

The crystal chemistry of nolanite, $(V,Fe,Ti,Al)_{10}O_{14}(OH)_2$, from Kalgoorlie, Western Australia

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Abstract

Nolanite crystals associated with gold mineralization in the "green leader" deposits of Kalgoorlie, Western Australia, show large local variations in vanadium, titanium and iron contents. The structures have been refined for two compositions with $V/\Sigma M$ atomic fractions of 0.69 and 0.52. Cell parameters (space group $P6_3mc$, $Z = 1$) are $a = 5.890(4)$, $c = 9.255(5)\text{\AA}$ and $a = 5.897(2)$, $c = 9.256(3)\text{\AA}$ respectively. Final weighted R factors were 0.039 and 0.049 for 737 and 604 reflections with $F > 4\sigma(F)$, collected on an automatic diffractometer using $MoK\alpha$ radiation. The structure is based on a closest-packed anion framework with a double hexagonal stacking sequence, ABCBA, *i.e.*, (*ch*) and with cations ordered into 2 tetrahedral and 8 octahedral sites. Valence sum calculations are consistent with nolanite being an oxyhydroxide, $(V,Fe,Ti,Al)_{10}O_{14}(OH)_2$, and with predominately trivalent vanadium and mixed divalent and trivalent iron. Based on a comparison of refined site occupancies and bond lengths for the two structures, plausible cation ordering schemes have been proposed and the intergrain compositional variations have been confirmed to be due to substitutions of the type $V^{3+} \leftrightarrow Fe^{3+}$ and $2(V^{3+},Fe^{3+}) \leftrightarrow (Fe^{2+}+Ti^{4+})$ in the octahedral sites.

Introduction

A new iron vanadate with hexagonal symmetry, $a = 5.854$ and $c = 9.295\text{\AA}$ from Goldfields, Saskatchewan, was first reported by Barnes and Qurashi (1952). The mineral was subsequently described in detail and named nolanite by Robinson *et al.* (1957). Chemical analyses led to inconclusive results regarding the formula because of the difficulty of removing impurities, but Robinson *et al.* used crystal-chemical arguments to propose that the structure was based on a closest-packed anion lattice with 16 anions and 10 cations per unit cell. They suggested unit cell compositions in the range $Fe_{2.5}^{2+}V_{1.5}^{3+}O_{16}$ to $Fe_{2.8}^{2+}V_{1.5}^{3+}O_{16}$. Subsequently their model was confirmed by Hanson (1958) from a single-crystal structure analysis using Weissenberg intensity data. He showed that the structure comprised a closest-packed anion framework with a stacking sequence ABCBA, and with metal ions occupying one 6-fold octahedrally coordinated site and

two 2-fold sites, one of octahedral and one of tetrahedral coordination. He proposed an ordering of cations $(V^{4+})_6^{[6]}(0.78Fe^{2+} + 0.22V^{3+})_2^{[6]}(0.47Fe^{2+} + 0.53V^{3+})_2^{[4]}O_{16}$ but noted that the unit cell composition was unbalanced by 1.5 electrons.

A new occurrence of nolanite, in metamorphosed greenstones associated with native gold and tellurides at Kalgoorlie, was reported by Taylor and Radtke (1967). They carried out electron microprobe analyses, supported by wet chemical analysis on purified material which gave the valence states of vanadium as V^{4+} and V^{5+} with $V_2O_5/V_2O_4 = 1.57$, and proposed a unit cell composition based on 18 anions and a cation to anion ratio of 1:2 *i.e.*, $Al_{0.17}Si_{0.05}Ti_{0.27}V_{5.16}Fe_{3.31}Zn_{0.04}Sn_{0.01}O_{18}$. This composition was in conflict with the results of the structure refinement of Hanson (1958).

Our interest in this material arose from a systematic study of hōgbomite–nigerite polytypes (Grey and Gatehouse, 1979; Gatehouse and Grey, 1982), which we have

| Atom | U_{11} | U_{22} | U_{33} | U_{12} | U_{13} | U_{23} |
|------|----------|----------|----------|----------|----------|----------|
|------|----------|----------|----------|----------|----------|----------|

Crystal 1

| | | | | | | |
|------|--------|--------|--------|--------|--------|-------|
| M(1) | 51 (3) | 51 (3) | 45 (2) | 20 (2) | -1 (3) | 1 (3) |
| M(2) | 48 (5) | 48 (5) | 36 (3) | 24 (3) | 0 | 0 |
| M(3) | 58 (5) | 58 (5) | 68 (3) | 29 (3) | 0 | 0 |
| O(1) | 60(20) | 60(20) | 60(15) | 30(10) | 0 | 0 |
| O(2) | 64(20) | 64(20) | 31(16) | 32(10) | 0 | 0 |
| O(3) | 81(20) | 81(20) | 96(11) | 46(13) | -2(11) | 2(11) |
| O(4) | 65(16) | 65(16) | 62 (9) | 36(10) | -4 (8) | 4 (8) |

Crystal 2

| | | | | | | |
|------|---------|---------|---------|---------|---------|--------|
| M(1) | 49 (3) | 49 (3) | 49 (3) | 24 (3) | -7 (4) | 7 (4) |
| M(2) | 44 (8) | 44 (8) | 41 (7) | 22 (4) | 0 | 0 |
| M(3) | 55 (7) | 55 (7) | 70 (7) | 27 (4) | 0 | 0 |
| O(1) | 139(35) | 139(35) | 41(33) | 69(17) | 0 | 0 |
| O(2) | -37(22) | -37(22) | 112(38) | -19(11) | 0 | 0 |
| O(3) | 116(23) | 116(23) | 89(21) | 23(32) | -10(15) | 10(15) |
| O(4) | 25(15) | 25(15) | 95(21) | 12(18) | 3 (9) | -3 (9) |

* The temperature factors are of the form
 $\exp [-2\pi^2 (U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} +$
 $2U_{12}hka^*b^* + U_{13}hla^*c^* + 2U_{23}klb^*c^*)]$

