**Table S1.** Powder X–ray diffraction data (*d* in Å) for natromarkeyite. Only calculated lines with *I* ≥ 2 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* |
| 7 | 12.91 |  | 12.7907 | 7 | 1 1 0 |  |  |  |  | 2.8338 | 3 | 6 2 0 |  | 23 | 2.0289 | bracket | 2.0336 | 4 | 2 8 2 |
| 88 | 10.21 |  | 10.2249 | 100 | 0 0 1 |  | 21 | 2.816 | bracket | 2.8240 | 6 | 2 5 2 |  | 2.0315 | 6 | 7 1 3 |
| 7 | 8.81 |  | 8.9410 | 3 | 2 0 0 |  | 2.8153 | 8 | 3 2 3 |  | 2.0279 | 2 | 5 2 4 |
| 4 | 8.07 |  | 7.9866 | 3 | 1 1 1 |  |  |  |  | 2.7785 | 5 | 2 6 1 |  | 2.0209 | 4 | 2 7 3 |
|  |  |  | 6.7307 | 2 | 2 0 1 |  | 31 | 2.726 | bracket | 2.7309 | 14 | 6 2 1 |  |  |  |  | 1.9974 | 2 | 4 8 1 |
| 92 | 6.40 | bracket | 6.3954 | 45 | 2 2 0 |  | 2.7111 | 9 | 4 4 2 |  | 24 | 1.9833 | bracket | 1.9958 | 6 | 0 2 5 |
| 6.3716 | 14 | 1 2 1 |  |  |  |  | 2.7020 | 3 | 1 4 3 |  | 1.9935 | 4 | 2 0 5 |
| 29 | 5.72 | bracket | 5.7742 | 11 | 1 3 0 |  | 10 | 2.638 | bracket | 2.6622 | 4 | 3 3 3 |  | 1.9834 | 2 | 1 2 5 |
| 5.6677 | 13 | 3 1 0 |  | 2.6416 | 6 | 5 3 2 |  | 1.9823 | 2 | 1 9 1 |
| 100 | 5.43 |  | 5.4221 | 70 | 2 2 1 |  | 2.6196 | 4 | 0 6 2 |  | 1.9772 | 3 | 3 5 4 |
| 42 | 5.07 | bracket | 5.1495 | 11 | 3 0 1 |  |  |  |  | 2.6139 | 2 | 2 4 3 |  | 1.9708 | 5 | 8 4 1 |
| 5.1125 | 9 | 0 0 2 |  |  |  |  | 2.5497 | 2 | 6 1 2 |  | 25 | 1.9414 | bracket | 1.9510 | 6 | 5 7 2 |
| 5.0279 | 23 | 1 3 1 |  | 22 | 2.513 | bracket | 2.5305 | 4 | 1 0 4 |  | 1.9403 | 3 | 6 0 4 |
| 19 | 4.94 | bracket | 4.9571 | 7 | 3 1 1 |  | 2.5198 | 3 | 4 6 0 |  | 1.9385 | 5 | 7 5 2 |
| 4.9155 | 8 | 1 0 2 |  | 2.5139 | 5 | 2 6 2 |  | 1.9247 | 4 | 3 9 0 |
| 30 | 4.535 | bracket | 4.5758 | 11 | 0 4 0 |  | 2.5082 | 6 | 1 7 1 |  | 13 | 1.8991 | bracket | 1.8996 | 2 | 0 8 3 |
| 4.5203 | 2 | 2 3 1 |  |  |  |  | 2.4785 | 3 | 6 2 2 |  | 1.8915 | 2 | 3 9 1 |
|  |  |  | 4.4878 | 2 | 3 2 1 |  | 17 | 2.451 | bracket | 2.4678 | 3 | 5 4 2 |  | 1.8892 | 2 | 9 3 0 |
| 15 | 4.362 | bracket | 4.4705 | 8 | 4 0 0 |  | 2.4560 | 3 | 7 1 1 |  | 17 | 1.8576 | bracket | 1.8691 | 2 | 8 0 3 |
| 4.4632 | 2 | 0 2 2 |  | 2.4452 | 5 | 5 1 3 |  | 1.8664 | 3 | 7 4 3 |
| 4.3304 | 6 | 1 2 2 |  | 2.4390 | 3 | 1 2 4 |  | 1.8581 | 6 | 2 8 3 |
| 55 | 4.141 |  | 4.1766 | 23 | 0 4 1 |  | 2.4373 | 3 | 2 7 1 |  |  |  |  | 1.8425 | 2 | 9 1 2 |
|  |  |  | 4.0961 | 28 | 4 0 1 |  |  |  |  | 2.4260 | 2 | 6 4 1 |  |  |  |  | 1.8303 | 2 | 0 10 0 |
|  |  |  | 4.0671 | 8 | 1 4 1 |  |  |  |  | 2.3823 | 2 | 5 2 3 |  | 12 | 1.8190 | bracket | 1.8276 | 4 | 2 4 5 |
| 42 | 4.009 |  | 3.9933 | 28 | 2 2 2 |  |  |  |  | 2.3736 | 2 | 2 2 4 |  | 1.8224 | 2 | 4 2 5 |
