

Table 5 (for deposit). Anisotropic displacement parameters of *P4nc* vesuvianite from N’chwaning (displacement parameters of sites related by *P4/nnc* pseudo-symmetry were constrained to each other)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Al1	0.0067(4)	0.0055(4)	0.0111(4)	0.0001(3)	0.0005(3)	0.0007(3)
Al2a	0.0067(3)	0.0074(3)	0.0077(4)	0.0000(2)	0.0011(2)	- 0.0002(2)
Al2b	0.0067(3)	0.0074(3)	0.0077(4)	0.0000(2)	0.0011(2)	0.0002(2)
Ca1	0.0123(5)	0.0095(5)	0.0084(5)	0	0	0
Ca2a	0.0082(2)	0.0112(2)	0.0087(3)	0.0007(2)	- 0.0004(2)	- 0.0001(2)
Ca2b	0.0082(2)	0.0112(2)	0.0087(3)	- 0.0007(2)	- 0.0004(2)	0.0001(2)
Ca3a	0.0127(2)	0.0121(2)	0.0184(3)	0.0028(2)	0.0034(2)	0.0046(2)
Ca3b	0.0121(2)	0.0127(2)	0.0184(3)	- 0.0028(2)	- 0.0046(2)	0.0034(2)
O1a	0.0092(7)	0.0079(7)	0.0082(7)	0.0000(5)	0.0009(5)	0.0003(6)
O1b	0.0092(7)	0.0079(7)	0.0082(7)	0.0000(5)	0.0009(5)	- 0.0003(6)
O2a	0.0098(7)	0.0096(7)	0.0083(7)	0.0007(5)	- 0.0002(6)	0.0002(5)
O2b	0.0096(7)	0.0098(7)	0.0083(7)	- 0.0007(5)	0.0002(5)	0.0002(6)
O3a	0.0079(7)	0.0098(7)	0.0079(7)	- 0.0001(5)	0.0001(6)	0.0006(5)
O3b	0.0079(7)	0.0098(7)	0.0079(7)	0.0001(5)	0.0001(6)	- 0.0006(5)
O4a	0.0074(7)	0.0080(7)	0.0089(8)	- 0.0010(5)	- 0.0006(5)	- 0.0002(5)
O4b	0.0074(7)	0.0080(7)	0.0089(8)	0.0010(5)	- 0.0006(5)	0.0002(5)
O5a	0.0089(7)	0.0099(7)	0.0095(8)	- 0.0012(5)	0.0009(6)	- 0.0009(6)
O5b	0.0089(7)	0.0099(7)	0.0095(8)	0.0012(5)	0.0009(6)	0.0009(6)
O6a	0.0099(7)	0.0170(9)	0.0125(8)	0.0033(6)	- 0.0027(6)	- 0.0027(7)
O6b	0.0099(7)	0.0170(9)	0.0125(8)	- 0.0033(6)	- 0.0027(6)	0.0027(7)

Table 6 (for deposit)

O7a	0.0104(7)	0.0178(8)	0.0135(8)	0.0028(6)	0.0016(6)	0.0015(6)
O7b	0.0104(7)	0.0178(8)	0.0135(8)	0.0028(6)	0.0016(6)	0.0015(6)
O8a	0.0065(7)	0.0085(7)	0.0110(8)	- 0.0003(5)	- 0.0006(6)	0.0016(6)
O8b	0.0065(7)	0.0085(7)	0.0110(8)	0.0003(5)	- 0.0006(6)	- 0.0016(6)
O9	0.0113(6)	0.0113(6)	0.008(1)	- 0.0011(8)	- 0.0010(6)	0.0010(6)
O10b	0.014(1)	0.014(1)	0.017(2)	0	0	0
O10a	0.014(1)	0.014(1)	0.017(2)	0	0	0
O11a	0.0086(7)	0.0092(7)	0.0066(7)	0.0001(6)	- 0.0010(5)	- 0.0005(5)
O11b	0.0086(7)	0.0092(7)	0.0066(7)	- 0.0001(6)	- 0.0010(5)	0.0005(5)
Y'3a	0.0059(4)	0.0059(4)	0.0111(9)	0	0	0
X'4a	0.0080(5)	0.0080(5)	0.021(1)	0	0	0

