

Table 2: Positional and thermal parameters from $\bar{I}1$ refinement of Monte Somma/6.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M ₀₀₀	0.2665(4)	0.9860(4)	0.0854(4)	0.0034(4)	0.0068(4)	0.0030(3)	-0.0017(3)	0.0015(3)	-0.0030(3)	2.50
M _{z00}	0.2693(4)	0.0290(5)	0.5481(7)	0.0031(3)	0.0025(2)	0.0021(3)	0.0006(2)	0.0004(2)	-0.0010(2)	1.34
M _{o10}	0.7741(3)	0.5356(2)	0.5436(2)	0.0032(4)	0.0020(1)	0.0018(1)	0.0010(2)	0.0007(2)	-0.0001(1)	1.13
M _{z10}	0.7631(8)	0.497 (2)	0.080 (1)	0.0032(8)	0.0051(8)	0.0015(5)	-0.0001(5)	0.0012(4)	-0.0012(6)	1.67
T ₁₀₀	0.0073(2)	0.1585(1)	0.1047(1)	0.0036(3)	0.0014(1)	0.0009(1)	-0.0002(1)	0.0009(1)	0.0001(1)	0.76
T _{10z}	0.0031(2)	0.1637(1)	0.6116(1)	0.0029(3)	0.0012(1)	0.0009(1)	-0.0003(1)	0.0006(1)	-0.0000(1)	0.69
T _{1m0}	0.0002(2)	0.8150(1)	0.1193(1)	0.0037(3)	0.0012(1)	0.0009(1)	0.0006(1)	0.0009(1)	0.0000(1)	0.70
T _{1mz}	0.0036(2)	0.8170(1)	0.6121(1)	0.0030(3)	0.0014(1)	0.0008(1)	0.0007(1)	0.0004(1)	0.0002(1)	0.73
T ₂₀₀	0.6874(2)	0.1123(1)	0.1597(1)	0.0028(3)	0.0011(1)	0.0016(1)	0.0001(1)	0.0008(1)	0.0001(1)	0.82
T _{20z}	0.6772(2)	0.1059(1)	0.6574(1)	0.0028(3)	0.0012(1)	0.0019(1)	0.0001(1)	0.0008(1)	-0.0000(1)	0.89
T _{2m0}	0.6763(2)	0.8812(1)	0.1809(1)	0.0028(3)	0.0010(1)	0.0017(1)	0.0002(1)	0.0006(1)	0.0002(1)	0.83
T _{2mz}	0.6829(2)	0.8755(1)	0.6779(1)	0.0027(3)	0.0010(1)	0.0013(1)	0.0004(1)	0.0007(1)	0.0003(1)	0.71
O _{a10}	0.0067(6)	0.1257(3)	-0.0090(3)	0.0095(9)	0.0023(2)	0.0014(2)	0.0005(4)	0.0022(4)	0.0000(2)	1.44
O _{a1z}	0.9990(6)	0.1259(3)	0.4897(3)	0.0099(9)	0.0020(2)	0.0015(2)	0.0005(4)	0.0023(4)	0.0002(2)	1.40
O _{a20}	0.5743(5)	0.9895(3)	0.1393(3)	0.0034(7)	0.0013(2)	0.0017(2)	-0.0000(3)	0.0006(4)	0.0002(2)	0.97
O _{a2z}	0.5739(5)	0.9911(3)	0.6386(3)	0.0028(7)	0.0009(2)	0.0020(2)	0.0002(3)	0.0007(4)	0.0001(2)	0.88
O _{b00}	0.8194(5)	0.0992(3)	0.0913(3)	0.0054(7)	0.0017(2)	0.0038(3)	-0.0005(3)	0.0035(4)	-0.0002(2)	1.43
O _{b0z}	0.8002(6)	0.1013(3)	0.5926(3)	0.0056(8)	0.0017(2)	0.0044(3)	-0.0012(3)	0.0038(4)	-0.0011(2)	1.57
O _{bm0}	0.8069(6)	0.8563(3)	0.1248(4)	0.0055(8)	0.0021(2)	0.0056(3)	-0.0001(3)	0.0036(4)	-0.0009(2)	1.99
O _{bmz}	0.8228(6)	0.8554(3)	0.6171(4)	0.0071(9)	0.0026(3)	0.0056(3)	0.0011(4)	0.0053(5)	0.0002(2)	1.98
O _{c00}	0.0125(5)	0.2796(3)	0.1373(3)	0.0050(7)	0.0018(2)	0.0024(2)	-0.0005(3)	0.0017(4)	-0.0002(2)	1.26
O _{c0z}	0.0165(5)	0.2925(3)	0.6490(3)	0.0062(8)	0.0014(2)	0.0024(2)	-0.0006(3)	0.0018(4)	-0.0001(2)	1.26
O _{cm0}	0.0067(5)	0.6805(3)	0.1071(3)	0.0048(7)	0.0016(2)	0.0020(2)	0.0004(3)	0.0010(4)	0.0002(2)	1.19
O _{cmz}	0.0070(6)	0.6908(3)	0.6004(3)	0.0054(7)	0.0019(2)	0.0017(2)	0.0011(3)	0.0003(4)	-0.0002(2)	1.30
O _{d00}	0.1922(6)	0.1059(3)	0.1865(3)	0.0055(8)	0.0023(2)	0.0017(2)	0.0010(3)	0.0003(4)	0.0001(2)	1.43
O _{d0z}	0.2016(6)	0.1028(3)	0.6921(3)	0.0061(8)	0.0015(2)	0.0019(2)	0.0001(3)	-0.0010(4)	0.0003(2)	1.50
O _{dmo}	0.1963(6)	0.8672(3)	0.2203(3)	0.0060(8)	0.0025(3)	0.0037(3)	0.0007(4)	-0.0007(4)	-0.0008(2)	2.19
O _{dmoz}	0.1868(6)	0.8623(3)	0.7099(3)	0.0078(9)	0.0030(3)	0.0026(3)	0.0009(4)	-0.0022(4)	-0.0012(2)	2.40

Table 2: Positional and thermal parameters from $\bar{1}\bar{1}$ refinement of Monte Somma/7.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M _{ooo}	0.2670(5)	0.9854(5)	0.0862(4)	0.0050(7)	0.0069(4)	0.0028(3)	-0.0012(4)	0.0020(3)	-0.0026(3)	2.52
M _{zoo}	0.2688(5)	0.0298(5)	0.5472(9)	0.0032(4)	0.0023(2)	0.0018(3)	0.0007(2)	0.0008(3)	-0.0004(2)	1.19
M _{oio}	0.7742(3)	0.5353(2)	0.5436(2)	0.0033(4)	0.0018(2)	0.0010(2)	0.0008(2)	0.0006(2)	-0.0003(1)	1.14
M _{zio}	0.7643(8)	0.500 (3)	0.078 (2)	0.0012(8)	0.006 (1)	0.0019(7)	-0.0005(5)	0.0005(5)	-0.0019(8)	1.89
T _{1oo}	0.0074(2)	0.1585(1)	0.1046(1)	0.0027(3)	0.0014(1)	0.0010(1)	-0.0004(1)	0.0007(1)	-0.0001(1)	0.74
T _{1oz}	0.0032(3)	0.1636(1)	0.6117(1)	0.0037(3)	0.0011(1)	0.0010(1)	-0.0003(1)	0.0011(2)	0.0001(1)	0.70
T _{1mo}	0.0002(3)	0.8147(1)	0.1196(1)	0.0037(4)	0.0012(1)	0.0010(1)	0.0002(1)	0.0009(2)	0.0001(1)	0.74
T _{1mz}	0.0038(2)	0.8172(1)	0.6119(1)	0.0032(3)	0.0011(1)	0.0010(1)	0.0006(1)	0.0007(1)	0.0002(1)	0.69
T _{2oo}	0.6875(3)	0.1125(1)	0.1595(1)	0.0024(3)	0.0009(1)	0.0017(1)	0.0000(1)	0.0008(2)	0.0001(1)	0.78
T _{2oz}	0.6771(2)	0.1058(1)	0.6574(1)	0.0031(3)	0.0009(1)	0.0019(1)	-0.0001(1)	0.0009(1)	-0.0001(1)	0.85
T _{2mo}	0.6763(2)	0.8816(1)	0.1809(1)	0.0025(3)	0.0010(1)	0.0018(1)	0.0003(1)	0.0008(2)	0.0003(1)	0.80
T _{2mz}	0.6831(2)	0.8753(1)	0.6778(1)	0.0030(3)	0.0009(1)	0.0012(1)	0.0001(1)	0.0008(2)	0.0003(1)	0.68
O _{a1o}	0.0062(6)	0.1253(3)	-0.0095(3)	0.010 (1)	0.0027(3)	0.0015(3)	0.0006(4)	0.0028(5)	0.0002(2)	1.47
O _{a1z}	0.0000(6)	0.1263(3)	0.4902(3)	0.011 (1)	0.0011(2)	0.0017(3)	0.0003(4)	0.0027(5)	0.0004(2)	1.31
O _{a2o}	0.5749(6)	0.9897(3)	0.1391(3)	0.0032(8)	0.0010(2)	0.0018(3)	-0.0000(3)	0.0009(4)	0.0002(2)	0.87
O _{a2z}	0.5723(6)	0.9910(3)	0.6381(3)	0.0035(8)	0.0013(2)	0.0021(3)	0.0002(3)	0.0009(4)	0.0002(2)	1.03
O _{boo}	0.8198(6)	0.0991(3)	0.0917(4)	0.0062(9)	0.0018(3)	0.0039(3)	-0.0011(4)	0.0035(5)	-0.0005(2)	1.53
O _{boz}	0.7997(6)	0.1009(3)	0.5924(4)	0.0058(9)	0.0012(2)	0.0039(3)	-0.0009(4)	0.0033(5)	-0.0006(2)	1.42
O _{bmo}	0.8075(7)	0.8563(3)	0.1247(4)	0.0075(9)	0.0020(3)	0.0062(4)	0.0004(4)	0.0050(6)	-0.0002(3)	2.09
O _{b mz}	0.8217(7)	0.8546(3)	0.6172(4)	0.007 (1)	0.0025(3)	0.0051(4)	0.0004(4)	0.0041(5)	-0.0003(3)	1.98
O _{coo}	0.0141(6)	0.2788(3)	0.1375(3)	0.0063(9)	0.0014(2)	0.0023(3)	-0.0006(4)	0.0019(4)	-0.0002(2)	1.22
O _{coz}	0.0161(6)	0.2932(3)	0.6491(4)	0.0051(8)	0.0012(2)	0.0027(3)	-0.0004(3)	0.0019(4)	-0.0004(2)	1.20
O _{cmo}	0.0075(6)	0.6803(3)	0.1074(3)	0.0048(8)	0.0016(2)	0.0017(3)	0.0011(4)	0.0012(4)	0.0001(2)	1.07
O _{cmz}	0.0050(6)	0.6905(3)	0.5999(3)	0.0051(9)	0.0015(2)	0.0017(3)	0.0003(4)	0.0006(4)	-0.0000(2)	1.18
O _{doo}	0.1912(6)	0.1063(3)	0.1860(4)	0.0057(9)	0.0019(3)	0.0021(3)	0.0006(4)	0.0005(4)	0.0001(2)	1.42
O _{doz}	0.2020(6)	0.1025(3)	0.6922(4)	0.0046(9)	0.0019(3)	0.0021(3)	0.0003(4)	-0.0013(4)	0.0002(2)	1.56
O _{dmo}	0.1968(7)	0.8675(3)	0.2212(4)	0.0052(9)	0.0023(3)	0.0032(3)	0.0001(4)	-0.0016(4)	-0.0008(2)	2.06
O _{d mz}	0.1850(7)	0.8623(4)	0.7095(4)	0.006 (1)	0.0027(3)	0.0027(3)	0.0010(4)	-0.0021(4)	-0.0009(2)	2.19

