Powder X-ray data (*d* in Å) for donowensite.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *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* |
| 100 | 9.88 | 9.8474 | 100 |  0 0 1 |  | 12 | 2.414 | 2.4241 | 4 |  0 4 0 |  | 2 | 1.7043 | 1.7013 | 3 | -3-2 4 |
|   |   | 9.6965 | 3 |  0 1 0 |  | 2.4154 | 2 |  0-4 1 |  |   |   | 1.6605 | 2 | -1 0 6 |
| 24 | 7.12 | 7.1163 | 22 |  1 0 0 |  | 2.3982 | 4 | -3 0 1 |  |   |   | 1.6558 | 1 | -3 0 5 |
|   |   | 6.5630 | 2 |  0 1 1 |  | 8 | 2.285 | 2.2979 | 4 |  0-2 4 |  | 6 | 1.6119 | 1.6185 | 1 |  4-2 2 |
| 15 | 6.33 | 6.3824 | 3 | -1 1 0 |  | 2.2902 | 1 | -3 0 2 |  | 1.6138 | 4 |  2 0 5 |
| 6.2819 | 11 | -1 0 1 |  | 2.2747 | 1 |  0-4 2 |  | 15 | 1.5916 | 1.6039 | 1 |  3-2 4 |
|   |   | 5.5546 | 1 | -1 1 1 |  | 9 | 2.257 | 2.2673 | 4 |  1 2 3 |  | 1.5956 | 3 | -4 4 0 |
| 4 | 5.39 | 5.3623 | 3 |  1 0 1 |  | 2.2602 | 5 | -2-2 3 |  | 1.5946 | 6 | -4 4 1 |
| 2 | 5.16 | 5.1771 | 2 |  1-1 1 |  | 2.2410 | 1 |  1-4 2 |  | 1.5939 | 3 | -2 0 6 |
|   |   | 5.0289 | 1 | -1-1 1 |  | 6 | 2.217 | 2.2254 | 4 | -1-2 4 |  | 1.5912 | 2 |  4 0 2 |
| 2 | 4.94 | 4.9237 | 2 |  0 0 2 |  | 2.2048 | 1 |  2-2 3 |  | 1.5825 | 1 |  3 0 4 |
| 5 | 4.55 | 4.5493 | 3 |  0-2 1 |  | 2.1965 | 1 | -3 2 2 |  | 8 | 1.5675 | 1.5730 | 2 |  3 2 3 |
|   |   | 4.4446 | 1 | -1 2 0 |  |   |   | 2.1834 | 1 | -1-4 1 |  | 1.5714 | 3 | -3-4 1 |
| 4 | 4.40 | 4.4040 | 3 | -1 0 2 |  | 9 | 2.1681 | 2.1696 | 1 | -2 4 1 |  | 1.5705 | 1 | -4 0 4 |
|   |   | 4.2099 | 1 |  0 1 2 |  | 2.1655 | 1 |  1 4 0 |  | 1.5687 | 1 | -2 6 1 |
| 17 | 4.176 | 4.1742 | 11 |  0 2 1 |  | 2.1614 | 6 |  2 2 2 |  | 1.5567 | 3 | -3-4 2 |
| 8 | 4.059 | 4.0571 | 4 | -1 2 1 |  | 2 | 2.1009 | 2.1050 | 3 |  0 2 4 |  | 7 | 1.5396 | 1.5469 | 1 |  3 4 0 |
|   |   | 4.0451 | 1 |  1-2 1 |  |   |   | 2.0595 | 1 |  0-4 3 |  | 1.5440 | 4 | -4 2 4 |
|   |   | 3.9687 | 1 | -1-1 2 |  | 9 | 2.0254 | 2.0285 | 1 | -2 4 2 |  | 1.5343 | 2 |  2-6 2 |
