 1.4755 | 1.0000 | |
| 5 | 33 | 12.413 | 11.005 | 11.002 | *025 | 1.407 | 1.1504 | 1.0000 | |
| 5 | 34 | 9.960 | 9.620 | -9.619 | -0.97 | *0340 | 2.0389 | 1.0000 | |
| 5 | 35 | 16.073 | 15.269 | 15.267 | *258 | *0803 | *4697 | 1.0000 | |
| 5 | 36 | 5.745 | 5.660 | 5.679 | *095 | *065 | *3122 | 1.0000 | |
| 5 | 37 | 10.694 | 9.430 | 9.427 | *237 | 1.264 | 8.6911 | 1.0000 | |
| 5 | 38 | 8.402 | 8.501 | -8.500 | -0.086 | -0.5403 | 1.5403 | 1.0000 | |
| 5 | 39 | 9.552 | 9.351 | 9.349 | *223 | *200 | 1.1008 | 1.0000 | |
| 5 | 40 | 21.033 | 20.820 | 20.819 | *186 | *213 | *8837 | 1.0000 | |
| 5 | 41 | 2.474 | 2.953 | 2.951 | -0.093 | -0.479 | -1.0201 | 1.0000 | |
| 5 | 42 | 2.510 | *3.59 | -3.311 | -1.178 | 2.151 | 4.6873 | 1.0000 | |
| 5 | 43 | 1.644 | 1.176 | -1.150 | *090 | 1.4668 | 2.0937 | 1.0000 | |
| 5 | 44 | 15.858 | 15.639 | 15.638 | *173 | *219 | 1.1560 | 1.0000 | |
| 5 | 45 | 2.168 | 2.641 | -2.640 | -0.092 | -0.474 | -0.7376 | 1.0000 | |
| 5 | 46 | 2.091 | *6.34 | -6.115 | -1.154 | 1.457 | 2.0952 | 1.0000 | |
| 5 | 47 | 27.776 | 28.268 | -28.267 | *279 | -0.492 | -1.4492 | 1.0000 | |
| 5 | 48 | 1.610 | 2.624 | 2.623 | *057 | -1.014 | -1.3809 | 1.0000 | |
| 5 | 49 | 25.256 | 25.077 | 25.076 | *210 | *179 | *7195 | 1.0000 | |
| 5 | 50 | 1.352 | *803 | -8.01 | -0.053 | *549 | *5686 | 1.0000 | |
| 5 | 51 | 21.531 | 21.805 | -21.805 | -0.276 | -1.3745 | 1.0000 | | |
| 5 | 52 | 2.848 | 3.009 | 3.009 | *052 | -0.162 | -3.3179 | 1.0000 | |
| 5 | 53 | 3.5976 | -35.976 | -35.976 | *522 | -0.522 | *6601 | 1.0000 | |

SILLIMANITE (GRANDYINE SPRINGS) AT 25 DEGREES C.

STRUCTURE FACTORS

PAGE 9

| R | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|----|----------|---------|---------|---------|---------|-------------|-------------|
| 5 | 5 | 8 | 1.377 * | 2.719 | 2.718 | 0.056 | -1.343 | -1.3645 | 1.0000 |
| 5 | 5 | 6 | 1.7360 | 1.7477 | 1.7469 | 0.518 | -0.117 | -0.6061 | 1.0000 |
| 5 | 5 | 3 | 3.867 | 2.880 | 2.860 | -0.633 | 1.007 | 2.7554 | 1.0000 |
| 5 | 5 | 8 | 2.8306 | 2.8175 | 2.8171 | -0.485 | 0.131 | 0.4606 | 1.0000 |
| 5 | 5 | 4 | 1.6444 * | 1.6210 | 1.6209 | 0.059 | 0.234 | 0.2265 | 1.0000 |
| 5 | 5 | 5 | 2.028 * | 2.054 | 2.0437 | 0.217 | 0.575 | 0.7952 | 1.0000 |
| 5 | 5 | 9 | 2.6447 * | 2.008 | 2.007 | 0.044 | 0.439 | 0.7294 | 1.0000 |
| 5 | 5 | 9 | 10.656 | 10.731 | 10.728 | 0.240 | -0.073 | -0.4284 | 1.0000 |
| 5 | 5 | 9 | 1.798 * | 2.084 | 2.083 | -0.041 | -0.206 | -0.3369 | 1.0000 |
| 5 | 5 | 10 | 25.360 | 24.636 | 24.637 | 0.232 | 0.722 | 2.9787 | 1.0000 |
| 5 | 5 | 10 | 3.245 | 2.936 | 2.936 | 0.035 | 0.309 | 0.6288 | 1.0000 |
| 5 | 5 | 10 | 9.563 | 9.752 | 9.749 | -0.222 | -0.222 | -0.8656 | 1.0000 |
| 5 | 5 | 10 | 8.8177 | 8.8706 | 8.8703 | -0.733 | -0.529 | -0.529 | 1.0000 |
| 5 | 6 | 0 | 30.945 | 31.160 | 31.159 | -0.189 | -0.214 | -0.7771 | 1.0000 |
| 5 | 6 | 0 | 65.503 | 65.198 | 65.195 | -0.680 | -0.304 | 1.0340 | 1.0000 |
| 5 | 6 | 0 | 18.798 | 17.669 | 17.668 | -0.9162 | -0.925 | 4.4356 | 1.0000 |
| 5 | 6 | 0 | 45.664 | 42.911 | 42.910 | -0.672 | -0.672 | 2.6322 | 1.0000 |
| 5 | 6 | 0 | 12.919 | 13.187 | 13.187 | -0.031 | -0.268 | -1.3993 | 1.0000 |
| 5 | 6 | 1 | 1.869 * | 1.864 | 1.864 | -0.312 | -0.312 | -1.9029 | 1.0000 |
| 5 | 6 | 2 | 9.318 | 9.638 | 9.637 | -0.031 | -0.320 | -2.0328 | 1.0000 |
| 5 | 6 | 3 | 30.534 | 30.244 | 30.243 | -0.296 | -0.296 | -0.9175 | 1.0000 |
| 5 | 5 | 8 | 8.518 | 8.124 | 8.124 | -0.027 | -0.394 | 2.3655 | 1.0000 |
| 5 | 5 | 5 | 1.407 * | 1.138 | 1.121 | -0.269 | -0.731 | -0.7272 | 1.0000 |
| 5 | 6 | 6 | 4.074 | 3.944 | 3.944 | -0.027 | -0.130 | -0.3596 | 1.0000 |
| 5 | 6 | 7 | 23.079 | 23.621 | 23.621 | -0.081 | -0.542 | -1.8333 | 1.0000 |
| 5 | 6 | 6 | 30.534 | 30.244 | 30.243 | -0.296 | -0.376 | -1.7469 | 1.0000 |
| 5 | 6 | 6 | 8.518 | 8.124 | 8.124 | -0.027 | -0.504 | 1.7267 | 1.0000 |
| 5 | 6 | 6 | 1.407 * | 1.138 | 1.121 | -0.269 | -0.640 | -2.2407 | 1.0000 |
| 5 | 6 | 7 | 4.074 | 3.944 | 3.944 | -0.027 | -0.675 | 3.6842 | 1.0000 |
| 5 | 6 | 0 | 23.079 | 23.621 | 23.621 | -0.081 | -0.376 | -1.7469 | 1.0000 |
| 5 | 6 | 1 | 8.635 | 8.035 | 8.034 | -0.127 | -0.504 | 1.7267 | 1.0000 |
| 5 | 6 | 2 | 26.680 | 25.976 | 25.972 | -0.466 | -0.640 | -2.2407 | 1.0000 |
| 5 | 6 | 3 | 7.339 | 7.378 | 7.377 | -0.123 | -0.675 | 3.6842 | 1.0000 |
| 5 | 6 | 4 | 17.053 | 16.365 | 16.365 | -0.075 | -0.376 | -1.7469 | 1.0000 |
| 5 | 6 | 5 | 5.846 | 5.830 | 5.829 | -0.113 | -0.376 | -1.7469 | 1.0000 |
| 5 | 6 | 6 | 16.467 | 16.290 | 16.285 | -0.385 | -0.177 | -0.9504 | 1.0000 |
| 5 | 6 | 6 | 5.270 | 4.545 | 4.544 | -0.102 | -0.726 | 2.4116 | 1.0000 |
| 5 | 6 | 7 | 26.767 | 27.183 | 27.183 | -0.071 | -0.6416 | -1.4404 | 1.0000 |
| 5 | 6 | 0 | 3.747 | 3.780 | 3.780 | -0.045 | -0.334 | -1.1714 | 1.0000 |
| 5 | 6 | 1 | 7.003 | 6.734 | 6.734 | -0.067 | -0.269 | 1.6145 | 1.0000 |
| 5 | 6 | 2 | 1.244 * | 1.540 | 1.538 | -0.042 | -0.704 | -0.7920 | 1.0000 |
| 5 | 6 | 3 | 17.790 | 18.116 | 18.116 | -0.065 | -0.326 | -1.7221 | 1.0000 |
| 5 | 6 | 4 | 4.800 | 4.712 | 4.712 | -0.041 | -0.088 | 1.6765 | 1.0000 |
| 5 | 6 | 5 | 4.1549 | 4.1247 | 4.1247 | -0.045 | -0.978 | 2.6680 | 1.0000 |
| 5 | 6 | 6 | 3.966 | 2.986 | 2.986 | -0.057 | -0.269 | 1.6145 | 1.0000 |
| 5 | 6 | 6 | 1.463 * | 1.268 | 1.267 | -0.034 | -0.675 | -0.7920 | 1.0000 |
| 5 | 6 | 6 | 17.790 | 18.116 | 18.116 | -0.065 | -0.326 | -1.7221 | 1.0000 |
| 5 | 6 | 6 | 4.800 | 4.712 | 4.712 | -0.041 | -0.088 | 1.6765 | 1.0000 |
| 5 | 6 | 6 | 3.966 | 2.986 | 2.986 | -0.057 | -0.269 | 1.6145 | 1.0000 |
| 5 | 6 | 6 | 1.463 * | 1.268 | 1.267 | -0.034 | -0.675 | -0.7920 | 1.0000 |
| 5 | 6 | 6 | 1.290 * | 6.610 | 6.617 | -0.034 | -0.133 | 2.8908 | 1.0000 |
| 5 | 6 | 5 | 6.637 | 2.6235 | 1.543 | -0.036 | -0.281 | 1.6762 | 1.0000 |
| 5 | 6 | 4 | 9.344 | 9.062 | 9.062 | -0.121 | -0.302 | 1.0268 | 1.0000 |
| 5 | 6 | 4 | 4.1549 | 4.1247 | 4.1247 | -0.045 | -0.978 | 2.6680 | 1.0000 |
| 5 | 6 | 4 | 8.441 | 8.182 | 8.182 | -0.116 | -0.259 | 1.6356 | 1.0000 |
| 5 | 6 | 4 | 1.290 * | 6.610 | 6.617 | -0.034 | -0.133 | 2.8908 | 1.0000 |
| 5 | 6 | 4 | 6.637 | 2.6235 | 1.543 | -0.036 | -0.281 | 1.6762 | 1.0000 |
| 5 | 6 | 4 | 2.787 | 22.932 | 22.929 | -0.146 | -0.748 | 3.1941 | 1.0000 |
| 5 | 6 | 4 | 2.046 * | 2.711 | 2.711 | -0.013 | -0.672 | 0.7293 | 1.0000 |
| 5 | 6 | 5 | 4.0607 | 4.1597 | 4.1595 | -0.349 | -0.133 | 0.5973 | 1.0000 |
| 5 | 6 | 5 | 1.289 * | 1.361 | 1.361 | -0.012 | -0.092 | -0.0999 | 1.0000 |
| 5 | 6 | 3 | 1.289 * | 1.361 | 1.361 | -0.012 | -0.491 | 2.5004 | 1.0000 |
| 5 | 6 | 3 | 18.377 | -16.376 | -16.376 | -0.325 | -0.492 | -1.2717 | 1.0000 |
| 5 | 6 | 4 | 4.274 | -4.274 | -4.274 | -0.013 | -0.492 | -1.2717 | 1.0000 |

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS PAGE 10

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|----|--------|---------|---------|---------|---------|-------------|-------------|
| 5 | 6 | 6 | 26.010 | 25.360 | 25.356 | *300 | *650 | 2.703 | 1.0000 |
| 6 | 6 | 0 | 44.330 | 44.480 | 44.475 | *656 | -0.150 | -0.4788 | 1.0000 |
| 6 | 6 | 1 | 3.930 | 3.498 | 3.496 | *011 | *333 | 1.0541 | 1.0000 |
| 6 | 6 | 2 | 5.506 | 5.340 | -5.338 | -1.182 | *166 | *7135 | 1.0000 |
| 6 | 6 | 3 | 2.544 | 2.924 | -2.924 | -0.009 | -0.380 | -0.7384 | 1.0000 |
| 5 | 6 | 4 | 34.257 | 34.561 | 34.555 | *609 | -0.304 | *8431 | 1.0000 |
| 6 | 6 | 5 | 3.255 | 2.795 | 2.795 | *010 | *460 | *9948 | 1.0000 |
| 6 | 6 | 0 | 13.718 | 12.485 | 12.485 | *200 | 1.232 | 6.6328 | 1.0000 |
| 6 | 6 | 1 | 9.229 | -9.229 | -9.229 | -0.052 | -0.000 | *0016 | 1.0000 |
| 6 | 6 | 2 | 20.554 | 20.364 | -20.363 | -0.191 | *189 | *9481 | 1.0000 |
| 6 | 6 | 3 | 12.095 | 11.853 | 11.853 | *051 | *242 | 1.3699 | 1.0000 |
| 6 | 6 | 4 | 9.813 | 10.068 | 10.066 | *186 | *254 | -1.4157 | 1.0000 |
| 6 | 6 | 5 | 3.646 | 3.171 | -3.170 | -0.456 | *275 | *6097 | 1.0000 |
| 6 | 6 | 0 | 11.171 | 11.120 | 11.120 | *192 | *053 | *053 | 1.0000 |
| 6 | 6 | 1 | 3.583 | 3.633 | -3.831 | -0.125 | -0.249 | -0.5975 | 1.0000 |
| 6 | 6 | 2 | 16.632 | 16.628 | 16.625 | *275 | *005 | *0244 | 1.0000 |
| 6 | 6 | 3 | 1.470 | 3.472 | 3.470 | *121 | *2.002 | -1.9068 | 1.0000 |
| 6 | 6 | 4 | 9.067 | 8.608 | 8.606 | *179 | *460 | *2857 | 1.0000 |
| 6 | 6 | 5 | 17.376 | 17.287 | 17.287 | *171 | *589 | *8625 | 1.0000 |
| 6 | 6 | 9 | 8.510 | 7.933 | -7.933 | *013 | *577 | 2.8366 | 1.0000 |
| 6 | 6 | 10 | 16.094 | 15.236 | -15.235 | -0.160 | *858 | *9351 | 1.0000 |
| 6 | 6 | 11 | 4.772 | 3.904 | -3.904 | -0.012 | *868 | *5745 | 1.0000 |
| 6 | 6 | 12 | 16.975 | 17.220 | 17.219 | *166 | *245 | -1.2462 | 1.0000 |
| 6 | 6 | 13 | 18.275 | 18.630 | -18.630 | -0.158 | *355 | -1.6981 | 1.0000 |
| 6 | 6 | 14 | 8.632 | 8.490 | -8.489 | *149 | *142 | *7651 | 1.0000 |
| 6 | 6 | 15 | 12.624 | 13.023 | 13.023 | *046 | -0.399 | -2.3084 | 1.0000 |
| 6 | 6 | 16 | 1.212 | *042 | *014 | *040 | *170 | *3514 | 1.0000 |
| 6 | 6 | 17 | 3.696 | 3.6314 | 3.6310 | *567 | *650 | 2.1681 | 1.0000 |
| 6 | 6 | 18 | 2.920 | 3.587 | 3.587 | *038 | *667 | -1.6398 | 1.0000 |
| 6 | 6 | 19 | 9.066 | 9.202 | 9.202 | *043 | *136 | *8541 | 1.0000 |
| 6 | 6 | 20 | 4.367 | 3.514 | 3.514 | *036 | *853 | 2.6141 | 1.0000 |
| 6 | 6 | 21 | 22.014 | 21.698 | 21.693 | *489 | *316 | 1.4769 | 1.0000 |
| 6 | 6 | 22 | 11.279 | 11.132 | 11.131 | *125 | *147 | *8609 | 1.0000 |
| 6 | 6 | 23 | 1.238 | *426 | *425 | -1.388 | -1.3429 | *8609 | 1.0000 |
| 6 | 6 | 24 | 3.388 | 3.149 | -3.147 | -0.121 | *239 | *6865 | 1.0000 |
| 6 | 6 | 25 | 2.394 | *946 | *945 | *068 | *447 | *9205 | 1.0000 |
| 6 | 6 | 26 | 8.812 | 8.527 | 8.526 | *116 | *285 | 1.7188 | 1.0000 |
| 6 | 6 | 27 | 4.322 | 3.625 | 3.625 | *061 | *497 | 1.4801 | 1.0000 |
| 6 | 6 | 28 | 1.651 | 2.351 | -2.349 | -0.104 | *700 | *7616 | 1.0000 |
| 6 | 6 | 29 | 55.235 | 55.176 | 55.170 | *811 | *059 | *2036 | 1.0000 |
| 6 | 6 | 30 | 2.525 | *666 | -2.666 | -0.015 | *141 | *3098 | 1.0000 |
| 6 | 6 | 31 | 22.348 | 22.448 | -22.446 | -0.263 | *100 | -4.210 | 1.0000 |
| 6 | 6 | 32 | 1.283 | *847 | *847 | *036 | *4761 | 1.0000 | * * * |
| 6 | 6 | 33 | 42.795 | 43.258 | 43.252 | *753 | *463 | *3832 | 1.0000 |
| 6 | 6 | 34 | 4.060 | 4.108 | -4.108 | *013 | *048 | *7614 | 1.0000 |
| 6 | 6 | 35 | 14.744 | 14.111 | -14.109 | -0.243 | *632 | 3.9905 | 1.0000 |
| 6 | 6 | 36 | 14.916 | 14.915 | -14.915 | -1.106 | *001 | *057 | 1.0000 |
| 6 | 6 | 37 | 1.280 | *955 | -0.950 | -0.102 | *324 | *3546 | 1.0000 |
| 6 | 6 | 38 | 1.851 | 2.331 | 2.328 | *108 | *480 | *7614 | 1.0000 |
| 6 | 6 | 39 | 1.316 | 1.569 | -1.566 | *099 | *253 | *2690 | 1.0000 |
| 6 | 6 | 40 | 11.366 | 11.343 | -11.343 | -0.098 | *023 | *1491 | 1.0000 |
| 6 | 6 | 41 | 3.707 | *148 | -3.147 | -0.090 | *559 | 1.4112 | 1.0000 |
| 6 | 6 | 42 | 2.010 | * | *800 | *093 | *2706 | 1.0000 | * * * |

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS

PAGE 11

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|---|--------|---------|---------|---------|---------|-------------|-------------|
| 7 | 7 | 5 | 0 | 4.150 | 4.148 | .126 | * 256 | * 8923 | 1.0000 |
| 5 | 1 | 4 | 4.06 | 5.661 | 5.661 | -.032 | -.085 | -.3647 | 1.0000 |
| 7 | 5 | 1 | 5.576 | 4.268 | 4.266 | +.372 | +.645 | -.19693 | 1.0000 |
| 2 | 2 | 3 | 4.5523 | 2.656 | 2.656 | -.2656 | -.032 | 1.7797 | 1.0000 |
| 3 | 3 | 2 | 3.372 | 2.914 | 2.912 | +.117 | +.434 | .9832 | 1.0000 |
| 5 | 3 | 4 | 3.348 | 3.88 | 3.88 | -.028 | -.277 | .9816 | 1.0000 |
| 4 | 5 | 0 | 5.666 | 6.138 | 6.138 | -.022 | -.027 | .1171 | 1.0000 |
| 5 | 0 | 1 | 6.165 | 15.249 | 15.249 | +.148 | -.164 | -.9176 | 1.0000 |
| 1 | 1 | 2 | 15.085 | 8.425 | 8.425 | +.028 | +.189 | -.9827 | 1.0000 |
| 2 | 2 | 3 | 8.236 | 8.887 | 8.887 | +.065 | +.077 | -.677 | 1.0000 |
| 3 | 3 | 0 | 11.590 | 11.688 | 11.687 | -.141 | -.098 | -.5679 | 1.0000 |
| 4 | 4 | 6 | 5.218 | 4.683 | 4.683 | -.021 | -.021 | 1.7395 | 1.0000 |
| 5 | 5 | 6 | 12.459 | 12.265 | 12.264 | +.133 | +.194 | 1.1868 | 1.0000 |
| 0 | 0 | 7 | 29.597 | -29.817 | -29.816 | -.165 | -.219 | -.5833 | 1.0000 |
| 1 | 1 | 7 | 8.810 | 8.887 | 8.887 | +.065 | +.077 | -.4016 | 1.0000 |
| 2 | 2 | 7 | 41.135 | 41.974 | 41.969 | +.634 | -.839 | -.2739 | 1.0000 |
| 3 | 3 | 7 | 6.932 | 8.962 | 8.962 | -.061 | -.030 | 1.1509 | 1.0000 |
| 4 | 4 | 7 | 24.966 | 23.999 | 23.998 | +.153 | +.968 | 3.9337 | 1.0000 |
| 5 | 5 | 8 | 3.803 | 3.362 | 3.362 | +.123 | 3.6441 | 8.5842 | 1.0000 |
| 0 | 0 | 1 | 1.470 | 2.513 | 2.513 | -.026 | -.043 | -.9932 | 1.0000 |
| 1 | 1 | 2 | 13.055 | 12.725 | 12.725 | -.113 | -.030 | 1.9903 | 1.0000 |
| 2 | 2 | 3 | 1.487 | 2.970 | 2.970 | +.026 | -.16483 | -1.3968 | 1.0000 |
| 3 | 3 | 0 | 3.630 | 3.360 | 3.360 | +.035 | +.536 | 3.7632 | 1.0000 |
| 0 | 0 | 1 | 1.495 | * 319 | * 317 | -.031 | 1.176 | 1.1014 | 1.0000 |
| 1 | 1 | 0 | 66.675 | 67.849 | 67.848 | -.463 | -.176 | -3.9735 | 1.0000 |
| 2 | 2 | 0 | 3.432 | 4.516 | 4.516 | +.040 | -.084 | -2.9473 | 1.0000 |
| 3 | 3 | 0 | 51.063 | 51.469 | 51.467 | +.449 | -.406 | -1.1796 | 1.0000 |
| 0 | 0 | 1 | 4.617 | 1.936 | 1.935 | -.035 | 2.681 | 7.5831 | 1.0000 |
| 1 | 1 | 0 | 26.401 | 26.245 | 26.242 | -.440 | -.156 | 4.722 | 1.0000 |
| 2 | 2 | 1 | 11.339 | 11.359 | 11.359 | -.070 | -.026 | -.020 | 1.0000 |
| 3 | 3 | 1 | 23.875 | 24.149 | 24.145 | +.433 | -.274 | -1.1202 | 1.0000 |
| 0 | 0 | 2 | 9.764 | 10.057 | 10.057 | +.069 | -.294 | -1.7867 | 1.0000 |
| 1 | 1 | 3 | 20.764 | 20.627 | 20.622 | -.068 | -.408 | .7096 | 1.0000 |
| 2 | 2 | 4 | 8.141 | 7.730 | 7.730 | -.061 | -.144 | -.141 | 1.0000 |
| 3 | 3 | 5 | 15.550 | 15.060 | 15.056 | -.373 | -.490 | 2.8959 | 1.0000 |
| 0 | 0 | 6 | 9.972 | 8.368 | 8.366 | +.178 | 1.604 | 10.1205 | 1.0000 |
| 1 | 1 | 0 | 7.540 | 7.537 | 7.536 | +.115 | -.004 | -.0209 | 1.0000 |
| 2 | 2 | 1 | 4.060 | 3.654 | 3.638 | -.335 | -.406 | 1.3259 | 1.0000 |
| 3 | 3 | 2 | 4.974 | 5.078 | 5.077 | -.110 | -.104 | -.3774 | 1.0000 |
| 4 | 4 | 3 | 6.662 | 6.925 | 6.923 | -.166 | -.264 | -1.1372 | 1.0000 |
| 5 | 5 | 2 | 6.435 | 6.327 | 6.327 | +.103 | -.107 | -.4155 | 1.0000 |
| 6 | 6 | 1 | 2.551 | 2.555 | 2.538 | -.289 | -.004 | -.0051 | 1.0000 |
| 7 | 7 | 0 | 5.630 | 5.603 | 5.603 | -.080 | -.027 | 1.1211 | 1.0000 |
| 8 | 8 | 1 | 2.498 | 1.563 | 1.556 | -.140 | -.935 | 1.9425 | 1.0000 |
| 9 | 9 | 2 | 4.833 | 4.781 | 4.781 | +.082 | 1.052 | 1.1870 | 1.0000 |
| 0 | 0 | 3 | 2.019 | * 985 | * 976 | -.133 | 1.034 | 1.5360 | 1.0000 |
| 1 | 1 | 4 | 3.434 | 4.429 | 4.428 | -.074 | -.472 | 1.5051 | 1.0000 |
| 2 | 2 | 5 | 1.455 | * 588 | * 574 | -.126 | -.867 | 1.9350 | 1.0000 |
| 3 | 3 | 6 | 16.009 | 16.097 | 16.096 | -.099 | -.088 | -.4693 | 1.0000 |
| 4 | 4 | 7 | 6.869 | 6.908 | 6.907 | -.079 | -.039 | -.1926 | 1.0000 |
| 5 | 5 | 8 | 37.967 | 38.337 | 38.334 | -.401 | -.370 | -.0714 | 1.0000 |
| 6 | 6 | 9 | 3.434 | 3.516 | 3.515 | -.077 | -.082 | -.1911 | 1.0000 |
| 7 | 7 | 0 | 12.154 | 12.153 | 12.153 | -.092 | -.304 | 1.7859 | 1.0000 |
| 8 | 8 | 1 | 6.909 | 6.811 | 6.811 | -.070 | -.097 | -.3979 | 1.0000 |

