|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Table S1a**. Calculated X-ray powder diffraction data (*I*calc. > 1, *d* in Å) for silesiaite from Szklarska Poręba, Poland. | | | | | | | | |
| *d*calc. | *Ic*alc. | *h k l* | *d*calc. | *Ic*alc. | *h k l* | *d*calc. | *Ic*alc. | *h k l* |
| 6.284 | 1.7 | 0 0 2 | 2.059 | 11.7 | -4 2 0, 4 2 0 | 1.519 | 5.0 | 5 1 3, 5 -1 3 |
| 6.166 | 3.2 | -1 1 1, -1 -1 1 | 2.003 | 13.3 | -4 -2 4, -4 2 4 | 1.516 | 1.5 | -2 -4 6, -2 4 6 |
| **5.178** | **63.7** | **1 1 1, 1 -1 1** | 1.992 | 4.2 | 3 3 1, 3 -3 1 | 1.504 | 6.3 | 3 1 6, 3 -1 6, 5 -3 1, 5 3 1 |
| 5.013 | 3.3 | -1 1 2, -1 -1 2 | 1.950 | 2.6 | 1 -3 4, 1 3 4 | 1.494 | 10.9 | -3 5 1, -3 -5 1, -1 -5 4, -1 5 4 |
| 4.729 | 7.7 | 2 0 0 | 1.947 | 15.3 | -2 -2 6, -2 2 6 | 1.481 | 2.1 | -4 4 5, -4 -4 5 |
| **4.563** | **30.0** | **-2 0 2** | 1.931 | 2.3 | -5 1 3, -5 -1 3 | 1.478 | 1.2 | -3 5 0, 3 5 0 |
| 4.181 | 7.3 | 0 2 0 | 1.929 | 1.9 | -2 -4 2, -2 4 2 | 1.471 | 3.0 | 0 -2 8, 0 2 8 |
| 4.023 | 2.4 | 1 1 2, 1 -1 2 | 1.915 | 6.5 | -5 -1 1, -5 1 1 | 1.466 | 12.7 | -4 -2 8, -4 2 8 |
| 3.968 | 1.1 | 0 -2 1, 0 2 1 | 1.901 | 3.5 | -2 -4 2, -2 4 2 | 1.457 | 1.2 | -5 -3 6, -5 3 6 |
| 3.894 | 16.4 | -1 1 3, -1 -1 3 | 1.873 | 3.5 | 0 2 6, 0 -2 6 | 1.452 | 2.5 | 1 -1 8, 1 1 8 |
| 3.482 | 5.2 | 0 2 2, 0 -2 2 | 1.871 | 10.3 | 0 4 3, 0 -4 3 | 1.448 | 1.3 | 4 4 2, 4 -4 2 |
| 3.296 | 4.3 | 2 0 2 | 1.835 | 5.0 | -1 1 7, -1 -1 7 | 1.445 | 1.5 | -3 1 9, -3 -1 9 |
| 3.207 | 10.4 | -2 2 1, -2 -2 1 | 1.811 | 6.1 | -3 3 5, -3 -3 5 | 1.434 | 1.2 | 2 -4 5, 2 4 5 |
| 3.179 | 6.6 | 1 1 3, 1 -1 3 | 1.810 | 5.0 | 4 2 2, 4 -2 2 | 1.431 | 8.1 | 5 -3 2, 5 3 2, 1 3 7, 1 -3 7 |
| **3.142** | **64.2** | **0 0 4** | 1.781 | 6.4 | 2 2 5, 2 -2 5 | 1.430 | 3.2 | -1 1 9, -1 -1 9 |
| 3.133 | 2.1 | 2 2 0, -2 2 0, -2 0 4 | 1.766 | 1.4 | 2 -4 2, 2 4 2 | 1.429 | 1.4 | -6 -2 6, -6 2 6 |
| **3.090** | **25.3** | **-3 1 1, -3 -1 1** | 1.753 | 1.7 | 1 -3 5, 1 3 5 | 1.416 | 1.3 | 6 2 1, 6 -2 1 |
| **3.083** | **100.0** | **-2 -2 2, -2 2 2** | 1.741 | 1.2 | 0 -4 4, 0 4 4 | 1.409 | 3.1 | -7 -1 3, -7 1 3 |
| 3.056 | 16.9 | -3 1 2, -3 -1 2 | 1.739 | 1.2 | -2 4 4, -2 -4 4 | 1.400 | 4.2 | -7 1 2, -7 -1 2 |
| 2.960 | 1.4 | 0 -2 3, 0 2 3 | 1.729 | 3.0 | -1 -3 6, -1 3 6 | 1.394 | 2.6 | 0 6 0 |
| 2.896 | 26.5 | 2 2 1, 2 -2 1 | 1.728 | 1.6 | -2 -2 7, -2 2 7 | 1.379 | 15.3 | -5 3 7, -5 -3 7 |
| 2.859 | 1.6 | -3 -1 3, -3 1 3 | 1.726 | 9.2 | 3 3 3, 3 -3 3 | 1.377 | 2.0 | -7 1 5, -7 -1 5 |
| 2.819 | 11.8 | -2 -2 3, -2 2 3 | 1.718 | 3.4 | 2 0 6 | 1.374 | 3.1 | -7 1 1, -7 -1 1 |
