Supplementary Table. Powder X–ray data for cuyaite for calculated lines with *I* > 1.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *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* |
| 11 | 13.33 | 13.1616 | 9 | –1 0 1 |  |   |   | 2.4955 | 2 |  2 2 1 |  | 6 | 1.7008 | 1.7056 | 2 | –2 3 4 |
| 10 | 8.93 | 8.8574 | 11 |  1 0 1 |  | 8 | 2.479 | 2.4779 | 2 |  0 2 3 |  | 1.6967 | 2 |  6 2 1 |
| 7 | 6.78 | 6.8036 | 6 |  2 0 0 |  | 2.4727 | 5 | –2 2 3 |  | 1.6902 | 2 |  0 3 4 |
|   |   | 6.5808 | 3 | –2 0 2 |  | 16 | 2.438 | 2.4466 | 2 |  5 1 0 |  | 9 | 1.6784 | 1.6741 | 5 | –3 3 4 |
| 6 | 5.81 | 5.8056 | 5 | –1 0 3 |  | 2.4396 | 12 | –6 0 2 |  | 1.6724 | 4 | –7 0 9 |
| 19 | 5.297 | 5.2782 | 16 |  0 1 1 |  | 2.4249 | 4 | –1 0 7 |  | 5 | 1.6636 | 1.6623 | 2 | –3 1 10 |
| 4 | 5.136 | 5.1429 | 6 | –1 1 1 |  | 7 | 2.398 | 2.3995 | 5 | –4 1 6 |  | 1.6614 | 2 | –4 3 2 |
| 7 | 4.869 | 4.8791 | 3 | –3 0 1 |  | 7 | 2.355 | 2.3564 | 2 | –3 2 3 |  | 10 | 1.641 | 1.6493 | 2 | –4 3 3 |
| 45 | 4.73 | 4.7255 | 34 |  1 1 1 |  | 2.3483 | 4 | –1 2 4 |  | 1.6406 | 2 | –2 3 5 |
| 4.6677 | 8 | –1 1 2 |  |   |   | 2.2246 | 2 | –5 0 7 |  | 1.6390 | 2 | –7 2 1 |
|   |   | 4.5898 | 3 |  0 1 2 |  | 10 | 2.217 | 2.2115 | 7 | –4 2 1 |  | 1.6367 | 2 |  3 3 2 |
|   |   | 4.4287 | 3 |  2 0 2 |  | 7 | 2.183 | 2.1936 | 3 | –6 0 6 |  | 1.6336 | 2 |  4 3 0 |
| 20 | 4.323 | 4.3178 | 16 |  2 1 0 |  | 2.1827 | 2 | –4 1 7 |  | 6 | 1.6224 | 1.6256 | 2 |  3 2 6 |
| 9 | 4.207 | 4.2467 | 8 | –2 0 4 |  | 2.1752 | 2 | –2 2 5 |  | 1.6206 | 3 |  4 2 5 |
| 17 | 4.036 | 4.0246 | 19 |  0 0 4 |  | 2.1689 | 2 | –1 2 5 |  | 5 | 1.5781 | 1.5821 | 3 | –2 2 9 |
| 7 | 3.891 | 3.9384 | 5 |  2 1 1 |  | 6 | 2.136 | 2.1449 | 2 |  5 1 2 |  | 1.5780 | 2 | –4 2 9 |
| 3.8702 | 3 |  0 1 3 |  | 2.1276 | 2 | –3 2 5 |  | 19 | 1.562 | 1.5663 | 3 |  1 3 5 |
|   |   | 3.8505 | 5 | –2 1 3 |  |   |   | 2.0586 | 2 |  4 1 4 |  | 1.5628 | 3 |  8 1 1 |
| 21 | 3.665 | 3.6750 | 5 | –3 1 1 |  | 14 | 2.0453 | 2.0452 | 4 | –7 0 5 |  | 1.5606 | 9 |  5 1 6 |
| 3.6477 | 21 | –3 1 2 |  | 2.0439 | 4 |  2 2 4 |  | 1.5598 | 3 | –7 2 7 |
| 13 | 3.497 | 3.5214 | 5 |  3 1 0 |  | 2.0419 | 2 | –6 1 6 |  | 10 | 1.5461 | 1.5528 | 2 | –1 2 9 |
| 3.4789 | 11 |  1 1 3 |  | 15 | 2.0225 | 2.0248 | 12 | –3 1 8 |  | 1.5517 | 2 | –5 3 4 |
|   |   | 3.3809 | 4 | –2 1 4 |  |   |   | 2.0103 | 3 |  1 2 5 |  | 1.5488 | 2 |  8 0 2 |
|   |   | 3.2904 | 3 | –4 0 4 |  | 8 | 1.9925 | 2.0017 | 2 | –5 2 1 |  | 1.5452 | 2 | –5 2 9 |
