**Table S1. Anisotropic displacement parameters of atoms for the crystal structure of horákite**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Atom | *U*11 | *U*22 | *U*33 | *U*12 | *U*13 | *U*23 |
| Bi1 | 0.0138(6) | 0.0127(7) | 0.0148(6) | −0.0035(5) | 0.0075(5) | −0.0021(5) |
| Bi2 | 0.0177(9) | 0.0106(9) | 0.0149(9) | 0 | 0.0089(8) | 0 |
| U1 | 0.0147(6) | 0.0125(7) | 0.0110(6) | 0.0002(5) | 0.0053(5) | 0.0001(5) |
| Bi3 | 0.0145(6) | 0.0204(7) | 0.0139(6) | −0.0009(6) | 0.0035(5) | 0.0045(6) |
| Bi4 | 0.0148(6) | 0.0242(8) | 0.0135(6) | −0.0048(6) | 0.0033(5) | −0.0016(6) |
| U2 | 0.0309(8) | 0.0160(7) | 0.0218(7) | −0.0043(6) | 0.0149(6) | −0.0029(6) |
| As1/P1 | 0.011(3) | 0.011(3) | 0.013(3) | −0.0047(19) | 0.008 (2) | −0.0022(19) |
| P2/As2 | 0.013(4) | 0.009(5) | 0.019(5) | 0.000(3) | 0.010(4) | −0.002(3) |