SUPPLEMENTARY Table s1. Calculated powder X-ray diffraction data (*d* in Å) for pseudodickthomssenite

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |  | *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |  | *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |
| **100** | **8.971** | 8.9868 | 37 | 0 0 1 |  |  |  | 2.6997 | 1 | -1 3 1 |  | **12** | **1.8405** | 1.8458 | 1 | 2-4 3 |
| 8.9242 | 63 | 0 1 0 |  |  |  | 2.6899 | 1 | 1-1 3 |  | 1.8387 | 6 | -4 1 1 |
| **10** | **7.494** | 7.5041 | 8 | 0-1 1 |  | 7 | 2.649 | 2.6416 | 8 | 2 1 1 |  | 7 | 1.8064 | 1.8083 | 2 | -4 0 1 |
| 2 | 6.319 | 6.3263 | 1 | -1 0 1 |  | 8 | 2.614 | 2.6213 | 3 | 0 1 3 |  | 1.8054 | 1 | -4 1 0 |
| 6.2790 | 2 | -1 1 0 |  | 2.6121 | 1 | -2 0 3 |  | 1.7974 | 2 | 0 0 5 |
| 5 | 4.958 | 4.9825 | 3 | 1 0 1 |  | 7 | 2.567 | 2.5897 | 5 | -2 2 2 |  | 1.7936 | 1 | -4 2 1 |
| **15** | **4.578** | 4.5775 | 1 | 0-1 2 |  | 2.5610 | 2 | -2-1 3 |  | 6 | 1.7871 | 1.7848 | 1 | 0 5 0 |
| 4.5527 | 15 | 0-2 1 |  | 2.5578 | 3 | 2-2 2 |  | 1.7821 | 3 | 0-3 5 |
| **21** | **4.473** | 4.4621 | 18 | 0 2 0 |  |  |  | 2.5352 | 1 | 1 3 0 |  | 3 | 1.7115 | 1.7141 | 1 | -4-1 2 |
| 6 | 4.103 | 4.0782 | 3 | -1-1 2 |  |  |  | 2.4317 | 1 | -3 1 1 |  | 1.7126 | 1 | -4-1 1 |
|  |  | 4.0403 | 1 | 1-2 1 |  | 3 | 2.292 | 2.2888 | 2 | 0-2 4 |  | 1.7113 | 1 | 2 4 0 |
| 6 | 3.738 | 3.7520 | 4 | 0-2 2 |  | 2.2763 | 1 | 0-4 2 |  |  |  | 1.6959 | 1 | -4 3 0 |
|  |  | 3.6771 | 1 | -1 1 2 |  | 3 | 2.231 | 2.2311 | 2 | 0 4 0 |  | 2 | 1.6847 | 1.6878 | 1 | -4 3 1 |
|  |  | 3.6592 | 1 | -1 2 1 |  |  |  | 2.2193 | 1 | 2 2 1 |  | 1.6820 | 1 | -2 5 1 |
| 8 | 3.615 | 3.6168 | 4 | 0 1 2 |  | 4 | 2.204 | 2.2100 | 1 | 0 2 3 |  | 4 | 1.6531 | 1.6634 | 1 | 2 2 3 |
|  |  | 3.5784 | 1 | -2 0 1 |  | 2.2053 | 2 | 0 3 2 |  | 1.6616 | 1 | 0 5 1 |
| **15** | **3.502** | 3.5135 | 9 | 2 0 0 |  | 2.2009 | 1 | -3-1 2 |  | 1.6510 | 2 | 0-4 5 |
| 3.4723 | 6 | -2 1 1 |  |  |  | 2.1885 | 1 | 3-2 1 |  | 1.6459 | 1 | 4-3 1 |
| 9 | 3.173 | 3.1755 | 5 | 2-1 1 |  | 5 | 2.154 | 2.1594 | 1 | 2-1 3 |  |  |  | 1.6386 | 1 | -2 3 4 |
| 3.1632 | 4 | -2 0 2 |  | 2.1532 | 1 | 2-2 3 |  | 4 | 1.5828 | 1.5877 | 1 | 4-2 2 |
| 8 | 3.122 | 3.1242 | 6 | 0-1 3 |  | 2.1484 | 1 | -2-1 4 |  | 1.5854 | 1 | 2 4 1 |
| 3.1031 | 2 | 0-3 1 |  |  |  | 2.1421 | 1 | -2 0 4 |  | 1.5841 | 1 | 0 4 3 |
|  |  | 3.0541 | 1 | -1-1 3 |  | 2 | 2.118 | 2.1243 | 1 | -1 1 4 |  | 1.5816 | 1 | -4 0 4 |
| 9 | 3.028 | 3.0366 | 2 | 2 1 0 |  | 2.1090 | 1 | -1 4 1 |  | 1.5787 | 1 | -4-2 1 |
| 3.0333 | 1 | 2 0 1 |  | 2 | 2.045 | 2.0484 | 1 | 2 0 3 |  | 1.5749 | 1 | 4-1 2 |
| 3.0232 | 1 | 1-3 1 |  | 2.0469 | 1 | 2 3 0 |  | 3 | 1.5607 | 1.5610 | 1 | -4-2 3 |
| 3.0025 | 1 | -1 3 0 |  | 2.0429 | 1 | -2-3 3 |  | 1.5593 | 1 | -4 1 4 |
| 2.9956 | 8 | 0 0 3 |  |  |  | 1.9871 | 1 | -1-4 3 |  | 3 | 1.5453 | 1.5516 | 2 | 0-6 2 |
| **31** | **2.979** | 2.9884 | 1 | -2 1 2 |  | **10** | **1.8633** | 1.8692 | 1 | 0-1 5 |  | 1.5498 | 1 | -4 4 1 |
| 2.9747 | 21 | 0 3 0 |  | 1.8635 | 2 | 0-2 5 |  | 5 | 1.5236 | 1.5291 | 1 | 2-3 5 |
| 2.9518 | 4 | 2-2 1 |  | 1.8600 | 4 | 0 3 3 |  | 1.5271 | 2 | 2-1 5 |
| **12** | **2.906** | 2.9045 | 1 | -1 2 2 |  | 1.8587 | 1 | -2-3 4 |  | 1.5162 | 2 | -2 0 6 |
| 2.8933 | 9 | 0-3 2 |  | 1.8517 | 2 | 0-5 2 |  | 1 | 1.5021 | 1.5008 | 1 | 0-5 5 |
| 2.8897 | 1 | 1 2 1 |  |  |  |  |  |  |  | 1.4942 | 1 | -4 2 4 |