Table S1. Powder X-ray diffraction data (*d* in Å) for flaggite. Only calculated lines with *I* > 2.5 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* |
|  |  | 10.0676 | 4 | 0 0 1 |  | 13 | 2.426 | 2.4295 | 10 | -1-3 2 |  | 16 | 1.7553 | 1.7607 | 3 | 2-2 4 |
| 65 | 9.41 | 9.4126 | 75 | 0 1 0 |  | 2.4275 | 10 | 1 4 2 |  | 1.7590 | 6 | -2 4 4 |
|  |  | 8.0240 | 3 | 0 1 1 |  |  |  | 2.3967 | 5 | 1 0 4 |  | 1.7569 | 3 | -3 3 4 |
| 15 | 5.04 | 5.0338 | 12 | 0 0 2 |  | 11 | 2.373 | 2.3886 | 5 | 4 1 0 |  |  |  | 1.7453 | 3 | 3-3 2 |
|  |  | 4.7063 | 6 | 0 2 0 |  | 2.3531 | 16 | 0 4 0 |  | 19 | 1.7295 | 1.7318 | 10 | 5 3 2 |
| 93 | 4.59 | 4.6724 | 22 | 2 0 0 |  | 16 | 2.335 | 2.3362 | 6 | 4 0 0 |  | 1.7208 | 8 | 5 0 2 |
| 4.5894 | 27 | 2 1 0 |  | 2.3133 | 4 | -3 2 2 |  | 15 | 1.6675 | 1.6600 | 8 | -1-5 2 |
| 4.5388 | 44 | 1 1 2 |  |  |  | 2.3067 | 5 | 2 4 0 |  | 1.6590 | 8 | 1 6 2 |
| 49 | 4.34 | 4.3283 | 37 | 1-1-2 |  | 15 | 2.287 | 2.2947 | 4 | 4 2 0 |  | 20 | 1.6377 | 1.6356 | 13 | 2-1-6 |
| 8 | 4.04 | 4.0162 | 5 | 0-1 2 |  | 2.2802 | 3 | 1-2 3 |  | 1.6307 | 5 | -2 5 0 |
| 4.0120 | 5 | 0 2 2 |  | 2.2733 | 6 | -1-1 4 |  | 1.6283 | 4 | 5 4 2 |
| 14 | 3.898 | 3.8822 | 4 | -1-2-2 |  | 2.2716 | 6 | 1 3 4 |  | 30 | 1.6135 | 1.6126 | 24 | -5 2 2 |
| 3.8717 | 9 | -2 1 0 |  | 41 | 2.167 | 2.1684 | 10 | 1-1 4 |  |  |  | 1.6082 | 3 | -2 0 6 |
| 34 | 3.744 | 3.7340 | 40 | 2 2 0 |  | 2.1664 | 28 | -1 3 4 |  | 22 | 1.5879 | 1.5917 | 15 | 6 1 0 |
| 53 | 3.519 | 3.5250 | 24 | 2 1 2 |  |  |  | 2.1642 | 3 | -2 2 4 |  | 1.5817 | 4 | 6 2 0 |
| 3.5213 | 15 | 1-1 2 |  |  |  | 2.1630 | 5 | -4 1 0 |  | 1.5807 | 3 | 0-1 6 |
| 3.5179 | 15 | -1 2 2 |  | 29 | 2.100 | 2.0984 | 17 | 4 3 0 |  | 16 | 1.5531 | 1.5509 | 5 | 1-5 2 |
| 9 | 3.251 | 3.2713 | 5 | 1 1 3 |  | 2.0960 | 14 | 3 4 2 |  | 1.5426 | 5 | 5 0-4 |
| 3.2293 | 4 | -1 1 3 |  |  |  | 2.0603 | 3 | 0 2 5 |  | 15 | 1.5306 | 1.5273 | 5 | -3 1 6 |
|  |  | 3.2164 | 5 | -1 0 3 |  | 31 | 2.016 | 2.0202 | 6 | -1-2 4 |  | 23 | 1.5146 | 1.5198 | 3 | 3-4 2 |
| 16 | 3.163 | 3.1375 | 16 | 0 3 0 |  | 2.0182 | 5 | 1 4 4 |  | 1.5189 | 6 | -3 5 2 |
