Table S1. Powder X-ray data (*d* in Å) for paramarkeyite. 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 | 11.31 | 11.4071 | 2 | -1 1 1 |  |  |  | 3.1829 | 3 | -4 4 1 |  | 12 | 2.181 | 2.1873 | 4 | 2 8 0 |
|  |  | 10.6685 | 2 | 1 0 1 |  |  |  | 3.0771 | 3 | -5 3 2 |  | 2.1858 | 2 | 5 6 1 |
|  |  | 9.0515 | 3 | 0 2 0 |  | 18 | 3.045 | 3.0598 | 2 | -2 0 6 |  | 2.1834 | 2 | 0 0 8 |
|  |  | 8.7334 | 6 | 0 0 2 |  | 3.0563 | 2 | -2 5 3 |  | 2.1742 | 2 | -8 2 3 |
| 100 | 8.54 | 8.5347 | 100 | 2 0 0 |  | 3.0536 | 7 | -3 4 4 |  |  |  | 2.1484 | 2 | -2 6 6 |
|  |  | 8.0472 | 4 | -1 1 2 |  | 3.0172 | 3 | 0 6 0 |  | 12 | 2.118 | 2.1254 | 2 | -3 6 6 |
| 9 | 7.83 | 7.9967 | 4 | 1 2 0 |  |  |  | 2.9975 | 2 | 3 1 4 |  | 2.1190 | 2 | 5 1 5 |
| 7.7198 | 2 | 2 1 0 |  | 22 | 2.970 | 2.9913 | 5 | -6 0 2 |  | 2.1045 | 4 | 4 1 6 |
| 9 | 6.85 | 6.9020 | 2 | 1 2 1 |  | 2.9748 | 8 | 1 4 4 |  | 17 | 2.079 | 2.0950 | 3 | 0 6 6 |
| 6.8063 | 11 | -2 1 2 |  | 2.9713 | 6 | 5 3 0 |  | 2.0920 | 2 | -7 5 2 |
| 91 | 6.31 | 6.3763 | 35 | -1 2 2 |  | 2.9544 | 3 | -3 1 6 |  | 2.0902 | 2 | 6 1 4 |
| 6.2849 | 54 | 0 2 2 |  | 38 | 2.858 | 2.8986 | 6 | -2 2 6 |  | 2.0720 | 3 | -4 6 6 |
| 6.2096 | 5 | 2 2 0 |  | 2.8727 | 7 | -1 2 6 |  | 2.0699 | 2 | 6 6 0 |
|  |  | 5.7973 | 2 | -1 1 3 |  | 2.8602 | 5 | -1 6 2 |  | 2.0687 | 3 | -6 0 8 |
| 45 | 5.66 | 5.7035 | 30 | -2 2 2 |  | 2.8518 | 9 | 0 6 2 |  | 20 | 2.046 | 2.0553 | 3 | -6 1 8 |
| 5.6893 | 7 | 1 3 0 |  | 2.8430 | 6 | -3 2 6 |  | 2.0444 | 4 | -7 2 7 |
| 46 | 5.52 | 5.5131 | 48 | 1 2 2 |  | 2.8157 | 4 | -4 1 6 |  | 2.0427 | 4 | -3 4 8 |
|  |  | 5.4280 | 2 | 3 1 0 |  | 27 | 2.785 | 2.7963 | 4 | -6 2 3 |  | 25 | 2.0085 | 2.0255 | 3 | 1 6 6 |
| 5 | 5.07 | 5.1168 | 8 | 2 1 2 |  | 2.7909 | 5 | -2 6 2 |  | 2.0209 | 4 | -2 8 4 |
| 5.0534 | 4 | 1 0 3 |  | 2.7818 | 2 | -6 1 4 |  | 2.0186 | 2 | -1 4 8 |
|  |  | 4.9272 | 3 | 2 3 0 |  | 2.7713 | 6 | 0 2 6 |  | 2.0167 | 2 | -6 2 8 |
|  |  | 4.8171 | 2 | 3 2 0 |  | 2.7677 | 6 | 1 6 2 |  | 2.0091 | 5 | 0 8 4 |
| 45 | 4.759 | 4.7810 | 29 | -3 2 2 |  |  |  | 2.7536 | 2 | 5 2 2 |  | 1.9992 | 7 | 4 8 0 |
| 4.7269 | 7 | -3 1 3 |  | 10 | 2.724 | 2.7254 | 4 | 5 4 0 |  | 15 | 1.9726 | 1.9797 | 3 | -8 4 1 |
| 29 | 4.542 | 4.5956 | 21 | 2 2 2 |  | 2.7187 | 2 | -4 2 6 |  | 1.9737 | 3 | 2 0 8 |
| 4.5569 | 2 | 1 3 2 |  | 2.7138 | 2 | -4 5 3 |  |  |  | 1.9564 | 2 | -6 7 2 |
| 4.4918 | 22 | -2 0 4 |  |  |  | 2.7038 | 3 | 4 3 3 |  | 24 | 1.9359 | 1.9514 | 4 | -9 0 1 |