Table 6 (for deposit). Interatomic distances of *P4nc* vesuvianite from N'chwaning

Si1- O1b 2x 1.644(4)

O1a 2x 1.649(4)

mean 1.647

Si2a- O7b 1.621(4)

O3a 1.642(4)

O2a 1.640(4)

O4a 1.682(4)

mean 1.646

Si2b- O7a 1.613(4)

O3b 1.638(3)

O2b 1.645(4)

O4b 1.675(4)

Table 6 (for deposit)

mean 1.643

Si3a O6b 1.590(3)

O8a 1.608(4)

O5b 1.632(4)

O9 1.662(4)

mean 1.623

Si3b- O6a 1.612(3)

O8b 1.634(4)

O5a 1.638(4)

O9 1.654(4)

mean 1.635

Al1- O8b 1.850(4)

O8a 1.876(4)

O11a 1.859(4)

O11b 1.885(4)

O4b 1.950(4)

O4a 1.946(4)

mean 1.894

Al2a- O2b 1.870(4)

O11a 1.889(4)

O1b 1.879(4)

O3a 1.915(4)

O5b 1.935(4)

O4b 2.051(4)

mean 1.923

Al2b- O2a 1.878(4)

O11b 1.885(3)

O1a 1.893(4)

O3b 1.926(3)

O5a 1.979(4)

O4a 2.036(4)

mean 1.933

Ca1a- O1a 2x 2.335(4)

O1b 2x 2.327(4)

Table 6 (for deposit)

O2a 2x 2.526(4)

O2b 2x 2.508(2)

mean 2.424

Ca2a- O8b 2.313(3)

O5a 2.320(3)

O3a 2.384(4)

O2b 2.433(4)

O5b 2.423(4)

O4b 2.425(4)

O1a 2.461(3)

O6a 2.999(3)

mean 2.470

Ca2b- O8a 2.316(4)

O5b 2.332(4)

O3b 2.374(4)

O2a 2.411(4)

O5a 2.438(4)

O4a 2.463(4)

O1b 2.502(3)

O6b 2.834(4)

mean 2.459

Ca3a- O7b 2.363(4)

O6a 2.460(4)

O3a 2.446(3)

O11a 2.462(4)

O7b 2.507(4)

O10a 2.570(2)

O8b 2.575(4)

O7a 2.576(4)

O6a 2.935(4)

mean 2.544

Ca3b- O7a 2.364(4)

O6b 2.425(3)

Table 6 (for deposit)

O3b 2.458(3)

O11b 2.516(4)

O7a 2.518(4)

O10b 2.544(2)

O8a 2.569(4)

O7b 2.615(4)

O6b 2.964(3)

mean 2.553

X'4a- O6b 4x 2.361(4)

O9 4x 2.590(3)

mean 2.476

X'4b- O6a 4x 2.266(8)

O9 4x 2.617(7)

mean 2.442

Y'3a- O6a 4x 2.002(3)

O10a 2.327(8)

mean 2.067

Y'3b- O6b 4x 2.125(4)

O10b 2.14(1)

mean 2.128

O11a- H11a 1.08(5)

H11a- H11b 1.53(7)

H11a- O7b 2.10(5)

H11a- O7a 2.24(5)

H11a O11b 2.12(5)

O11b- H11b 0.89(5)

H11b- O11a 2.30(5)

H11b- O5a 2.54(5)

Table 8 (for deposit). Anisotropic displacement parameters of *P4/n* vesuvianite from Asbestos

