**Table S1.** Crystallographic data and reﬁnement parameters for ‘minasgeraisite-(Y)’

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Temperature, °C | 27 | 27 | 150 | 300 | 450 | 600 | 700 | 800 | 900 | 1000 |
| Temperature point |  | T01 | T02 | T03 | T04 | T05 | T06 | T07 | T08 | T09 |
| Space group, Z | *P*21/*c*, 2 | | | | | | | | | |
| *a*, Å | 4.7476(4) | 4.7560(4) | 4.7587(3) | 4.7640(3) | 4.7649(4) | 4.7727(4) | 4.7727(4) | 4.7789(5) | 4.7756(7) | 4.7513(10) |
| *b*, Å | 7.6586(5) | 7.6721(5) | 7.6796(4) | 7.6938(4) | 7.7003(5) | 7.7191(6) | 7.7220(5) | 7.7317(7) | 7.6917(12) | 7.6230(18) |
| *c*, Å | 9.9467(9) | 9.9678(7) | 9.9669(6) | 9.9735(7) | 9.9767(7) | 9.9881(8) | 9.9878(8) | 10.0003(9) | 10.0012(14) | 10.0282(18) |
| β, ° | 90.230(7) | 90.265(7) | 90.263(6) | 90.294(6) | 90.347(7) | 90.336(8) | 90.425(7) | 90.396(8) | 90.218(13) | 90.276(18) |
| Volume, Å3 | 361.66(5) | 363.71(5) | 364.24(4) | 365.56(4) | 366.05(4) | 367.97(5) | 368.09(5) | 369.49(6) | 367.37(9) | 363.21(13) |
| Data collection |  |  |  |  |  |  |  |  |  |  |
| Wavelength, Å | 0.71073 | | | | | | | | | |
| Max. *θ*° | 30.467 | 29.416 | 29.083 | 29.066 | 29.283 | 29.330 | 29.268 | 29.171 | 29.161 | 29.015 |
| Index ranges | –6 ≤ h ≤ 5 | –5 ≤ h ≤ 6 | –5 ≤ h ≤ 6 | –6 ≤ h ≤ 5 | –5 ≤ h ≤ 6 | –6 ≤ h ≤ 5 | –6 ≤ h ≤ 6 | –6 ≤ h ≤ 6 | –6 ≤ h ≤ 6 | –6 ≤ h ≤ 6 |
|  | –9 ≤ k ≤ 9 | –8 ≤ k ≤ 10 | –7 ≤ k ≤ 10 | –7 ≤ k ≤ 10 | –7 ≤ k ≤ 10 | –8 ≤ k ≤ 10 | –7 ≤ k ≤ 10 | –7 ≤ k ≤ 10 | –7 ≤ k ≤ 10 | –7 ≤ k ≤ 10 |
|  | –13 ≤ l ≤ 12 | –12 ≤ l ≤ 13 | –12 ≤ l ≤ 13 | –13 ≤ l ≤ 12 | –12 ≤ l ≤ 13 | –13 ≤ l ≤ 12 | –13 ≤ l ≤ 13 | –13 ≤ l ≤ 13 | –13 ≤ l ≤ 13 | –13 ≤ l ≤ 13 |
| No. meas. reﬂ. | 3528 | 3555 | 3535 | 3561 | 3576 | 3587 | 3665 | 3597 | 3448 | 3420 |
| No. uniq. reﬂ. | 894 | 872 | 873 | 874 | 879 | 880 | 897 | 897 | 889 | 872 |
| No. obs. reﬂ. | 782 | 752 | 767 | 706 | 705 | 671 | 658 | 637 | 484 | 430 |
| (I > 2σ(I)) |  |  |  |  |  |  |  |  |  |  |
| Reﬁnement of the structure | | |  |  |  |  |  |  |  |  |
| No. of variables | 77 | 81 | 77 | 76 | 77 | 77 | 77 | 76 | 76 | 76 |
| Rint | 0.880 | 0.0965 | 0.0638 | 0.1067 | 0.0709 | 0.0864 | 0.1145 | 0.1014 | 0.1510 | 0.2129 |