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 1

PAGE 1

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|----|---|-----|----|----|----|---|-----|----|----|----|---|-----|----|----|----|----|-----|----|----|
| 0 | 0 | -18 | 39 | 42 | -3 | 6 | -14 | 9 | 9 | -1 | 7 | -12 | 8 | 8 | -2 | 6 | -10 | 35 | 35 |
| 0 | 1 | -18 | 8 | 7 | -2 | 6 | -14 | 10 | 11 | 0 | 7 | -12 | 10 | 10 | -1 | 6 | -10 | 14 | 13 |
| -1 | 2 | -18 | 17 | 15 | 0 | 6 | -14 | 23 | 23 | -4 | 8 | -12 | 18 | 18 | 0 | 6 | -10 | 53 | 53 |
| 0 | 2 | -18 | 22 | 22 | -2 | 7 | -14 | 8 | 11 | -3 | 8 | -12 | 9 | 7 | -3 | 7 | -10 | 11 | 11 |
| 0 | 1 | -17 | 10 | 12 | 0 | 1 | -13 | 25 | 25 | -2 | 8 | -12 | 14 | 15 | -2 | 7 | -10 | 21 | 21 |
| 0 | 2 | -17 | 24 | 24 | 0 | 2 | -13 | 42 | 42 | -1 | 8 | -12 | 18 | 18 | -1 | 7 | -10 | 11 | 10 |
| -1 | 3 | -17 | 14 | 14 | -1 | 3 | -13 | 21 | 22 | 0 | 1 | -11 | 11 | 14 | 0 | 7 | -10 | 10 | 10 |
| -1 | 4 | -17 | 10 | 11 | -1 | 4 | -13 | 23 | 22 | 0 | 2 | -11 | 40 | 39 | -4 | 8 | -10 | 49 | 48 |
| 0 | 0 | -16 | 33 | 34 | 0 | 4 | -13 | 58 | 38 | -1 | 3 | -11 | 15 | 13 | -3 | 8 | -10 | 12 | 13 |
| 0 | 1 | -16 | 9 | 8 | -2 | 5 | -13 | 23 | 23 | -1 | 4 | -11 | 13 | 12 | -2 | 8 | -10 | 28 | 28 |
| -1 | 2 | -16 | 15 | 17 | 0 | 5 | -13 | 17 | 18 | 0 | 4 | -11 | 34 | 34 | -1 | 8 | -10 | 15 | 16 |
| 0 | 2 | -16 | 12 | 10 | -2 | 6 | -13 | 34 | 34 | -2 | 5 | -11 | 11 | 12 | 0 | 8 | -10 | 25 | 24 |
| -1 | 3 | -16 | 9 | 7 | -1 | 6 | -13 | 16 | 18 | 0 | 5 | -11 | 14 | 13 | -4 | 9 | -10 | 10 | 10 |
| 0 | 3 | -16 | 16 | 17 | -3 | 7 | -13 | 15 | 16 | -2 | 6 | -11 | 29 | 31 | -3 | 9 | -10 | 16 | 17 |
| -2 | 4 | -16 | 33 | 31 | -2 | 7 | -13 | 8 | 5 | -1 | 6 | -11 | 10 | 10 | 0 | 1 | -9 | 17 | 16 |
| -1 | 4 | -16 | 9 | 8 | -1 | 7 | -13 | 20 | 19 | -3 | 7 | -11 | 11 | 11 | 0 | 2 | -9 | 17 | 16 |
| 0 | 4 | -16 | 10 | 9 | 0 | 7 | -13 | 20 | 19 | -1 | 7 | -11 | 9 | 10 | -1 | 3 | -9 | 34 | 33 |
| -1 | 5 | -16 | 14 | 15 | -3 | 8 | -13 | 16 | 17 | 0 | 7 | -11 | 9 | 10 | -1 | 4 | -9 | 15 | 14 |
| 0 | 5 | -16 | 8 | 5 | 0 | 8 | -13 | 26 | 24 | -3 | 8 | -11 | 9 | 9 | 0 | 4 | -9 | 13 | 13 |
| 0 | 1 | -15 | 23 | 24 | 0 | 1 | -12 | 13 | 12 | -2 | 8 | -11 | 24 | 25 | -2 | 5 | -9 | 29 | 28 |
| 0 | 2 | -15 | 38 | 39 | -1 | 2 | -12 | 30 | 28 | -1 | 8 | -11 | 8 | 1 | 0 | 5 | -9 | 12 | 11 |
| -1 | 3 | -15 | 19 | 21 | 0 | 2 | -12 | 27 | 27 | 0 | 8 | -11 | 23 | 24 | -2 | 6 | -9 | 25 | 25 |
| -1 | 4 | -15 | 21 | 21 | -1 | 3 | -12 | 10 | 11 | -4 | 9 | -11 | 8 | 9 | -1 | 6 | -9 | 11 | 10 |
| 0 | 4 | -15 | 34 | 36 | 0 | 3 | -12 | 27 | 27 | 0 | 0 | -10 | 78 | 77 | -3 | 7 | -9 | 9 | 10 |
| -2 | 5 | -15 | 21 | 21 | -2 | 4 | -12 | 23 | 22 | 0 | 1 | -10 | 17 | 17 | -1 | 7 | -9 | 8 | 8 |
| 0 | 5 | -15 | 16 | 18 | -1 | 4 | -12 | 12 | 11 | -1 | 2 | -10 | 29 | 30 | 0 | 7 | -9 | 13 | 13 |
| -2 | 6 | -15 | 31 | 32 | 0 | 4 | -12 | 22 | 23 | 0 | 2 | -10 | 51 | 50 | -3 | 8 | -9 | 8 | 8 |
| -1 | 6 | -15 | 17 | 18 | -2 | 5 | -12 | 11 | 11 | -1 | 3 | -10 | 15 | 15 | -2 | 8 | -9 | 21 | 21 |
| 0 | 0 | -14 | 34 | 33 | -1 | 5 | -12 | 24 | 24 | 0 | 3 | -10 | 28 | 28 | 0 | 8 | -9 | 19 | 19 |
| 0 | 1 | -14 | 8 | 5 | 0 | 5 | -12 | 11 | 9 | -2 | 4 | -10 | 66 | 66 | -4 | 9 | -9 | 9 | 9 |
| -1 | 2 | -14 | 15 | 13 | -3 | 6 | -12 | 22 | 23 | -1 | 4 | -10 | 15 | 15 | -2 | 9 | -9 | 8 | 8 |
| 0 | 2 | -14 | 12 | 13 | -2 | 6 | -12 | 19 | 20 | 0 | 4 | -10 | 42 | 41 | -1 | 9 | -9 | 17 | 17 |
| 0 | 3 | -14 | 14 | 13 | -1 | 6 | -12 | 9 | 8 | -2 | 5 | -10 | 13 | 13 | -4 | 10 | -9 | 8 | 8 |
| -2 | 4 | -14 | 29 | 29 | 0 | 6 | -12 | 19 | 19 | -1 | 5 | -10 | 24 | 24 | 0 | 10 | -9 | 17 | 17 |
| 0 | 4 | -14 | 10 | 12 | -3 | 7 | -12 | 7 | 8 | 0 | 5 | -10 | 12 | 12 | -4 | 10 | -8 | 83 | 81 |
| -1 | 5 | -14 | 12 | 11 | -2 | 7 | -12 | 22 | 21 | -3 | 6 | -10 | 19 | 19 | 0 | 3 | -7 | 29 | 28 |
| 0 | 3 | -14 | 29 | 29 | 0 | 6 | -12 | 19 | 20 | -2 | 5 | -10 | 42 | 41 | -4 | 10 | -9 | 17 | 17 |
| -2 | 4 | -14 | 10 | 12 | -3 | 7 | -12 | 7 | 8 | 0 | 5 | -10 | 12 | 12 | -4 | 10 | -8 | 83 | 81 |
| -1 | 5 | -14 | 12 | 11 | -2 | 7 | -12 | 22 | 21 | -3 | 6 | -10 | 19 | 19 | 0 | 3 | -7 | 29 | 28 |