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Si1a	0.0068(8)	0.0068(8)	0.006(1)	0	0	0
Si1b	0.0102(8)	0.0102(8)	0.005(1)	0	0	0
Si2a	0.0064(8)	0.0071(8)	0.0075(7)	0.0010(6)	0.0003(5)	0.0001(6)

Table 6 (for deposit)

Si2b	0.0079(8)	0.0044(8)	0.0060(7)	0.0005(6)	- 0.0007(5)	0.0003(6)
Si3a	0.0087(8)	0.0053(7)	0.0074(6)	- 0.0007(6)	- 0.0002(5)	0.0004(5)
Si3b	0.0095(7)	0.0052(7)	0.0055(6)	0.0004(5)	- 0.0005(5)	- 0.0005(6)
Al1a	0.007(1)	0.007(1)	0.0074(9)	0.0006(9)	0.0010(9)	- 0.0015(9)
Al1b	0.006(1)	0.005(1)	0.0076(9)	- 0.0005(8)	- 0.0002(9)	- 0.0005(9)
Al2a	0.0081(8)	0.0067(9)	0.0086(7)	- 0.0003(7)	0.0001(6)	0.0010(6)
Al2b	0.0056(8)	0.0069(9)	0.0069(7)	0.0000(6)	0.0008(6)	0.0013(6)
Ca1	0.0115(4)	0.0064(4)	0.0062(4)	- 0.0010(9)	0	0
Ca2a	0.0095(6)	0.0070(6)	0.0076(5)	0.0005(5)	- 0.0003(4)	0.0000(4)
Ca2b	0.0067(6)	0.0099(6)	0.0082(5)	- 0.0001(5)	- 0.0015(4)	0.0007(4)
Ca3a	0.0103(6)	0.0101(6)	0.0185(5)	0.0021(4)	- 0.0033(4)	- 0.0034(4)
Ca3b	0.0096(6)	0.0110(5)	0.0166(5)	- 0.0017(4)	- 0.0052(4)	0.0028(4)
O1a	0.010(2)	0.007(2)	0.006(1)	0.001(1)	0.001(1)	-0.002(1)
O1b	0.008(2)	0.013(2)	0.006(1)	0.000(1)	-0.001(1)	-0.001(1)
O2a	0.008(2)	0.009(2)	0.007(1)	0.002(2)	-0.001(1)	-0.001(1)
O2b	0.008(2)	0.010(2)	0.011(2)	0.000(2)	-0.003(2)	0.003(1)
O3a	0.009(2)	0.007(2)	0.009(2)	0.003(1)	0.000(1)	-0.001(1)
O3b	0.010(2)	0.008(2)	0.008(2)	0.001(2)	0.001(1)	0.000(1)
O4a	0.009(2)	0.006(2)	0.010(2)	0.000(2)	0.004(1)	0.000(1)
O4b	0.011(2)	0.009(2)	0.005(2)	-0.001(2)	0.001(1)	0.001(1)
O5a	0.016(2)	0.011(2)	0.008(2)	-0.002(2)	-0.003(1)	-0.001(1)
O5b	0.013(2)	0.006(2)	0.009(2)	0.004(1)	0.000(1)	0.001(1)
O6a	0.015(2)	0.010(2)	0.014(2)	0.004(1)	0.000(1)	0.002(1)
O6b	0.016(2)	0.009(2)	0.011(2)	-0.001(1)	-0.004(1)	0.002(1)
O7a	0.008(2)	0.012(2)	0.014(2)	0.001(1)	0.002(1)	0.000(1)

Table 6 (for deposit)