Table 2: Positional and thermal parameters from $\bar{I}1$ refinement of Monte Somma/8.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2662(4)	0.9862(4)	0.0854(3)	0.0038(5)	0.0057(3)	0.0023(2)	-0.0008(2)	0.0012(2)	-0.0021(2)	2.12
Mzoo	0.2686(4)	0.0294(5)	0.5473(7)	0.0035(3)	0.0021(2)	0.0018(2)	0.0006(1)	0.0000(2)	-0.0000(1)	1.18
Moio	0.7744(2)	0.5353(2)	0.5434(2)	0.0028(3)	0.0019(1)	0.0013(1)	0.0007(1)	0.0002(1)	-0.0002(1)	1.02
Mzio	0.7629(7)	0.500 (2)	0.078 (2)	0.0026(7)	0.0045(7)	0.0014(5)	-0.0005(4)	0.0007(4)	-0.0015(5)	1.55
Tloo	0.0073(2)	0.1581(1)	0.1044(1)	0.0028(2)	0.0010(1)	0.0008(1)	-0.0002(1)	0.0006(1)	-0.0000(1)	0.64
Tloz	0.0024(2)	0.1636(1)	0.6116(1)	0.0034(3)	0.0010(1)	0.0009(1)	-0.0003(1)	0.0008(1)	0.0000(1)	0.68
Tlmo	0.0003(2)	0.8147(1)	0.1196(1)	0.0039(3)	0.0011(1)	0.0007(1)	0.0004(1)	0.0008(1)	0.0001(1)	0.69
Tlmz	0.0039(2)	0.8173(1)	0.6118(1)	0.0027(2)	0.0010(1)	0.0007(1)	0.0003(1)	0.0004(1)	-0.0000(1)	0.64
T2oo	0.6878(2)	0.1125(1)	0.1596(1)	0.0023(2)	0.0009(1)	0.0016(1)	-0.0000(1)	0.0006(1)	-0.0000(1)	0.77
T2oz	0.6766(2)	0.1058(1)	0.6572(1)	0.0025(2)	0.0008(1)	0.0017(1)	-0.0000(1)	0.0007(1)	-0.0000(1)	0.79
T2mo	0.6760(2)	0.8813(1)	0.1808(1)	0.0030(2)	0.0008(1)	0.0014(1)	0.0003(1)	0.0005(1)	0.0001(1)	0.77
T2mz	0.6829(2)	0.8752(1)	0.6776(1)	0.0026(3)	0.0009(1)	0.0013(1)	0.0000(1)	0.0008(1)	0.0001(1)	0.71
Oa1o	0.0067(5)	0.1250(2)	-0.0089(2)	0.0095(9)	0.0017(2)	0.0012(2)	0.0001(3)	0.0025(3)	0.0000(1)	1.21
Oa1z	0.9988(5)	0.1260(2)	0.4898(3)	0.011 (1)	0.0013(2)	0.0017(2)	0.0001(3)	0.0030(4)	0.0002(1)	1.36
Oa2o	0.5750(5)	0.9899(2)	0.1393(2)	0.0027(7)	0.0008(2)	0.0019(2)	-0.0001(2)	0.0007(3)	0.0003(1)	0.85
Oa2z	0.5722(5)	0.9909(2)	0.6380(2)	0.0023(6)	0.0009(2)	0.0016(2)	0.0002(2)	0.0001(3)	0.0002(1)	0.83
Oboo	0.8212(5)	0.0992(2)	0.0924(3)	0.0054(7)	0.0012(2)	0.0035(2)	-0.0007(3)	0.0028(4)	-0.0005(2)	1.37
Oboz	0.7995(5)	0.1011(2)	0.5919(3)	0.0051(7)	0.0018(2)	0.0041(3)	-0.0012(3)	0.0037(4)	-0.0009(2)	1.51
Obmo	0.8080(6)	0.8560(3)	0.1253(3)	0.0069(8)	0.0020(2)	0.0055(3)	0.0007(3)	0.0039(4)	-0.0002(2)	2.02
Obmz	0.8220(6)	0.8560(3)	0.6163(3)	0.0078(9)	0.0026(2)	0.0050(3)	0.0006(3)	0.0051(4)	0.0000(2)	1.94
Ocoo	0.0136(5)	0.2790(2)	0.1368(3)	0.0060(7)	0.0013(2)	0.0021(2)	-0.0004(3)	0.0016(3)	-0.0002(1)	1.20
Ocoz	0.0155(5)	0.2935(2)	0.6491(3)	0.0046(7)	0.0011(2)	0.0017(2)	-0.0005(2)	0.0009(3)	0.0000(1)	1.02
Ocmo	0.0076(5)	0.6799(2)	0.1074(3)	0.0049(7)	0.0010(2)	0.0018(2)	0.0006(3)	0.0009(3)	-0.0001(1)	1.04
Ocmz	0.0059(5)	0.6910(2)	0.6001(3)	0.0053(7)	0.0012(2)	0.0018(2)	0.0006(3)	0.0006(3)	0.0001(1)	1.17
Odoo	0.1911(5)	0.1058(2)	0.1855(3)	0.0054(8)	0.0018(2)	0.0016(2)	0.0007(3)	-0.0000(3)	0.0000(1)	1.33
Odoz	0.2013(5)	0.1029(3)	0.6919(3)	0.0054(8)	0.0018(2)	0.0018(2)	0.0000(3)	-0.0010(3)	-0.0000(1)	1.53
Odmo	0.1961(6)	0.8675(3)	0.2201(3)	0.0066(8)	0.0019(2)	0.0034(3)	0.0005(3)	-0.0013(4)	-0.0009(2)	2.15
Odmz	0.1860(6)	0.8618(3)	0.7092(3)	0.0063(8)	0.0025(2)	0.0026(2)	0.0012(3)	-0.0026(4)	-0.0010(2)	2.23

Table 2: Positional and thermal parameters from $\bar{1}\bar{1}$ refinement of 115082a/1.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M _{ooo}	0.2663(4)	0.9855(4)	0.0860(3)	0.0039(5)	0.0050(3)	0.0022(2)	-0.0008(3)	0.0015(3)	-0.0019(2)	1.91
M _{zoo}	0.2685(4)	0.0305(6)	0.5462(9)	0.0033(3)	0.0020(2)	0.0014(3)	0.0009(2)	0.0007(2)	-0.0027(2)	1.03
M _{oio}	0.7746(3)	0.5352(2)	0.5439(2)	0.0040(4)	0.0022(1)	0.0015(1)	0.0010(2)	0.0005(2)	-0.0005(1)	1.18
M _{zio}	0.7645(7)	0.503 (2)	0.076 (2)	0.0039(6)	0.0049(7)	0.0025(6)	0.0006(4)	0.0009(4)	-0.0015(7)	2.03
T _{1oo}	0.0074(2)	0.1583(1)	0.1044(1)	0.0034(2)	0.0012(1)	0.0007(1)	-0.0001(1)	0.0009(1)	0.0001(1)	0.65
T _{1oz}	0.0028(2)	0.1636(1)	0.6119(1)	0.0034(3)	0.0011(1)	0.0008(1)	-0.0002(1)	0.0009(1)	-0.0000(1)	0.65
T _{1mo}	0.0004(2)	0.8151(1)	0.1197(1)	0.0036(3)	0.0012(1)	0.0007(1)	0.0004(1)	0.0007(1)	0.0000(1)	0.67
T _{1mz}	0.0044(2)	0.8173(1)	0.6118(1)	0.0036(2)	0.0012(1)	0.0007(1)	0.0007(1)	0.0007(1)	0.0001(1)	0.68
T _{2oo}	0.6876(2)	0.1126(1)	0.1594(1)	0.0032(3)	0.0009(1)	0.0016(1)	0.0001(1)	0.0008(1)	0.0000(1)	0.80
T _{2oz}	0.6770(2)	0.1056(1)	0.6576(1)	0.0027(2)	0.0009(1)	0.0018(1)	0.0001(1)	0.0010(1)	-0.0001(1)	0.80
T _{2mo}	0.6759(2)	0.8815(1)	0.1807(1)	0.0027(2)	0.0010(1)	0.0014(1)	0.0002(1)	0.0006(1)	0.0002(1)	0.74
T _{2mz}	0.6834(2)	0.8753(1)	0.6776(1)	0.0034(3)	0.0010(1)	0.0013(1)	0.0004(1)	0.0012(1)	0.0004(1)	0.69
O _{a1o}	0.0068(5)	0.1254(3)	-0.0087(3)	0.0107(9)	0.0020(2)	0.0014(2)	0.0007(3)	0.0026(4)	-0.0000(2)	1.41
O _{a1z}	0.9987(5)	0.1259(3)	0.4895(3)	0.0097(8)	0.0018(2)	0.0012(2)	0.0009(3)	0.0024(4)	0.0003(2)	1.24
O _{a2o}	0.5752(5)	0.9896(2)	0.1393(3)	0.0025(6)	0.0010(2)	0.0017(2)	0.0002(3)	0.0007(3)	0.0002(2)	0.80
O _{a2z}	0.5726(5)	0.9908(2)	0.6381(3)	0.0035(6)	0.0009(2)	0.0018(2)	0.0003(3)	0.0008(3)	0.0002(2)	0.89
O _{boo}	0.8213(5)	0.0996(3)	0.0922(3)	0.0059(7)	0.0018(2)	0.0035(3)	-0.0011(2)	0.0033(4)	-0.0006(2)	1.42
O _{boz}	0.7989(5)	0.1011(3)	0.5926(3)	0.0062(7)	0.0016(2)	0.0043(3)	-0.0005(3)	0.0039(4)	-0.0003(2)	1.54
O _{bmo}	0.8065(5)	0.8557(3)	0.1256(3)	0.0061(7)	0.0024(2)	0.0058(3)	0.0002(3)	0.0044(4)	0.0044(4)	2.05
O _{bmoz}	0.8255(5)	0.8557(3)	0.6171(3)	0.0080(8)	0.0021(2)	0.0051(3)	0.0009(3)	0.0047(4)	0.0002(2)	1.87
O _{coo}	0.0129(5)	0.2790(3)	0.1366(3)	0.0059(7)	0.0012(2)	0.0023(2)	-0.0001(3)	0.0021(3)	-0.0003(2)	1.12
O _{coz}	0.0158(5)	0.2936(2)	0.6489(3)	0.0046(6)	0.0012(2)	0.0020(2)	-0.0001(3)	0.0013(3)	0.0000(2)	1.02
O _{cmo}	0.0074(5)	0.6801(2)	0.1073(3)	0.0053(7)	0.0013(2)	0.0017(2)	0.0006(3)	0.0010(3)	0.0000(2)	1.07
O _{cmz}	0.0058(5)	0.6908(3)	0.5999(3)	0.0051(7)	0.0014(2)	0.0016(2)	0.0009(3)	0.0009(3)	-0.0001(2)	1.08
O _{do}	0.1912(5)	0.1064(3)	0.1856(3)	0.0050(7)	0.0020(2)	0.0016(2)	0.0003(3)	0.0000(3)	-0.0002(2)	1.33
O _{doz}	0.2021(5)	0.1032(3)	0.6920(3)	0.0066(7)	0.0018(2)	0.0013(2)	0.0012(3)	-0.0010(3)	0.0004(2)	1.44
O _{dmo}	0.1965(5)	0.8678(3)	0.2204(3)	0.0061(8)	0.0020(2)	0.0032(3)	0.0008(3)	-0.0014(4)	-0.0009(2)	2.05
O _{dmz}	0.1860(6)	0.8616(3)	0.7092(3)	0.0073(8)	0.0028(2)	0.0024(2)	0.0005(4)	-0.0022(4)	-0.0012(2)	2.24

Table 2: Positional and thermal parameters from $\text{I}\bar{1}$ refinement of 87975a/1.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M _{ooo}	0.2662(6)	0.9819(6)	0.0867(5)	0.0051(8)	0.0064(5)	0.0028(3)	-.0024(4)	0.0025(4)	-.0018(3)	2.34
M _{zoo}	0.268 (1)	0.0317(6)	0.5431(6)	0.0040(9)	0.0012(5)	0.0008(4)	0.0013(4)	0.0005(4)	0.0009(3)	0.75
M _{oio}	0.7747(4)	0.5340(3)	0.5454(3)	0.0042(6)	0.0030(2)	0.0022(2)	0.0007(3)	0.0003(3)	-.0009(2)	1.61
M _{zio}	0.7677(9)	0.512 (2)	0.066 (2)	0.0037(8)	0.0101(7)	0.0063(8)	0.0017(6)	-.0001(6)	-.0060(6)	4.39
T _{1oo}	0.0076(3)	0.1591(2)	0.1047(2)	0.0031(4)	0.0013(1)	0.0009(1)	-.0004(2)	0.0007(2)	0.0000(1)	0.72
T _{1oz}	0.0034(3)	0.1638(2)	0.6112(2)	0.0037(4)	0.0014(1)	0.0011(1)	-.0002(2)	0.0010(2)	0.0001(1)	0.79
T _{1mo}	0.0011(3)	0.8154(2)	0.1192(2)	0.0046(4)	0.0015(1)	0.0009(1)	0.0005(2)	0.0011(2)	0.0000(1)	0.86
T _{1mz}	0.0038(3)	0.8171(1)	0.6121(2)	0.0034(4)	0.0013(1)	0.0009(1)	0.0008(2)	0.0004(2)	0.0002(1)	0.76
T _{2oo}	0.6874(3)	0.1120(2)	0.1592(2)	0.0032(4)	0.0010(1)	0.0015(1)	-.0001(2)	0.0007(2)	-.0001(1)	0.81
T _{2oz}	0.6785(3)	0.1059(2)	0.6580(2)	0.0031(4)	0.0011(1)	0.0018(1)	0.0004(2)	0.0007(2)	0.0000(1)	0.89
T _{2mo}	0.6766(3)	0.8816(2)	0.1807(2)	0.0027(4)	0.0011(1)	0.0015(1)	0.0001(1)	0.0008(2)	-.0000(1)	0.78
T _{2mz}	0.6834(3)	0.8751(2)	0.6774(2)	0.0037(4)	0.0010(1)	0.0013(1)	0.0007(2)	0.0008(2)	0.0005(1)	0.78
O _{a1o}	0.0087(8)	0.1266(4)	-.0087(4)	0.009 (1)	0.0027(4)	0.0010(3)	0.0003(5)	0.0015(5)	0.0002(3)	1.47
O _{a1z}	0.9985(7)	0.1268(4)	0.4896(4)	0.009 (1)	0.0023(3)	0.0015(3)	0.0012(5)	0.0023(6)	0.0004(3)	1.40
O _{a2o}	0.5754(7)	0.9897(4)	0.1389(4)	0.004 (1)	0.0011(3)	0.0023(4)	-.0008(4)	0.0012(5)	-.0003(3)	1.09
O _{a2z}	0.5756(7)	0.9913(4)	0.6388(4)	0.003 (1)	0.0015(3)	0.0021(3)	0.0008(4)	0.0010(5)	0.0009(3)	0.99
O _{bo}	0.8207(8)	0.1005(4)	0.0918(4)	0.006 (1)	0.0021(3)	0.0032(4)	-.0011(5)	0.0026(5)	-.0007(3)	1.53
O _{boz}	0.8005(8)	0.1017(4)	0.5933(4)	0.006 (1)	0.0015(3)	0.0040(4)	-.0005(4)	0.0030(5)	0.0001(3)	1.53
O _{bmo}	0.8093(8)	0.8558(4)	0.1260(5)	0.007 (1)	0.0023(3)	0.0052(5)	-.0002(5)	0.0034(6)	-.0009(3)	2.10
O _{bmz}	0.8198(8)	0.8550(4)	0.6162(5)	0.006 (1)	0.0028(3)	0.0048(4)	0.0017(5)	0.0037(6)	0.0005(3)	1.94
O _{co}	0.0129(7)	0.2808(4)	0.1369(4)	0.0053(9)	0.0021(3)	0.0019(3)	-.0005(4)	0.0015(5)	-.0001(2)	1.24
O _{coz}	0.0174(8)	0.2933(4)	0.6485(4)	0.006 (1)	0.0016(3)	0.0028(3)	-.0002(4)	0.0021(5)	-.0003(3)	1.38
O _{cmo}	0.0095(8)	0.6808(4)	0.1080(4)	0.006 (1)	0.0023(3)	0.0019(3)	0.0011(5)	0.0007(5)	0.0004(3)	1.39
O _{cmz}	0.0073(8)	0.6911(4)	0.6010(4)	0.005 (1)	0.0014(3)	0.0021(3)	0.0011(4)	0.0010(5)	0.0000(2)	1.20
O _{do}	0.1925(8)	0.1067(4)	0.1874(4)	0.006 (1)	0.0023(3)	0.0023(3)	0.0011(5)	0.0005(5)	-.0004(3)	1.58
O _{doz}	0.2018(8)	0.1040(4)	0.6917(4)	0.006 (1)	0.0018(3)	0.0014(3)	0.0003(5)	-.0007(5)	0.0008(2)	1.39
O _{dmo}	0.1966(8)	0.8673(4)	0.2193(4)	0.006 (1)	0.0025(3)	0.0027(4)	-.0008(5)	-.0013(5)	-.0009(3)	2.04
O _{dmz}	0.1856(8)	0.8627(4)	0.7102(4)	0.007 (1)	0.0026(4)	0.0028(4)	0.0007(5)	-.0013(5)	-.0008(3)	2.10