| 17 | 3.830 | bracket | 3.8806 | 8 | 3 0 2 |  |  |  |  | 2.3722 | 2 | 6 3 2 |  | 1.8152 | 2 | 9 2 2 |
| 3.8277 | 3 | 1 3 2 |  | 6 | 2.320 | bracket | 2.3320 | 4 | 4 4 3 |  | 1.8082 | 2 | 5 5 4 |
| 3.7962 | 7 | 3 1 2 |  | 2.3084 | 4 | 1 7 2 |  | 1.8069 | 2 | 7 0 4 |
|  |  |  | 3.7841 | 2 | 2 4 1 |  |  |  |  | 2.2879 | 2 | 0 8 0 |  |  |  |  | 1.8013 | 3 | 3 9 2 |
| 16 | 3.582 | bracket | 3.5890 | 10 | 2 3 2 |  | 19 | 2.273 | bracket | 2.2852 | 5 | 7 0 2 |  | 25 | 1.7881 | bracket | 1.7982 | 3 | 7 1 4 |
| 3.5727 | 4 | 3 2 2 |  | 2.2797 | 3 | 2 3 4 |  | 1.7908 | 2 | 2 7 4 |
| 28 | 3.370 | bracket | 3.4096 | 8 | 0 4 2 |  | 2.2755 | 3 | 3 2 4 |  | 1.7873 | 6 | 8 5 2 |
| 3.3841 | 2 | 1 5 1 |  | 2.2676 | 4 | 7 1 2 |  | 1.7847 | 4 | 7 5 3 |
| 3.3653 | 8 | 4 0 2 |  | 2.2602 | 2 | 4 6 2 |  | 1.7721 | 3 | 9 3 2 |
| 3.3492 | 8 | 1 4 2 |  |  |  |  | 2.2528 | 3 | 2 7 2 |  |  |  |  | 1.7615 | 2 | 10 0 1 |
|  |  |  | 3.3199 | 4 | 5 1 1 |  | 9 | 2.221 | bracket | 2.2316 | 3 | 0 4 4 |  | 11 | 1.7479 | bracket | 1.7464 | 3 | 0 9 3 |
|  |  |  | 3.2744 | 2 | 3 3 2 |  | 2.2191 | 2 | 4 0 4 |  | 1.7405 | 3 | 4 9 2 |
|  |  |  | 3.2158 | 2 | 2 5 1 |  | 2.2171 | 3 | 7 2 2 |  | 7 | 1.7099 | bracket | 1.7232 | 2 | 0 10 2 |
| 19 | 3.196 | bracket | 3.1977 | 7 | 4 4 0 |  |  |  |  | 2.2030 | 3 | 2 6 3 |  | 1.7144 | 2 | 6 5 4 |
| 3.1940 | 6 | 0 2 3 |  | 12 | 2.171 | bracket | 2.1783 | 5 | 4 5 3 |  | 1.7090 | 2 | 9 1 3 |
|  |  |  | 3.1442 | 3 | 1 2 3 |  | 2.1652 | 6 | 2 4 4 |  | 14 | 1.6753 | bracket | 1.6871 | 2 | 9 2 3 |
| 15 | 3.075 | bracket | 3.0854 | 7 | 5 3 0 |  |  |  |  | 2.1566 | 3 | 4 2 4 |  | 1.6754 | 4 | 0 2 6 |
| 3.0519 | 6 | 4 4 1 |  | 20 | 2.097 | bracket | 2.1108 | 4 | 5 7 0 |  | 1.6740 | 4 | 2 0 6 |
| 36 | 2.975 | bracket | 3.0078 | 6 | 2 2 3 |  | 2.0949 | 7 | 7 5 0 |  | 1.6711 | 2 | 4 10 1 |
| 2.9836 | 8 | 3 5 1 |  | 2.0899 | 2 | 3 4 4 |  | 6 | 1.6114 |  | 1.6123 | 2 | 8 7 2 |
| 2.9803 | 6 | 6 0 0 |  | 2.0816 | 3 | 1 5 4 |  | 11 | 1.5923 | bracket | 1.5973 | 4 | 5 5 5 |
| 2.9588 | 7 | 3 0 3 |  | 24 | 2.065 | bracket | 2.0742 | 2 | 1 8 2 |  | 1.5911 | 3 | 7 9 0 |
| 2.9538 | 7 | 5 3 1 |  | 2.0672 | 11 | 5 7 1 |  | 1.5879 | 2 | 4 6 5 |
| 25 | 2.897 | bracket | 2.9232 | 4 | 0 6 1 |  | 2.0560 | 2 | 8 3 1 |  | 10 | 1.5797 | bracket | 1.5820 | 5 | 9 7 0 |
| 2.9208 | 2 | 3 1 3 |  |  |  |  | 2.0460 | 2 | 5 5 3 |  | 1.5721 | 6 | 7 9 1 |
| 2.8937 | 3 | 5 1 2 |  |  |  |  | 2.0441 | 3 | 7 0 3 |  | 11 | 1.5658 | bracket | 1.5688 | 2 | 4 2 6 |
| 2.8871 | 6 | 2 6 0 |  |  |  |  |  |  |  |  | 1.5634 | 4 | 9 7 1 |
| 2.8849 | 4 | 1 6 1 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 2.8613 | 4 | 6 0 1 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |