Supplementary Table S3. Powder X-ray diffraction data (*d* in Å) for sulfatoredmondite. The calculated intensities have been scaled so that the combined intensity of the 200 and -201 lines is 100. Only calculated lines with scaled *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* |
| 35 | 11.87 | 11.9116 | 28 |  0 0 1 |  | 26 | 2.536 | 2.5520 | 8 | -5 1 4 |  |  |  | 1.8386 | 3 | -8 2 1 |
| 100 | 8.10 | 8.1625 | 36 | -2 0 1 |  | 2.5452 | 9 | -4 2 3 |  |  |  | 1.8365 | 3 |  3 3 3 |
| 8.0929 | 64 |  2 0 0 |  | 2.5283 | 18 |  4 2 1 |  |  |  | 1.8348 | 3 |  1 3 4 |
| 18 | 6.75 | 6.7050 | 15 |  1 1 0 |  |  |  | 2.5217 | 4 |  2 0 4 |  | 46 | 1.8268 | 1.8233 | 10 | -4 2 6 |
| 48 | 6.23 | 6.2454 | 60 | -1 1 1 |  | 15 | 2.482 | 2.4807 | 13 | -6 0 4 |  | 1.8206 | 24 |  2 2 5 |
|  |  | 5.9558 | 4 |  0 0 2 |  |  |  | 2.4678 | 4 | -4 0 5 |  | 22 | 1.7925 | 1.7958 | 4 |  2 4 0 |
| 46 | 5.86 | 5.8879 | 24 | -2 0 2 |  |  |  | 2.4076 | 3 | -2 2 4 |  | 1.7879 | 9 |  2 0 6 |
| 5.8101 | 21 |  2 0 1 |  |  |  | 2.4039 | 4 | -1 3 1 |  | 1.7850 | 5 | -8 2 4 |
| 24 | 5.51 | 5.5094 | 18 |  1 1 1 |  | 19 | 2.394 | 2.3951 | 16 |  2 2 3 |  | 7 | 1.7570 | 1.7634 | 3 | -3 3 5 |
| 19 | 4.80 | 4.8153 | 21 | -1 1 2 |  |  |  | 2.3823 | 3 |  0 0 5 |  | 1.7556 | 3 |  2 4 1 |
|  |  | 4.5237 | 6 | -3 1 1 |  |  |  | 2.3547 | 4 |  1 3 1 |  |  |  | 1.7230 | 3 | -10 0 2 |
| 27 | 4.344 | 4.3528 | 26 |  3 1 0 |  | 19 | 2.308 | 2.3158 | 12 |  0 2 4 |  | 21 | 1.7139 | 1.7204 | 6 |  6 0 4 |
| 76 | 4.108 | 4.1496 | 34 |  2 0 2 |  | 2.3129 | 4 | -7 1 1 |  | 1.7142 | 10 |  6 2 3 |
| 4.0813 | 53 | -4 0 2 |  | 2.2909 | 9 | -1 3 2 |  | 1.7017 | 5 |  0 0 7 |
|  |  | 4.0465 | 3 |  4 0 0 |  | 14 | 2.256 | 2.2574 | 13 | -6 2 1 |  | 36 | 1.6802 | 1.6834 | 6 |  2 4 2 |
| 23 | 3.732 | 3.7585 | 25 |  3 1 1 |  |  |  | 2.2350 | 5 |  3 3 0 |  | 1.6801 | 16 |  8 2 1 |
|  |  | 3.6834 | 4 |  0 2 0 |  | 17 | 2.180 | 2.1854 | 8 |  3 1 4 |  | 1.6787 | 9 | -4 4 2 |
|  |  | 3.6585 | 12 | -1 1 3 |  | 2.1764 | 10 |  6 2 0 |  | 1.6741 | 3 |  3 3 4 |
| 35 | 3.516 | 3.5190 | 55 |  0 2 1 |  |  |  | 2.1616 | 5 | -8 0 2 |  | 6 | 1.6379 | 1.6400 | 4 | -7 1 7 |
