

Deposit item. Anisotropic atomic displacement parameters (\AA^2) for menzerite-(Y) and almandine

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Menzerite-(Y)						
$x_{\text{Ca, Y}}$	0.0088(2)	0.01361(18)	0.01361(18)	0.0030(2)	0	0
$y_{\text{Fe, Mg}}$	0.0069(2)	0.0069(2)	0.0069(2)	-0.0002(2)	-0.0002(2)	-0.0002(2)
z_{Si}	0.0099(5)	0.0087(4)	0.0087(4)	0	0	0
O1	0.0169(8)	0.0152(8)	0.0135(8)	0.0015(5)	0.0005(5)	0.0014(5)
Almandine						
$x_{\text{Ca, Fe}}$	0.0114(2)	0.0169(2)	0.0169(2)	0.0007(2)	0	0
$y_{\text{Al, Fe}}$	0.0113(4)	0.0113(4)	0.0113(4)	0.0001(2)	0.0001(2)	0.0001(2)
z_{Si}	0.0103(5)	0.0092(4)	0.0092(4)	0	0	0
O1	0.0147(8)	0.0149(8)	0.0119(7)	0.0005(5)	-0.0011(5)	0.0008(5)

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$