Table S2. Powder X-ray diffraction data (*d* in Å) for hayelasdiite. Only calculated lines with *I* > 1.5 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* |
| 84 | 14.38 | 14.3024 | 100 |  0 1 0 |  | 58 | 2.868 | 2.9084 | 18 | -2-1 4 |  | 8 | 1.9100 | 1.9154 | 2 |  2-2 8 |
| 5 | 8.63 | 8.5450 | 4 |  0-1 2 |  | 2.8869 | 5 |  1 1 5 |  | 1.9097 | 3 | -2 3 6 |
| 72 | 6.88 | 6.9369 | 18 | -1 0 1 |  | 2.8608 | 22 |  2-1 4 |  | 1.9036 | 2 | -1 7 1 |
| 6.8472 | 20 |  1 0 1 |  | 2.8575 | 3 | -2 0 4 |  | 1.8967 | 3 |  1 7 1 |
| 17 | 6.57 | 6.5877 | 16 |  0 1 2 |  | 2.8427 | 6 | -2-2 4 |  | 32 | 1.8805 | 1.8830 | 5 |  2 3 6 |
| 6.4974 | 8 |  0-2 2 |  | 10 | 2.800 | 2.8077 | 2 |  2 0 4 |  | 1.8799 | 10 |  4 0 0 |
| 14 | 5.95 | 5.9867 | 7 | -1 1 1 |  | 2.8028 | 4 |  2-2 4 |  | 1.8700 | 3 |  2-6 6 |
| 5.9070 | 3 |  1 1 1 |  | 13 | 2.684 | 2.6704 | 6 |  0 1 6 |  | 1.8688 | 2 | -2-4 8 |
| 14 | 5.29 | 5.2799 | 7 | -1-2 1 |  | 2.6677 | 2 | -2 3 2 |  | 9 | 1.8572 | 1.8673 | 2 |  1-4 9 |
| 5.2704 | 6 |  1-2 1 |  | 14 | 2.644 | 2.6402 | 4 |  0-4 6 |  | 1.8625 | 2 |  4 1 0 |
| 20 | 4.79 | 4.8574 | 7 |  0 2 2 |  | 2.6356 | 6 |  2 3 2 |  | 1.8603 | 2 |  0-8 2 |
| 4.7970 | 10 |  0-3 2 |  |  |  | 2.5983 | 2 | -2 4 0 |  | 1.8470 | 2 |  1 0 9 |
| 4.7246 | 4 | -1 2 1 |  | 15 | 2.524 | 2.5469 | 6 | -1 5 1 |  | 1.8461 | 2 |  2-4 8 |
| 7 | 4.66 | 4.6744 | 5 |  1 2 1 |  | 2.5339 | 3 |  1 5 1 |  | 16 | 1.7991 | 1.8113 | 4 | -1-8 3 |
| 4.4963 | 3 |  0-1 4 |  | 2.5073 | 17 |  0 5 2 |  | 1.7965 | 3 | 0 -2 10 |
| 23 | 4.28 | 4.3064 | 7 |  0 0 4 |  | 16 | 2.494 | 2.4977 | 3 | -2 2 4 |  | 1.7908 | 3 | -2-5 8 |
| 4.2725 | 3 |  0-2 4 |  | 2.4889 | 8 |  0-6 2 |  | 17 | 1.7645 | 1.7750 | 2 | -3 3 5 |
| 54 | 3.797 | 3.8304 | 15 |  0 1 4 |  | 11 | 2.420 | 2.4331 | 4 |  0 2 6 |  | 1.7719 | 3 |  2-5 8 |
| 3.7829 | 21 |  0-3 4 |  | 2.4012 | 2 |  0-5 6 |  | 1.7616 | 5 | -2 4 6 |
|  |  | 3.7669 | 2 | -1-3 3 |  | 23 | 2.343 | 2.3623 | 2 | -2 4 2 |  | 1.7528 | 2 | -4-3 2 |
|  |  | 3.7400 | 2 |  1-3 3 |  | 2.3457 | 2 | -1-6 3 |  | 20 | 1.7377 | 1.7395 | 6 |  2 4 6 |
|  |  | 3.7100 | 5 |  1 3 1 |  | 2.3397 | 4 |  1-6 1 |  | 1.7365 | 2 | -2-7 6 |
| 12 | 3.632 | 3.7011 | 3 |  0-4 2 |  | 2.3375 | 7 | -2-5 2 |  | 1.7270 | 4 |  2-7 6 |
|  |  | 3.6413 | 2 | -2 1 0 |  | 2.3230 | 2 | -3 2 1 |  | 12 | 1.6996 | 1.6993 | 2 | -4 1 4 |
