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Crystal structures of the {011}, {610} and {010} growth sectors in brewsterite

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Table 5 Anisotropic displacement parameters of {011}, {610} and {010} sector

{011} sector

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
TA	0.009(1)	0.021(1)	0.0069(9)	0.0014(8)	-0.0013(8)	0.0014(8)
TA'	0.009(1)	0.022(1)	0.0089(10)	-0.0015(8)	-0.0005(8)	0.0002(8)
TB	0.011(1)	0.016(1)	0.0100(10)	0.0014(8)	-0.0013(8)	0.0030(8)
TB'	0.012(1)	0.015(1)	0.0101(10)	-0.0014(8)	-0.0001(8)	-0.0015(8)
TC	0.012(1)	0.013(1)	0.0093(10)	0.0024(8)	0.0004(8)	0.0015(8)
TC'	0.014(1)	0.013(1)	0.0076(9)	-0.0011(8)	0.0012(8)	0.0000(8)
TD	0.0081(10)	0.015(1)	0.015(1)	0.0011(8)	-0.0015(8)	0.0004(8)
TD'	0.0080(10)	0.016(1)	0.0120(10)	0.0001(8)	-0.0010(8)	0.0019(8)
O1	0.021(3)	0.023(3)	0.009(3)	0.001(2)	-0.003(2)	0.004(2)
O1'	0.021(3)	0.022(3)	0.010(3)	-0.001(2)	-0.001(2)	-0.003(2)
O2	0.022(3)	0.036(4)	0.019(3)	0.010(3)	-0.006(2)	-0.004(3)
O2'	0.022(3)	0.040(4)	0.014(3)	-0.010(3)	-0.004(2)	0.007(2)
O3	0.018(3)	0.024(3)	0.022(3)	0.010(2)	0.004(2)	0.006(2)
O3'	0.016(3)	0.021(3)	0.020(3)	-0.007(2)	0.002(2)	-0.001(2)
O4	0.022(3)	0.034(3)	0.018(3)	0.006(3)	0.007(2)	0.008(2)
O4'	0.025(3)	0.034(4)	0.017(3)	-0.004(3)	0.006(2)	-0.006(2)
O5	0.012(3)	0.040(4)	0.027(3)	0.004(2)	-0.008(2)	-0.012(3)
O5'	0.014(3)	0.036(4)	0.026(3)	-0.004(2)	-0.008(2)	0.011(3)
O6	0.021(3)	0.030(4)	0.048(4)	-0.004(3)	0.003(3)	0.023(3)
O6'	0.023(3)	0.026(3)	0.046(4)	0.008(3)	0.003(3)	-0.016(3)
O7	0.014(3)	0.020(3)	0.015(3)	0.004(2)	0.001(2)	-0.003(2)
O7'	0.015(3)	0.022(3)	0.016(3)	-0.005(2)	-0.002(2)	0.005(2)

Table 5 continued

Atom	{011} sector U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O8	0.028(5)	0.048(6)	0.030(5)	0.018(4)	-0.010(4)	-0.025(4)
O8'	0.023(5)	0.046(6)	0.035(5)	-0.016(4)	-0.009(4)	0.026(4)
O9	0.050(4)	0.021(3)	0.029(3)	0.003(3)	0.022(3)	0.000(3)
M	0.0228(3)	0.0198(3)	0.0235(3)	0.0006(3)	0.0012(3)	0.0012(2)
O10	0.054(5)	0.056(5)	0.032(4)	0.001(4)	0.011(3)	0.003(3)
O11	0.042(4)	0.057(5)	0.083(6)	0.003(4)	0.011(4)	0.021(4)
O11'	0.040(4)	0.060(5)	0.086(6)	-0.002(4)	0.017(4)	-0.018(4)
O12	0.030(4)	0.054(5)	0.072(5)	-0.001(3)	0.019(4)	0.002(4)
O13	0.094(6)	0.028(4)	0.029(4)	0.002(4)	-0.007(4)	0.001(3)

Refined M site contents for {011} sector :$Sr_{0.50}Ba_{0.45}K_{0.01}$
O10~O13 are H_2O oxygens.