SILLIMANITE (GRANDY MINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS

PAGE 12

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|----|---------|---------|---------|---------|---------|-------------|-------------|
| 6 | 5 | 0 | 36.0232 | 36.0929 | .484 | -.698 | -1.9730 | 1.0000 | |
| 8 | 5 | 1 | 11.095 | 10.617 | -.066 | .478 | 3.0842 | 1.0000 | |
| 0 | 5 | 2 | 34.0245 | 33.964 | -.469 | .280 | .7601 | 1.0000 | |
| 3 | 5 | 3 | 9.0919 | 9.644 | .064 | .064 | 1.5589 | 1.0000 | |
| 4 | 5 | 4 | 29.0452 | 29.442 | .449 | .009 | 0.0334 | 1.0000 | |
| 0 | 6 | 0 | 15.0152 | 15.0194 | .428 | -.042 | -.1960 | 1.0000 | |
| 6 | 6 | 1 | 2.0914 | 2.0251 | -.051 | 2.663 | 5.2865 | 1.0000 | * |
| 6 | 6 | 2 | 3.0657 | 3.0184 | -.057 | .472 | 1.1510 | 1.0000 | * |
| 6 | 6 | 3 | 2.0980 | 2.0866 | .050 | .114 | 2.2204 | 1.0000 | * |
| 6 | 6 | 4 | 11.0787 | 11.0809 | -.102 | -.5955 | 1.0000 | | |
| 7 | 7 | 0 | 16.0816 | 17.0225 | -.291 | -.126 | -.6037 | 1.0000 | |
| 7 | 7 | 1 | 5.0936 | 5.0795 | -.073 | 1.141 | 1.5104 | 1.0000 | * |
| 7 | 7 | 2 | 14.0929 | 15.0433 | -.053 | -.503 | 2.9361 | 1.0000 | |
| 7 | 7 | 3 | 3.0906 | 5.0131 | .072 | 1.225 | 2.6770 | 1.0000 | |
| 8 | 7 | 0 | 13.0816 | 13.0299 | -.239 | -.518 | 2.8647 | 1.0000 | |
| 8 | 7 | 1 | 7.020 | 7.0201 | -.105 | -.161 | -.7156 | 1.0000 | |
| 8 | 7 | 2 | 3.0355 | 3.0377 | -.024 | -.022 | -.0563 | 1.0000 | |
| 9 | 7 | 3 | 1.0440 | 0.076 | -.024 | 1.354 | 1.3638 | 1.0000 | * |
| 9 | 7 | 4 | 4.0765 | 5.0036 | -.020 | -.273 | -.090 | 1.0000 | |
| 9 | 7 | 5 | 25.0236 | 25.0555 | -.0408 | -.319 | -.273 | 1.0000 | |
| 9 | 7 | 6 | 9.0290 | 9.0523 | -.170 | -.225 | -.3482 | 1.0000 | |
| 9 | 7 | 7 | 12.0304 | 12.0380 | -.104 | -.076 | -.4567 | 1.0000 | |
| 9 | 7 | 8 | 11.0339 | 11.0429 | -.164 | -.090 | -.5590 | 1.0000 | |
| 9 | 7 | 9 | 19.0681 | 20.0689 | -.379 | -.408 | -.0660 | 1.0000 | |
| 9 | 7 | 10 | 5.0202 | 4.0513 | -.152 | -.690 | 2.01920 | 1.0000 | |
| 9 | 7 | 11 | 35.0406 | 36.0080 | -.436 | -.674 | -.9572 | 1.0000 | |
| 9 | 7 | 12 | 4.0531 | 4.0044 | -.002 | -.025 | -.4806 | 1.0000 | |
| 9 | 7 | 13 | 30.0816 | 30.0999 | -.625 | -.165 | -.165 | 1.0000 | |
| 9 | 7 | 14 | 5.0712 | 6.0076 | -.003 | -.364 | -.3292 | 1.0000 | |
| 9 | 7 | 15 | 28.0012 | 28.0811 | -.404 | -.690 | -.7096 | 1.0000 | |
| 9 | 7 | 16 | 1.0471 | 1.0345 | -.000 | 1.201 | 1.0728 | 1.0000 | * |
| 9 | 7 | 17 | 6.0196 | 5.0745 | -.022 | -.451 | 1.65598 | 1.0000 | |
| 9 | 7 | 18 | 2.0716 | 4.0004 | -.021 | -.172 | -.3289 | 1.0000 | |
| 9 | 7 | 19 | 29.057 | 29.0761 | -.076 | -.518 | -.5995 | 1.0000 | |
| 9 | 7 | 20 | 1.0444 | 0.0160 | -.0158 | 1.284 | 1.2453 | 1.0000 | * |
| 9 | 7 | 21 | 3.082 | 3.0345 | -.000 | 1.127 | 1.0000 | * | |
| 9 | 7 | 22 | 4.0745 | 5.0745 | -.022 | -.022 | 1.0000 | | |
| 9 | 7 | 23 | 3.0620 | 3.0437 | -.02546 | -.021 | 1.0000 | | |
| 9 | 7 | 24 | 4.0833 | 5.0350 | -.033 | -.0517 | 1.0000 | | |
| 9 | 7 | 25 | 13.0893 | 14.0117 | -.328 | -.224 | 1.2776 | 1.0000 | |
| 9 | 7 | 26 | 2.0802 | 2.0443 | -.030 | -.639 | 1.2027 | 1.0000 | |
| 9 | 7 | 27 | 4.0254 | 4.0664 | -.020 | 1.793 | 4.6216 | 1.0000 | |
| 9 | 7 | 28 | 23.0702 | 23.0766 | -.0329 | -.064 | 2.2663 | 1.0000 | |
| 9 | 7 | 29 | 9.0417 | 9.0466 | -.0180 | -.045 | -.2619 | 1.0000 | |
| 9 | 7 | 30 | 15.0603 | 15.0672 | -.160 | -.069 | -.3972 | 1.0000 | |
| 9 | 7 | 31 | 6.0626 | 6.0605 | -.172 | -.022 | -.0849 | 1.0000 | |
| 9 | 7 | 32 | 14.0319 | 13.0784 | -.151 | -.0535 | 2.9009 | 1.0000 | |
| 9 | 7 | 33 | 1.0474 | 1.0499 | -.007 | -.025 | -.0240 | 1.0000 | |
| 9 | 7 | 34 | 1.0489 | 1.0781 | -.765 | .156 | -.6657 | 1.0000 | * |
| 9 | 7 | 35 | 15.0797 | 15.0556 | -.419 | -.2462 | 1.2469 | 1.0000 | |
| 9 | 7 | 36 | 25.0373 | 25.0788 | -.281 | -.415 | 1.4931 | 1.0000 | |
| 9 | 7 | 37 | 52.030 | 53.0398 | -.771 | -.368 | -.7562 | 1.0000 | |
| 9 | 7 | 38 | 21.0965 | 21.0102 | -.260 | -.863 | 4.3420 | 1.0000 | |
| 9 | 7 | 39 | 10.0829 | 10.0898 | -.043 | -.4069 | -.4069 | 1.0000 | |

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

STRUCTURE FACTORS PAGE 13

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|----|---|---|---------|---------|---------|---------|---------|-------------|-------------|
| 10 | 1 | 1 | 2.552 * | 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 | 2 | 0 | 21.338 | 22.065 | 22.061 | .463 | .726 | -3.010 | 1.0000 |
| 10 | 2 | 1 | 3.357 | 3.350 | 3.349 | .048 | .007 | .0165 | 1.0000 |
| 10 | 2 | 2 | 8.023 | 8.359 | 8.359 | .037 | .337 | -1.5384 | 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 | .4330 | 1.0000 |
| 10 | 3 | 1 | 16.874 | 16.879 | -16.878 | .184 | .005 | .0284 | 1.0000 |
| 10 | 3 | 2 | 4.723 | 4.191 | 4.191 | .024 | .532 | .5516 | 1.0000 |
| 10 | 3 | 3 | 13.626 | 13.525 | 13.524 | .178 | .103 | .6322 | 1.0000 |
| 10 | 4 | 0 | 34.859 | 36.284 | 36.279 | .592 | -1.425 | -3.555 | 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 | .385 | .7986 | 1.0000 |
| 10 | 5 | 0 | 2.519 * | 0.93 | -.073 | .058 | 2.426 | 3.8411 | 1.0000 |
| 10 | 5 | 1 | 4.246 | 3.609 | -3.608 | .042 | .635 | 1.6790 | 1.0000 |
| 11 | 0 | 1 | 3.755 | 3.047 | -3.046 | .205 | .707 | 1.6571 | 1.0000 |
| 11 | 1 | 0 | 12.232 | 13.037 | 13.030 | .439 | .806 | 4.3952 | 1.0000 |
| 11 | 1 | 1 | 5.604 | 5.599 | 5.599 | .063 | .005 | .0169 | 1.0000 |
| 11 | 1 | 2 | 10.324 | 10.754 | 10.754 | .053 | .430 | -2.2458 | 1.0000 |
| 11 | 2 | 0 | 21.211 | 21.874 | -21.871 | .342 | .662 | -2.8720 | 1.0000 |
| 11 | 2 | 1 | 9.615 | 9.215 | -9.214 | .091 | .206 | .9953 | 1.0000 |

SILLIMANITE (BRANDYWINE SPRINGS) AT 25 DEGREES C

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS

NUMERATOR

DENOMINATOR

NUMBER

R

WEIGHTED R 13353.63

7158729.14

659

.041

UNWEIGHTED R 403.97

9822.30

659

.041

RANGES OF F(OBS)

| | | | |
|---------|------------|-----|------|
| 3739.33 | 920855.41 | .80 | .064 |
| 1544.22 | 1142885.87 | 105 | .037 |
| 541.15 | 1048900.95 | 45 | .023 |
| 967.42 | 1422697.21 | 17 | .026 |
| 279.34 | 963603.21 | 6 | .017 |
| 2363.39 | 993524.77 | 4 | .049 |
| 113.66 | 263468.62 | 1 | .021 |
| 3765.32 | 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 |
| 387.79 | 672276.37 | 54 | .024 |
| 509.94 | 407748.14 | 90 | .035 |
| 352.70 | 443261.88 | 98 | .028 |
| 468.56 | 447939.16 | 113 | .032 |
| 692.37 | 349125.92 | 113 | .045 |

UNREJECTED REFLECTIONS

WEIGHTED R 7103.74

6349655.55

537

.032

UNWEIGHTED R 299.52

9396.36

537

.032

RANGES OF F(OBS)

| | | | |
|---------|------------|-----|------|
| 3542.44 | 919946.82 | 360 | .062 |
| 1544.22 | 1142885.87 | 165 | .037 |
| 541.15 | 1048900.95 | 45 | .023 |
| 967.42 | 1422697.21 | 17 | .026 |
| 279.34 | 963608.21 | 6 | .017 |
| 115.51 | 588147.67 | 3 | .014 |
| 113.66 | 263468.82 | 1 | .021 |
| .00 | .00 | 0 | .000 |

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

| | | | |
|---------|------------|----|------|
| 2928.39 | 1826972.51 | 37 | .040 |
| 979.65 | 1410459.18 | 50 | .026 |
| 961.87 | 792698.64 | 56 | .035 |
| 361.83 | 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 STANDARD DEV OF UNIT WEIGHT OBS

9748.97

3.80

17.30.50. 03/28/78 XLLGGYP TRR68ZU2 40 PM

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

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

John K. Winter

and

Subrata Ghose

Department of Geological Sciences
University of Washington
Seattle, Washington 98195

Table 4. Sillimanite, andalusite and kyanite: observed and
calculated structure factors at various temperatures.

END OF THE LOAD
LINE 1 OF THE LOAD

111
74743

TRANSFER ADDRESS --- REFINE

112

***** REFINER SUMMARY

RE4105// COMMON PLANK COMMON TRUNCATED BY 207000 WORDS

PROGRAM AND BLOCK ASSIGNMENTS.

| BLOCK | ADDRESS | LENGTH | FILE | DATA | PROGESS | VER | LEVEL | HARDWARE | COMMENTS |
|----------|---------|--------|-----------|----------|---------|-----|-------|----------|----------|
| REFINE | 111 | 10575 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /E/ | 10706 | 1355 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /C/ | 12263 | 457 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /D/ | 12742 | 3244 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /E/ | 16205 | 10 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /F/ | 16216 | 174 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /G/ | 16412 | 2307 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /LSV/ | 20721 | 334 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /TAP/E/ | 21255 | 6 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| /DEGEN/ | 21263 | 311 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| REFINE | 21574 | 5726 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| SODA&I | 27522 | 1147 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| ELVIBL | 30671 | 1312 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| INPUT | 32203 | 241 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| MATRIX | 32444 | 231 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| MODIFY | 32675 | 115 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| RCALC | 33012 | 152 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| RESET | 33164 | 73 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| SFAC | 33257 | 476 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| SYMINV | 33755 | 361 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| WEIGHT | 34336 | 12 | REFINE | 05/14/76 | RUN | F | 74 | F | 646X T |
| ASIN COS | 34350 | 130 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| EXP | 34506 | 55 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| SINCOS | 34563 | 72 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| SORT | 34655 | 46 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| ACGDR | 34721 | 12 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| ENDFILE | 34733 | 57 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| GTRBA | 35012 | 17 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| INPUTB | 35031 | 256 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| KRAKER | 35307 | 1052 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| OUTPTB | 36361 | 244 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| SIDS | 36625 | 1504 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| INPUTC | 40331 | 121 | SL-RUN2P3 | 03/17/75 | COMPASS | 3. | 74190 | | |
| KODER | 40452 | 1310 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| OUTPTC | 41762 | 71 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| REWIND | 42053 | 63 | SL-RUN2P3 | 02/19/75 | COMPASS | 3. | 74190 | | |
| SYSTEM | 42136 | 1122 | SL-RUN2P3 | 03/10/75 | COMPASS | 3. | 74190 | | |
| | 43260 | 31463 | | | | | | | |

STRUCTURE FACTORS AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 1

| L | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|-----|---------|---------|---------|---------|-------------|-------------|
| 2 | 62.754 | 64.659 | -64.658 | -0.351 | -1.895 | 1.0000 |
| 4 | 135.513 | 145.697 | 145.695 | -0.832 | -12.164 | 1.0000 |
| 6 | 27.106 | 26.542 | -26.541 | -0.283 | 0.563 | 1.0000 |
| 8 | 45.146 | 53.272 | 53.268 | 0.615 | 1.875 | 1.0000 |
| 10 | 15.151 | 13.185 | 13.185 | 0.027 | 1.966 | 1.0000 |
| 12 | 4.607 | 4.347 | -4.347 | -0.055 | 0.260 | 1.0000 |
| 14 | 22.634 | 14.835 | -14.828 | 3.708 | 19.207 | 1.0000 |
| 16 | 6.555 | 6.293 | 6.293 | 0.063 | 2.01 | 1.0000 |
| 18 | 8.232 | 7.279 | 7.279 | 0.026 | 0.953 | 1.0000 |
| 20 | 1.049 | 0.886 | 0.866 | 1.011 | 5.372 | 1.0000 |
| 22 | 6.315 | 7.884 | 7.872 | 0.419 | 1.2860 | 1.0000 |
| 24 | 4.785 | 4.594 | 4.593 | 0.053 | 0.192 | 1.0000 |
| 26 | 1.369 | 2.658 | 2.657 | 0.022 | -1.288 | 1.0000 |
| 28 | 21.922 | 19.946 | 19.945 | -1.152 | 1.477 | 1.0000 |
| 30 | 6.301 | 6.398 | 6.397 | 0.082 | -1.965 | 1.0000 |
| 32 | 88.466 | 90.392 | 90.390 | 0.664 | -9.6356 | 1.0000 |
| 34 | 10.033 | 10.712 | 10.711 | -0.076 | -0.675 | 1.0000 |
| 36 | 4.642 | 6.475 | 6.475 | -0.136 | -1.835 | 1.0000 |
| 38 | 2.183 | 2.926 | 2.925 | -0.073 | 1.255 | 1.0000 |
| 40 | 4.667 | 4.234 | 4.233 | -0.543 | -1.767 | 1.0000 |
| 42 | 7.194 | 7.543 | 7.543 | -0.063 | -1.350 | 1.0000 |
| 44 | 1.379 | 2.50 | 2.50 | -0.097 | 1.126 | 1.0000 |
| 46 | 51.637 | 51.225 | 51.219 | -0.73 | 4.12 | 1.0000 |
| 48 | 7.887 | 7.887 | 7.887 | -0.020 | 0.060 | 1.0000 |
| 50 | 7.947 | 7.887 | 7.887 | -0.273 | -1.201 | 1.0000 |
| 52 | 23.055 | 24.356 | 24.354 | -0.020 | -0.386 | 1.0000 |
| 54 | 10.093 | 7.078 | 7.07 | -0.231 | -5.564 | 1.0000 |
| 56 | 38.054 | 39.618 | 39.611 | -0.599 | -5.3699 | 1.0000 |
| 58 | 6.051 | 7.992 | 7.992 | -0.016 | 0.412 | 1.0000 |
| 60 | 11.606 | 12.554 | 12.552 | -0.221 | -0.3533 | 1.0000 |
| 62 | 3.352 | 1.999 | 1.999 | -0.015 | -1.201 | 1.0000 |
| 64 | 19.652 | 18.542 | 18.541 | -0.197 | -0.564 | 1.0000 |
| 66 | 2.242 | 2.536 | 2.536 | -0.070 | -0.297 | 1.0000 |
| 68 | 23.117 | 23.816 | 23.815 | -0.243 | -0.609 | 1.0000 |
| 70 | 5.406 | 6.013 | 6.012 | -0.058 | -0.648 | 1.0000 |
| 72 | 12.365 | 13.225 | 13.224 | -0.178 | -0.647 | 1.0000 |
| 74 | 2.357 | 2.299 | 2.299 | -0.062 | -0.110 | 1.0000 |
| 76 | 13.917 | 14.629 | 14.628 | -0.020 | -0.712 | 1.0000 |
| 78 | 5.949 | 6.201 | 6.197 | -0.204 | -0.255 | 1.0000 |
| 80 | 4.752 | 4.978 | 4.977 | -0.091 | -0.255 | 1.0000 |
| 82 | 29.487 | 30.537 | 30.532 | -1.085 | -1.051 | 1.0000 |
| 84 | 1.366 | 1.130 | -1.127 | -0.183 | 4.051 | 1.0000 |
| 86 | 10.203 | 5.152 | -5.149 | -0.183 | 2.175 | 1.0000 |
| 88 | 13.049 | 12.227 | -12.226 | -0.077 | -0.7661 | 1.0000 |
| 90 | 1.955 | 1.954 | -1.954 | -0.074 | -4.030 | 1.0000 |
| 92 | 9.232 | 9.449 | 9.449 | -0.069 | -0.217 | 1.0000 |
| 94 | 2.273 | 2.229 | 2.229 | -0.060 | -0.044 | 1.0000 |
| 96 | 25.957 | 24.335 | 24.335 | -0.068 | 1.622 | 1.0000 |
| 98 | 4.617 | 6.825 | 6.825 | -0.028 | 3.791 | 1.0000 |
| 100 | 62.318 | 63.253 | 63.251 | -0.476 | -5.935 | 1.0000 |
| 102 | 8.610 | 8.561 | 8.561 | -0.027 | 0.2907 | 1.0000 |
| 104 | 13.645 | 14.181 | 14.180 | -0.063 | -2.9880 | 1.0000 |
| 106 | 4.990 | 5.117 | 5.117 | -0.026 | -0.6692 | 1.0000 |
| 108 | 30.232 | 29.312 | 29.312 | -0.390 | 0.917 | 1.0000 |

SILVIMITE (EPHYDITE) SPRINGS. AT 400 DEGREES C.

STRUCTURE FACTORS

PAGE 2

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|---|--------|---------|---------|---------|---------|-------------|-------------|
| 1 | 1 | 1 | 7 | 4.566 | 4.813 | 4.813 | -0.23 | -0.246 | -0.9359 |
| 1 | 1 | 1 | 8 | 6.340 | 6.274 | 6.273 | 0.050 | 0.066 | 1.0000 |
| 1 | 1 | 2 | C | 80.357 | 82.439 | 82.438 | -1.052 | -1.17003 | 1.0000 |
| 1 | 1 | 2 | 1 | 8.253 | 7.932 | 7.932 | -0.044 | 0.321 | 1.0000 |
| 1 | 1 | 2 | 2 | 86.087 | 86.196 | 86.195 | -0.41 | -0.106 | 1.0000 |
| 1 | 1 | 2 | 3 | 1.242 | 2.007 | 2.007 | -2.707 | -0.043 | -0.765 |
| 1 | 1 | 2 | 4 | 46.917 | 48.160 | 48.159 | -4.18 | -1.243 | -1.243 |
| 1 | 1 | 2 | 5 | 7.626 | 8.102 | 8.101 | -0.33 | -0.476 | -5.3521 |
| 1 | 1 | 2 | 6 | 37.341 | 37.638 | 37.636 | -3.67 | -0.297 | -3.4866 |
| 1 | 1 | 2 | 7 | 2.166 | 2.199 | 2.199 | -0.023 | -0.023 | -0.9914 |
| 1 | 1 | 2 | 8 | 20.571 | 20.331 | 20.329 | -0.307 | -0.240 | 1.1450 |
| 1 | 1 | 3 | C | 46.149 | 47.111 | 47.106 | -0.634 | -0.662 | -5.8618 |
| 1 | 1 | 3 | 1 | 5.563 | 5.623 | 5.623 | -0.010 | -0.060 | -0.3148 |
| 1 | 1 | 3 | 2 | 2.943 | 3.695 | 3.696 | -0.090 | -0.090 | -3.4295 |
| 1 | 1 | 3 | 3 | 2.783 | 2.257 | 2.257 | -2.257 | -0.010 | -0.526 |
| 1 | 1 | 3 | 4 | 39.336 | 39.284 | 39.280 | -0.774 | -0.447 | -5.7958 |
| 1 | 1 | 3 | 5 | 5.617 | 6.131 | 6.131 | -0.008 | -0.514 | -2.9236 |
| 1 | 1 | 3 | 6 | 3.676 | 3.575 | 3.576 | -0.071 | -0.123 | -0.4303 |
| 1 | 1 | 3 | 7 | 2.933 | 3.089 | 3.089 | -0.006 | -0.156 | -0.3799 |
| 1 | 1 | 3 | 8 | 19.469 | 19.168 | 19.168 | -0.425 | -0.286 | 1.4969 |
| 1 | 1 | 4 | 0 | 2.119 | * 0.949 | -0.982 | -0.350 | 1.171 | 3.1655 |
| 1 | 1 | 4 | 1 | 3.510 | 3.125 | -3.125 | -0.031 | -0.384 | 1.8172 |
| 1 | 1 | 4 | 2 | 26.579 | 27.178 | 27.176 | -0.342 | -0.596 | -2.6599 |
| 1 | 1 | 4 | 3 | 6.978 | 7.240 | 7.240 | -0.630 | -0.262 | -1.4555 |
| 1 | 1 | 4 | 4 | 6.857 | 6.366 | -6.359 | -0.316 | -0.491 | 3.2180 |
| 1 | 1 | 4 | 5 | 2.777 | 3.950 | -0.950 | -0.027 | 1.827 | 5.3590 |
| 1 | 1 | 4 | 6 | 14.974 | 15.343 | 15.340 | -0.379 | -0.369 | -2.1125 |
| 1 | 1 | 4 | 7 | 4.850 | 5.550 | 5.549 | -0.026 | -0.695 | -2.5433 |
| 1 | 1 | 4 | 8 | 4.934 | 4.957 | -4.090 | -0.233 | -0.887 | 3.1600 |
| 1 | 1 | 5 | 0 | 10.970 | 10.049 | 10.047 | -0.179 | -0.921 | 4.6070 |
| 1 | 1 | 5 | 1 | 6.601 | 6.489 | -0.024 | -0.024 | -0.112 | 5.693 |
| 1 | 1 | 5 | 2 | 63.055 | 65.305 | 65.304 | -0.323 | -2.219 | -9.7492 |
| 1 | 1 | 5 | 3 | 2.155 | 1.130 | -1.130 | -0.024 | 1.025 | 2.0250 |
| 1 | 1 | 5 | 4 | 9.155 | 9.067 | -9.066 | -0.163 | -0.667 | 0.691 |
| 1 | 1 | 5 | 5 | 4.093 | 5.178 | -5.176 | -0.021 | -1.085 | -4.1904 |
| 1 | 1 | 5 | 6 | 30.310 | 31.105 | 31.104 | -0.266 | -0.795 | -2.3488 |
| 1 | 1 | 5 | 7 | 2.836 | 1.607 | -1.607 | -0.021 | -1.229 | 2.7201 |
| 1 | 1 | 6 | 0 | 24.291 | 24.284 | -24.284 | -0.154 | -0.007 | 0.0241 |
| 1 | 1 | 6 | 1 | 3.575 | 2.845 | -2.844 | -0.082 | -0.730 | 2.5171 |
| 1 | 1 | 6 | 2 | 1.153 | * 0.819 | -0.805 | -0.150 | -0.334 | 0.4059 |
| 1 | 1 | 6 | 3 | 5.041 | -5.041 | -0.079 | -0.079 | -0.034 | 0.1770 |
| 1 | 1 | 6 | 4 | 16.485 | -16.484 | -16.484 | -0.138 | -0.045 | -0.2586 |
| 1 | 1 | 6 | 5 | 1.537 | * 1.006 | -1.003 | -0.073 | -0.521 | 1.7806 |
| 1 | 1 | 6 | 6 | 1.307 | * * | -0.902 | -0.122 | -0.396 | 0.4245 |
| 1 | 1 | 6 | 7 | 3.847 | 4.171 | -4.171 | -0.063 | -0.324 | -0.9134 |
| 1 | 1 | 6 | 8 | 26.523 | 27.728 | -27.726 | -0.026 | -1.205 | -4.1713 |
| 1 | 1 | 7 | 1 | 6.459 | 6.712 | -6.712 | -0.044 | -0.253 | -1.5315 |
| 1 | 1 | 7 | 2 | 42.860 | 43.839 | -43.836 | -0.482 | -0.979 | -3.5151 |
| 1 | 1 | 7 | 3 | 6.817 | 7.158 | -7.158 | -0.041 | -0.341 | -2.0091 |
| 1 | 1 | 7 | 4 | 17.537 | 18.320 | -18.320 | -0.022 | -0.684 | -3.2507 |
| 1 | 1 | 7 | 5 | 4.413 | 4.423 | -3.423 | -0.040 | -0.991 | 3.6019 |
| 1 | 1 | 7 | 6 | 24.452 | 24.850 | -24.847 | -0.394 | -0.398 | 1.0000 |
| 1 | 1 | 7 | 7 | 33.916 | 33.895 | -33.893 | -0.405 | -0.672 | 1.0000 |

SILLIMANITE (GRANDYING SPRINGS) AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 3

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|-----|-----|---------|---------|---------|---------|---------|-------------|-------------|
| 1 | 8 | 1 | 1.766 * | 1.291 | 1.290 | -0.052 | +474 | +7956 | 1.CCCC * |
| 1 | 8 | 2 | 13.360 | 13.503 | -13.497 | -0.394 | +357 | 2.0071 | 1.GCCC * |
| 1 | 8 | 3 | 1.225 * | 3.16 | -3.12 | +0.050 | +909 | 1.0395 | 1.CCCC * |
| 1 | 8 | 4 | 23.735 | 25.327 | 25.324 | +0.366 | -1.591 | -6.2022 | 1.CCCC * |
| 1 | 8 | 5 | 1.344 * | 1.224 | 1.224 | -0.045 | +115 | +1244 | 1.CCCC * |
| 1 | 8 | 6 | 7.674 | 8.460 | -8.474 | -0.321 | +806 | -3.5410 | 1.CCCC |
| 1 | 8 | 7 | 3.434 | 3.501 | 3.578 | +0.453 | -732 | +2.2410 | 1.CCCC |
| 1 | 8 | 8 | 1.269 * | 5.59 | -5.59 | -0.016 | +710 | +7931 | 1.GCCC * |
| 1 | 8 | 9 | 12.237 | 12.110 | 12.109 | -0.034 | +127 | +8334 | 1.CCCC * |
| 1 | 8 | 10 | 2.643 * | 7.715 | -7.714 | +0.015 | +1325 | 2.1915 | 1.0000 |
| 1 | 8 | 11 | 25.531 | 25.783 | 25.780 | +0.410 | +152 | +6949 | 1.0000 |
| 1 | 8 | 12 | 2.033 * | 0.629 | -0.26 | -0.012 | +2064 | 3.0474 | 1.0000 |
| 1 | 8 | 13 | 21.574 | 21.506 | -21.506 | -0.160 | +067 | +2660 | 1.0000 |
| 1 | 8 | 14 | 4.780 | 4.493 | -4.493 | -0.634 | +286 | +5908 | 1.CCCC |
| 1 | 8 | 15 | 6.707 | 7.035 | -7.033 | +0.157 | +328 | -1.4711 | 1.0000 |
| 1 | 8 | 16 | 4.112 | 3.562 | -3.562 | +0.033 | +549 | +549 | 1.0000 |
| 1 | 8 | 17 | 16.797 | 16.707 | -16.706 | -0.145 | +090 | +090 | 1.0000 |
| 1 | 8 | 18 | 5.772 | 5.341 | -5.336 | +0.215 | +432 | +432 | 1.0000 |
| 1 | 8 | 19 | 3.484 | 3.251 | -3.251 | +0.034 | +233 | +5522 | 1.CCCC |
| 1 | 8 | 20 | 3.845 | 3.108 | -3.105 | +0.143 | +736 | +736 | 1.0000 |
| 1 | 8 | 21 | 11.0 | 11.2 | -11.0 | +0.143 | +9076 | +9076 | 1.0000 |
| 1 | 8 | 22 | 0 | 0 | 32.070 | +0.098 | +875 | 12.2905 | 1.0000 |
| 1 | 8 | 23 | 45.274 | 44.755 | -44.753 | +0.445 | +519 | +6747 | 1.0000 |
| 1 | 8 | 24 | 16.519 | 16.387 | -16.387 | +0.990 | +132 | +6347 | 1.0000 |
| 1 | 8 | 25 | 26.296 | 25.794 | -25.794 | +0.365 | +499 | 1.5811 | 1.0000 |
| 1 | 8 | 26 | 5.592 | 5.176 | -5.175 | +0.69 | +517 | 2.0061 | 1.0000 |
| 1 | 8 | 27 | 87.597 | 93.934 | -93.933 | -0.504 | +6336 | +5202 | 1.0000 |
| 1 | 8 | 28 | 7.296 | 7.088 | -7.088 | -0.027 | +208 | +6990 | 1.0000 |
| 1 | 8 | 29 | 5.117 | 1.298 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 30 | 6.107 | 6.082 | -6.082 | +0.028 | +029 | +5522 | 1.0000 |
| 1 | 8 | 31 | 32.070 | -53.179 | -53.179 | +0.029 | +1420 | +1420 | 1.0000 |
| 1 | 8 | 32 | 44.753 | -44.753 | -44.753 | +0.029 | +6025 | -4.4357 | 1.0000 |
| 1 | 8 | 33 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 34 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 35 | 5.175 | -5.175 | -5.175 | +0.69 | +025 | +1925 | 1.0000 |
| 1 | 8 | 36 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 37 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 38 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 39 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 40 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 41 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 42 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 43 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 44 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 45 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 46 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 47 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 48 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 49 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 50 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 51 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 52 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 53 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 54 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 55 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 56 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 57 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 58 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 59 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 60 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 61 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 62 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 63 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 64 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 65 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 66 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 67 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 68 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 69 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 70 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 71 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 72 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 73 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 74 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 75 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 76 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 77 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 78 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 79 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 80 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 81 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 82 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 83 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 84 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 85 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 86 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 87 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 88 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 89 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 90 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 91 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 92 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 93 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 94 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 95 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 96 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 97 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 98 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 99 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 100 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 101 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 102 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 103 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 104 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 105 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 106 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 107 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 108 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 109 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8 | 110 | 1.298 | -1.202 | -1.202 | +0.491 | +819 | +6747 | 1.0000 |
| 1 | 8 | 111 | 6.082 | -6.082 | -6.082 | +0.028 | +029 | +1420 | 1.0000 |
| 1 | 8 | 112 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 113 | 44.753 | -44.753 | -44.753 | +0.029 | +363 | +2742 | 1.0000 |
| 1 | 8 | 114 | 16.387 | -16.387 | -16.387 | +0.990 | +155 | +1925 | 1.0000 |
| 1 | 8 | 115 | 25.794 | -25.794 | -25.794 | +0.365 | +363 | +2742 | 1.0000 |
| 1 | 8 | 116 | 5.175 | -5.175 | -5.175 | +0.69 | +155 | +1925 | 1.0000 |
| 1 | 8 | 117 | 93.934 | -93.933 | -93.933 | +0.504 | +6336 | +5196 | 1.0000 |
| 1 | 8 | 118 | 7.088 | -7.088 | -7.088 | +0.027 | +208 | +6747 | 1.0000 |
| 1 | 8</ | | | | | | | | |

