**Electronic Supplementary Material ESM1** The calculated powder patterns for alfredcasparite (Cu*K*α= 1.5406 Å, Bragg-Brentano geometry, fixed slit, no anomalous dispersion). Lines with relative intensities below 2 % are omitted

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| I[%] | d[Å] | *h* | *k* | *l* |  | I[%] | d[Å] | *h* | *k* | *l* |
| 5.5 | 5.024 | 0 | 0 | 1 |  | 7.5 | 1.573 | 4 | 1 | 2 |
| 2.5 | 4.160 | 2 | 0 | 0 |  | 4.6 | 1.553 | 2 | 0 | 3 |
| 11.3 | 3.820 | 1 | 1 | 1 |  | 5.0 | 1.552 | 5 | 1 | 1 |
| 4.5 | 3.721 | 2 | 1 | 0 |  | 6.2 | 1.546 | 3 | 3 | 2 |
| **39.8** | 3.204 | 2 | 0 | 1 |  | 11.8 | 1.527 | 2 | 1 | 3 |
| **100.0** | 2.990 | 2 | 1 | 1 |  | 2.9 | 1.495 | 4 | 2 | 2 |
| 11.8 | 2.942 | 2 | 2 | 0 |  | 7.8 | 1.477 | 5 | 2 | 1 |
| **28.9** | 2.631 | 3 | 1 | 0 |  | 2.2 | 1.471 | 4 | 4 | 0 |
| **17.7** | 2.512 | 0 | 0 | 2 |  | 2.9 | 1.427 | 5 | 3 | 0 |
| 6.6 | 2.331 | 3 | 1 | 1 |  | 4.2 | 1.387 | 6 | 0 | 0 |
| 3.5 | 2.150 | 2 | 0 | 2 |  | 2.3 | 1.373 | 5 | 3 | 1 |
| 2.2 | 2.097 | 3 | 2 | 1 |  | 6.7 | 1.289 | 4 | 1 | 3 |
| **16.5** | 2.082 | 2 | 1 | 2 |  | 3.2 | 1.273 | 3 | 3 | 3 |
| 2.3 | 2.080 | 4 | 0 | 0 |  | 4.9 | 1.273 | 6 | 2 | 1 |
| **15.3** | 2.018 | 4 | 1 | 0 |  | 3.5 | 1.258 | 5 | 4 | 1 |
| 6.6 | 1.961 | 3 | 3 | 0 |  | 2.9 | 1.241 | 5 | 3 | 2 |
| 2.4 | 1.922 | 4 | 0 | 1 |  | 4.2 | 1.214 | 6 | 0 | 2 |
| 4.1 | 1.910 | 2 | 2 | 2 |  | 2.4 | 1.169 | 5 | 1 | 3 |
| 14.9 | 1.872 | 4 | 1 | 1 |  | 2.3 | 1.154 | 5 | 4 | 2 |
| 8.0 | 1.860 | 4 | 2 | 0 |  | 4.0 | 1.136 | 5 | 2 | 3 |
| 13.5 | 1.827 | 3 | 3 | 1 |  | 3.2 | 1.133 | 3 | 1 | 4 |
| **15.7** | 1.817 | 3 | 1 | 2 |  | 2.4 | 1.114 | 7 | 2 | 1 |