| R1, all data | 0.0891 | 0.0938 | 0.0738 | 0.1048 | 0.0789 | 0.0841 | 0.1069 | 0.0916 | 0.1531 | 0.2167 |
| R1, I > 2σ(I) | 0.0788 | 0.0630 | 0.0627 | 0.0642 | 0.0588 | 0.0611 | 0.0631 | 0.0569 | 0.0696 | 0.1095 |
| wR2, all data | 0.1716 | 0.1388 | 0.1347 | 0.1507 | 0.1335 | 0.1421 | 0.1433 | 0.1334 | 0.1753 | 0.3310 |
| wR2, I > 2σ(I) | 0.1680 | 0.1255 | 0.1312 | 0.1343 | 0.1265 | 0.1323 | 0.1261 | 0.1203 | 0.1368 | 0.2747 |
| GooF | 1.220 | 1.222 | 1.211 | 1.267 | 1.087 | 1.060 | 1.027 | 0.921 | 1.033 | 1.042 |

**Table S2.** Bond distances (Å) and polyhedral volumes (Å3) in the crystal structure of ‘minasgeraisite-(Y)’

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Temperature, °C | | 27 | 27 | 150 | 300 | 450 | 600 | 700 | 800 | 900 | 1000 |
| Temperature point | |  | T01 | T02 | T03 | T04 | T05 | T06 | T07 | T08 | T09 |
| SiO4 tetrahedra | | | | | | | | | | | |
| **Si–O4** | | 1.612(12) | 1.639(9) | 1.623(9) | 1.629(10) | 1.629(9) | 1.633(10) | 1.628(10) | 1.625(9) | 1.622(11) | 1.63(3) |
| **Si–O3** | | 1.623(11) | 1.631(10) | 1.629(9) | 1.632(10) | 1.631(9) | 1.634(10) | 1.623(10) | 1.634(9) | 1.636(10) | 1.62(3) |
| **Si–O2** | | 1.618(10) | 1.605(9) | 1.611(9) | 1.612(10) | 1.600(9) | 1.609(10) | 1.598(10) | 1.595(9) | 1.601(11) | 1.59(3) |
| **Si–O1** | | 1.650(11) | 1.647(10) | 1.643(10) | 1.646(11) | 1.650(10) | 1.654(10) | 1.660(10) | 1.658(10) | 1.651(10) | 1.69(3) |
| **<Si–O>** | | 1.63 | 1.631 | 1.626 | 1.630 | 1.623 | 1.633 | 1.627 | 1.628 | 1.628 | 1.63 |
| **Volume** | | 2.20 | 2.218 | 2.202 | 2.215 | 2.208 | 2.228 | 2.205 | 2.208 | 2.203 | 2.21 |
|  | *T2*O4 tetrahedra | | | | | | | | | | |
| ***T2*–O5** | | 1.552(18) | 1.570(14) | 1.574(13) | 1.598(14) | 1.573(13) | 1.593(14) | 1.591(13) | 1.589(13) | 1.590(18) | 1.62(5) |
| ***T2*–O1** | | 1.628(18) | 1.629(15) | 1.622(14) | 1.620(15) | 1.629(14) | 1.629(15) | 1.628(15) | 1.635(15) | 1.653(16) | 1.76(5) |
| ***T2*–O3** | | 1.635(18) | 1.630(15) | 1.639(14) | 1.637(15) | 1.650(14) | 1.621(15) | 1.648(15) | 1.661(14) | 1.641(16) | 1.57(5) |
| ***T2*–O4** | | 1.638(18) | 1.618(14) | 1.630(14) | 1.617(15) | 1.617(14) | 1.634(15) | 1.624(15) | 1.632(14) | 1.649(17) | 1.64(5) |
