Table S2. 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* |
|  |  |  | 12.5402 | 3 |  1 1 0 |  | 22 | 3.044 | brace | 3.0593 | 11 | -3 5 1 |  | 20 | 2.130 | brace | 2.1410 | 2 | -2 3 4 |
|  |  |  | 9.2775 | 6 |  0 2 0 |  | 3.0396 | 2 | -5 1 2 |  | 2.1344 | 2 | -4 2 4 |
| 86 | 8.73 |  | 8.7729 | 100 | -1 0 1 |  | 3.0245 | 5 | -3 4 2 |  | 2.1327 | 6 | -8 2 1 |
|  |  |  | 8.1452 | 3 |  1 2 0 |  |  |  |  | 2.9814 | 5 |  5 3 0 |  | 2.1314 | 4 | -3 8 1 |
|  |  |  | 7.9958 | 4 |  0 1 1 |  |  |  |  | 2.9536 | 3 |  0 0 3 |  | 2.1193 | 2 | -3 3 4 |
|  |  |  | 7.1815 | 6 |  1 0 1 |  |  |  |  | 2.9477 | 4 |  5 0 1 |  | 2.1178 | 4 | -4 7 2 |
| 100 | 6.28 | brace | 6.4078 | 17 |  0 2 1 |  | 27 | 2.917 | brace | 2.9242 | 5 | -5 2 2 |  |  |  |  | 2.1052 | 2 | -5 5 3 |
| 6.2701 | 76 |  2 2 0 |  | 2.9198 | 2 |  0 6 1 |  | 18 | 2.0884 | brace | 2.1026 | 2 | -5 0 4 |
| 72 | 5.70 | brace | 5.8128 | 17 |  1 3 0 |  | 2.9166 | 5 | -1 6 1 |  | 2.0911 | 6 |  5 7 0 |
| 5.6789 | 49 |  1 2 1 |  | 2.9064 | 5 |  2 6 0 |  | 2.0893 | 3 | -5 1 4 |
|  |  |  | 5.6098 | 9 | -2 2 1 |  |  |  |  | 2.8854 | 3 | -1 2 3 |  | 2.0750 | 2 |  1 6 3 |
|  |  |  | 5.5089 | 5 |  2 0 1 |  |  |  |  | 2.8770 | 4 | -6 1 1 |  | 23 | 2.0389 | brace | 2.0548 | 5 |  0 8 2 |
| 24 | 5.41 | brace | 5.4236 | 12 |  3 1 0 |  |  |  |  | 2.8449 | 2 |  0 5 2 |  | 2.0506 | 3 | -5 2 4 |
| 5.4048 | 4 | -3 0 1 |  | 59 | 2.811 | brace | 2.8395 | 10 |  2 4 2 |  | 2.0333 | 5 |  7 5 0 |
|  |  |  | 5.2810 | 3 |  2 1 1 |  | 2.8357 | 2 |  6 0 0 |  | 2.0278 | 4 |  2 0 4 |
|  |  |  | 5.1891 | 2 | -3 1 1 |  | 2.8316 | 4 | -2 6 1 |  | 2.0263 | 4 |  3 7 2 |
| 22 | 5.07 |  | 5.0717 | 14 |  0 3 1 |  | 2.8144 | 8 |  0 2 3 |  | 20 | 2.0027 | brace | 2.0112 | 2 |  8 3 0 |
|  |  |  | 4.8388 | 3 |  3 2 0 |  | 2.8093 | 12 |  5 2 1 |  | 2.0078 | 3 | -7 5 2 |
|  |  |  | 4.7368 | 3 |  2 2 1 |  | 2.8020 | 4 |  3 3 2 |  | 2.0041 | 4 |  5 0 3 |
| 80 | 4.65 | brace | 4.6701 | 35 | -3 2 1 |  | 2.7969 | 9 | -4 5 1 |  | 1.9968 | 3 | -1 7 3 |