Table 5 continued

{610} sector

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
TA	0.0110(9)	0.0158(9)	0.0092(9)	0.0005(7)	0.0018(7)	-0.0005(7)
TA'	0.0108(9)	0.0162(9)	0.0092(9)	0.0000(7)	0.0014(7)	0.0003(7)
TB	0.0161(10)	0.0138(9)	0.0118(9)	0.0004(8)	0.0020(7)	0.0016(7)
TB'	0.0154(10)	0.0154(10)	0.0109(9)	-0.0001(8)	0.0027(7)	-0.0002(7)
TC	0.0161(10)	0.0127(9)	0.0097(9)	0.0018(7)	0.0025(7)	0.0010(7)
TC'	0.0138(10)	0.0113(9)	0.0097(9)	-0.0007(7)	0.0033(7)	0.0001(7)
TD	0.0105(9)	0.0122(9)	0.0133(9)	0.0010(7)	0.0018(7)	-0.0010(7)
TD'	0.0099(9)	0.0124(9)	0.0119(9)	-0.0007(7)	0.0018(7)	0.0011(7)
O1	0.025(3)	0.022(3)	0.011(2)	0.001(2)	0.003(2)	0.001(2)
O1'	0.023(3)	0.019(3)	0.012(2)	0.002(2)	0.002(2)	0.001(2)
O2	0.023(3)	0.034(3)	0.019(3)	0.008(2)	0.000(2)	-0.007(2)
O2'	0.020(3)	0.033(3)	0.019(3)	-0.004(2)	-0.001(2)	0.008(2)
O3	0.024(3)	0.024(3)	0.019(3)	0.009(2)	0.005(2)	0.008(2)
O3'	0.017(3)	0.021(3)	0.020(3)	-0.006(2)	0.005(2)	-0.007(2)
O4	0.027(3)	0.027(3)	0.016(3)	0.003(2)	0.010(2)	0.006(2)
O4'	0.027(3)	0.025(3)	0.017(3)	0.000(2)	0.011(2)	-0.004(2)
O5	0.014(3)	0.031(3)	0.030(3)	0.002(2)	-0.005(2)	-0.013(2)
O5'	0.015(3)	0.030(3)	0.027(3)	-0.005(2)	-0.005(2)	0.012(2)
O6	0.030(3)	0.027(3)	0.043(4)	-0.010(2)	0.007(3)	0.013(3)
O6'	0.030(3)	0.024(3)	0.043(4)	0.007(2)	0.009(3)	-0.013(3)
O7	0.015(3)	0.021(3)	0.024(3)	0.003(2)	0.002(2)	-0.003(2)
O7'	0.015(3)	0.021(3)	0.020(3)	-0.003(2)	0.001(2)	0.002(2)

Table 5 continued

Atom	{610} sector U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O8	0.036(5)	0.047(5)	0.029(5)	0.016(4)	0.001(4)	-0.022(4)
O8'	0.029(5)	0.048(5)	0.031(5)	-0.016(4)	0.003(4)	0.025(4)
O9	0.043(3)	0.013(3)	0.038(3)	-0.001(2)	0.023(3)	0.001(2)
M	0.0240(3)	0.0170(3)	0.0199(3)	0.0000(2)	0.0034(2)	0.0005(2)
O10	0.058(4)	0.046(4)	0.036(4)	0.000(3)	0.020(3)	0.004(3)
O11	0.044(4)	0.060(5)	0.084(6)	0.001(4)	0.017(4)	0.023(4)
O11'	0.046(4)	0.068(5)	0.086(6)	-0.004(4)	0.021(4)	-0.022(4)
O12	0.039(4)	0.053(4)	0.066(5)	0.001(3)	0.019(3)	0.000(4)
O13	0.082(5)	0.028(3)	0.034(4)	-0.002(3)	0.000(3)	-0.003(3)

Refined M site contents for {610} sector :$Sr_{0.40}Ba_{0.55}K_{0.01}$
O10~O13 are H_2O oxygens.

