

Table 4. Anisotropic displacement parameters for non-hydrogen atoms of Tutton's salts

| | atom | U^{11} | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} |
|----|------------|-------------|-------------|-------------|--------------|-------------|--------------|
| Mg | <i>M</i> | 0.0154(3) | 0.0168(3) | 0.0157(3) | 0.0002(2) | 0.0037(2) | -0.0011(2) |
| Fe | | 0.0152(2) | 0.0171(3) | 0.0157(2) | 0.00022(15) | 0.00047(16) | -0.00117(14) |
| Co | | 0.01264(15) | 0.01578(13) | 0.01555(13) | 0.00029(10) | 0.00331(11) | -0.00105(11) |
| Ni | | 0.01271(12) | 0.01479(13) | 0.01434(13) | 0.00014(10) | 0.00391(9) | -0.00095(10) |
| Cu | | 0.01541(11) | 0.01697(12) | 0.01406(11) | 0.00068(9) | 0.00367(8) | -0.00243(9) |
| Zn | | 0.0164(2) | 0.01722(18) | 0.01629(17) | 0.00033(16) | 0.00369(14) | -0.00150(17) |
| Mg | <i>K</i> | 0.03259(16) | 0.03123(16) | 0.02921(16) | -0.00037(12) | 0.01124(12) | -0.00269(12) |
| Fe | | 0.0335(4) | 0.0321(4) | 0.0281(3) | -0.0002(2) | 0.0088(3) | -0.0024(2) |
| Co | | 0.0301(2) | 0.0304(2) | 0.02903(19) | -0.00041(15) | 0.01121(18) | -0.00223(16) |
| Ni | | 0.03046(19) | 0.0295(2) | 0.02847(19) | -0.00026(16) | 0.01221(16) | -0.00189(16) |
| Cu | | 0.02998(19) | 0.03057(19) | 0.02703(17) | -0.00043(14) | 0.01086(14) | -0.00119(14) |
| Zn | | 0.0311(4) | 0.0299(3) | 0.0281(3) | -0.0003(2) | 0.0115(2) | -0.0025(3) |
| Mg | <i>S</i> | 0.01540(12) | 0.01931(13) | 0.01754(13) | -0.00196(11) | 0.00382(9) | -0.00266(10) |
| Fe | | 0.0166(3) | 0.0206(3) | 0.0174(3) | -0.00192(19) | 0.0016(2) | -0.00235(18) |
| Co | | 0.01455(18) | 0.01910(17) | 0.01763(16) | -0.00191(13) | 0.00404(15) | -0.00239(14) |
| Ni | | 0.01451(15) | 0.01763(17) | 0.01711(16) | -0.00185(14) | 0.00410(13) | -0.00207(13) |
| Cu | | 0.01673(15) | 0.01915(16) | 0.01706(14) | -0.00135(12) | 0.00465(11) | -0.00278(12) |
| Zn | | 0.0154(3) | 0.0183(2) | 0.0174(2) | -0.0014(2) | 0.0042(2) | -0.0026(2) |
| Mg | <i>O1</i> | 0.0511(7) | 0.0242(5) | 0.0240(5) | 0.0023(4) | 0.0083(5) | -0.0128(5) |
| Fe | | 0.0515(15) | 0.0258(10) | 0.0242(11) | 0.0041(8) | 0.0038(10) | -0.0121(10) |
| Co | | 0.0462(9) | 0.0242(6) | 0.0244(6) | 0.0023(5) | 0.0074(6) | -0.0119(6) |
| Ni | | 0.0466(8) | 0.0221(6) | 0.0236(6) | 0.0021(5) | 0.0103(6) | -0.0101(6) |
| Cu | | 0.0466(8) | 0.0233(6) | 0.0245(6) | 0.0035(5) | 0.0079(5) | -0.0109(5) |
| Zn | | 0.0506(14) | 0.0238(10) | 0.0228(9) | 0.0030(7) | 0.0076(9) | -0.0123(9) |
| Mg | <i>O2</i> | 0.0185(5) | 0.0552(8) | 0.0456(7) | -0.0102(6) | 0.0016(5) | 0.0099(5) |
| Fe | | 0.0202(9) | 0.0598(19) | 0.0410(15) | -0.0133(13) | -0.0016(9) | 0.0109(11) |
| Co | | 0.0176(7) | 0.0523(10) | 0.0427(8) | -0.0103(8) | 0.0013(7) | 0.0096(7) |
| Ni | | 0.0172(6) | 0.0486(10) | 0.0429(9) | -0.0096(8) | 0.0017(6) | 0.0090(6) |
| Cu | | 0.0193(6) | 0.0482(9) | 0.0381(7) | -0.0076(6) | 0.0033(5) | 0.0076(6) |
| Zn | | 0.0187(11) | 0.0518(14) | 0.0430(12) | -0.0104(11) | 0.0023(10) | 0.0100(10) |
| Mg | <i>O3</i> | 0.0214(4) | 0.0240(4) | 0.0257(5) | -0.0059(4) | 0.0064(4) | -0.0080(3) |
| Fe | | 0.0230(9) | 0.0261(10) | 0.0263(10) | -0.0056(8) | 0.0051(7) | -0.0083(7) |
| Co | | 0.0189(6) | 0.0246(6) | 0.0265(6) | -0.0051(5) | 0.0068(5) | -0.0076(5) |
| Ni | | 0.0192(5) | 0.0238(6) | 0.0248(6) | -0.0049(3) | 0.0073(5) | -0.0080(5) |
| Cu | | 0.0201(5) | 0.0258(6) | 0.0236(5) | -0.0052(4) | 0.0062(4) | -0.0076(4) |
| Zn | | 0.0189(10) | 0.0260(9) | 0.0255(9) | -0.0068(7) | 0.0070(8) | -0.0078(8) |
| Mg | <i>O4</i> | 0.0377(6) | 0.0261(5) | 0.0193(4) | -0.0048(4) | 0.0103(4) | -0.0045(4) |
| Fe | | 0.0377(12) | 0.0280(10) | 0.0199(9) | -0.0040(8) | 0.0081(8) | -0.0031(9) |
| Co | | 0.0355(8) | 0.0250(6) | 0.0189(5) | -0.0034(5) | 0.0096(6) | -0.0039(5) |
| Ni | | 0.0355(7) | 0.0257(6) | 0.0177(5) | -0.0035(5) | 0.0100(5) | -0.0035(5) |
| Cu | | 0.0357(7) | 0.0295(6) | 0.0188(5) | -0.0044(4) | 0.0100(5) | -0.0031(5) |
| Zn | | 0.0339(12) | 0.0257(9) | 0.0190(8) | -0.0046(7) | 0.0103(8) | -0.0033(8) |
| Mg | <i>OW1</i> | 0.0219(4) | 0.0284(5) | 0.0208(5) | -0.0005(4) | 0.0029(4) | -0.0074(4) |
| Fe | | 0.0228(9) | 0.0309(11) | 0.0214(9) | 0.0004(8) | -0.0013(7) | -0.0072(7) |
| Co | | 0.0201(7) | 0.0277(6) | 0.0207(6) | -0.0004(5) | 0.0028(6) | -0.0068(5) |
| Ni | | 0.0200(5) | 0.0245(6) | 0.0191(6) | -0.0013(5) | 0.0043(5) | -0.0061(5) |
| Cu | | 0.0238(6) | 0.0346(7) | 0.0192(5) | 0.0026(5) | 0.0043(4) | -0.0058(5) |
| Zn | | 0.0209(11) | 0.0271(10) | 0.0210(9) | -0.0004(8) | 0.0042(9) | -0.0065(8) |
| Mg | <i>OW2</i> | 0.0192(4) | 0.0208(4) | 0.0272(5) | 0.0010(4) | 0.0058(4) | 0.0013(3) |
| Fe | | 0.0210(8) | 0.0237(9) | 0.0284(10) | 0.0011(8) | 0.0043(7) | 0.0028(7) |
| Co | | 0.0177(6) | 0.0214(6) | 0.0274(6) | 0.0004(5) | 0.0058(6) | 0.0011(5) |
| Ni | | 0.0177(5) | 0.0191(6) | 0.0246(6) | -0.0005(5) | 0.0061(5) | 0.0007(4) |