TABLE

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 1

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|----|----|----|----|----|----|----|----|-----|-----|----|----|----|----|----|----|----|----|----|----|
| -2 | 5 | -7 | 39 | 38 | -4 | 9 | -6 | 7 | 3 | 0 | 4 | -4 | 41 | 41 | -2 | 8 | -3 | 20 | 21 |
| -1 | 5 | -7 | 7 | 5 | 0 | 9 | -6 | 8 | 4 | 0 | 5 | -4 | 10 | 9 | 0 | 8 | -3 | 19 | 19 |
| 0 | 5 | -7 | 25 | 25 | -4 | 10 | -6 | 16 | 16 | -1 | 5 | -4 | 13 | 13 | -4 | 9 | -3 | 23 | 22 |
| -2 | 6 | -7 | 25 | 23 | -3 | 10 | -6 | 8 | 2 | 0 | 5 | -4 | 6 | 5 | -2 | 9 | -3 | 31 | 32 |
| -1 | 6 | -7 | 25 | 26 | -2 | 10 | -6 | 29 | 29 | -3 | 6 | -4 | 15 | 14 | -1 | 9 | -3 | 27 | 27 |
| -3 | 7 | -7 | 23 | 22 | 0 | 1 | -5 | 36 | 34 | -2 | 6 | -4 | 32 | 31 | -4 | 10 | -3 | 18 | 17 |
| -1 | 7 | -7 | 28 | 27 | 0 | 2 | -5 | 134 | 132 | -1 | 6 | -4 | 6 | 2 | -3 | 10 | -3 | 23 | 23 |
| 0 | 7 | -7 | 28 | 29 | -1 | 3 | -5 | 32 | 31 | 0 | 6 | -4 | 30 | 29 | -1 | 10 | -3 | 18 | 19 |
| -3 | 8 | -7 | 24 | 23 | 0 | 3 | -5 | 5 | 7 | -2 | 7 | -4 | 8 | 8 | 0 | 10 | -3 | 14 | 14 |
| -2 | 8 | -7 | 18 | 18 | -1 | 4 | -5 | 25 | 24 | -1 | 7 | -4 | 8 | 9 | -5 | 11 | -3 | 24 | 25 |
| 0 | 8 | -7 | 14 | 15 | 0 | 4 | -5 | 95 | 94 | 0 | 7 | -4 | 6 | 4 | -3 | 11 | -3 | 16 | 17 |
| -4 | 9 | -7 | 25 | 25 | -2 | 5 | -5 | 21 | 21 | -4 | 8 | -4 | 27 | 27 | 0 | 0 | -2 | 67 | 67 |
| -3 | 9 | -7 | 8 | 5 | 0 | 5 | -5 | 24 | 23 | -3 | 8 | -4 | 6 | 8 | 0 | 1 | -2 | 53 | 53 |
| -2 | 9 | -7 | 17 | 16 | -2 | 6 | -5 | 76 | 76 | -2 | 8 | -4 | 22 | 22 | -1 | 2 | -2 | 52 | 52 |
| -1 | 9 | -7 | 16 | 17 | -1 | 6 | -5 | 20 | 19 | -1 | 8 | -4 | 11 | 10 | 0 | 2 | -2 | 90 | 90 |
| 0 | 9 | -7 | 9 | 6 | -3 | 7 | -5 | 19 | 19 | 0 | 8 | -4 | 19 | 19 | -1 | 3 | -2 | 61 | 59 |
| -4 | 10 | -7 | 14 | 14 | -1 | 7 | -5 | 15 | 15 | -4 | 9 | -4 | 8 | 8 | 0 | 0 | -2 | 38 | 38 |
| -3 | 10 | -7 | 16 | 17 | 0 | 7 | -5 | 12 | 14 | -3 | 9 | -4 | 10 | 8 | -2 | 3 | -2 | 71 | 71 |
| 0 | 10 | -6 | 91 | 89 | -3 | 8 | -5 | 14 | 15 | 0 | 9 | -4 | 8 | 6 | -1 | 4 | -2 | 38 | 38 |
| 0 | 1 | -6 | 6 | 5 | -2 | 8 | -5 | 56 | 57 | -5 | 10 | -4 | 11 | 10 | 0 | 4 | -2 | 32 | 32 |
| -1 | 2 | -6 | 12 | 11 | 0 | 8 | -5 | 51 | 52 | -4 | 10 | -4 | 17 | 17 | -2 | 5 | -2 | 30 | 30 |
| 0 | 2 | -6 | 41 | 41 | -4 | 9 | -5 | 51 | 52 | -4 | 10 | -4 | 17 | 17 | -2 | 5 | -2 | 29 | 29 |
| -1 | 3 | -6 | 5 | 5 | -2 | 9 | -5 | 11 | 13 | -2 | 10 | -4 | 22 | 22 | -1 | 5 | -2 | 29 | 29 |
| 0 | 3 | -6 | 9 | 9 | -1 | 9 | -5 | 11 | 13 | 0 | 1 | -3 | 77 | 76 | -1 | 5 | -2 | 51 | 51 |
| -2 | 4 | -6 | 68 | 65 | -4 | 10 | -5 | 47 | 47 | -1 | 2 | -3 | 62 | 61 | 0 | 5 | -2 | 23 | 23 |
| -1 | 4 | -6 | 6 | 2 | -3 | 10 | -5 | 13 | 12 | -1 | 3 | -3 | 71 | 70 | -3 | 6 | -2 | 46 | 46 |
| 0 | 4 | -6 | 31 | 30 | -1 | 10 | -5 | 11 | 11 | 0 | 3 | -3 | 8 | 7 | -1 | 6 | -2 | 20 | 20 |
| -1 | 5 | -6 | 9 | 8 | -5 | 11 | -5 | 11 | 11 | -1 | 4 | -3 | 51 | 51 | 0 | 6 | -2 | 22 | 22 |
| -3 | 6 | -6 | 10 | 10 | -5 | 11 | -5 | 10 | 12 | 0 | 4 | -3 | 38 | 38 | -3 | 7 | -2 | 19 | 18 |
| -2 | 6 | -6 | 23 | 25 | 0 | 0 | -4 | 48 | 45 | -2 | 5 | -3 | 41 | 39 | -2 | 7 | -2 | 38 | 38 |
| 0 | 6 | -6 | 45 | 45 | -1 | 2 | -4 | 15 | 13 | 0 | 5 | -3 | 49 | 49 | -1 | 7 | -2 | 19 | 19 |
| -2 | 7 | -6 | 6 | 6 | 0 | 2 | -4 | 21 | 21 | -2 | 6 | -3 | 29 | 29 | 0 | 7 | -2 | 18 | 19 |
| -4 | 8 | -6 | 40 | 39 | -1 | 3 | -4 | 63 | 63 | -4 | 8 | -2 | 39 | 39 | -4 | 8 | -2 | 19 | 19 |
| -3 | 8 | -6 | 7 | 1 | 0 | 3 | -4 | 7 | 7 | -3 | 7 | -3 | 41 | 40 | 0 | 8 | -2 | 40 | 40 |
| -2 | 8 | -6 | 18 | 19 | -2 | 4 | -4 | 15 | 16 | -1 | 7 | -3 | 27 | 28 | -3 | 8 | -2 | 28 | 28 |
| 0 | 8 | -6 | 15 | 17 | -1 | 4 | -4 | 41 | 38 | 0 | 7 | -3 | 25 | 24 | -2 | 8 | -2 | 24 | 24 |
| -2 | 8 | -6 | 15 | 17 | -1 | 4 | -4 | 7 | 6 | -3 | 8 | -3 | 29 | 28 | -1 | 8 | -2 | 31 | 31 |
| 0 | 8 | -6 | 15 | 17 | -1 | 4 | -4 | 7 | 6 | -3 | 8 | -3 | 29 | 28 | -1 | 8 | -2 | 31 | 31 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 1