Table 5 continued

{010} sector

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
TA	0.015(1)	0.025(1)	0.012(1)	0.0003(10)	0.0020(9)	0.0004(10)
TA'	0.015(1)	0.024(1)	0.014(1)	-0.0011(10)	0.0016(9)	-0.0003(10)
TB	0.018(1)	0.022(1)	0.014(1)	-0.0016(10)	0.0021(9)	0.0010(9)
TB'	0.018(1)	0.021(1)	0.014(1)	-0.0007(10)	0.0016(9)	-0.0007(9)
TC	0.019(1)	0.019(1)	0.014(1)	0.0000(10)	0.0028(10)	0.0016(9)
TC'	0.019(1)	0.019(1)	0.013(1)	-0.0017(10)	0.0028(9)	-0.0004(9)
TD	0.016(1)	0.019(1)	0.018(1)	-0.0001(10)	0.0023(10)	-0.0003(10)
TD'	0.015(1)	0.020(1)	0.017(1)	-0.0017(9)	0.0016(10)	0.0015(10)
O1	0.032(4)	0.032(4)	0.010(3)	-0.003(3)	0.001(3)	0.005(3)
O1'	0.031(4)	0.029(4)	0.013(3)	-0.001(3)	0.002(3)	-0.002(3)
O2	0.033(4)	0.049(5)	0.020(3)	0.004(3)	0.000(3)	-0.013(3)
O2'	0.032(4)	0.047(4)	0.019(3)	-0.007(3)	0.000(3)	0.013(3)
O3	0.026(4)	0.033(4)	0.030(4)	0.010(3)	0.009(3)	0.011(3)
O3'	0.022(3)	0.035(4)	0.027(4)	-0.011(3)	0.007(3)	-0.006(3)
O4	0.032(4)	0.039(4)	0.025(4)	0.001(3)	0.013(3)	0.008(3)
O4'	0.033(4)	0.037(4)	0.026(4)	-0.003(3)	0.014(3)	-0.009(3)
O5	0.017(3)	0.044(4)	0.033(4)	0.000(3)	-0.003(3)	-0.011(3)
O5'	0.017(3)	0.041(4)	0.032(4)	-0.001(3)	-0.005(3)	0.009(3)
O6	0.032(4)	0.032(4)	0.055(5)	-0.011(3)	0.008(4)	0.015(4)
O6'	0.033(4)	0.029(4)	0.053(5)	0.008(3)	0.011(4)	-0.016(3)
O7	0.021(3)	0.028(4)	0.023(3)	0.005(3)	0.003(3)	0.000(3)
O7'	0.021(3)	0.030(4)	0.025(3)	-0.007(3)	0.001(3)	0.004(3)

Table 5 continued

{010} sector

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O8	0.041(7)	0.063(8)	0.040(6)	0.016(6)	0.002(5)	-0.033(6)
O8'	0.040(6)	0.058(7)	0.035(6)	-0.017(5)	0.000(5)	0.034(5)
O9	0.053(5)	0.022(4)	0.039(4)	-0.002(3)	0.023(4)	0.001(3)
M	0.0176(4)	0.0152(4)	0.0150(4)	-0.0007(3)	0.0019(3)	0.0004(3)
O10	0.059(6)	0.063(6)	0.036(5)	-0.002(4)	0.017(4)	0.002(4)
O11	0.050(6)	0.080(7)	0.085(7)	0.000(5)	0.021(5)	0.021(6)
O11'	0.056(6)	0.077(7)	0.083(7)	-0.008(5)	0.027(5)	-0.019(5)
O12	0.043(5)	0.067(6)	0.088(7)	-0.002(4)	0.024(5)	0.005(5)
O13	0.114(8)	0.032(5)	0.036(5)	-0.002(5)	-0.002(5)	0.001(4)

Refined M site contents for {010} sector :$Sr_{0.67}Ba_{0.24}K_{0.01}$
O10~O13 are H_2O oxygens.