Table 2: Positional and thermal parameters from $\bar{I}\bar{1}$ refinement of 21704a/1.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2677(6)	0.9828(7)	0.0857(5)	0.0030(7)	0.0078(6)	0.0030(3)	-0.0014(4)	0.0014(4)	0.0014(4)	2.63
Mzoo	0.2697(6)	0.0299(6)	0.5475(7)	0.0032(5)	0.0027(3)	0.0022(3)	0.0014(2)	0.0004(3)	-0.0004(2)	1.42
Moio	0.7743(4)	0.5341(3)	0.5451(3)	0.0049(6)	0.0029(2)	0.0022(2)	0.0010(3)	0.0004(3)	-0.0008(2)	1.63
Mzio	0.763 (1)	0.495 (3)	0.078 (2)	0.006 (1)	0.007 (1)	0.0039(9)	-0.0014(7)	0.0018(7)	-0.003 (1)	3.07
Tloo	0.0071(2)	0.1597(1)	0.1047(1)	0.0033(3)	0.0013(1)	0.0011(1)	-0.0002(1)	0.0008(2)	0.0001(1)	0.78
Tloz	0.0040(3)	0.1640(1)	0.6106(1)	0.0028(4)	0.0012(1)	0.0008(1)	-0.0004(1)	0.0006(2)	-0.0000(1)	0.68
Tlmo	0.0003(3)	0.8153(1)	0.1183(2)	0.0036(4)	0.0014(1)	0.0010(1)	0.0007(2)	0.0009(2)	0.0001(1)	0.79
Tlmz	0.0040(2)	0.8171(1)	0.6126(1)	0.0034(4)	0.0014(1)	0.0010(1)	0.0008(1)	0.0006(2)	0.0001(1)	0.79
T2oo	0.6875(3)	0.1114(1)	0.1592(1)	0.0028(4)	0.0010(1)	0.0014(1)	0.0001(1)	0.0004(2)	0.0001(1)	0.79
T2oz	0.6793(3)	0.1065(1)	0.6583(1)	0.0028(3)	0.0011(1)	0.0016(1)	0.0002(1)	0.0007(2)	0.0000(1)	0.84
T2mo	0.6778(3)	0.8810(1)	0.1808(1)	0.0028(3)	0.0010(1)	0.0015(1)	0.0002(1)	0.0006(2)	0.0001(1)	0.77
T2mz	0.6830(3)	0.8758(1)	0.6775(1)	0.0029(4)	0.0010(1)	0.0013(1)	0.0004(1)	0.0008(2)	0.0003(1)	0.73
Oa1o	0.0073(6)	0.1278(3)	-0.0084(3)	0.009 (1)	0.0024(2)	0.0013(3)	0.0009(4)	0.0019(5)	0.0004(2)	1.41
Oa1z	-0.0010(7)	0.1273(3)	0.4893(3)	0.011 (1)	0.0023(3)	0.0014(3)	0.0011(5)	0.0022(5)	0.0004(2)	1.55
Oa2o	0.5776(6)	-0.0098(3)	0.1393(3)	0.0035(9)	0.0013(3)	0.0020(3)	0.0002(4)	0.0007(4)	0.0003(2)	1.04
Oa2z	0.5749(6)	-0.0088(3)	0.6383(3)	0.0028(9)	0.0013(3)	0.0024(3)	0.0005(4)	0.0005(4)	0.0005(2)	1.07
Oboo	0.8185(7)	0.1018(3)	0.0919(4)	0.0056(9)	0.0017(3)	0.0033(3)	-0.0005(4)	0.0024(5)	-0.0007(2)	1.44
Oboz	0.8023(7)	0.1030(3)	0.5934(4)	0.0057(9)	0.0019(3)	0.0037(3)	-0.0009(4)	0.0027(5)	-0.0001(3)	1.55
Obmo	0.8077(7)	0.8549(4)	0.1247(4)	0.007 (1)	0.0023(3)	0.0059(4)	0.0002(4)	0.0046(6)	-0.0009(3)	2.16
Obmz	0.8211(7)	0.8548(4)	0.6175(4)	0.0048(9)	0.0028(3)	0.0054(4)	0.0009(4)	0.0036(5)	-0.0002(3)	1.99
Ocoo	0.0142(7)	0.2825(3)	0.1381(4)	0.0058(9)	0.0020(3)	0.0025(3)	-0.0003(4)	0.0017(5)	0.0003(2)	1.39
Ocoz	0.0157(7)	0.2939(3)	0.6473(4)	0.0056(9)	0.0019(3)	0.0029(3)	-0.0007(4)	0.0018(5)	-0.0001(2)	1.48
Ocmo	0.0089(6)	0.6816(3)	0.1076(4)	0.0047(9)	0.0019(3)	0.0022(3)	0.0013(4)	0.0006(4)	0.0000(2)	1.32
Ocmz	0.0084(7)	0.6903(4)	0.6014(4)	0.0056(9)	0.0020(3)	0.0021(3)	0.0008(4)	0.0007(4)	-0.0003(2)	1.41
Odoo	0.1928(6)	0.1072(3)	0.1881(4)	0.0038(9)	0.0021(3)	0.0018(3)	0.0006(4)	-0.0003(4)	0.0001(2)	1.33
Odoo	0.2017(7)	0.1044(4)	0.6923(4)	0.007 (1)	0.0022(3)	0.0022(3)	0.0005(4)	0.0001(5)	0.0003(2)	1.63
Odmo	0.1966(7)	0.8676(4)	0.2190(4)	0.0045(9)	0.0023(3)	0.0032(3)	0.0003(4)	-0.0006(5)	-0.0010(3)	1.88
Odmoz	0.1862(7)	0.8629(4)	0.7118(4)	0.008 (1)	0.0027(3)	0.0027(3)	0.0010(5)	-0.0012(5)	-0.0009(3)	2.20

Table 2: Positional and thermal parameters from \bar{H} refinement of 101377a/1.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2664(6)	0.9842(9)	0.0841(7)	0.0033(8)	0.0086(8)	0.0036(5)	-0.0026(5)	0.0018(4)	-0.0034(5)	3.02
Mzoo	0.2709(6)	0.0298(6)	0.5485(6)	0.0039(5)	0.0036(3)	0.0022(3)	0.0015(3)	0.0006(3)	-0.0009(2)	1.68
Moi0	0.7740(5)	0.5331(4)	0.5457(4)	0.0052(6)	0.0028(3)	0.0024(3)	0.0009(3)	0.0008(3)	-0.0004(2)	1.63
Mzio	0.765 (1)	0.488 (2)	0.082 (1)	0.009 (1)	0.010 (1)	0.0037(7)	-0.0027(9)	0.0034(7)	-0.0030(9)	3.75
Tl0o	0.0073(3)	0.1604(2)	0.1059(2)	0.0036(3)	0.0014(1)	0.0011(1)	-0.0002(2)	0.0008(2)	0.0002(1)	0.80
Tl0z	0.0046(3)	0.1644(2)	0.6099(2)	0.0046(4)	0.0018(1)	0.0011(1)	-0.0007(2)	0.0011(2)	-0.0000(1)	0.97
Tlmo	0.0004(3)	0.8153(2)	0.1177(2)	0.0051(4)	0.0015(1)	0.0012(1)	0.0005(2)	0.0012(2)	0.0004(1)	0.92
Tl mz	0.0042(3)	0.8171(2)	0.6132(2)	0.0036(3)	0.0019(1)	0.0008(1)	0.0009(2)	0.0006(2)	-0.0001(1)	0.88
T20o	0.6874(3)	0.1109(2)	0.1592(2)	0.0036(4)	0.0013(1)	0.0014(1)	0.0005(2)	0.0006(2)	0.0002(1)	0.91
T20z	0.6805(3)	0.1069(2)	0.6583(2)	0.0034(4)	0.0013(1)	0.0016(1)	-0.0002(2)	0.0009(2)	-0.0002(1)	0.92
T2mo	0.6786(3)	0.8805(2)	0.1798(2)	0.0037(4)	0.0012(1)	0.0016(1)	0.0000(2)	0.0009(2)	0.0001(1)	0.88
T2 mz	0.6821(3)	0.8766(2)	0.6779(2)	0.0041(4)	0.0014(1)	0.0014(1)	0.0005(2)	0.0009(2)	0.0005(1)	0.90
Oa1o	0.0073(7)	0.1276(4)	-0.0090(4)	0.011 (1)	0.0026(4)	0.0014(3)	0.0011(5)	0.0024(5)	0.0008(3)	1.61
Oa1z	0.0003(7)	0.1280(4)	0.4896(4)	0.010 (1)	0.0032(4)	0.0018(3)	0.0008(5)	0.0024(6)	-0.0001(3)	1.80
Oa2o	0.5765(7)	0.9905(4)	0.1390(4)	0.006 (1)	0.0017(3)	0.0020(3)	-0.0003(4)	0.0013(5)	0.0000(3)	1.24
Oa2z	0.5783(6)	0.9912(4)	0.6389(4)	0.0037(9)	0.0016(3)	0.0021(3)	0.0007(4)	0.0006(5)	0.0007(3)	1.15
Obo0	0.8187(7)	0.1021(4)	0.0936(4)	0.0061(9)	0.0020(3)	0.0030(3)	-0.0002(4)	0.0019(5)	0.0002(3)	1.52
Oboz	0.8043(8)	0.1023(4)	0.5933(4)	0.0074(9)	0.0026(3)	0.0034(4)	-0.0010(5)	0.0034(5)	-0.0006(3)	1.73
Obmo	0.8109(7)	0.8535(4)	0.1239(5)	0.008 (1)	0.0028(4)	0.0051(4)	-0.0002(5)	0.0037(6)	-0.0006(3)	2.21
Ob mz	0.8192(7)	0.8550(4)	0.6194(5)	0.008 (1)	0.0035(4)	0.0050(4)	0.0014(5)	0.0040(6)	-0.0001(3)	2.32
Oco0	0.0125(7)	0.2841(4)	0.1373(4)	0.006 (1)	0.0034(3)	0.0022(3)	0.0001(5)	0.0019(5)	0.0007(3)	1.62
Ocoz	0.0158(7)	0.2920(4)	0.6454(4)	0.007 (1)	0.0017(3)	0.0027(3)	-0.0017(4)	0.0015(5)	-0.0004(3)	1.52
Ocmo	0.0106(7)	0.6822(4)	0.1080(4)	0.007 (1)	0.0024(3)	0.0022(3)	0.0011(5)	0.0008(5)	-0.0002(3)	1.63
Ocmz	0.0109(7)	0.6905(4)	0.6034(4)	0.006 (1)	0.0025(3)	0.0018(3)	0.0015(4)	0.0007(5)	0.0001(2)	1.49
Odo0	0.1933(7)	0.1073(4)	0.1883(4)	0.008 (1)	0.0024(3)	0.0028(3)	0.0003(5)	0.0015(5)	0.0002(3)	1.76
Odoz	0.2005(7)	0.1048(4)	0.6917(4)	0.006 (1)	0.0028(3)	0.0009(3)	0.0007(5)	-0.0007(4)	0.0004(2)	1.44
Odmo	0.1918(8)	0.8677(4)	0.2166(4)	0.009 (1)	0.0025(4)	0.0032(4)	0.0001(5)	-0.0000(6)	-0.0000(3)	2.22
Od mz	0.1891(8)	0.8634(4)	0.7125(4)	0.007 (1)	0.0034(4)	0.0027(3)	0.0009(5)	-0.0010(5)	-0.0003(3)	2.19

Table 2 (supplement). M site occupancies from $\bar{1}\bar{1}$ refinements.

