Tab. S1: Atom coordinates, equivalent displacement parameters (Å2) and occupation factors for the structure of zippeite.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom | *Occupancy* | *x/a* | *y/b* | *z/c* | *U*eq |
| U1 |  | 0.66924(3) | 0.265705(16) | 0.17190(2) | 0.01214(8) |
| S1 |  | 0.5 | 0.24745(17) | 0.5 | 0.0188(8) |
| K1 | 0.548(5) | 0.8881(6) | 0 | 0.1568(7) | 0.0432(9)\* |
| K1' | 0.452(5) | 0.9363(9) | 0 | 0.2672(8) | 0.0432(9)\* |
| O1 |  | 0.9503(9) | 0.5 | 0.2590(11) | 0.040(3) |
| K2 | 0.045(7) | 0.577(9) | 0.5 | 0.530(11) | 0.082(4)\* |
| K2' | 0.356(7) | 0.7504(11) | 0.5 | 0.4974(12) | 0.082(4)\* |
| O2 |  | 0.6921(6) | 0.1420(3) | 0.2255(5) | 0.0252(16) |
| O3 |  | 0.5687(5) | 0.3096(4) | 0.3997(5) | 0.0233(17) |
| O4 |  | 0.3965(8) | 0.2422(4) | 0.0890(5) | 0.0306(18) |
| O5 |  | 0.6520(6) | 0.3925(3) | 0.1357(5) | 0.0256(17) |
| O6 |  | 0.3783(5) | 0.1851(4) | 0.4022(5) | 0.0229(17) |
| O7 | 0.188(13) | 0.970(4) | 0.5 | 0.034(4) | 0.022(5)\* |
| O7' | 0.312(13) | 0.931(3) | 0.5 | 0.113(3) | 0.022(5)\* |

\* – refined with isotropic displacement parameters.

**Tab. S2:** Anisotropic displacement parameters (Å2) for the structure of zippeite.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Atom | *U*11 | *U*22 | *U*33 | *U*12 | *U*13 | *U*23 |
| U1 | 0.01075(12) | 0.01856(13) | 0.00693(12) | −0.00232(11) | 0.00185(11) | 0.00013(9) |
| S1 | 0.0072(10) | 0.0415(16) | 0.0072(10) | 0 | 0.0006(13) | 0 |
| O1 | 0.006(3) | 0.013(3) | 0.103(7) | 0 | 0.018(4) | 0 |
| O2 | 0.022(2) | 0.027(3) | 0.025(3) | 0.004(2) | 0.003(2) | 0.001(2) |
| O3 | 0.017(2) | 0.043(3) | 0.013(3) | −0.005(2) | 0.011(2) | −0.002(2) |
| O4 | 0.005(2) | 0.074(4) | 0.011(2) | −0.006(2) | −0.002(3) | −0.003(2) |
| O5 | 0.024(3) | 0.026(3) | 0.023(3) | −0.002(2) | 0.000(3) | 0.005(2) |
| O6 | 0.015(2) | 0.037(3) | 0.014(3) | −0.002(2) | −0.002(2) | 0.003(2) |