| 2.695 | 5.0 | 3 1 1, 3 -1 1 | 1.677 | 11.9 | 3 -1 5, 3 1 5 | 1.369 | 8.0 | -3 -5 5, -3 5 5 |
| 2.674 | 4.6 | -1 3 0, 1 3 0 | 1.675 | 2.1 | -5 1 6, -5 -1 6 | 1.363 | 1.8 | -6 -2 7, -6 2 7 |
| 2.666 | 1.3 | -1 -3 1, -1 3 1 | 1.663 | 6.0 | -6 0 2 | 1.362 | 2.0 | 0 4 7, 0 -4 7 |
| 2.593 | 14.0 | 1 -1 4, 1 1 4 | 1.659 | 1.0 | 2 -4 3, 2 4 3 | 1.347 | 2.2 | 6 -2 2, 6 2 2 |
| **2.589** | **28.3** | **2 -2 2, 2 2 2** | 1.647 | 9.1 | 4 0 4, 1 5 0, 1 -5 0 | 1.343 | 9.3 | 1 -5 5, 1 5 5 |
| 2.581 | 10.5 | -3 -1 4, -3 1 4 | 1.635 | 2.9 | 1 -1 7, 1 1 7 | 1.341 | 1.5 | 3 -3 6, 3 3 6 |
| 2.568 | 21.6 | 1 -3 1, 1 3 1 | 1.621 | 15.2 | 1 -5 1, 1 5 1 | 1.338 | 1.3 | -7 1 6, -7 -1 6 |
| 2.547 | 1.1 | -1 3 2, -1 -3 2 | 1.617 | 15.7 | -5 3 3, -5 -3 3 | 1.337 | 1.4 | 2 6 0 , -2 6 0 |
| 2.530 | 6.3 | -1 1 5, -1 -1 5 | 1.608 | 1.3 | 0 -4 5, 0 4 5 | 1.331 | 2.3 | 3 -5 3, 3 5 3 |
| 2.512 | 2.8 | 0 -2 4, 0 2 4 | 1.604 | 2.6 | -4 -4 2, -4 4 2 | 1.328 | 5.1 | 2 -4 6, 2 4 6, -2 0 10 |
| 2.403 | 2.2 | 3 1 2, 3 -1 2 | 1.598 | 2.1 | -4 -4 1, -4 4 1 | 1.316 | 2.1 | 2 6 1, 2 -6 1 |
| 2.364 | 16.6 | 4 0 0 | 1.597 | 1.8 | -4 2 7, -4 -2 7 | 1.301 | 1.5 | -2, 4 8, -2 -4 8 |
| 2.355 | 5.5 | -1 3 3, -1 -3 3 | 1.590 | 5.6 | 2 -2 6, 2 2 6 | 1.298 | 1.7 | -3 3 9, -3 -3 9 |
| 2.290 | 2.5 | -3 1 5, -3 -1 5 | 1.584 | 1.6 | -4 4 3, -4 -4 3 | 1.295 | 4.8 | 4 2 6, 4 -2 6 |
| 2.283 | 1.4 | 2 -2 3, 2 2 3 | 1.583 | 1.2 | -5 -3 4, -5 3 4 | 1.284 | 1.8 | 7 -1 1, 7 1 1 |
| 2.282 | 2.4 | -4 0 4 | 1.576 | 2.1 | 6 0 0 | 1.274 | 2.4 | 0 6 4, 0 -6 4 |
| 2.208 | 4.3 | -2 2 5, -2 -2 5 | 1.571 | 4.1 | 0 0 8 | 1.265 | 1.8 | 3 5 4, 3 -5 4 |
| 2.200 | 19.3 | -2 0 6 | 1.567 | 3.0 | -4 4 0, 4 4 0 | 1.259 | 1.3 | 6 4 0, -6 4 0 |
| 2.176 | 8.6 | 1 1 5, 1 -1 5 | 1.566 | 3.3 | -4 0 8 | 1.254 | 2.1 | 6 0 4 |
| 2.155 | 3.4 | 0 -2 5, 0 2 5 | 1.563 | 6.6 | -1 -5 3, -1 5 3 | 1.250 | 2.2 | -1 -5 7, -1 5 7 |
| **2.137** | **29.2** | **-3 3 1, -3 -3 1** | 1.559 | 7.7 | -1 3 7, -1 -3 7 | 1.249 | 2.7 | -8 0 4 |
| 2.136 | 2.0 | -1 3 4, -1 -3 4 | 1.546 | 5.5 | 2 4 4, 2 -4 4 | 1.227 | 2.5 | 7 -1 2, 7 1 2 |
| 2.131 | 6.8 | -4 -2 1, -4 2 1 | 1.545 | 11.4 | -6 2 2, -6 -2 2, -2 2 8,-2 -2 8 | 1.206 | 2.2 | -2 4 9, -2 -4 9 |
| 2.099 | 3.8 | -4 2 3, -4 -2 3 | 1.542 | 2.6 | -4 -4 4, -4 4 4 | 1.197 | 1.1 | -8 2 4, -8 -2 4 |
| 2.095 | 2.3 | 0 0 6 | 1.536 | 2.9 | -3 3 7, -3 -3 7 | 1.192 | 1.9 | 5 -3 5, 5 3 5 |
| 2.091 | 1.3 | 0 4 0 | 1.533 | 3.0 | 4 -2 4, 4 2 4 | 1.191 | 3.0 | -6 0 10 |
| 2.062 | 4.4 | 0 4 1, 0 -4 1 | 1.521 | 7.1 | -6 0 6 | 1.184 | 1.6 | 2 2 9, 2 -2 9 |
| Note: seven strongest reflections are given in bold. | | | | | | | | |