|  |  | 3.5756 | 6 |  0 4 0 |  |  |  | 2.3016 | 2 | -2 0 6 |  | 1.6910 | 3 | -4-3 4 |
| 100 | 3.331 | 3.3357 | 30 | -2 2 0 |  |  |  | 2.2861 | 2 | -2-3 6 |  | 22 | 1.6705 | 1.6824 | 2 | -2 6 4 |
| 3.3320 | 2 | -1-4 1 |  | 38 | 2.261 | 2.2751 | 2 | -3-2 3 |  | 1.6809 | 2 | -2 7 2 |
| 3.3202 | 24 |  2 2 0 |  | 2.2711 | 2 | -2 3 4 |  | 1.6761 | 3 |  4-3 4 |
| 3.2938 | 10 |  0 2 4 |  | 2.2625 | 5 |  2 0 6 |  | 1.6689 | 5 |  2 7 2 |
|  |  | 3.2884 | 2 | -2 1 2 |  | 2.2550 | 3 |  2-3 6 |  | 1.6662 | 2 |  2 6 4 |
| 55 | 3.243 | 3.2638 | 10 | -1-1 5 |  | 2.2482 | 7 |  0-2 8 |  | 1.6615 | 3 | -2-8 4 |
| 3.2487 | 17 |  0-4 4 |  | 2.2417 | 2 | -2-5 4 |  | 1.6591 | 3 |  2-8 4 |
| 3.2427 | 3 |  2-2 2 |  |  |  | 2.2289 | 3 |  2-5 4 |  | 13 | 1.6223 | 1.6330 | 2 | -4-4 4 |
| 3.2206 | 10 |  1-1 5 |  |  |  | 2.2162 | 3 |  0-3 8 |  | 1.6213 | 3 |  4-4 4 |
|  |  | 3.1978 | 2 | -1-4 3 |  |  |  | 2.1954 | 2 | -2 1 6 |  | 1.6191 | 3 |  0 6 6 |
|  |  | 3.1112 | 4 |  1 0 5 |  | 12 | 2.174 | 2.1732 | 4 | -2-4 6 |  | 6 | 1.6012 | 1.6023 | 2 | -4 4 2 |
|  |  | 3.0439 | 3 | -1 4 1 |  | 2.1658 | 2 |  0-6 6 |  | 1.5990 | 2 |  0-9 6 |
|  |  | 3.0246 | 2 |  1 4 1 |  |  |  | 2.0911 | 2 |  1 4 5 |  | 1.5907 | 3 | -4-5 2 |
| 73 | 3.006 | 3.0175 | 10 | -1-3 5 |  | 27 | 2.071 | 2.0761 | 3 |  2-6 2 |  | 11 | 1.5816 | 1.5867 | 2 |  4 4 2 |
| 3.0097 | 7 |  0 4 2 |  | 2.0747 | 3 | -2-6 2 |  | 1.5767 | 3 | -2 0 10 |
| 2.9933 | 7 | -2 2 2 |  | 2.0725 | 6 | -3-1 5 |  | 1.5746 | 4 | 0 2 10 |
| 2.9889 | 9 |  1-3 5 |  | 21 | 2.037 | 2.0432 | 6 |  0 7 0 |  | 8 | 1.5505 | 1.5556 | 4 | 2 0 10 |
| 2.9837 | 7 |  0-5 2 |  | 2.0395 | 3 |  3-1 5 |  | 1.5501 | 2 | -4 1 6 |
|  |  | 2.9770 | 2 |  0-2 6 |  | 2.0260 | 2 | -2-6 4 |  | 8 | 1.5181 | 1.5247 | 2 |  4 1 6 |
| 72 | 2.941 | 2.9653 | 6 | -2-3 2 |  | 2.0182 | 2 |  2-6 4 |  | 1.5115 | 2 | -4 5 2 |
| 2.9603 | 7 | -2 3 0 |  |  |  | 2.0032 | 2 | -3-3 5 |  | 23 | 1.4965 | 1.5017 | 2 |  0-9 8 |
| 2.9535 | 13 |  2 2 2 |  | 4 | 1.9790 | 1.9782 | 3 |  3-3 5 |  | 1.4969 | 3 |  4 5 2 |
| 2.9442 | 7 |  2 3 0 |  | 9 | 1.9343 | 1.9447 | 3 |  3 1 5 |  | 1.4919 | 2 | 0 -10 4 |
| 2.9231 | 10 | -1 1 5 |  | 1.9393 | 3 | -1-2 9 |  | 1.4889 | 2 | 0 3 10 |
|  |  |  |  |  |  | 1.9301 | 2 | -2-1 8 |  | 10 | 1.4709 | 1.4756 | 2 |  4 2 6 |
|  |  |  |  |  |  |  |  |  |  |  |  | 1.4729 | 2 | -3 4 7 |