|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Table S1b**. Calculated X-ray powder diffraction data (*I*calc. > 1, *d* in Å) for silesiaite from Häiviäntien, Finland. | | | | | | | | |
| *d*calc. | *Ic*alc. | *h k l* | *d*calc. | *Ic*alc. | *h k l* | *d*calc. | *Ic*alc. | *h k l* |
| 6.272 | 2.7 | 0 0 2 | 2.056 | 11.7 | -4 2 0, 4 2 0 | 1.513 | 1.6 | -2 -4 6, -2 4 6 |
| 6.157 | 5.1 | -1 1 1, -1 -1 1 | 2.001 | 13.5 | -4 -2 4, -4 2 4 | 1.502 | 6.3 | 3 1 6, 3 -1 6, 5 -3 1, 5 3 1 |
| **5.188** | **67.7** | **1 1 1, 1 -1 1** | 1.988 | 4.4 | 3 3 1, 3 -3 1 | 1.492 | 10.9 | -3 5 1, -3 -5 1, -1 -5 4, -1 5 4 |
| 5.005 | 3.1 | -1 1 2, -1 -1 2 | 1.945 | 2.5 | 1 -3 4, 1 3 4 | 1.479 | 2.1 | -4 4 5, -4 -4 5 |
| 4.723 | 8.6 | 2 0 0 | 1.944 | 15.3 | -2 -2 6, -2 2 6 | 1.475 | 1.2 | -3 5 0, 3 5 0 |
| **4.558** | **30.6** | **-2 0 2** | 1.929 | 2.2 | -5 1 3, -5 -1 3 | 1.468 | 3.1 | 0 -2 8, 0 2 8 |
| 4.172 | 7.6 | 0 2 0 | 1.925 | 1.9 | -2 -4 2, -2 4 2 | 1.464 | 12.8 | -4 -2 8, -4 2 8 |
| 4.015 | 2.3 | 1 1 2, 1 -1 2 | 1.913 | 6.7 | -5 -1 1, -5 1 1 | 1.455 | 1.3 | -5 -3 6, -5 3 6 |
| 3.959 | 1.0 | 0 -2 1, 0 2 1 | 1.897 | 3.6 | -2 -4 2, -2 4 2 | 1.449 | 2.5 | 1 -1 8, 1 1 8 |
| 3.888 | 16.8 | -1 1 3, -1 -1 3 | 1.871 | 1.2 | -5 1 4, -5 -1 4 | 1.445 | 1.3 | 4 4 2, 4 -4 2 |
| 3.474 | 5.9 | 0 2 2, 0 -2 2 | 1.869 | 3.6 | 0 2 6, 0 -2 6 | 1.442 | 1.6 | -3 1 9, -3 -1 9 |
| 3.291 | 4.5 | 2 0 2 | 1.867 | 10.4 | 0 4 3, 0 -4 3 | 1.430 | 1.2 | 2 -4 5, 2 4 5 |
| 3.202 | 10.2 | -2 2 1, -2 -2 1 | 1.861 | 1.2 | 3 3 2, 3 -3 2 | 1.429 | 1.3 | 5 -3 2, 5 3 2 |
| 3.173 | 7.3 | 1 1 3, 1 -1 3 | 1.831 | 5.1 | -1 1 7, -1 -1 7 | 1.428 | 11.7 | -6 -2 6, -6 2 6, 1 3 7, 1 -3 7, -1 1 9, -1 -1 9 |
| **3.136** | **63.5** | **0 0 4** | 1.808 | 6.0 | -3 3 5, -3 -3 5 | 1.414 | 1.4 | 6 2 1, 6 -2 1 |
| 3.128 | 2.8 | 2 2 0, -2 2 0, -2 0 4 | 1.807 | 5.3 | 4 2 2, 4 -2 2 | 1.408 | 3.2 | -7 -1 3, -7 1 3 |
| **3.087** | **25.1** | **-3 1 1, -3 -1 1** | 1.778 | 6.2 | 2 2 5, 2 -2 5 | 1.407 | 1.0 | -4 4 6, -4 -4 6 |
| **3.078** | **100.0** | **-2 -2 2, -2 2 2** | 1.762 | 1.5 | 2 -4 2, 2 4 2 | 1.398 | 4.2 | -7 1 2, -7 -1 2 |
| 3.051 | 16.6 | -3 1 2, -3 -1 2 | 1.749 | 3.3 | 1 -3 5, 1 3 5 | 1.391 | 2.6 | 0 6 0 |
| 2.954 | 1.3 | 0 -2 3, 0 2 3 | 1.737 | 1.3 | 0 -4 4, 0 4 4 | 1.377 | 15.3 | -5 3 7, -5 -3 7 |
| 2.891 | 26.2 | 2 2 1, 2 -2 1 | 1.736 | 1.3 | -2 4 4, -2 -4 4 | 1.375 | 1.9 | -7 1 5, -7 -1 5 |
| 2.856 | 2.0 | -3 -1 3, -3 1 3 | 1.725 | 4.7 | -1 -3 6, -1 3 6, -2 -2 7, -2 2 7 | 1.372 | 3.1 | -7 1 1, -7 -1 1 |
| 2.814 | 11.6 | -2 -2 3, -2 2 3 | 1.723 | 9.0 | 3 3 3, 3 -3 3 | 1.366 | 8.1 | -3 -5 5, -3 5 5 |
