CHALCOPHANITE, ZnMn3O7-3H2O: New Crystal-structure determinations

Post and Appleman

To be deposited: Tables 2, 3

American Mineralogist, 73, 11-12, 1401-1404
Table 2. Observed and calculated structure factors for chalcophanite from Bisbee, AZ.

Note: Reflections tagged as unobserved are indicated by "<" and those rejected during merging of equivalent reflections by "M". This table does not include corrections for anomalous dispersion. Items are listed in the order k, F^o, F^c, sigma(F^o).

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Table 3-1. Observed and calculated structure factors for calcophanite from Sterling Hill, N.J.

Note: Reflections tagged as unobserved are indicated by "<" and those rejected during merging of equivalent reflections by "M". This table does not include corrections for anomalous dispersion. Items are listed in the order $k$, $F_{\text{obs}}$, $F_{\text{calc}}$, sigma($F_{\text{obs}}$).

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| 10,K,9 |   | -4 | 50 | 46 | 5 |   | 0,K,12 |   | 2 | 56 | 55 | 2 | -2 | 155 | 155 | 10 |   |   |   |
| -7 | 26 | 25 | 4 |   |   |   |   |   | 5 | 38 | 35 | 3 | -5 | 72 | 68 | 5 |   |   |   |
| -5 | 0 | 0 | 1M | 0,K,11 |   | 3 | 31 | 29 | 2 | -1 | 55 | 56 | 2 |
| 0,K,10 |   | 6 | 20 | 21 | 3 | -4 | 54 | 53 | 5 |   |   |   | 1,K,14 |
| 2 | 70 | 72 | 3 | 4 | 36 | 34 | 3 | -3 | 25 | 22 | 1 | -1 | 77 | 80 | 9 |
| 5 | 77 | 73 | 10 | 7 | 217 | 206 | 27 |   |   |   |   | 1,K,13 |   |   |   |   | 2 | 124 | 124 | 11 |
| 8 | 53 | 50 | 7 | -2 | 58 | 57 | 4 |   |   |   |   | 1,K,12 |   |   |   |   | -4 | 90 | 91 | 8 |
| -1 | 69 | 72 | 2 | -5 | 46 | 45 | 4 |   |   |   |   |   |   |   |   |   | -7 | 84 | 82 | 6 |
| -4 | 41 | 41 | 4 | -8 | 36 | 34 | 3 |   |   |   |   | 2 | 20 | 22 | 3 | 3 | 61 | 61 | 6 |
| -7 | 247 | 254 | 10 |   |   |   |   |   |   |   | 4 | 173 | 169 | 25 | -3 | 124 | 120 | 11 | 2,K,14 |
| 1,K,10 |   | -5 | -3 | 32 | 31 | 3 |   | -8 | 20 | 21 | 6 | 2,K,13 |   | 6 | 57 | 56 | 10 |
| 3 | 14 | 12 | 3< | 5 | 63 | 61 | 9 |   |   |   |   |   |   |   |   |   | -6 | 208 | 204 | 18 |
| 6 | 28 | 27 | 3 | -4 | 57 | 58 | 5 |   | 2,K,12 |   | 4 | 34 | 31 | 5 |
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| -9 | 0 | 0 | 3M | 2,K,11 |   | 5 | 21 | 16 | 5 | -8 | 42 | 42 | 4 | 4 | 117 | 113 | 16 |
| 2,K,10 |   | 3 | 51 | 48 | 6 | -7 | 0 | 0 | 1M | 3,K,13 |   |   |   |   |
| 4 | 61 | 59 | 10 | -6 | 266 | 263 | 22 | 3,K,12 |   | 5 | 91 | 89 | 14 |
| 7 | 0 | 11 | 0< | -9 | 35 | 35 | 3 |   | -1 | 66 | 67 | 4 |
| 3,K,14 |   | 4,K,15 |   |   | 6,K,16 |   | 8,K,17 |   |   | -7 | 94 | 94 | 7 | 1,K,19 |
| -2 | 300 | 298 | 7 | 4 | 70 | 68 | 6 | -1 | 64 | 60 | 5 | -3 | 129 | 121 | 10 |   |   |   |
| -8 | 79 | 80 | 7 | -2 | 120 | 118 | 5 | -4 | 65 | 63 | 6 | -6 | 35 | 29 | 3 | 3 | 34 | 34 | 1 |
| 4,K,14 |   | 5,K,15 |   |   |   |   | 0,K,18 |   |   | -3 | 126 | 130 | 7 |
| 5 | 40 | 35 | 4 | -1 | 63 | 59 | 6 | -3 | 82 | 78 | 8 | 0 | 325 | 332 | 4 |
| -1 | 116 | 116 | 8 | -4 | 110 | 110 | 10 | -6 | 67 | 63 | 9 | 3 | 25 | 22 | 3 | 2,K,19 |
| 5,K,14 |   | 6,K,15 |   |   | 8,K,16 |   | -3 | 0 | 4 | 0< | 4 | 25 | 24 | 3 |
| -3 | 135 | 131 | 10 | -3 | 89 | 85 | 6 | -2 | 48 | 46 | 5 |   | -5 | 72 | 69 | 4 |   |   | 1,K,18 |
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| -2 | 58 | 55 | 5 | -2 | 93 | 89 | 10 |   |   |   |   |   |   |   |   |   | 4 | 242 | 238 | 22 |
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| 7,K,14 |   | 8,K,15 |   |   |   | 126 | 121 | 14 | 2,K,18 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| -1 | 95 | 95 | 7 | -1 | 49 | 49 | 2 | -5 | 48 | 46 | 4 | 2 | 21 | 19 | 3 | -3 | 34 | 31 | 2 |
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| -3 | 169 | 158 | 18 |   |   |   |   |   |   | 5 | 32 | 28 | 4 |   |   | 3,K,18 |   |   |   |   |   |   |   |   |
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| 9,K,14 |   | -1 | 117 | 117 | 3 | -4 | 90 | 88 | 6 | 2,K,17 |   |   |   |   |   | 4,K,18 |   | -4 | 112 | 110 | 7 |
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Table 3-6