	Val Pasmaeda	Monte Somma	115082a	87975a	21704a	101377a	Crystal Bay
Mooo	0.486(4)	0.469(5)	0.488(4)	0.519(6)	0.519(6)	0.461(4)	0.42(2)
Moio	0.513(4)	0.519(5)	0.473(4)	0.415(6)	0.385(6)	0.411(4)	0.44(2)
Ca	1.00	0.97	0.91	0.85	0.79	0.72	0.69
Na	0.00	0.03	0.09	0.15	0.21	0.28	0.31
Mzoo	0.57 (2)	0.59 (3)	0.67 (2)	0.73 (3)	0.74 (2)	0.63 (2)	0.49(9)
Mzio	0.43 (2)	0.41 (3)	0.33 (2)	0.23 (3)	0.23 (2)	0.28 (2)	0.40(9)
Ca	1.00	1.00	1.00	0.91	0.93	0.80	0.76
Na	0.00	0.00	0.00	0.09	0.07	0.20	0.24
	Lake Co.	Val Pas- meda/3	Val Pas- meda/6	Val Pas- meda/7	Val Pas- meda/8	Monte Somma/1	Monte Somma/6
Mooo	0.41 (1)	0.433(9)	0.41(1)	0.410(7)	0.417(5)	0.434(4)	0.432(7)
Moio	0.43 (1)	0.569(9)	0.60(1)	0.599(7)	0.584(5)	0.555(4)	0.572(7)
Ca	0.65	1.00	1.00	1.00	1.00	0.98	1.00
Na	0.35	0.00	0.00	0.00	0.00	0.02	0.00
Mzoo	0.57 (2)	0.63 (6)	0.60 (1)	0.70 (3)	0.604(4)	0.67 (2)	0.70 (3)
Mzio	0.30 (2)	0.37 (6)	0.39 (1)	0.29 (3)	0.395(5)	0.32 (2)	0.28 (3)
Ca	0.71	1.00	1.00	1.00	1.00	0.98	0.97
Na	0.29	0.00	0.00	0.00	0.00	0.02	0.03
	Monte Somma/7	Monte Somma/8	115082a /1	87975a /1	21704a /1	101377a /1	
Mooo	0.415(8)	0.418(7)	0.401(6)	0.39(1)	0.40(1)	0.39(1)	
Moio	0.585(8)	0.577(7)	0.575(6)	0.56(1)	0.53(1)	0.48(1)	
Ca	1.00	0.99	0.95	0.89	0.84	0.71	
Na	0.00	0.01	0.05	0.11	0.16	0.29	

Mzoo	0.65 (4)	0.67 (4)	0.61 (4)	0.36(5)	0.62(4)	0.58(3)
Mzio	0.33 (4)	0.31 (4)	0.38 (4)	0.59(5)	0.33(4)	0.33(3)
Ca	0.97	0.96	0.98	0.84	0.89	0.80
Na	0.03	0.04	0.02	0.16	0.11	0.20

Note: M site occupancies are refined calcium content constrained to a total of $1.1 + 0.9n_{AN}$ for an asymmetric unit. Ca and Na contents for each pair of sites are calculated assuming that each has a total occupancy of unity, so that $x_{Na} = 20/9 (1 - X_{Ca})$, where X_{Ca} is the refined Ca occupancy of the pair.

Table 3a: Tetrahedral bond lengths from $P\bar{1}$ refinements (natural samples).

	Val Pasmada		Monte Somma		115082a	
	o	i	o	i	o	i
T1oo - Oa1o	1.637(4)	1.643(4)	1.646(6)	1.634(6)	1.631(6)	1.635(6)
Oboo	1.632(4)	1.610(4)	1.634(6)	1.613(6)	1.627(6)	1.612(6)
Ocoo	1.582(4)	1.593(4)	1.591(6)	1.587(6)	1.591(6)	1.584(6)
Odoe	1.623(4)	1.633(4)	1.620(6)	1.643(6)	1.627(6)	1.637(6)
Ave.	1.619	1.620	1.623	1.619	1.619	1.617
T1oz - Oa1z	1.758(4)	1.780(4)	1.769(6)	1.765(6)	1.770(6)	1.771(6)
Oboz	1.750(4)	1.756(4)	1.746(6)	1.749(6)	1.740(6)	1.758(6)
Ocoz	1.699(4)	1.722(4)	1.707(6)	1.722(6)	1.713(6)	1.713(6)
Odoz	1.755(4)	1.759(4)	1.764(6)	1.779(6)	1.759(6)	1.767(6)
Ave.	1.741	1.754	1.747	1.754	1.746	1.752
T1mo - Oa1o	1.771(4)	1.770(4)	1.770(6)	1.760(6)	1.778(6)	1.763(6)
Obmo	1.700(4)	1.752(4)	1.696(6)	1.754(6)	1.698(6)	1.740(6)
Ocmo	1.749(4)	1.745(4)	1.745(6)	1.736(6)	1.728(6)	1.762(6)
Odmoe	1.773(4)	1.699(4)	1.773(6)	1.702(6)	1.745(6)	1.698(6)
Ave.	1.748	1.742	1.746	1.738	1.737	1.741
T1mz - Oa1z	1.646(4)	1.649(4)	1.647(6)	1.648(6)	1.645(6)	1.647(6)
Obmz	1.621(4)	1.589(4)	1.622(6)	1.582(6)	1.616(6)	1.592(6)
Ocmz	1.633(4)	1.603(4)	1.638(6)	1.603(6)	1.616(6)	1.622(6)
Odmz	1.578(4)	1.621(4)	1.579(6)	1.621(6)	1.586(6)	1.611(6)
Ave.	1.620	1.616	1.622	1.614	1.616	1.618
T2oo - Oa2o	1.767(4)	1.768(4)	1.772(6)	1.769(6)	1.756(6)	1.754(6)
Oboo	1.755(4)	1.749(4)	1.760(6)	1.741(6)	1.757(6)	1.741(6)
Ocmz	1.734(5)	1.748(4)	1.733(6)	1.739(6)	1.714(6)	1.754(6)
Odmz	1.708(4)	1.727(4)	1.702(6)	1.723(6)	1.687(6)	1.698(6)
Ave.	1.741	1.748	1.742	1.743	1.729	1.737
T2oz - Oa2z	1.640(4)	1.630(4)	1.643(6)	1.628(6)	1.643(6)	1.628(6)
Oboz	1.615(4)	1.636(4)	1.614(6)	1.631(6)	1.620(6)	1.633(6)
Ocmo	1.612(4)	1.610(4)	1.623(6)	1.615(6)	1.597(6)	1.627(6)
Odmoe	1.615(4)	1.582(4)	1.604(6)	1.581(6)	1.622(6)	1.574(6)
Ave.	1.621	1.615	1.621	1.614	1.621	1.616
T2mo - Oa2o	1.632(4)	1.648(4)	1.627(6)	1.644(6)	1.630(6)	1.648(6)
Obmo	1.585(4)	1.621(4)	1.600(6)	1.614(6)	1.583(6)	1.617(6)
Ocoz	1.608(4)	1.603(4)	1.618(6)	1.592(6)	1.593(6)	1.607(6)
Odoz	1.643(4)	1.638(4)	1.641(6)	1.616(6)	1.650(6)	1.621(6)
Ave.	1.617	1.628	1.622	1.617	1.614	1.623
T2mz - Oa2z	1.758(4)	1.758(4)	1.750(6)	1.758(6)	1.744(6)	1.765(6)
Obmz	1.748(4)	1.704(4)	1.747(6)	1.704(6)	1.745(6)	1.700(6)
Ocoo	1.713(4)	1.734(5)	1.729(6)	1.723(6)	1.711(6)	1.733(6)
Odoe	1.749(4)	1.784(4)	1.752(6)	1.770(6)	1.739(6)	1.751(6)
Ave.	1.742	1.745	1.745	1.739	1.735	1.737
<Si _{rich} - O>		1.620		1.619		1.618
<Al _{rich} - O>		1.745		1.744		1.739
<T - O>		1.682		1.682		1.679

Table 3b: Tetrahedral bond lengths from \bar{H} refinements.

	Val Pasmada	Monte Somma	115082a	87975a	21704a	101377a	Crystal Bay
T1oo - Oa1o	1.635(3)	1.640(4)	1.634(3)	1.633(3)	1.631(3)	1.634(2)	1.627(7)
Oboo	1.614(3)	1.617(4)	1.616(3)	1.622(4)	1.625(4)	1.632(2)	1.618(9)
Ocoo	1.586(3)	1.587(4)	1.587(3)	1.588(4)	1.594(3)	1.603(2)	1.640(9)
Odoe	1.621(3)	1.624(4)	1.627(3)	1.626(4)	1.624(4)	1.635(2)	1.639(9)
Ave.	1.614	1.617	1.616	1.617	1.619	1.626	1.631
T1oz - Oa1z	1.760(3)	1.754(4)	1.762(3)	1.751(4)	1.756(3)	1.750(2)	1.758(8)
Oboz	1.743(3)	1.741(4)	1.744(3)	1.741(4)	1.738(4)	1.734(2)	1.749(9)
Ocoz	1.710(3)	1.713(4)	1.711(3)	1.711(4)	1.714(4)	1.703(2)	1.677(9)
Odoz	1.753(3)	1.768(4)	1.761(3)	1.763(4)	1.761(3)	1.753(2)	1.758(9)
Ave.	1.742	1.744	1.745	1.742	1.742	1.735	1.736
T1oo - Oa1o	1.768(3)	1.763(4)	1.765(3)	1.759(4)	1.755(3)	1.737(2)	1.731(8)
Obmo	1.709(3)	1.712(4)	1.708(3)	1.702(4)	1.696(4)	1.690(2)	1.659(9)
Ocmo	1.746(3)	1.740(4)	1.744(3)	1.742(4)	1.740(3)	1.726(2)	1.746(8)
Odmno	1.721(4)	1.723(4)	1.712(3)	1.721(4)	1.719(4)	1.702(2)	1.685(9)
Ave.	1.736	1.734	1.732	1.731	1.728	1.714	1.705
T1mz - Oa1z	1.642(3)	1.642(4)	1.646(3)	1.640(4)	1.638(3)	1.641(2)	1.631(8)
Obmz	1.591(3)	1.594(4)	1.600(3)	1.606(4)	1.600(4)	1.608(2)	1.650(9)
Ocmz	1.619(3)	1.620(4)	1.619(3)	1.622(4)	1.624(3)	1.621(2)	1.596(8)
Odmz	1.585(4)	1.586(4)	1.590(3)	1.586(4)	1.593(4)	1.598(2)	1.621(9)
Ave.	1.609	1.611	1.614	1.614	1.614	1.617	1.625
T2oo - Oa2o	1.758(3)	1.763(4)	1.748(3)	1.742(4)	1.749(3)	1.730(2)	1.731(8)
Oboo	1.750(3)	1.749(4)	1.747(3)	1.733(4)	1.724(4)	1.712(2)	1.725(8)
Ocmz	1.738(3)	1.734(4)	1.734(3)	1.721(4)	1.715(4)	1.710(2)	1.711(9)
Odmz	1.711(4)	1.704(5)	1.688(4)	1.685(4)	1.683(4)	1.674(2)	1.648(9)
Ave.	1.739	1.738	1.729	1.720	1.718	1.707	1.704
T2oz - Oa2z	1.633(3)	1.634(4)	1.635(3)	1.640(3)	1.632(3)	1.641(2)	1.628(8)
Oboz	1.622(3)	1.617(4)	1.624(3)	1.613(4)	1.621(4)	1.622(2)	1.600(8)
Ocmo	1.610(3)	1.620(4)	1.613(3)	1.612(4)	1.612(4)	1.614(2)	1.599(9)
Odmno	1.596(4)	1.593(4)	1.601(3)	1.596(4)	1.598(4)	1.602(2)	1.619(9)
Ave.	1.615	1.616	1.618	1.615	1.616	1.620	1.612
T2mo - Oa2o	1.640(3)	1.637(3)	1.639(3)	1.637(3)	1.634(3)	1.639(2)	1.614(7)
Obmo	1.602(4)	1.602(4)	1.603(3)	1.599(4)	1.598(4)	1.603(2)	1.642(9)
Ocoz	1.604(3)	1.606(4)	1.604(3)	1.606(4)	1.602(3)	1.612(2)	1.627(9)
Odoz	1.638(4)	1.627(4)	1.631(3)	1.635(4)	1.630(4)	1.630(2)	1.628(9)
Ave.	1.621	1.618	1.619	1.619	1.616	1.621	1.628
T2mz - Oa2z	1.758(3)	1.749(3)	1.754(3)	1.743(3)	1.751(3)	1.733(2)	1.726(8)
Obmz	1.722(4)	1.724(3)	1.725(3)	1.722(4)	1.726(4)	1.705(2)	1.673(8)
Ocoo	1.722(3)	1.727(4)	1.721(3)	1.720(4)	1.720(3)	1.705(2)	1.681(9)
Odoe	1.760(3)	1.757(4)	1.748(3)	1.748(4)	1.746(4)	1.728(2)	1.717(8)
Ave.	1.741	1.739	1.737	1.733	1.736	1.718	1.699
<<Si _{rich} - O>>	1.615	1.616	1.617	1.616	1.616	1.621	1.624
<<Al _{rich} - O>>	1.739	1.739	1.736	1.732	1.731	1.718	1.711
<<T - O>>	1.677	1.677	1.676	1.674	1.674	1.670	1.667

Table 3b (contd): Tetrahedral bond lengths from $\bar{I}\bar{1}$ refinements.