SILLIMANITE CRYSTALLIZING SPRINGS AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 6

| H | K | L | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR | | | |
|---|----|---|---------|---------|---------|---------|-------------|-------------|---------|--------|---|
| 2 | 2 | 4 | 4.694 | -4.994 | -0.952 | -0.300 | -1.4200 | 1.0000 | | | |
| 2 | 2 | 6 | 4.104 | 4.560 | 0.146 | 0.256 | 0.5813 | 1.0000 | | | |
| 2 | 3 | 4 | 4.594 | 4.337 | 0.051 | 0.257 | 1.1941 | 1.0000 | | | |
| 2 | 4 | 4 | 37.657 | 38.306 | 0.339 | -0.045 | -2.4469 | 1.0000 | | | |
| 2 | 5 | 4 | 3.409 | 3.126 | -3.126 | -0.053 | 0.283 | 0.5522 | 1.0000 | | |
| 2 | 6 | 5 | 5.037 | 4.763 | 4.761 | 0.121 | 0.274 | 1.1933 | 1.0000 | | |
| 2 | 7 | R | 1.906 | 2.401 | 2.401 | 0.040 | -0.496 | -0.7272 | 1.0000 | * | |
| 2 | 8 | R | 16.520 | 15.727 | 15.725 | 0.052 | 0.293 | 1.6382 | 1.0000 | * | |
| 2 | 9 | C | 0.150 | 0.898 | 0.540 | -0.046 | 0.245 | 1.1092 | 1.0000 | | |
| 2 | 10 | C | 11.709 | 11.486 | -11.486 | -0.053 | 0.222 | 1.2464 | 1.0000 | | |
| 2 | 11 | C | 74.648 | 76.444 | -76.442 | -0.526 | -1.796 | -7.7310 | 1.0000 | | |
| 2 | 12 | C | 13.727 | 14.274 | 14.274 | 0.052 | -0.546 | -3.2614 | 1.0000 | | |
| 2 | 13 | C | 36.426 | 37.297 | 37.294 | 0.094 | -0.871 | -3.6774 | 1.0000 | | |
| 2 | 14 | C | 2.682 | 2.771 | -2.770 | -0.046 | 0.121 | *.3332 | 1.0000 | | |
| 2 | 15 | C | 27.207 | 39.518 | -39.516 | -0.428 | -2.311 | -6.7793 | 1.0000 | | |
| 2 | 16 | C | 9.439 | 6.822 | 6.822 | 0.041 | 0.617 | 3.66330 | 1.0000 | | |
| 2 | 17 | O | 2.945 | 2.734 | 2.733 | 0.094 | 0.722 | 2.5426 | 1.0000 | | |
| 2 | 18 | O | 1.439 | 1.772 | -1.772 | -0.005 | -0.335 | -0.335 | 1.0000 | | |
| 2 | 19 | O | 23.084 | 22.752 | 22.748 | 0.394 | -0.323 | 1.1751 | 1.0000 | | |
| 2 | 20 | O | 1.156 | 1.489 | 1.489 | 0.056 | -0.323 | -0.3874 | 1.0000 | | |
| 2 | 21 | O | 14.608 | 14.942 | 14.942 | 0.056 | -0.334 | -1.7643 | 1.0000 | | |
| 2 | 22 | O | 2.676 | 1.084 | -1.084 | -0.004 | 1.094 | 1.094 | 1.0000 | | |
| 2 | 23 | O | 13.657 | 14.355 | 14.352 | 0.315 | -0.699 | -4.0298 | 1.0000 | | |
| 2 | 24 | O | 1.372 | *.835 | *.835 | 0.005 | *.537 | *.5477 | 1.0000 | * | |
| 2 | 25 | O | 20.058 | 19.468 | -19.466 | -0.298 | *.589 | 2.6647 | 1.0000 | | |
| 2 | 26 | O | 5.670 | -1.019 | -1.019 | -0.019 | 1.094 | 5.2199 | 1.0000 | | |
| 2 | 27 | O | 30.711 | 31.013 | 31.011 | 0.292 | -0.301 | -1.0227 | 1.0000 | | |
| 2 | 28 | O | 3.991 | 4.399 | -4.399 | *.019 | -0.408 | -1.4087 | 1.0000 | | |
| 2 | 29 | O | 14.978 | 15.170 | -15.116 | -0.269 | -0.143 | -0.143 | 1.0000 | | |
| 2 | 30 | O | 2.530 | 3.638 | -3.638 | -0.17 | -1.105 | -2.1051 | 1.0000 | | |
| 2 | 31 | O | 17.284 | 17.728 | 17.726 | .238 | -0.444 | -2.2723 | 1.0000 | | |
| 2 | 32 | O | 27.775 | 26.404 | 26.403 | *.237 | 1.370 | 4.3282 | 1.0000 | | |
| 2 | 33 | O | 2.130 | 1.973 | 1.972 | *.093 | *.157 | *.3040 | 1.0000 | | |
| 2 | 34 | O | 9.201 | 9.107 | 0.104 | *.199 | *.094 | *.6476 | 1.0000 | | |
| 2 | 35 | O | 1.921 | * | 1.736 | -1.735 | -0.049 | *.185 | *.3149 | 1.0000 | * |
| 2 | 36 | O | 18.973 | 19.348 | 19.348 | *.215 | -0.376 | -1.6905 | 1.0000 | | |
| 2 | 37 | O | 1.358 | * | 1.525 | 1.524 | *.047 | -0.167 | -0.1720 | 1.0000 | * |
| 2 | 38 | O | 6.030 | 5.608 | 5.805 | *.164 | *.222 | *.8982 | 1.0000 | | |
| 2 | 39 | O | 24.324 | 23.349 | -23.348 | -0.231 | *.975 | 3.9423 | 1.0000 | | |
| 2 | 40 | O | 9.554 | 9.672 | 9.672 | *.082 | -0.079 | -0.4894 | 1.0000 | | |
| 2 | 41 | O | 19.786 | 19.621 | 19.620 | *.226 | *.165 | *.7544 | 1.0000 | | |
| 2 | 42 | O | 4.612 | 5.028 | -5.027 | -0.078 | -0.416 | -1.4169 | 1.0000 | | |
| 2 | 43 | O | 17.770 | 18.015 | -18.014 | -0.208 | -0.245 | -1.4049 | 1.0000 | | |
| 2 | 44 | O | 9.934 | 10.082 | 10.082 | *.072 | -0.146 | -0.8365 | 1.0000 | | |
| 2 | 45 | O | 22.109 | 21.581 | 21.579 | *.302 | *.527 | 2.2792 | 1.0000 | | |
| 2 | 46 | O | 1.392 | * | 1.962 | -1.962 | -0.040 | -0.570 | -0.5725 | 1.0000 | * |
| 2 | 47 | O | 1.402 | * | 1.743 | 1.741 | *.084 | -0.341 | -0.3409 | 1.0000 | * |
| 2 | 48 | O | 2.371 | 1.859 | 1.859 | *.039 | *.512 | *.8691 | 1.0000 | | |
| 2 | 49 | O | 15.369 | 16.553 | 16.550 | -0.184 | -1.1028 | 1.0000 | | | |
| 2 | 50 | O | 15.714 | 15.502 | 15.497 | *.389 | 1.1654 | 1.0000 | | | |
| 2 | 51 | O | 1.448 | * | 1.253 | -0.247 | -0.055 | 1.1557 | 1.0000 | * | |
| 2 | 52 | O | 17.844 | -17.840 | -17.840 | -0.378 | -0.245 | 1.3091 | 1.0000 | | |
| 2 | 53 | O | 6.293 | 5.862 | -5.862 | -0.033 | *.432 | 2.1841 | 1.0000 | | |

SILVERNITE IS A MOUNTAIN SPRINGS. AT 400 DEGREES C

STRUCTURE FACTORS

94

| | F(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | FXT. | FACTOR |
|---|---------|---------|----------|-------------|---------|---------|
| 3 | 4.838 | 4.718 | 4.032 | *1.21 | *143 | 1.0000 |
| 3 | 4.940 | 5.135 | -0.076 | *1.195 | -9324 | 1.0000 |
| 3 | 4.664 | 5.073 | 0.025 | *1.195 | 1.5683 | 1.0000 |
| 3 | 4.590 | 4.529 | -0.093 | *1.195 | 2.825 | 1.0000 |
| 3 | 4.70 | 4.711 | -0.045 | 1.756 | 0.042 | 1.0000 |
| 3 | 1.140 | 3.132 | *0.045 | 1.007 | 0.256 | 1.0000 |
| 3 | 1.129 | 2.539 | *0.535 | 1.590 | 5.7608 | 1.0000 |
| 3 | 1.154 | 2.533 | -0.075 | *1.196 | -1.3086 | 1.0000 |
| 3 | 1.129 | 2.532 | -0.024 | *1.196 | 1.5511 | 1.0000 |
| 3 | 1.901 | 2.136 | -0.2137 | *0.667 | -3.5667 | 1.0000 |
| 3 | 1.901 | 2.136 | -0.2137 | *0.237 | *0.237 | *0.237 |
| 3 | 1.291 | 2.286 | 1.20262 | *0.997 | *0.003 | *0.155 |
| 3 | 2.900 | 2.849 | 2.86648 | *0.551 | *0.2263 | *0.2263 |
| 3 | 5.160 | 5.296 | *0.006 | *1.136 | *0.6481 | 1.0000 |
| 3 | 3.710 | 3.690 | -0.192 | *0.202 | *0.991 | 1.0000 |
| 3 | 9.967 | 9.787 | -0.1807 | *1.180 | *0.9431 | 1.0000 |
| 3 | 18.142 | 19.106 | 1.9105 | *0.178 | -4.4609 | 1.0000 |
| 3 | 2.973 | 1.820 | -1.1620 | *0.008 | 1.153 | 1.0000 |
| 3 | 17.573 | 17.686 | -0.1156 | *0.112 | -6.6161 | 1.0000 |
| 3 | 3.710 | 2.690 | -1.003 | *0.003 | 3.0826 | 1.0000 |
| 3 | 6.192 | 5.498 | -0.695 | *0.695 | 1.02072 | 1.0000 |
| 3 | 8.684 | 8.453 | -0.232 | *0.232 | *0.006 | *0.006 |
| 3 | 33.963 | 33.968 | -0.005 | *0.005 | *0.225 | 1.0000 |
| 3 | 5.046 | 4.250 | -0.796 | *0.796 | 3.4776 | 1.0000 |
| 3 | 52.858 | 52.858 | -0.156 | *0.156 | -6.6161 | 1.0000 |
| 3 | 2.097 | * | -0.003 | *0.003 | 3.0826 | 1.0000 |
| 3 | 1.911 | 1.911 | -0.007 | *0.007 | *0.9431 | 1.0000 |
| 3 | 21.949 | 22.730 | -0.22728 | *1.176 | -4.4609 | 1.0000 |
| 3 | 4.710 | 5.204 | -0.007 | *0.007 | 1.153 | 1.0000 |
| 3 | 30.858 | 30.858 | -0.1156 | *0.112 | -6.6161 | 1.0000 |
| 3 | 5.303 | 5.303 | -0.003 | *0.003 | 3.0826 | 1.0000 |
| 3 | 2.964 | 2.974 | -0.005 | *0.005 | *0.232 | *0.232 |
| 3 | 10.450 | 9.771 | -0.190 | *0.190 | *0.679 | *0.679 |
| 3 | 9.569 | 6.895 | -1.142 | *1.142 | 2.6693 | 1.0000 |
| 3 | 7.375 | 7.217 | -0.028 | *0.028 | 13.7870 | 1.0000 |
| 3 | 14.729 | 14.708 | -0.139 | *0.139 | 7.957 | 1.0000 |
| 3 | 1.729 | * | -0.026 | *0.026 | 0.917 | 1.0000 |
| 3 | 1.785 | 1.753 | -0.128 | *0.128 | 0.9965 | 1.0000 |
| 3 | 6.631 | 6.340 | -0.025 | *0.025 | 0.613 | 1.0000 |
| 3 | 7.761 | 7.430 | -0.113 | *0.113 | 1.6672 | 1.0000 |
| 3 | 2.419 | 1.853 | -0.018 | *0.018 | 1.8850 | 1.0000 |
| 3 | 30.835 | 9.685 | -0.566 | *0.566 | 1.0378 | 1.0000 |
| 3 | 3.819 | 2.682 | -0.150 | *0.150 | 1.0000 | 1.0000 |
| 3 | 2.703 | 2.703 | -0.115 | *0.115 | 1.0000 | 1.0000 |
| 3 | 2.983 | 2.964 | -0.510 | *0.510 | 1.0000 | 1.0000 |
| 3 | 3.476 | 2.747 | -0.274 | *0.274 | 1.0000 | 1.0000 |
| 3 | 1.317 | * | -0.073 | *0.073 | 1.0000 | 1.0000 |
| 3 | 4.085 | 2.424 | -0.063 | *0.063 | 1.0000 | 1.0000 |
| 3 | 17.514 | 17.682 | -0.075 | *0.075 | 1.0000 | 1.0000 |
| 3 | 2.405 | 1.308 | -0.020 | *0.020 | 1.0000 | 1.0000 |
| 3 | 2.694 | -2.963 | -0.075 | *0.075 | 1.0000 | 1.0000 |
| 3 | 1.194 | * | -0.910 | *0.910 | 1.0000 | 1.0000 |
| 3 | 12.053 | * | -11.895 | *11.895 | -0.068 | *0.068 |
| 3 | 2.662 | 2.537 | -0.015 | *0.015 | 1.0000 | 1.0000 |
| 3 | 1.356 | * | -0.988 | *0.988 | 0.361 | *0.361 |

SILVIANITE-CASSITERITE SPRINGS AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 6

| R | L | F (CRSS) | F (CALC) | A (CALC) | B (CALC) | C (CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR | PAGE | |
|---|---|----------|----------|----------|----------|----------|---------|-------------|-------------|--------|---|
| 3 | 3 | 6 | 7 | 1.412 | 1.460 | -1.480 | -0.615 | -0.665 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.412 | 1.460 | -1.480 | -0.622 | -0.626 | 1.0000 | 6 | |
| 3 | 3 | 6 | 6 | 5.98 | 5.177 | 6.174 | -0.622 | -0.527 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 7.15 | 6.19 | -11.618 | -0.644 | -0.647 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 5.56 | 5.723 | -5.721 | -0.644 | -0.267 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 11.76 | 11.242 | 11.241 | -0.644 | -0.165 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 7.53 | 6.611 | 4.608 | -0.644 | -0.065 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 7.630 | 6.688 | -6.987 | -0.644 | -0.350 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 4.290 | 4.676 | -4.675 | -0.644 | -0.712 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 16.71 | 16.535 | 16.525 | -0.644 | -0.225 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 3.75 | 3.462 | 3.462 | -0.644 | -0.287 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.254 | 1.757 | 0.739 | -0.644 | -0.497 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.312 | 1.981 | -1.981 | -0.644 | -0.669 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 12.105 | 12.295 | 12.294 | -0.644 | -0.267 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 3.295 | 2.619 | 2.618 | -0.644 | -0.225 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 19.356 | 19.974 | -18.973 | -0.644 | -0.165 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.332 | 1.462 | -1.462 | -0.644 | -0.287 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 2.919 | 2.947 | 2.947 | -0.644 | -0.267 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.379 | 1.574 | -1.574 | -0.644 | -0.267 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 14.141 | 14.200 | -14.199 | -0.644 | -0.165 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.421 | 1.463 | -1.463 | -0.644 | -0.065 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 13.750 | 12.963 | -12.963 | -0.644 | -0.532 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 3.920 | 5.773 | -5.773 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 2.932 | 5.574 | -5.574 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 5.309 | 6.059 | -6.059 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.309 | 4.909 | -4.909 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 7.539 | 7.947 | -7.947 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 6.522 | 5.859 | -5.859 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 7.836 | 7.694 | -7.694 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 6.201 | 6.405 | -6.405 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 4.919 | 6.740 | -6.740 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 41.202 | 46.241 | -46.237 | -0.644 | -0.251 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 7.529 | 7.947 | -7.947 | -0.644 | -0.560 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 20.105 | 18.627 | -18.627 | -0.644 | -0.278 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 22.946 | 22.903 | -22.901 | -0.644 | -0.443 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 3.317 | 2.611 | -2.610 | -0.644 | -0.706 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 21.793 | 21.371 | -21.360 | -0.644 | -0.269 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.159 | 1.613 | -1.612 | -0.644 | -0.564 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 17.625 | 17.421 | -17.421 | -0.644 | -0.278 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.544 | 1.614 | -1.611 | -0.644 | -0.530 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 12.725 | 12.406 | -12.404 | -0.644 | -0.220 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 1.368 | *.821 | -.820 | -0.642 | -0.547 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 8.464 | 7.980 | 7.978 | -0.642 | -0.194 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 77.795 | 76.973 | 76.972 | -0.642 | -0.461 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 2.512 | 1.720 | -1.720 | 0.613 | -0.345 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 16.793 | 37.267 | 37.267 | 0.613 | -0.592 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 2.825 | 2.201 | -2.201 | 0.613 | -0.624 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 20.976 | 19.788 | 19.755 | 0.310 | -0.195 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 6.097 | 4.513 | 4.513 | 0.511 | -0.573 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 12.197 | 11.873 | -11.873 | -0.112 | -0.324 | 1.0000 | 6 | |
| 3 | 3 | 7 | 7 | 5.350 | 4.388 | -4.388 | -0.489 | -0.962 | 4.1019 | 1.0000 | 6 |
| 3 | 3 | 7 | 7 | 9.412 | 9.921 | -9.921 | -0.108 | -0.505 | -2.5031 | 1.0000 | 6 |

SILLIMANITE (KANDYKINE) SPRINGS. AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 7

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|----|----|--------|---------|---------|---------|---------|-------------|-------------|
| 4 | 3 | 4 | 3.941 | 2.060 | -2.059 | .046 | 1.881 | 7.2985 | 1.0000 |
| 4 | 3 | 5 | 6.659 | 6.777 | -6.777 | -.096 | -.114 | -.6500 | 1.0000 |
| 4 | 3 | 6 | 2.552 | * 1.520 | 1.520 | -.039 | 1.031 | 2.1985 | 1.0000 |
| 4 | 3 | 7 | 5.042 | 4.907 | 4.907 | .087 | .135 | .4754 | 1.0000 |
| 4 | 0 | 0 | 56.599 | 56.716 | 56.715 | -.591 | -.119 | -.5146 | 1.0000 |
| 4 | 1 | 1 | 1.963 | 1.219 | 1.218 | -.034 | -.744 | 1.3974 | 1.0000 |
| 4 | 2 | 2 | 3.478 | 3.6214 | 3.6214 | -.080 | -.736 | -.2.6418 | 1.0000 |
| 4 | 3 | 3 | 4.619 | 5.311 | 5.311 | -.033 | -.962 | -.3.1204 | 1.0000 |
| 4 | 4 | 4 | 4.650 | 4.584 | 4.584 | .535 | .666 | .2297 | 1.0000 |
| 4 | 5 | 5 | 2.323 | * 1.507 | 1.506 | -.030 | .114 | 1.7141 | 1.0000 |
| 4 | 6 | 6 | 16.785 | 16.583 | 16.583 | -.063 | .202 | .0202 | 1.0000 |
| 4 | 7 | 7 | 5.964 | 4.957 | 4.957 | .028 | .028 | 4.020 | 1.0000 |
| 4 | 8 | 6 | 30.560 | 30.033 | 30.032 | -.292 | -.292 | 5.26 | 1.0000 |
| 4 | 9 | 5 | 1.462 | * .675 | .674 | .049 | .786 | 1.0853 | 1.0000 |
| 4 | 10 | 5 | 27.003 | 26.565 | 26.563 | .286 | .438 | 1.609 | 1.0000 |
| 4 | 11 | 2 | 1.364 | * 1.000 | 1.000 | -.045 | .964 | .9676 | 1.0000 |
| 4 | 12 | 3 | 22.664 | 22.061 | 22.079 | -.263 | -.263 | .583 | 1.0000 |
| 4 | 13 | 4 | 1.659 | * 1.236 | 1.235 | .043 | .423 | .615 | 1.0000 |
| 4 | 14 | 5 | 15.369 | 15.349 | 15.347 | .233 | .211 | .1152 | 1.0000 |
| 4 | 15 | 6 | 1.666 | * 1.082 | 1.081 | -.034 | .0585 | .6673 | 1.0000 |
| 4 | 16 | 7 | 1.666 | * 1.082 | 1.081 | -.034 | .0585 | .6673 | 1.0000 |
| 4 | 17 | 0 | 15.777 | 16.117 | 16.116 | -.181 | -.240 | -.1.7085 | 1.0000 |
| 4 | 18 | 1 | 4.614 | * 4.902 | 4.902 | .027 | .286 | -.1.2331 | 1.0000 |
| 4 | 19 | 2 | 43.030 | 41.697 | 41.697 | .639 | 1.333 | 4.6899 | 1.0000 |
| 4 | 20 | 3 | 1.225 | * .087 | -.084 | .024 | 1.138 | 1.3007 | 1.0000 |
| 4 | 21 | 4 | 9.704 | * 9.591 | 9.686 | -.162 | .013 | .0647 | 1.0000 |
| 4 | 22 | 5 | 6.575 | 6.115 | 6.115 | .023 | .611 | 2.1904 | 1.0000 |
| 4 | 23 | 6 | 24.144 | 24.530 | 24.524 | .522 | -.386 | -.1.6783 | 1.0000 |
| 4 | 24 | 7 | 15.709 | 15.135 | 15.134 | .177 | .577 | 3.0865 | 1.0000 |
| 4 | 25 | 8 | 2.665 | * .545 | -.544 | .061 | .2126 | .0959 | 1.0000 |
| 4 | 26 | 9 | 12.569 | 12.233 | 12.232 | -.170 | -.337 | 1.9422 | 1.0000 |
| 4 | 27 | 10 | 1.260 | * 2.279 | 2.273 | -.057 | .581 | 1.0910 | 1.0000 |
| 4 | 28 | 11 | 11.744 | 11.338 | 11.337 | .160 | .407 | 2.6450 | 1.0000 |
| 4 | 29 | 12 | 1.382 | * 3.67 | 3.63 | .055 | .015 | 1.0285 | 1.0000 |
| 4 | 30 | 13 | 7.590 | 7.233 | 7.231 | -.139 | .357 | 1.6360 | 1.0000 |
| 4 | 31 | 14 | 23.152 | 22.909 | 22.908 | .225 | .243 | .0891 | 1.0000 |
| 4 | 32 | 15 | 3.927 | * 4.089 | 4.089 | .023 | .163 | -.5196 | 1.0000 |
| 4 | 33 | 16 | 2.754 | * 1.909 | 1.899 | .198 | .844 | 1.6736 | 1.0000 |
| 4 | 34 | 17 | 6.570 | 7.051 | 7.051 | -.021 | .681 | -.2.1921 | 1.0000 |
| 4 | 35 | 18 | 17.079 | 17.237 | 17.236 | -.024 | .159 | -.8079 | 1.0000 |
| 4 | 36 | 19 | 1.411 | * 5.510 | 5.500 | .022 | .660 | -.8539 | 1.0000 |
| 4 | 37 | 20 | 9.886 | 9.534 | 9.533 | .114 | .355 | 2.0334 | 1.0000 |
| 4 | 38 | 21 | 9.392 | * 9.372 | 9.371 | -.095 | .020 | .1124 | 1.0000 |
| 4 | 39 | 22 | 10.729 | 10.423 | 10.422 | -.108 | .306 | 1.8013 | 1.0000 |
| 4 | 40 | 23 | 8.376 | * 8.365 | 8.365 | .093 | .010 | .0508 | 1.0000 |
| 4 | 41 | 24 | 7.986 | * 7.376 | 7.376 | .102 | .116 | 2.4244 | 1.0000 |
| 4 | 42 | 25 | 30.812 | 29.970 | 29.966 | .512 | .642 | 3.6608 | 1.0000 |
| 4 | 43 | 26 | 3.542 | * 2.783 | 2.782 | -.055 | .759 | 1.7799 | 1.0000 |
| 4 | 44 | 27 | 8.018 | * 8.358 | 8.357 | -.132 | .341 | -.1.6211 | 1.0000 |
| 4 | 45 | 28 | 1.436 | * 3.07 | 3.07 | .054 | .130 | 1.1010 | 1.0000 |
| 5 | 46 | 29 | 3.844 | * 4.217 | 4.216 | -.084 | .374 | -.2.7765 | 1.0000 |
| 5 | 47 | 30 | 7.540 | * 6.862 | 6.862 | -.083 | .676 | 3.7598 | 1.0000 |
| 5 | 48 | 31 | 3.332 | * 3.021 | 3.020 | -.073 | .310 | -.9012 | 1.0000 |
| 5 | 49 | 32 | 3.735 | * 3.282 | 3.282 | -.070 | .452 | 1.1300 | 1.0000 |

SILLIMANITE CRYSTALLINE SPRINGS AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 6

| | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|--------|---------|---------|---------|---------|-------------|-------------|
| 5 | 1 | 0 | 14.567 | -13.027 | 13.024 | .237 | 1.639 | 7.4666 |
| 5 | 1 | 1 | 8.116 | 7.875 | 7.875 | .0F2 | 24C | 1.0000 |
| 5 | 1 | 2 | 34.034 | 34.294 | 34.293 | .233 | 26C | 1.0000 |
| 5 | 1 | 3 | 34.447 | 31.711 | -11.711 | -.078 | 264 | 1.0000 |
| 5 | 1 | 4 | 13.356 | 12.491 | 12.488 | .260 | 4729 | 1.0000 |
| 5 | 1 | 5 | 2.177 * | 1.633 | 1.631 | .070 | 2034 | 1.0000 |
| 5 | 1 | 6 | 17.634 | 17.252 | 17.251 | .192 | 545 | 1.0000 |
| 5 | 1 | 7 | 8.109 | 7.674 | 7.674 | -.060 | 383 | 1.0000 |
| 5 | 2 | 0 | 6.926 | 6.052 | -6.050 | -.535 | 126 | 1.0000 |
| 5 | 2 | 1 | 14.718 | 14.569 | 14.569 | .049 | 474 | 1.0000 |
| 5 | 2 | 2 | 6.9189 | 7.0416 | 7.0416 | .522 | 6402 | 1.0000 |
| 5 | 2 | 3 | 6.686 | 6.759 | -6.759 | -.045 | 1791 | 1.0000 |
| 5 | 2 | 4 | 46.452 | 46.788 | -46.785 | -.493 | 4359 | 1.0000 |
| 5 | 2 | 5 | 10.576 | 10.737 | 10.737 | .045 | 736 | 1.0000 |
| 5 | 2 | 6 | 38.455 | 37.211 | 37.208 | .425 | 9067 | 1.0000 |
| 5 | 2 | 7 | 1.403 * | .922 | -.921 | -.035 | 4801 | 1.0000 |
| 5 | 3 | 0 | 21.629 | 21.125 | 21.123 | .505 | 7758 | 1.0000 |
| 5 | 3 | 1 | 4.635 | 4.463 | .016 | .173 | 6786 | 1.0000 |
| 5 | 3 | 2 | 39.701 | 39.986 | .284 | -.286 | 1079 | 1.0000 |
| 5 | 3 | 3 | 1.362 * | .476 | -.015 | .687 | 2257 | 1.0000 |
| 5 | 3 | 4 | 15.453 | 15.955 | 15.954 | .200 | 6501 | 1.0000 |
| 5 | 3 | 5 | 4.693 | 5.284 | .014 | -.791 | 5497 | 1.0000 |
| 5 | 3 | 6 | 20.253 | 20.332 | 20.330 | .233 | 934 | 1.0000 |
| 5 | 3 | 7 | 4.173 | 2.187 | 2.187 | -.011 | 986 | 1.0000 |
| 5 | 3 | 8 | 8.620 | 7.200 | 7.188 | -.405 | 420 | 1.0000 |
| 5 | 3 | 9 | 9.573 | 10.248 | 10.248 | .034 | 6020 | 1.0000 |
| 5 | 3 | 10 | 24.592 | 23.429 | -23.425 | -.393 | 7209 | 1.0000 |
| 5 | 3 | 11 | 10.582 | 10.959 | -10.958 | -.031 | 6121 | 1.0000 |
| 5 | 3 | 12 | 12.571 | 2.187 | 2.187 | -.011 | 5241 | 1.0000 |
| 5 | 3 | 13 | 8.214 | 8.079 | 8.071 | .365 | 2637 | 1.0000 |
| 5 | 3 | 14 | 4.440 | 3.984 | 3.984 | .033 | 627 | 1.0000 |
| 5 | 3 | 15 | 15.019 | 13.633 | -13.633 | -.320 | 5935 | 1.0000 |
| 5 | 3 | 16 | 7.360 | 6.809 | 6.809 | -.025 | 151 | 1.0000 |
| 5 | 3 | 17 | 11.068 | 11.066 | 11.066 | -.031 | 377 | 1.0000 |
| 5 | 3 | 18 | 8.577 | 8.318 | 8.317 | -.066 | 335 | 1.0000 |
| 5 | 3 | 19 | 4.420 | 3.984 | 3.984 | -.033 | 456 | 1.0000 |
| 5 | 3 | 20 | 13.482 | 13.637 | -13.633 | -.320 | 493 | 1.0000 |
| 5 | 3 | 21 | 5.615 | 6.809 | 6.809 | -.025 | 8935 | 1.0000 |
| 5 | 3 | 22 | 10.304 | 10.959 | -10.958 | -.031 | 1164 | 1.0000 |
| 5 | 3 | 23 | 12.571 | 2.187 | 2.187 | -.011 | 5241 | 1.0000 |
| 5 | 3 | 24 | 8.214 | 8.079 | 8.071 | .365 | 2637 | 1.0000 |
| 5 | 3 | 25 | 4.440 | 3.984 | 3.984 | .033 | 627 | 1.0000 |
| 5 | 3 | 26 | 15.019 | 14.526 | 14.524 | .242 | 5935 | 1.0000 |
| 5 | 3 | 27 | 7.360 | 6.627 | 6.626 | .082 | 151 | 1.0000 |
| 5 | 3 | 28 | 11.068 | 9.452 | 9.450 | .212 | 377 | 1.0000 |
| 5 | 3 | 29 | 8.577 | 7.276 | -7.276 | -.073 | 106 | 1.0000 |
| 5 | 3 | 30 | 4.420 | 8.275 | 8.272 | -.200 | 5301 | 1.0000 |
| 5 | 3 | 31 | 13.482 | 18.625 | 18.625 | .200 | 4043 | 1.0000 |
| 5 | 3 | 32 | 5.615 | 1.972 | 1.970 | -.061 | 4043 | 1.0000 |
| 5 | 3 | 33 | 10.304 | 7.60 | -.760 | -.174 | 4043 | 1.0000 |
| 5 | 3 | 34 | 12.571 | .512 | .504 | .089 | 4043 | 1.0000 |
| 5 | 3 | 35 | 8.214 | 13.705 | 13.704 | .163 | 8357 | 1.0000 |
| 5 | 3 | 36 | 4.440 | 1.93 | 1.93 | -.061 | 8357 | 1.0000 |
| 5 | 3 | 37 | 13.482 | 1.331 | 1.331 | -.078 | 8357 | 1.0000 |
| 5 | 3 | 38 | 5.615 | 2.124 | 2.124 | -.061 | 8357 | 1.0000 |
| 5 | 3 | 39 | 10.304 | 9.452 | 9.450 | .212 | 1751 | 1.0000 |
| 5 | 3 | 40 | 12.571 | 7.276 | -7.276 | -.073 | 1751 | 1.0000 |
| 5 | 3 | 41 | 8.214 | 8.275 | 8.272 | -.200 | 1751 | 1.0000 |
| 5 | 3 | 42 | 4.440 | 13.705 | 13.704 | .163 | 7237 | 1.0000 |
| 5 | 3 | 43 | 13.482 | 1.331 | 1.331 | -.078 | 7237 | 1.0000 |
| 5 | 3 | 44 | 5.615 | 2.124 | 2.124 | -.061 | 7131 | 1.0000 |
| 5 | 3 | 45 | 10.304 | 9.452 | 9.450 | .212 | 5715 | 1.0000 |
| 5 | 3 | 46 | 12.571 | 7.276 | -7.276 | -.073 | 5715 | 1.0000 |
| 5 | 3 | 47 | 8.214 | 8.275 | 8.272 | -.200 | 1639 | 1.0000 |
| 5 | 3 | 48 | 4.440 | 13.705 | 13.704 | .163 | 1714 | 1.0000 |
| 5 | 3 | 49 | 13.482 | 1.331 | 1.331 | -.078 | 1714 | 1.0000 |
| 5 | 3 | 50 | 5.615 | 2.124 | 2.124 | -.061 | 1640 | 1.0000 |
| 5 | 3 | 51 | 10.304 | 9.452 | 9.450 | .212 | 4749 | 1.0000 |
| 5 | 3 | 52 | 12.571 | 7.276 | -7.276 | -.073 | 1356 | 1.0000 |
| 5 | 3 | 53 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 54 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 55 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 56 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 57 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 58 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 59 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 60 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 61 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 62 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 63 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 64 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 65 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 66 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 67 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 68 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 69 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 70 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 71 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 72 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 73 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 74 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 75 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 76 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 77 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 78 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 79 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 80 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 81 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 82 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 83 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 84 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 85 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 86 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 87 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 88 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 89 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 90 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 91 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 92 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 93 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 94 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 95 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 96 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 97 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 98 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 99 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 100 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 101 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 102 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 103 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 104 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 105 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 106 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 107 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 108 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 109 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 110 | 5.615 | 2.124 | 2.124 | -.061 | 1441 | 1.0000 |
| 5 | 3 | 111 | 10.304 | 9.452 | 9.450 | .212 | 1441 | 1.0000 |
| 5 | 3 | 112 | 12.571 | 7.276 | -7.276 | -.073 | 1441 | 1.0000 |
| 5 | 3 | 113 | 8.214 | 8.275 | 8.272 | -.200 | 1441 | 1.0000 |
| 5 | 3 | 114 | 4.440 | 13.705 | 13.704 | .163 | 1441 | 1.0000 |
| 5 | 3 | 115 | 13.482 | 1.331 | 1.331 | -.078 | 1441 | 1.0000 |
| 5 | 3 | 116 | 5.615 | 2.124 | 2.1 | | | |

