**Supplementary tables**

Table S1. Calculated X-ray powder diffraction pattern for deynekoite (Cu*K*α1)\*.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *h* | *k* | *l* | *d*calc [Å] | *I*calc [%] |  | *h* | *k* | *l* | *d*calc [Å] | *I*calc [%] |
| 0 | 1 | 2 | 8.074 | 14 |  | 5 | 0 | 2 | 1.785 | 5 |
| **1** | **0** | **4** | **6.451** | **51** |  | 4 | 1 | 9 | 1.768 | 3 |
| 0 | 0 | 6 | 6.193 | 6 |  | 0 | 5 | 4 | 1.760 | 10 |
| 1 | 1 | 0 | 5.176 | 17 |  | 3 | 3 | 0 | 1.725 | 2 |
| 2 | 0 | 2 | 4.357 | 8 |  | **2** | **0** | **20** | **1.716** | **28** |
| 0 | 1 | 8 | 4.124 | 4 |  | 3 | 0 | 18 | 1.699 | 5 |
| 0 | 2 | 4 | 4.037 | 18 |  | 1 | 3 | 16 | 1.697 | 3 |
| 1 | 1 | 6 | 3.972 | 2 |  | 5 | 0 | 8 | 1.673 | 6 |
| **1** | **0** | **10** | **3.433** | **25** |  | 2 | 4 | 4 | 1.667 | 3 |
| 2 | 1 | 1 | 3.374 | 3 |  | 4 | 1 | 12 | 1.654 | 2 |
| 1 | 2 | 2 | 3.333 | 7 |  | 1 | 2 | 20 | 1.629 | 2 |
| 1 | 1 | 9 | 3.228 | 3 |  | 2 | 3 | 14 | 1.626 | 4 |
| **2** | **1** | **4** | **3.183** | **64** |  | 4 | 0 | 16 | 1.613 | 2 |
| 3 | 0 | 0 | 2.988 | 7 |  | 3 | 3 | 9 | 1.592 | 2 |
| **0** | **2** | **10** | **2.861** | **100** |  | 5 | 1 | 4 | 1.586 | 3 |
| **1** | **2** | **8** | **2.737** | **24** |  | 2 | 4 | 10 | 1.542 | 9 |
| 0 | 3 | 6 | 2.691 | 4 |  | 3 | 2 | 16 | 1.540 | 7 |
| 1 | 1 | 12 | 2.657 | 6 |  | 1 | 5 | 8 | 1.521 | 4 |
| **2** | **2** | **0** | **2.588** | **81** |  | 2 | 1 | 22 | 1.512 | 4 |
| 0 | 1 | 14 | 2.545 | 3 |  | 3 | 3 | 12 | 1.507 | 2 |
| 2 | 2 | 3 | 2.533 | 5 |  | 6 | 0 | 0 | 1.494 | 5 |
| 2 | 1 | 10 | 2.504 | 12 |  | 4 | 3 | 4 | 1.456 | 5 |
| 1 | 3 | 1 | 2.481 | 3 |  | 0 | 4 | 20 | 1.430 | 3 |
| 1 | 2 | 11 | 2.392 | 2 |  | 1 | 4 | 18 | 1.420 | 2 |
| 2 | 2 | 6 | 2.388 | 6 |  | 3 | 4 | 8 | 1.405 | 6 |
| 3 | 1 | 5 | 2.358 | 4 |  | 5 | 2 | 6 | 1.398 | 3 |
| 1 | 0 | 16 | 2.248 | 7 |  | 2 | 5 | 6 | 1.398 | 2 |
| 1 | 1 | 15 | 2.235 | 2 |  | 2 | 3 | 20 | 1.379 | 3 |
| 4 | 0 | 4 | 2.179 | 8 |  | 1 | 2 | 26 | 1.317 | 2 |
| 3 | 0 | 12 | 2.150 | 10 |  | 4 | 4 | 0 | 1.294 | 5 |
| 0 | 3 | 12 | 2.150 | 2 |  | 3 | 5 | 1 | 1.280 | 2 |
| 1 | 2 | 14 | 2.090 | 3 |  | 5 | 3 | 2 | 1.278 | 2 |
| 1 | 3 | 10 | 2.066 | 2 |  | 4 | 2 | 20 | 1.252 | 6 |
| 0 | 0 | 18 | 2.064 | 3 |  | 2 | 6 | 2 | 1.240 | 2 |
| 3 | 2 | 1 | 2.054 | 2 |  | 0 | 0 | 30 | 1.239 | 2 |
| 2 | 3 | 2 | 2.044 | 4 |  | 5 | 3 | 8 | 1.235 | 2 |
| 0 | 4 | 8 | 2.019 | 11 |  | 6 | 2 | 4 | 1.232 | 2 |
| 3 | 2 | 4 | 2.008 | 4 |  | 7 | 1 | 0 | 1.187 | 2 |
| 2 | 2 | 12 | 1.986 | 7 |  | 2 | 5 | 18 | 1.179 | 2 |
| **4** | **0** | **10** | **1.919** | **24** |  | 7 | 0 | 16 | 1.121 | 3 |
| 2 | 3 | 8 | 1.881 | 11 |  | 5 | 0 | 26 | 1.118 | 3 |
| 4 | 1 | 6 | 1.865 | 7 |  | 2 | 2 | 30 | 1.117 | 6 |
| 1 | 4 | 6 |  | 3 | 2 | 28 | 1.115 | 2 |
| 0 | 1 | 20 | 1.819 | 4 |  | 7 | 1 | 12 | 1.109 | 2 |
| 3 | 2 | 10 | 1.799 | 6 |  |  |  |  |  |  |

\*Calculated using PowderCell 2.4 (Krause and Noltze, 1996) on the basis of atomic coordinates and unit-cell parameters obtained from the structure refinement. Reflections with the relative intensity less than 2 have been omitted.

**Table S2.** Structural parameters and optical data for the merrillite group minerals.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Structural data | | | | Optical data | | |
|  | *a* Å | *c* Å | *V* Å3 | *M-Omean* Å |  | *ω* | *ε* |
| Merrillite | 10.3444(3) | 37.0182(11) | 3430.5(2) | 2.080 | (-) | 1.635(1) | 1.634(1) |
| Ferromerrillite | 10.372(2) | 37.217(13) | 3467.34(3) | 2.117 | (-) | 1.623(1) | 1.621(1) |
| Keplerite | 10.3330(4) | 37.0668(24) | 3427.4(3) | 2.080 | (-) | 1.622(1) | 1.619(1) |
| Matyhite | 10.456(7) | 37.408(34) | 3541.6(5) |  |  |  |  |
| Deynekoite | 10.3516(3) | 37.1599(17) | 3448.4(3) | 2.041 | (-) | 1.658(3) | 1.652(3) |
| Whitlockite | 10.33(1) | 37.103(1) | 3428.79(1) | 2.082 | (-) | 1.629(2) | 1.626(2) |
| Changesite-(Y) | 10.3957(4) | 37.207(2) |  |  |  |  |  |

Krause, W. and Nolze, G. (1996) Powder Cell - a program for the representation and manipulation of crystal structures and calculation of the resulting X-ray powder patterns. *J. Appl. Crystallogr.*, **29**, 301–303.