O7b	0.006(2)	0.013(2)	0.013(2)	0.004(2)	0.002(1)	-0.003(1)
O8a	0.004(2)	0.007(2)	0.014(2)	-0.003(2)	0.000(1)	0.002(1)
O8b	0.012(2)	0.007(2)	0.010(2)	0.000(2)	-0.003(1)	-0.005(1)
O9	0.010(2)	0.013(2)	0.007(1)	0.001(1)	0.001(1)	0.003(1)
O10a	0.015(2)	0.015(2)	0.004(3)	0	0	0
O10b	0.014(2)	0.014(2)	0.023(4)	0	0	0
O11a	0.013(2)	0.012(2)	0.007(2)	-0.003(2)	-0.003(2)	-0.002(2)
O11b	0.008(2)	0.014(2)	0.008(2)	-0.001(2)	-0.001(2)	-0.001(2)
X'4a	0.0064(8)	0.0064(8)	0.015(1)	0	0	0
Y'3a	0.0049(6)	0.0049(6)	0.016(1)	0	0	0

Table 9 (for deposit). Interatomic distances of *P4/n* vesuvianite from Quebec

Si1a - O1a 4x 1.642(3)

Si1b - O1b 4x 1.649(3)

Si2a - O7a 1.622(4)

O3a 1.641(4)

O2a 1.656(4)

O4a 1.673(4)

mean 1.648

Si2b- O7b 1.613(4)

O3b 1.638(4)

O2b 1.634(4)

O4b 1.676(3)

mean 1.643

Si3a- O6a 1.615(4)

O8a 1.622(4)

O5a 1.629(4)

O9 1.677(4)

mean 1.638

Si3b- O6b 1.589(3)

O8b 1.614(4)

O5b 1.633(4)

O9 1.646(4)

mean 1.621

Al1a- O11a 2x 1.863(3)

O8a 2x 1.883(3)

O4a 2x 1.950(3)

mean 1.899

Al1b- O11b 2x 1.862(3)

O8b 2x 1.872(3)

O4b 2x 1.941(3)

mean 1.892

Al2a- O1a 1.918(4)

O11a 1.935(4)

O2b 1.936(4)

O3a 1.966(4)

O5a 2.026(4)

O4a 2.076(4)

mean 1.976

Al2b- O1b 1.899(4)

O11b 1.903(4)

O2a 1.872(4)

O3b 1.929(4)

O5b 1.957(4)

O4b 2.051(3)

mean 1.935

Ca1- O1a 2x 2.324(3)

O1b 2x 2.338(3)

O2a 2x 2.499(4)

O2b 2x 2.533(4)

mean 2.424

Ca2a- O8a 2.316(3)

O5a 2.329(4)

O3a 2.368(4)

O4a 2.412(4)

O5b 2.429(3)

O2a 2.448(4)

O1a 2.455(4)

O6a 3.037(4)

mean 2.474

Ca2b O8b 2.329(4)

O5b 2.340(4)

O3b 2.379(4)

O4b 2.476(4)

O5a 2.455(3)

O2b 2.409(4)

O1b 2.497(4)

O6b 2.842(4)

mean 2.465

Ca3a O7a 2.357(4)

O3a 2.435(4)

O11a 2.454(4)

O7a 2.487(4)

O7b 2.531(4)

O6a 2.579(3)

O10a 2.593(1)

O8a 2.635(3)

O6a 3.019(4)

mean 2.566

Ca3b- O7b 2.408(4)

O3b 2.466(4)

O11b 2.564(4)

O7b 2.497(4)

O7a 2.630(3)

O6b 2.390(3)

O10b 2.526(2)

O8b 2.612(4)

O6b 2.973(3)

Table 6 (for deposit)

mean 2.563

X'4a- O6b 4x 2.375(4)

O9 4x 2.593(3)

mean 2.487

X'4b- O6a 4x 2.251(7)

O9 4x 2.599(7)

mean 2.44

Y'3a- O10a 1.884(6)

O6a 4x 1.994(4)

mean 1.972

Y'3b- O10b 2.14(1)

O6b 4x 2.148(4)

mean 2.146

O11a- H11a 0.97(4)

H11a- H11b 1.71(7)

H11a- O11b 2.35(5)

H11a- O5a 2.43(5)

O11b- H11b 0.82(5)

H11b- O7b 2.23(5)

H11b- O7a 2.46(5)

H11b- O11a 2.32(5)