SILLIMANITE (GRANDY WINE SPRINGS) AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 9

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|-------|-----|---------|---------|---------|---------|---------|-------------|-------------|
| 5 | 8 | 1 | 1.0357 | 2.0323 | 2.0322 | 0.059 | -0.9976 | 3.0000 | * * * |
| 5 | 6 | 2 | 16.151 | 16.7763 | 16.757 | 0.459 | -0.613 | -3.01742 | 1.0000 |
| 5 | 5 | 3 | 3.028 | 2.079 | -2.078 | -0.544 | .549 | 2.0530 | 1.0000 |
| 5 | 4 | 4 | 25.050 | 24.962 | -24.959 | -0.422 | .477 | .3727 | 1.0000 |
| 5 | 3 | 5 | 2.394 | 1.055 | 1.054 | .052 | 1.0335 | 2.01262 | 1.0000 |
| 5 | 2 | 6 | 2.176 | 1.548 | 1.537 | .184 | .628 | .9516 | 1.0000 |
| 5 | 1 | 7 | 2.0205 | 2.278 | 2.276 | .034 | -0.073 | -0.1108 | 1.0000 |
| 5 | 0 | 8 | 9.357 | 9.082 | 9.079 | .025 | .275 | 1.4683 | 1.0000 |
| 5 | 9 | 2 | 2.671 | 2.286 | -2.286 | -.031 | 3.0384 | .6911 | 1.0000 |
| 5 | 8 | 3 | 2.605 | 1.500 | 1.491 | .168 | 1.0104 | .0546 | 1.0000 |
| 5 | 7 | 4 | 19.877 | 19.424 | 19.423 | .185 | .453 | 2.0330 | 1.0000 |
| 5 | 6 | 5 | 1.955 | * | 2.371 | .039 | -0.406 | -0.5201 | * * * |
| 5 | 5 | 6 | 7.100 | 7.437 | -7.434 | -.177 | -.337 | -1.4208 | 1.0000 |
| 5 | 4 | 0 | 8.2767 | 8.3603 | 8.3601 | .692 | -.036 | -3.0462 | 1.0000 |
| 5 | 3 | 1 | 28.941 | 29.308 | -29.307 | -.173 | -.367 | -1.3291 | 1.0000 |
| 5 | 2 | 0 | 60.111 | 59.661 | 59.598 | .626 | .510 | 1.7567 | 1.0000 |
| 5 | 1 | 1 | 16.082 | 15.318 | -15.317 | -.139 | .765 | 4.02151 | 1.0000 |
| 5 | 0 | 0 | 46.0782 | 39.981 | 39.981 | .308 | 2.9639 | 1.0000 | 1.0000 |
| 5 | 9 | 1 | 11.259 | 11.464 | -11.464 | -.026 | -.205 | -.9974 | 1.0000 |
| 5 | 8 | 2 | 1.201 | * | 7.54 | -.300 | -.692 | 4.47 | 1.0000 |
| 5 | 7 | 3 | 8.006 | 8.083 | 8.083 | .027 | -.677 | -.6804 | 1.0000 |
| 5 | 6 | 4 | 1.455 | * | 27.864 | .278 | -.697 | -.3039 | 1.0000 |
| 5 | 5 | 5 | 2.587 | 23.267 | 23.267 | .080 | -.679 | -.6624 | 1.0000 |
| 5 | 4 | 6 | 27.767 | 27.862 | -6.228 | -.019 | -.134 | 1.0000 | 1.0000 |
| 5 | 3 | 7 | 6.367 | 6.228 | -6.228 | -.244 | -.207 | 1.207 | 1.0000 |
| 5 | 2 | 8 | 1.412 | 2.619 | -2.608 | -.021 | -.157 | 1.1136 | 1.0000 |
| 5 | 1 | 9 | 2.612 | 2.612 | 2.612 | -.021 | -.060 | -.3241 | 1.0000 |
| 5 | 0 | 10 | 2.2 | 2.2 | 2.2 | -.104 | -.983 | -.1673 | 1.0000 |
| 5 | 9 | 11 | 25.319 | 8.133 | 8.133 | -.119 | -.0341 | -.241 | 1.0000 |
| 5 | 8 | 12 | 1.473 | 24.592 | 24.588 | .416 | -.726 | 2.05083 | 1.0000 |
| 5 | 7 | 13 | 7.078 | 7.340 | 7.340 | .114 | -.263 | -.1966 | 1.0000 |
| 5 | 6 | 14 | 1.455 | 2.619 | -2.608 | -.244 | -.157 | 1.1136 | 1.0000 |
| 5 | 5 | 15 | 2.612 | 2.612 | 2.612 | -.021 | -.060 | -.679 | 1.0000 |
| 5 | 4 | 16 | 2.587 | 23.267 | 23.267 | -.073 | -.265 | 1.3600 | 1.0000 |
| 5 | 3 | 17 | 8.103 | 8.133 | -8.133 | -.119 | -.983 | -.4481 | 1.0000 |
| 5 | 2 | 18 | 2.2 | 2 | 2 | -.026 | -.241 | -.2487 | 1.0000 |
| 5 | 1 | 19 | 2.2 | 2 | 2 | -.026 | -.091 | -.4659 | 1.0000 |
| 5 | 0 | 20 | 23.659 | 23.936 | -23.936 | -.073 | -.932 | -.9533 | 1.0000 |
| 5 | 9 | 21 | 2.891 | 3.823 | 3.823 | .037 | -.932 | -.841 | 1.0000 |
| 5 | 8 | 22 | 7.348 | 6.910 | -6.909 | -.070 | -.439 | 2.7707 | 1.0000 |
| 5 | 7 | 23 | 1.242 | * | 15.014 | -.032 | -.536 | -.6067 | 1.0000 |
| 5 | 6 | 24 | 1.242 | * | 15.014 | -.032 | -.066 | -.4657 | 1.0000 |
| 5 | 5 | 25 | 4.450 | 4.284 | 4.283 | -.266 | -.0821 | -.0821 | 1.0000 |
| 5 | 4 | 26 | 4.450 | 4.284 | 4.283 | -.024 | -.662 | 1.7191 | 1.0000 |
| 5 | 3 | 27 | 15.149 | 15.435 | 15.435 | -.032 | -.593 | -.5676 | 1.0000 |
| 5 | 2 | 28 | 4.607 | 4.631 | 4.631 | -.032 | -.255 | 1.4657 | 1.0000 |
| 5 | 1 | 29 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.5935 | 1.0000 |
| 5 | 0 | 30 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.4283 | 1.0000 |
| 5 | 9 | 31 | 1.242 | * | 1.208 | -.034 | -.034 | 1.7147 | 1.0000 |
| 5 | 8 | 32 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 7 | 33 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 6 | 34 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 5 | 35 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 4 | 36 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 3 | 37 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 2 | 38 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 1 | 39 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 0 | 40 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 9 | 41 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 8 | 42 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 7 | 43 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 6 | 44 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 5 | 45 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 4 | 46 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 3 | 47 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 2 | 48 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 1 | 49 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 0 | 50 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 9 | 51 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 8 | 52 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 7 | 53 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 6 | 54 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 5 | 55 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 4 | 56 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 3 | 57 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 2 | 58 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 1 | 59 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 0 | 60 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 9 | 61 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 8 | 62 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 7 | 63 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 6 | 64 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 5 | 65 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 4 | 66 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 3 | 67 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 2 | 68 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 1 | 69 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 0 | 70 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 9 | 71 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 8 | 72 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 7 | 73 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 6 | 74 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 5 | 75 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 4 | 76 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 3 | 77 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 2 | 78 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 1 | 79 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 0 | 80 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 9 | 81 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 8 | 82 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 7 | 83 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 6 | 84 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 5 | 85 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 4 | 86 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 3 | 87 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 2 | 88 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 1 | 89 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 0 | 90 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 9 | 91 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 8 | 92 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 7 | 93 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 6 | 94 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 5 | 95 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 4 | 96 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 3 | 97 | 7.997 | 7.746 | 7.745 | .112 | -.099 | 1.0366 | 1.0000 |
| 5 | 2 | 98 | 4.607 | 4.631 | 4.631 | .113 | -.024 | 1.0842 | 1.0000 |
| 5 | 1 | 99 | 3.790 | 3.129 | -3.128 | -.057 | -.057 | 1.0366 | 1.0000 |
| 5 | 0 | 100 | 1.463 | 1.870 | 1.870 | -.020 | -.020 | 1.0366 | 1.0000 |
| 5 | 9 | 101 | 1.242 | * | 1.208 | -.034 | -.034 | 1.0366 | 1.0000 |
| 5 | 8</td | | | | | | | | |

SILLIMANITE (BEPANDYKING SPRINGS) AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 10

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|----|--------|---------|---------|---------|---------|-------------|-------------|
| 5 | 5 | 5 | -2.207 | 2.967 | -2.967 | .013 | -760 | -1.1979 | 1.0000 |
| 5 | 5 | 6 | 21.850 | 22.097 | 22.096 | .266 | -247 | -1.1384 | 1.0000 |
| 5 | 6 | 6 | 39.950 | 40.257 | 40.253 | .589 | -307 | -0.9913 | 1.0000 |
| 6 | 6 | 1 | ?-4.01 | 2.656 | 2.656 | .010 | -745 | 2.1356 | 1.0000 |
| 6 | 6 | 2 | 3.084 | 3.750 | -3.746 | -1.134 | -666 | -1.6599 | 1.0000 |
| 6 | 6 | 3 | 1.832 | 2.257 | -2.257 | -0.09 | -425 | -0.6125 | 1.0000 |
| 6 | 6 | 4 | 30.436 | 30.340 | 30.336 | .533 | -0.98 | -2.930 | 1.0000 |
| 6 | 6 | 5 | 2.524 | *-1.139 | 2.139 | .010 | -385 | -6770 | 1.0000 |
| 6 | 7 | 0 | 11.416 | 10.455 | 10.494 | .171 | -923 | 5.2908 | 1.0000 |
| 6 | 7 | 1 | 7.779 | 7.159 | -7.199 | -0.038 | -560 | 2.9704 | 1.0000 |
| 6 | 7 | 2 | 18.426 | 18.144 | -18.143 | .164 | -2.112 | -2.112 | 1.0000 |
| 6 | 7 | 3 | 9.261 | 9.391 | 9.391 | .038 | -1.130 | -7349 | 1.0000 |
| 6 | 7 | 4 | 6.391 | 6.070 | 6.066 | .155 | -0.320 | -1.6306 | 1.0000 |
| 6 | 7 | 5 | 2.961 | 1.712 | -1.712 | -0.29 | -2.469 | 2.4281 | 1.0000 |
| 6 | 8 | 0 | 9.396 | 8.658 | 8.657 | .171 | -736 | 4.1191 | 1.0000 |
| 6 | 8 | 1 | 4.042 | 3.647 | -3.645 | -0.112 | -3.95 | 1.0964 | 1.0000 |
| 6 | 8 | 2 | 14.228 | 14.231 | 14.229 | .232 | -0.03 | -0.03 | 1.0000 |
| 6 | 8 | 3 | 2.994 | *-3.21 | 3.320 | .108 | -2.27 | -6556 | 1.0000 |
| 6 | 8 | 4 | 7.124 | 6.422 | 6.420 | .155 | -702 | 2.4809 | 1.0000 |
| 6 | 9 | 0 | 15.024 | 15.897 | 15.896 | .160 | -2.93 | -1.4494 | 1.0000 |
| 6 | 9 | 1 | 6.766 | 6.352 | -6.352 | .004 | -414 | 1.6966 | 1.0000 |
| 6 | 9 | 2 | 14.001 | 13.026 | -13.025 | -1.152 | -976 | -0.03 | -0.03 |
| 6 | 9 | 3 | 2.765 | *-2.998 | 2.998 | -0.02 | -2.33 | -4091 | 1.0000 |
| 6 | 9 | 4 | 15.024 | 15.189 | 15.188 | .150 | -1.163 | -0.9391 | 1.0000 |
| 6 | 9 | 5 | 15.922 | 16.084 | -16.083 | -1.140 | -1.162 | -8660 | 1.0000 |
| 6 | 9 | 6 | 7.035 | 6.872 | -6.871 | -0.132 | -1.163 | -7753 | 1.0000 |
| 7 | 0 | 0 | 11.549 | 12.257 | 12.257 | -0.047 | -708 | -3.9763 | 1.0000 |
| 7 | 1 | 1 | 1.205 | *-2.624 | 2.620 | .041 | -942 | 1.0937 | 1.0000 |
| 7 | 1 | 2 | 3.253 | 3.329 | 3.325 | .530 | -0.683 | 3.0128 | 1.0000 |
| 7 | 1 | 3 | 8.278 | 2.693 | -2.693 | -0.040 | -560 | -5.6228 | 1.0000 |
| 7 | 1 | 4 | 8.562 | 8.562 | -8.562 | -0.041 | -285 | -1.6773 | 1.0000 |
| 7 | 1 | 5 | 3.155 | 3.199 | 3.199 | .038 | -0.644 | -1.0100 | 1.0000 |
| 7 | 1 | 6 | 19.262 | 18.859 | 18.854 | .434 | -4.03 | -4.03 | 1.0000 |
| 7 | 1 | 7 | 9.032 | 9.210 | 9.209 | .107 | -1.177 | -1.1211 | 1.0000 |
| 7 | 2 | 1 | 1.914 | *-6.666 | 1.664 | -0.062 | -246 | -4.474 | 1.0000 |
| 7 | 2 | 2 | 2.792 | 2.764 | -2.762 | -0.103 | -0.26 | -0.675 | 1.0000 |
| 7 | 2 | 3 | 2.303 | *-5.534 | 2.534 | -0.062 | -2.32 | -4.621 | 1.0000 |
| 7 | 2 | 4 | 7.158 | 6.919 | -6.919 | .097 | -2.38 | -2.2666 | 1.0000 |
| 7 | 2 | 5 | 3.261 | 2.792 | -2.792 | -0.061 | -469 | -0.906 | 1.0000 |
| 7 | 2 | 6 | 3.818 | 2.073 | -2.072 | -0.085 | -745 | 4.4015 | 1.0000 |
| 7 | 3 | 0 | 51.843 | 52.142 | 52.136 | .751 | -2.93 | -1.0404 | 1.0000 |
| 7 | 3 | 1 | 2.500 | -2.060 | -2.060 | -0.012 | -740 | 1.8162 | 1.0000 |
| 7 | 3 | 2 | 20.431 | -20.948 | -20.946 | -0.262 | -517 | -2.1191 | 1.0000 |
| 7 | 3 | 3 | 1.715 | *-7.766 | -7.766 | .012 | -929 | 1.3533 | 1.0000 |
| 7 | 3 | 4 | 39.523 | 39.959 | 39.959 | .679 | -442 | -1.3096 | 1.0000 |
| 7 | 4 | 2 | 2.657 | *-1.575 | -1.575 | -0.089 | -296 | -3.234 | 1.0000 |
| 7 | 4 | 3 | 2.053 | *-1.713 | -1.713 | .093 | -442 | 1.0823 | 1.0000 |
| 7 | 4 | 4 | 9.093 | *-5.66 | -5.66 | -0.056 | -359 | -6.990 | 1.0000 |
| 7 | 4 | 5 | 2.524 | -9.142 | -9.142 | -0.084 | -282 | -2.822 | 1.0000 |
| 7 | 4 | 6 | 12.238 | -12.439 | -12.439 | -0.093 | -202 | -1.1426 | 1.0000 |
| 7 | 4 | 7 | 1.279 | *-1.575 | -1.575 | -0.089 | -296 | -3.234 | 1.0000 |
| 7 | 4 | 8 | 2.053 | *-1.713 | -1.713 | -0.093 | -442 | 1.0823 | 1.0000 |
| 7 | 4 | 9 | 9.093 | -9.142 | -9.142 | -0.084 | -282 | -2.822 | 1.0000 |
| 7 | 4 | 10 | 5.524 | -3.446 | -3.446 | -0.074 | -15897 | -1.5897 | 1.0000 |

SILLIMANITE EXPANDING SPRINGS AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 11

| M | K | L | F(CS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|-----|-------|---------|----------|---------|---------|-------------|-------------|
| 7 | 7 | 4 | 6 | 3.126 | 1.585 | .076 | 1.539 | 3.1941 | 1.0000 |
| 7 | 7 | 0 | 6 | 4.957 | 4.431 | .122 | 4.465 | 1.6052 | 1.0000 |
| 7 | 5 | 1 | 6 | 4.866 | 4.955 | .036 | 4.955 | 2.652 | 1.0000 |
| 7 | 5 | 2 | 3 | 3.936 | 3.830 | .069 | 3.829 | 3.952 | 1.0000 |
| 7 | 5 | 3 | 2 | 1.552 | 2.435 | .325 | 2.435 | 1.0423 | 1.0000 |
| 7 | 5 | 4 | 3 | 3.299 | 3.322 | .036 | 3.320 | 0.663 | * * * |
| 7 | 5 | 5 | 4 | 3.030 | 3.330 | .111 | 3.330 | 0.032 | -0.032 |
| 7 | 5 | 6 | 0 | 4.075 | 4.075 | .023 | 4.075 | 0.743 | -0.743 |
| 7 | 6 | 0 | 6 | 4.476 | 4.621 | .014 | 4.621 | 1.369 | 1.0000 |
| 7 | 6 | 1 | 6 | 5.622 | 5.461 | .161 | 5.461 | 6.616 | 1.0000 |
| 7 | 6 | 2 | 1 | 1.237 | 1.234 | .129 | 1.234 | 1.0000 | 1.0000 |
| 7 | 6 | 3 | 2 | 6.150 | 6.123 | .017 | 6.123 | 0.557 | -0.557 |
| 7 | 6 | 4 | 3 | 8.569 | 8.939 | .120 | 8.938 | 2.403 | -2.403 |
| 7 | 6 | 5 | 4 | 3.831 | 4.072 | .013 | 4.072 | 1.7820 | 1.0000 |
| 7 | 6 | 6 | 5 | 9.925 | 9.467 | .014 | 9.467 | 6.104 | -6.104 |
| 7 | 7 | 0 | 6 | 25.92 | 25.869 | .157 | 25.898 | 4.435 | -4.435 |
| 7 | 7 | 1 | 0 | 6.156 | 6.633 | .057 | 6.633 | 3.464 | -3.464 |
| 7 | 7 | 2 | 1 | 36.403 | 37.075 | .077 | 37.071 | 4.014 | -4.014 |
| 7 | 7 | 3 | 2 | 8.591 | 8.195 | .013 | 8.195 | 1.7820 | 1.0000 |
| 7 | 7 | 4 | 3 | 20.492 | 20.050 | .057 | 20.050 | 6.104 | -6.104 |
| 7 | 7 | 5 | 4 | 1.462 | 1.288 | .098 | 1.288 | 3.464 | -3.464 |
| 7 | 7 | 6 | 5 | 1.447 | * 1.161 | .024 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 7 | 6 | 10.307 | 10.181 | .091 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 8 | 7 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 9 | 8 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 10 | 9 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 11 | 10 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 12 | 11 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 13 | 12 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 14 | 13 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 15 | 14 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 16 | 15 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 17 | 16 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 18 | 17 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 19 | 18 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 20 | 19 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 21 | 20 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 22 | 21 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 23 | 22 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 24 | 23 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 25 | 24 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 26 | 25 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 27 | 26 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 28 | 27 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 29 | 28 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 30 | 29 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 31 | 30 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 32 | 31 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 33 | 32 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 34 | 33 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 35 | 34 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 36 | 35 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 37 | 36 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 38 | 37 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 39 | 38 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 40 | 39 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 41 | 40 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 42 | 41 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 43 | 42 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 44 | 43 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 45 | 44 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 46 | 45 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 47 | 46 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 48 | 47 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 49 | 48 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 50 | 49 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 51 | 50 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 52 | 51 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 53 | 52 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 54 | 53 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 55 | 54 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 56 | 55 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 57 | 56 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 58 | 57 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 59 | 58 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 60 | 59 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 61 | 60 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 62 | 61 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 63 | 62 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 64 | 63 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 65 | 64 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 66 | 65 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 67 | 66 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 68 | 67 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 69 | 68 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 70 | 69 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 71 | 70 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 72 | 71 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 73 | 72 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 74 | 73 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 75 | 74 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 76 | 75 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 77 | 76 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 78 | 77 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 79 | 78 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 80 | 79 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 81 | 80 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 82 | 81 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 83 | 82 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 84 | 83 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 85 | 84 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 86 | 85 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 87 | 86 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 88 | 87 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 89 | 88 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 90 | 89 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 91 | 90 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 92 | 91 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 93 | 92 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 94 | 93 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 95 | 94 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 96 | 95 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 97 | 96 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 98 | 97 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000 |
| 7 | 7 | 99 | 98 | 20.492 | 29.088 | .157 | 29.083 | 1.9382 | -1.9382 |
| 7 | 7 | 100 | 99 | 30.029 | * 29.083 | .098 | 29.083 | 1.0000 | 1.0000 |
| 7 | 7 | 101 | 100 | 2.533 | * 1.126 | .174 | 1.126 | 1.3324 | -1.3324 |
| 7 | 7 | 102 | 101 | 1.447 | * 1.161 | .266 | 1.161 | 2.570 | 1.0000 |
| 7 | 7 | 103 | 102 | 10.307 | 10.181 | .026 | 10.181 | 0.037 | -0.037 |
| 7 | 7 | 104 | 103 | 1.463 | * 1.532 | .025 | 1.532 | 1.0000 | 1.0000</td |

SILLIMANITE-CRABBYWINE SPRINGS AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 12

| | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|----|---|----|--------|---------|---------|---------|---------|-------------|-------------|
| 10 | 4 | 5 | 5.0284 | 5.0648 | -5.647 | -0.056 | .237 | .8462 | 1.0000 |
| 10 | 5 | 0 | 23.166 | 33.786 | 33.783 | .427 | -6.616 | -1.7616 | 1.0000 |
| 10 | 5 | 1 | 9.026 | 9.043 | -9.043 | -0.059 | -0.015 | -0.0875 | 1.0000 |
| 10 | 6 | 2 | 30.301 | 30.000 | -29.997 | -0.413 | .301 | 1.1689 | 1.0000 |
| 10 | 6 | 3 | 8.150 | 8.086 | 8.086 | .058 | .064 | .3146 | 1.0000 |
| 10 | 6 | 4 | 25.977 | 26.118 | 26.115 | .386 | -0.141 | -0.6090 | 1.0000 |
| 10 | 6 | 5 | 13.74 | 13.604 | 13.598 | .378 | .140 | .7471 | 1.0000 |
| 10 | 6 | 6 | 1.423 | *.104 | -0.996 | -0.039 | 1.316 | 1.2981 | 1.0000 |
| 10 | 6 | 7 | 2.103 | *.2487 | 2.487 | .044 | -0.384 | -0.5495 | 1.0000 |
| 10 | 6 | 8 | 1.540 | *.2554 | 2.554 | .038 | -1.014 | -1.0385 | 1.0000 |
| 10 | 6 | 9 | 10.227 | 10.265 | 10.279 | .342 | -0.056 | -0.3198 | 1.0000 |
| 10 | 7 | 0 | 13.911 | 14.269 | -14.267 | -0.245 | -0.246 | -1.8201 | 1.0000 |
| 10 | 7 | 1 | 4.028 | 4.026 | -4.925 | -0.667 | -0.012 | *.012 | 1.0000 |
| 10 | 7 | 2 | 11.481 | 11.669 | 11.667 | .243 | -1.014 | -1.1401 | 1.0000 |
| 10 | 7 | 3 | 4.193 | 4.387 | 4.387 | .067 | -0.105 | -0.5090 | 1.0000 |
| 10 | 7 | 4 | 4.191 | 1.2139 | 12.137 | .211 | .352 | 1.9416 | 1.0000 |
| 10 | 7 | 5 | 4.761 | 4.899 | 4.899 | .079 | -0.136 | -1.4025 | 1.0000 |
| 10 | 7 | 6 | 1.347 | *.651 | 2.651 | .013 | -1.303 | -3.3543 | 1.0000 |
| 10 | 7 | 7 | 1.604 | *.224 | *.224 | .015 | 1.386 | *.C370 | 1.0000 |
| 10 | 7 | 8 | 4.336 | 3.713 | 3.713 | -.006 | 1.625 | 1.5754 | 1.0000 |
| 10 | 7 | 9 | 21.332 | 21.989 | 21.956 | -.360 | -0.657 | -3.0567 | 1.0000 |
| 10 | 8 | 0 | 8.058 | 8.132 | -8.130 | -.149 | -0.074 | -0.4001 | 1.0000 |
| 10 | 8 | 1 | 11.141 | 11.398 | 11.398 | .098 | -0.257 | -0.257 | 1.0000 |
| 10 | 8 | 2 | 9.677 | 9.667 | 9.666 | .142 | 0.010 | *.010 | 1.0000 |
| 10 | 8 | 3 | 16.689 | 16.945 | 16.942 | .326 | -0.216 | -0.216 | 1.0000 |
| 10 | 8 | 4 | 4.354 | 3.756 | -3.753 | -.125 | .599 | 1.5943 | 1.0000 |
| 10 | 8 | 5 | 32.660 | 32.006 | 32.904 | .306 | -0.247 | -0.247 | 1.0000 |
| 10 | 8 | 6 | 2.556 | *.734 | 2.734 | -.003 | -0.178 | -0.7236 | 1.0000 |
| 10 | 8 | 7 | 3.5477 | 3.5566 | -3.5564 | -.34 | -0.089 | -0.3406 | 1.0000 |
| 10 | 8 | 8 | 3.507 | 3.957 | -3.957 | -.007 | -0.449 | -1.0569 | 1.0000 |
| 10 | 8 | 9 | 25.580 | 25.499 | 25.497 | .357 | 0.081 | *.081 | 1.0000 |
| 10 | 9 | 0 | 1.476 | *.217 | 0.217 | -.001 | 1.256 | 1.1942 | 1.0000 |
| 10 | 9 | 1 | 5.047 | 4.298 | -4.298 | -.011 | 1.549 | 1.5263 | 1.0000 |
| 10 | 9 | 2 | 1.399 | *.1562 | -1.562 | -.017 | 1.162 | -0.2541 | 1.0000 |
| 10 | 9 | 3 | 26.050 | 26.476 | 26.473 | .447 | -0.427 | -1.05925 | 1.0000 |
| 10 | 9 | 4 | 1.436 | *.656 | -6.56 | .017 | 0.780 | .7602 | 1.0000 |
| 10 | 9 | 5 | 4.525 | 3.306 | -3.306 | -.009 | 1.219 | 3.5530 | 1.0000 |
| 10 | 9 | 6 | 4.797 | 3.551 | -3.530 | -.298 | 1.246 | 4.0993 | 1.0000 |
| 10 | 9 | 7 | 3.745 | 3.315 | 3.315 | .022 | 0.430 | 1.0889 | 1.0000 |
| 10 | 9 | 8 | 11.390 | 11.757 | 11.754 | .284 | -0.368 | -2.0662 | 1.0000 |
| 10 | 9 | 9 | 1.453 | *.000 | -1.000 | -.017 | 0.452 | *.4359 | 1.0000 |
| 10 | 9 | 10 | 3.150 | 2.567 | -2.554 | -.260 | 0.583 | 1.1646 | 1.0000 |
| 10 | 9 | 11 | 19.379 | 19.832 | 19.830 | .281 | -0.453 | -2.0729 | 1.0000 |
| 10 | 9 | 12 | 9.376 | 8.664 | 8.662 | .153 | -0.288 | -1.4076 | 1.0000 |
| 10 | 9 | 13 | 12.582 | 12.795 | 12.795 | .137 | -0.213 | -1.1761 | 1.0000 |
| 10 | 9 | 14 | 5.861 | 6.068 | -6.066 | -.145 | -0.206 | -0.7320 | 1.0000 |
| 10 | 9 | 15 | 12.662 | 11.914 | -11.913 | -.144 | .746 | 4.2860 | 1.0000 |
| 10 | 9 | 16 | 1.019 | 1.019 | 1.019 | .004 | 2.467 | 5.6781 | 1.0000 |
| 10 | 9 | 17 | 2.307 | * | 1.800 | 1.794 | .145 | *.507 | *.507 |
| 10 | 9 | 18 | 14.095 | 13.717 | 13.713 | .344 | .377 | 2.1211 | 1.0000 |
| 10 | 9 | 19 | 22.792 | 22.507 | -22.506 | -.245 | *.285 | 1.2562 | 1.0000 |
| 10 | 9 | 20 | 45.784 | 46.940 | -46.935 | -.668 | -1.156 | -3.2075 | 1.0000 |
| 10 | 9 | 21 | 18.700 | 17.879 | -17.878 | -.220 | .821 | 4.3037 | 1.0000 |

