Supplementary Table S1. Powder X-ray data (*d* in Å) for scenicite. 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* |
| 8 | 10.63 | 10.6072 | 7 | 2 0 0 |  | 7 | 2.268 | 2.2785 | 3 | 4 2 3 |  |  |  | 1.7523 | 3 | 3 1 6 |
| 70 | 7.69 | 7.7194 | 70 | 2 0 1 |  | 2.2496 | 3 | 6 2 2 |  | 13 | 1.7477 | 1.7466 | 11 | 9 1 4 |
| 9 | 6.46 | 6.4917 | 9 | 1 1 0 |  | 13 | 2.226 | 2.2281 | 5 | 7 1 3 |  | 7 | 1.7136 | 1.7161 | 5 | 8 0 5 |
|  |  | 5.7359 | 5 | 2 1 0 |  | 2.2225 | 3 | 2 3 0 |  | 15 | 1.6979 | 1.7058 | 3 | 8 3 1 |
| 100 | 5.63 | 5.6234 | 88 | 1 1 1 |  | 2.2175 | 2 | 5 1 4 |  | 1.6992 | 5 | 1 4 0 |
|  |  | 5.3036 | 4 | 4 0 0 |  | 2.2158 | 2 | 1 3 1 |  | 1.6866 | 2 | 12 0 2 |
| 7 | 5.13 | 5.1105 | 7 | 2 1 1 |  | 17 | 2.203 | 2.2017 | 12 | 6 0 4 |  | 1.6802 | 2 | 1 4 1 |
| 84 | 4.92 | 4.9713 | 26 | 2 0 2 |  | 25 | 2.169 | 2.1804 | 9 | 2 3 1 |  | 5 | 1.6629 | 1.6634 | 2 | 11 1 3 |
| 4.9085 | 51 | 3 1 0 |  | 2.1655 | 8 | 8 0 3 |  | 1.6589 | 3 | 6 2 5 |
| 93 | 4.80 | 4.7977 | 100 | 4 0 1 |  |  |  | 2.1639 | 2 | 3 3 0 |  | 1.6571 | 2 | 6 0 6 |
| 11 | 4.50 | 4.4993 | 12 | 3 1 1 |  | 23 | 2.121 | 2.1261 | 9 | 2 2 4 |  | 5 | 1.6388 | 1.6396 | 2 | 3 4 1 |
| 22 | 4.26 | 4.2523 | 19 | 1 1 2 |  | 2.1250 | 2 | 3 3 1 |  | 1.6267 | 2 | 1 4 2 |
| 4 | 3.992 | 4.0171 | 5 | 2 1 2 |  | 2.1214 | 2 | 10 0 0 |  | 5 | 1.6234 | 1.6242 | 3 | 2 2 6 |
|  |  | 3.8597 | 4 | 4 0 2 |  | 2.1075 | 4 | 0 3 2 |  | 8 | 1.5937 | 1.6009 | 2 | 3 2 6 |
| 48 | 3.699 | 3.6992 | 44 | 3 1 2 |  | 20 | 2.087 | 2.0972 | 3 | 1 3 2 |  | 1.5967 | 3 | 7 2 5 |
| 24 | 3.539 | 3.5371 | 23 | 2 0 3 |  | 2.0932 | 4 | 8 2 0 |  | 1.5897 | 3 | 3 4 2 |
| 55 | 3.398 | 3.4310 | 7 | 5 1 1 |  | 2.0847 | 2 | 10 0 1 |  |  |  | 1.5814 | 2 | 6 3 4 |
| 3.4094 | 24 | 0 2 0 |  | 2.0747 | 4 | 3 2 4 |  | 12 | 1.5679 | 1.5715 | 3 | 13 1 1 |
| 3.3732 | 7 | 6 0 1 |  | 26 | 2.062 | 2.0714 | 8 | 9 1 2 |  | 1.5664 | 5 | 5 4 1 |
| 3.3662 | 13 | 1 2 0 |  | 2.0671 | 5 | 2 3 2 |  | 1.5608 | 2 | 1 1 7 |
| 30 | 3.244 | 3.2483 | 23 | 1 1 3 |  | 2.0538 | 6 | 6 2 3 |  | 6 | 1.5486 | 1.5479 | 2 | 1 4 3 |
| 3.2251 | 8 | 1 2 1 |  | 6 | 2.024 | 2.0462 | 5 | 3 1 5 |  | 17 | 1.5301 | 1.5388 | 2 | 4 0 7 |
|  |  | 3.1398 | 3 | 2 1 3 |  | 2.0197 | 2 | 3 3 2 |  | 1.5329 | 3 | 8 2 5 |
| 12 | 3.116 | 3.1188 | 5 | 2 2 1 |  | 7 | 1.9802 | 1.9851 | 3 | 10 0 2 |  | 1.5313 | 6 | 4 3 5 |