	Lake Co.	Val Pas- meda/3	Val Pas- meda/6	Val Pas- meda/7	Val Pas- meda/8	Monte Somma/1	Monte Somma/6
T1oo - Oa1o	1.648(4)	1.632(5)	1.650(6)	1.647(4)	1.635(3)	1.637(3)	1.640(4)
Oboo	1.639(4)	1.625(6)	1.630(6)	1.619(4)	1.623(3)	1.618(3)	1.632(4)
Ocoo	1.615(4)	1.599(6)	1.602(7)	1.589(4)	1.595(3)	1.590(3)	1.595(4)
Odoe	1.645(4)	1.627(6)	1.632(7)	1.646(4)	1.630(4)	1.634(3)	1.642(4)
Ave.	1.637	1.621	1.628	1.625	1.621	1.620	1.627
T1oz - Oa1z	1.733(4)	1.756(5)	1.749(6)	1.755(4)	1.757(3)	1.756(3)	1.754(4)
Oboz	1.723(4)	1.738(6)	1.737(7)	1.741(4)	1.765(4)	1.744(3)	1.734(4)
Ocoz	1.704(4)	1.701(5)	1.697(7)	1.706(4)	1.744(4)	1.709(3)	1.698(4)
Odoz	1.740(4)	1.761(6)	1.757(7)	1.755(4)	1.707(3)	1.759(3)	1.759(4)
Ave.	1.725	1.739	1.735	1.739	1.743	1.742	1.736
T1mo - Oa1o	1.720(4)	1.770(5)	1.753(6)	1.752(4)	1.740(4)	1.763(3)	1.758(4)
Obmo	1.680(4)	1.706(6)	1.708(7)	1.713(4)	1.764(3)	1.709(3)	1.711(4)
Ocmo	1.716(4)	1.740(6)	1.733(7)	1.736(4)	1.712(4)	1.746(3)	1.734(4)
Odmo	1.683(5)	1.716(6)	1.709(7)	1.711(4)	1.715(4)	1.717(3)	1.710(4)
Ave.	1.700	1.733	1.726	1.728	1.733	1.734	1.728
T1mz - Oa1z	1.644(4)	1.643(5)	1.648(6)	1.648(4)	1.641(3)	1.647(3)	1.647(4)
Obmz	1.616(4)	1.598(6)	1.608(7)	1.604(4)	1.605(4)	1.603(3)	1.599(4)
Ocmz	1.630(4)	1.628(5)	1.634(7)	1.626(4)	1.629(3)	1.625(3)	1.626(4)
Odmz	1.619(5)	1.590(7)	1.605(8)	1.593(5)	1.597(4)	1.588(3)	1.605(5)
Ave.	1.627	1.614	1.624	1.618	1.618	1.616	1.619
T2oo - Oa2o	1.713(4)	1.764(5)	1.774(6)	1.755(4)	1.761(3)	1.760(3)	1.759(4)
Oboo	1.701(4)	1.741(6)	1.736(6)	1.746(4)	1.745(3)	1.749(3)	1.742(4)
Ocmz	1.692(4)	1.737(6)	1.727(7)	1.732(4)	1.734(4)	1.739(3)	1.728(4)
Odmz	1.658(4)	1.706(7)	1.679(7)	1.696(5)	1.693(4)	1.700(3)	1.689(5)
Ave.	1.691	1.737	1.729	1.732	1.733	1.737	1.729
T2oz - Oa2z	1.647(4)	1.620(5)	1.628(6)	1.641(4)	1.641(3)	1.640(3)	1.637(4)
Oboz	1.629(4)	1.629(6)	1.634(6)	1.628(4)	1.615(3)	1.625(3)	1.631(4)
Ocmo	1.621(4)	1.620(6)	1.622(7)	1.621(4)	1.625(3)	1.613(3)	1.625(4)
Odmo	1.607(5)	1.591(6)	1.600(7)	1.599(5)	1.595(4)	1.592(3)	1.598(5)
Ave.	1.626	1.615	1.621	1.622	1.619	1.618	1.623
T2mo - Oa2o	1.647(4)	1.636(5)	1.633(6)	1.640(4)	1.641(3)	1.641(3)	1.642(4)
Obmo	1.612(4)	1.614(6)	1.612(7)	1.607(4)	1.609(4)	1.609(3)	1.613(4)
Ocoz	1.606(4)	1.609(5)	1.612(6)	1.604(4)	1.605(3)	1.608(3)	1.609(4)
Odoz	1.634(4)	1.627(6)	1.634(7)	1.635(4)	1.636(4)	1.632(3)	1.634(4)
Ave.	1.625	1.621	1.623	1.632	1.623	1.623	1.625
T2mz - Oa2z	1.714(4)	1.757(5)	1.752(6)	1.742(4)	1.742(3)	1.745(3)	1.741(4)
Obmz	1.688(4)	1.718(6)	1.715(7)	1.720(4)	1.715(4)	1.721(3)	1.722(4)
Ocoo	1.692(4)	1.714(6)	1.706(7)	1.724(4)	1.719(3)	1.718(3)	1.719(4)
Odoe	1.708(4)	1.753(6)	1.749(7)	1.743(4)	1.753(4)	1.749(3)	1.739(4)
Ave.	1.701	1.736	1.731	1.732	1.732	1.733	1.730
<Si _{rich} - O>	1.629	1.618	1.624	1.622	1.620	1.619	1.624
<Al _{rich} - O>	1.704	1.736	1.730	1.733	1.735	1.737	1.731
<T - O>	1.667	1.677	1.677	1.678	1.678	1.678	1.677

Table 3 (contd): Tetrahedral bond lengths from $\bar{I}\bar{I}$ refinements.

	Monte Somma/7	Monte Somma/8	115082a /1	87975a /1	21704a /1	101377a /1
T1oo - Oa1o	1.645(4)	1.637(4)	1.633(3)	1.640(5)	1.634(4)	1.660(5)
Oboo	1.633(5)	1.621(4)	1.620(4)	1.624(6)	1.636(5)	1.640(5)
Ocoo	1.585(4)	1.591(4)	1.588(3)	1.598(5)	1.616(5)	1.622(6)
Odoo	1.632(5)	1.629(4)	1.627(4)	1.640(6)	1.648(5)	1.646(5)
Ave.	1.624	1.620	1.617	1.626	1.634	1.642
T1oz - Oa1z	1.751(4)	1.754(4)	1.760(3)	1.743(5)	1.741(4)	1.727(5)
Oboz	1.739(5)	1.757(4)	1.739(4)	1.736(6)	1.728(5)	1.728(6)
Ocoz	1.707(5)	1.730(4)	1.712(4)	1.704(6)	1.710(5)	1.678(6)
Odoz	1.763(5)	1.711(4)	1.757(4)	1.746(6)	1.747(5)	1.734(5)
Ave.	1.740	1.738	1.742	1.732	1.732	1.716
T1mo - Oa1o	1.761(4)	1.738(4)	1.766(4)	1.743(5)	1.739(4)	1.725(5)
Obmo	1.707(5)	1.767(4)	1.714(4)	1.700(6)	1.701(5)	1.667(5)
Ocmo	1.734(5)	1.702(4)	1.740(4)	1.733(6)	1.725(5)	1.716(6)
Odmo	1.718(5)	1.707(5)	1.709(4)	1.698(6)	1.709(5)	1.676(6)
Ave.	1.730	1.729	1.732	1.719	1.719	1.696
T1mz - Oa1z	1.646(4)	1.642(4)	1.638(3)	1.641(5)	1.641(4)	1.645(5)
Obmz	1.606(5)	1.603(4)	1.608(4)	1.613(6)	1.608(5)	1.631(5)
Ocmz	1.631(4)	1.625(4)	1.627(4)	1.620(5)	1.633(5)	1.630(6)
Odmz	1.593(5)	1.592(5)	1.589(4)	1.599(6)	1.610(5)	1.624(6)
Ave.	1.619	1.616	1.616	1.618	1.623	1.633
T2oo - Oa2o	1.757(4)	1.753(4)	1.757(3)	1.750(5)	1.735(5)	1.730(5)
Oboo	1.739(5)	1.738(4)	1.740(4)	1.737(5)	1.720(5)	1.701(5)
Ocmz	1.735(5)	1.733(4)	1.733(4)	1.723(6)	1.715(5)	1.700(6)
Odmz	1.696(5)	1.694(5)	1.698(4)	1.687(6)	1.672(5)	1.659(6)
Ave.	1.732	1.730	1.732	1.724	1.711	1.698
T2oz - Oa2z	1.640(4)	1.639(6)	1.638(3)	1.632(5)	1.647(5)	1.647(5)
Oboz	1.630(4)	1.611(4)	1.626(4)	1.623(5)	1.635(5)	1.639(5)
Ocmo	1.620(5)	1.635(4)	1.619(4)	1.615(6)	1.625(5)	1.619(5)
Odmo	1.587(5)	1.601(5)	1.593(4)	1.597(6)	1.596(5)	1.627(6)
Ave.	1.619	1.622	1.619	1.617	1.626	1.633
T2mo - Oa2o	1.640(4)	1.642(4)	1.637(3)	1.635(5)	1.644(4)	1.656(5)
Obmo	1.619(5)	1.615(4)	1.604(4)	1.614(6)	1.611(5)	1.627(5)
Ocoz	1.607(4)	1.603(4)	1.601(4)	1.600(5)	1.608(5)	1.623(5)
Odoz	1.632(5)	1.634(4)	1.635(4)	1.635(6)	1.629(5)	1.647(5)
Ave.	1.625	1.624	1.619	1.621	1.623	1.638
T2mz - Oa2z	1.750(4)	1.747(4)	1.746(3)	1.739(5)	1.733(4)	1.708(5)
Obmz	1.712(5)	1.719(4)	1.712(4)	1.700(6)	1.703(5)	1.677(5)
Ocoo	1.716(5)	1.713(4)	1.721(4)	1.705(5)	1.691(5)	1.689(6)
Odoo	1.747(5)	1.753(4)	1.753(4)	1.730(6)	1.723(5)	1.714(6)
Ave.	1.731	1.733	1.733	1.719	1.713	1.697
<Si _{rich} - O>	1.622	1.620	1.618	1.620	1.626	1.636
<Al _{rich} - O>	1.733	1.732	1.735	1.723	1.718	1.702
<T - O>	1.678	1.676	1.676	1.672	1.672	1.669

Table 4a: M-O bond lengths from $P\bar{1}$ refinements (natural samples).

	Val Pasmeda	Monte Somma	115082a
Mo ₀₀ - Oa ₁₀₀	2.620(4)	2.624(6)	2.629(6)
Oa ₁₀₀	2.512(4)	2.506(6)	2.501(6)
Oa ₂₀₀	2.303(4)	2.301(6)	2.310(6)
Ob ₀₀₀	2.371(4)	2.369(6)	2.381(6)
Od ₀₀	2.395(4)	2.378(6)	2.377(6)
Od _{m0}	2.528(4)	2.556(6)	2.583(6)
Ave.	2.455	2.456	2.464
Mo ₁₀ - Oa _{10i}	2.453(4)	2.433(6)	2.409(6)
Oa _{10i}	2.806(4)	2.838(6)	2.832(6)
Oa _{20i}	2.328(4)	2.332(7)	2.327(6)
Ob _{00i}	2.428(4)	2.424(6)	2.401(6)
Ob _{m0i}	2.493(4)	2.508(6)	2.581(6)
Oc _{mz0}	2.549(4)	2.561(6)	2.590(6)
Od _{00i}	2.412(4)	2.424(6)	2.465(6)
Ave.	2.496	2.503	2.515
Mz ₀₀ - Oa _{1z0}	2.492(4)	2.500(6)	2.485(6)
Oa _{1z0}	2.728(4)	2.717(6)	2.720(6)
Oa _{2z0}	2.343(4)	2.346(6)	2.332(6)
Ob _{0z0}	2.441(4)	2.447(6)	2.443(6)
Ob _{mz0}	2.479(4)	2.498(5)	2.519(6)
Oc _{m0i}	2.570(4)	2.569(6)	2.554(6)
Od _{0z0}	2.371(4)	2.371(5)	2.377(6)
Ave.	2.489	2.493	2.490
Mz ₁₀ - Oa _{1zi}	2.445(4)	2.434(6)	2.407(6)
Oa _{1zi}	2.586(4)	2.614(6)	2.641(6)
Oa _{2zi}	2.287(4)	2.294(7)	2.283(6)
Ob _{0zi}	2.401(4)	2.410(6)	2.386(6)
Oc _{m00}	2.826(4)	2.801(6)	2.738(6)
Od _{0zi}	2.422(4)	2.432(6)	2.440(6)
Od _{mzi}	2.704(4)	2.782(6)	2.999(6)
Ave.	2.524	2.538	2.556

Table 4b: M-O bond lengths from $\bar{I}\bar{I}$ refinements.