SILVIANITE-COPPERYLINE SPRINGS AT 400 DEGREES C

STRUCTURE FACTORS

PAGE 13

| μ | κ | ℓ | $F(\text{CALS})$ | $F(\text{CALC})$ | $L(\text{CALC})$ | $B(\text{CALC})$ | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|-------|----------|--------|------------------|------------------|------------------|------------------|---------|-------------|-------------|
| 10 | 1 | 0 | 9.084 | 8.904 | -6.904 | -0.047 | *1FC | *973.2 | 1.0000 |
| 20 | 1 | 1 | 3.657 | 2.457 | 2.456 | *0.07 | 1.200 | 2.0091 | 1.0000 |
| 20 | 1 | 2 | 3.657 | 2.457 | 2.456 | *0.07 | 1.200 | 2.0591 | 1.0000 |
| 20 | 1 | 0 | 6.084 | 5.904 | -8.904 | -0.047 | *1FC | *973.2 | 1.0000 |
| 20 | 1 | 0 | 3.657 | 2.457 | 2.456 | *0.07 | 1.200 | 2.0737 | 1.0000 |
| 20 | 1 | 1 | 3.657 | 2.457 | 2.456 | *0.07 | 1.200 | 2.0691 | 1.0000 |
| 20 | 1 | 2 | 3.657 | 2.457 | 2.456 | *0.07 | 1.200 | 2.0699 | 1.0000 |
| 20 | 1 | 0 | 7.678 | 7.811 | -7.811 | *0.045 | *152 | *1.999 | 1.0000 |
| 20 | 1 | 1 | 2.950 | 1.632 | -1.626 | *0.079 | 1.228 | 2.2945 | 1.0000 |
| 20 | 1 | 2 | 7.014 | 6.700 | -6.700 | -0.042 | *314 | 1.2716 | 1.0000 |
| 20 | 1 | 0 | 17.955 | 16.274 | 16.269 | *2.99 | -419 | -3.8966 | 1.0000 |
| 20 | 1 | 1 | 2.959 | 3.249 | 3.248 | *0.031 | *371 | *705.3 | 1.0000 |
| 20 | 1 | 2 | 7.014 | 7.372 | 7.372 | *0.35 | -111 | -4.6234 | 1.0000 |
| 20 | 1 | 0 | 4.492 | 3.069 | -3.068 | -0.077 | 1.423 | 4.0774 | 1.0000 |
| 20 | 1 | 0 | 10.772 | 11.136 | 11.136 | -0.025 | -364 | -2.0046 | 1.0000 |
| 20 | 1 | 0 | 12.927 | 13.172 | -13.171 | -1.10 | -944 | -1.8980 | 1.0000 |
| 20 | 1 | 1 | 4.122 | 3.316 | 3.316 | *0.026 | *806 | 2.1202 | 1.0000 |
| 20 | 1 | 2 | 15.391 | 16.398 | 16.398 | *145 | -667 | -0.409 | 1.0000 |
| 20 | 1 | 0 | 30.085 | 31.407 | 31.403 | *510 | -1322 | -4.7263 | 1.0000 |
| 20 | 1 | 0 | 5.961 | 5.367 | -5.366 | -0.052 | *594 | 2.1670 | 1.0000 |
| 20 | 1 | 1 | 6.311 | 6.375 | -6.375 | -0.01 | *665 | -0.2381 | 1.0000 |
| 20 | 1 | 2 | 2.562 | 1.545 | *1.545 | *0.60 | 2.014 | 3.2616 | 1.0000 |
| 20 | 1 | 0 | 2.503 | 2.033 | -2.033 | *0.35 | *670 | *741.7 | 1.0000 |
| 20 | 1 | 1 | 3.388 | 3.710 | -3.706 | -1.172 | -322 | -6.934 | 1.0000 |
| 20 | 1 | 2 | 11.034 | 11.467 | 11.461 | *380 | *633 | -2.3441 | 1.0000 |
| 20 | 1 | 0 | 4.946 | 4.555 | 4.558 | *0.62 | *356 | 1.1850 | 1.0000 |
| 20 | 1 | 1 | 8.721 | 8.963 | 8.963 | *0.37 | -242 | -1.1552 | 1.0000 |
| 20 | 1 | 2 | 17.951 | 17.924 | -17.922 | -2.82 | *227 | *1396 | 1.0000 |
| 20 | 1 | 0 | 6.059 | 6.857 | -6.857 | -0.77 | -3420 | -2.8420 | 1.0000 |

SILLIMASITE CEPANDYKINE SPRINGS AT 400 DEGREES C

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS

NUMERATOR

NUMBER

F

WEIGHTED P

13043.96

6769665.02

663

.044

UNWEIGHTED Q

414.41

9046.41

663

.046

RANGES OF F(OBS)

| | | | |
|----------|------------|------|------|
| 3.958.73 | 860028.97 | .500 | .068 |
| 1516.55 | 1031711.35 | .96 | .038 |
| 465.75 | 936724.79 | .39 | .022 |
| 1010.45 | 1287897.29 | .16 | .028 |
| 339.22 | 1119416.66 | .7 | .017 |
| 2290.45 | 633196.54 | .3 | .051 |
| 133.35 | 252093.75 | .1 | .023 |
| 3319.49 | 393595.58 | .1 | .091 |

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

| | | | |
|---------|------------|------|------|
| 4911.98 | 2270501.37 | .54 | .046 |
| 4349.56 | 1758178.94 | .56 | .050 |
| 756.98 | 792074.36 | .67 | .032 |
| 512.05 | 592085.10 | .86 | .029 |
| 435.24 | 346936.45 | .88 | .027 |
| 478.87 | 396333.17 | .99 | .035 |
| 378.81 | 379558.88 | .117 | .032 |
| 1170.48 | 264596.74 | .112 | .066 |

UNREJECTED REFLECTIONS

WEIGHTED R

| | | | |
|---------|------------|------|------|
| 7325.73 | 5956055.56 | .524 | .035 |
| 301.06 | 2585.23 | .524 | .025 |

UNWEIGHTED R

| | | | |
|---------|------------|------|------|
| 3767.14 | 858764.02 | .363 | .066 |
| 1515.55 | 1031711.35 | .06 | .038 |
| 465.75 | 936724.79 | .29 | .022 |
| 1010.45 | 1287897.28 | .16 | .028 |
| 339.22 | 1119416.66 | .7 | .017 |
| 93.27 | 463447.70 | .2 | .014 |
| 133.35 | 252093.75 | .1 | .023 |
| .00 | .00 | .00 | .000 |

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

| | | | |
|---------|------------|-----|------|
| 2704.79 | 1859694.20 | .35 | .038 |
| 1026.34 | 1359544.01 | .51 | .027 |
| 737.36 | 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 | .96 | .031 |
| 1108.74 | 264718.23 | .83 | .065 |

SUM F(CAL)

8931.90

STANDARD DEV OF UNIT WEIGHT OBS

3.91

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

John K. Winter

and

Subrata Ghose

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Seattle, Washington 98195

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

Sillimanite 600°C

ULLGOSLI

LOAD MAP - SECTION

GY-
32
n
20
LOADER 1-3-460

02/19/78 16.46.C1

-5-

FWD OF THE LOAD
LWA+1 OF THE LOAD 111
TRANSFER ADDRESS --- SEEING 74743
112

中華書局影印
宋史卷一百一十五

PROGRAM AND BLOCK ASSIGNMENTS

| | | | | | | | | | |
|---------|-------|------|-----------|----------|---------|---|----|----|---|
| REFINE | 21374 | 5726 | RFINE | 05/14/76 | RUN | F | E5 | 74 | B |
| BODANI | 27522 | 1147 | RFINE | 05/14/76 | RUN | F | E5 | 74 | B |
| FLVIRI | 30671 | 1312 | RFINE | 05/14/76 | RUN | F | FR | 74 | S |
| INPUT | 32203 | 241 | RFINE | 05/14/76 | RUN | F | FS | 74 | E |
| MATRIX | 32444 | 231 | RFINE | 05/14/76 | RUN | F | FB | 74 | E |
| NODIFY | 32675 | 115 | RFINE | 05/14/76 | RUN | F | FB | 74 | E |
| RCALC | 33012 | 152 | RFINE | 05/14/76 | RUN | F | FR | 74 | S |
| RESET | 33164 | 73 | RFINE | 05/14/76 | RUN | F | FB | 74 | E |
| SFAC | 33257 | 476 | RFINE | 05/14/76 | RUN | F | FR | 74 | E |
| SYMMY | 33755 | 361 | RFINE | 05/14/76 | RUN | F | FB | 74 | B |
| WEIGHT | 34336 | 12 | RFINE | 05/14/76 | RUN | F | FB | 74 | B |
| ASINCOS | 34350 | 136 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| EXP | 34506 | 55 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| SINCOS | 34563 | 72 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| SORT | 34655 | 44 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| ACGDEP | 34721 | 12 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| ENDFILE | 34733 | 57 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| GETBA | 35012 | 17 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| INPUTB | 35031 | 256 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| KRAKER | 35307 | 1052 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| OUTPTB | 36361 | 244 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| S10S | 36625 | 1504 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| INPUTC | 40331 | 121 | SL-RUN2P3 | 03/17/75 | COMPASS | F | EB | 74 | E |
| KODER | 40452 | 1310 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| OUTPTC | 41762 | 71 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| REWIND | 42053 | 63 | SL-RUN2P3 | 02/19/75 | COMPASS | F | EB | 74 | E |
| SYSTEM | 42136 | 1122 | SL-RUN2P3 | 03/04/75 | COMPASS | F | EB | 74 | E |

SILLIMANITE (BRANDYWINE SPRINGS, PA) 600 DEGREES C

STRUCTURE FACTORS
PAGE 1

| 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 | -350 | -1.307 | -9.0549 | 1.0000 |
| 0 | 0 | 4 | 132.414 | 143.860 | 143.858 | .823 | -11.446 | -55.4853 | 1.0000 * |
| 0 | 0 | 6 | 26.044 | 25.632 | -25.630 | .278 | .412 | 1.3745 | 1.0000 |
| 0 | 0 | 8 | 51.315 | 50.630 | -50.626 | .590 | .485 | 1.3929 | 1.0000 |
| 0 | 2 | 0 | 15.490 | 13.241 | 13.241 | .029 | 2.245 | 10.3365 | 1.0000 |
| 0 | 2 | 1 | 4.719 | 4.311 | -4.311 | .065 | 4.07 | 1.0210 | 1.0000 |
| 0 | 2 | 2 | 23.005 | 18.752 | -18.745 | .507 | 4.253 | 23.045 | 1.0000 |
| 0 | 2 | 3 | 6.270 | 6.072 | -6.072 | .063 | 1.196 | 1.0857 | 1.0000 |
| 0 | 2 | 4 | 7.542 | 6.839 | -6.839 | .027 | 7.04 | 3.7835 | 1.0000 |
| 0 | 2 | 5 | 1.074 | *207 | -207 | .050 | 7.76 | 1.0131 | 1.0000 |
| 0 | 2 | 6 | 8.576 | 8.015 | -8.005 | .407 | 4.583 | 4.2086 | 1.0000 |
| 0 | 2 | 7 | 6.326 | 4.522 | -4.522 | .054 | 1.105 | -6.7314 | 1.0000 |
| 0 | 2 | 8 | 3.063 | 2.142 | -2.142 | .021 | 1.723 | 5.3016 | 1.0000 |
| 0 | 4 | 0 | 21.330 | 19.565 | -19.565 | .153 | 1.765 | 8.5537 | 1.0000 |
| 0 | 4 | 1 | 6.364 | 6.630 | -6.629 | .081 | .265 | -1.5897 | 1.0000 |
| 0 | 4 | 2 | 89.402 | 89.780 | -89.777 | .657 | -1.375 | -7.0651 | 1.0000 |
| 0 | 4 | 3 | 9.629 | 10.359 | -10.359 | -1.077 | -7.730 | -4.3189 | 1.0000 |
| 0 | 4 | 4 | 4.172 | 5.801 | -5.799 | -1.326 | -1.629 | -7.4488 | 1.0000 |
| 0 | 4 | 5 | 2.563 | 1.226 | -1.224 | .072 | 1.337 | 3.9280 | 1.0000 |
| 0 | 4 | 6 | 43.044 | 45.230 | -45.227 | .527 | -2.185 | -7.1607 | 1.0000 |
| 0 | 4 | 7 | 6.979 | 6.978 | -6.978 | .062 | .3565 | 1.0000 | * |
| 0 | 4 | 8 | 1.822 | *335 | -6.322 | -.095 | 1.486 | 2.0928 | 1.0000 |
| 0 | 6 | 0 | 50.143 | 49.563 | -49.556 | .751 | .579 | 2.4954 | 1.0000 |
| 0 | 6 | 1 | 7.411 | 7.338 | -7.338 | -.021 | 0.72 | 1.366 | 1.0000 |
| 0 | 6 | 2 | 22.505 | 23.704 | -23.703 | .264 | -1.202 | *4200 | 1.0000 |
| 0 | 6 | 3 | 1.083 | *707 | -6.707 | -.020 | 4.376 | 4.667 | 1.0000 |
| 0 | 6 | 4 | 36.086 | 37.862 | -37.856 | .672 | -1.776 | -6.1539 | 1.0000 |
| 0 | 6 | 5 | 7.267 | 7.246 | -7.246 | -.015 | *C21 | *1366 | 1.0000 |
| 0 | 6 | 6 | 10.996 | 11.744 | -11.742 | -.210 | -.747 | -5.1785 | 1.0000 |
| 0 | 6 | 7 | 2.606 | *18.968 | -1.725 | -.014 | *451 | 1.8212 | 1.0000 |
| 0 | 6 | 8 | 18.968 | 18.505 | -18.505 | .194 | .462 | 1.9890 | 1.0000 |
| 0 | 8 | 0 | 1.425 | *2.270 | -2.269 | -.067 | -.845 | -1.1865 | 1.0000 |
| 0 | 8 | 1 | 21.876 | 22.511 | -22.510 | -.225 | -.635 | -2.8041 | 1.0000 |
| 0 | 8 | 2 | 4.129 | 5.361 | -5.361 | -.055 | -1.232 | -4.6716 | 1.0000 |
| 0 | 8 | 3 | 12.765 | 12.899 | -12.897 | .174 | -.133 | -9.9246 | 1.0000 |
| 0 | 8 | 4 | 2.870 | 2.037 | -2.036 | -.049 | -.733 | 1.7625 | 1.0000 |
| 0 | 8 | 5 | 12.960 | 13.555 | -13.554 | -.181 | -.595 | -4.0003 | 1.0000 |
| 0 | 8 | 6 | 5.840 | 6.362 | -6.359 | -.192 | -.521 | -2.1924 | 1.0000 |
| 0 | 10 | 0 | 4.087 | 4.596 | -4.595 | -.085 | -.500 | -1.5542 | 1.0000 |
| 0 | 10 | 1 | 27.669 | 28.481 | -28.476 | .541 | -.813 | -3.1759 | 1.0000 |
| 0 | 10 | 2 | 1.343 | *1.211 | -1.118 | -.080 | *221 | *2310 | 1.0000 |
| 0 | 10 | 3 | 6.977 | 5.225 | -5.222 | -.171 | 1.752 | 8.0512 | 1.0000 |
| 0 | 10 | 4 | 12.625 | 12.107 | -12.107 | .077 | .516 | 2.3560 | 1.0000 |
| 0 | 10 | 5 | 1.668 | 1.668 | -1.666 | -.074 | .746 | 2.4500 | 1.0000 |
| 0 | 10 | 6 | 9.175 | 9.239 | -9.239 | .069 | -.064 | -.4086 | 1.0000 |
| 0 | 10 | 7 | 1.249 | *1.795 | -1.795 | -.060 | -.547 | -.6131 | 1.0000 |
| 1 | 1 | 0 | 25.479 | 24.008 | -24.003 | .067 | 1.471 | 11.8640 | 1.0000 |
| 1 | 1 | 1 | 4.635 | *846 | -.846 | .029 | 3.769 | 6.1904 | 1.0000 |
| 1 | 1 | 2 | 62.253 | 62.849 | -62.848 | .475 | -.597 | -3.9200 | 1.0000 |
| 1 | 1 | 3 | 8.424 | 8.313 | -8.313 | -.028 | .111 | .6546 | 1.0000 |
| 1 | 1 | 4 | 13.107 | 14.234 | -14.234 | -.061 | -1.127 | -6.2896 | 1.0000 |
| 1 | 1 | 5 | 4.328 | 4.959 | -4.959 | -.026 | -.632 | -2.9648 | 1.0000 |
| 1 | 1 | 6 | 29.023 | 28.242 | -28.242 | .381 | -.779 | 2.6485 | 1.0000 |

SILLIMANITE CERANDYLINE SPRINGS AT 600 DEGREES C

STRUCTURE FACTORS

PAGE 2

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA SIGN. | EATI, FACTOR |
|---|---|---|--------|---------|---------|---------|---------|-------------|-------------------|
| 1 | 1 | 1 | 7 | 4.666 | 4.487 | 4.487 | -0.024 | +1.78 | *7220 1.0000 |
| 1 | 1 | 6 | 6 | 6.350 | 6.238 | 6.238 | +0.046 | +1.12 | *5091 1.0000 |
| 1 | 2 | 0 | 81 | 2.09 | 2.211 | 2.210 | -0.461 | -1.003 | -7.6022 1.0000 |
| 1 | 2 | 1 | 7 | 5.31 | 7.818 | 7.818 | -0.044 | +2.87 | -1.1726 1.0000 |
| 1 | 2 | 2 | 85 | 4.02 | 5.522 | 5.522 | -0.48 | +1.20 | -0.7365 1.0000 |
| 1 | 2 | 3 | 2 | 3.42 | 1.862 | 1.862 | +0.42 | +0.61 | 1.5564 1.0000 |
| 1 | 2 | 4 | 46 | 7.21 | 4.7560 | 4.7558 | +0.412 | +0.39 | -3.7016 1.0000 |
| 1 | 2 | 5 | 7 | 1.58 | 7.855 | 7.854 | -0.038 | +0.96 | -4.3204 1.0000 |
| 1 | 2 | 6 | 36 | 1.20 | 7.709 | 7.707 | -0.358 | +5.81 | -1.5656 1.0000 |
| 1 | 2 | 7 | 1 | 2.55 | 1.987 | 1.986 | +0.34 | +7.32 | -0.6170 1.0000 |
| 1 | 2 | 8 | 20 | 0.64 | 19.499 | 19.497 | +0.295 | +5.65 | 2.6140 1.0000 |
| 1 | 3 | 0 | 46 | 5.65 | 4.069 | 4.069 | +0.630 | +0.65 | -3.1725 1.0000 |
| 1 | 3 | 1 | 5 | 4.78 | 5.554 | 5.554 | -0.011 | +0.75 | -0.3946 1.0000 |
| 1 | 3 | 2 | 3 | 4.34 | 6.06 | 6.06 | -0.090 | +1.73 | -0.8604 1.0000 |
| 1 | 3 | 3 | 2 | 8.45 | 2.155 | 2.155 | -0.2155 | +0.10 | +0.691 1.0000 |
| 1 | 3 | 4 | 38 | 2.17 | 3.9031 | 3.9027 | +0.564 | +0.14 | -3.3902 1.0000 |
| 1 | 3 | 5 | 5 | 6.76 | 6.003 | 6.003 | +0.008 | +3.28 | -1.5902 1.0000 |
| 1 | 3 | 6 | 3 | 6.26 | 3.636 | 3.636 | -0.070 | +2.08 | -0.7337 1.0000 |
| 1 | 3 | 7 | 2 | 5.98 | 2.639 | 2.639 | +0.007 | +2.41 | +0.5297 1.0000 |
| 1 | 3 | 8 | 18 | 7.17 | 18.569 | 18.569 | +0.405 | +0.46 | +0.7923 1.0000 |
| 1 | 4 | 0 | 2 | 1.25 | *770 | *689 | +0.344 | +3.55 | 1.355 1.0000 |
| 1 | 4 | 1 | 3 | 0.46 | 2.672 | 2.672 | +0.027 | +0.30 | +0.174 1.0000 |
| 1 | 4 | 2 | 25 | 6.69 | 26.555 | 26.553 | +0.334 | +0.66 | -3.1031 1.0000 |
| 1 | 4 | 3 | 6 | 1.82 | 6.972 | 6.972 | +0.029 | +0.29 | +0.790 1.0000 |
| 1 | 4 | 4 | 6 | 6.505 | 6.266 | 6.261 | +0.303 | +0.37 | +0.5947 1.0000 |
| 1 | 4 | 5 | 1 | 3.59 | *866 | *865 | +0.027 | +0.27 | 3.6306 1.0000 |
| 1 | 4 | 6 | 14 | 4.57 | 14.775 | 14.772 | +0.30 | +0.30 | +0.694 1.0000 |
| 1 | 4 | 7 | 25 | 6.06 | 26.53 | 26.53 | +0.318 | +0.318 | +0.686 1.0000 |
| 1 | 4 | 8 | 6 | 3.927 | 6.182 | 6.182 | +0.025 | +0.25 | +0.8082 1.0000 |
| 1 | 5 | 0 | 10 | 9.90 | 10.054 | 10.052 | +0.261 | +0.26 | +0.5947 1.0000 |
| 1 | 5 | 1 | 6 | 6.739 | 6.400 | 6.400 | +0.23 | +0.23 | +0.7389 1.0000 |
| 1 | 5 | 2 | 61 | 9.02 | 5.329 | 5.329 | +0.025 | +0.25 | +1.8423 1.0000 |
| 1 | 5 | 3 | 63 | 2.129 | *2.129 | *2.129 | +0.030 | +0.30 | +0.7516 1.0000 |
| 1 | 5 | 4 | 1 | 1.011 | -1.011 | -1.011 | +0.024 | +0.24 | +0.665 1.0000 |
| 1 | 5 | 5 | 9 | 1.189 | 9.189 | 9.187 | +0.161 | +1.79 | +0.7429 1.0000 |
| 1 | 5 | 6 | 4 | 4.977 | 4.977 | 4.977 | +0.021 | +0.21 | +0.7986 1.0000 |
| 1 | 5 | 7 | 29 | 3.311 | 29.311 | 29.310 | +0.252 | +0.25 | +1.375 1.0000 |
| 1 | 5 | 8 | 1 | 6.666 | 1.666 | 1.666 | +0.022 | +0.22 | +0.645 1.0000 |
| 1 | 6 | 0 | 23 | 3.92 | -23.962 | -23.962 | +0.153 | +0.571 | +0.667 1.0000 |
| 1 | 6 | 1 | 3 | 1.70 | 2.849 | 2.849 | +0.080 | +0.80 | +0.9996 1.0000 |
| 1 | 6 | 2 | 1 | 1.42 | *2.93 | *2.93 | +0.252 | +1.49 | +0.849 1.0000 |
| 1 | 6 | 3 | 5 | 5.90 | -5.023 | -5.023 | +0.076 | +0.76 | +0.0400 1.0000 |
| 1 | 6 | 4 | 16 | 1.573 | -1.159 | -1.158 | +0.137 | +0.66 | +0.3602 1.0000 |
| 1 | 6 | 5 | 1 | 1.87 | *9.17 | *9.17 | +0.070 | +0.70 | +0.3155 1.0000 |
| 1 | 6 | 6 | 1 | 2.79 | 1.125 | 1.119 | +0.125 | +0.125 | +0.155 1.0000 |
| 1 | 6 | 7 | 2 | 8.08 | *4.001 | -4.001 | +0.061 | +0.061 | +1.193 1.0000 |
| 1 | 6 | 8 | 0 | 8.47 | -26.576 | -26.576 | +0.027 | +0.27 | +0.5326 1.0000 |
| 1 | 6 | 9 | 1 | 2.07 | 6.379 | 6.379 | +0.043 | +0.43 | +0.5963 1.0000 |
| 1 | 7 | 2 | 41 | 2.41 | 42.312 | 42.309 | +0.43 | +1.72 | +1.0547 1.0000 |
| 1 | 7 | 3 | 6 | 9.12 | 6.966 | 6.966 | +0.041 | +0.41 | +0.9435 1.0000 |
| 1 | 7 | 4 | 16 | 8.86 | -17.267 | -17.267 | +0.023 | +0.23 | +0.3378 1.0000 |
| 1 | 7 | 5 | 3 | 5.94 | 3.137 | 3.137 | +0.039 | +0.39 | +2.1231 1.0000 |
| 1 | 7 | 6 | 23 | 2.79 | 23.276 | 23.276 | +0.374 | +0.374 | +0.4011 1.0000 |
| 1 | 7 | 7 | 24 | 4.45 | 22.445 | 22.445 | +0.634 | +0.634 | +3.7564 1.0000 |
| 1 | 7 | 8 | 31 | 7.71 | 32.071 | 32.071 | +0.386 | +0.386 | +1.6544 1.0000 |

