ESM 1 Anisotropic displacement parameters (Å2) in giftgrubeite

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| Atom | *U*11 | *U*22 | *U*33 | *U*12 | *U*13 | *U*23 |
| As1 | 0.0359(15) | 0.0255(14) | 0.0343(13) | 0.0001(11) | −0.0031(10) | 0.0005(10) |
| As2 | 0.0386(16) | 0.0266(15) | 0.0348(13) | −0.0001(12) | 0.0019(10) | −0.0002(10) |
| Mn1/Mg1 | 0.041(3) | 0.022(3) | 0.035(3) | −0.005(2) | −0.0008(19) | 0.0041(17) |
| Ca2 | 0.030(4) | 0.030(4) | 0.028(3) | 0 | 0.003(3) | 0 |
| Ca3 | 0.041(3) | 0.024(3) | 0.037(3) | 0.001(2) | −0.001(2) | 0.0045(19) |
| O1 | 0.045(11) | 0.019(10) | 0.044(9) | −0.004(8) | −0.004(7) | −0.005(7) |
| O2 | 0.044(10) | 0.021(9) | 0.034(8) | −0.007(8) | −0.012(7) | 0.005(6) |
| O3 | 0.033(9) | 0.031(10) | 0.030(8) | 0.008(8) | 0.012(6) | −0.009(7) |
| O4 | 0.063(12) | 0.027(10) | 0.030(8) | 0.004(8) | −0.010(7) | −0.009(7) |
| O5 | 0.041(10) | 0.025(10) | 0.050(10) | 0.004(8) | 0.007(7) | 0.009(7) |
| O6 | 0.042(10) | 0.063(14) | 0.047(10) | 0.010(9) | −0.007(8) | −0.011(9) |
| O7 | 0.060(12) | 0.025(10) | 0.055(10) | −0.014(9) | −0.016(8) | 0.016(8) |
| O8 | 0.040(10) | 0.039(11) | 0.032(8) | 0.002(9) | 0.004(7) | −0.005(7) |
| O9 | 0.064(13) | 0.048(13) | 0.046(10) | −0.015(10) | 0.013(8) | 0.012(8) |
| O10 | 0.045(11) | 0.049(12) | 0.029(9) | 0.007(9) | 0.001(7) | −0.005(7) |