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| TABLE D. ANISOTROPIC DISPLACEMENT PARAMETERS FOR BULGAKITE |
| Atom |  *U*11 |  *U*22 |  *U*33 |  *U*23 |  *U*13 |  *U*12 |
|  |  |  |  |  |  |  |
| M(1) | 0.00847(17) | 0.00763(17) | 0.01272(17) | 0.00529(12) |  0.00334(11) |  0.00341(12) |
| M(2) | 0.00854(16) | 0.00865(17) | 0.01315(16) | 0.00610(12)  |  0.00378(10) |  0.00371(11) |
| M(3) | 0.00889(16) | 0.00843(16) | 0.01362(16) | 0.00631(11)  |  0.00408(10) |  0.00441(11) |
| M(4) | 0.00769(19) | 0.0071(2) | 0.0126(2) | 0.00496(15) |  0.00219(13) |  0.00293(14) |
| D | 0.00547(14) | 0.00744(15) | 0.01042(15) | 0.00438(11) |  0.00213(10) |  0.00306(10) |
| A(1) | 0.0423(6) | 0.0423(8) | 0.0263(5) | 0.0117(5) |  0.0050(4) |  0.0102(6) |
| A(2) | 0.045(6) | 0.021(4) | 0.029(5) | 0.011(4) |  0.005(4) |  0.006(4) |
| B | 0.0181(3) | 0.0129(3) | 0.0123(3) | 0.0056(2) |  0.0028(2) |  0.0053(2) |
| T(1) | 0.0078(2) | 0.0079(2) | 0.0106(2) | 0.00538(18) |  0.00240(17) |  0.00326(17) |
| T(2) | 0.0085(2) | 0.0072(2) | 0.0113(2) | 0.00498(18) |  0.00234(17) |  0.00296(17) |
| T(3) | 0.0083(2) | 0.0071(2) | 0.0109(2) | 0.00518(18) |  0.00234(17) |  0.00313(17) |
| T(4) | 0.0079(2) | 0.0068(2) | 0.0104(2) | 0.00494(18) |  0.00231(16) |  0.00296(17) |
| O(1) | 0.0099(6) | 0.0103(6) | 0.0109(6) | 0.0054(5) |  0.0025(5) |  0.0036(5) |
| O(2) | 0.0103(6) | 0.0104(6) | 0.0120(6) | 0.0046(5) |  0.0015(5) |  0.0033(5) |
| O(3) | 0.0096(6) | 0.0088(6) | 0.0106(6) | 0.0043(5) |  0.0021(5) |  0.0035(5) |
| O(4) | 0.0115(6) | 0.0114(6) | 0.0134(6) | 0.0058(5) |  0.0035(5) |  0.0045(5) |
| O(5) | 0.0117(6) | 0.0119(6) | 0.0131(6) | 0.0058(5) |  0.0027(5) |  0.0045(5) |
| O(6) | 0.0098(6) | 0.0093(6) | 0.0103(6) | 0.0052(5) |  0.0023(5) |  0.0037(5) |
| O(7) | 0.0106(6) | 0.0097(6) | 0.0103(6) | 0.0044(5) |  0.0024(5) |  0.0038(5) |
| O(8) | 0.0137(6) | 0.0193(7) | 0.0151(7) | 0.0068(6) |  0.0031(5) | -0.0011(5) |
| O(9) | 0.0140(6) | 0.0190(7) | 0.0157(7) | 0.0061(6) |  0.0056(5) | -0.0014(5) |
| O(10) | 0.0200(7) | 0.0188(7) | 0.0153(7) | 0.0066(6) |  0.0025(5) |  0.0126(6) |
| O(11) | 0.0232(7) | 0.0212(7) | 0.0167(7) | 0.0095(6) |  0.0078(6) |  0.0171(6) |
| O(12) | 0.0198(7) | 0.0174(7) | 0.0164(7) | 0.0053(6) | -0.0010(5) |  0.0130(6) |
| O(13) | 0.0279(8) | 0.0086(6) | 0.0149(6) | 0.0064(5) |  0.0028(6) |  0.0036(5) |
| O(14) | 0.0285(8) | 0.0098(6) | 0.0160(7) | 0.0078(5) |  0.0040(6) |  0.0046(6) |
| O(15) | 0.0124(6) | 0.0190(7) | 0.0154(6) | 0.0078(6) |  0.0011(5) | -0.0026(5) |
| X*P*D | 0.0142(7) | 0.0119(7) | 0.0081(7) | 0.0042(6) |  0.0017(6) |  0.0040(6) |
| W | 0.045(3) | 0.035(3) | 0.034(3) | 0.015(3) |  0.006(2) |  0.011(3) |

