Supplementary Table S1. Powder X-ray data (*d* in Å) for thebaite-(NH4).

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |  | *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |
| 19 | 10.70 | 10.8733 | 27 | 1 0 0 |  | 13 | 2.486 | 2.5164 | 5 | 2 2 2 |
| 88 | 9.21 | 9.0892 | 100 | 0 0 2 |  | 2.4917 | 7 | 4 1 0 |
| 24 | 7.88 | 7.8969 | 30 | -1 0 2 |  | 6 | 2.423 | 2.4335 | 3 | 1 2 4 |
| 7 | 6.20 | 6.3132 | 4 | 1 0 2 |  | 2.3972 | 2 | 0 1 7 |
| 44 | 5.39 | 5.4366 | 8 | 2 0 0 |  |  |  | 2.3856 | 2 | -1 2 5 |
| 5.4082 | 22 | 1 1 0 |  |  |  | 2.3731 | 2 | 2 2 3 |
| 5.3489 | 6 | -1 1 1 |  | 13 | 2.294 | 2.2864 | 8 | -2 0 8 |
|  |  | 5.2070 | 2 | -2 0 2 |  | 18 | 2.212 | 2.2179 | 4 | 2 2 4 |
| 26 | 4.93 | 5.0328 | 3 | 1 1 1 |  | 2.1747 | 5 | 5 0 0 |
| 4.8931 | 11 | -1 1 2 |  |  |  | 2.1533 | 2 | -4 1 6 |
| 32 | 4.56 | 4.5728 | 4 | -1 0 4 |  |  |  | 2.1322 | 3 | 4 0 4 |
| 4.5446 | 14 | 0 0 4 |  |  |  | 2.1308 | 2 | 1 0 8 |
| 4.4358 | 6 | 1 1 2 |  |  |  | 2.1005 | 2 | -5 1 2 |
|  |  | 4.3451 | 4 | 0 1 3 |  | 19 | 2.0521 | 2.0750 | 2 | -4 2 2 |
|  |  | 4.2783 | 2 | -1 1 3 |  | 2.0487 | 6 | 4 2 0 |
| 9 | 3.928 | 3.9963 | 8 | -2 1 2 |  | 2.0411 | 2 | 1 3 0 |
| 3.9484 | 3 | -2 0 4 |  |  |  | 2.0252 | 2 | -1 2 7 |
| 3.8945 | 5 | 1 0 4 |  | 12 | 2.0185 | 2.0163 | 7 | 1 1 8 |
|  |  | 3.8599 | 2 | 2 1 1 |  |  |  | 1.9982 | 2 | -4 2 4 |
|  |  | 3.6244 | 5 | 3 0 0 |  |  |  | 1.9817 | 2 | 3 2 4 |
| 19 | 3.474 | 3.5197 | 25 | 2 1 2 |  | 13 | 1.9795 | 1.9738 | 7 | 1 3 2 |
| 39 | 3.350 | 3.3357 | 15 | -2 1 4 |  | 13 | 1.8519 | 1.8620 | 3 | -1 0 10 |
|  |  | 3.3030 | 2 | 1 1 4 |  | 1.8588 | 2 | -6 0 2 |
|  |  | 3.2045 | 17 | -3 0 4 |  | 1.8436 | 3 | -2 2 8 |
|  |  | 3.1563 | 7 | -3 1 2 |  |  |  | 1.8362 | 2 | 0 2 8 |
|  |  | 3.1406 | 3 | 0 1 5 |  | 10 | 1.8107 | 1.8122 | 2 | 6 0 0 |
| 100 | 3.112 | 3.1333 | 15 | 3 1 0 |  | 1.8027 | 2 | 3 3 0 |
| 3.1170 | 43 | 0 2 0 |  | 8 | 1.7604 | 1.7841 | 3 | -1 1 10 |
| 3.1036 | 19 | -1 0 6 |  | 1.7559 | 4 | 4 1 6 |
|  |  | 3.0722 | 3 | 0 2 1 |  | 9 | 1.7316 | 1.7402 | 4 | 6 1 0 |
|  |  | 3.0297 | 3 | 0 0 6 |  | 1.7319 | 2 | 3 3 2 |
|  |  | 2.9861 | 2 | -1 2 1 |  |  |  | 1.6966 | 2 | -4 0 10 |
| 42 | 2.964 | 2.9484 | 32 | 0 2 2 |  |  |  | 1.6774 | 2 | -5 2 6 |
| 2.9410 | 8 | -2 0 6 |  |  |  | 1.6646 | 2 | -4 3 2 |
| 17 | 2.808 | 2.8001 | 13 | 3 1 2 |  | 8 | 1.6455 | 1.6509 | 2 | 4 3 0 |
| 2.7807 | 11 | -4 0 2 |  | 1.6451 | 2 | 6 1 2 |
|  |  | 2.7250 | 5 | 0 1 6 |  |  |  | 1.6152 | 2 | 3 3 4 |
|  |  | 2.7183 | 2 | 4 0 0 |  | 10 | 1.5590 | 1.5585 | 4 | 0 4 0 |
|  |  | 2.6324 | 2 | 2 2 1 |  | 1.5518 | 2 | -2 0 12 |
| 12 | 2.538 | 2.5756 | 5 | -1 2 4 |  | 1.5485 | 2 | -1 0 12 |
| 2.5674 | 6 | 3 0 4 |  | 19 | 1.5336 | 1.5361 | 4 | 0 4 2 |
| 2.5261 | 8 | 1 1 6 |  | 1.5335 | 2 | 0 3 8 |
|  |  |  |  |  |  | 1.5280 | 2 | -7 0 6 |