| 100 | 3.162 | 3.1538 | 100 | –3 1 4 |  | 1.9963 | 3 |  1 1 7 |  | 1.5428 | 2 | –9 1 6 |
|   |   | 3.0716 | 6 | –4 1 2 |  |   |   | 1.9745 | 5 | –1 1 8 |  | 12 | 1.5276 | 1.5342 | 3 | –8 2 3 |
| 28 | 3.035 | 3.0378 | 3 | –4 1 1 |  | 5 | 1.9588 | 1.9582 | 2 | –7 1 4 |  | 1.5268 | 6 |  2 1 9 |
| 3.0249 | 28 |  2 1 3 |  | 15 | 1.9328 | 1.9351 | 10 |  0 2 6 |  | 1.5251 | 2 | –4 3 6 |
| 37 | 3.004 | 2.9983 | 38 |  2 0 4 |  | 1.9253 | 5 | –4 2 6 |  | 1.5203 | 2 | –5 3 5 |
|   |   | 2.9525 | 2 |  3 0 3 |  |   |   | 1.9103 | 2 | –6 0 8 |  | 1.5189 | 2 | –8 2 2 |
| 90 | 2.931 | 2.9458 | 11 | –2 1 5 |  | 7 | 1.8822 | 1.8802 | 5 | –7 0 7 |  | 11 | 1.5076 | 1.5102 | 6 | –7 1 10 |
| 2.9302 | 2 | –1 1 5 |  |   |   | 1.8680 | 2 | –1 0 9 |  | 1.5010 | 2 | –2 1 11 |
| 2.9235 | 76 |  3 1 2 |  | 23 | 1.8536 | 1.8548 | 4 | –5 0 9 |  | 1.4999 | 2 | –7 2 8 |
| 2.9179 | 5 | –5 0 3 |  | 1.8534 | 10 |  4 2 3 |  | 5 | 1.4909 | 1.4960 | 4 |  5 2 5 |
|   |   | 2.9056 | 3 |  4 1 0 |  | 1.8477 | 3 |  7 0 1 |  | 1.4865 | 2 | –8 0 10 |
|   |   | 2.8952 | 5 |  1 0 5 |  | 26 | 1.8318 | 1.8375 | 10 | –6 2 2 |  | 1.4774 | 2 | 1 1 10 |
|   |   | 2.8695 | 5 | –5 0 1 |  | 1.8359 | 2 |  7 1 0 |  | 6 | 1.4624 | 1.4658 | 2 | –9 1 8 |
| 28 | 2.799 | 2.7935 | 24 |  0 2 0 |  | 1.8312 | 6 | –1 2 7 |  | 1.4624 | 2 | –8 2 7 |
| 12 | 2.717 | 2.7365 | 3 |  1 2 0 |  | 1.8238 | 6 | –6 2 4 |  | 1.4594 | 4 |  9 1 0 |
| 2.7091 | 9 |  4 1 1 |  | 1.8225 | 3 |  1 3 1 |  |   |   | 1.4476 | 2 | 2 0 10 |
| 11 | 2.686 | 2.6830 | 15 |  0 0 6 |  | 7 | 1.8057 | 1.8093 | 2 | –4 1 9 |  | 3 | 1.4287 | 1.4349 | 3 | –7 2 9 |
| 15 | 2.661 | 2.6571 | 8 | –4 0 6 |  | 1.7963 | 3 |  2 3 0 |  | 10 | 1.4126 | 1.4224 | 2 | –10 1 5 |
| 2.6537 | 8 | –1 2 2 |  |   |   | 1.7755 | 2 |  0 2 7 |  | 1.4197 | 3 | –6 3 6 |
| 8 | 2.636 | 2.6323 | 2 | –5 0 5 |  | 13 | 1.774 | 1.7715 | 8 |  5 0 5 |  | 1.4156 | 2 | –6 0 12 |
| 2.6245 | 8 | –4 1 5 |  | 6 | 1.7482 | 1.7559 | 2 |  2 0 8 |  | 1.4110 | 2 | –10 1 3 |
| 8 | 2.61 | 2.6115 | 4 | –2 2 1 |  | 1.7543 | 2 |  7 1 1 |  | 10 | 1.3988 | 1.4041 | 6 |  1 3 7 |
|   |   | 2.5842 | 2 |  2 2 0 |  | 1.7441 | 3 | –8 1 3 |  | 1.4029 | 2 | –10 0 8 |
| 5 | 2.569 | 2.5706 | 5 |  1 1 5 |  | 16 | 1.719 | 1.7177 | 5 |  1 3 3 |  | 1.3965 | 2 | –1 3 8 |
| 20 | 2.533 | 2.5365 | 2 | –1 1 6 |  | 1.7167 | 2 |  2 3 2 |  | 1.3906 | 5 | –10 1 7 |
| 2.5323 | 9 |  1 2 2 |  | 1.7149 | 5 | –3 2 8 |  |  |  |  |  |  |
| 2.5293 | 3 |  5 0 1 |  |  |  |  |  |  |  |  |  |  |  |  |
| 2.5254 | 7 | –3 1 6 |  |  |  |  |  |  |  |  |  |  |  |  |