| 4.6474 | 17 | -2 3 1 |  | 2.7890 | 5 | -3 2 3 |  |  |  |  | 1.9840 | 2 | -6 5 3 |
| 4.6388 | 24 |  0 4 0 |  |  |  |  | 2.7780 | 3 | -5 4 1 |  | 11 | 1.9605 | brace | 1.9640 | 2 | -3 7 3 |
|  |  |  | 4.5641 | 2 | -1 0 2 |  |  |  |  | 2.7580 | 3 | -5 3 2 |  | 1.9603 | 5 | -6 7 1 |
|  |  |  | 4.4304 | 2 |  0 0 2 |  | 13 | 2.726 | brace | 2.7254 | 2 | -1 3 3 |  | 1.9541 | 2 | -8 1 3 |
|  |  |  | 4.3864 | 5 | -2 0 2 |  | 2.7118 | 5 |  6 2 0 |  | 12 | 1.9312 | brace | 1.9376 | 5 |  3 9 0 |
| 55 | 4.293 | brace | 4.3265 | 22 |  3 0 1 |  | 7 | 2.660 | brace | 2.6842 | 5 | -3 6 1 |  | 1.9269 | 2 |  2 3 4 |
| 4.2688 | 2 | -2 1 2 |  | 2.6431 | 3 | -4 2 3 |  |  |  |  | 1.9130 | 2 |  3 0 4 |
| 4.2535 | 18 |  4 0 0 |  | 2.6405 | 4 |  4 2 2 |  | 14 | 1.8988 | brace | 1.9031 | 4 | -9 1 2 |
| 47 | 4.082 | brace | 4.1479 | 10 | -4 1 1 |  |  |  |  | 2.6348 | 4 | -6 3 1 |  | 1.9021 | 3 |  0 5 4 |
| 4.1137 | 4 |  2 3 1 |  |  |  |  | 2.5395 | 4 |  0 7 1 |  | 1.8881 | 2 | -4 5 4 |
| 4.1008 | 15 | -1 4 1 |  |  |  |  | 2.5358 | 3 |  0 6 2 |  | 1.8869 | 2 | -8 5 1 |
| 4.0953 | 3 | -1 2 2 |  | 23 | 2.512 | brace | 2.5275 | 3 | -2 6 2 |  | 19 | 1.8622 | brace | 1.8738 | 3 | -9 2 2 |
| 4.0698 | 4 | -3 3 1 |  | 2.5159 | 4 |  3 6 1 |  | 1.8685 | 2 | -7 1 4 |
| 4.0556 | 5 |  1 0 2 |  | 2.5080 | 2 |  5 5 0 |  | 1.8659 | 2 | -2 9 2 |
| 25 | 3.973 |  | 3.9979 | 29 |  0 2 2 |  | 2.5063 | 5 |  6 1 1 |  | 1.8590 | 2 | -7 5 3 |
|  |  |  | 3.9889 | 3 | -3 0 2 |  |  |  |  | 2.5013 | 2 |  4 6 0 |  | 1.8580 | 2 |  2 4 4 |
|  |  |  | 3.9655 | 4 | -2 2 2 |  | 7 | 2.480 | brace | 2.4867 | 2 |  1 7 1 |  | 1.8555 | 5 | 0 10 0 |
|  |  |  | 3.8966 | 4 |  1 4 1 |  | 2.4808 | 6 | -2 7 1 |  | 1.8533 | 2 |  7 3 2 |
|  |  |  | 3.8740 | 3 | -2 4 1 |  | 2.4738 | 3 | -3 4 3 |  | 15 | 1.8332 | brace | 1.8398 | 2 |  5 4 3 |
|  |  |  | 3.7160 | 2 |  1 2 2 |  |  |  |  | 2.4166 | 3 | -7 2 1 |  | 1.8294 | 2 | -5 5 4 |