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|----|----|---|-----|-----|----|----|---|----|----|----|----|---|----|----|----|----|---|-----|-----|----|----|---|----|----|
| -1 | 0 | 3 | 17 | 18 | -2 | 6 | 1 | 45 | 44 | -4 | 9 | 2 | 16 | 17 | -1 | 10 | 3 | 18 | 19 | 0 | 5 | 5 | 22 | 24 |
| 0 | 3 | 0 | 32 | 31 | -2 | 7 | 1 | 7 | 9 | -3 | 9 | 2 | 28 | 30 | 0 | 10 | 3 | 13 | 13 | -2 | 6 | 5 | 76 | 76 |
| -2 | 4 | 0 | 172 | 179 | -1 | 7 | 1 | 7 | 5 | -2 | 9 | 2 | 14 | 14 | -5 | 11 | 3 | 24 | 25 | -1 | 6 | 5 | 21 | 19 |
| -1 | 4 | 0 | 11 | 11 | -3 | 8 | 1 | 7 | 2 | -1 | 9 | 2 | 12 | 12 | -3 | 11 | 3 | 16 | 17 | -3 | 7 | 5 | 20 | 20 |
| 0 | 4 | 0 | 48 | 49 | -2 | 8 | 1 | 34 | 33 | 0 | 9 | 2 | 25 | 26 | 0 | 0 | 4 | 47 | 49 | -2 | 7 | 5 | 6 | 6 |
| -2 | 5 | 0 | 11 | 11 | 0 | 8 | 1 | 28 | 28 | -5 | 10 | 2 | 27 | 28 | 0 | 1 | 4 | 13 | 13 | -1 | 7 | 5 | 15 | 15 |
| -1 | 5 | 0 | 25 | 25 | -2 | 9 | 1 | 7 | 5 | -4 | 10 | 2 | 11 | 10 | 0 | 2 | 4 | 20 | 21 | 0 | 7 | 5 | 13 | 13 |
| 0 | 5 | 0 | 12 | 13 | 0 | 9 | 1 | 9 | 7 | -3 | 10 | 2 | 13 | 12 | -1 | 2 | 4 | 63 | 63 | -3 | 8 | 5 | 13 | 15 |
| -3 | 6 | 0 | 24 | 25 | -4 | 10 | 1 | 26 | 26 | -2 | 10 | 2 | 16 | 14 | 0 | 2 | 4 | 9 | 7 | -2 | 8 | 5 | 56 | 57 |
| -2 | 6 | 0 | 39 | 39 | -3 | 10 | 1 | 7 | 1 | -1 | 10 | 2 | 12 | 12 | 0 | 3 | 4 | 16 | 16 | -2 | 8 | 5 | 51 | 52 |
| -1 | 6 | 0 | 6 | 7 | 0 | 10 | 1 | 23 | 23 | 0 | 10 | 2 | 8 | 8 | -2 | 4 | 4 | 42 | 40 | -4 | 9 | 5 | 13 | 12 |
| 0 | 6 | 0 | 98 | 99 | 0 | 0 | 2 | 66 | 67 | -5 | 11 | 2 | 12 | 11 | -1 | 4 | 4 | 7 | 6 | -4 | 9 | 5 | 13 | 16 |
| -3 | 7 | 0 | 12 | 9 | 0 | 1 | 2 | 51 | 53 | -4 | 11 | 2 | 23 | 24 | 0 | 4 | 4 | 41 | 41 | -2 | 9 | 5 | 13 | 16 |
| -2 | 7 | 0 | 15 | 16 | -1 | 2 | 2 | 90 | 90 | -3 | 11 | 2 | 14 | 12 | -2 | 5 | 4 | 10 | 9 | -1 | 9 | 5 | 14 | 13 |
| -4 | 8 | 0 | 82 | 84 | 0 | 2 | 2 | 62 | 60 | 0 | 11 | 3 | 75 | 76 | -1 | 5 | 4 | 14 | 14 | -4 | 10 | 5 | 47 | 47 |
| -2 | 8 | 0 | 29 | 31 | -1 | 3 | 2 | 38 | 38 | 0 | 12 | 3 | 61 | 61 | -1 | 5 | 4 | 6 | 5 | -3 | 10 | 5 | 11 | 12 |
| -1 | 8 | 0 | 17 | 18 | 0 | 3 | 2 | 71 | 70 | -1 | 12 | 3 | 71 | 71 | -3 | 6 | 4 | 12 | 14 | 0 | 11 | 6 | 90 | 90 |
| 0 | 8 | 0 | 26 | 28 | -2 | 4 | 2 | 37 | 38 | 0 | 13 | 3 | 7 | 7 | -2 | 6 | 4 | 31 | 31 | 0 | 12 | 6 | 11 | 11 |
| -3 | 9 | 0 | 14 | 8 | -1 | 4 | 2 | 31 | 32 | -1 | 13 | 3 | 51 | 51 | 0 | 6 | 4 | 30 | 31 | -1 | 13 | 6 | 5 | 5 |
| -2 | 9 | 0 | 7 | 10 | 0 | 4 | 2 | 30 | 31 | 0 | 14 | 3 | 38 | 38 | -2 | 7 | 4 | 8 | 9 | -2 | 14 | 6 | 40 | 39 |
| 0 | 9 | 0 | 9 | 10 | -2 | 5 | 2 | 30 | 29 | -2 | 14 | 3 | 41 | 39 | -4 | 8 | 4 | 30 | 28 | 0 | 15 | 6 | 7 | 7 |
| -5 | 10 | 0 | 13 | 18 | -1 | 5 | 2 | 52 | 51 | 0 | 15 | 3 | 49 | 50 | -4 | 8 | 4 | 21 | 22 | -1 | 16 | 6 | 5 | 5 |
| -4 | 10 | 0 | 26 | 26 | 0 | 5 | 2 | 23 | 23 | -2 | 15 | 3 | 29 | 29 | -2 | 8 | 4 | 21 | 22 | 0 | 17 | 6 | 10 | 9 |
| -3 | 10 | 0 | 7 | 2 | -3 | 6 | 2 | 47 | 46 | -1 | 16 | 3 | 40 | 39 | -1 | 8 | 4 | 10 | 10 | -2 | 18 | 6 | 66 | 65 |
| -2 | 10 | 0 | 56 | 59 | -2 | 6 | 2 | 20 | 21 | -3 | 16 | 3 | 40 | 40 | 0 | 8 | 4 | 17 | 19 | 0 | 19 | 6 | 29 | 28 |
| 0 | 10 | 0 | 22 | 22 | -1 | 6 | 2 | 21 | 20 | -2 | 17 | 3 | 6 | 4 | -4 | 9 | 4 | 7 | 6 | -4 | 20 | 6 | 6 | 8 |
| -4 | 11 | 0 | 10 | 10 | 0 | 6 | 2 | 23 | 22 | -1 | 17 | 3 | 28 | 27 | -3 | 9 | 4 | 10 | 8 | 0 | 21 | 6 | 5 | 5 |
| 0 | 11 | 1 | 13 | 12 | -3 | 7 | 2 | 19 | 18 | -5 | 10 | 4 | 24 | 23 | -5 | 10 | 4 | 12 | 10 | -2 | 22 | 6 | 23 | 23 |
| 0 | 12 | 1 | 79 | 80 | -2 | 7 | 2 | 38 | 38 | 0 | 10 | 4 | 28 | 28 | -4 | 10 | 4 | 15 | 17 | 0 | 23 | 6 | 44 | 45 |
| -1 | 13 | 1 | 8 | 8 | -1 | 7 | 2 | 17 | 19 | -3 | 11 | 4 | 20 | 20 | -2 | 10 | 4 | 21 | 22 | -2 | 24 | 7 | 7 | 6 |
| 0 | 13 | 1 | 12 | 12 | 0 | 7 | 2 | 18 | 19 | -4 | 11 | 4 | 21 | 21 | 0 | 11 | 5 | 35 | 34 | 0 | 25 | 8 | 3 | 3 |
| -1 | 14 | 1 | 6 | 6 | -4 | 8 | 2 | 19 | 20 | 0 | 12 | 5 | 21 | 19 | -1 | 11 | 5 | 131 | 132 | -4 | 26 | 8 | 41 | 39 |
| 0 | 14 | 1 | 57 | 57 | -3 | 8 | 2 | 17 | 16 | -2 | 12 | 5 | 32 | 32 | 0 | 12 | 5 | 33 | 32 | -2 | 27 | 8 | 19 | 18 |
| -2 | 15 | 1 | 9 | 10 | -2 | 8 | 2 | 13 | 13 | -1 | 13 | 5 | 25 | 27 | 0 | 13 | 5 | 26 | 24 | -4 | 28 | 8 | 17 | 16 |
| -1 | 15 | 1 | 6 | 7 | -1 | 8 | 2 | 30 | 32 | -4 | 13 | 5 | 18 | 17 | 0 | 14 | 5 | 8 | 7 | 0 | 29 | 8 | 16 | 15 |
| 0 | 15 | 1 | 8 | 8 | -3 | 8 | 2 | 10 | 11 | -3 | 14 | 5 | 25 | 27 | -1 | 14 | 5 | 95 | 94 | -2 | 30 | 9 | 29 | 29 |
| 0 | 16 | 1 | 8 | 8 | -4 | 9 | 2 | 18 | 16 | -4 | 14 | 5 | 18 | 17 | 0 | 15 | 5 | 20 | 20 | 0 | 31 | 9 | 50 | 49 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 1

