

Table 5 to be deposited

Table 5a. Atomic displacement parameters (standard deviations in parentheses) for henritermierite at 100 K

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn1	0.00299(9)	0.00320(9)	0.00265(8)	0.00041(6)	$\bar{0.00043(5)}$	$\bar{0.00043(5)}$
Ca1	0.0034(1)	0.0041(1)	0.0042(1)	0	0	$\bar{0.00074(6)}$
Ca2	0.00454(9)	0.00454(9)	0.0043(1)	-0.0011(1)	0	0
Si1	0.0027(2)	0.0037(2)	0.0030(1)	0	0	-0.0004(1)
O1	0.0057(3)	0.0045(3)	0.0034(2)	-0.0005(2)	0.0002(2)	-0.0008(2)
O2	0.0047(3)	0.0050(3)	0.0049(2)	-0.0011(2)	0.0007(2)	0.0008(2)
O3	0.0058(5)	0.0054(5)	0.0052(4)	-0.0006(3)	0.0013(3)	-0.0003(3)

Table 5b. Atomic displacement parameters (standard deviations in parentheses) for henritermierite at 293 K

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn1	0.00571(7)	0.00572(7)	0.00478(6)	0.00100(5)	$\bar{0.00063(4)}$	$\bar{0.00075(4)}$
Ca1	0.00605(8)	0.00740(9)	0.00775(8)	0	0	$\bar{0.00111(6)}$
Ca2	0.00918(7)	0.00918(7)	0.0072(1)	$\bar{0.00300(9)}$	0	0
Si1	0.0045(1)	0.0057(1)	0.0046(1)	0	0	$\bar{0.00035(8)}$
O1	0.0094(2)	0.0070(2)	0.0056(2)	-0.0009(2)	0.0003(2)	-0.0011(2)
O2	0.0071(2)	0.0085(2)	0.0074(2)	-0.0018(2)	0.0008(2)	0.0012(2)
O3	0.0093(3)	0.0071(3)	0.0083(3)	-0.0014(2)	0.0022(2)	-0.0007(2)

Anisotropic displacement parameters are given in the form $\exp (-2^2[h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \dots + 2hka^*b^*U_{12}])$

Table 5c. Atomic displacement parameters (standard deviations in parentheses) for henritermierite at 8.6 GPa.

atom	11	22	33	12	13	23
Mn1	0.00133(10)	0.00149(10)	0.00164(10)	0.00018(35)	$\bar{0.00015(35)}$	0.00009(22)
Ca1	0.00149(21)	0.00172(22)	0.00190(28)	0	0	0.00009(38)
Ca2	0.00172(16)	0.00172(16)	0.00173(25)	$\bar{0.00090(65)}$	0	0

Anisotropic displacement parameters are given in the form $\exp [-(h^2_{11} + k^2_{22} + l^2_{33} + 2hk_{12} + 2hl_{13} + 2kl_{23})]$