SILLIMANITE (B-PANDYWIN SPRINGS) AT 600 DEGREES C

STRUCTURE FACTORS

PAGE 3

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | FXT | FACTCP |
|----|-------|----|----------|---------|---------|---------|---------|-------------|--------|--------|
| 1 | 8 | 1 | 2.170 * | 1.105 | -1.104 | -0.051 | 1.06* | 2.2604 | 1.0000 | * * * |
| 1 | 8 | 2 | 14.119 * | 12.980 | -12.974 | -0.375 | 1.135 | 6.8275 | 1.0000 | * * * |
| 1 | 8 | 3 | 1.213 * | 0.655 | -0.026 | 0.048 | 1.156 | 1.3566 | 1.0000 | * * * |
| 1 | 8 | 4 | 22.919 | 23.656 | -23.853 | -0.345 | 1.110 | -3.6591 | 1.0000 | * * * |
| 1 | 8 | 5 | 2.032 * | 1.110 | -0.043 | 0.922 | 1.15318 | 1.0000 | * * * | |
| 1 | 8 | 6 | 7.580 | 7.999 | -7.933 | -0.300 | 1.116 | -1.6337 | 1.0000 | * * * |
| 1 | 8 | 0 | 32.626 | 31.558 | -31.555 | -0.424 | 1.068 | 3.2599 | 1.0000 | * * * |
| 1 | 9 | 1 | 1.636 * | 0.688 | -0.686 | -0.016 | 0.947 | 1.3939 | 1.0000 | * * * |
| 1 | 9 | 2 | 11.177 | 11.305 | -11.305 | -0.029 | 1.128 | -0.6162 | 1.0000 | * * * |
| 1 | 9 | 3 | 1.648 * | 0.974 | -0.974 | -0.016 | 0.674 | 0.9442 | 1.0000 | * * * |
| 1 | 9 | 4 | 23.621 | 24.101 | -24.096 | -0.350 | 0.481 | -2.2221 | 1.0000 | * * * |
| 1 | 9 | 5 | 2.241 * | 1.055 | -1.044 | -0.012 | 2.136 | 3.6514 | 1.0000 | * * * |
| 1 | 10 | 0 | 20.069 | 19.635 | -19.634 | -0.144 | 0.434 | 1.9337 | 1.0000 | * * * |
| 1 | 10 | 1 | 4.100 | 3.960 | -3.959 | -0.031 | 0.140 | 0.4366 | 1.0000 | * * * |
| 1 | 10 | 2 | 6.263 | 6.277 | -6.275 | -0.140 | 0.006 | 0.0285 | 1.0000 | * * * |
| 1 | 10 | 3 | 2.212 * | 3.252 | -3.252 | -0.030 | 0.040 | -1.7249 | 1.0000 | * * * |
| 1 | 10 | 4 | 14.910 | 15.083 | -15.083 | -0.129 | 0.265 | -1.5906 | 1.0000 | * * * |
| 1 | 11 | 0 | 5.207 | 5.172 | -5.169 | -0.020 | 0.034 | 0.1190 | 1.0000 | * * * |
| 1 | 11 | 1 | 4.668 * | 3.046 | -3.047 | -0.031 | 0.375 | -0.7070 | 1.0000 | * * * |
| 11 | 1 | 2 | 2.694 * | 2.654 | -2.651 | -0.126 | 0.641 | 0.6772 | 1.0000 | * * * |
| 11 | 0 | 3 | 34.423 | 32.276 | -32.276 | -0.100 | 2.147 | 14.5386 | 1.0000 | * * * |
| 0 | 0 | 4 | 45.504 | 44.656 | -44.654 | -0.441 | 0.848 | 5.1503 | 1.0000 | * * * |
| 0 | 0 | 5 | 15.920 | 15.927 | -15.927 | -0.006 | -0.07 | -0.0334 | 1.0000 | * * * |
| 0 | 0 | 6 | 2.660 | 2.545 | -2.545 | -0.356 | 1.214 | 3.9902 | 1.0000 | * * * |
| 0 | 0 | 7 | 5.506 | 4.606 | -4.605 | -0.056 | 0.900 | 3.5160 | 1.0000 | * * * |
| 0 | 0 | 8 | 40.400 | 43.422 | -43.421 | -0.502 | -3.032 | -22.9867 | 1.0000 | * * * |
| 0 | 0 | 9 | 7.859 | 7.145 | -7.146 | -0.289 | 0.714 | 3.0898 | 1.0000 | * * * |
| 0 | 0 | 10 | 15.920 | 15.927 | -15.927 | -0.006 | -0.07 | -0.0334 | 1.0000 | * * * |
| 0 | 0 | 11 | 2.660 | 2.545 | -2.545 | -0.356 | 1.214 | 3.9902 | 1.0000 | * * * |
| 0 | 0 | 12 | 4.606 | 4.605 | -4.605 | -0.056 | 0.900 | 3.5160 | 1.0000 | * * * |
| 0 | 0 | 13 | 51.339 | 52.427 | -52.425 | -0.27 | 0.375 | 3.5160 | 1.0000 | * * * |
| 1 | 1.102 | * | 1.102 | 1.226 | -1.226 | -0.025 | -1.088 | -4.6013 | 1.0000 | * * * |
| 5 | 5 | 6 | 11.356 | 10.810 | -10.803 | -0.300 | -1.124 | -1.1574 | 1.0000 | * * * |
| 6 | 6 | 7 | 4.915 | 4.934 | -4.934 | -0.488 | -0.577 | 3.7353 | 1.0000 | * * * |
| 7 | 7 | 8 | 1.357 | 1.357 | -1.357 | -0.266 | -0.053 | -0.1200 | 1.0000 | * * * |
| 8 | 8 | 9 | 5.172 | 5.792 | -5.792 | -0.027 | 0.375 | 2.0641 | 1.0000 | * * * |
| 9 | 9 | 10 | 51.339 | 52.427 | -52.425 | -0.27 | -1.088 | -4.6013 | 1.0000 | * * * |
| 10 | 10 | 11 | 62.235 | 61.102 | -61.101 | -0.343 | -1.133 | -1.1574 | 1.0000 | * * * |
| 11 | 11 | 12 | 5.116 | 5.116 | -5.116 | -0.056 | -0.201 | -0.9541 | 1.0000 | * * * |
| 12 | 12 | 13 | 13.720 | 13.224 | -13.224 | -0.196 | -0.406 | 2.9329 | 1.0000 | * * * |
| 13 | 13 | 14 | 2.670 | 2.700 | -2.700 | -0.024 | -0.053 | -0.1200 | 1.0000 | * * * |
| 14 | 14 | 15 | 20.834 | 20.087 | -20.085 | -0.321 | -0.747 | 3.7206 | 1.0000 | * * * |
| 15 | 15 | 16 | 61.102 | 61.102 | -61.101 | -0.343 | -1.133 | 7.6133 | 1.0000 | * * * |
| 16 | 16 | 17 | 11.356 | 10.810 | -10.803 | -0.300 | -0.201 | -0.9541 | 1.0000 | * * * |
| 17 | 17 | 18 | 4.915 | 4.934 | -4.934 | -0.488 | -0.406 | 2.9329 | 1.0000 | * * * |
| 18 | 18 | 19 | 1.357 | 1.357 | -1.357 | -0.266 | -0.053 | -0.1200 | 1.0000 | * * * |
| 19 | 19 | 20 | 5.172 | 5.792 | -5.792 | -0.027 | -0.321 | -0.6000 | 1.0000 | * * * |
| 20 | 20 | 21 | 51.339 | 52.427 | -52.425 | -0.27 | -0.449 | -4.6013 | 1.0000 | * * * |
| 21 | 21 | 22 | 62.235 | 61.102 | -61.101 | -0.343 | -1.226 | -1.1574 | 1.0000 | * * * |
| 22 | 22 | 23 | 5.116 | 5.116 | -5.116 | -0.056 | -0.577 | 3.7353 | 1.0000 | * * * |
| 23 | 23 | 24 | 13.720 | 13.224 | -13.224 | -0.196 | -0.406 | -0.1200 | 1.0000 | * * * |
| 24 | 24 | 25 | 2.670 | 2.700 | -2.700 | -0.024 | -0.053 | -0.6000 | 1.0000 | * * * |
| 25 | 25 | 26 | 20.834 | 20.087 | -20.085 | -0.321 | -0.747 | 3.7206 | 1.0000 | * * * |
| 26 | 26 | 27 | 61.102 | 61.102 | -61.101 | -0.343 | -1.133 | 7.6133 | 1.0000 | * * * |
| 27 | 27 | 28 | 11.356 | 10.810 | -10.803 | -0.300 | -0.201 | -0.9541 | 1.0000 | * * * |
| 28 | 28 | 29 | 4.915 | 4.934 | -4.934 | -0.488 | -0.406 | 2.9329 | 1.0000 | * * * |
| 29 | 29 | 30 | 1.357 | 1.357 | -1.357 | -0.266 | -0.053 | -0.1200 | 1.0000 | * * * |
| 30 | 30 | 31 | 5.172 | 5.792 | -5.792 | -0.027 | -0.321 | -0.6000 | 1.0000 | * * * |
| 31 | 31 | 32 | 51.339 | 52.427 | -52.425 | -0.27 | -0.449 | -4.6013 | 1.0000 | * * * |
| 32 | 32 | 33 | 62.235 | 61.102 | -61.101 | -0.343 | -1.226 | -1.1574 | 1.0000 | * * * |
| 33 | 33 | 34 | 5.116 | 5.116 | -5.116 | -0.056 | -0.577 | 3.7353 | 1.0000 | * * * |
| 34 | 34 | 35 | 13.720 | 13.224 | -13.224 | -0.196 | -0.406 | -0.1200 | 1.0000 | * * * |
| 35 | 35 | 36 | 2.670 | 2.700 | -2.700 | -0.024 | -0.053 | -0.6000 | 1.0000 | * * * |
| 36 | 36 | 37 | 20.834 | 20.087 | -20.085 | -0.321 | -0.747 | 3.7206 | 1.0000 | * * * |
| 37 | 37 | 38 | 61.102 | 61.102 | -61.101 | -0.343 | -1.133 | 7.6133 | 1.0000 | * * * |
| 38 | 38 | 39 | 11.356 | 10.810 | -10.803 | -0.300 | -0.201 | -0.9541 | 1.0000 | * * * |
| 39 | 39 | 40 | 4.915 | 4.934 | -4.934 | -0.488 | -0.406 | 2.9329 | 1.0000 | * * * |
| 40 | 40 | 41 | 1.357 | 1.357 | -1.357 | -0.266 | -0.053 | -0.1200 | 1.0000 | * * * |
| 41 | 41 | 42 | 5.172 | 5.792 | -5.792 | -0.027 | -0.321 | -0.6000 | 1.0000 | * * * |
| 42 | 42 | 43 | 51.339 | 52.427 | -52.425 | -0.27 | -0.449 | -4.6013 | 1.0000 | * * * |
| 43 | 43 | 44 | 62.235 | 61.102 | -61.101 | -0.343 | -1.226 | -1.1574 | 1.0000 | * * * |
| 44 | 44 | 45 | 5.116 | 5.116 | -5.116 | -0.056 | -0.577 | 3.7353 | 1.0000 | * * * |
| 45 | 45 | 46 | 13.720 | 13.224 | -13.224 | -0.196 | -0.406 | -0.1200 | 1.0000 | * * * |
| 46 | 46 | 47 | 2.670 | 2.700 | -2.700 | -0.024 | -0.053 | -0.6000 | 1.0000 | * * * |
| 47 | 47 | 48 | 20.834 | 20.087 | -20.085 | -0.321 | -0.747 | 3.7206 | 1.0000 | * * * |
| 48 | 48 | 49 | 61.102 | 61.102 | -61.101 | -0.343 | -1.133 | 7.6133 | 1.0000 | * * * |
| 49 | 49 | 50 | 11.356 | 10.810 | -10.803 | -0.300 | -0.201 | -0.9541 | 1.0000 | * * * |
| 50 | 50 | 51 | 4.915 | 4.934 | -4.934 | -0.488 | -0.406 | 2.9329 | 1.0000 | * * * |
| 51 | 51 | 52 | 1.357 | 1.357 | -1.357 | -0.266 | -0.053 | -0.1200 | 1.0000 | * * * |
| 52 | 52 | 53 | 5.172 | 5.792 | -5.792 | -0.027 | -0.321 | -0.6000 | 1.0000 | * * * |
| 53 | 53 | 54 | 51.339 | 52.427 | -52.425 | -0.27 | -0.449 | -4.6013 | 1.0000 | * * * |
| 54 | 54 | 55 | 62.235 | 61.102 | -61.101 | -0.343 | -1.226 | -1.1574 | 1.0000 | * * * |
| 55 | 55 | 56 | 5.116 | 5.116 | -5.116 | -0.056 | -0.577 | 3.7353 | 1.0000 | * * * |
| 56 | 56 | 57 | 13.720 | 13.224 | -13.224 | -0.196 | -0.406 | -0.1200 | 1.0000 | * * * |
| 57 | 57 | 58 | 2.670 | 2.700 | -2.700 | -0.024 | -0.053 | -0.6000 | 1.0000 | * * * |
| 58 | 58 | 59 | 20.834 | 20.087 | -20.085 | -0.321 | -0.747 | 3.7206 | 1.0000 | * * * |
| 59 | 59 | 60 | 61.102 | 61.102 | -61.101 | -0.343 | -1.133 | 7.6133 | 1.0000 | * * * |
| 60 | 60 | 61 | 11.356 | 10.810 | -10.803 | -0.300 | -0.201 | -0.9541 | 1.0000 | * * * |
| 61 | 61 | 62 | 4.915 | 4.934 | -4.934 | -0.488 | -0.406 | 2.9329 | 1.0000 | * * * |
| 62 | 62 | 63 | 1.357 | 1.357 | -1.357 | -0.266 | -0.053 | -0.1200 | 1.0000 | * * * |
| 63 | 63 | 64 | 5.172 | 5.792 | -5.792 | -0.027 | -0.321 | -0.6000 | 1.0000 | * * * |
| 64 | 64 | 65 | 51.339 | 52.427 | -52.425 | -0.27 | -0.449 | -4.6013 | 1.0000 | * * * |
| 65 | 65 | 66 | 62.235 | 61.102 | -61.101 | -0.343 | -1.226 | -1.1574 | 1.0000 | * * * |
| 66 | 66 | 67 | 5.116 | 5.116 | -5.116 | -0.056 | -0.577 | 3.7353 | 1.0000 | * * * |
| 67 | 67 | 68 | 13.720 | 13.224 | -13.224 | -0.196 | -0.406 | -0.1200 | 1.0000 | * * * |
| 68 | 68 | 69 | 2.670 | 2.700 | -2.700 | -0.024 | -0.053 | -0.6000 | 1.0000 | * * * |
| 69 | 69 | 70 | 20.834 | 20.087 | -20.085 | -0.321 | -0.747 | 3.7206 | 1.0000 | * * * |
| 70 | 70 | 71 | 61.102 | 61.102 | -61.101 | -0.343 | -1.133 | 7.6133 | 1.0000 | * * * |
| 71 | 71 | 72 | 11.356 | 10.810 | -10.803 | -0.300 | -0.201 | -0.9541 | 1.0000 | * * * |
| 72 | 72 | 73 | 4.915 | 4.934 | -4.934 | -0.488 | -0.406 | 2.9329 | 1.0000 | * * * |
| 73 | 73 | 74 | 1.357 | 1.357 | -1.357 | -0.266 | -0.053 | -0.1200 | 1.0000 | * * * |
| 74 | 74 | 75 | 5.172 | 5.792 | -5.792 | -0.027 | -0.321 | -0.6000 | 1.0000 | * * * |
| 75 | 75 | 76 | 51.339 | 52.427 | -52.425 | -0.27 | -0.449 | -4.6013 | 1.0000 | * * * |
| 76 | 76 | 77 | 62.235 | 61.102 | -61.101 | -0.343 | -1.226 | -1.1574 | 1.0000 | * * * |
| 77 | 77 | 78 | 5.116 | 5.116 | -5.116 | -0.056 | -0.577 | 3.7353 | 1.0000 | * * * |
| 78 | 78 | 79 | | | | | | | | |

STRUCTURE, ACTORS
STILLMANNITE (B-CRYSTAL)
SPOTINGS AT 600 DEGREES C

STRUCTURE, ACTORS

PAGE 4

| | H | K | L | F (CALC) | A (CALC) | B (CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|---|----|----------|----------|----------|---------|-------------|-------------|
| 0 | 2 | 4 | 1 | 4.573 | 4.788 | -4.788 | -0.051 | -0.215 | -0.9076 |
| 0 | 2 | 4 | 2 | 4.554 | 4.704 | 4.703 | +0.144 | +0.250 | -1.1250 |
| 0 | 2 | 4 | 3 | 4.156 | 4.148 | 4.147 | +0.049 | +0.009 | 1.0000 |
| 0 | 2 | 4 | 4 | 3.797 | 3.075 | 3.076 | +0.330 | +0.376 | 0.0376 |
| 0 | 2 | 4 | 5 | 3.299 | 2.961 | 2.961 | +0.336 | +0.276 | -1.0624 |
| 0 | 2 | 4 | 6 | 5.97 | 9.662 | 9.662 | +0.116 | +0.043 | 1.1461 |
| 0 | 2 | 4 | 7 | 1.320 | 2.250 | 2.250 | +0.365 | +0.365 | 1.5063 |
| 0 | 2 | 4 | 8 | 14.969 | 14.564 | 14.562 | +0.039 | +0.039 | 1.0000 |
| 0 | 2 | 4 | 9 | 49.252 | 48.900 | 48.897 | +0.228 | +0.401 | 1.0000 |
| 0 | 2 | 4 | 10 | 11.389 | 11.259 | 11.259 | +0.052 | +0.052 | 1.0000 |
| 0 | 2 | 4 | 11 | 73.439 | 75.102 | 75.100 | +0.515 | +0.515 | 1.0000 |
| 0 | 2 | 4 | 12 | 13.206 | 13.572 | 13.572 | +0.366 | +0.366 | 1.0000 |
| 0 | 2 | 4 | 13 | 35.405 | 36.205 | 36.202 | +0.401 | +0.401 | 1.0000 |
| 0 | 2 | 4 | 14 | 2.419 | 2.935 | 2.935 | +0.045 | +0.045 | 1.0000 |
| 0 | 2 | 4 | 15 | 37.938 | -37.938 | -37.938 | +0.412 | +0.412 | 1.0000 |
| 0 | 2 | 4 | 16 | 8.196 | 8.094 | 8.094 | +0.040 | +0.040 | 1.0000 |
| 0 | 2 | 4 | 17 | 22.950 | 22.047 | 22.047 | +0.003 | +0.003 | 1.0000 |
| 0 | 2 | 4 | 18 | 2.059 | 1.567 | 1.567 | +0.004 | +0.004 | 1.0000 |
| 0 | 2 | 4 | 19 | 22.456 | 21.930 | 21.927 | +0.371 | +0.371 | 1.0000 |
| 0 | 2 | 4 | 20 | 1.134 | 1.319 | 1.319 | +0.005 | +0.005 | 1.0000 |
| 0 | 2 | 4 | 21 | 14.139 | 14.157 | 14.157 | +0.033 | +0.033 | 1.0000 |
| 0 | 2 | 4 | 22 | 1.210 | 0.944 | 0.944 | +0.003 | +0.003 | 1.0000 |
| 0 | 2 | 4 | 23 | 29.398 | 29.387 | 29.385 | +0.275 | +0.275 | 1.0000 |
| 0 | 2 | 4 | 24 | 4.163 | 4.160 | 4.160 | +0.018 | +0.018 | 1.0000 |
| 0 | 2 | 4 | 25 | 13.364 | 13.729 | 13.729 | +0.005 | +0.005 | 1.0000 |
| 0 | 2 | 4 | 26 | 1.344 | 1.344 | 1.344 | +0.005 | +0.005 | 1.0000 |
| 0 | 2 | 4 | 27 | 16.306 | 17.914 | 17.912 | +0.203 | +0.203 | 1.0000 |
| 0 | 2 | 4 | 28 | 1.663 | *.274 | *.273 | +0.013 | +0.013 | 1.0000 |
| 0 | 2 | 4 | 29 | 29.387 | 29.385 | 29.385 | +0.013 | +0.013 | 1.0000 |
| 0 | 2 | 4 | 30 | 4.163 | -4.190 | -4.190 | +0.018 | +0.018 | 1.0000 |
| 0 | 2 | 4 | 31 | 13.952 | 13.967 | 13.967 | +0.253 | +0.253 | 1.0000 |
| 0 | 2 | 4 | 32 | 3.691 | -13.965 | -13.965 | +0.015 | +0.015 | 1.0000 |
| 0 | 2 | 4 | 33 | 16.731 | 16.470 | 16.470 | +0.017 | +0.017 | 1.0000 |
| 0 | 2 | 4 | 34 | 25.594 | 25.250 | 25.249 | +0.220 | +0.220 | 1.0000 |
| 0 | 2 | 4 | 35 | 2.935 | 1.847 | 1.846 | +0.649 | +0.649 | 1.0000 |
| 0 | 2 | 4 | 36 | 8.748 | 8.862 | 8.860 | +0.190 | +0.190 | 1.0000 |
| 0 | 2 | 4 | 37 | 1.735 | * | 1.625 | +0.625 | +0.625 | 1.0000 |
| 0 | 2 | 4 | 38 | 17.601 | 18.172 | 18.172 | +0.020 | +0.020 | 1.0000 |
| 0 | 2 | 4 | 39 | 2.737 | * | 1.417 | +0.643 | +0.643 | 1.0000 |
| 0 | 2 | 4 | 40 | 5.654 | 5.655 | 5.653 | +0.153 | +0.153 | 1.0000 |
| 0 | 2 | 4 | 41 | 22.386 | -22.332 | -22.332 | +0.553 | +0.553 | 1.0000 |
| 0 | 2 | 4 | 42 | 9.122 | 9.012 | 9.012 | +0.223 | +0.223 | 1.0000 |
| 0 | 2 | 4 | 43 | 17.660 | 16.228 | 16.227 | +0.217 | +0.217 | 1.0000 |
| 0 | 2 | 4 | 44 | 4.861 | 4.813 | 4.813 | +0.074 | +0.074 | 1.0000 |
| 0 | 2 | 4 | 45 | 16.572 | 17.029 | 17.028 | +0.199 | +0.199 | 1.0000 |
| 0 | 2 | 4 | 46 | 9.194 | 9.196 | 9.195 | +0.066 | +0.066 | 1.0000 |
| 0 | 2 | 4 | 47 | 20.342 | 19.879 | 19.877 | +0.012 | +0.012 | 1.0000 |
| 0 | 2 | 4 | 48 | 2.049 | * | 1.864 | +0.374 | +0.374 | 1.0000 |
| 0 | 2 | 4 | 49 | 10.225 | -1.864 | -4.812 | +0.078 | +0.078 | 1.0000 |
| 0 | 2 | 4 | 50 | 1.367 | 1.609 | 1.607 | +0.076 | +0.076 | 1.0000 |
| 0 | 2 | 4 | 51 | 14.661 | 15.005 | 15.003 | +0.366 | +0.366 | 1.0000 |
| 0 | 2 | 4 | 52 | 14.926 | 14.502 | 14.497 | +0.516 | +0.516 | 1.0000 |
| 0 | 2 | 4 | 53 | 1.461 | * | 1.518 | +0.052 | +0.052 | 1.0000 |
| 0 | 2 | 4 | 54 | 16.572 | 16.194 | 16.190 | +0.343 | +0.343 | 1.0000 |
| 0 | 2 | 4 | 55 | 6.034 | 5.764 | 5.764 | +0.031 | +0.031 | 1.0000 |

SULFURATE (BANDYKIE SPRINGS) AT 600 DEGREES C

| | | F (OBS) | F (CALC) | $\Delta (C', C)$ | B (CALC) | DELTA F | DELTA/SIGMA | STRUCTURE FACTORS | PAGE |
|---|---|---------|----------|------------------|----------|---------|-------------|-------------------|------|
| 0 | 0 | 5.252 | 4.553 | -0.30 | 0.98 | -0.164 | -0.684 | 1.0000 | 1 |
| 0 | 0 | 4.676 | 4.860 | +0.24 | -0.21 | -0.467 | -1.525 | 1.0000 | |
| 0 | 0 | 4.054 | 4.736 | +0.21 | -0.21 | -0.310 | -1.2416 | 1.0000 | |
| 0 | 0 | 4.463 | 4.453 | -0.09 | -0.09 | -0.452 | -0.482 | 1.0000 | |
| 0 | 0 | 3.901 | 3.151 | -0.35 | -0.45 | -0.839 | -0.7124 | 1.0000 | |
| 0 | 0 | 3.895 | 2.856 | -1.03 | -0.92 | -0.736 | -0.8752 | 1.0000 | |
| 0 | 0 | 2.643 | 2.549 | -0.52 | -0.72 | -0.726 | -0.8752 | 1.0000 | |
| 0 | 0 | 2.915 | 2.643 | -0.27 | -0.27 | -0.046 | -0.436 | 1.0000 | |
| 0 | 0 | 1.045 | 0.946 | -0.075 | -0.075 | -0.046 | -0.067 | 1.0000 | |
| 0 | 0 | 1.045 | 1.048 | +0.03 | -0.03 | -0.046 | -0.067 | 1.0000 | |
| 0 | 0 | 1.048 | 1.046 | -0.02 | -0.02 | -0.046 | -0.067 | 1.0000 | |
| 0 | 0 | 1.048 | 1.046 | -0.02 | -0.02 | -0.046 | -0.067 | 1.0000 | |
| 0 | 0 | 1.047 | 1.041 | -0.06 | -0.06 | -0.015 | -0.036 | 1.0000 | |
| 0 | 0 | 2.915 | 2.643 | -0.27 | -0.27 | -0.046 | -0.436 | 1.0000 | |
| 0 | 0 | 5.120 | 4.947 | -0.075 | -0.075 | -0.179 | -0.179 | 1.0000 | |
| 0 | 0 | 3.621 | 3.620 | -0.01 | -0.01 | -0.202 | -0.202 | 1.0000 | |
| 0 | 0 | 9.521 | 9.334 | -0.086 | -0.086 | -0.181 | -0.181 | 1.0000 | |
| 0 | 0 | 6.492 | 6.334 | -0.156 | -0.156 | -0.334 | -0.334 | 1.0000 | |
| 0 | 0 | 6.373 | 6.147 | -0.226 | -0.226 | -0.573 | -0.573 | 1.0000 | |
| 0 | 0 | 3.779 | 3.484 | -0.286 | -0.286 | -0.779 | -0.779 | 1.0000 | |
| 0 | 0 | 4.439 | 4.247 | -0.09 | -0.09 | -0.192 | -0.192 | 1.0000 | |
| 0 | 0 | 10.247 | 10.431 | -1.26 | -1.26 | -0.560 | -0.560 | 1.0000 | |
| 0 | 0 | 2.144 | 1.649 | -0.007 | -0.007 | -0.485 | -0.485 | 1.0000 | |
| 0 | 0 | 21.314 | 21.930 | -0.255 | -0.255 | -0.615 | -0.615 | 1.0000 | |
| 0 | 0 | 5.200 | 5.061 | -0.07 | -0.07 | -0.136 | -0.136 | 1.0000 | |
| 0 | 0 | 50.651 | 51.082 | -0.032 | -0.032 | -0.286 | -0.286 | 1.0000 | |
| 0 | 0 | 2.738 | 2.601 | -0.034 | -0.034 | -0.137 | -0.137 | 1.0000 | |
| 0 | 0 | 9.599 | 9.012 | -0.010 | -0.010 | -0.597 | -0.597 | 1.0000 | |
| 0 | 0 | 6.140 | 5.956 | -0.140 | -0.140 | -0.194 | -0.194 | 1.0000 | |
| 0 | 0 | 7.010 | 6.959 | -0.027 | -0.027 | -0.052 | -0.052 | 1.0000 | |
| 0 | 0 | 14.711 | 14.487 | -0.136 | -0.136 | -0.256 | -0.256 | 1.0000 | |
| 0 | 0 | 2.386 | 1.931 | -0.024 | -0.024 | -0.236 | -0.236 | 1.0000 | |
| 0 | 0 | 1.125 | 1.285 | -0.125 | -0.125 | -0.166 | -0.166 | 1.0000 | |
| 0 | 0 | 5.787 | 5.891 | -0.022 | -0.022 | -0.104 | -0.104 | 1.0000 | |
| 0 | 0 | 6.936 | 7.166 | -0.109 | -0.109 | -0.230 | -0.230 | 1.0000 | |
| 0 | 0 | 2.796 | 1.945 | -0.1016 | -0.1016 | -0.856 | -0.856 | 1.0000 | |
| 0 | 0 | 2.9676 | 2.760 | -0.361 | -0.361 | -1.916 | -1.916 | 1.0000 | |
| 0 | 0 | 3.673 | 3.428 | -0.079 | -0.079 | -0.246 | -0.246 | 1.0000 | |
| 0 | 0 | 1.179 | 0.799 | -0.790 | -0.790 | -1.25 | -1.25 | 1.0000 | |
| 0 | 0 | 1.119 | 0.672 | -0.668 | -0.668 | -0.447 | -0.447 | 1.0000 | |
| 0 | 0 | 21.515 | 22.163 | -0.324 | -0.324 | -0.643 | -0.643 | 1.0000 | |
| 0 | 0 | 2.337 | 2.410 | -2.409 | -2.409 | -0.073 | -0.073 | 1.0000 | |
| 0 | 0 | 1.291 | 0.352 | -0.337 | -0.337 | -0.935 | -0.935 | 1.0000 | |
| 0 | 0 | 3.049 | 2.474 | -2.473 | -2.473 | -0.661 | -0.661 | 1.0000 | |
| 0 | 0 | 17.240 | 17.675 | -1.675 | -1.675 | -0.435 | -0.435 | 1.0000 | |
| 0 | 0 | 1.166 | 1.075 | -1.075 | -1.075 | -0.091 | -0.091 | 1.0000 | |
| 0 | 0 | 1.614 | 2.077 | -2.076 | -2.076 | -0.463 | -0.463 | 1.0000 | |
| 0 | 0 | 1.818 | 1.157 | -1.157 | -1.157 | -0.017 | -0.017 | 1.0000 | |
| 0 | 0 | 11.923 | 11.779 | -1.779 | -1.779 | -0.069 | -0.069 | 1.0000 | |
| 0 | 0 | 2.562 | 2.498 | -2.498 | -2.498 | -0.013 | -0.013 | 1.0000 | |
| 0 | 0 | 1.320 | 0.589 | -0.586 | -0.586 | -0.731 | -0.731 | 1.0000 | |