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|----|----|----|----|----|----|----|---|----|----|----|----|----|----|----|----|---|----|----|----|
| 0 | 2 | 2 | 36 | 37 | -1 | 6 | 8 | 17 | 18 | -4 | 9 | 9 | 10 | 9 | 0 | 4 | 11 | 34 | 34 |
| -1 | 3 | 3 | 37 | 37 | 0 | 6 | 8 | 42 | 42 | -2 | 9 | 9 | 10 | 9 | -2 | 5 | 11 | 13 | 11 |
| 0 | 3 | 3 | 8 | 7 | -3 | 7 | 8 | 16 | 15 | -1 | 9 | 9 | 9 | 7 | 0 | 5 | 11 | 13 | 11 |
| -1 | 4 | 4 | 37 | 37 | -2 | 7 | 8 | 31 | 30 | -4 | 10 | 9 | 17 | 18 | -2 | 6 | 11 | 30 | 30 |
| 0 | 4 | 4 | 28 | 29 | -1 | 7 | 8 | 18 | 17 | 0 | 0 | 10 | 76 | 76 | -1 | 6 | 11 | 11 | 10 |
| -2 | 5 | 5 | 38 | 38 | 0 | 7 | 8 | 17 | 16 | 0 | 1 | 10 | 17 | 17 | -3 | 7 | 11 | 12 | 12 |
| 0 | 5 | 5 | 24 | 25 | -4 | 8 | 8 | 36 | 37 | -1 | 2 | 10 | 30 | 30 | -1 | 7 | 11 | 10 | 9 |
| -2 | 6 | 6 | 24 | 24 | -3 | 8 | 8 | 17 | 16 | 0 | 2 | 10 | 50 | 51 | 0 | 7 | 11 | 9 | 9 |
| -1 | 6 | 6 | 25 | 26 | -2 | 8 | 8 | 11 | 11 | -1 | 3 | 10 | 16 | 16 | -3 | 8 | 11 | 9 | 9 |
| -3 | 7 | 7 | 22 | 22 | -1 | 8 | 8 | 23 | 24 | 0 | 3 | 10 | 28 | 28 | -2 | 8 | 11 | 23 | 24 |
| -2 | 7 | 7 | 9 | 7 | 0 | 8 | 8 | 11 | 11 | -2 | 4 | 10 | 65 | 65 | 0 | 8 | 11 | 23 | 24 |
| -1 | 7 | 7 | 27 | 27 | -4 | 9 | 8 | 14 | 15 | -1 | 4 | 10 | 15 | 15 | -4 | 9 | 11 | 8 | 8 |
| 0 | 7 | 7 | 28 | 29 | -3 | 9 | 8 | 24 | 24 | 0 | 4 | 10 | 42 | 42 | 0 | 9 | 11 | 25 | 26 |
| -3 | 8 | 8 | 24 | 23 | -2 | 9 | 8 | 10 | 11 | -2 | 5 | 10 | 12 | 13 | 0 | 1 | 12 | 12 | 12 |
| -2 | 8 | 8 | 19 | 20 | -1 | 9 | 8 | 13 | 12 | -1 | 5 | 10 | 23 | 24 | -1 | 2 | 12 | 29 | 28 |
| 0 | 8 | 8 | 17 | 16 | 0 | 9 | 8 | 22 | 22 | 0 | 5 | 10 | 10 | 12 | 0 | 2 | 12 | 27 | 27 |
| -4 | 9 | 9 | 26 | 25 | -5 | 10 | 8 | 20 | 20 | -3 | 6 | 10 | 22 | 21 | -1 | 3 | 12 | 12 | 11 |
| -2 | 9 | 9 | 15 | 16 | -4 | 10 | 8 | 10 | 10 | -2 | 6 | 10 | 36 | 36 | 0 | 3 | 12 | 26 | 26 |
| -1 | 9 | 9 | 15 | 16 | -3 | 10 | 8 | 14 | 13 | -1 | 6 | 10 | 13 | 13 | -2 | 4 | 12 | 23 | 24 |
| 0 | 9 | 9 | 18 | 17 | -3 | 10 | 8 | 14 | 13 | 0 | 6 | 10 | 53 | 52 | -1 | 4 | 12 | 10 | 10 |
| -4 | 10 | 10 | 15 | 15 | 0 | 1 | 9 | 16 | 16 | -3 | 7 | 10 | 11 | 12 | 0 | 4 | 12 | 23 | 23 |
| -3 | 10 | 10 | 16 | 17 | -1 | 2 | 9 | 33 | 34 | -2 | 7 | 10 | 20 | 21 | -2 | 5 | 12 | 11 | 11 |
| 0 | 1 | 1 | 82 | 82 | 0 | 3 | 9 | 7 | 5 | -1 | 7 | 10 | 13 | 12 | -1 | 5 | 12 | 24 | 24 |
| -1 | 2 | 2 | 28 | 28 | -1 | 4 | 9 | 13 | 13 | 0 | 7 | 10 | 9 | 10 | 0 | 5 | 12 | 9 | 9 |
| -1 | 2 | 2 | 48 | 48 | 0 | 4 | 9 | 28 | 29 | -4 | 8 | 10 | 46 | 48 | -3 | 6 | 12 | 22 | 22 |
| 0 | 2 | 2 | 16 | 15 | -2 | 5 | 9 | 14 | 13 | -3 | 8 | 10 | 12 | 13 | -2 | 6 | 12 | 20 | 20 |
| -1 | 3 | 3 | 24 | 24 | -1 | 5 | 9 | 8 | 4 | -2 | 8 | 10 | 28 | 28 | -1 | 6 | 12 | 9 | 8 |
| 0 | 3 | 3 | 44 | 43 | 0 | 5 | 9 | 13 | 12 | -1 | 8 | 10 | 15 | 16 | 0 | 6 | 12 | 21 | 21 |
| -2 | 4 | 4 | 61 | 61 | -2 | 6 | 9 | 26 | 25 | -4 | 9 | 10 | 26 | 25 | -3 | 7 | 12 | 9 | 8 |
| -1 | 4 | 4 | 22 | 23 | -1 | 6 | 9 | 10 | 10 | 0 | 9 | 10 | 9 | 9 | -2 | 7 | 12 | 21 | 21 |
| 0 | 4 | 4 | 15 | 14 | -3 | 7 | 9 | 10 | 11 | -3 | 9 | 10 | 15 | 16 | -1 | 7 | 12 | 11 | 11 |
| -2 | 5 | 5 | 22 | 21 | -1 | 7 | 9 | 9 | 10 | -2 | 9 | 10 | 9 | 9 | 0 | 7 | 12 | 9 | 9 |
| -1 | 5 | 5 | 36 | 35 | 0 | 7 | 9 | 10 | 11 | 0 | 1 | 11 | 13 | 13 | -4 | 8 | 12 | 18 | 19 |
| 0 | 5 | 5 | 17 | 17 | -3 | 8 | 9 | 8 | 8 | -1 | 2 | 11 | 38 | 39 | -3 | 8 | 12 | 8 | 8 |
| -3 | 6 | 6 | 31 | 32 | -2 | 8 | 9 | 22 | 21 | 0 | 3 | 11 | 14 | 13 | -2 | 8 | 12 | 14 | 15 |
| -2 | 6 | 6 | 14 | 13 | 0 | 8 | 9 | 19 | 19 | -1 | 3 | 11 | 10 | 11 | -1 | 8 | 12 | 18 | 18 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 1

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|----|---|----|----|----|----|---|----|----|----|---|---|----|----|----|----|---|----|----|----|
| 0 | 1 | 16 | 9 | 8 | 0 | 3 | 16 | 17 | 17 | 0 | 5 | 16 | 8 | 5 | -1 | 3 | 17 | 13 | 14 |
| -1 | 2 | 16 | 15 | 17 | -2 | 4 | 16 | 29 | 29 | 0 | 1 | 17 | 12 | 12 | -1 | 4 | 17 | 14 | 11 |
| 0 | 2 | 16 | 10 | 11 | 0 | 4 | 16 | 11 | 10 | 0 | 2 | 17 | 24 | 24 | 0 | 0 | 18 | 40 | 41 |
| -1 | 3 | 16 | 8 | 7 | -1 | 5 | 16 | 12 | 14 | | | | | | 0 | 2 | 18 | 21 | 23 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 2

