Table D. Anisotropic displacement parameters (Å2) for jinshajiangite

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | *U*11 | *U*22 | *U*33 | *U*23 | *U*13 | *U*12 | *U*eq |
| MO(1) | 0.0124(7) | 0.0122(7) | 0.0138(8) | -0.0001(6) | 0.0001(5) | 0.0016(6) | 0.0129(5) |
| MO(2) | 0.0058(4) | 0.0079(4) | 0.0148(4) | -0.0023(4) | 0.0045(3) | -0.0012(4) | 0.0093(3) |
| MO(3) | 0.0052(4) | 0.0077(4) | 0.0138(4) | 0.0001(4) | 0.0023(3) | -0.0003(4) | 0.0088(3) |
| MO(4) | 0.0083(4) | 0.0102(4) | 0.0108(4) | -0.0012(4) | 0.0040(3) | -0.0004(4) | 0.0096(3) |
| MO(5) | 0.0114(8) | 0.0196(8) | 0.0266(10) | 0.0088(7) | 0.0075(6) | 0.0053(6) | 0.0188(5) |
| MO(6) | 0.0074(4) | 0.0105(4) | 0.0116(4) | 0.0004(4) | 0.0024(3) | 0.0002(4) | 0.0097(3) |
| MO(7) | 0.0090(4) | 0.0098(4) | 0.0091(4) | 0.0006(5) | -0.0002(3) | 0.0010(5) | 0.0094(3) |
| MO(8) | 0.0133(8) | 0.0221(9) | 0.0253(10) | 0.0119(8) | 0.0100(6) | 0.0090(7) | 0.0198(6) |
| MO(9) | 0.0057(7) | 0.0105(7) | 0.0192(8) | 0.0008(6) | 0.0022(5) | 0.0014(6) | 0.0117(5) |
| MO(10) | 0.0070(4) | 0.0075(4) | 0.0115(4) | -0.0007(5) | 0.0003(3) | -0.0003(5) | 0.0087(3) |
| MH(1) | 0.0041(4) | 0.0031(5) | 0.0074(4) | 0.0013(4) | -0.0004(3) | -0.0006(4) | 0.0049(3) |
| MH(2) | 0.0037(4) | 0.0062(6) | 0.0091(4) | -0.0012(4) | 0.0005(3) | -0.0003(3) | 0.0063(3) |
| MH(3) | 0.0045(4) | 0.0030(6) | 0.0063(4) | 0.0002(4) | 0.0006(3) | 0.0004(4) | 0.0046(3) |
| MH(4) | 0.0051(4) | 0.0062(5) | 0.0075(5) | -0.0013(3) | 0.0009(3) | 0.0005(3) | 0.0062(3) |
| Si(1) | 0.0107(7) | 0.0068(7) | 0.0070(7) | -0.0001(6) | 0.0008(5) | 0.0032(5) | 0.0082(3) |
| Si(2) | 0.0081(7) | 0.0067(6) | 0.0034(6) | 0.0001(5) | -0.0007(5) | -0.0002(5) | 0.0061(3) |
| Si(3) | 0.0035(6) | 0.0053(7) | 0.0082(6) | -0.0016(5) | -0.0003(5) | -0.0028(5) | 0.0057(3) |
| Si(4) | 0.0084(7) | 0.0071(7) | 0.0036(6) | 0.0002(5) | 0.0008(5) | 0.0005(5) | 0.0063(3) |
| Si(5) | 0.0060(6) | 0.0054(7) | 0.0113(7) | -0.0015(6) | 0.0016(5) | 0.0006(5) | 0.0075(3) |
| Si(6) | 0.0063(6) | 0.0057(6) | 0.0065(6) | -0.0009(5) | -0.0003(5) | -0.0013(5) | 0.0062(3) |
| Si(7) | 0.0056(6) | 0.0074(7) | 0.0088(7) | -0.0010(5) | 0.0016(5) | 0.0005(5) | 0.0072(3) |
| Si(8) | 0.0080(7) | 0.0046(7) | 0.0118(7) | -0.0019(6) | 0.0004(5) | 0.0002(5) | 0.0082(3) |
| A*P*(1) | 0.01125(9) | 0.01269(10) | 0.01145(10) | -0.00051(13) | 0.00083(6) | -0.00060(14) | 0.01181(6) |
| A*P*(21) | 0.0071(6) | 0.090(2) | 0.0235(8) | -0.0009(11) | 0.0029(5) | 0.0104(10) | 0.0400(8) |
| A*P*(22) | 0.0292(11) | 0.0249(12) | 0.0193(10) | 0.0001(10) | 0.0006(8) | -0.0023(11) | 0.0246(5) |
| B*P*(1) | 0.0210(6) | 0.0185(6) | 0.0052(5) | -0.0013(10) | 0.0003(4) | 0.0103(10) | 0.0149(4) |
| B*P*(2) | 0.0225(7) | 0.0209(7) | 0.0062(5) | -0.0011(10) | -0.0002(4) | -0.0127(11) | 0.0166(4) |
| O(1) | 0.0063(16) | 0.0094(19) | 0.0037(17) | 0.0001(15) | 0.0012(13) | 0.0006(15) | 0.0064(8) |
| O(3) | 0.0069(15) | 0.0074(16) | 0.0156(17) | 0.0001(14) | -0.0014(13) | -0.0027(14) | 0.0101(9) |
| O(4) | 0.0121(19) | 0.0103(19) | 0.012(2) | -0.0045(18) | 0.0024(15) | -0.0039(17) | 0.0114(9) |
| O(5) | 0.0120(18) | 0.016(2) | 0.017(2) | -0.002(2) | -0.0022(16) | 0.0020(18) | 0.0153(10) |
| O(6) | 0.0118(18) | 0.0052(18) | 0.0097(19) | 0.0009(16) | 0.0005(15) | 0.0022(16) | 0.0090(9) |