SILLIMANITE CRYSTALLINE SPRINGS AT 600 DEGREES C

STRUCTURE FACTORS

PAGE 6

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTR |
|---|----|---|--------|---------|----------|---------|---------|-------------|------------|
| 3 | 6 | 7 | 1.651 | 1.506 | -1.506 | .012 | .146 | .1825 | 1.0000 |
| 3 | 7 | 0 | 63.173 | 62.586 | 62.584 | .568 | .566 | 2.1760 | 1.0000 |
| 3 | 7 | 1 | 11.301 | 10.870 | -10.870 | .920 | .920 | 2.8080 | 1.0000 |
| 3 | 7 | 2 | 6.227 | 5.756 | -5.754 | 1.53 | 1.53 | 2.6465 | 1.0000 |
| 3 | 7 | 3 | 10.353 | 10.661 | 10.660 | .087 | .087 | -1.6663 | 1.0000 |
| 3 | 7 | 4 | 45.726 | 46.351 | 46.348 | .536 | .536 | -1.6223 | 1.0000 |
| 3 | 7 | 5 | 6.572 | 6.437 | -6.437 | .077 | .077 | 1.35 | 1.0000 |
| 3 | 7 | 6 | 4.394 | 4.699 | -4.698 | .121 | .121 | -2.305 | 1.0000 |
| 3 | 7 | 7 | 15.663 | 15.459 | 15.458 | .165 | .165 | 1.205 | 1.0000 |
| 3 | 7 | 8 | 2.985 | 3.336 | -3.336 | .015 | .015 | -1.358 | 1.0000 |
| 3 | 8 | 9 | 2.998 | 5.346 | -5.340 | .160 | .160 | 1.764 | 1.0000 |
| 3 | 8 | 9 | 2.646 | 1.726 | -1.725 | .015 | .015 | 5.206 | 1.0000 |
| 3 | 8 | 9 | 11.394 | 11.430 | 11.429 | .147 | .147 | -1.429 | 1.0000 |
| 3 | 8 | 9 | 3.125 | 2.713 | -2.713 | .012 | .012 | 4.12 | 1.0000 |
| 3 | 9 | 0 | 17.707 | 17.357 | -17.357 | .159 | .159 | 3.350 | 1.0000 |
| 3 | 9 | 1 | 1.309 | .172 | -.172 | .029 | .029 | 1.137 | 1.0000 |
| 3 | 9 | 2 | 26.974 | 27.521 | 27.315 | .528 | .528 | -1.346 | 1.0000 |
| 3 | 9 | 3 | 1.334 | .218 | -.218 | .007 | .007 | 1.116 | 1.0000 |
| 3 | 9 | 4 | 13.002 | 12.810 | -12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 9 | 5 | 1.389 | .403 | -.402 | .007 | .007 | 1.1252 | 1.0000 |
| 3 | 9 | 6 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 9 | 7 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 9 | 8 | 2.956 | 2.819 | -.2.819 | .045 | .045 | -1.346 | 1.0000 |
| 3 | 9 | 9 | 5.348 | 4.531 | -.4.531 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 10 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 10 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 10 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 10 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 11 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 11 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 11 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 11 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 11 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 11 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 11 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 11 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 12 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 12 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 12 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 12 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 12 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 12 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 12 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 12 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 13 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 13 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 13 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 13 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 13 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 13 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 13 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 13 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 14 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 14 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 14 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 14 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 14 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 14 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 14 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 14 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 15 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 15 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 15 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 15 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 15 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 15 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 15 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 15 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 16 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 16 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 16 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 16 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 16 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 16 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 16 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 16 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 17 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 17 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 17 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 17 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 17 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 17 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 17 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 17 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 18 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 18 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 18 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 18 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 18 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 18 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 18 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 18 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 19 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 19 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 19 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 19 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 19 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 19 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 19 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 19 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 20 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 20 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 20 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 20 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 20 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 20 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 20 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 20 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 21 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 21 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 21 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 21 | 3 | 13.002 | 12.810 | -.12.817 | .142 | .142 | 1.184 | 1.0000 |
| 3 | 21 | 4 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 21 | 5 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 21 | 6 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0000 |
| 3 | 21 | 7 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 22 | 0 | 1.389 | .403 | -.4.03 | .019 | .019 | 1.1530 | 1.0000 |
| 3 | 22 | 1 | 12.475 | 11.846 | -.11.846 | .047 | .047 | 1.2167 | 1.0000 |
| 3 | 22 | 2 | 5.180 | 5.142 | -.5.142 | .021 | .021 | 2.0771 | 1.0 |

SILLIMINITE (GRANULITE SPRINGS) AT 600 DEGREES C

STRUCTURE FACTORS

PAGE 7

| H | K | L | F(CBS) | F(CALC) | A(CALC) | S(CALC) | DELTA F | DELTA/SIGMA | FXT. FACTOR | |
|---|---|----|--------|---------|---------|----------|---------|-------------|-------------|--------|
| 4 | 4 | 3 | 2.958 | 1.814 | -1.814 | .044 | 1.144 | 3.5472 | 1.0000 | |
| 4 | 4 | 4 | 5.457 | 6.522 | -6.522 | -.093 | -.065 | -.3652 | 1.0000 | |
| 4 | 3 | 0 | 1.743 | 1.431 | 1.431 | -.038 | .331 | .5024 | 1.0000 | |
| 4 | 3 | 7 | 4.946 | 4.553 | 4.553 | .083 | .393 | 1.4118 | 1.0000 | |
| 4 | 4 | 0 | 5.046 | 5.571 | 5.571 | .582 | .276 | 1.2221 | 1.0000 | |
| 4 | 4 | 1 | 2.167 | 1.794 | 1.794 | -.035 | .373 | .7851 | 1.0000 | |
| 4 | 4 | 2 | 3.456 | 3.562 | 3.562 | -.082 | -.1.016 | -.4.0432 | 1.0000 | |
| 4 | 4 | 3 | 5.043 | 5.334 | 5.334 | .034 | -.291 | -.1.4737 | 1.0000 | |
| 4 | 4 | 4 | 39.738 | 40.354 | 40.354 | .521 | -.616 | -.2.1772 | 1.0000 | |
| 4 | 4 | 5 | 1.660 | .981 | .981 | -.051 | .675 | 1.0111 | 1.0000 | |
| 4 | 4 | 6 | 16.205 | 15.836 | 15.836 | -.064 | .367 | 2.0208 | 1.0000 | |
| 4 | 4 | 7 | 5.079 | 4.568 | 4.568 | .030 | -.291 | 1.7636 | 1.0000 | |
| 4 | 4 | 8 | 29.804 | 29.120 | 29.118 | -.282 | -.616 | 2.0114 | 1.0000 | |
| 4 | 4 | 9 | 1.368 | .611 | .609 | .047 | .757 | 1.0103 | 1.0000 | |
| 4 | 4 | 10 | 25.389 | 25.160 | 25.159 | .274 | -.225 | .8287 | 1.0000 | |
| 4 | 4 | 11 | 2.326 | * | 1.049 | -.044 | 1.275 | 3.0747 | 1.0000 | |
| 4 | 4 | 12 | 21.435 | 21.236 | 21.236 | -.216 | -.252 | 1.197 | 1.0000 | |
| 4 | 4 | 13 | 1.243 | * | 1.264 | 1.263 | .041 | -.020 | -.0227 | 1.0000 |
| 4 | 4 | 14 | 14.161 | 14.371 | 14.369 | .220 | -.210 | -.21264 | 1.0000 | |
| 4 | 4 | 15 | 1.376 | * | 1.211 | -.1.211 | -.033 | .1.67 | 1.0000 | |
| 4 | 4 | 16 | 15.074 | 15.538 | 15.537 | -.174 | -.464 | -.2.3937 | 1.0000 | |
| 4 | 4 | 17 | 3.782 | 4.732 | 4.732 | .026 | -.4.22 | -.3.5126 | 1.0000 | |
| 4 | 4 | 18 | 42.156 | 40.407 | 40.403 | .613 | 1.749 | 6.3319 | 1.0000 | |
| 4 | 4 | 19 | 1.472 | * | .174 | -.023 | 1.298 | 1.8251 | 1.0000 | |
| 4 | 4 | 20 | 8.772 | 9.026 | 9.025 | -.155 | -.2.56 | -.1.7198 | 1.0000 | |
| 4 | 4 | 21 | 5.165 | 5.587 | 5.587 | .022 | -.4.22 | -.1.6576 | 1.0000 | |
| 4 | 4 | 22 | 23.021 | 23.381 | 23.376 | .491 | -.3.60 | -.1.5753 | 1.0000 | |
| 4 | 4 | 23 | 14.583 | 14.599 | 14.598 | .165 | -.023 | 1.298 | 1.0000 | |
| 4 | 4 | 24 | 1.719 | * | .172 | -.017 | 1.298 | 1.8251 | 1.0000 | |
| 4 | 4 | 25 | 9.026 | 9.025 | 9.025 | -.057 | -.1.56 | -.1.7198 | 1.0000 | |
| 4 | 4 | 26 | 11.446 | 11.506 | 11.507 | -.160 | -.1.61 | -.3.7877 | 1.0000 | |
| 4 | 4 | 27 | 1.993 | * | .110 | -.096 | 1.883 | 3.4024 | 1.0000 | |
| 4 | 4 | 28 | 10.250 | 10.772 | 10.771 | .148 | -.5.22 | -.3.2179 | 1.0000 | |
| 4 | 4 | 29 | 1.376 | * | .481 | .051 | -.8.93 | .9519 | 1.0000 | |
| 4 | 4 | 30 | 6.469 | 6.648 | 6.647 | -.129 | -.1.79 | -.7.702 | 1.0000 | |
| 4 | 4 | 31 | 21.012 | 20.904 | 20.903 | .207 | -.1.08 | .4355 | 1.0000 | |
| 4 | 4 | 32 | 3.939 | 3.741 | 3.741 | .023 | .1.98 | .6612 | 1.0000 | |
| 4 | 4 | 33 | 2.625 | * | 2.200 | 2.192 | .193 | .4.25 | .9407 | 1.0000 |
| 4 | 4 | 34 | 6.469 | 6.319 | 6.319 | -.022 | -.0.59 | -.2.772 | 1.0000 | |
| 4 | 4 | 35 | 15.560 | 15.491 | 15.490 | -.186 | -.0.69 | .3855 | 1.0000 | |
| 4 | 4 | 36 | 1.376 | * | 4.488 | 4.488 | .023 | .888 | .9037 | 1.0000 |
| 4 | 4 | 37 | 9.473 | 8.866 | 8.865 | .105 | -.607 | 3.6654 | 1.0000 | |
| 4 | 4 | 38 | 8.814 | 8.464 | 8.464 | -.6.69 | -.3.50 | 2.0027 | 1.0000 | |
| 4 | 4 | 39 | 10.567 | 10.192 | 10.191 | -.10.191 | -.1.02 | .375 | 1.0000 | |
| 4 | 4 | 40 | 7.541 | 7.483 | 7.483 | -.085 | .058 | .2925 | 1.0000 | |
| 4 | 4 | 41 | 7.393 | 6.757 | 6.756 | .094 | .636 | 3.0807 | 1.0000 | |
| 4 | 4 | 42 | 29.058 | 28.102 | 28.096 | .475 | .6.957 | 3.5514 | 1.0000 | |
| 4 | 4 | 43 | 3.088 | 2.599 | 2.598 | -.0.52 | .489 | 1.0623 | 1.0000 | |
| 4 | 4 | 44 | 7.379 | 7.692 | 7.691 | -.125 | -.3.13 | -.1.4528 | 1.0000 | |
| 4 | 4 | 45 | 2.355 | * | .155 | -.1.47 | 2.0200 | 3.6474 | 1.0000 | |
| 5 | 0 | 46 | 0 | 3.924 | 4.013 | 4.012 | -.085 | -.0.69 | -.3.028 | 1.0000 |
| 5 | 0 | 47 | 5.088 | 6.226 | 6.226 | .083 | -.5.55 | 3.1978 | 1.0000 | |
| 5 | 0 | 48 | 3.045 | -3.244 | -3.244 | -.074 | -.2.38 | -.6.611 | 1.0000 | |
| 5 | 0 | 49 | 2.762 | * | 2.483 | -.069 | -.2.78 | -.5.609 | 1.0000 | |

SILLIMANITE (BRANDYWINE SPRINGS) AT 600 DEGREES C

STRUCTURE FACTORS

PAGE 8

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|----|---------|---------|---------|---------|---------|-------------|--------------|
| 1 | 1 | 0 | 14.0369 | 13.364 | 13.361 | .285 | 1.505 | 7.00996 | 1.0000 |
| 1 | 1 | 1 | 7.921 | 7.603 | 7.603 | .078 | .316 | 1.4863 | 1.0000 |
| 1 | 1 | 2 | 32.952 | 33.244 | 33.244 | .225 | -.292 | -1.1950 | 1.0000 |
| 1 | 1 | 3 | 11.150 | 11.251 | 11.250 | -.074 | -.101 | -.1120 | 1.0000 |
| 1 | 1 | 4 | 13.613 | 12.649 | 12.646 | .255 | .964 | 5.3791 | 1.0000 |
| 1 | 1 | 5 | 1.692 | 1.545 | 1.544 | .066 | .147 | .2354 | 1.0000 * *** |
| 1 | 1 | 6 | 16.276 | 16.167 | 16.166 | .182 | .105 | .6059 | 1.0000 |
| 1 | 1 | 7 | 7.681 | 7.158 | 7.157 | -.055 | .523 | 2.6656 | 1.0000 |
| 1 | 2 | 0 | 64.258 | 65.059 | 65.057 | -.525 | -.800 | -3.6794 | 1.0000 |
| 1 | 2 | 1 | 13.94 | 14.158 | 14.158 | .049 | -.164 | -.8574 | 1.0000 |
| 1 | 2 | 2 | 67.571 | 68.926 | 68.924 | .511 | -.135 | -5.8634 | 1.0000 |
| 1 | 2 | 3 | 6.176 | 6.651 | 6.650 | -.045 | -.504 | -2.7785 | 1.0000 |
| 1 | 2 | 4 | 45.0309 | 45.589 | 45.587 | -.470 | -.260 | -1.0282 | 1.0000 |
| 1 | 2 | 5 | 10.068 | 9.930 | 9.930 | .048 | .137 | .8764 | 1.0000 |
| 1 | 2 | 6 | 35.681 | 35.731 | 35.729 | -.408 | -.050 | -.1504 | 1.0000 |
| 1 | 2 | 7 | 1.379 | * .912 | -.911 | -.035 | .467 | .4742 | 1.0000 * ** |
| 1 | 0 | 1 | 20.242 | 20.305 | 20.304 | .211 | -.063 | -.2203 | 1.0000 |
| 1 | 0 | 2 | 3.832 | 4.378 | 4.376 | .015 | -.546 | -1.6646 | 1.0000 |
| 1 | 0 | 3 | 38.595 | 38.754 | 38.753 | .280 | -.159 | -.6307 | 1.0000 |
| 1 | 0 | 4 | 1.150 | * .452 | -.452 | -.014 | .698 | .6491 | 1.0000 |
| 1 | 0 | 5 | 15.192 | 15.346 | 15.346 | .190 | -.154 | -.8470 | 1.0000 |
| 1 | 0 | 6 | 4.632 | 5.060 | 5.060 | .013 | -.428 | -1.7043 | 1.0000 |
| 1 | 0 | 7 | 19.110 | 19.155 | 19.154 | .224 | -.045 | -.2306 | 1.0000 |
| 1 | 0 | 8 | 2.858 | * .047 | 2.047 | -.010 | .611 | 1.6928 | 1.0000 |
| 1 | 0 | 9 | 8.511 | 6.580 | 6.577 | .391 | 1.922 | 9.6346 | 1.0000 |
| 1 | 1 | 0 | 9.219 | 9.756 | 9.756 | .034 | -.537 | -2.8720 | 1.0000 |
| 1 | 1 | 1 | 23.479 | 22.333 | 22.330 | -.360 | 1.145 | 4.0801 | 1.0000 |
| 1 | 1 | 2 | 9.837 | 10.350 | 10.350 | -.032 | 4.93 | -.9363 | 1.0000 |
| 1 | 1 | 3 | 11.944 | 11.944 | 11.944 | -.225 | 1.018 | 5.3439 | 1.0000 |
| 1 | 1 | 4 | 7.345 | 7.350 | 7.350 | -.205 | -.205 | -.2295 | 1.0000 |
| 1 | 1 | 5 | 4.191 | 3.685 | 3.685 | .032 | .506 | 1.7695 | 1.0000 |
| 1 | 1 | 6 | 13.024 | 12.917 | 12.913 | -.304 | .327 | 2.0026 | 1.0000 |
| 1 | 1 | 7 | 6.646 | 6.235 | 6.235 | -.025 | .412 | 1.7642 | 1.0000 |
| 1 | 1 | 8 | 10.045 | 10.926 | 10.924 | -.225 | 1.018 | 5.3439 | 1.0000 |
| 1 | 1 | 9 | 6.0875 | 6.908 | 6.908 | -.067 | -.072 | .4867 | 1.0000 |
| 1 | 1 | 10 | 14.0391 | 14.273 | 14.276 | .235 | .613 | 3.5105 | 1.0000 |
| 1 | 1 | 11 | 4.367 | 4.264 | 4.263 | .077 | .103 | .4096 | 1.0000 |
| 1 | 1 | 12 | 9.267 | 9.265 | 9.265 | .201 | .776 | 4.8597 | 1.0000 |
| 1 | 1 | 13 | 17.154 | 17.624 | 17.623 | -.177 | .531 | 2.7051 | 1.0000 |
| 1 | 1 | 14 | 1.551 | 1.567 | 1.565 | -.088 | -.016 | -.0239 | 1.0000 |
| 1 | 1 | 15 | 1.391 | * .963 | -.947 | -.171 | .675 | 1.6136 | 1.0000 |
| 1 | 1 | 16 | 2.4386 | * .754 | -.749 | -.085 | 1.751 | 4.0344 | 1.0000 |
| 1 | 1 | 17 | 13.031 | 12.958 | 12.957 | .158 | .074 | .4026 | 1.0000 |
| 1 | 1 | 18 | 2.586 | * .695 | -.892 | -.077 | 1.691 | 3.3106 | 1.0000 |
| 1 | 1 | 19 | 1.878 | * .037 | 1.094 | -.085 | .2996 | 1.0000 | ** ** |
| 1 | 1 | 20 | 2.037 | * .968 | -.967 | -.137 | 1.028 | 1.0140 | 1.0000 |
| 1 | 1 | 21 | 17.832 | * .386 | 24.383 | -.250 | -.003 | .5609 | 1.0000 |
| 1 | 1 | 22 | 2.277 | * .868 | 2.839 | -.045 | .211 | .5609 | 1.0000 |
| 1 | 1 | 23 | 19.807 | * .039 | 19.805 | .165 | .071 | .3458 | 1.0000 |
| 1 | 1 | 24 | 2.037 | * .968 | -.967 | -.042 | 1.069 | 1.8203 | 1.0000 |
| 1 | 1 | 25 | 18.380 | * .379 | 18.379 | -.224 | -.498 | -.7121 | 1.0000 |
| 1 | 1 | 26 | 2.277 | * .868 | 2.868 | -.039 | -.591 | -.9823 | 1.0000 |
| 1 | 1 | 27 | 31.905 | * .117 | 31.117 | -.440 | -.787 | 2.3282 | 1.0000 |

SILLIMANITE (GRANDYMIKE SPRINGS) AT 600 DEGREES C

STRUCTURE FACTORS

PAGE 9

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | FXT. | FACTOR |
|----|----|---|--------|---------|---------|---------|---------|-------------|--------|--------|
| 5 | 8 | 1 | 2.834 | 2.255 | .254 | .055 | .579 | 1.2806 | 1.0000 | |
| 5 | 5 | 2 | 15.637 | 16.057 | 16.051 | 4.428 | -3.76 | -2.1299 | 1.0000 | |
| 5 | 6 | 3 | 2.606 | 2.076 | -2.077 | -.052 | .726 | 1.5195 | 1.0000 | * |
| 6 | 8 | 4 | 23.429 | 23.443 | -23.439 | -.303 | .014 | -.0506 | 1.0000 | * |
| 5 | 5 | 5 | 2.151 | *.914 | .912 | .048 | 1.266 | 1.9354 | 1.0000 | * |
| 5 | 9 | 0 | 1.405 | 1.387 | 1.376 | .170 | *.016 | *.0179 | 1.0000 | * |
| 5 | 9 | 1 | 2.375 | 2.329 | 2.329 | .031 | .046 | .0775 | 1.0000 | * |
| 5 | 9 | 2 | 8.367 | 8.671 | 8.669 | .190 | -.284 | -1.4811 | 1.0000 | * |
| 5 | 9 | 3 | 2.497 | 2.455 | -2.455 | -.028 | .042 | .0744 | 1.0000 | * |
| 5 | 9 | 4 | 1.414 | *.393 | .384 | .153 | *.621 | *.0204 | 1.0000 | * |
| 10 | 10 | 0 | 17.487 | 17.033 | 17.032 | .162 | *.454 | 1.9738 | 1.0000 | |
| 10 | 11 | 1 | 2.709 | *.934 | .934 | .035 | .775 | 1.4141 | 1.0000 | * |
| 10 | 10 | 2 | 6.526 | 6.447 | -6.445 | -.158 | .078 | .3261 | 1.0000 | |
| 6 | 0 | 0 | 81.035 | 81.063 | 81.060 | .672 | -.028 | -.0192 | 1.0000 | |
| 6 | 0 | 0 | 28.648 | 28.265 | -28.264 | -.166 | .216 | -.7997 | 1.0000 | |
| 6 | 0 | 0 | 57.890 | 57.133 | 57.133 | .602 | -.754 | 2.6766 | 1.0000 | |
| 5 | 5 | 0 | 15.113 | 14.368 | -14.367 | -.132 | .745 | 4.1314 | 1.0000 | |
| 5 | 6 | 0 | 38.947 | 38.979 | 38.978 | .303 | .968 | 3.8199 | 1.0000 | |
| 5 | 6 | 1 | 11.074 | 10.668 | -10.668 | -.023 | .606 | 2.0225 | 1.0000 | |
| 5 | 6 | 1 | 2.789 | 1.226 | -1.190 | -.294 | .563 | 4.2795 | 1.0000 | |
| 5 | 6 | 1 | 7.275 | 7.364 | 7.363 | .023 | .086 | -.5471 | 1.0000 | |
| 5 | 6 | 1 | 26.597 | 26.912 | 26.910 | .270 | -.235 | -.6950 | 1.0000 | |
| 5 | 5 | 1 | 5.923 | 5.571 | -5.571 | .017 | .332 | 1.6697 | 1.0000 | |
| 5 | 5 | 1 | 3.259 | 2.764 | -2.754 | -.235 | .465 | 1.2121 | 1.0000 | |
| 5 | 6 | 1 | 1.419 | *.154 | .2154 | .017 | -.734 | -.7248 | 1.0000 | * |
| 5 | 6 | 1 | 22.297 | 22.924 | 22.924 | .079 | -.627 | -.1993 | 1.0000 | * |
| 5 | 5 | 2 | 7.537 | 7.996 | -7.995 | -.116 | .406 | -.2014 | 1.0000 | |
| 5 | 5 | 2 | 24.530 | 23.966 | 23.963 | .402 | .564 | 2.0023 | 1.0000 | |
| 5 | 5 | 2 | 7.034 | 7.198 | 7.197 | .111 | -.164 | -.0036 | 1.0000 | |
| 5 | 6 | 2 | 15.194 | 14.872 | 14.871 | .072 | .323 | 1.9475 | 1.0000 | |
| 5 | 6 | 2 | 5.737 | 5.536 | -5.535 | -.100 | .201 | .9128 | 1.0000 | |
| 5 | 6 | 2 | 14.561 | 14.422 | 14.416 | .323 | .139 | .7612 | 1.0000 | |
| 5 | 6 | 2 | 4.807 | 4.168 | 4.168 | .087 | .638 | 2.0587 | 1.0000 | |
| 5 | 6 | 2 | 22.009 | 22.553 | -22.553 | .074 | -.545 | -1.9031 | 1.0000 | |
| 5 | 6 | 3 | 3.008 | 3.505 | 3.505 | .031 | -.696 | -.4620 | 1.0000 | |
| 5 | 6 | 3 | 7.563 | 7.107 | -7.107 | -.071 | .455 | 2.0767 | 1.0000 | |
| 5 | 6 | 3 | 1.482 | *.817 | -.816 | -.027 | .666 | -.9432 | 1.0000 | * |
| 5 | 6 | 4 | 14.220 | 14.382 | -14.382 | .066 | -.161 | -.9235 | 1.0000 | * |
| 5 | 6 | 4 | 4.443 | 4.182 | 4.182 | .025 | .260 | *.9132 | 1.0000 | |
| 5 | 6 | 4 | 3.940 | 3.153 | -3.152 | -.057 | .767 | 2.2819 | 1.0000 | |
| 5 | 6 | 4 | 1.402 | * | .549 | .016 | .854 | .8528 | 1.0000 | * |
| 5 | 6 | 4 | 1.867 | *.839 | -.032 | 1.028 | 1.9231 | 1.0000 | * | |
| 5 | 6 | 4 | 7.375 | 7.142 | 7.141 | .109 | .028 | 1.4323 | 1.0000 | * |
| 5 | 6 | 4 | 36.566 | 36.015 | 36.011 | .486 | .551 | 1.9404 | 1.0000 | |
| 5 | 6 | 4 | 7.225 | 6.485 | -6.484 | -.103 | .739 | 4.4316 | 1.0000 | |
| 5 | 6 | 4 | 1.256 | * | .071 | -.066 | 1.185 | 1.3202 | 1.0000 | * |
| 5 | 6 | 4 | 5.272 | 5.085 | 5.084 | .094 | 1.187 | .7283 | 1.0000 | * |
| 5 | 6 | 4 | 21.632 | 21.198 | 21.198 | .390 | .431 | 1.2687 | 1.0000 | |
| 5 | 6 | 4 | 20.577 | 20.515 | -20.513 | -.324 | .061 | 1.0000 | 1.0000 | |
| 5 | 6 | 5 | 1.649 | * | 1.646 | .013 | .003 | .0041 | 1.0000 | * |
| 5 | 6 | 5 | 35.969 | 36.283 | 36.281 | .315 | -.314 | 1.0471 | 1.0000 | * |
| 5 | 6 | 5 | 2.890 | 1.705 | -1.705 | -.011 | 1.185 | 3.0661 | 1.0000 | |
| 5 | 6 | 5 | 15.742 | 15.871 | -15.868 | -.290 | 1.128 | -.7034 | 1.0000 | |

SILLIMANITE (BRANDYWINE SPRINGS). AT 600 DEGREES C.

