Table S1. Powder X-ray data for shinkolobweite (*d* values in Å). Only calculated lines with *I* ≥ 1.5 are listed.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |  | *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |
| 27 | 7.27 | 7.2404 | 100 |  2 0 0 |  | 5 | 1.8312 | 1.8427 | 2 |  5 0 5 |
|  |  | 6.3518 | 2 |  1 1 0 |  | 1.8101 | 5 |  8 0 0 |
| 9 | 6.06 | 6.0826 | 6 |  0 1 1 |  | 16 | 1.7710 | 1.7690 | 15 |  4 3 3 |
|  |  | 5.9712 | 3 |  0 0 2 |  | 1.7670 | 4 |  0 4 0 |
|  |  | 4.6067 | 3 |  2 0 2 |  | 10 | 1.7330 | 1.7442 | 5 |  4 0 6 |
| 7 | 4.494 | 4.4752 | 5 |  3 0 1 |  | 1.7342 | 4 |  0 2 6 |
| 15 | 3.614 | 3.6202 | 38 |  4 0 0 |  | 1.7166 | 8 |  2 4 0 |
| 49 | 3.486 | 3.5341 | 28 |  0 2 0 |  | 10 | 1.6910 | 1.6865 | 8 |  2 2 6 |
| 3.4685 | 41 |  0 1 3 |  | 8 | 1.6558 | 1.6584 | 3 |  0 1 7 |
|  |  | 3.3153 | 3 |  3 1 2 |  | 9 | 1.6213 | 1.6340 | 3 |  2 3 5 |
| 100 | 3.149 | 3.1759 | 42 |  2 2 0 |  | 1.6166 | 4 |  2 1 7 |
| 3.1281 | 75 |  2 1 3 |  | 1.6111 | 4 |  8 2 0 |
|  |  | 2.8040 | 2 |  2 2 2 |  | 4 | 1.5947 | 1.6047 | 7 |  8 1 3 |
| 7 | 2.777 | 2.7601 | 6 |  2 0 4 |  | 1.5880 | 4 |  4 4 0 |
| 15 | 2.519 | 2.5289 | 10 |  4 2 0 |  | 6 | 1.5632 | 1.5640 | 5 |  4 2 6 |
| 2.5045 | 18 |  4 1 3 |  | 1.5524 | 6 |  6 3 3 |
|  |  | 2.4450 | 2 |  5 1 2 |  | 3 | 1.5354 | 1.5356 | 2 |  6 0 6 |
|  |  | 2.4135 | 5 |  6 0 0 |  | 5 | 1.5135 | 1.5173 | 3 |  9 1 2 |
| 8 | 2.282 | 2.2807 | 5 |  0 2 4 |  | 1.5077 | 3 |  4 1 7 |
| 2.2628 | 3 |  0 1 5 |  |  |  | 1.5044 | 2 |  7 3 2 |
| 5 | 2.174 | 2.2017 | 3 |  5 2 1 |  | 3 | 1.4302 | 1.4300 | 2 |  7 2 5 |
| 2.1753 | 3 |  2 2 4 |  | 1.4257 | 3 |  6 4 0 |
| 2.1597 | 2 |  2 1 5 |  | 3 | 1.4113 | 1.4084 | 3 |  6 2 6 |
| 15 | 2.032 | 2.0383 | 3 |  7 0 1 |  | 3 | 1.3759 | 1.3668 | 2 |  6 1 7 |
| 2.0275 | 18 |  0 3 3 |  | 6 | 1.3513 | 1.3573 | 2 |  2 3 7 |
| 23 | 1.9931 | 1.9931 | 9 |  6 2 0 |  |  | 1.3503 | 5 |  8 3 3 |
| 1.9904 | 5 |  0 0 6 |  |  |  | 1.3400 | 2 | 10 2 0 |
| 1.9811 | 18 |  6 1 3 |  |  |  | 1.3363 | 3 | 10 1 3 |
| 14 | 1.9521 | 1.9524 | 16 |  2 3 3 |  |  |  | 1.3321 | 2 |  0 5 3 |
| 10 | 1.9200 | 1.9297 | 3 |  4 2 4 |  |  |  | 1.3214 | 2 |  0 4 6 |
| 1.9192 | 10 |  2 0 6 |  | 5 | 1.3100 | 1.3101 | 4 |  2 5 3 |
| 4 | 1.8776 | 1.8840 | 3 |  7 1 2 |  |  |  |  |  |  |