| OBSERVED | | CALCULATED | | STRUCTURE FACTORS FOR | | CRYSTAL 2 | | O | | | |
|----------|------|------------|----|-----------------------|------|-----------|----|----|------|----|----|
| H | K L | FO | FC | H | K L | FO | FC | H | K L | FO | FC |
| -1 | 2-18 | 21 | 17 | 0 | 1-12 | 10 | 10 | -1 | 5-10 | 22 | 22 |
| 0 | 2-18 | 20 | 21 | -1 | 2-12 | 28 | 26 | -3 | 6-10 | 16 | 20 |
| 0 | 2-17 | 21 | 23 | 0 | 2-12 | 26 | 26 | -2 | 6-10 | 36 | 36 |
| 0 | 1-16 | 13 | 8 | -1 | 3-12 | 11 | 9 | -1 | 6-10 | 52 | 53 |
| -1 | 2-16 | 20 | 20 | 0 | 3-12 | 27 | 25 | 0 | 7-10 | 21 | 21 |
| 0 | 3-16 | 23 | 19 | -2 | 4-12 | 23 | 25 | -1 | 7-10 | 15 | 10 |
| -2 | 4-16 | 32 | 30 | 0 | 4-12 | 25 | 22 | -4 | 8-10 | 51 | 48 |
| -2 | 5-16 | 17 | 6 | -1 | 5-12 | 22 | 22 | -2 | 8-10 | 27 | 28 |
| -1 | 5-16 | 18 | 17 | -3 | 6-12 | 21 | 21 | 0 | 8-10 | 18 | 16 |
| 0 | 1-15 | 19 | 21 | -2 | 6-12 | 16 | 19 | 0 | 8-10 | 27 | 25 |
| 0 | 2-15 | 41 | 39 | 0 | 6-12 | 21 | 21 | -3 | 9-10 | 19 | 17 |
| -1 | 3-15 | 23 | 18 | -3 | 7-12 | 14 | 8 | -2 | 9-10 | 13 | 9 |
| -1 | 4-15 | 21 | 19 | -2 | 7-12 | 17 | 19 | 0 | 9-10 | 16 | 18 |
| 0 | 4-15 | 35 | 35 | -4 | 8-12 | 25 | 20 | 0 | 9-10 | 32 | 32 |
| -2 | 5-15 | 19 | 20 | -2 | 8-12 | 16 | 15 | -1 | 3-9 | 12 | 16 |
| -2 | 6-15 | 29 | 32 | -1 | 8-12 | 15 | 17 | -1 | 4-9 | 13 | 15 |
| 0 | 3-14 | 14 | 15 | 0 | 1-11 | 12 | 16 | 0 | 4-9 | 29 | 28 |
| -2 | 4-14 | 29 | 29 | 0 | 2-11 | 43 | 41 | -2 | 5-9 | 17 | 15 |
| -1 | 5-14 | 17 | 13 | -1 | 3-11 | 13 | 14 | -2 | 6-9 | 25 | 25 |
| -2 | 6-14 | 14 | 11 | -1 | 4-11 | 11 | 14 | 0 | 6-9 | 13 | 13 |
| -1 | 6-14 | 13 | 6 | 0 | 4-11 | 36 | 36 | -1 | 7-9 | 15 | 13 |
| 0 | 6-14 | 20 | 24 | -2 | 5-11 | 14 | 14 | -1 | 7-9 | 14 | 13 |
| -2 | 7-14 | 16 | 12 | 0 | 5-11 | 15 | 12 | 0 | 8-9 | 14 | 14 |
| 0 | 1-13 | 26 | 27 | -2 | 6-11 | 32 | 33 | -3 | 8-9 | 14 | 11 |
| 0 | 2-13 | 42 | 41 | -1 | 6-11 | 16 | 11 | 0 | 8-9 | 24 | 20 |
| -1 | 3-13 | 23 | 23 | -3 | 7-11 | 13 | 11 | 0 | 8-9 | 16 | 19 |
| -1 | 4-13 | 21 | 24 | -2 | 8-11 | 28 | 27 | -2 | 9-9 | 17 | 17 |
| 0 | 4-13 | 38 | 36 | 0 | 8-11 | 23 | 27 | -1 | 10-9 | 29 | 29 |
| -2 | 5-13 | 24 | 25 | -4 | 9-11 | 13 | 10 | -1 | 1-8 | 29 | 50 |
| 0 | 5-13 | 17 | 18 | 0 | 1-10 | 15 | 16 | -1 | 2-8 | 17 | 15 |
| -2 | 6-13 | 33 | 33 | -1 | 2-10 | 30 | 28 | 0 | 3-8 | 25 | 26 |
| -1 | 6-13 | 18 | 19 | 0 | 2-10 | 51 | 49 | -1 | 3-8 | 47 | 45 |
| -3 | 7-13 | 15 | 17 | -1 | 3-10 | 15 | 15 | -2 | 4-8 | 58 | 59 |
| -1 | 7-13 | 21 | 20 | 0 | 3-10 | 24 | 26 | 0 | 4-8 | 23 | 24 |
| 0 | 7-13 | 19 | 21 | -2 | 4-10 | 66 | 65 | -1 | 4-8 | 12 | 13 |
| -3 | 8-13 | 15 | 18 | 0 | 4-10 | 39 | 41 | -2 | 5-8 | 20 | 21 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 2

0

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| | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|----|----|---|-----|-----|----|----|---|----|----|
| -2 | 9 | -5 | 14 | 17 | 0 | 5 | -3 | 51 | 50 | -4 | 8 | -2 | 23 | 20 | -1 | 5 | 0 | 26 | 26 | -1 | 3 | 2 | 40 | 40 |
| -1 | 9 | -5 | 16 | 15 | -2 | 6 | -3 | 30 | 28 | -3 | 8 | -2 | 15 | 16 | -3 | 6 | 0 | 27 | 26 | 0 | 3 | 2 | 71 | 70 |
| -4 | 10 | -5 | 47 | 48 | -1 | 6 | -3 | 41 | 40 | -2 | 8 | -2 | 16 | 14 | -2 | 6 | 0 | 41 | 40 | -2 | 4 | 2 | 38 | 38 |
| -5 | 11 | -5 | 19 | 14 | -3 | 7 | -3 | 40 | 41 | -1 | 8 | -2 | 31 | 32 | 0 | 6 | 0 | 31 | 32 | -1 | 4 | 2 | 31 | 32 |
| 0 | 1 | -4 | 14 | 13 | -1 | 7 | -3 | 30 | 29 | -4 | 9 | -2 | 18 | 15 | -2 | 7 | 0 | 18 | 16 | 0 | 4 | 2 | 29 | 30 |
| -1 | 2 | -4 | 21 | 23 | 0 | 7 | -3 | 25 | 24 | -3 | 9 | -2 | 31 | 29 | -1 | 7 | 0 | 13 | 13 | -2 | 5 | 2 | 28 | 27 |
| 0 | 2 | -4 | 61 | 62 | -3 | 8 | -3 | 30 | 30 | -2 | 9 | -2 | 18 | 16 | 0 | 8 | 0 | 14 | 14 | -1 | 5 | 2 | 52 | 51 |
| -1 | 3 | -4 | 11 | 10 | -2 | 8 | -3 | 22 | 20 | 0 | 10 | -2 | 27 | 25 | -4 | 8 | 0 | 86 | 86 | 0 | 5 | 2 | 25 | 25 |
| 0 | 3 | -4 | 18 | 18 | 0 | 8 | -3 | 20 | 19 | -5 | 10 | -2 | 28 | 28 | -2 | 8 | 0 | 34 | 31 | -3 | 6 | 2 | 49 | 46 |
| -2 | 4 | -4 | 38 | 39 | -4 | 9 | -3 | 22 | 22 | -4 | 10 | -2 | 14 | 10 | -1 | 8 | 0 | 18 | 20 | -2 | 6 | 2 | 21 | 20 |
| -1 | 4 | -4 | 9 | 7 | -2 | 9 | -3 | 32 | 32 | -2 | 10 | -2 | 15 | 15 | 0 | 8 | 0 | 15 | 15 | -1 | 6 | 2 | 22 | 22 |
| 0 | 4 | -4 | 41 | 41 | -1 | 9 | -3 | 24 | 27 | -5 | 11 | -2 | 16 | 13 | -3 | 9 | 0 | 13 | 16 | 0 | 6 | 2 | 21 | 23 |
| -2 | 5 | -4 | 11 | 8 | -4 | 10 | -3 | 21 | 17 | -4 | 11 | -2 | 26 | 23 | -5 | 10 | 0 | 26 | 20 | -3 | 7 | 2 | 21 | 21 |
| -1 | 5 | -4 | 15 | 15 | -3 | 10 | -3 | 27 | 24 | -3 | 11 | -2 | 16 | 11 | -4 | 10 | 0 | 11 | 11 | -2 | 7 | 2 | 38 | 38 |
| 0 | 5 | -4 | 11 | 9 | -1 | 10 | -3 | 19 | 20 | 0 | 11 | -1 | 12 | 12 | -2 | 10 | 0 | 12 | 12 | -1 | 7 | 2 | 16 | 18 |
| -3 | 6 | -4 | 16 | 17 | -5 | 11 | -3 | 27 | 26 | 0 | 12 | -1 | 82 | 82 | 0 | 10 | 0 | 12 | 24 | 0 | 7 | 2 | 16 | 18 |
| -2 | 6 | -4 | 31 | 31 | -3 | 11 | -3 | 16 | 18 | -1 | 12 | -1 | 10 | 8 | -3 | 11 | 0 | 14 | 7 | -4 | 8 | 2 | 21 | 19 |
| -1 | 6 | -4 | 11 | 4 | 0 | 11 | -2 | 51 | 52 | 0 | 13 | -1 | 9 | 10 | 0 | 11 | 1 | 12 | 12 | -3 | 8 | 2 | 17 | 17 |
| 0 | 6 | -4 | 30 | 30 | -1 | 12 | -2 | 89 | 89 | -1 | 14 | -1 | 9 | 8 | 0 | 12 | 1 | 9 | 84 | -2 | 8 | 2 | 13 | 13 |
| -3 | 7 | -4 | 11 | 7 | 0 | 12 | -2 | 62 | 61 | 0 | 14 | -1 | 61 | 59 | -1 | 13 | 1 | 7 | 10 | -1 | 8 | 2 | 33 | 33 |
| -4 | 8 | -4 | 28 | 28 | -1 | 13 | -2 | 40 | 40 | -2 | 15 | -1 | 47 | 46 | 0 | 14 | 1 | 7 | 10 | -4 | 9 | 2 | 16 | 15 |
| -2 | 8 | -4 | 21 | 22 | 0 | 13 | -2 | 39 | 39 | -2 | 16 | -1 | 37 | 35 | -1 | 14 | 1 | 9 | 8 | -3 | 9 | 2 | 28 | 28 |
| -1 | 8 | -4 | 15 | 13 | -2 | 14 | -2 | 32 | 31 | 0 | 16 | -1 | 30 | 29 | 0 | 15 | 1 | 60 | 60 | -3 | 9 | 2 | 16 | 16 |
| 0 | 8 | -4 | 19 | 19 | -1 | 14 | -2 | 32 | 31 | 0 | 17 | -1 | 30 | 27 | -2 | 16 | 1 | 12 | 12 | -2 | 9 | 2 | 15 | 15 |
| -3 | 9 | -4 | 12 | 12 | 0 | 15 | -2 | 30 | 32 | -4 | 18 | -1 | 26 | 27 | -3 | 17 | 1 | 25 | 25 | -1 | 9 | 2 | 25 | 25 |
| -5 | 10 | -4 | 16 | 16 | -2 | 16 | -2 | 27 | 27 | 0 | 19 | -1 | 25 | 25 | -2 | 18 | 1 | 11 | 11 | 0 | 9 | 2 | 27 | 27 |
| -4 | 10 | -4 | 22 | 22 | -1 | 17 | -2 | 51 | 51 | -4 | 20 | -1 | 23 | 25 | -3 | 19 | 1 | 13 | 13 | -5 | 10 | 2 | 15 | 13 |
| -2 | 10 | -4 | 22 | 23 | 0 | 18 | -2 | 27 | 26 | 0 | 21 | -1 | 23 | 25 | -3 | 20 | 1 | 14 | 14 | 0 | 11 | 2 | 26 | 26 |
| 0 | 1 | -3 | 78 | 79 | -3 | 19 | -2 | 48 | 46 | -1 | 22 | 0 | 44 | 44 | -2 | 21 | 1 | 66 | 67 | -4 | 11 | 2 | 30 | 26 |
| 0 | 2 | -3 | 60 | 60 | -2 | 20 | -2 | 21 | 22 | 0 | 23 | 0 | 17 | 17 | -4 | 22 | 1 | 17 | 17 | 0 | 11 | 2 | 28 | 28 |
| -1 | 3 | -3 | 71 | 72 | -1 | 21 | -2 | 20 | 21 | -1 | 24 | 0 | 17 | 17 | 0 | 23 | 1 | 66 | 67 | 0 | 11 | 2 | 61 | 61 |
| 0 | 3 | -3 | 9 | 10 | 0 | 22 | -2 | 23 | 23 | 0 | 25 | 0 | 32 | 32 | 0 | 24 | 1 | 32 | 32 | 0 | 12 | 2 | 72 | 72 |
| -1 | 4 | -3 | 53 | 53 | -3 | 23 | -2 | 22 | 23 | -3 | 26 | 0 | 180 | 182 | 0 | 25 | 1 | 182 | 182 | -1 | 13 | 2 | 8 | 8 |
| 0 | 4 | -3 | 37 | 37 | -2 | 24 | -2 | 39 | 37 | -1 | 27 | 0 | 13 | 13 | 0 | 26 | 1 | 13 | 13 | 0 | 14 | 2 | 53 | 53 |
| -2 | 5 | -3 | 42 | 41 | -1 | 25 | -2 | 16 | 18 | 0 | 28 | 0 | 51 | 49 | -1 | 27 | 1 | 51 | 49 | -1 | 15 | 2 | 37 | 38 |
| -1 | 5 | -3 | 10 | 6 | 0 | 26 | -2 | 18 | 18 | -2 | 29 | 0 | 16 | 15 | 0 | 28 | 1 | 15 | 15 | 0 | 16 | 2 | 37 | 38 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 2