| 2.691 | 5.4 | 3 1 1, 3 -1 1 | 1.715 | 3.4 | 2 0 6 | 1.361 | 1.8 | -6 -2 7, -6 2 7 |
| 2.669 | 4.6 | -1 3 0, 1 3 0 | 1.674 | 12.1 | 3 -1 5, 3 1 5 | 1.359 | 2.0 | 0 4 7, 0 -4 7 |
| 2.661 | 1.5 | -1 -3 1, -1 3 1 | 1.673 | 2.0 | -5 1 6, -5 -1 6 | 1.349 | 1.1 | 5 -3 3, 5 3 3 |
| 2.587 | 14.1 | 1 -1 4, 1 1 4 | 1.661 | 5.9 | -6 0 2 | 1.345 | 2.2 | 6 -2 2, 6 2 2 |
| **2.584** | **28.4** | **2 -2 2, 2 2 2** | 1.655 | 1.0 | 2 -4 3, 2 4 3 | 1.340 | 9.3 | 1 -5 5, 1 5 5 |
| 2.578 | 10.5 | -3 -1 4, -3 1 4 | 1.645 | 8.9 | 4 0 4, -1 5 0, 1 5 0 | 1.338 | 1.6 | 3 -3 6, 3 3 6 |
| 2.562 | 21.3 | 1 -3 1, 1 3 1 | 1.632 | 3.1 | 1 -1 7, 1 1 7 | 1.336 | 1.3 | -7 1 6, -7 -1 6 |
| 2.542 | 1.0 | -1 3 2, -1 -3 2 | 1.618 | 15.3 | 1 -5 1, 1 5 1 | 1.334 | 1.4 | 2 6 0 , -2 6 0 |
| 2.525 | 6.6 | -1 1 5, -1 -1 5 | 1.615 | 15.8 | -5 3 3, -5 -3 3 | 1.328 | 2.3 | 3 -5 3, 3 5 3 |
| 2.507 | 2.9 | 0 -2 4, 0 2 4 | 1.604 | 1.2 | 0 -4 5, 0 4 5 | 1.325 | 5.1 | 2 -4 6, 2 4 6, -2 0 10 |
| 2.399 | 2.2 | 3 1 2, 3 -1 2 | 1.601 | 2.7 | -4 -4 2, -4 4 2 | 1.314 | 2.2 | 2 6 1, 2 -6 1 |
| 2.362 | 16.7 | 4 0 0 | 1.595 | 3.9 | -4 -4 1, -4 4 1, -4 2 7, -4 -2 7 | 1.299 | 1.5 | -2, 4 8, -2 -4 8 |
| 2.350 | 5.5 | -1 3 3, -1 -3 3 | 1.586 | 5.5 | 2 -2 6, 2 2 6 | 1.296 | 1.8 | -3 3 9, -3 -3 9 |
| 2.287 | 2.6 | -3 1 5, -3 -1 5 | 1.582 | 1.7 | -4 4 3, -4 -4 3 | 1.293 | 4.8 | 4 2 6, 4 -2 6 |
| 2.279 | 3.7 | -4 0 4, 2 -2 3, 2 2 3 | 1.580 | 1.2 | -5 -3 4, -5 3 4 | 1.282 | 1.9 | 7 -1 1, 7 1 1 |
| 2.204 | 4.2 | -2 2 5, -2 -2 5 | 1.575 | 2.2 | 6 0 0 | 1.271 | 2.4 | 0 6 4, 0 -6 4 |
| 2.197 | 19.3 | -2 0 6 | 1.568 | 4.1 | 0 0 8 | 1.262 | 1.8 | 3 5 4, 3 -5 4 |
| 2.171 | 8.4 | 1 1 5, 1 -1 5 | 1.564 | 3.0 | -4 4 0, 4 4 0 | 1.257 | 1.4 | 6 4 0, -6 4 0 |
| 2.150 | 3.3 | 0 -2 5, 0 2 5 | 1.563 | 3.3 | -4 0 8 | 1.252 | 2.1 | 6 0 4 |
| 2.143 | 1.2 | -4 -2 2, -4 2 2 | 1.560 | 6.7 | -1 -5 3, -1 5 3 | 1.248 | 2.7 | -8 0 4 |
| **2.133** | **29.0** | **-3 3 1, -3 -3 1** | 1.556 | 7.7 | -1 3 7, -1 -3 7 | 1.247 | 2.3 | -1 -5 7, -1 5 7 |
| 2.132 | 2.0 | -1 3 4, -1 -3 4 | 1.543 | 9.8 | -6 2 2, -6 -2 2 | 1.225 | 2.5 | 7 -1 2, 7 1 2 |
| 2.128 | 6.7 | -4 -2 1, -4 2 1 | 1.542 | 7.3 | -2 2 8,-2 -2 8, 2 4 4, 2 -4 4 | 1.204 | 2.2 | -2 4 9, -2 -4 9 |
| 2.097 | 3.8 | -4 2 3, -4 -2 3, -4 0 5 | 1.539 | 2.6 | -4 -4 4, -4 4 4 | 1.196 | 1.0 | -8 2 4, -8 -2 4 |
| 2.091 | 2.3 | 0 0 6 | 1.533 | 2.9 | -3 3 7, -3 -3 7 | 1.190 | 1.8 | 5 -3 5, 5 3 5 |
| 2.086 | 1.3 | 0 4 0 | 1.519 | 7.1 | -6 0 6 | 1.189 | 3.1 | -6 0 10 |
| 2.058 | 4.4 | 0 4 1, 0 -4 1 | 1.517 | 5.1 | 5 1 3, 5 -1 3 | 1.181 | 1.6 | 2 2 9, 2 -2 9 |
| Note: seven strongest reflections are given in bold. | | | | | | | | |