| 3 | 3.780 | 3.7680 | 3 |  1 0 2 |  | 2.0225 | 2 |  2-4 2 |  |   |   | 1.5184 | 1 |  1-6 3 |
| 20 | 3.671 | 3.6771 | 4 |  1 2 0 |  | 2.0172 | 1 |  3-2 2 |  | 9 | 1.5073 | 1.5116 | 1 |  1 6 0 |
| 3.6584 | 9 |  0-2 2 |  | 2.0149 | 1 |  1-4 3 |  | 1.5058 | 1 |  0 2 6 |
| 3.6512 | 5 | -1-2 1 |  | 2.0110 | 1 |  3 0 2 |  | 1.5050 | 1 | -2 6 2 |
| 5 | 3.593 | 3.5582 | 3 |  2 0 0 |  | 3 | 1.9864 | 1.9843 | 2 | -2-2 4 |  | 1.5038 | 2 | -1-6 2 |
|   |   | 3.5386 | 1 | -2 0 1 |  | 1.9793 | 1 |  3 2 0 |  | 1.4946 | 2 |  4-2 3 |
|   |   | 3.3057 | 3 | -1 2 2 |  | 1 | 1.9363 | 1.9437 | 2 | -1-4 3 |  | 1.4847 | 2 |  4-4 2 |
| 44 | 3.283 | 3.2927 | 4 |  1-2 2 |  |   |   | 1.9158 | 1 | -1 4 3 |  | 7 | 1.4759 | 1.4806 | 1 | -4 4 3 |
| 3.2825 | 15 |  0 0 3 |  | 10 | 1.8879 | 1.8978 | 3 |  0-2 5 |  | 1.4769 | 1 | -2 4 5 |
| 3.2699 | 12 |  1 2 1 |  | 1.8840 | 1 |  2 0 4 |  | 1.4711 | 3 |  2-4 5 |
| 22 | 3.202 | 3.2159 | 13 | -1-2 2 |  | 1.8828 | 2 |  1 4 2 |  | 7 | 1.4556 | 1.4659 | 1 |  4 0 3 |
| 3.1912 | 2 | -2 2 0 |  | 1.8805 | 2 |  2-2 4 |  | 1.4645 | 2 |  1 6 1 |
| 3.1825 | 4 |  2 0 1 |  | 1.8794 | 2 | -3 4 1 |  | 1.4553 | 1 |  2-6 3 |
|   |   | 3.1410 | 3 | -2 0 2 |  | 15 | 1.8597 | 1.8696 | 1 | -3 0 4 |  | 1.4503 | 2 | -1-6 3 |
| 19 | 3.110 | 3.1067 | 15 | -2 2 1 |  | 1.8646 | 1 | -2-4 1 |  | 6 | 1.4346 | 1.4466 | 1 | -5 2 0 |
|   |   | 3.0420 | 1 | -1-1 3 |  | 1.8582 | 1 | -2 0 5 |  | 1.4443 | 1 | -4 0 5 |
|   |   | 2.9769 | 1 |  0 3 1 |  | 1.8563 | 6 |  0 4 3 |  | 1.4419 | 1 | -5 2 2 |
| 26 | 2.973 | 2.9695 | 22 |  2-2 1 |  | 11 | 1.8347 | 1.8465 | 1 |  3-4 1 |  | 1.4328 | 2 | -1 6 3 |
|   |   | 2.8660 | 2 |  0-2 3 |  | 1.8436 | 3 | -2 4 3 |  | 1.4286 | 1 | -3-4 4 |
|   |   | 2.8478 | 1 |  2 1 1 |  | 1.8368 | 1 |  2-4 3 |  | 9 | 1.4172 | 1.4236 | 1 |  0-6 4 |
|   |   | 2.8093 | 1 |  1 0 3 |  | 1.8292 | 5 |  0-4 4 |  | 1.4202 | 1 | -3 6 2 |
| 15 | 2.775 | 2.7773 | 12 | -2 2 2 |  | 1.8223 | 1 |  1 0 5 |  | 1.4184 | 2 |  1-6 4 |
| 2.7347 | 5 |  1 2 2 |  |   |   | 1.8050 | 1 |  3-2 3 |  | 1.4171 | 2 | -4 2 5 |