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | | | | | |
|----|----|---|----|----|----|----|---|-----|-----|----|----|---|----|----|----|----|---|----|----|----|----|----|----|----|
| -2 | 5 | 3 | 42 | 41 | -4 | 8 | 4 | 28 | 27 | -2 | 6 | 6 | 25 | 26 | 0 | 4 | 8 | 12 | 14 | -2 | 9 | 9 | 13 | 11 |
| -1 | 5 | 3 | 10 | 6 | -2 | 8 | 4 | 20 | 22 | 0 | 6 | 6 | 49 | 48 | -2 | 5 | 8 | 21 | 21 | -4 | 10 | 9 | 18 | 17 |
| 0 | 5 | 3 | 50 | 49 | -1 | 8 | 4 | 14 | 13 | -4 | 8 | 6 | 39 | 43 | -1 | 5 | 8 | 37 | 37 | 0 | 0 | 10 | 77 | 78 |
| -2 | 6 | 3 | 28 | 29 | 0 | 8 | 4 | 16 | 19 | -2 | 8 | 6 | 22 | 20 | 0 | 5 | 8 | 21 | 19 | 0 | 1 | 10 | 16 | 15 |
| -1 | 6 | 3 | 40 | 40 | -4 | 10 | 4 | 17 | 16 | 0 | 8 | 6 | 20 | 19 | -3 | 6 | 8 | 33 | 34 | -1 | 2 | 10 | 25 | 28 |
| -3 | 7 | 3 | 40 | 40 | -2 | 10 | 4 | 19 | 22 | -4 | 10 | 6 | 18 | 17 | -3 | 6 | 8 | 33 | 33 | -1 | 2 | 10 | 25 | 28 |
| -1 | 7 | 3 | 31 | 29 | 0 | 1 | 5 | 33 | 33 | -2 | 10 | 6 | 31 | 32 | 0 | 6 | 8 | 21 | 19 | 0 | 2 | 10 | 51 | 49 |
| 0 | 7 | 3 | 23 | 25 | 0 | 2 | 5 | 133 | 133 | -1 | 1 | 5 | 47 | 48 | -1 | 6 | 8 | 39 | 41 | 0 | 3 | 10 | 26 | 26 |
| -3 | 8 | 3 | 30 | 29 | -1 | 3 | 5 | 32 | 31 | 0 | 2 | 7 | 36 | 36 | -3 | 6 | 8 | 31 | 32 | -1 | 3 | 10 | 14 | 15 |
| -2 | 8 | 3 | 19 | 21 | -1 | 4 | 5 | 24 | 24 | -1 | 3 | 7 | 35 | 35 | -2 | 7 | 8 | 31 | 32 | -2 | 4 | 10 | 65 | 66 |
| 0 | 8 | 3 | 21 | 19 | 0 | 4 | 5 | 97 | 95 | -1 | 4 | 7 | 36 | 36 | -1 | 7 | 8 | 19 | 17 | -1 | 4 | 10 | 41 | 41 |
| -4 | 9 | 3 | 21 | 22 | -2 | 5 | 5 | 19 | 20 | 0 | 4 | 7 | 29 | 29 | 0 | 7 | 8 | 15 | 15 | 0 | 4 | 10 | 12 | 11 |
| -2 | 9 | 3 | 31 | 32 | 0 | 5 | 5 | 23 | 24 | -2 | 5 | 7 | 37 | 37 | -4 | 7 | 8 | 25 | 25 | -2 | 5 | 10 | 21 | 23 |
| -1 | 9 | 3 | 27 | 27 | -2 | 6 | 5 | 76 | 77 | 0 | 5 | 7 | 25 | 23 | -3 | 8 | 8 | 37 | 37 | -1 | 5 | 10 | 11 | 12 |
| -4 | 10 | 3 | 19 | 17 | -1 | 6 | 5 | 17 | 20 | -2 | 6 | 7 | 23 | 23 | -3 | 8 | 8 | 17 | 17 | 0 | 5 | 10 | 17 | 20 |
| -3 | 10 | 3 | 24 | 24 | -3 | 7 | 5 | 17 | 20 | -1 | 6 | 7 | 26 | 25 | -2 | 8 | 8 | 26 | 25 | -3 | 6 | 10 | 16 | 16 |
| -1 | 10 | 3 | 20 | 20 | -1 | 7 | 5 | 19 | 16 | -3 | 7 | 7 | 18 | 20 | 0 | 8 | 8 | 18 | 20 | -1 | 6 | 10 | 11 | 13 |
| 0 | 10 | 3 | 15 | 14 | 0 | 7 | 5 | 13 | 14 | -2 | 7 | 7 | 11 | 11 | -3 | 8 | 8 | 11 | 6 | 0 | 6 | 10 | 51 | 53 |
| -5 | 11 | 3 | 25 | 25 | -3 | 8 | 5 | 13 | 16 | -1 | 7 | 7 | 26 | 27 | -1 | 8 | 8 | 15 | 13 | -2 | 7 | 10 | 17 | 21 |
| -3 | 11 | 3 | 15 | 18 | -2 | 8 | 5 | 57 | 58 | 0 | 7 | 7 | 29 | 29 | 0 | 9 | 8 | 29 | 29 | 0 | 7 | 10 | 12 | 10 |
| 0 | 11 | 3 | 44 | 43 | 0 | 8 | 5 | 52 | 53 | -3 | 8 | 7 | 22 | 23 | -5 | 9 | 8 | 22 | 23 | -4 | 8 | 10 | 46 | 49 |
| 0 | 11 | 3 | 13 | 13 | -1 | 9 | 5 | 15 | 15 | -2 | 8 | 7 | 19 | 19 | 0 | 10 | 8 | 19 | 14 | -2 | 8 | 10 | 28 | 27 |
| -1 | 12 | 4 | 22 | 23 | -4 | 10 | 5 | 48 | 48 | 0 | 8 | 7 | 17 | 17 | 0 | 1 | 9 | 17 | 15 | -1 | 8 | 10 | 15 | 16 |
| -1 | 12 | 4 | 63 | 62 | -3 | 10 | 5 | 15 | 14 | -4 | 9 | 7 | 25 | 26 | 0 | 2 | 9 | 32 | 32 | 0 | 8 | 10 | 23 | 25 |
| 0 | 12 | 4 | 18 | 17 | -5 | 11 | 5 | 14 | 14 | -2 | 9 | 7 | 18 | 18 | -1 | 3 | 9 | 16 | 16 | 0 | 1 | 11 | 15 | 15 |
| -2 | 14 | 4 | 37 | 37 | -4 | 11 | 5 | 16 | 14 | -4 | 10 | 7 | 19 | 19 | 0 | 4 | 9 | 14 | 14 | -1 | 3 | 11 | 42 | 42 |
| -1 | 14 | 4 | 41 | 41 | 0 | 1 | 6 | 92 | 94 | -3 | 10 | 7 | 18 | 17 | -2 | 5 | 9 | 17 | 17 | -1 | 4 | 11 | 17 | 14 |
| 0 | 14 | 4 | 10 | 8 | 0 | 1 | 6 | 9 | 7 | 0 | 10 | 7 | 78 | 79 | 0 | 5 | 9 | 18 | 17 | 0 | 4 | 11 | 15 | 14 |
| -2 | 15 | 4 | 15 | 15 | 0 | 2 | 6 | 41 | 42 | 0 | 1 | 8 | 30 | 29 | -2 | 6 | 9 | 25 | 24 | -2 | 5 | 11 | 35 | 37 |
| -1 | 15 | 4 | 10 | 9 | 0 | 3 | 6 | 9 | 10 | -1 | 2 | 8 | 30 | 30 | -1 | 6 | 9 | 29 | 29 | -2 | 6 | 11 | 12 | 12 |
| 0 | 15 | 4 | 13 | 13 | -2 | 3 | 6 | 70 | 69 | 0 | 2 | 8 | 15 | 16 | -2 | 6 | 9 | 50 | 50 | -1 | 6 | 11 | 31 | 34 |
| -3 | 16 | 4 | 30 | 31 | -1 | 4 | 6 | 10 | 10 | -1 | 3 | 8 | 26 | 26 | 0 | 7 | 9 | 26 | 26 | 0 | 6 | 11 | 13 | 13 |
| -2 | 16 | 4 | 31 | 29 | 0 | 4 | 6 | 31 | 31 | -1 | 3 | 8 | 46 | 45 | -2 | 7 | 9 | 46 | 45 | -3 | 8 | 11 | 28 | 28 |
| 0 | 16 | 4 | 13 | 9 | -1 | 5 | 6 | 10 | 7 | -2 | 4 | 8 | 59 | 59 | 0 | 8 | 9 | 59 | 59 | 0 | 8 | 11 | 24 | 27 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CRYSTAL 2