|  |  | 3.1034 | 4 | 1 0 3 |  | 2.0154 | 4 | 3-2 2 |  | 1.5183 | 3 | 4 5 4 |
|  |  | 3.0768 | 5 | 1 2 3 |  | 2.0142 | 14 | -3 3 2 |  | 1.5132 | 10 | -3 0 6 |
| 99 | 3.070 | 3.0636 | 52 | -1-2 2 |  |  |  | 2.0081 | 3 | 0-2 4 |  | 1.5063 | 6 | -4 4 0 |
| 3.0609 | 52 | 1 3 2 |  |  |  | 2.0060 | 4 | 0 4 4 |  | 1.5021 | 3 | -5-4 2 |
|  |  | 3.0557 | 7 | 0-2 2 |  |  |  | 2.0014 | 4 | 3 1 4 |  | 14 | 1.4709 | 1.4705 | 5 | -1-2 6 |
|  |  | 3.0525 | 7 | 0 3 2 |  | 25 | 1.9747 | 1.9740 | 12 | 2-1 4 |  | 1.4628 | 3 | -3-1 6 |
| 87 | 3.023 | 3.0126 | 78 | -2 2 0 |  | 1.9723 | 12 | -2 3 4 |  | 1.4622 | 6 | 3 4 6 |
|  |  | 2.9149 | 3 | -1 2 3 |  | 17 | 1.9367 | 1.9431 | 4 | -2 4 0 |  | 11 | 1.4553 | 1.4607 | 4 | 0 5 6 |
| 24 | 2.902 | 2.9045 | 26 | 2 3 0 |  | 1.9385 | 3 | -3-3-4 |  | 1.4522 | 3 | 4 6 0 |
|  |  | 2.8867 | 3 | -1-1 3 |  | 1.9359 | 7 | -4 2 0 |  | 1.4472 | 4 | 6 4 0 |
|  |  | 2.8607 | 4 | 2-1 2 |  | 1.9331 | 3 | -2-4 2 |  | 10 | 1.4278 | 1.4342 | 3 | -6-3 2 |
|  |  | 2.8585 | 4 | -2 2 2 |  | 1.9319 | 3 | 2 5 2 |  | 1.4235 | 5 | -1-6 2 |
|  |  | 2.7854 | 3 | -2-2 2 |  | 10 | 1.9029 | 1.9100 | 6 | 2 2 5 |  | 1.4228 | 5 | 1 7 2 |
| 15 | 2.771 | 2.7676 | 15 | 1-2 2 |  | 13 | 1.8878 | 1.8902 | 12 | 2 5 0 |  | 6 | 1.4003 | 1.4051 | 3 | -4 1 6 |
| 2.7650 | 15 | -1 3 2 |  | 1.8825 | 8 | 0 5 0 |  | 1.4005 | 5 | -2 6 0 |
| 100 | 2.724 | 2.7184 | 100 | 3 1 2 |  | 6 | 1.8664 | 1.8670 | 4 | 4 4 0 |  | 6 | 1.3773 | 1.3838 | 3 | 2-4 4 |
|  |  | 2.7037 | 3 | 1-1 3 |  | 20 | 1.8266 | 1.8315 | 9 | 1-4 2 |  | 1.3825 | 3 | -2 6 4 |
| 27 | 2.619 | 2.6402 | 13 | -3-1 2 |  | 1.8302 | 9 | -1 5 2 |  | 1.3706 | 4 | 5 6 2 |
| 2.6112 | 23 | 0 1 4 |  | 1.8160 | 7 | -3-4 2 |  | 15 | 1.3521 | 1.3590 | 5 | -6 0 4 |
|  |  | 2.5835 | 4 | 3-1-2 |  | 1.8151 | 7 | 3 5 2 |  | 1.3529 | 5 | -6-1 4 |
| 17 | 2.516 | 2.5169 | 6 | 0 0 4 |  | 12 | 1.7995 | 1.8023 | 4 | -3-2 4 |  | 1.3482 | 6 | 6 5 0 |
| 2.5151 | 18 | 1 1 4 |  | 1.8012 | 4 | 3 4 4 |  |  |  |  |  |  |
|  |  | 2.4653 | 3 | -1 0 4 |  | 1.7895 | 4 | -5-1 2 |  |  |  |  |  |  |
|  |  |  |  |  |  | 1.7823 | 3 | 0 4 5 |  |  |  |  |  |  |