Table S2. Powder X-ray data (*d* in Å) for epiebnerite compared with the pattern calculated from the structure of ABW-type NH4ZnPO4 (Bu *et al*., 1997). 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* |
| 9 | 8.86 | 8.9653 | 3 | 0 0 1 |  |  |  | 1.8791 | 3 | -2 1 4 |
|  |  |  |  |  |  |  |  |  |  |  |
| 60 | 6.25 | 6.2966 | 100 | -1 0 1 |  |  |  | 1.8344 | 2 | -2 2 3 |
| 48 | 4.643 | 4.6611 | 95 | 0 1 1 |  |  |  | 1.8292 | 4 | 2 2 3 |
| 50 | 4.406 | 4.4826 | 37 | 0 0 2 |  | 6 | 1.7671 | 1.7825 | 7 | 0 3 1 |
| 4.3982 | 76 | 2 0 0 |  | 1.7760 | 3 | -4 0 3 |
| 6 | 4.112 | 4.1136 | 10 | 1 1 1 |  | 1.7550 | 2 | 1 0 5 |
| 7 | 3.949 | 3.9849 | 7 | 1 0 2 |  |  |  | 1.7466 | 4 | 1 3 1 |
| 3.9399 | 6 | 2 0 1 |  | 8 | 1.7290 | 1.7318 | 5 | 0 2 4 |
| 7 | 3.429 | 3.4637 | 4 | 0 1 2 |  | 1.7282 | 3 | -5 0 1 |
| 3.4243 | 10 | 2 1 0 |  | 1.7245 | 5 | 5 0 1 |
| 100 | 3.195 | 3.2276 | 59 | -1 1 2 |  | 6 | 1.6974 | 1.7034 | 4 | 0 1 5 |
| 3.1942 | 50 | -2-1-1 |  | 1.6970 | 19 | -3 1 4 |
| 19 | 3.137 | 3.1483 | 12 | -2 0 2 |  | 28 | 1.6791 | 1.6887 | 16 | 3 1 4 |
| 3.1306 | 14 | 2 0 2 |  | 1.6804 | 4 | 4 2 1 |
|  |  | 2.9884 | 8 | 0 0 3 |  | 1.6707 | 8 | 1 1 5 |
| 32 | 2.776 | 2.7915 | 40 | -3 0 1 |  | 13 | 1.6509 | 1.6559 | 11 | -1 3 2 |
| 38 | 2.723 | 2.7283 | 48 | 0 2 0 |  | 1.6514 | 3 | 2 3 1 |
| 2.7154 | 3 | 2 1 2 |  | 8 | 1.6362 | 1.6444 | 7 | 5 1 1 |
| 33 | 2.601 | 2.6211 | 53 | 0 1 3 |  | 1.6345 | 3 | 5 0 2 |
| 2.6058 | 2 | 1 2 0 |  | 1.6138 | 3 | -2 2 4 |
| 13 | 2.487 | 2.5034 | 21 | -1 2 1 |  |  |  | 1.6090 | 3 | 2 2 4 |
| 2.4783 | 10 | -2 0 3 |  |  |  | 1.6018 | 2 | -4 2 2 |
| 10 | 2.453 | 2.4654 | 4 | 2 0 3 |  | 9 | 1.5635 | 1.5713 | 7 | -5 1 2 |
| 2.4475 | 2 | 3 0 2 |  | 1.5658 | 9 | 5 1 2 |
|  |  | 2.3184 | 4 | 2 2 0 |  | 9 | 1.5489 | 1.5537 | 13 | 0 3 3 |
| 39 | 2.233 | 2.2428 | 51 | -3 1 2 |  | 1.5336 | 5 | -3 0 5 |
| 2.2331 | 13 | 3 1 2 |  | 6 | 1.5143 | 1.5259 | 5 | 3 0 5 |
|  |  | 2.1991 | 2 | 4 0 0 |  | 1.5224 | 2 | 3 3 1 |
|  |  | 2.1690 | 5 | 1 0 4 |  | 1.4942 | 4 | 0 0 6 |
|  |  | 2.1386 | 2 | -4 0 1 |  |  |  | 1.4884 | 2 | -4 2 3 |
|  |  | 2.0732 | 4 | 0 1 4 |  |  |  | 1.4828 | 2 | 4 2 3 |
| 9 | 2.048 | 2.0397 | 7 | 4 1 0 |  |  |  | 1.4783 | 5 | -1 2 5 |
|  |  | 2.0149 | 4 | 0 2 3 |  | 22 | 1.4589 | 1.4661 | 10 | 6 0 0 |
| 6 | 1.9909 | 1.9974 | 3 | 3 2 0 |  | 1.4625 | 6 | -3 3 2 |
| 1.9911 | 3 | -4 1 1 |  | 1.4577 | 14 | 5 2 1 |
| 25 | 1.9443 | 1.9590 | 2 | -3 1 3 |  |  |  |  |  |  |
| 1.9512 | 31 | -3 2 1 |  |  |  |  |  |  |

Note that intensity and *d*-value mismatches are attributable to the differing compositions and cell parameters between epiebnerite and synthetic ABW-type NH4ZnPO4, as well as to sample orientation effects. The whole-pattern-fitting refinement largely compensates for these factors resulting in the excellent fit observed in Figure 6.