

AM-96-611

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Crystal structure of a $P2_1/m$ ferromagnesian cummingtonite at 140 K

Hexiong Yang and Joseph R. Smyth

For deposit: Table 3

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(Table 3 is for deposit)

Table 3. Atomic anisotropic ($\times 10^4$) displacement factors for NMNH 118125 cummingtonite at 295 and 140 K

| | | 295 K | 140 K | |
|-----|--------------|--------|--------|--------|
| | | | A set | B set |
| M1 | β_{11} | 21(2) | | 13(1) |
| | β_{22} | 4(1) | | 2(1) |
| | β_{33} | 36(5) | | 22(4) |
| | β_{12} | 0 | | -1(1) |
| | β_{13} | 8(2) | | 5(2) |
| | β_{23} | 0 | | 1(1) |
| M2 | β_{11} | 17(2) | | 14(1) |
| | β_{22} | 4(1) | | 3(1) |
| | β_{33} | 48(6) | | 22(4) |
| | β_{12} | 0 | | -1(1) |
| | β_{13} | 4(4) | | 2(2) |
| | β_{23} | 0 | | 0(1) |
| M3 | β_{11} | 20(3) | | 13(2) |
| | β_{22} | 4(1) | | 3(1) |
| | β_{33} | 46(8) | | 24(6) |
| | β_{13} | 1(3) | | 2(2) |
| M4 | β_{11} | 24(1) | | 14(1) |
| | β_{22} | 7(1) | | 4(1) |
| | β_{33} | 56(3) | | 15(2) |
| | β_{12} | 0 | | 0(1) |
| | β_{13} | 14(1) | | 6(1) |
| | β_{23} | 0 | | 0(1) |
| Si1 | β_{11} | 14(1) | 8(2) | 14(2) |
| | β_{22} | 3(1) | 2(1) | 2(1) |
| | β_{33} | 36(3) | 20(4) | 17(4) |
| | β_{12} | -1(1) | 0(1) | -1(1) |
| | β_{13} | 2(2) | -1(2) | 4(2) |
| | β_{23} | -1(1) | 0(1) | 0(1) |

Table 3. (continued 1)

| | | | | |
|-----|--------------|--------|--------|--------|
| Si2 | β_{11} | 12(1) | 13(2) | 8(1) |
| | β_{22} | 3(1) | 2(1) | 3(1) |
| | β_{33} | 34(3) | 21(4) | 15(2) |
| | β_{12} | -1(1) | -1(1) | -1(1) |
| | β_{13} | 1(2) | 1(2) | -3(1) |
| | β_{23} | 0(1) | 0(1) | 1(1) |
| O1 | β_{11} | 13(3) | 8(5) | 19(5) |
| | β_{22} | 5(1) | 4(1) | 1(1) |
| | β_{33} | 45(9) | 19(11) | 44(11) |
| | β_{12} | 0(1) | 0(2) | 1(2) |
| | β_{13} | 4(4) | 2(5) | 5(6) |
| | β_{23} | -1(2) | -2(3) | 4(3) |
| O2 | β_{11} | 16(3) | 14(5) | 9(5) |
| | β_{22} | 5(1) | 3(1) | 3(1) |
| | β_{33} | 57(9) | 47(11) | 43(10) |
| | β_{12} | 0(1) | -2(2) | 1(2) |
| | β_{13} | 3(4) | 10(5) | 2(5) |
| | β_{23} | 4(2) | 0(3) | 4(3) |
| O3 | β_{11} | 22(5) | 24(8) | 15(6) |
| | β_{22} | 4(1) | 4(2) | 2(2) |
| | β_{33} | 73(14) | 35(17) | 36(16) |
| | β_{13} | 9(7) | 10(8) | 1(8) |
| O4 | β_{11} | 30(3) | 10(5) | 25(5) |
| | β_{22} | 6(1) | 2(1) | 6(1) |
| | β_{33} | 76(10) | 47(10) | 37(10) |
| | β_{12} | -4(1) | -2(2) | -3(2) |
| | β_{13} | 5(5) | -5(5) | 9(6) |
| | β_{23} | 2(2) | 3(3) | -4(3) |

Table 3. (continued 2)

| | | | | |
|----|--------------|---------|--------|--------|
| O5 | β_{11} | 19(3) | 13(4) | 16(4) |
| | β_{22} | 9(1) | 5(1) | 3(1) |
| | β_{33} | 65(10) | 36(10) | 25(10) |
| | β_{12} | -1(1) | -1(2) | 1(2) |
| | β_{13} | 5(4) | 3(5) | 1(5) |
| | β_{23} | 14(2) | 10(3) | 2(3) |
| O6 | β_{11} | 22(3) | 15(4) | 11(4) |
| | β_{22} | 13(1) | 6(1) | 6(1) |
| | β_{33} | 77(10) | 39(11) | 29(10) |
| | β_{12} | 3(2) | 2(2) | 2(2) |
| | β_{13} | -1(5) | -5(5) | -2(5) |
| | β_{23} | -12(3) | -4(3) | -3(3) |
| O7 | β_{11} | 27(5) | 21(7) | 12(7) |
| | β_{22} | 2(1) | 5(2) | 2(2) |
| | β_{33} | 125(16) | 32(16) | 58(16) |
| | β_{13} | 10(7) | -2(8) | 16(8) |