STRUCTURE FACTORS

PAGE TWO

SILLIMANITE (BRANDYWINE SPRINGS) AT 600 DEGREES C

STRUCTURE FACTORS

PAGE 11

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | PXT. | FACTOR |
|---|---|----|--------|---------|---------|---------|---------|-------------|---------|--------------|
| 7 | 7 | 4 | 6 | 1.614 * | 1.451 | 1.450 | .059 | .163 | 1.832 | 1.0000 * *** |
| 7 | 5 | 6 | 6 | 5.069 | 4.499 | 4.497 | .120 | .571 | 2.3883 | 1.0000 |
| 7 | 5 | 1 | 1 | 4.216 | 4.744 | 4.744 | -.038 | .526 | -1.8442 | 1.0000 |
| 7 | 5 | 2 | 2 | 3.92 | 3.278 | 3.277 | -.304 | .286 | -.8945 | 1.0000 |
| 7 | 5 | 3 | 3 | 3.236 | 2.337 | 2.337 | -.037 | .899 | 2.3057 | 1.0000 |
| 7 | 5 | 4 | 4 | 3.43 | 3.407 | 3.405 | .108 | .035 | .0856 | 1.0000 |
| 7 | 5 | 5 | 5 | 3.34 | 3.613 | 3.613 | -.034 | .220 | .5767 | 1.0000 |
| 7 | 6 | 0 | 0 | 4.535 | 4.987 | 4.987 | -.012 | .452 | -1.5554 | 1.0000 |
| 7 | 6 | 1 | 1 | 1.155 | 1.206 | 1.206 | -.102 | .65 | -.3234 | 1.0000 |
| 7 | 6 | 2 | 2 | 4.842 | 5.245 | 5.245 | -.012 | .403 | -1.4304 | 1.0000 |
| 7 | 6 | 3 | 3 | 7.799 | 8.020 | 8.020 | -.111 | .221 | -1.1264 | 1.0000 |
| 7 | 6 | 4 | 4 | 3.790 | 3.729 | 3.729 | -.011 | .060 | -.1601 | 1.0000 |
| 7 | 6 | 5 | 5 | 8.457 | 8.521 | 8.521 | -.102 | .65 | -.3234 | 1.0000 |
| 7 | 6 | 6 | 6 | 24.741 | 24.224 | 24.223 | -.151 | .517 | 1.9866 | 1.0000 |
| 7 | 7 | 1 | 1 | 8.577 | 8.258 | 8.258 | -.059 | .279 | 1.5201 | 1.0000 |
| 7 | 7 | 2 | 2 | 3.3.618 | 3.4.801 | 3.4.801 | -.163 | .3.2490 | 1.0000 | 1.0000 |
| 7 | 7 | 3 | 3 | 7.805 | 7.798 | 7.798 | -.055 | .007 | .0357 | 1.0000 |
| 7 | 7 | 4 | 4 | 19.536 | 18.535 | 18.535 | -.134 | .485 | 2.2082 | 1.0000 |
| 7 | 7 | 5 | 5 | 1.426 * | .594 | .585 | .085 | .832 | .8175 | 1.0000 * *** |
| 7 | 7 | 6 | 6 | 1.423 * | .837 | .837 | -.022 | .526 | .586 | 1.0000 * *** |
| 7 | 7 | 7 | 7 | 8.343 | 8.957 | 8.957 | -.082 | .114 | -.5827 | 1.0000 |
| 7 | 7 | 8 | 8 | 2.451 * | 1.317 | 1.316 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 7 | 9 | 9 | 27.168 | 26.239 | 26.234 | -.479 | .929 | 3.2328 | 1.0000 |
| 7 | 7 | 10 | 10 | 1.946 * | 1.157 | 1.157 | -.016 | .791 | 1.0239 | 1.0000 * *** |
| 7 | 8 | 0 | 0 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 8 | 1 | 1 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 8 | 2 | 2 | 3.581 | 3.350 | 3.350 | -.020 | .232 | 1.9019 | 1.0000 |
| 7 | 8 | 3 | 3 | 2.451 * | 1.317 | 1.317 | -.022 | .134 | 1.551 | 1.0000 |
| 7 | 8 | 4 | 4 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 8 | 5 | 5 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 8 | 6 | 6 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 8 | 7 | 7 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 8 | 8 | 8 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 8 | 9 | 9 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 8 | 10 | 10 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 11 | 11 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 12 | 12 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 13 | 13 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 14 | 14 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 15 | 15 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 16 | 16 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 17 | 17 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 18 | 18 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 19 | 19 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 20 | 20 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 21 | 21 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 22 | 22 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 23 | 23 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 24 | 24 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 25 | 25 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 26 | 26 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 27 | 27 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 28 | 28 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 29 | 29 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 30 | 30 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 31 | 31 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 32 | 32 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 33 | 33 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 34 | 34 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 35 | 35 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 36 | 36 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 37 | 37 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 38 | 38 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 39 | 39 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 40 | 40 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 41 | 41 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 42 | 42 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 43 | 43 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 44 | 44 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 45 | 45 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 46 | 46 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 47 | 47 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 48 | 48 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 49 | 49 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 50 | 50 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 51 | 51 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 52 | 52 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 53 | 53 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 54 | 54 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 55 | 55 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 56 | 56 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 57 | 57 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 58 | 58 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 59 | 59 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 60 | 60 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 61 | 61 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 62 | 62 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 63 | 63 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 64 | 64 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 65 | 65 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 66 | 66 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 67 | 67 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 68 | 68 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 69 | 69 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 70 | 70 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 71 | 71 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 72 | 72 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 73 | 73 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 74 | 74 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 75 | 75 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 76 | 76 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 77 | 77 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 78 | 78 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 79 | 79 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1.329 | 1.0000 |
| 7 | 9 | 80 | 80 | 9.035 | 8.957 | 8.957 | -.082 | .082 | -.5827 | 1.0000 |
| 7 | 9 | 81 | 81 | 2.451 * | 1.317 | 1.317 | -.022 | .022 | 1.134 | 1.0000 * *** |
| 7 | 9 | 82 | 82 | 42.885 | 42.701 | 42.701 | -.029 | .093 | 5.551 | 1.0000 |
| 7 | 9 | 83 | 83 | 3.534 | 3.067 | 3.067 | -.016 | .016 | 5.8671 | 1.0000 |
| 7 | 9 | 84 | 84 | 1.946 * | 1.157 | 1.157 | -.016 | .016 | 1.0239 | 1.0000 * *** |
| 7 | 9 | 85 | 85 | 57.298 | 58.627 | 58.627 | -.022 | .329 | -1 | |

| | F (CALC) | A (CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|----|----------|----------|---------|-------------|-------------|
| 4 | 4.118 | 4.0864 | -4.084 | -0.49 | -766 |
| 5 | 4.712 | 4.070 | 32.066 | 0.356 | -1.0447 |
| 6 | 3.992 | 6.338 | -8.336 | -0.55 | -1.8463 |
| 7 | 6.644 | 2.020 | -26.199 | -0.388 | 1.7508 |
| 8 | 7.413 | 7.318 | 7.317 | -0.054 | -0.095 |
| 9 | 24.557 | 24.508 | 24.505 | -0.357 | -0.050 |
| 10 | 12.966 | 12.999 | 12.995 | -0.355 | -0.334 |
| 11 | 2.100 * | 2.241 | -0.239 | -0.035 | 1.855 |
| 12 | 1.674 | 2.097 | 2.096 | -0.038 | 1.423 |
| 13 | 3.637 | 2.263 | 2.283 | -0.034 | 1.324 |
| 14 | 6.635 | 9.711 | 9.706 | -0.318 | -0.077 |
| 15 | 13.145 | 13.104 | -13.102 | -0.225 | 0.041 |
| 16 | 5.246 | 4.677 | -4.677 | -0.225 | 2.8427 |
| 17 | 9.216 | 10.044 | 10.041 | -0.063 | -4.677 |
| 18 | 2.650 | 4.091 | 4.090 | -0.062 | -4.625 |
| 19 | 11.501 | 11.668 | 11.666 | -0.198 | -1.441 |
| 20 | 4.045 | 3.923 | 3.922 | -0.068 | 0.122 |
| 21 | 1.453 | 2.404 | 2.404 | -0.006 | -0.951 |
| 22 | 1.381 | 0.029 | 0.029 | -0.007 | 2.342 |
| 23 | 2.313 | 3.178 | 3.178 | -0.001 | -1.3384 |
| 24 | 19.777 | 20.584 | 20.581 | -0.338 | -0.807 |
| 25 | 7.121 | 7.587 | -7.586 | -0.139 | -4.467 |
| 26 | 10.673 | 10.811 | 10.810 | -0.094 | -1.136 |
| 27 | 8.759 | 8.967 | 8.966 | -0.132 | -1.196 |
| 28 | 15.336 | 15.731 | 15.728 | -0.303 | -0.393 |
| 29 | 3.923 | 3.518 | -3.516 | -0.119 | -0.405 |
| 30 | 30.765 | 31.169 | 31.166 | -0.377 | -4.403 |
| 31 | 2.155 | 2.172 | 2.172 | -0.006 | -0.017 |
| 32 | 8.751 | 3.575 | -3.573 | -0.366 | -7.724 |
| 33 | 32.551 | 33.575 | 33.573 | -0.006 | -0.676 |
| 34 | 2.746 | 3.216 | -3.216 | -0.356 | -0.9276 |
| 35 | 24.778 | 23.922 | 23.920 | -0.356 | 0.157 |
| 36 | 1.570 | 0.801 | -0.801 | -0.004 | -0.9363 |
| 37 | 2.909 | 2.824 | -2.824 | -0.007 | -0.570 |
| 38 | 2.663 | 1.213 | -1.213 | -0.016 | 1.0445 |
| 39 | 24.778 | 24.883 | 24.880 | -0.105 | -0.476 |
| 40 | 1.570 | 0.801 | -0.801 | -0.016 | -0.769 |
| 41 | 2.909 | 2.824 | -2.824 | -0.006 | -0.084 |
| 42 | 3.102 | 3.635 | -3.625 | -0.270 | -0.533 |
| 43 | 3.348 | 2.833 | 2.833 | -0.016 | -0.515 |
| 44 | 10.957 | 10.932 | 10.929 | -0.025 | 1.2254 |
| 45 | 1.418 | 0.809 | -0.808 | -0.013 | -0.610 |
| 46 | 2.803 | 2.609 | -2.597 | -0.242 | -0.195 |
| 47 | 17.751 | 18.192 | 18.190 | -0.261 | -0.441 |
| 48 | 8.247 | 8.469 | 8.468 | -0.141 | -0.222 |
| 49 | 11.265 | 11.658 | 11.657 | -0.127 | -0.393 |
| 50 | 5.935 | -5.926 | -5.926 | -0.133 | 0.007 |
| 51 | 12.233 | -11.325 | -11.325 | -0.140 | -0.907 |
| 52 | 1.438 | 1.358 | 1.358 | -0.008 | 0.080 |
| 53 | 2.147 | * | 2.013 | -0.008 | 0.135 |
| 54 | 12.919 | 12.722 | 12.718 | -0.310 | -0.198 |
| 55 | 4.257 | 4.032 | -4.031 | -0.099 | -0.224 |
| 56 | 20.621 | -20.900 | -20.900 | -0.229 | -0.286 |
| 57 | 43.816 | -43.816 | -43.816 | -1.259 | -3.5463 |

SILLIMANITE (BERNARDINE SPRINGS) AT 600 DEGREES C

STRUCTURE FACTORS

PAGE 13

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR | |
|----|---|---|--------|---------|---------|---------|---------|-------------|-------------|---|
| 10 | 0 | 4 | 17.132 | 16.493 | -16.492 | -.204 | .639 | 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 | .078 | .394 | 1.0000 | |
| 10 | 1 | 2 | 7.328 | 6.797 | -6.797 | -.531 | .4812 | 1.0000 | * | |
| 10 | 1 | 3 | 2.713 | * | 1.509 | -1.508 | 1.204 | 2.2065 | 1.0000 | |
| 10 | 1 | 4 | 6.946 | 6.136 | -6.136 | -.072 | .042 | .813 | 1.0000 | |
| 10 | 2 | 0 | 16.076 | 16.517 | 16.517 | -.370 | .741 | -3.7139 | 1.0000 | |
| 10 | 2 | 1 | 4.207 | 3.024 | 3.024 | -.080 | 1.183 | 3.4263 | 1.0000 | |
| 10 | 2 | 2 | 7.015 | 6.652 | 6.652 | -.034 | .163 | *.7133 | 1.0000 | |
| 10 | 2 | 3 | 3.302 | 2.884 | -2.883 | -.076 | .498 | 1.1273 | 1.0000 | |
| 10 | 3 | 0 | 9.746 | 9.807 | 9.807 | -.027 | .676 | -.3410 | 1.0000 | |
| 10 | 3 | 1 | 11.247 | 11.914 | 11.914 | -.134 | .667 | -.3.5703 | 1.0000 | |
| 10 | 3 | 2 | 3.795 | 3.011 | 3.011 | -.026 | .784 | 1.9598 | 1.0000 | |
| 10 | 3 | 3 | 9.016 | 9.343 | 9.342 | -.129 | .327 | -1.6760 | 1.0000 | |
| 10 | 4 | 0 | 27.946 | 29.125 | 29.125 | -.472 | .179 | -.4.2532 | 1.0000 | |
| 10 | 4 | 1 | 5.807 | 5.344 | 5.344 | -.079 | .462 | 1.6801 | 1.0000 | |
| 10 | 4 | 2 | 6.405 | 5.688 | -5.687 | -.085 | .718 | 2.8417 | 1.0000 | |
| 10 | 5 | 0 | 1.454 | * | .676 | -.059 | .778 | .7490 | 1.0000 | |
| 10 | 5 | 1 | 2.929 | * | 1.838 | -1.837 | .032 | 1.091 | 2.0947 | * |
| 11 | 0 | 1 | 4.344 | 3.716 | -3.712 | -.160 | .629 | 1.7426 | 1.0000 | |
| 11 | 1 | 0 | 9.956 | 10.831 | 10.825 | -.353 | .875 | -4.7599 | 1.0000 | |
| 11 | 1 | 1 | 2.502 | * | 3.855 | -.051 | -1.053 | -1.8987 | 1.0000 | |
| 11 | 1 | 2 | 7.686 | 8.034 | 8.034 | -.031 | .346 | -1.5624 | 1.0000 | |
| 11 | 2 | 0 | 16.152 | -16.212 | 16.214 | -.257 | .662 | -.3185 | 1.0000 | |
| 11 | 2 | 1 | 5.440 | 6.046 | 6.045 | -.071 | .606 | -.2.0505 | 1.0000 | |

SILLIMANITE (BRANDYWINE SPRINGS) AT 600 DEGREES C

RESULTS OF STRUCTURE FACTOR CALCULATIONS

ALL REFLECTIONS

NUMERATOR DENOMINATOR NUMBER R

WEIGHTED R 10290.26

6837009.55

661

.039

UNWEIGHTED R 392.22

6673.66

661

.045

RANGES OF F(OBS)

| | | | |
|---------|------------|------|------|
| 3271.40 | ±49969.78 | 5.05 | .062 |
| 1423.07 | 947286.35 | 9.3 | .039 |
| 660.26 | 1020445.83 | 3.7 | .025 |
| 839.56 | 1233409.19 | 14 | .026 |
| 377.91 | 1159598.69 | 7 | .016 |
| 578.84 | 652097.52 | 3 | .025 |
| 60.48 | 262178.52 | 1 | .015 |
| 3078.61 | 412023.68 | 1 | .066 |

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

| | | | |
|---------|------------|------|------|
| 3134.37 | 2412865.09 | 3.9 | .036 |
| 3971.44 | 1810921.26 | 5.5 | .047 |
| 688.64 | 746692.98 | 6.7 | .030 |
| 485.53 | 575794.10 | 8.7 | .029 |
| 587.98 | 326726.53 | 6.7 | .042 |
| 349.08 | 379722.52 | 1.04 | .030 |
| 410.04 | 342917.40 | 1.10 | .035 |
| 652.98 | 239369.67 | 1.12 | .052 |

UNREJECTED REFLECTIONS

WEIGHTED R

| | | | |
|---------|------------|------|------|
| 6383.09 | 6423122.52 | 5.09 | .023 |
|---------|------------|------|------|

UNWEIGHTED R

| | | | |
|--------|---------|------|------|
| 275.85 | 8261.04 | 5.09 | .033 |
|--------|---------|------|------|

RANGES OF F(OBS)

| | | | |
|---------|------------|------|------|
| 2942.85 | 848106.43 | 3.54 | .059 |
| 1423.07 | 947286.35 | 9.3 | .039 |
| 660.38 | 1020445.83 | 3.7 | .025 |
| 839.56 | 1233409.19 | 14 | .026 |
| 377.91 | 1159598.69 | 7 | .018 |
| 578.84 | 652097.52 | 3 | .025 |
| 60.48 | 262178.52 | 1 | .015 |
| .00 | .00 | 0 | .000 |

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

| | | | |
|---------|------------|-----|------|
| 3121.19 | 2412832.65 | 3.9 | .036 |
| 885.89 | 1398823.26 | 4.9 | .025 |
| 663.72 | 746597.44 | 5.5 | .030 |
| 429.47 | 575560.22 | 6.6 | .027 |
| 528.43 | 326504.62 | 6.6 | .040 |
| 318.53 | 379423.41 | 8.2 | .029 |
| 363.55 | 342532.84 | 8.0 | .033 |
| 572.31 | 238848.07 | 7.3 | .049 |

SUM FCAL
STANDARD DEV OF UNIT WEIGHT OBS

8553.24
3.86

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

John K. Winter

and

Subrata Chose

Department of Geological Sciences
University of Washington
Seattle, Washington 98195

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

Sillimanite 800°C

FWD OF THE LOAD
LWA+1 OF THE LOAD

TRANSFER ADDRESS --- REFINER

2

***** ERROR SUMMARY

NE4105/// CM BLANK COMMON TRUNCATED BY 20700 WORDS

PROGRAM AND BLOCK ASSIGNMENTS

SILLIMANITE (GRANDVIEW SPRINGS) AT 800 DEGREES C

STRUCTURE FACTORS

PAGE 1

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|-----|---------|---------|---------|---------|---------|-------------|-------------|
| 0 | 0 | 2 | 62.536 | 63.711 | -63.710 | -348 | -1.175 | -8.4051 | 1.0000 |
| 0 | 0 | 4 | 130.200 | 140.702 | 140.700 | 808 | -10.502 | -53.0573 | * |
| 0 | 0 | 6 | 24.387 | 23.851 | -23.850 | 265 | -2.265 | 1.6632 | 1.0000 |
| 0 | 0 | 8 | 48.033 | 46.654 | 46.650 | 536 | -536 | 1.379 | 1.0000 |
| 0 | 0 | 10 | 15.565 | 13.221 | 13.221 | 548 | -548 | 4.1399 | 1.0000 |
| 0 | 0 | 12 | 4.310 | 4.536 | -4.535 | 565 | -4.565 | 11.4636 | 1.0000 |
| 0 | 0 | 14 | 22.575 | 18.624 | -18.617 | 575 | -4.525 | -5.396 | 1.0000 |
| 0 | 0 | 16 | 6.311 | 6.168 | 6.168 | 502 | -502 | 22.1377 | 1.0000 |
| 0 | 0 | 18 | 7.318 | 6.341 | 6.341 | 502 | -502 | 8.383 | 1.0000 |
| 0 | 0 | 20 | 1.045 | .056 | .010 | 528 | -528 | 5.8275 | 1.0000 |
| 0 | 0 | 22 | 8.202 | 8.015 | 8.005 | 586 | -586 | 1.3245 | 1.0000 |
| 0 | 0 | 24 | 4.461 | 4.121 | 4.121 | 502 | -502 | 1.3517 | 1.0000 |
| 0 | 0 | 26 | 2.491 | 1.696 | 1.696 | 521 | -521 | 1.3952 | 1.0000 |
| 0 | 0 | 28 | 21.220 | 19.142 | 19.142 | 575 | -575 | 1.6293 | 1.0000 |
| 0 | 0 | 30 | 6.211 | 6.217 | 6.217 | 513 | -513 | 10.4979 | 1.0000 |
| 0 | 0 | 32 | 87.435 | 88.736 | 88.734 | 547 | -547 | 1.3517 | 1.0000 |
| 0 | 0 | 34 | 9.898 | 10.109 | -10.109 | 502 | -502 | 1.3777 | 1.0000 |
| 0 | 0 | 36 | 4.127 | 5.457 | 5.456 | 521 | -521 | 1.3952 | 1.0000 |
| 0 | 0 | 38 | 1.070 | *.055 | *.070 | 502 | -502 | 1.6293 | 1.0000 |
| 0 | 0 | 40 | 4.1029 | 4.3162 | 4.3159 | 549 | -549 | 1.6293 | 1.0000 |
| 0 | 0 | 42 | 6.702 | 6.633 | -6.633 | 506 | -506 | 1.6293 | 1.0000 |
| 0 | 0 | 44 | 1.023 | *.286 | *.272 | 587 | -587 | 1.6293 | 1.0000 |
| 0 | 0 | 46 | 48.261 | 47.537 | 47.532 | 523 | -523 | 1.6293 | 1.0000 |
| 0 | 0 | 48 | 6.726 | 6.928 | -6.928 | 520 | -520 | 1.6293 | 1.0000 |
| 0 | 0 | 50 | 21.560 | 23.051 | -23.050 | 555 | -555 | 1.6293 | 1.0000 |
| 0 | 0 | 52 | 1.056 | *.264 | *.263 | 520 | -520 | 1.6293 | 1.0000 |
| 0 | 0 | 54 | 34.718 | 35.680 | 35.675 | 539 | -539 | 1.6293 | 1.0000 |
| 0 | 0 | 56 | 6.839 | 6.863 | -6.863 | 514 | -514 | 1.6293 | 1.0000 |
| 0 | 0 | 58 | 10.556 | 11.047 | -11.045 | 595 | -595 | 1.6293 | 1.0000 |
| 0 | 0 | 60 | 2.677 | *.014 | *.014 | 575 | -575 | 1.6293 | 1.0000 |
| 0 | 0 | 62 | 1.925 | *.176 | *.176 | 563 | -563 | 1.6293 | 1.0000 |
| 0 | 0 | 64 | 20.605 | 21.389 | -21.388 | 514 | -514 | 1.6293 | 1.0000 |
| 0 | 0 | 66 | 4.307 | 4.805 | -4.805 | 564 | -564 | 1.6293 | 1.0000 |
| 0 | 0 | 68 | 11.928 | 12.179 | 12.178 | 564 | -564 | 1.6676 | 1.0000 |
| 0 | 0 | 70 | 2.516 | *.247 | -2.247 | 555 | -555 | 1.5770 | 1.0000 |
| 0 | 0 | 72 | 12.298 | 12.513 | 12.512 | 512 | -512 | -3.5360 | 1.0000 |
| 0 | 0 | 74 | 6.648 | 6.704 | -6.701 | 506 | -506 | -3.3152 | 1.0000 |
| 0 | 0 | 76 | 4.550 | 4.397 | 4.396 | 581 | -581 | 1.6210 | 1.0000 |
| 0 | 0 | 78 | 25.948 | 26.254 | -26.249 | 597 | -597 | 1.6210 | 1.0000 |
| 0 | 0 | 80 | 2.320 | *.053 | -1.051 | 574 | -574 | 4.1476 | 1.0000 |
| 0 | 0 | 82 | 7.474 | 5.445 | -5.453 | 519 | -519 | 1.822 | 1.0000 |
| 0 | 0 | 84 | 12.630 | 12.073 | -12.072 | 577 | -577 | 1.5675 | 1.0000 |
| 0 | 0 | 86 | 2.613 | 2.009 | -2.008 | 572 | -572 | 1.2796 | 1.0000 |
| 0 | 0 | 88 | 8.755 | 8.831 | -8.831 | 566 | -566 | 1.5490 | 1.0000 |
| 0 | 0 | 90 | 2.918 | 2.126 | -2.128 | 555 | -555 | 1.2280 | 1.0000 |
| 0 | 0 | 92 | 7.474 | 5.445 | -5.453 | 519 | -519 | 1.4299 | 1.0000 |
| 0 | 0 | 94 | 13.619 | 14.066 | -14.065 | 564 | -564 | 1.6645 | 1.0000 |
| 0 | 0 | 96 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 0 | 0 | 98 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 0 | 0 | 100 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 11 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 13 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 15 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 17 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 19 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 21 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 23 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 25 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 27 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 29 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 31 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 33 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 35 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 37 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 39 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 41 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 43 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 45 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 47 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 49 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 51 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 53 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 55 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 57 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 59 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 61 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 63 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 65 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 67 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 69 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 71 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 73 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 75 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 77 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 79 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 81 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 83 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 85 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 87 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 89 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 91 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 93 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 95 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 97 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 99 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 101 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 103 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 105 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 107 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 109 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 111 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 113 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 115 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 117 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 119 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 121 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 123 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 125 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 127 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 129 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 131 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 133 | 8.338 | 8.265 | -8.265 | 573 | -573 | 1.4991 | 1.0000 |
| 1 | 1 | 135 | 13.619 | 14.066 | -14.065 | 564 | -564 | 2.1609 | 1.0000 |
| 1 | 1 | 137 | 4.505 | 5.054 | -5.053 | 532 | -532 | 1.6645 | 1.0000 |
| 1 | 1 | 139 | 26.454 | 26.934 | -26.932 | 566 | -566 | 2.6712 | 1.0000 |
| 1 | 1 | 141 | 5.263 | 1.091 | -1.091 | 572 | -572 | 2.1814 | 1.0000 |
| 1 | 1 | 143 | 61.614 | 62.320 | -62.320 | 574 | -574 | 1.2280 | 1.0000 |
| 1 | 1 | 145 | 8.338 | 8.265 | -8.265 | 573 | -57 | | |

SILLIMANITE (BRANDYWINE SPRINGS) AT 800 DEGREES C

STRUCTURE FACTORS

PAGE 2

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) | DELTA F | DELTA/SIGMA | EXT. FACTOR |
|---|---|---|--------|---------|----------|---------|---------|-------------|-------------|
| 1 | 1 | 1 | 7 | 4.407 | 4.0331 | 4.331 | -0.021 | 0.076 | 1.0000 |
| 1 | 1 | 1 | 6 | 6.122 | 5.868 | 5.868 | +0.043 | +0.254 | 1.1564 |
| 1 | 1 | 2 | 0 | 81.321 | 81.924 | 81.922 | +0.459 | +0.603 | 1.0000 |
| 1 | 1 | 2 | 1 | 7.872 | 7.968 | 7.968 | +0.044 | +0.116 | 0.5190 |
| 1 | 1 | 2 | 2 | 84.441 | 84.504 | 84.502 | +0.444 | +0.062 | 0.4007 |
| 1 | 1 | 2 | 3 | 0.981 | * 1.0768 | -1.0767 | +0.042 | +0.786 | -1.1221 |
| 1 | 1 | 2 | 4 | 45.400 | 46.372 | 46.370 | +0.403 | +0.972 | -4.4479 |
| 1 | 1 | 2 | 5 | 7.415 | 7.816 | -7.818 | +0.037 | +0.404 | -3.0336 |
| 1 | 1 | 2 | 6 | 34.532 | 34.772 | -34.770 | +0.342 | +0.240 | -0.8523 |
| 1 | 1 | 2 | 7 | 1.4220 | * 1.0865 | -1.0865 | +0.032 | +0.645 | -0.7402 |
| 1 | 1 | 2 | 8 | 18.643 | 17.835 | 17.833 | +0.272 | +0.808 | 4.5812 |
| 1 | 1 | 3 | 0 | 46.497 | 47.174 | 47.170 | +0.625 | +0.677 | -4.4413 |
| 1 | 1 | 3 | 1 | 5.140 | 5.269 | -5.269 | +0.010 | +0.129 | -0.6695 |
| 1 | 1 | 3 | 2 | 2.522 | 3.064 | -3.063 | +0.089 | +1.161 | -4.0362 |
| 1 | 1 | 3 | 3 | 2.695 | 2.404 | -2.404 | +0.019 | -1.162 | 1.0246 |
| 1 | 1 | 3 | 4 | 37.369 | 38.531 | 38.528 | +0.549 | +0.291 | -5.0220 |
| 1 | 1 | 3 | 5 | 5.105 | 5.676 | -5.678 | +0.007 | +0.573 | -3.2473 |
| 1 | 1 | 3 | 6 | 4.156 | 3.837 | -3.837 | +0.067 | +0.316 | 1.3379 |
| 1 | 1 | 3 | 7 | 3.049 | 2.880 | -2.880 | +0.008 | +0.169 | 0.4662 |
| 1 | 1 | 3 | 8 | 17.234 | 17.456 | 17.452 | +0.373 | +0.223 | -1.2032 |
| 1 | 1 | 4 | 0 | 1.857 | * 0.652 | -0.558 | +0.338 | +1.205 | 1.0000 |
| 1 | 1 | 4 | 1 | 2.513 | 0.882 | -3.048 | +0.029 | +0.151 | -0.5421 |
| 1 | 1 | 4 | 2 | 2.898 | 2.5162 | 25.917 | +0.327 | +0.755 | -3.5421 |
| 1 | 1 | 4 | 3 | 5.956 | 5.200 | 5.964 | +0.29 | +0.158 | -0.8678 |
| 1 | 1 | 4 | 4 | 6.469 | 6.211 | -6.204 | +0.296 | +0.258 | 1.5509 |
| 1 | 1 | 4 | 5 | 2.513 | 0.882 | -8.82 | +0.025 | +1.630 | 0.7847 |
| 1 | 1 | 4 | 6 | 13.956 | 13.976 | 13.973 | +0.252 | +0.019 | -0.1184 |
| 1 | 1 | 4 | 7 | 4.964 | 4.964 | 4.964 | +0.023 | +0.237 | 1.0184 |
| 1 | 1 | 4 | 8 | 3.775 | 3.773 | -3.773 | +0.200 | +0.032 | 1.032 |
| 1 | 1 | 4 | 9 | 10.499 | 10.063 | 10.061 | +0.176 | +0.416 | 2.1267 |
| 1 | 1 | 4 | 10 | 6.969 | 6.508 | 6.508 | +0.024 | +0.461 | 2.6992 |
| 1 | 1 | 4 | 11 | 59.178 | 60.846 | 60.845 | +0.303 | +1.668 | -7.8301 |
| 1 | 1 | 4 | 12 | 1.105 | * | 1.061 | -1.061 | +0.044 | +0.0560 |
| 1 | 1 | 4 | 13 | 9.053 | 9.238 | 9.236 | +0.156 | +0.184 | -1.3011 |
| 1 | 1 | 4 | 14 | 4.826 | 4.948 | 4.948 | +0.020 | +0.122 | -0.6100 |
| 1 | 1 | 4 | 15 | 2.6232 | 2.6887 | 2.6886 | +0.235 | +0.655 | -2.8307 |
| 1 | 1 | 4 | 16 | 2.656 | * | 1.555 | +0.021 | +1.102 | 2.4905 |
| 1 | 1 | 4 | 17 | 23.040 | -23.322 | -23.322 | +0.151 | +0.283 | -1.0932 |
| 1 | 1 | 4 | 18 | 3.413 | 2.678 | 2.677 | +0.079 | +0.735 | 2.6432 |
| 1 | 1 | 4 | 19 | 1.104 | * | 0.150 | +0.033 | +0.146 | +0.000 |
| 1 | 1 | 4 | 20 | 4.445 | 4.745 | -4.745 | +0.074 | +0.300 | -1.4994 |
| 1 | 1 | 4 | 21 | 15.280 | 15.410 | -15.410 | +0.132 | +0.130 | -0.7932 |
| 1 | 1 | 4 | 22 | 2.038 | * | 0.881 | +0.081 | +0.067 | 1.157 |
| 1 | 1 | 4 | 23 | 1.596 | * | 1.182 | +1.182 | +1.176 | 2.4202 |
| 1 | 1 | 4 | 24 | 4.197 | 3.677 | -3.677 | +0.056 | +0.056 | 0.5860 |
| 1 | 1 | 4 | 25 | 24.422 | -25.281 | -25.281 | +0.030 | +0.859 | 1.7088 |
| 1 | 1 | 4 | 26 | 6.200 | 6.495 | 6.495 | +0.043 | +0.295 | -3.1898 |
| 1 | 1 | 4 | 27 | 3.017 | 4.0213 | 4.0211 | +0.446 | +1.196 | -4.5317 |
| 1 | 1 | 4 | 28 | 6.635 | -6.806 | -6.806 | +0.039 | +1.172 | -1.0862 |
| 1 | 1 | 4 | 29 | 15.368 | -15.954 | -15.954 | +0.025 | +0.586 | -3.6885 |
| 1 | 1 | 4 | 30 | 3.169 | 3.088 | 3.088 | +0.038 | +0.081 | 0.2339 |
| 1 | 1 | 4 | 31 | 2.082 | 2.1211 | 2.1208 | +0.345 | +0.929 | -4.2325 |
| 1 | 1 | 4 | 32 | 4.016 | 4.116 | 4.116 | +0.028 | +0.054 | 1.0000 |