|  |  | 3.0711 | 3 | 3 2 0 |  | 1.9826 | 2 | 4 1 5 |  | 1.5280 | 3 | 3 1 7 |
|  |  | 3.0629 | 3 | 4 0 3 |  |  |  | 1.9619 | 3 | 8 2 2 |  | 11 | 1.4986 | 1.5018 | 3 | 14 0 1 |
| 21 | 3.036 | 3.0341 | 10 | 5 1 2 |  |  |  | 1.9586 | 2 | 4 3 2 |  | 1.4969 | 5 | 12 0 4 |
|  |  | 3.0235 | 2 | 6 1 1 |  | 11 | 1.9467 | 1.9391 | 6 | 7 2 3 |  |  |  | 1.4711 | 2 | 8 3 4 |
| 33 | 2.983 | 2.9939 | 16 | 6 0 2 |  | 29 | 1.9090 | 1.9122 | 6 | 2 3 3 |  | 13 | 1.4624 | 1.4683 | 2 | 5 1 7 |
| 2.9808 | 15 | 3 1 3 |  | 1.9090 | 16 | 5 1 5 |  | 1.4637 | 2 | 6 0 7 |
|  |  | 2.9628 | 3 | 3 2 1 |  | 1.8989 | 3 | 6 0 5 |  | 1.4617 | 4 | 13 1 3 |
| 15 | 2.887 | 2.9160 | 4 | 0 2 2 |  | 8 | 1.8760 | 1.8850 | 3 | 6 3 1 |  | 1.4595 | 2 | 13 2 1 |
| 2.8889 | 5 | 1 2 2 |  | 1.8759 | 2 | 0 0 6 |  | 1.4573 | 2 | 6 3 5 |
| 2.8679 | 3 | 4 2 0 |  | 1.8745 | 2 | 3 3 3 |  | 11 | 1.4389 | 1.4416 | 2 | 11 2 4 |
| 43 | 2.791 | 2.8117 | 13 | 2 2 2 |  | 1.8712 | 2 | 1 2 5 |  | 1.4349 | 4 | 9 1 6 |
| 2.7940 | 4 | 4 1 3 |  | 23 | 1.8506 | 1.8558 | 6 | 11 1 0 |  | 6 | 1.4239 | 1.4280 | 3 | 3 4 4 |
| 2.7791 | 19 | 4 2 1 |  | 1.8498 | 6 | 2 2 5 |  | 8 | 1.3997 | 1.4025 | 2 | 4 2 7 |
|  |  | 2.7413 | 2 | 6 1 2 |  | 1.8467 | 5 | 10 0 3 |  | 1.3955 | 2 | 12 3 0 |
| 42 | 2.693 | 2.7198 | 7 | 2 0 4 |  | 21 | 1.8240 | 1.8331 | 3 | 9 2 2 |  | 1.3905 | 2 | 7 1 7 |
| 2.6958 | 6 | 3 2 2 |  | 1.8311 | 2 | 11 1 1 |  |  |  | 1.3848 | 2 | 15 1 0 |
| 2.6892 | 18 | 7 1 1 |  | 1.8279 | 3 | 8 2 3 |  | 17 | 1.3775 | 1.3814 | 5 | 7 4 3 |
|  |  | 2.6518 | 4 | 8 0 0 |  | 1.8253 | 9 | 4 3 3 |  | 1.3757 | 2 | 5 2 7 |
|  |  | 2.6011 | 2 | 0 1 4 |  | 1.8103 | 5 | 6 3 2 |  | 1.3745 | 4 | 15 1 1 |
| 51 | 2.590 | 2.5985 | 17 | 5 1 3 |  | 14 | 1.8012 | 1.8022 | 6 | 1 1 6 |  | 1.3706 | 3 | 12 2 4 |
| 2.5865 | 9 | 5 2 1 |  | 1.8012 | 2 | 10 2 0 |  | 6 | 1.3561 | 1.3582 | 2 | 10 3 4 |
| 2.5818 | 16 | 1 1 4 |  | 1.7951 | 2 | 7 3 1 |  | 1.3544 | 2 | 12 3 2 |
|  |  | 2.5731 | 3 | 6 0 3 |  |  |  | 1.7786 | 2 | 10 2 1 |  | 1.3525 | 3 | 3 1 8 |
| 12 | 2.497 | 2.5055 | 3 | 1 2 3 |  | 22 | 1.7658 | 1.7681 | 6 | 0 3 4 |  | 10 | 1.3447 | 1.3450 | 3 | 6 2 7 |
| 2.4848 | 8 | 7 1 2 |  | 1.7673 | 2 | 5 3 3 |  | 1.3430 | 2 | 2 5 1 |
| 14 | 2.456 | 2.4547 | 8 | 2 2 3 |  | 1.7624 | 7 | 11 1 2 |  | 1.3415 | 2 | 9 4 2 |
| 11 | 2.399 | 2.3988 | 7 | 8 0 2 |  |  |  |  |  |  |  |  |  |  |  |  |