	Val Pasmeda	Monte Somma	115082a	87975a	21704a	101377a	Crystal Bay
Mooo - Oa1o	2.726(4)	2.724(5)	2.719(4)	2.716(5)	2.721(5)	2.758(4)	2.80 (2)
Oa1o	2.387(4)	2.402(5)	2.404(4)	2.427(5)	2.447(4)	2.435(3)	2.42 (1)
Oa2o	2.298(3)	2.297(5)	2.304(3)	2.310(4)	2.303(4)	2.311(3)	2.31 (1)
Oboo	2.500(3)	2.493(5)	2.477(4)	2.470(4)	2.474(4)	2.480(3)	2.49 (1)
Odoe	2.294(4)	2.294(5)	2.317(3)	2.334(4)	2.349(4)	2.360(3)	2.38 (1)
Odmo	2.716(5)	2.723(5)	2.709(4)	2.678(6)	2.688(6)	2.703(4)	2.68 (2)
Ave.	2.487	2.488	2.488	2.489	2.497	2.508	2.514
Moio - Oa1o	2.328(4)	2.325(4)	2.324(3)	2.310(5)	2.316(5)	2.342(3)	2.36 (1)
Oa1o	2.906(4)	2.911(4)	2.911(4)	2.928(5)	2.946(5)	2.946(3)	2.93 (1)
Oa2o	2.342(3)	2.344(4)	2.344(3)	2.345(5)	2.340(4)	2.336(3)	2.34 (1)
Oboo	2.343(3)	2.344(4)	2.344(3)	2.353(4)	2.365(4)	2.386(3)	2.40 (1)
Obmo	2.670(4)	2.676(5)	2.707(4)	2.742(6)	2.759(6)	2.756(4)	2.80 (2)
Ocmz	2.583(3)	2.591(4)	2.591(3)	2.595(5)	2.600(5)	2.607(3)	2.65 (1)
Odoe	2.541(4)	2.533(4)	2.548(4)	2.549(5)	2.557(5)	2.542(3)	2.54 (1)
Ave.	2.530	2.532	2.538	2.546	2.555	2.559	2.573
Mzoo - Oa1z	2.376(4)	2.381(5)	2.391(4)	2.419(5)	2.425(4)	2.406(3)	2.39 (1)
Oa1z	2.787(7)	2.790(9)	2.771(7)	2.761(7)	2.761(6)	2.791(4)	2.83 (2)
Oa2z	2.330(4)	2.340(5)	2.325(3)	2.332(4)	2.333(4)	2.336(3)	2.36 (1)
Oboz	2.361(4)	2.375(5)	2.383(4)	2.413(5)	2.419(4)	2.418(3)	2.43 (1)
Obmz	2.63 (1)	2.63 (1)	2.624(9)	2.61 (1)	2.620(9)	2.649(6)	2.65 (2)
Ocmo	2.541(6)	2.544(8)	2.545(6)	2.567(6)	2.577(5)	2.583(4)	2.59 (2)
Odoz	2.515(8)	2.508(9)	2.491(6)	2.460(7)	2.464(6)	2.480(5)	2.49 (2)
Ave.	2.506	2.510	2.504	2.509	2.514	2.523	2.533
Mzio - Oa1z	2.586(8)	2.59 (1)	2.61 (1)	2.66 (2)	2.68 (2)	2.66 (2)	2.62 (6)
Oa1z	2.469(8)	2.48 (1)	2.45 (1)	2.44 (2)	2.41 (2)	2.44 (1)	2.51 (6)
Oa2z	2.295(4)	2.299(5)	2.289(4)	2.29 (1)	2.297(8)	2.302(4)	2.31 (2)
Oboz	2.526(7)	2.525(9)	2.527(8)	2.56 (1)	2.56 (1)	2.527(6)	2.52 (2)
Ocmo	2.89 (1)	2.88 (2)	2.89 (1)	2.92 (3)	2.96 (3)	2.97 (2)	2.92 (8)
Odoz	2.249(6)	2.259(8)	2.254(7)	2.24 (1)	2.253(7)	2.287(5)	2.31 (2)
Odmz	2.88 (2)	2.91 (2)	2.93 (2)	2.95 (4)	2.93 (4)	2.94 (2)	3.01 (9)
Ave.	2.556	2.564	2.565	2.580	2.585	2.589	2.600

Table 4b (contd): Ca-O bond lengths from $\bar{I}\bar{I}$ refinements.

	Lake Co	Val Pas- meda/3	Val Pas- meda/6	Val Pas- meda/7	Val Pas- meda/8	Monte Somma/1	Monte Somma/6
Mooo - Oa1o	2.772(9)	2.742(8)	2.738(9)	2.745(6)	2.738(4)	2.728(4)	2.738(7)
Oa1o	2.431(7)	2.400(7)	2.399(9)	2.402(5)	2.405(4)	2.408(4)	2.415(6)
Oa2o	2.320(5)	2.287(6)	2.289(8)	2.298(5)	2.286(4)	2.297(3)	2.291(5)
Oboo	2.488(6)	2.492(7)	2.480(8)	2.483(5)	2.480(4)	2.485(3)	2.469(5)
Odoe	2.381(5)	2.300(6)	2.311(8)	2.305(5)	2.303(4)	2.307(3)	2.313(5)
Odmoe	2.73 (1)	2.729(9)	2.74 (1)	2.739(7)	2.739(6)	2.737(4)	2.752(8)
Ave.	2.521	2.492	2.492	2.495	2.492	2.494	2.496
Moio - Oa1o	2.361(5)	2.335(6)	2.328(7)	2.334(4)	2.333(4)	2.333(3)	2.340(4)
Oa1o	2.936(7)	2.905(7)	2.920(8)	2.921(5)	2.917(4)	2.918(3)	2.923(5)
Oa2o	2.341(5)	2.341(6)	2.343(7)	2.345(5)	2.336(4)	2.339(3)	2.341(4)
Oboo	2.404(5)	2.352(6)	2.366(6)	2.362(4)	2.354(4)	2.354(3)	2.355(4)
Obmo	2.744(8)	2.675(8)	2.664(9)	2.669(6)	2.666(5)	2.675(4)	2.666(6)
Ocmz	2.624(7)	2.563(6)	2.553(8)	2.567(5)	2.565(4)	2.570(3)	2.569(5)
Odoe	2.541(6)	2.525(6)	2.514(7)	2.515(4)	2.519(4)	2.534(3)	2.524(4)
Ave.	2.564	2.528	2.527	2.530	2.527	2.532	2.531
Mzoo - Oa1z	2.402(5)	2.381(8)	2.397(9)	2.388(5)	2.392(5)	2.394(4)	2.401(5)
Oa1z	2.812(8)	2.80 (1)	2.82 (2)	2.789(8)	2.801(9)	2.773(7)	2.787(8)
Oa2z	2.344(5)	2.334(8)	2.324(8)	2.329(5)	2.333(4)	2.333(3)	2.332(4)
Oboz	2.432(5)	2.380(8)	2.38 (1)	2.387(5)	2.377(6)	2.379(4)	2.389(5)
Obmz	2.71 (1)	2.64 (2)	2.64 (2)	2.67 (1)	2.64 (1)	2.66 (1)	2.68 (1)
Ocmo	2.604(7)	2.53 (1)	2.53 (1)	2.546(7)	2.535(7)	2.554(6)	2.554(7)
Odoz	2.489(7)	2.50 (1)	2.50 (2)	2.482(8)	2.495(9)	2.491(7)	2.482(9)
Ave.	2.542	2.510	2.513	2.513	2.510	2.511	2.517
Mzio - Oa1z	2.74 (2)	2.60 (2)	2.61 (4)	2.64 (2)	2.60 (2)	2.62 (1)	2.65 (2)
Oa1z	2.40 (2)	2.48 (2)	2.48 (4)	2.44 (2)	2.48 (2)	2.46 (1)	2.43 (2)
Oa2z	2.314(7)	2.304(9)	2.30 (1)	2.304(7)	2.299(5)	2.298(4)	2.311(7)
Oboz	2.515(8)	2.51 (1)	2.47 (2)	2.520(9)	2.50 (1)	2.527(7)	2.517(8)
Ocmo	3.09 (2)	2.89 (3)	2.90 (5)	2.94 (2)	2.88 (2)	2.91 (1)	2.96 (2)
Odoz	2.344(8)	2.26 (1)	2.29 (1)	2.260(7)	2.264(9)	2.257(6)	2.268(7)
Odmz	2.82 (3)	2.90 (5)	2.94 (7)	2.85 (3)	2.94 (4)	2.88 (2)	2.85 (3)
Ave.	2.602	2.564	2.571	2.565	2.566	2.564	2.570

Table 4b (contd): M-O bond lengths from $\bar{I}\bar{I}$ refinements.

	Monte Somma/7	Monte Somma/8	115082a /1	87975a /1	21704a /1	101377a /1
Mooo - Oa1o	2.748(7)	2.725(6)	2.737(6)	2.767(9)	2.780(9)	2.75 (1)
Oa1o	2.407(6)	2.407(6)	2.405(5)	2.399(7)	2.420(7)	2.422(9)
Oa2o	2.294(6)	2.296(5)	2.299(4)	2.302(7)	2.305(6)	2.302(6)
Oboo	2.478(6)	2.482(5)	2.484(4)	2.472(7)	2.476(6)	2.486(7)
Odoe	2.315(5)	2.303(5)	2.311(4)	2.343(6)	2.363(6)	2.359(6)
Odmo	2.748(9)	2.746(8)	2.736(7)	2.692(9)	2.72 (1)	2.73 (1)
Ave.	2.498	2.493	2.495	2.500	2.510	2.509
Moio - Oa1o	2.342(5)	2.336(4)	2.341(4)	2.339(6)	2.353(5)	2.351(6)
Oa1o	2.916(5)	2.914(5)	2.916(4)	2.926(7)	2.933(6)	2.923(8)
Oa2o	2.342(5)	2.337(4)	2.338(4)	2.326(6)	2.344(5)	2.328(6)
Oboo	2.355(5)	2.360(4)	2.366(4)	2.370(6)	2.384(5)	2.398(6)
Obmo	2.668(6)	2.671(6)	2.685(5)	2.710(8)	2.706(8)	2.718(9)
Ocmz	2.559(5)	2.565(5)	2.563(4)	2.586(7)	2.591(6)	2.617(8)
Odoe	2.529(5)	2.520(5)	2.520(4)	2.521(6)	2.534(6)	2.527(7)
Ave.	2.530	2.529	2.533	2.540	2.549	2.552
Mzoo - Oa1z	2.390(5)	2.394(5)	2.387(5)	2.38 (1)	2.401(6)	2.400(6)
Oa1z	2.800(9)	2.785(9)	2.796(9)	2.82 (1)	2.82 (1)	2.84 (1)
Oa2z	2.328(5)	2.324(5)	2.334(5)	2.36 (1)	2.333(6)	2.343(6)
Oboz	2.383(7)	2.378(6)	2.383(6)	2.37 (1)	2.410(6)	2.408(6)
Obmz	2.67 (1)	2.65 (1)	2.64 (1)	2.595(9)	2.68 (1)	2.71 (1)
Ocmo	2.551(8)	2.549(8)	2.541(8)	2.55 (1)	2.569(9)	2.582(9)
Odoz	2.49 (1)	2.486(9)	2.49 (1)	2.52 (1)	2.497(9)	2.487(8)
Ave.	2.515	2.509	2.511	2.515	2.529	2.537
Mzio - Oa1z	2.62 (3)	2.62 (2)	2.60 (2)	2.53 (2)	2.67 (3)	2.75 (2)
Oa1z	2.47 (2)	2.45 (2)	2.48 (2)	2.60 (2)	2.43 (2)	2.40 (2)
Oa2z	2.291(8)	2.298(7)	2.290(6)	2.293(9)	2.310(9)	2.319(8)
Oboz	2.51 (1)	2.511(9)	2.51 (1)	2.46 (1)	2.51 (1)	2.500(9)
Ocmo	2.92 (3)	2.92 (3)	2.88 (3)	2.77 (2)	3.00 (3)	3.09 (3)
Odoz	2.269(8)	2.259(7)	2.272(9)	2.34 (1)	2.306(8)	2.330(9)
Odmz	2.90 (4)	2.89 (3)	2.94 (4)	2.88 (4)	2.88 (4)	2.78 (3)
Ave.	2.569	2.564	2.569	2.551	2.586	2.596

Table 5a: T - O - T bond angles from $P\bar{1}$ refinements.

	Val		Monte		115082a	
	Pasmeda		Somma			
	o	i	o	i	o	i
Oa1o	137.0(3)	138.4(3)	136.8(4)	135.3(4)	138.0(4)	138.8(4)
Oa1z	136.9(3)	134.5(3)	136.5(4)	135.3(4)	136.8(4)	135.0(4)
Oa2o	127.0(3)	122.2(3)	126.7(4)	122.5(4)	127.0(4)	123.1(4)
Oa2z	123.4(3)	125.1(3)	123.6(4)	125.2(4)	123.7(4)	124.7(4)
Oboo	129.3(3)	137.5(3)	128.8(4)	137.5(4)	129.9(4)	136.5(4)
Oboz	138.9(3)	126.7(3)	139.0(4)	128.2(4)	138.4(4)	128.3(4)
Obmo	170.2(3)	145.7(3)	168.8(4)	145.8(4)	167.8(4)	148.9(4)
Obmz	143.3(3)	166.7(3)	144.4(4)	165.2(4)	145.2(4)	163.0(4)
Ocoo	133.9(3)	130.3(3)	133.5(4)	130.4(4)	131.5(4)	132.3(4)
Ocoz	131.9(3)	130.5(3)	132.0(4)	130.3(4)	130.2(4)	132.3(4)
Ocmo	130.5(3)	131.4(3)	130.1(4)	131.1(4)	130.9(4)	130.0(4)
Ocmz	127.2(3)	130.6(3)	127.5(4)	130.7(4)	128.1(4)	129.8(4)
Odoz	136.0(3)	125.6(3)	135.1(4)	126.4(4)	135.4(4)	128.7(4)
Odmz	123.9(3)	134.5(3)	123.6(4)	134.5(4)	124.2(4)	133.1(4)
Odmz	139.3(3)	164.6(3)	140.1(4)	163.5(4)	140.8(4)	161.4(5)
Odmz	163.8(3)	135.9(3)	162.3(4)	137.5(4)	160.7(5)	142.2(5)

Table 5b: O-T-O bond angles from $P\bar{1}$ refinements.