| | | | | | | | |
|----|-----|------------|-----------|-----------|-----------|-----------|------------|
| Cu | | 0.0235(6) | 0.0282(6) | 0.0282(6) | 0.0031(5) | 0.0045(5) | -0.0021(5) |
| Zn | | 0.0199(11) | 0.0219(9) | 0.0248(9) | 0.0001(7) | 0.0056(8) | 0.0005(8) |
| Mg | OW3 | 0.0280(5) | 0.0219(4) | 0.0225(4) | 0.0037(4) | 0.0114(4) | 0.0028(4) |
| Fe | | 0.0307(10) | 0.0253(9) | 0.0214(9) | 0.0037(7) | 0.0084(8) | 0.0032(8) |
| Co | | 0.0270(7) | 0.0217(6) | 0.0215(5) | 0.0036(5) | 0.0107(5) | 0.0034(5) |
| Ni | | 0.0252(6) | 0.0197(6) | 0.0195(5) | 0.0028(4) | 0.0100(5) | 0.0013(5) |
| Cu | | 0.0222(5) | 0.0220(5) | 0.0188(5) | 0.0033(4) | 0.0081(4) | 0.0014(4) |
| Zn | | 0.0272(13) | 0.0220(9) | 0.0206(8) | 0.0019(7) | 0.0104(8) | 0.0025(8) |
