TABLE S1. X-RAY POWDER-DIFFRACTION DATA OF CHIYOKOITE. THE STRONGEST REFLECTIONS ARE GIVEN IN BOLD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *I*obs | *d*obs | *I*calc1 | *d*calc2 | *h k l* |
| **100** | **9.53** | 100 | 9.54 | 100 |
| **24** | **5.50** | 31 | 5.51 | 110 |
| 7 | 4.880 | 10 | 4.879 | 111 |
| 2 | 4.766 | 3 | 4.768 | 200 |
| **11** | **4.618** | 20 | 4.608 | 102 |
| 1 | 4.342 | 1 | 4.343 | 201 |
| **23** | **3.812** | 39 | 3.804 | 112 |
| 8 | 3.540 | 7 | 3.534 | 202 |
| **15** | **3.412** | 21 | 3.410 | 211 |
| 6 | 3.180 | 8 | 3.179 | 300 |
| 2 | 3.041 | 2 | 3.043 | 301 |
| 4 | 2.970 | 3 | 2.959 | 113 |
| 3 | 2.755 | 2 | 2.753 | 220 |
| **14** | **2.726** | 24 | 2.721 | 302 |
| 4 | 2.646 | 2 | 2.645 | 310 |
| 7 | 2.568 | 10 | 2.565 | 131 |
| **19** | **2.521** | 29 | 2.514 | 123 |
| 1 | 2.445 | 2 | 2.439 | 222 |
| 3 | 2.368 | 1; 2 | 2.374; 2.363 | 114; 132 |
| 2 | 2.312 | 4 | 2.304 | 204 |
| **13** | **2.172** | 3; 1; 24 | 2.188; 2.172; 2.166 | 320; 402; 223 |
| 4 | 2.146 | 6 | 2.142 | 231 |
| 8 | 2.118 | 15 | 2.112 | 313 |
| 2 | 2.085 | 2 | 2.081 | 410 |
| 2 | 2.042 | 3 | 2.042 | 411 |
| 4 | 2.024 | 4 | 2.020 | 322 |
| 1 | 1.970 | 2 | 1.966 | 115 |
| 2 | 1.939 | 4 | 1.935 | 412 |
| 4 | 1.911 | 5 | 1.907 | 500 |
| 1 | 1.872 | 1 | 1.877; 1.865 | 501; 134 |
| 3 | 1.825 | 6 | 1.818 | 215 |
| 3 | 1.812 | 5 | 1.808 | 331 |
| 2 | 1.796 | 4; 1 | 1.793; 1.790 | 502; 143 |
| 2 | 1.774 | 3 | 1.776 | 421 |
| 2 | 1.763 | 4; 2 | 1.767; 1.754 | 404; 006 |
| 2 | 1.736 | 5 | 1.733 | 332 |
| 1 | 1.694 | 1 | 1.691 | 151 |
| 2 | 1.654 | 4 | 1.647 | 315 |
| 3 | 1.638 | 9 | 1.632 | 144 |
| 2 | 1.592 | 4 | 1.589 | 600 |
| 1 | 1.568 | 1 | 1.568 | 430 |
| 2 | 1.550 | 2; 4 | 1.551; 1.544 | 341; 504 |

1 for the calculated pattern, only reflections with intensities ≥1 are given;

2 for the unit-cell parameters calculated from single-crystal data.