	$O_A - O_B$	$O_A - O_C$	$O_A - O_D$	$O_B - O_C$	$O_B - O_D$	$O_C - O_D$
<u>Val Pasmada</u>						
T1ooo	101.0(2)	118.1(2)	102.0(2)	111.6(2)	114.1(2)	109.7(2)
T1ooi	102.7(2)	116.7(2)	101.7(2)	110.9(2)	113.6(2)	110.8(2)
T1ozo	99.7(2)	117.8(2)	98.9(2)	112.3(2)	115.9(2)	111.2(2)
T1ozi	96.8(2)	121.1(2)	96.3(2)	113.3(2)	116.1(2)	111.7(2)
T1moo	108.0(2)	111.9(2)	98.8(2)	114.1(2)	111.7(2)	111.3(2)
T1moi	98.2(1)	113.5(2)	107.8(2)	113.2(2)	113.6(2)	109.3(2)
T1mzo	100.5(2)	113.8(2)	108.2(2)	111.5(2)	114.2(2)	108.6(2)
T1mzi	106.0(2)	112.7(2)	101.9(2)	112.5(2)	111.9(2)	111.3(2)
T2ooo	108.5(2)	104.4(2)	107.0(2)	112.9(2)	109.1(2)	114.5(2)
T2ooi	100.6(2)	98.9(2)	107.9(2)	112.9(2)	115.7(2)	117.7(2)
T2ozo	104.8(2)	101.5(2)	110.7(2)	112.5(2)	112.1(2)	114.4(2)
T2ozi	109.4(2)	102.1(2)	110.4(2)	113.0(2)	107.3(2)	114.5(2)
T2moo	111.8(2)	104.5(2)	109.7(2)	112.5(2)	106.7(2)	111.8(2)
T2moi	108.8(2)	106.7(2)	108.1(2)	112.1(2)	108.9(2)	112.1(2)
T2mzo	107.9(2)	105.4(2)	103.4(2)	110.9(2)	112.4(2)	116.0(2)
T2mzi	111.4(2)	104.9(2)	107.2(2)	111.6(2)	109.1(2)	112.7(2)
<u>Monte Somma</u>						
T1ooo	100.2(3)	118.6(3)	101.6(3)	112.2(3)	113.7(3)	110.1(3)
T1ooi	103.7(3)	116.2(3)	101.7(3)	110.2(3)	114.3(3)	110.5(3)
T1ozo	99.2(3)	118.1(3)	98.9(3)	112.7(3)	115.7(3)	111.4(3)
T1ozi	98.0(3)	120.8(3)	96.6(3)	112.7(3)	116.5(3)	111.1(3)
T1moo	107.3(3)	112.5(3)	98.9(1)	114.0(3)	111.9(3)	111.6(3)
T1moi	98.6(3)	113.6(3)	108.3(3)	113.6(3)	113.7(3)	109.2(3)
T1mzo	101.5(3)	113.7(3)	107.1(3)	111.7(3)	114.2(3)	108.5(3)
T1mzi	105.4(3)	113.2(3)	103.0(3)	112.6(3)	111.8(3)	110.5(3)
T2ooo	107.8(3)	103.9(3)	107.1(3)	113.5(3)	110.0(3)	114.0(3)
T2ooi	101.3(3)	99.3(3)	107.7(3)	112.4(3)	115.9(3)	117.3(3)
T2ozo	105.0(3)	101.4(3)	110.5(3)	113.0(3)	111.8(3)	114.1(3)
T2ozi	109.6(3)	102.3(3)	110.2(3)	112.7(3)	107.3(3)	114.6(3)
T2moo	111.2(3)	104.4(3)	109.8(3)	112.2(3)	107.3(3)	112.0(3)
T2moi	108.7(3)	106.5(3)	108.0(3)	112.6(3)	109.9(3)	111.1(3)
T2mzo	107.8(3)	105.5(3)	103.6(3)	110.3(3)	112.3(3)	116.5(3)
T2mzi	111.2(3)	104.8(3)	106.5(3)	112.5(3)	109.8(3)	111.8(3)
<u>115082a</u>						
T1ooo	100.9(3)	118.4(3)	102.0(3)	111.0(3)	113.6(3)	110.5(3)
T1ooi	102.4(3)	116.5(3)	102.4(3)	111.6(3)	113.6(3)	110.0(3)
T1ozo	99.1(3)	118.6(3)	98.2(3)	112.0(3)	115.4(3)	112.4(3)
T1ozi	97.0(3)	120.4(3)	96.7(3)	114.1(3)	116.1(3)	111.0(3)

T1moo	107.1(3)	111.8(3)	99.4(1)	113.8(3)	112.3(3)	111.4(3)
T1moi	100.3(3)	113.6(3)	107.4(3)	112.2(3)	113.7(3)	109.4(3)
T1mzo	101.2(3)	113.2(3)	106.9(3)	112.1(3)	113.7(3)	109.4(3)
T1mzi	105.0(3)	113.4(3)	103.9(3)	111.5(3)	112.5(3)	110.2(3)
T2ooo	107.8(3)	103.5(3)	106.4(3)	113.0(3)	119.9(3)	115.5(3)
T2ooi	102.4(3)	100.3(3)	108.7(3)	112.3(3)	115.1(3)	116.1(3)
T2ozo	105.6(3)	101.0(3)	110.0(3)	112.7(3)	111.5(3)	115.2(3)
T2ozi	108.3(3)	102.2(3)	111.6(3)	112.0(3)	108.9(3)	113.6(3)
T2moo	111.4(3)	105.5(3)	109.0(3)	111.8(3)	107.3(3)	111.8(3)
T2moi	108.9(3)	105.8(3)	108.4(3)	112.2(3)	109.6(3)	111.9(3)
T2mzo	107.8(3)	106.0(3)	104.2(3)	110.2(3)	112.0(3)	116.0(3)
T2mzi	110.6(3)	104.5(3)	106.5(3)	111.8(3)	110.0(3)	113.2(3)

Table 5c: O-T-O bond angles from \bar{I} refinements.

	$O_A - O_B$	$O_A - O_C$	$O_A - O_D$	$O_B - O_C$	$O_B - O_D$	$O_C - O_D$
<u>Val Paseda</u>						
T1oo	101.7(2)	117.6(2)	101.9(2)	111.3(2)	113.7(2)	110.3(2)
T1oz	98.2(2)	119.5(2)	97.4(2)	112.9(1)	115.8(2)	111.8(2)
T1mo	103.1(2)	112.8(2)	102.8(2)	113.8(2)	113.1(2)	110.6(2)
T1mz	102.7(2)	113.3(2)	104.6(2)	112.2(2)	113.4(2)	110.2(2)
T2oo	104.5(2)	102.0(1)	107.2(2)	112.9(2)	112.7(2)	116.1(2)
T2oz	106.9(2)	101.9(2)	110.3(2)	112.9(2)	110.1(1)	114.2(2)
T2mo	110.0(2)	105.6(2)	108.8(2)	112.0(2)	108.5(2)	112.0(2)
T2mz	109.3(2)	105.2(2)	105.3(2)	111.1(2)	111.2(2)	114.3(2)
<u>Monte Somma</u>						
T1oo	101.8(2)	117.6(2)	101.7(2)	111.2(2)	113.8(2)	110.4(2)
T1oz	98.5(2)	119.3(2)	97.6(2)	112.7(2)	116.1(2)	111.5(2)
T1mo	102.7(2)	112.9(2)	102.9(2)	113.7(2)	113.2(2)	110.7(2)
T1mz	102.7(2)	113.4(2)	105.1(3)	112.1(2)	113.5(3)	109.6(2)
T2oo	104.5(2)	101.9(2)	107.4(2)	113.1(2)	112.6(3)	115.8(2)
T2oz	107.1(2)	102.1(2)	110.3(2)	112.9(2)	110.1(3)	114.0(2)
T2mo	109.9(2)	105.5(2)	108.5(2)	112.1(2)	109.1(3)	111.7(2)
T2mz	109.2(2)	105.2(2)	105.2(2)	111.0(2)	111.6(2)	114.2(2)
<u>115082a</u>						
T1oo	101.5(2)	117.5(2)	102.2(2)	111.2(2)	113.6(2)	110.4(2)
T1oz	98.0(2)	119.6(1)	97.4(2)	113.2(1)	115.6(2)	111.8(2)
T1mo	103.6(2)	112.8(1)	102.7(2)	113.1(2)	113.3(2)	110.7(2)
T1mz	102.5(2)	113.3(2)	105.5(2)	112.0(2)	113.4(2)	109.8(2)
T2oo	105.2(1)	102.0(1)	107.7(2)	112.7(2)	112.3(2)	115.7(2)
T2oz	106.9(1)	101.6(1)	110.3(2)	112.7(2)	110.5(2)	114.2(2)
T2mo	110.1(2)	105.5(2)	108.8(2)	111.7(2)	108.6(2)	112.0(2)
T2mz	108.9(2)	105.2(1)	105.2(1)	110.8(2)	111.5(2)	114.6(2)
<u>87975a</u>						
T1oo	102.2(2)	117.4(2)	102.1(2)	111.0(2)	113.6(2)	110.2(2)
T1oz	98.8(2)	119.1(2)	98.0(2)	113.0(2)	115.1(2)	111.7(2)
T1mo	103.8(2)	113.0(2)	102.7(2)	113.2(2)	113.7(2)	110.0(2)
T1mz	102.7(2)	112.8(2)	106.2(2)	112.4(2)	112.7(2)	109.8(2)
T2oo	106.0(2)	102.5(2)	107.8(2)	112.4(2)	111.3(2)	115.9(2)
T2oz	106.7(2)	101.8(2)	110.2(2)	112.7(2)	111.1(2)	113.8(2)
T2mo	109.8(2)	105.4(2)	108.8(2)	111.9(2)	109.1(2)	111.8(2)
T2mz	108.3(2)	105.6(2)	105.3(2)	111.2(2)	111.6(2)	114.4(2)
<u>21704a</u>						
T1oo	102.6(2)	116.8(2)	102.4(2)	111.0(2)	113.4(2)	110.4(2)
T1oz	98.6(2)	119.1(2)	98.4(2)	113.0(2)	115.5(2)	111.3(2)
T1mo	104.5(2)	112.6(2)	102.9(2)	113.1(2)	113.1(2)	110.2(2)

T1mz	102.8(2)	112.9(2)	106.0(2)	112.1(2)	113.6(2)	109.2(2)
T2oo	106.4(2)	102.5(2)	107.7(2)	112.8(2)	111.6(2)	115.0(2)
T2oz	107.0(2)	101.7(2)	110.0(2)	112.4(2)	111.0(2)	114.1(2)
T2mo	110.2(2)	105.2(2)	109.2(2)	112.0(2)	108.8(2)	111.3(2)
T2mz	108.4(2)	105.5(2)	105.3(2)	111.1(2)	111.6(2)	114.3(2)

101377a

T1oo	102.6(1)	116.6(1)	102.9(1)	111.1(1)	113.2(1)	110.1(1)
T1oz	99.0(1)	118.8(1)	98.8(1)	112.8(1)	114.7(1)	111.6(1)
T1mo	104.5(1)	112.5(1)	103.6(1)	112.6(1)	113.3(1)	110.0(1)
T1mz	103.2(1)	113.0(1)	106.1(1)	111.8(1)	113.1(1)	109.4(1)
T2oo	106.5(1)	102.6(1)	107.8(1)	112.6(1)	111.5(1)	115.0(1)
T2oz	107.2(1)	102.1(1)	110.1(1)	112.4(1)	110.6(1)	113.9(1)
T2mo	109.8(1)	105.7(1)	108.8(1)	111.6(1)	108.8(1)	111.8(1)
T2mz	108.6(1)	105.4(1)	106.0(1)	110.9(1)	111.5(1)	114.0(1)

Crystal Bay

T1oo	102.6(5)	116.2(4)	103.6(4)	111.2(4)	113.7(5)	109.3(5)
T1oz	100.1(4)	118.4(4)	98.3(4)	112.9(4)	114.1(4)	111.9(5)
T1mo	106.2(5)	112.5(4)	103.8(4)	111.9(4)	112.4(5)	109.8(4)
T1mz	103.0(4)	112.9(4)	106.1(5)	112.2(5)	113.0(5)	109.4(5)
T2oo	106.6(4)	103.6(4)	107.6(4)	111.2(4)	112.6(5)	114.5(4)
T2oz	107.6(4)	102.5(5)	109.7(4)	112.9(5)	109.7(5)	114.1(4)
T2mo	110.4(5)	105.4(5)	108.7(4)	111.6(5)	109.1(5)	111.6(5)
T2mz	108.1(4)	105.9(5)	106.4(4)	110.7(5)	111.5(5)	113.8(4)

