Supplementary Table S2. Powder X-ray diffraction data (*d* in Å) for hydroredmondite. The calculated intensities have been scaled so that the combined intensity of the (111) and (-111) 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* |
| 29 | 9.05 | 9.0746 | 52 | -1 0 1 |  | 44 | 2.888 | 2.8933 | 16 | -2 0 4 |  | 8 | 2.0323 | 2.0382 | 3 | -4 2 4 |
| 9.0047 | 10 |  1 0 1 |  | 2.8760 | 24 | -3 1 3 |  | 2.0255 | 4 |  4 2 4 |
| 12 | 7.51 | 7.4728 | 8 |  1 1 0 |  |  |  | 2.8421 | 3 | -4 0 2 |  | 6 | 1.9487 | 1.9362 | 4 |  3 4 2 |
| 100 | 6.49 | 6.4887 | 52 | -1 1 1 |  | 40 | 2.825 | 2.8340 | 12 | -2 2 3 |  | 6 | 1.8923 | 1.8994 | 4 | -2 3 5 |
| 6.4631 | 48 |  1 1 1 |  | 2.8212 | 13 |  2 2 3 |  | 1.8874 | 5 |  0 4 4 |
|  |  | 5.3180 | 4 |  0 1 2 |  | 27 | 2.794 | 2.8011 | 21 |  3 2 2 |  | 15 | 1.8699 | 1.8739 | 4 | -5 3 2 |
| 10 | 5.25 | 5.2123 | 7 |  2 1 0 |  | 2.7771 | 8 |  2 3 0 |  | 1.8682 | 11 |  4 4 0 |
| 34 | 4.83 | 4.8261 | 20 |  2 1 1 |  | 2.7623 | 12 | -2 1 4 |  | 8 | 1.8426 | 1.8449 | 3 | -4 2 5 |
|  |  | 4.5373 | 11 | -2 0 2 |  | 32 | 2.729 | 2.7246 | 4 |  1 3 2 |  | 4 | 1.8285 | 1.8358 | 4 |  3 4 3 |
| 14 | 4.396 | 4.3699 | 8 |  0 2 1 |  | 2.7175 | 19 | -2 3 1 |  | 13 | 1.8011 | 1.8009 | 6 |  5 0 5 |
| 4.3549 | 6 |  1 2 0 |  | 2.7137 | 3 |  2 3 1 |  | 1.7975 | 3 | -4 4 2 |
| 8 | 4.102 | 4.1319 | 3 | -1 2 1 |  | 9 | 2.605 | 2.6062 | 8 |  4 2 0 |  | 1.7931 | 4 |  4 4 2 |
| 4.0816 | 3 |  1 0 3 |  | 2.5983 | 6 |  1 2 4 |  | 12 | 1.7750 | 1.7809 | 3 |  7 0 1 |
| 16 | 3.955 | 4.0046 | 7 | -3 0 1 |  | 18 | 2.530 | 2.5381 | 3 |  1 0 5 |  | 1.7666 | 6 |  1 5 2 |
| 3.9208 | 15 |  0 1 3 |  | 2.5341 | 5 | -3 2 3 |  | 12 | 1.7577 | 1.7566 | 5 |  6 0 4 |
| 23 | 3.777 | 3.7748 | 10 |  0 2 2 |  | 2.5165 | 8 |  0 3 3 |  | 1.7542 | 3 | -6 2 3 |
|  |  | 3.7512 | 3 | -1 1 3 |  | 13 | 2.493 | 2.4995 | 12 |  0 1 5 |  | 9 | 1.7413 | 1.7490 | 3 |  7 1 1 |
| 21 | 3.720 | 3.7363 | 23 |  1 1 3 |  | 2.4909 | 3 |  3 3 0 |  | 1.7377 | 4 | -6 1 4 |
| 46 | 3.638 | 3.6770 | 12 | -3 1 1 |  | 2.4831 | 4 | -3 1 4 |  | 10 | 1.7201 | 1.7216 | 3 |  0 2 7 |
| 3.6630 | 11 |  3 1 1 |  | 20 | 2.461 | 2.4771 | 5 | -5 0 1 |  | 1.7206 | 3 |  6 3 1 |
| 3.6204 | 26 | -1 2 2 |  | 2.4659 | 6 |  3 1 4 |  | 16 | 1.6941 | 1.6911 | 5 |  3 0 7 |
|  |  | 3.5862 | 3 |  2 2 1 |  | 6 | 2.437 | 2.4441 | 12 |  2 2 4 |  | 1.6859 | 6 | -4 3 5 |
| 24 | 3.309 | 3.3183 | 15 |  2 1 3 |  | 3 | 2.331 | 2.3406 | 3 | -2 3 3 |  | 11 | 1.6800 | 1.6769 | 5 |  4 3 5 |
| 3.2857 | 5 |  3 1 2 |  | 2.3290 | 4 | -3 3 2 |  | 6 | 1.6675 | 1.6659 | 5 |  2 4 5 |
| 8 | 3.243 | 3.2444 | 4 | -2 2 2 |  |  |  | 2.2842 | 4 |  0 4 1 |  | 8 | 1.6503 | 1.6530 | 3 | -6 2 4 |
| 3.2315 | 5 |  2 2 2 |  | 8 | 2.268 | 2.2686 | 3 | -4 0 4 |  | 1.6438 | 5 | -3 5 2 |
| 14 | 3.131 | 3.1497 | 10 |  4 0 0 |  | 2.2652 | 4 |  0 2 5 |  | 9 | 1.6341 | 1.6294 | 7 |  3 3 6 |
| 3.1139 | 5 |  3 2 0 |  |  |  | 2.2512 | 4 |  4 0 4 |  | 1.6218 | 4 |  7 2 2 |
| 14 | 3.060 | 3.0731 | 4 | -1 2 3 |  | 5 | 2.238 | 2.2155 | 5 | -3 0 5 |  | 8 | 1.5730 | 1.5748 | 4 |  8 0 0 |
| 3.0626 | 9 |  0 1 4 |  | 12 | 2.192 | 2.2038 | 4 | -4 1 4 |  | 13 | 1.5532 | 1.5517 | 3 | -2 1 8 |
| 52 | 3.017 | 3.0240 | 13 |  3 2 1 |  | 2.1877 | 4 |  4 1 4 |  | 1.5470 | 3 |  0 6 0 |
| 3.0096 | 24 |  0 3 1 |  | 9 | 2.161 | 2.1538 | 8 | -1 4 2 |  | 1.5461 | 3 |  2 1 8 |
|  |  | 3.0016 | 4 |  3 0 3 |  |  |  | 2.1265 | 3 | -5 1 3 |  | 8 | 1.5373 | 1.5313 | 3 |  0 2 8 |
|  |  | 2.9709 | 4 |  1 1 4 |  | 23 | 2.107 | 2.1130 | 10 |  5 1 3 |  | 14 | 1.5089 | 1.5152 | 4 | -7 3 2 |
| 16 | 2.928 | 2.9284 | 8 | -1 3 1 |  | 2.1001 | 9 | -5 2 2 |  | 1.5020 | 3 | -4 5 3 |
| 2.9115 | 18 | -4 1 1 |  | 8 | 2.071 | 2.0801 | 3 | -1 1 6 |  | 1.4988 | 3 | -5 0 7 |
|  |  | 2.9022 | 12 |  4 1 1 |  | 2.0626 | 6 |  2 4 2 |  | 1.4981 | 3 |  4 5 3 |