Table S1. Powder X-ray diffraction data (*d* in Å) for naalasite. Only calculated lines with intensities > 1.5 are listed.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *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* |
| 20 | 9.04 | 9.0153 | 31 |  2 0 0 |  | 8 | 2.494 | 2.4983 | 8 |  4 0 4 |  | 5 | 1.7218 | 1.7162 | 3 | -10 2 2 |
| 89 | 7.23 | 7.2140 | 100 | -1 1 1 |  | 2.4955 | 2 | -1 3 3 |  | 1.7137 | 2 |  8 0 4 |
| 7.1447 | 46 |  0 0 2 |  | 2.4875 | 4 | -5 1 5 |  | 5 | 1.6982 | 1.6944 | 2 | -1 3 7 |
| 9 | 4.51 | 4.5076 | 17 |  4 0 0 |  |  |  | 2.4629 | 2 |  5 1 3 |  | 1.6891 | 2 | -4 2 8 |
| 30 | 4.33 | 4.3385 | 13 |  0 2 0 |  |  |  | 2.4601 | 2 | -7 1 3 |  | 14 | 1.6739 | 1.6732 | 2 |  7 3 3 |
| 4.2908 | 28 | -1 1 3 |  | 5 | 2.266 | 2.2538 | 6 |  8 0 0 |  | 1.6721 | 6 | -9 3 3 |
|  |  | 3.8726 | 2 | -3 1 3 |  | 6 | 2.190 | 2.1826 | 3 | -5 3 3 |  | 1.6701 | 2 | -3 5 1 |
| 7 | 3.710 | 3.7083 | 7 |  0 2 2 |  | 2.1742 | 2 |  5 3 1 |  | 1.6655 | 3 |  6 0 6 |
|  |  | 3.6676 | 5 | -2 0 4 |  | 8 | 2.166 | 2.1692 | 2 |  0 4 0 |  |  |  | 1.6632 | 2 | -10 0 6 |
| 9 | 3.617 | 3.6070 | 9 | -2 2 2 |  | 2.1663 | 3 |  2 0 6 |  | 7 | 1.6499 | 1.6552 | 2 | -5 3 7 |
|  |  | 3.5723 | 6 |  0 0 4 |  | 2.1650 | 2 |  4 2 4 |  | 1.6517 | 2 |  0 2 8 |
|  |  | 3.4324 | 2 | -5 1 1 |  |  |  | 2.1565 | 2 | -7 1 5 |  | 1.6372 | 2 | -1 5 3 |
|  |  | 3.2759 | 2 |  2 2 2 |  |  |  | 2.1454 | 5 | -2 2 6 |  | 6 | 1.6243 | 1.6294 | 2 | -2 4 6 |
|  |  | 3.1769 | 3 | -4 2 1 |  | 7 | 2.075 | 2.0757 | 2 |  0 4 2 |  | 1.6236 | 2 | -6 2 8 |
| 100 | 3.127 | 3.1259 | 40 |  4 2 0 |  | 2.0635 | 4 | -1 3 5 |  | 1.6167 | 2 | -3 1 9 |
| 3.1098 | 40 |  3 1 3 |  | 8 | 2.052 | 2.0574 | 2 | -2 4 2 |  |  |  | 1.6032 | 2 | -4 4 6 |
| 3.1060 | 41 | -5 1 3 |  | 2.0494 | 3 | -3 1 7 |  | 11 | 1.5964 | 1.5939 | 2 |  8 2 4 |
| 33 | 3.085 | 3.0771 | 31 | -4 2 2 |  | 2.0453 | 3 | -3 3 5 |  | 1.5897 | 2 | -11 1 5 |
| 3.0573 | 15 |  2 0 4 |  |  |  | 2.0326 | 3 | -1 1 7 |  | 1.5885 | 3 | -8 4 2 |
|  |  | 3.0051 | 4 |  6 0 0 |  | 10 | 1.9996 | 2.0000 | 3 |  8 2 0 |  | 6 | 1.5731 | 1.5825 | 2 | -9 3 5 |
|  |  | 2.9437 | 2 |  4 2 1 |  | 1.9963 | 2 |  7 1 3 |  | 1.5780 | 2 |  5 1 7 |
| 4 | 2.846 | 2.8231 | 7 | -1 3 1 |  | 1.9943 | 3 | -9 1 3 |  | 9 | 1.5459 | 1.5549 | 2 |  6 2 6 |
| 15 | 2.809 | 2.8009 | 6 | -2 2 4 |  | 1.9898 | 3 |  2 4 2 |  | 1.5410 | 2 | 10 2 2 |
| 2.7886 | 7 | -1 1 5 |  | 5 | 1.9735 | 1.9793 | 3 |  1 3 5 |  | 8 | 1.5302 | 1.5390 | 3 |  3 5 3 |
| 7 | 2.769 | 2.7783 | 3 |  1 3 1 |  | 1.9659 | 4 | -5 1 7 |  | 1.5328 | 2 |  2 4 6 |
| 2.7577 | 4 |  0 2 4 |  | 7 | 1.8639 | 1.8587 | 2 |  7 3 1 |  | 1.5249 | 2 |  3 3 7 |
|  |  | 2.7441 | 4 | -3 1 5 |  | 1.8532 | 2 |  6 2 4 |  |  |  | 1.5212 | 2 | -7 1 9 |
| 5 | 2.690 | 2.6894 | 9 |  4 2 2 |  | 9 | 1.8345 | 1.8472 | 3 | -9 1 5 |  |  |  | 1.5199 | 2 | -8 2 8 |
|  |  | 2.6714 | 3 | -6 0 4 |  | 1.8330 | 3 |  4 4 2 |  |  |  | 1.4718 | 2 |  8 4 2 |
| 9 | 2.615 | 2.6171 | 4 | -3 3 1 |  | 1.8249 | 3 |  3 3 5 |  | 11 | 1.4589 | 1.4679 | 2 |  7 3 5 |
| 2.5988 | 4 | -4 2 4 |  | 4 | 1.8105 | 1.8137 | 4 | -7 1 7 |  | 1.4612 | 2 | -11 1 7 |
|  |  | 2.5907 | 5 |  1 1 5 |  |  |  | 1.8031 | 2 | 10 0 0 |  | 1.4432 | 2 | -9 3 7 |
|  |  | 2.5431 | 2 | -7 1 1 |  | 8 | 1.7705 | 1.7723 | 3 | -6 4 2 |  | 16 | 1.4171 | 1.4176 | 2 | -13 1 3 |
| 15 | 2.518 | 2.5138 | 3 |  3 3 1 |  | 1.7642 | 3 | -7 3 5 |  | 1.4158 | 2 | -10 4 2 |
| 2.5081 | 10 | -6 2 2 |  |  |  | 1.7574 | 3 |  3 1 7 |  | 1.4115 | 3 | -11 3 5 |