|  |  |  | 3.6645 | 4 | -3 2 2 |  |  |  |  | 2.4100 | 2 |  7 1 0 |  | 1.8228 | 2 |  5 8 1 |
|  |  |  | 3.6258 | 5 |  1 5 0 |  | 9 | 2.385 | brace | 2.3963 | 3 |  1 4 3 |  |  |  |  | 1.8172 | 3 | -3 8 3 |
|  |  |  | 3.6017 | 2 |  0 3 2 |  | 2.3799 | 3 | -3 7 1 |  | 15 | 1.8033 | brace | 1.8153 | 2 | -1 10 1 |
| 21 | 3.588 |  | 3.5908 | 13 |  2 0 2 |  | 2.3679 | 4 | -7 1 2 |  | 1.8079 | 2 |  9 3 0 |
|  |  |  | 3.5254 | 3 |  2 1 2 |  |  |  |  | 2.3625 | 3 | -5 3 3 |  | 1.8013 | 2 |  6 2 3 |
|  |  |  | 3.5200 | 3 | -3 4 1 |  |  |  |  | 2.3433 | 2 |  2 6 2 |  | 1.7971 | 2 | -7 3 4 |
| 12 | 3.468 | brace | 3.4688 | 9 | -5 0 1 |  | 9 | 2.330 | brace | 2.3350 | 2 | -6 4 2 |  | 1.7953 | 2 |  6 8 0 |
| 3.4229 | 7 |  0 5 1 |  | 2.3202 | 2 | -7 3 1 |  |  |  |  | 1.7879 | 2 |  2 9 2 |
|  |  |  | 3.3470 | 2 |  5 1 0 |  | 2.3179 | 4 |  3 2 3 |  | 15 | 1.7673 | brace | 1.7747 | 4 | -1 2 5 |
| 7 | 3.300 | brace | 3.2924 | 7 | -4 2 2 |  | 2.3121 | 2 | -7 2 2 |  | 1.7721 | 2 |  0 0 5 |
| 3.2832 | 4 | -2 5 1 |  |  |  |  | 2.2820 | 2 | -2 0 4 |  | 1.7634 | 4 |  5 5 3 |
|  |  |  | 3.2534 | 3 | -1 4 2 |  |  |  |  | 2.2747 | 2 |  0 7 2 |  | 14 | 1.7270 | brace | 1.7366 | 3 | -8 5 3 |
|  |  |  | 3.1872 | 3 | -2 4 2 |  |  |  |  | 2.2559 | 2 | -3 0 4 |  | 1.7294 | 2 | -2 7 4 |
|  |  |  | 3.1639 | 4 |  3 4 1 |  |  |  |  | 2.2377 | 2 |  2 8 0 |  | 1.7240 | 3 | -5 2 5 |
| 17 | 3.113 | brace | 3.1350 | 3 |  4 4 0 |  | 15 | 2.201 | brace | 2.2133 | 2 | -4 5 3 |  | 1.7204 | 2 |  1 0 5 |
| 3.1053 | 4 |  3 5 0 |  | 2.2119 | 2 |  7 0 1 |  | 1.7089 | 2 | -2 10 2 |
| 3.0925 | 5 |  0 6 0 |  | 2.2071 | 3 |  1 8 1 |  | 13 | 1.6954 | brace | 1.7053 | 2 | 3 10 1 |
| 3.0812 | 6 | -5 0 2 |  | 2.1912 | 7 |  4 0 3 |  | 1.7007 | 4 | 4 10 0 |
|  |  |  | 3.0778 | 3 |  2 5 1 |  |  |  |  | 2.1762 | 3 | -8 1 1 |  | 1.6958 | 2 |  2 6 4 |
|  |  |  |  |  |  |  |  |  |  | 2.1665 | 2 | -1 6 3 |  | 1.6850 | 2 | -3 9 3 |
|  |  |  |  |  |  |  |  |  |  | 2.1546 | 2 |  0 2 4 |  |  |  |  |  |  |  |