Table 5. Anisotropic displacement parameters U_{ij} [Å^2] for tuzlaite

(for deposit)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca	0.0119(3)	0.0128(3)	0.0109(3)	0.0020(3)	0.0003(3)	-0.0009(3)
Na	0.0219(8)	0.0274(9)	0.0223(8)	-0.0046(6)	0.0036(6)	-0.0050(7)
O1	0.008(1)	0.011(1)	0.011(1)	-0.0023(9)	0.0028(9)	0.001(1)
O2	0.019(1)	0.010(1)	0.015(1)	-0.001(1)	0.002(1)	0.000(1)
O3	0.008(1)	0.013(1)	0.015(1)	0.0008(9)	0.001(1)	0.003(1)
O4	0.010(1)	0.012(1)	0.020(1)	-0.0026(9)	0.003(1)	-0.003(1)
O5	0.007(1)	0.015(1)	0.015(1)	0.001(1)	-0.0005(9)	0.003(1)
O6	0.011(1)	0.017(1)	0.015(1)	0.002(1)	0.003(1)	0.003(1)
O7w	0.013(1)	0.021(1)	0.024(1)	0.000(1)	-0.001(1)	0.004(1)
O8hy	0.009(1)	0.020(1)	0.013(1)	0.000(1)	0.001(1)	0.004(1)
O9	0.006(1)	0.011(1)	0.020(1)	0.0001(9)	0.001(1)	0.003(1)
O10w	0.025(2)	0.021(1)	0.016(1)	-0.004(1)	0.003(1)	-0.003(1)
O11hy	0.023(2)	0.022(2)	0.012(1)	0.005(1)	-0.001(1)	-0.003(1)
O12	0.017(1)	0.012(1)	0.016(1)	-0.005(1)	0.007(1)	-0.003(1)
O13w	0.037(2)	0.023(2)	0.042(2)	-0.010(1)	0.016(1)	-0.013(1)
B1	0.013(2)	0.007(2)	0.010(2)	0.001(2)	0.001(2)	-0.002(2)
B2	0.009(2)	0.009(2)	0.013(2)	0.002(1)	0.001(1)	0.003(2)
B3	0.011(2)	0.012(2)	0.010(2)	-0.001(2)	-0.006(1)	0.002(2)
B4	0.015(2)	0.010(2)	0.011(2)	-0.001(2)	0.001(2)	0.001(2)
B5	0.009(2)	0.011(2)	0.011(2)	-0.002(2)	-0.001(1)	0.001(2)

Note: displacement parameters are of the form

$$\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)].$$