| 13 | 2.684 | 2.6812 | 10 |  2 0 2 |  | 7 | 1.7987 | 1.8037 | 2 | -4 0 1 |  | 1.4118 | 1 | -1-4 6 |
|   |   | 2.6455 | 1 | -1 2 3 |  | 1.8025 | 1 | -4 2 1 |  | 8 | 1.3935 | 1.4064 | 2 |  3 4 2 |
| 9 | 2.622 | 2.6400 | 5 | -2 0 3 |  | 1.7909 | 4 | -3 2 4 |  | 1.4046 | 1 |  2 0 6 |
| 2.6355 | 1 |  1-2 3 |  |   |   | 1.7791 | 1 |  4 0 0 |  | 1.4041 | 1 |  5-2 1 |
| 2.6274 | 1 |  2 2 0 |  | 3 | 1.7683 | 1.7693 | 1 | -4 0 2 |  | 1.3955 | 1 | -5 2 3 |
| 2.5909 | 4 |  0 2 3 |  | 1.7594 | 1 |  0 2 5 |  | 1.3925 | 1 | -5 0 3 |
|   |   | 2.5885 | 2 |  2-2 2 |  | 1.7551 | 1 |  2 4 1 |  | 1.3920 | 1 |  0-2 7 |
| 2 | 2.513 | 2.5145 | 4 | -2-2 2 |  | 4 | 1.7379 | 1.7368 | 2 | -2 2 5 |  | 1.3914 | 1 |  0 6 3 |
| 16 | 2.450 | 2.4619 | 1 |  0 0 4 |  | 1.7334 | 1 | -2-2 5 |  | 1.3891 | 1 | -2 0 7 |
| 2.4501 | 6 | -1 4 0 |  | 1.7327 | 1 | -2-4 3 |  | 1.3887 | 1 | -4 4 4 |
| 2.4314 | 5 |  2 2 1 |  | 1.7306 | 2 |  3 2 2 |  |  |  |  |  |  |

Powder X-ray data (*d* in Å) for mikehowardite.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |  | *I*obs | *d*obs | *d*calc | *I*calc | *hkl* |
| 86 | 8.80 | 8.7478 | 74 |  0 0 1 |  | 13 | 1.9456 | 1.9447 | 3 |  2 1 4 |
| 100 | 6.45 | 6.4245 | 100 |  1 0 0 |  | 1.9396 | 6 |  0-1 4 |
|   |   | 5.2795 | 4 |  1 0 1 |  | 2 | 1.8720 | 1.8607 | 2 | -3 1 1 |
| 27 | 5.16 | 5.1656 | 10 |  1 1 0 |  | 7 | 1.8454 | 1.8552 | 2 |  2 3 3 |
| 5.0823 | 11 | -1 0 1 |  | 1.8378 | 4 |  3-1 1 |
| 13 | 4.65 | 4.6525 | 10 |  0-1 1 |  |   |   | 1.8117 | 2 |  3 2 3 |
| 4 | 4.051 | 4.0318 | 3 | -1 1 0 |  | 9 | 1.7726 | 1.7751 | 6 | -2 0 4 |
| 6 | 3.844 | 3.8308 | 7 | -1 1 1 |  | 17 | 1.7555 | 1.7609 | 3 |  3 3 1 |
| 29 | 3.693 | 3.6845 | 22 |  1 0 2 |  | 1.7556 | 3 | -3 1 2 |
| 34 | 3.273 | 3.2745 | 16 |  0-1 2 |  | 1.7491 | 5 |  0-3 2 |
|   |   | 3.2122 | 4 |  2 0 0 |  | 6 | 1.7210 | 1.7307 | 2 |  3 3 2 |
| 88 | 3.198 | 3.2077 | 41 |  1 2 1 |  | 1.7272 | 2 | -2 1 4 |
| 3.1921 | 12 |  2 1 0 |  | 1.7094 | 3 |  1 2 5 |