| 16 | 3.357 | 3.3574 | 5 | -2 2 1 |  | 8 | 2.147 | 2.1408 | 6 |  3 3 1 |  | 1.6269 | 5 | -4 2 7 |
| 3.3525 | 10 |  2 2 0 |  | 13 | 2.103 | 2.1075 | 5 | -2 0 6 |  | 19 | 1.6175 | 1.6155 | 14 | -2 2 7 |
| 45 | 3.176 | 3.1813 | 50 | -2 0 4 |  | 2.0984 | 5 | -4 0 6 |  | 19 | 1.5918 | 1.5948 | 3 |  1 1 7 |
|  |  | 3.1525 | 5 |  2 0 3 |  |  |  | 2.0808 | 4 |  2 2 4 |  | 1.5939 | 12 | -2 4 4 |
|  |  | 3.1327 | 3 |  0 2 2 |  |  |  | 2.0576 | 3 | -6 2 4 |  | 1.5907 | 3 | -4 0 8 |
| 78 | 3.115 | 3.1227 | 37 | -2 2 2 |  |  |  | 2.0502 | 3 | -4 2 5 |  | 1.5884 | 4 | -8 2 6 |
| 3.1109 | 55 |  2 2 1 |  | 30 | 2.033 | 2.0406 | 8 | -8 0 4 |  | 16 | 1.5630 | 1.5663 | 6 |  0 4 4 |
|  |  | 3.0786 | 4 | -5 1 2 |  | 2.0381 | 4 | -3 1 6 |  | 1.5632 | 9 | -10 2 3 |
| 24 | 2.969 | 2.9779 | 23 |  0 0 4 |  | 2.0326 | 8 |  4 2 3 |  | 29 | 1.5518 | 1.5555 | 16 |  4 4 2 |
| 2.9637 | 6 |  5 1 0 |  | 2.0232 | 13 |  8 0 0 |  | 1.5500 | 6 | -10 0 6 |
| 63 | 2.892 | 2.9051 | 48 |  4 0 2 |  | 11 | 1.9955 | 2.0004 | 11 |  0 2 5 |  | 1.5493 | 6 | -6 4 2 |
| 2.8820 | 9 | -1 1 4 |  |  |  | 1.9626 | 4 | -6 0 6 |  | 1.5479 | 3 | -6 4 1 |
| 41 | 2.853 | 2.8658 | 28 | -6 0 2 |  | 6 | 1.9479 | 1.9564 | 3 |  5 3 0 |  | 8 | 1.5196 | 1.5211 | 8 |  7 3 2 |
| 2.8574 | 31 | -5 1 3 |  | 1.9324 | 3 | -1 3 4 |  | 1.5120 | 4 | -9 3 2 |
| 63 | 2.779 | 2.8037 | 42 | -4 2 1 |  | 1.9249 | 6 | -5 3 3 |  | 14 | 1.4821 | 1.4890 | 4 |  0 0 8 |
| 2.7684 | 47 | -2 2 3 |  | 30 | 1.8959 | 1.8976 | 27 | -6 2 5 |  | 1.4787 | 4 | -6 4 4 |
|  |  | 2.7547 | 5 |  2 2 2 |  |  |  | 1.8793 | 4 |  6 2 2 |  | 1.4760 | 5 | -4 4 5 |
|  |  | 2.7344 | 5 | -4 2 2 |  |  |  | 1.8738 | 6 |  7 1 2 |  | 9 | 1.4636 | 1.4720 | 3 | -8 0 8 |
| 47 | 2.706 | 2.7208 | 6 | -6 0 3 |  | 19 | 1.8549 | 1.8568 | 7 | -9 1 2 |  | 1.4603 | 5 | -4 2 8 |
| 2.7004 | 36 |  0 2 3 |  | 1.8451 | 9 | -8 2 3 |  | 1.4525 | 3 |  8 0 4 |
| 2.6976 | 9 |  6 0 0 |  | 1.8417 | 18 |  0 4 0 |  |  |  |  |  |  |
| 7 | 2.576 | 2.5898 | 6 |  3 1 3 |  |  |  |  |  |  |  |  |  |  |  |  |
| 2.5852 | 8 |  1 1 4 |  |  |  |  |  |  |  |  |  |  |  |  |