| **<*T*2–O>** | | 1.61 | 1.612 | 1.616 | 1.618 | 1.617 | 1.619 | 1.623 | 1.629 | 1.633 | 1.64 |
| **Volume** | | 2.14 | 2.134 | 2.152 | 2.161 | 2.153 | 2.163 | 2.177 | 2.199 | 2.210 | 2.24 |
|  | *A*O8 polyhedra | | | | | | | | | | |
| ***A*–O3** | | 2.411(10) | 2.412(9) | 2.410(8) | 2.413(10) | 2.417(8) | 2.427(9) | 2.429(9) | 2.428(9) | 2.414(9) | 2.44(3) |
| ***A*–O4** | | 2.761(11) | 2.762(9) | 2.779(9) | 2.779(10) | 2.793(9) | 2.798(10) | 2.814(10) | 2.817(9) | 2.771(10) | 2.72(3) |
| ***A*–O2** | | 2.280(10) | 2.277(9) | 2.270(8) | 2.272(9) | 2.277(8) | 2.278(9) | 2.279(9) | 2.285(9) | 2.295(10) | 2.33(3) |
| ***A*–O5** | | 2.463(11) | 2.469(10) | 2.467(9) | 2.470(10) | 2.472(9) | 2.482(10) | 2.483(10) | 2.489(10) | 2.485(11) | 2.45(3) |
| ***A*–O5** | | 2.612(10) | 2.598(10) | 2.614(10) | 2.610(10) | 2.616(10) | 2.625(10) | 2.622(10) | 2.622(10) | 2.562(11) | 2.52(3) |
| ***A*–O2** | | 2.271(10) | 2.297(8) | 2.300(8) | 2.298(9) | 2.304(9) | 2.300(9) | 2.304(9) | 2.306(9) | 2.310(11) | 2.31(3) |
| ***A*–O1** | | 2.401(12) | 2.414(9) | 2.418(9) | 2.426(10) | 2.419(9) | 2.414(10) | 2.423(10) | 2.423(9) | 2.432(11) | 2.37(3) |
| ***A*–O4** | | 2.484(10) | 2.479(10) | 2.484(9) | 2.490(10) | 2.494(9) | 2.501(10) | 2.498(10) | 2.505(9) | 2.513(10) | 2.55(3) |
| **<*A*–O>** | | 2.46 | 2.463 | 2.468 | 2.470 | 2.474 | 2.478 | 2.482 | 2.485 | 2.473 | 2.46 |
| **Volume** | | 25.28 | 25.372 | 25.506 | 25.536 | 25.645 | 25.751 | 25.854 | 25.935 | 25.570 | 25.17 |
|  | MnO6 octahedra | | | | | | | | | | |
| **Mn–O3 (x2)** | | 2.291(10) | 2.295(9) | 2.303(8) | 2.315(10) | 2.309(8) | 2.312(9) | 2.324(9) | 2.323(8) | 2.333(9) | 2.26(3) |
| **Mn–O1 (x2)** | | 2.206(11) | 2.209(9) | 2.219(9) | 2.212(10) | 2.218(9) | 2.228(10) | 2.213(10) | 2.221(9) | 2.189(11) | 2.10(3) |
| **Mn–O5 (x2)** | | 2.034(11) | 2.047(9) | 2.026(9) | 2.019(10) | 2.019(9) | 2.011(10) | 2.004(9) | 1.992(9) | 1.996(10) | 1.99(3) |
| **<Mn–O>** | | 2.18 | 2.184 | 2.183 | 2.182 | 2.182 | 2.184 | 2.180 | 2.179 | 2.173 | 2.12 |
| **Volume** | | 12.94 | 13.062 | 13.031 | 12.990 | 12.987 | 13.010 | 12.938 | 12.908 | 12.789 | 11.96 |