| 97 | 4.371 | 4.3746 | 46 | 1 4 0 |  |  |  | 2.6671 | 2 | 4 0 4 |  | 1.9370 | 3 | -9 0 5 |
| 4.3667 | 24 | 0 0 4 |  |  |  | 2.6594 | 3 | -3 6 2 |  | 1.9348 | 2 | -3 5 8 |
|  |  | 4.3596 | 2 | -2 1 4 |  | 27 | 2.625 | 2.6338 | 2 | -4 4 5 |  | 1.9339 | 3 | -8 4 5 |
|  |  | 4.3069 | 2 | -3 2 3 |  | 2.6262 | 6 | 2 6 2 |  | 1.9265 | 4 | -4 8 4 |
|  |  | 4.2848 | 4 | -4 1 2 |  | 2.6212 | 7 | -5 4 4 |  | 22 | 1.9004 | 1.9136 | 3 | 6 7 0 |
|  |  | 4.2673 | 4 | 4 0 0 |  | 2.6163 | 5 | 1 2 6 |  | 1.9104 | 3 | -5 8 1 |
| 11 | 4.163 | 4.1535 | 3 | 4 1 0 |  | 2.6070 | 5 | 5 3 2 |  | 1.9028 | 2 | -8 2 7 |
| 4.1397 | 11 | 3 3 0 |  |  |  | 2.5692 | 2 | 6 2 1 |  | 1.8964 | 5 | 2 8 4 |
|  |  | 4.1167 | 2 | -3 3 2 |  | 6 | 2.539 | 2.5505 | 2 | -5 2 6 |  | 1.8944 | 3 | 1 4 8 |
| 9 | 3.962 | 3.9646 | 12 | -4 2 2 |  | 2.5232 | 7 | 3 4 4 |  | 8 | 1.8560 | 1.8457 | 2 | 3 1 8 |
|  |  | 3.8567 | 2 | 1 1 4 |  | 11 | 2.490 | 2.4902 | 4 | -4 6 2 |  |  |  | 1.8385 | 2 | 7 6 1 |
| 8 | 3.808 | 3.8163 | 10 | 3 2 2 |  | 2.4754 | 4 | -6 4 1 |  | 9 | 1.8199 | 1.8171 | 2 | -7 0 9 |
|  |  | 3.7802 | 2 | 2 4 1 |  | 11 | 2.450 | 2.4646 | 3 | 6 1 2 |  | 15 | 1.7893 | 1.8002 | 2 | -3 2 10 |
|  |  | 3.7344 | 2 | -4 2 3 |  | 2.4521 | 5 | 3 6 2 |  | 1.7928 | 3 | -5 8 5 |
| 10 | 3.630 | 3.6726 | 7 | -4 0 4 |  | 2.4336 | 4 | 2 2 6 |  | 1.7898 | 3 | -2 2 10 |
| 3.5993 | 8 | -4 1 4 |  |  |  | 2.4042 | 2 | -5 5 4 |  | 1.7746 | 2 | -1 10 2 |
|  |  | 3.5795 | 2 | -1 1 5 |  | 5 | 2.370 | 2.3783 | 3 | -5 1 7 |  | 14 | 1.7566 | 1.7605 | 2 | -1 2 10 |
| 41 | 3.544 | 3.5646 | 4 | -5 0 1 |  | 2.3739 | 2 | -7 0 5 |  | 1.7519 | 4 | 1 10 2 |
| 3.5419 | 26 | 3 4 0 |  |  |  | 2.3591 | 2 | -7 3 2 |  | 11 | 1.7212 | 1.7337 | 2 | -9 4 6 |
|  |  | 3.4841 | 2 | 4 3 0 |  |  |  | 2.3545 | 2 | 7 2 0 |  | 1.7234 | 2 | -3 10 2 |
| 15 | 3.445 | 3.4756 | 10 | 2 0 4 |  |  |  | 2.3271 | 2 | 2 7 2 |  | 1.7167 | 2 | 3 4 8 |
| 3.4520 | 3 | 3 3 2 |  |  |  | 2.2925 | 3 | -2 0 8 |  | 5 | 1.6699 | 1.6779 | 2 | -8 7 4 |
| 3.4352 | 4 | -3 1 5 |  | 7 | 2.268 | 2.2676 | 2 | 4 6 2 |  | 9 | 1.6355 | 1.6322 | 2 | 6 7 4 |
|  |  | 3.4133 | 3 | 2 1 4 |  | 2.2629 | 3 | 0 8 0 |  | 12 | 1.6054 | 1.6104 | 4 | -2 8 8 |
|  |  | 3.3770 | 3 | 4 1 2 |  | 2.2590 | 2 | 5 5 2 |  | 1.5941 | 2 | -4 8 8 |
|  |  | 3.3267 | 4 | -5 2 2 |  |  |  | 2.2447 | 4 | 3 2 6 |  | 1.5907 | 2 | 2 2 10 |
| 16 | 3.214 | 3.2209 | 11 | -1 4 4 |  | 9 | 2.224 | 2.2309 | 3 | -4 7 2 |  |  |  |  |  |  |
| 3.2135 | 5 | 4 2 2 |  | 2.2117 | 5 | 4 7 0 |  |  |  |  |  |  |