**Table S1.** Anisotropic displacement parameters (A2) for atomic sites in the crystal structure of halotrichite, sample **vk4-09**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Site** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| Fe | 0.0185(3) | 0.0189(3) | 0.0225(3) | 0.00147(18) | 0.00427(18) | -0.0003(2) |
| S1 | 0.0224(3) | 0.0190(3) | 0.0193(3) | 0.0009(2) | 0.0032(3) | -0.0022(3) |
| S2 | 0.0213(3) | 0.0193(3) | 0.0225(3) | -0.0016(3) | 0.0043(3) | 0.0019(3) |
| S3 | 0.0239(4) | 0.0192(3) | 0.0224(3) | -0.0008(3) | 0.0039(3) | -0.0045(3) |
| S4 | 0.0210(3) | 0.0224(3) | 0.0208(3) | 0.0024(3) | 0.0017(3) | -0.0029(3) |
| Al1 | 0.0177(4) | 0.0164(4) | 0.0196(4) | -0.0008(3) | 0.0030(3) | -0.0012(3) |
| Al2 | 0.0191(4) | 0.0173(4) | 0.0179(4) | 0.0003(3) | 0.0038(3) | -0.0001(3) |
| O1 | 0.0251(10) | 0.0217(9) | 0.0227(10) | -0.0018(7) | 0.0026(8) | -0.0052(8) |
| O2 | 0.0296(11) | 0.0234(10) | 0.0246(10) | 0.0002(8) | 0.0006(8) | -0.0091(8) |
| O3 | 0.0242(10) | 0.0174(9) | 0.0287(10) | -0.0006(7) | 0.0052(8) | 0.0005(8) |
| O4 | 0.0238(11) | 0.0276(10) | 0.0233(10) | 0.0011(8) | 0.0004(8) | 0.0048(8) |
| O5 | 0.0232(10) | 0.0238(10) | 0.0295(11) | -0.0019(8) | 0.0089(8) | -0.0028(8) |
| O6 | 0.0247(10) | 0.0232(10) | 0.0289(11) | -0.0060(8) | 0.0112(8) | -0.0050(8) |
| O7 | 0.0226(10) | 0.0260(10) | 0.0293(11) | 0.0053(8) | 0.0052(8) | 0.0040(8) |
| O8 | 0.0238(11) | 0.0268(10) | 0.0303(11) | -0.0036(8) | 0.0037(9) | 0.0047(8) |
| O9 | 0.0340(11) | 0.0263(10) | 0.0213(10) | 0.0033(8) | 0.0077(8) | -0.0022(9) |
| O10 | 0.0258(11) | 0.0204(10) | 0.0419(12) | 0.0002(8) | 0.0100(9) | 0.0045(8) |
| O11 | 0.0284(11) | 0.0247(10) | 0.0341(11) | -0.0012(8) | 0.0100(9) | 0.0024(8) |
| O12 | 0.0289(11) | 0.0362(12) | 0.0299(11) | 0.0031(9) | -0.0039(9) | -0.0151(9) |
| O13 | 0.0397(12) | 0.0231(10) | 0.0212(10) | -0.0023(8) | 0.0111(9) | -0.0048(9) |
| O14 | 0.0281(11) | 0.0194(10) | 0.0322(11) | 0.0025(8) | 0.0002(9) | -0.0014(8) |
| O15 | 0.0243(11) | 0.0296(10) | 0.0314(11) | 0.0086(8) | 0.0048(9) | 0.0050(8) |
| O16 | 0.0299(12) | 0.0318(11) | 0.0430(13) | -0.0081(9) | 0.0149(10) | -0.0053(9) |
| O17 | 0.0491(14) | 0.0264(11) | 0.0325(11) | -0.0068(8) | 0.0242(10) | -0.0101(9) |
| O18 | 0.0274(11) | 0.0196(10) | 0.0414(12) | 0.0042(8) | 0.0110(9) | 0.0013(8) |
| O19 | 0.0333(12) | 0.0365(12) | 0.0233(10) | 0.0022(8) | -0.0003(9) | 0.0126(9) |
| O20 | 0.0208(10) | 0.0349(11) | 0.0346(11) | 0.0077(9) | 0.0052(9) | 0.0007(9) |
| O21 | 0.0317(12) | 0.0305(11) | 0.0301(11) | 0.0117(8) | 0.0008(9) | 0.0015(9) |
| O22 | 0.0299(12) | 0.0273(11) | 0.0429(13) | 0.0064(9) | 0.0092(10) | 0.0036(9) |
| O23 | 0.0368(13) | 0.0441(13) | 0.0303(12) | 0.0034(9) | -0.0055(10) | -0.0212(10) |
| O24 | 0.0350(12) | 0.0326(11) | 0.0380(12) | -0.0062(9) | 0.0186(10) | -0.0041(9) |
| O25 | 0.0281(11) | 0.0358(11) | 0.0342(12) | -0.0156(9) | 0.0007(9) | 0.0023(9) |
| O26 | 0.0304(12) | 0.0415(12) | 0.0323(12) | 0.0117(9) | 0.0045(9) | 0.0067(9) |
| O27 | 0.0428(13) | 0.0239(11) | 0.0488(14) | -0.0053(9) | 0.0253(11) | -0.0117(9) |
| O28 | 0.0348(12) | 0.0365(12) | 0.0404(13) | -0.0146(9) | -0.0093(10) | 0.0062(10) |
| O29 | 0.0482(14) | 0.0238(11) | 0.0525(14) | 0.0002(9) | 0.0349(11) | -0.0009(10) |
| O30 | 0.0353(13) | 0.0377(12) | 0.0430(13) | -0.0127(10) | 0.0147(10) | -0.0116(10) |
| O31 | 0.0533(15) | 0.0411(13) | 0.0258(11) | 0.0102(9) | -0.0115(10) | -0.0162(11) |
| O32 | 0.0354(13) | 0.0474(14) | 0.0412(13) | 0.0195(10) | -0.0067(11) | -0.0048(10) |
| O33 | 0.0251(13) | 0.0852(19) | 0.0626(17) | 0.0491(14) | 0.0062(12) | 0.0057(12) |
| O34 | 0.0303(12) | 0.0456(13) | 0.0401(13) | 0.0097(10) | 0.0006(10) | 0.0072(10) |
| O35 | 0.0648(17) | 0.0366(12) | 0.0357(13) | 0.0013(10) | 0.0114(12) | 0.0103(11) |
| O36 | 0.112(3) | 0.077(2) | 0.0413(16) | -0.0224(14) | -0.0104(17) | 0.035(2) |
| O37 | 0.075(2) | 0.0540(16) | 0.0482(15) | -0.0021(12) | 0.0207(14) | -0.0150(14) |
| O38 | 0.0555(16) | 0.0745(18) | 0.0386(14) | 0.0216(12) | -0.0006(12) | -0.0105(14) |