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| TABLE D. ANISOTROPIC DISPLACEMENT PARAMETERS FOR NALIVKINITE |
| Atom |  *U*11 |  *U*22 |  *U*33 |  *U*23 |  *U*13 |  *U*12 |
|  |  |  |  |  |  |  |
| M(1) | 0.0059(3) | 0.0070(4) | 0.0099(3) | 0.0029(3) |  0.0018(2) |  0.0006(3) |
| M(2) | 0.0056(4) | 0.0083(4) | 0.0105(4) | 0.0036(3) |  0.0018(2) |  0.0012(3) |
| M(3) | 0.0067(4) | 0.0083(4) | 0.0109(4) | 0.0043(3) |  0.0032(2) |  0.0020(3) |
| M(4) | 0.0062(4) | 0.0067(4) | 0.0099(5) | 0.0030(4) |  0.0014(3) |  0.0007(3) |
| D | 0.0027(2) | 0.0063(3) | 0.0130(3) | 0.0043(3) |  0.00152(17) |  0.0008(2) |
| A(1) | 0.0414(16) | 0.041(2) | 0.0157(11) | 0.007(2) |  0.0026(10) |  0.006(2) |
| A(2) | 0.043(9) | 0.051(11) | 0.007(6) | 0.012(9) |  0.004(6) |  0.017(10) |
| B | 0.0155(8) | 0.0080(9) | 0.0049(7) | 0.0007(8) |  0.0005(6) |  0.0022(9) |
| T(1) | 0.0067(5) | 0.0082(5) | 0.0088(6) | 0.0048(5) |  0.0013(4) |  0.0011(4) |
| T(2) | 0.0060(5) | 0.0062(5) | 0.0085(5) | 0.0032(4) |  0.0010(4) |  0.0008(4) |
| T(3) | 0.0056(5) | 0.0060(5) | 0.0080(5) | 0.0033(5) |  0.0013(4) |  0.0010(4) |
| T(4) | 0.0076(5) | 0.0059(5) | 0.0078(6) | 0.0030(4) |  0.0007(4) |  0.0010(4) |
| O(1) | 0.0080(14) | 0.0106(15) | 0.0085(15) | 0.0051(12) |  0.0006(11) |  0.0005(12) |
| O(2) | 0.0087(12) | 0.0105(14) | 0.0079(11) | 0.0023(14) |  0.0010(9) |  0.0021(13) |
| O(3) | 0.0080(14) | 0.0069(15) | 0.0086(15) | 0.0021(13) |  0.0005(11) |  0.0012(12) |
| O(4) | 0.0091(14) | 0.0093(15) | 0.0134(17) | 0.0051(13) |  0.0025(13) | -0.0004(12) |
| O(5) | 0.0082(14) | 0.0109(15) | 0.0079(15) | 0.0020(13) |  0.0015(11) |  0.0013(13) |
| O(6) | 0.0077(12) | 0.0083(14) | 0.0060(12) | 0.0005(13) |  0.0007(9) |  0.0023(13) |
| O(7) | 0.0094(14) | 0.0100(15) | 0.0058(14) | 0.0019(12) |  0.0004(11) |  0.0009(12) |
| O(8) | 0.0090(15) | 0.0193(16) | 0.0101(16) | 0.0053(13) |  0.0024(12) | -0.0007(12) |
| O(9) | 0.0173(18) | 0.0203(17) | 0.0167(18) | 0.0028(14) |  0.0064(14) | -0.0064(14) |
| O(10) | 0.0176(17) | 0.0191(16) | 0.0133(17) | 0.0069(14) |  0.0010(13) |  0.0103(14) |
| O(11) | 0.031(2) | 0.0290(19) | 0.0158(18) | 0.0105(16) |  0.0092(16) |  0.0257(17) |
| O(12) | 0.0239(19) | 0.0225(17) | 0.0156(17) | 0.0027(15) | -0.0035(14) |  0.0163(15) |
| O(13) | 0.0284(19) | 0.0075(14) | 0.0127(16) | 0.0054(12) |  0.0025(14) |  0.0014(13) |
| O(14) | 0.0278(19) | 0.0096(14) | 0.0102(16) | 0.0046(12) |  0.0013(14) |  0.0006(13) |
| O(15) | 0.0144(17) | 0.0239(18) | 0.0156(17) | 0.0087(15) | -0.0012(14) | -0.0107(14) |
| X*P*D | 0.0143(15) | 0.0148(17) | 0.0082(13) | 0.0045(17) |  0.0005(11) |  0.0029(16) |
| W | 0.019(4) | 0.018(4) | 0.013(3) | 0.000(5) | -0.002(2) |  0.002(5) |