|   |   | 3.1481 | 2 | -1 1 2 |  | 16 | 1.6660 | 1.6652 | 10 |  1 4 1 |
| 25 | 3.130 | 3.1454 | 24 |  0 2 0 |  | 13 | 1.6304 | 1.6372 | 2 |  0-2 4 |
|   |   | 3.1425 | 2 |  1 2 0 |  | 1.6321 | 6 |  2-1 4 |
|   |   | 3.0550 | 5 |  2 0 1 |  | 19 | 1.6108 | 1.6213 | 2 |  1 4 0 |
| 50 | 2.982 | 2.9772 | 39 | -2 0 1 |  | 1.6141 | 4 |  2 4 1 |
| 59 | 2.909 | 2.9159 | 33 |  0 0 3 |  | 1.6131 | 4 |  1-3 2 |
| 2.8959 | 15 |  1 2 2 |  | 18 | 1.5990 | 1.6012 | 4 |  4 1 2 |
| 2.8642 | 7 |  0 2 2 |  | 1.5987 | 9 |  0-1 5 |
| 31 | 2.792 | 2.8096 | 6 |  1-1 2 |  | 1.5955 | 3 | -3 2 1 |
| 2.8034 | 4 |  1 1 3 |  | 12 | 1.5658 | 1.5686 | 2 | -4 0 1 |
| 2.7749 | 14 |  0-2 1 |  | 1.5670 | 4 | -2 3 2 |
| 4 | 2.694 | 2.6960 | 3 |  1 0 3 |  | 11 | 1.5434 | 1.5511 | 3 |  1-2 4 |
| 26 | 2.632 | 2.6397 | 7 |  2 0 2 |  | 1.5481 | 3 |  1 3 5 |
| 2.6315 | 7 |  2 2 1 |  | 1.5420 | 3 | -3 2 2 |
| 2.6163 | 6 | -1 0 3 |  | 6 | 1.5087 | 1.5044 | 2 |  4 1 3 |
| 12 | 2.576 | 2.5876 | 8 | -1 2 0 |  | 1.5005 | 2 | -3 0 4 |
| 2.5460 | 3 | -2 1 1 |  | 9 | 1.4854 | 1.4870 | 2 |  1 1 6 |
| 5 | 2.468 | 2.4669 | 3 |  2-1 1 |  | 1.4775 | 3 |  1 4 4 |
| 11 | 2.413 | 2.4147 | 6 |  0 2 3 |  | 16 | 1.4649 | 1.4671 | 4 |  4 3 2 |
| 2.4042 | 6 | -1 2 2 |  | 1.4605 | 3 | -1 4 2 |
| 4 | 2.333 | 2.3335 | 2 |  2 1 3 |  | 18 | 1.4509 | 1.4558 | 3 |  1-3 3 |
| 10 | 2.191 | 2.1870 | 5 |  0 0 4 |  | 1.4477 | 2 |  0 2 6 |
| 30 | 2.145 | 2.1472 | 6 |  0 3 1 |  | 1.4459 | 5 | -2-1 5 |
| 2.1415 | 15 |  3 0 0 |  | 8 | 1.4152 | 1.4164 | 2 | -1-4 2 |
|   |   | 2.1127 | 3 | -1 2 3 |  |   | 1.4101 | 3 |  3-1 4 |
| 23 | 2.085 | 2.0959 | 7 |  1 0 4 |  | 8 | 1.3818 | 1.3804 | 3 |  3 3 5 |
| 2.0741 | 8 | -3-1 1 |  | 4 | 1.3701 | 1.3685 | 2 | -1 2 6 |
| 2.0612 | 6 | -3 0 1 |  | 1.3659 | 2 |  1 3 6 |
| 16 | 2.047 | 2.0442 | 4 | -2-2 2 |  | 8 | 1.3260 | 1.3277 | 2 | -3 3 2 |
| 2.0338 | 2 |  1 2 4 |  | 1.3195 | 2 | -4-2 3 |
|   |   | 2.0152 | 2 | -2 2 1 |  | 8 | 1.3089 | 1.3072 | 3 |  4-1 3 |
|  |  |  |  |  |  | 1.3063 | 2 |  3-3 1 |