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| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | |
|----|---|----|----|----|----|---|----|----|----|----|---|----|----|----|----|---|----|----|----|----|----|----|----|----|----|
| 0 | 0 | 12 | 29 | 26 | 0 | 6 | 12 | 20 | 20 | -1 | 6 | 13 | 22 | 20 | -1 | 5 | 14 | 14 | 14 | 13 | 0 | 0 | 16 | 36 | 34 |
| 0 | 1 | 12 | 13 | 11 | -3 | 7 | 12 | 14 | 8 | -3 | 7 | 13 | 19 | 17 | -3 | 6 | 14 | 14 | 14 | 11 | -1 | 2 | 16 | 17 | 20 |
| -1 | 2 | 12 | 25 | 26 | -2 | 7 | 12 | 19 | 19 | -1 | 7 | 13 | 22 | 20 | 0 | 6 | 14 | 23 | 23 | 0 | 2 | 16 | 17 | 12 | 9 |
| 0 | 2 | 12 | 26 | 26 | -2 | 8 | 12 | 16 | 15 | 0 | 7 | 13 | 19 | 20 | -2 | 7 | 14 | 14 | 14 | -1 | 3 | 16 | 13 | 9 | 20 |
| -1 | 3 | 12 | 14 | 10 | -1 | 8 | 12 | 18 | 17 | -3 | 8 | 13 | 20 | 18 | 0 | 1 | 15 | 23 | 21 | 0 | 3 | 16 | 18 | 20 | 31 |
| 0 | 3 | 12 | 24 | 24 | 0 | 1 | 13 | 27 | 27 | 0 | 0 | 14 | 31 | 31 | 0 | 2 | 15 | 37 | 39 | -2 | 4 | 16 | 32 | 11 | |
| -2 | 4 | 12 | 24 | 24 | 0 | 2 | 13 | 42 | 41 | 0 | 1 | 14 | 11 | 6 | -1 | 3 | 15 | 19 | 18 | 0 | 4 | 16 | 13 | 11 | |
| -1 | 4 | 12 | 13 | 9 | -1 | 3 | 13 | 22 | 23 | -1 | 2 | 14 | 22 | 15 | -1 | 4 | 15 | 17 | 19 | 0 | 1 | 17 | 13 | 10 | |
| 0 | 4 | 12 | 22 | 22 | -1 | 4 | 13 | 22 | 24 | 0 | 2 | 14 | 12 | 13 | 0 | 4 | 15 | 35 | 35 | 0 | 2 | 17 | 19 | 23 | |
| -1 | 5 | 12 | 23 | 22 | 0 | 4 | 13 | 37 | 36 | 0 | 3 | 14 | 15 | 15 | -2 | 5 | 15 | 18 | 20 | -1 | 3 | 17 | 12 | 23 | |
| -3 | 6 | 12 | 23 | 21 | -2 | 5 | 13 | 31 | 34 | -2 | 4 | 14 | 24 | 28 | 0 | 5 | 15 | 15 | 15 | 0 | 0 | 18 | 39 | 40 | |
| -2 | 6 | 12 | 19 | 19 | 0 | 5 | 13 | 17 | 19 | 0 | 4 | 14 | 16 | 12 | -2 | 6 | 15 | 30 | 32 | 0 | 0 | 18 | 18 | 20 | |
| -1 | 6 | 12 | 12 | 7 | -2 | 6 | 13 | 32 | 33 | -2 | 5 | 14 | 12 | 6 | -1 | 6 | 15 | 15 | 15 | 0 | 2 | 18 | 18 | 20 | |