

Table 4 (for deposit). Anisotropic displacement parameters for vesuvianite NC14-2 in space group *P4/n*.

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Ca1	0.0116(6)	0.0070(6)	0.0073(6)	0.000(1)	0	0
Ca2a	0.0090(8)	0.0093(8)	0.0096(7)	0.0021(6)	-0.0004(6)	0.0008(6)
Ca2b	0.0066(8)	0.0145(9)	0.0053(7)	-0.0001(6)	-0.0016(6)	0.0002(5)
Ca3a	0.018(1)	0.0113(9)	0.0208(8)	0.0084(6)	-0.0061(7)	-0.0051(6)
Ca3b	0.0106(8)	0.0165(9)	0.0160(7)	-0.0010(6)	-0.0065(6)	0.0040(6)
O1a	0.007(3)	0.005(2)	0.011(2)	0.001(2)	-0.003(2)	-0.001(2)
O1b	0.012(3)	0.018(3)	0.007(2)	0.000(2)	0.004(2)	0.003(2)
O2a	0.009(3)	0.010(3)	0.006(2)	-0.001(2)	0.000(2)	0.000(2)
O2b	0.011(3)	0.011(3)	0.012(2)	0.000(2)	-0.002(2)	0.004(2)
O3a	0.009(3)	0.016(3)	0.009(2)	-0.001(2)	-0.002(2)	-0.003(2)
O3b	0.010(3)	0.007(3)	0.005(2)	-0.003(2)	-0.002(2)	0.001(2)
O4a	0.009(3)	0.009(3)	0.015(3)	0.005(2)	0.009(2)	0.000(2)
O4b	0.013(3)	0.013(3)	0.007(2)	0.002(2)	0.005(2)	0.001(2)
O5a	0.017(3)	0.013(3)	0.005(2)	-0.009(2)	0.002(2)	-0.003(2)
O5b	0.015(3)	0.010(3)	0.015(3)	0.005(2)	0.004(2)	0.000(2)
O6a	0.029(3)	0.004(3)	0.013(2)	0.002(2)	0.002(2)	0.007(2)
O6b	0.019(3)	0.014(3)	0.011(2)	-0.006(2)	-0.006(2)	-0.003(2)
O7a	0.011(3)	0.013(3)	0.019(3)	0.000(2)	0.003(2)	-0.006(2)
O7b	0.010(3)	0.023(3)	0.010(2)	0.005(2)	0.001(2)	0.005(2)
O8a	0.006(3)	0.009(3)	0.010(2)	-0.003(2)	0.001(2)	0.001(2)
O8b	0.014(3)	0.006(3)	0.013(2)	-0.001(2)	-0.001(2)	-0.005(2)
O9	0.013(3)	0.013(3)	0.005(1)	0.001(1)	0.002(2)	0.002(2)
O10a	0.031(4)	0.031(4)	0.010(5)	0	0	0
O10b	0.024(4)	0.024(4)	0.026(6)	0	0	0
O11a	0.015(3)	0.008(3)	0.004(2)	-0.001(2)	-0.004(2)	0.002(2)
O11b	0.009(3)	0.010(3)	0.011(2)	-0.002(2)	0.001(2)	0.005(2)
CaX'4a	0.010(1)	0.010(1)	0.019(2)	0	0	0
MnY'3a	0.014(1)	0.014(1)	0.017(1)	0	0	0

Table 5. (for deposit) Interatomic distances of *P4/n* vesuvianite NC14-2 from N'chwaning mine

Si1a - O1a 4x 1.659(5) Si1b - O1b 4x 1.670(5) Si2a - O7a 1.621(6) O3a 1.655(5) O2a 1.662(6) O4a 1.677(5) mean 1.654 Si2b- O7b 1.609(6) O3b 1.637(5) O2b 1.640(6) O4b 1.683(5) mean 1.642 Si3a- O6a 1.608(5) O8a 1.620(5) O5a 1.631(6) O9 1.668(6) mean 1.632 Si3b- O6b 1.606(5) O8b 1.618(5) O5b 1.627(5) O9 1.654(5) mean 1.626 Al1a- O11a 2x 1.871(5) O8a 2x 1.905(5) O4a 2x 1.970(5) mean 1.915 Al1b- O11b 2x 1.891(5) O8b 2x 1.874(5) O4b 2x 1.960(5) mean 1.908 Al2a- O1a 1.945(5) O11a 1.868(5) O2b 1.940(5) O3a 1.965(5) O5a 2.025(6) O4a 2.035(5) mean 1.963 Al2b- O1b 1.896(6) O11b 1.870(6) O2a 1.882(5) O3b 1.953(5) O5b 1.953(6) O4b 2.026(5) mean 1.930

Table 4 (for deposit)

Ca1- O1a 2x 2.330(5)

O1b 2x 2.332(5)

O2a 2x 2.490(6)

O2b 2x 2.539(6)

mean 2.423

Ca2a- O8a 2.320(5)

O5a 2.319(5)

O3a 2.366(5)

O4a 2.427(5)

O5b 2.414(5)

O2a 2.460(5)

O1a 2.478(5)

O6a 3.007(6)

mean 2.474

Ca2b O8b 2.308(5)

O5b 2.354(5)

O3b 2.381(5)

O4b 2.449(5)

O5a 2.446(5)

O2b 2.403(6)

O1b 2.520(6)

O6b 2.860(6)

mean 2.465

Ca3a O7a 2.373(5)

O3a 2.429(5)

O11a 2.443(5)

O7a 2.511(5)

O7b 2.543(5)

O6a 2.556(5)

O10a 2.633(1)

O8a 2.590(5)

O6a 3.03(1)

mean 2.490

Table 4 (for deposit)

Ca3b- O7b 2.381(5)

O3b 2.481(5)

O11b 2.497(5)

O7b 2.381(5)

O7a 2.563(5)

O6b 2.450(5)

O10b 2.582(2)

O8b 2.595(5)

O6b 2.996(5)

mean 2.468

X'4a- O6b 4x 2.347(6)

O9 4x 2.604(4)

mean 2.476

X'4b- O6a 4x 2.264(7)

O9 4x 2.609(6)

mean 2.437

Y'3a- O10a 2.09(1)

O6a 4x 2.009(6)

mean 2.025

Y'3b- O10b 2.25(1)

O6b 4x 2.118(6)

mean 2.144