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Mineralogical studies of the nitrate deposits of Chile: VII. Two new saline minerals with the composition $K_6(Na,K)_4Na_6Mg_{10}(XO_4)_{12}(IO_3)_{12} \cdot 12H_2O$: Fuenzalidaite (X = S) and carlosruizite (X = Se)

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For deposit: Tables 4 - 6

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Table 4. Anisotropic thermal parameters for fuenzalidaite and carlosruizite

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

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
<u>Fuenzalidaite</u>						
I	0.006(1)	0.008(1)	0.003(1)	0.002(1)	0.001(1)	0.001(1)
S	0.004(4)	0.011(4)	0.017(5)	0.004(3)	-0.005(4)	-0.003(4)
K1	0.016(4)	0.028(7)	0.027(7)	0.014(4)	0.001(3)	0.001(6)
M	0.034(11)	= U_{11}	0.033(14)	= $\frac{1}{2}U_{11}$	0	0
Na1	0.026(8)	= U_{11}	0.011(13)	= $\frac{1}{2}U_{11}$	0	0
Na2	0.004(10)	= U_{11}	0.018(6)	= $\frac{1}{2}U_{11}$	0	0
Mg1	0.017(6)	= U_{11}	0.004(10)	= $\frac{1}{2}U_{11}$	0	0
Mg2	0.026(8)	= U_{11}	0.004(11)	= $\frac{1}{2}U_{11}$	0	0
Mg3	0.005(8)	= U_{11}	0.004(13)	= $\frac{1}{2}U_{11}$	0	0
<u>Carlosruizite</u>						
I	0.008(1)	0.013(1)	0.012(1)	0.004(1)	-0.001(1)	-0.001(1)
Se(S)	0.011(3)	0.015(3)	0.015(3)	0.009(2)	-0.001(2)	-0.003(2)
K1	0.034(5)	0.021(6)	0.027(6)	0.011(3)	0.001(3)	0.002(6)
M	0.020(7)	= U_{11}	0.026(10)	= $\frac{1}{2}U_{11}$	0	0
Na1	0.015(7)	= U_{11}	0.029(13)	= $\frac{1}{2}U_{11}$	0	0
NA2	0.015(10)	= U_{11}	0.010(15)	= $\frac{1}{2}U_{11}$	0	0
Mg1	0.008(6)	= U_{11}	0.012(8)	= $\frac{1}{2}U_{11}$	0	0
Mg2	0.012(6)	= U_{11}	0.020(10)	= $\frac{1}{2}U_{11}$	0	0
Mg3	0.001(7)	= U_{11}	0.037(15)	= $\frac{1}{2}U_{11}$	0	0