| O(7) | 0.0083(17) | 0.0080(18) | 0.0049(17) | 0.0033(15) | 0.0005(13) | -0.0008(16) | 0.0071(8) |
| O(8) | 0.0114(18) | 0.020(2) | 0.0026(17) | -0.0024(18) | 0.0008(14) | -0.0009(18) | 0.0112(9) |
| O(9) | 0.0079(14) | 0.0074(16) | 0.0265(17) | -0.0028(15) | 0.0004(12) | -0.0024(12) | 0.0140(7) |
| O(10) | 0.0085(15) | 0.0152(18) | 0.0113(16) | -0.0001(14) | -0.0033(13) | -0.0008(14) | 0.0119(7) |
| O(11) | 0.0103(15) | 0.0130(18) | 0.0128(16) | -0.0007(14) | 0.0021(13) | -0.0031(14) | 0.0120(7) |
| O(12) | 0.0112(16) | 0.0139(18) | 0.0160(18) | 0.0037(15) | 0.0029(14) | -0.0057(14) | 0.0136(7) |
| O(13) | 0.0164(17) | 0.0094(17) | 0.0109(16) | -0.0055(14) | 0.0052(13) | 0.0039(14) | 0.0120(7) |
| O(14) | 0.0055(15) | 0.0144(18) | 0.0199(19) | 0.0006(15) | -0.0020(13) | 0.0024(14) | 0.0135(7) |
| O(15) | 0.0105(16) | 0.016(2) | 0.0152(18) | -0.0043(15) | 0.0000(14) | -0.0032(15) | 0.0140(8) |
| O(16) | 0.0124(16) | 0.0123(17) | 0.0079(15) | -0.0031(13) | 0.0046(13) | -0.0006(14) | 0.0107(7) |
| O(17) | 0.0158(16) | 0.0055(15) | 0.0267(18) | -0.0039(15) | 0.0023(14) | 0.0048(13) | 0.0160(7) |
| O(18) | 0.0111(14) | 0.0099(16) | 0.0094(13) | 0.0020(13) | 0.0034(11) | -0.0041(13) | 0.0100(6) |
| O(19) | 0.0104(15) | 0.0156(17) | 0.0095(15) | -0.0038(15) | -0.0024(12) | -0.0038(15) | 0.0120(7) |
| O(20) | 0.0106(15) | 0.0107(16) | 0.0169(16) | -0.0005(15) | 0.0041(13) | 0.0026(14) | 0.0126(7) |
| O(21) | 0.0045(14) | 0.0159(18) | 0.027(2) | 0.0110(17) | 0.0001(13) | -0.0027(15) | 0.0160(8) |
| O(22) | 0.0072(15) | 0.0137(17) | 0.0199(17) | -0.0060(16) | 0.0052(13) | 0.0018(14) | 0.0134(7) |
| O(23) | 0.0052(14) | 0.0165(18) | 0.0157(16) | -0.0065(16) | 0.0063(12) | -0.0040(15) | 0.0122(7) |
| O(24) | 0.0075(15) | 0.0171(18) | 0.0163(17) | -0.0018(16) | -0.0075(13) | 0.0010(15) | 0.0141(7) |
| O(25) | 0.0176(15) | 0.0074(16) | 0.0079(13) | 0.0020(13) | -0.0027(12) | 0.0034(13) | 0.0112(6) |
| O(26) | 0.0089(16) | 0.0104(18) | 0.026(2) | 0.0049(16) | -0.0021(15) | 0.0064(14) | 0.0152(8) |
| O(27) | 0.0137(16) | 0.0129(17) | 0.0148(16) | 0.0090(15) | 0.0046(13) | 0.0037(15) | 0.0136(7) |
| O(28) | 0.0152(16) | 0.0151(17) | 0.0154(17) | 0.0017(16) | 0.0027(13) | -0.0004(16) | 0.0151(7) |
| XOM(1) | 0.0081(16) | 0.016(2) | 0.0043(15) | -0.0028(16) | 0.0042(12) | -0.0013(16) | 0.0093(8) |
| XOM(2) | 0.0077(16) | 0.018(2) | 0.0063(16) | 0.0002(15) | -0.0028(13) | 0.0008(15) | 0.0109(9) |
| XOM(3) | 0.0108(16) | 0.013(2) | 0.0128(17) | 0.0010(16) | 0.0067(14) | 0.0017(16) | 0.0117(9) |
| XOM(4) | 0.0119(18) | 0.019(3) | 0.0164(19) | 0.0020(17) | -0.0010(15) | -0.0016(16) | 0.0160(10) |
| XOA(1) | 0.0096(17) | 0.012(2) | 0.0072(17) | -0.003(2) | 0.0076(14) | -0.004(2) | 0.0092(9) |
| XOA(2) | 0.0082(17) | 0.010(2) | 0.0120(19) | 0.002(2) | -0.0027(14) | 0.000(2) | 0.0102(9) |
| XOA(3) | 0.0110(18) | 0.011(2) | 0.017(2) | 0.005(2) | -0.0081(16) | -0.001(2) | 0.0134(10) |
| XOA(4) | 0.0112(18) | 0.014(2) | 0.0077(17) | -0.001(2) | 0.0024(14) | -0.006(2) | 0.0109(9) |
| X*P*M(1) | 0.0159(18) | 0.0192(13) | 0.0085(16) | 0.0030(11) | -0.0014(13) | -0.0028(12) | 0.0147(7) |
| X*P*M(2) | 0.0161(17) | 0.0197(14) | 0.0104(16) | -0.0026(11) | 0.0022(13) | 0.0026(12) | 0.0154(7) |