Lake County

T1oo	102.6(2)	116.4(2)	102.9(2)	111.3(2)	113.6(2)	109.7(2)
T1oz	99.9(2)	118.2(2)	100.1(2)	112.8(2)	113.8(2)	111.2(2)
T1mo	104.3(2)	112.4(2)	104.4(2)	112.2(2)	113.3(2)	110.0(2)
T1mz	103.9(2)	112.8(2)	105.7(2)	111.9(2)	112.9(2)	109.4(2)
T2oo	106.8(2)	102.9(2)	107.8(2)	112.1(2)	111.6(2)	114.8(2)
T2oz	107.7(2)	102.3(2)	109.8(2)	112.2(2)	110.4(2)	114.0(2)
T2mo	109.5(2)	105.8(2)	108.3(2)	111.3(2)	109.5(2)	112.4(2)
T2mz	108.8(2)	105.8(2)	106.6(2)	110.7(2)	111.2(2)	113.4(2)

Val Pasmada/3

T1oo	101.6(3)	117.9(3)	102.1(3)	110.8(3)	113.8(3)	110.3(3)
T1oz	98.4(3)	119.2(3)	97.7(3)	115.7(3)	113.1(3)	111.6(3)
T1mo	102.3(3)	112.5(3)	103.2(3)	114.1(3)	113.1(3)	110.8(3)
T1mz	102.6(3)	113.2(3)	105.1(3)	112.0(3)	113.6(4)	109.9(3)
T2oo	104.6(3)	101.2(3)	107.0(3)	113.3(3)	112.8(4)	116.3(3)
T2oz	106.9(3)	101.9(3)	110.8(3)	112.3(3)	109.9(4)	114.6(3)
T2mo	109.6(3)	105.8(3)	108.5(3)	112.0(3)	108.7(4)	112.1(3)
T2mz	108.5(3)	105.6(3)	105.3(3)	111.3(3)	111.3(3)	114.3(3)

Val Pasmada/6

T1oo	101.8(3)	117.6(3)	101.5(3)	111.5(3)	113.7(4)	110.2(4)
T1oz	98.4(3)	119.2(3)	97.9(3)	113.3(3)	115.6(4)	111.3(3)
T1mo	101.8(3)	112.8(3)	103.6(3)	113.8(3)	113.7(4)	110.5(4)
T1mz	102.5(4)	113.4(3)	105.4(4)	112.2(4)	113.6(4)	109.5(4)
T2oo	104.5(3)	100.8(3)	107.8(4)	113.4(3)	112.4(4)	116.4(3)
T2oz	106.7(3)	101.8(3)	110.3(4)	112.7(4)	110.5(4)	114.4(3)
T2mo	109.4(3)	105.3(4)	108.7(3)	112.3(3)	109.1(4)	111.9(3)
T2mz	108.2(3)	105.7(3)	106.0(3)	110.6(3)	111.4(4)	114.5(3)

Val Pasmada/7

T1oo	102.0(2)	117.8(2)	101.5(2)	111.3(2)	113.7(2)	110.2(2)
T1oz	98.5(2)	119.1(2)	97.9(2)	113.1(2)	115.7(2)	111.5(2)
T1mo	102.1(2)	113.2(2)	103.6(2)	110.3(2)	113.3(2)	110.3(2)
T1mz	102.1(2)	113.6(2)	105.2(2)	112.3(2)	114.1(2)	109.3(2)
T2oo	104.5(2)	101.4(2)	107.9(2)	113.3(2)	112.4(2)	115.9(2)
T2oz	106.8(2)	101.7(2)	110.8(2)	112.7(2)	109.9(2)	114.4(2)
T2mo	109.2(2)	105.9(2)	108.6(2)	111.7(2)	108.9(2)	112.4(2)
T2mz	108.5(2)	105.3(2)	105.8(2)	110.7(2)	111.8(2)	114.1(2)

Val Pasmada/8

T1oo	101.7(2)	117.8(2)	101.6(2)	111.3(2)	114.0(2)	110.1(2)
T1oz	98.3(2)	119.5(2)	97.8(2)	112.9(2)	115.8(2)	111.5(2)
T1mo	102.2(2)	112.9(2)	103.5(2)	113.9(2)	113.3(2)	110.3(2)
T1mz	102.7(2)	113.3(2)	105.1(2)	112.6(2)	113.6(2)	109.3(2)
T2oo	104.5(2)	101.2(2)	108.1(2)	112.8(2)	112.9(2)	116.0(2)
T2oz	107.0(2)	101.9(2)	110.4(2)	112.9(2)	109.8(2)	114.4(2)
T2mo	109.5(2)	105.7(2)	108.7(2)	112.0(2)	109.3(2)	111.6(2)
T2mz	108.9(2)	105.3(2)	105.7(2)	111.1(2)	111.2(2)	114.0(2)

Monte Somma/1

T1oo	101.9(2)	117.5(2)	101.8(2)	111.3(1)	113.8(2)	110.2(2)
T1oz	98.1(2)	119.4(1)	97.9(1)	112.9(1)	116.1(2)	111.4(1)
T1mo	102.4(2)	112.6(1)	103.5(2)	113.9(1)	113.3(2)	110.5(1)
T1mz	102.5(2)	113.5(1)	105.0(2)	112.2(2)	113.6(2)	109.8(2)
T2oo	104.5(1)	101.2(1)	107.9(2)	113.0(1)	112.6(2)	116.1(1)
T2oz	106.8(1)	101.8(1)	110.3(2)	112.6(2)	110.4(2)	114.3(2)
T2mo	109.6(2)	105.5(1)	108.9(1)	112.1(2)	108.9(2)	111.7(2)
T2mz	108.8(1)	105.4(1)	105.4(1)	111.0(2)	111.4(2)	114.5(1)

Monte Somma/6

T1oo	101.4(2)	117.8(2)	101.8(2)	111.3(2)	113.9(2)	110.3(2)
T1oz	98.4(2)	119.3(2)	98.1(2)	113.0(2)	115.7(2)	111.2(2)
T1mo	102.1(2)	112.6(2)	103.7(2)	113.5(2)	113.9(2)	110.5(2)
T1mz	102.7(2)	113.5(2)	105.0(2)	112.6(2)	113.6(2)	109.3(2)
T2oo	104.5(2)	101.3(2)	108.1(2)	112.6(2)	112.8(2)	116.1(2)
T2oz	107.2(2)	101.8(2)	110.2(2)	112.8(2)	110.2(2)	114.3(2)
T2mo	109.1(2)	105.8(2)	108.7(2)	111.7(2)	109.4(2)	112.0(2)
T2mz	108.6(2)	105.6(2)	105.6(2)	111.1(2)	111.2(2)	114.3(2)

Monte Somma/7

T1oo	101.4(2)	117.9(2)	101.9(2)	111.6(2)	113.7(2)	110.0(3)
T1oz	98.5(2)	119.1(2)	97.9(2)	113.1(2)	115.6(2)	111.5(3)
T1mo	101.9(2)	112.8(2)	103.6(2)	113.9(2)	113.6(3)	110.4(2)
T1mz	103.0(3)	113.4(2)	105.6(3)	111.5(2)	113.4(3)	109.8(3)
T2oo	104.3(2)	101.0(2)	108.1(2)	113.2(2)	112.3(3)	116.5(2)
T2oz	107.2(2)	101.5(2)	110.5(3)	112.8(2)	110.1(3)	114.2(2)
T2mo	109.1(2)	105.7(2)	108.8(2)	111.8(2)	109.5(3)	111.9(2)
T2mz	109.1(2)	105.7(2)	105.9(2)	110.5(2)	111.2(3)	114.1(2)

Monte Somma/8

T1oo	101.9(2)	117.7(2)	101.6(2)	111.5(2)	113.6(2)	110.3(2)
T1oz	98.2(2)	119.2(2)	98.0(2)	113.2(2)	115.9(2)	111.3(2)
T1mo	102.0(2)	112.7(2)	103.4(2)	113.8(2)	113.6(2)	110.6(2)
T1mz	102.4(2)	113.4(2)	105.3(2)	112.3(2)	113.8(3)	109.3(2)
T2oo	104.5(2)	101.2(2)	108.1(2)	113.2(2)	112.4(3)	116.0(2)
T2oz	107.2(2)	101.6(2)	110.3(2)	112.7(2)	110.3(3)	114.3(2)
T2mo	109.2(2)	105.6(2)	108.6(2)	112.1(2)	109.0(3)	111.9(2)
T2mz	108.4(2)	105.5(2)	105.6(1)	110.8(2)	111.5(2)	114.4(2)

115082a/1

T1oo	101.9(2)	117.7(2)	101.7(2)	111.2(2)	113.7(2)	110.3(2)
T1oz	98.4(2)	119.0(2)	97.9(2)	113.0(2)	116.1(2)	111.3(2)
T1mo	102.4(2)	112.4(2)	103.6(2)	113.3(2)	113.8(2)	110.6(2)
T1mz	102.6(2)	113.6(2)	105.4(2)	112.1(2)	113.4(2)	109.4(2)
T2oo	104.6(2)	101.3(2)	108.0(2)	113.2(2)	112.4(2)	116.0(2)
T2oz	107.1(2)	101.7(2)	110.4(2)	112.4(2)	110.3(2)	114.3(2)
T2mo	109.5(2)	105.8(2)	108.8(2)	111.7(2)	109.3(2)	111.7(2)
T2mz	108.8(2)	105.3(2)	105.8(2)	111.0(2)	111.4(2)	114.2(2)

87975a/1

T1oo	102.2(3)	117.3(3)	101.9(3)	111.3(3)	113.6(3)	110.2(3)
T1oz	99.0(3)	118.7(3)	98.6(3)	113.0(3)	115.8(3)	110.8(3)
T1mo	102.5(3)	112.6(3)	104.2(3)	113.3(3)	113.7(3)	110.0(3)
T1mz	103.0(3)	113.4(3)	105.2(3)	112.0(3)	113.5(3)	109.5(3)
T2oo	105.2(2)	101.6(3)	108.1(3)	112.9(3)	112.1(3)	115.8(3)
T2oz	107.2(3)	102.2(3)	110.1(3)	112.3(3)	110.9(3)	113.7(3)
T2mo	109.4(3)	106.0(3)	109.4(3)	111.6(3)	109.0(3)	111.4(3)
T2mz	108.3(3)	105.5(3)	105.3(3)	111.1(3)	111.9(3)	114.2(3)

21704a/1

T1oo	102.3(2)	117.2(3)	102.4(2)	111.2(2)	113.9(3)	109.5(3)
T1oz	99.3(2)	118.6(2)	99.4(2)	112.3(2)	115.5(3)	111.0(3)
T1mo	103.3(3)	112.3(2)	104.0(3)	112.8(2)	113.9(3)	110.0(3)
T1mz	103.3(3)	113.1(2)	105.7(3)	112.1(3)	113.0(3)	109.4(3)
T2oo	105.7(2)	102.0(2)	108.3(3)	112.1(3)	112.0(2)	115.6(2)
T2oz	107.5(2)	101.8(2)	110.0(3)	111.9(3)	111.0(3)	114.1(2)
T2mo	108.9(3)	105.5(3)	108.8(2)	111.5(3)	110.0(3)	112.0(3)
T2mz	108.7(2)	105.4(2)	106.1(2)	111.4(3)	111.2(3)	113.6(2)

101377a/1

T1oo	102.4(3)	116.5(3)	101.9(3)	111.3(3)	113.7(3)	110.6(3)
T1oz	99.5(3)	118.3(3)	99.8(2)	112.9(3)	114.5(3)	111.1(3)
T1mo	103.3(3)	113.0(3)	103.6(3)	112.6(3)	113.6(3)	110.2(3)
T1mz	103.8(3)	113.2(3)	105.8(3)	112.1(3)	113.1(3)	108.9(3)
T2oo	106.5(3)	102.2(3)	108.3(3)	112.5(3)	112.1(3)	114.3(3)
T2oz	106.9(3)	102.5(3)	109.3(3)	112.4(3)	110.7(3)	114.4(3)
T2mo	109.9(3)	105.6(3)	108.4(3)	110.9(3)	110.0(3)	112.0(3)
T2mz	108.2(3)	105.9(3)	106.6(3)	111.2(3)	110.5(3)	114.1(3)

Table 5d: T - O - T bond angles from $\bar{I}1$ refinements.

	Val Pasmeda	Monte Somma	115082a	87975a	21704a	101377a	Crystal Bay
Oa1o	138.4(2)	138.5(2)	138.7(2)	138.9(2)	139.8(2)	140.4(1)	141.9(5)
Oa1z	136.8(2)	137.2(2)	136.6(2)	137.5(2)	137.6(2)	137.9(1)	138.2(6)
Oa2o	124.5(2)	124.7(2)	125.0(2)	125.7(2)	125.5(2)	126.0(1)	126.1(5)
Oa2z	124.1(2)	124.2(2)	124.1(2)	124.3(2)	124.5(2)	124.9(1)	126.0(6)
Oboo	133.9(2)	133.8(3)	133.5(2)	133.8(2)	134.0(2)	134.9(1)	135.4(6)
Oboz	133.3(2)	133.8(3)	133.7(2)	135.4(2)	135.6(2)	135.6(2)	136.3(5)
Obmo	157.2(3)	157.0(4)	158.1(3)	159.1(3)	160.0(3)	158.8(2)	160.2(8)
Obmz	154.7(3)	154.0(2)	152.9(3)	151.3(3)	151.0(3)	152.6(2)	153.1(6)
Ocoo	132.1(2)	132.1(2)	131.9(2)	132.0(2)	131.5(2)	131.7(1)	131.9(6)
Ocoz	131.2(2)	131.1(3)	131.3(2)	131.3(2)	131.5(2)	131.1(1)	130.9(6)
Ocmo	130.9(2)	130.7(3)	130.4(2)	131.0(2)	130.9(2)	131.2(1)	131.8(6)
Ocmz	129.0(2)	129.0(2)	129.0(2)	129.3(2)	129.6(2)	129.9(2)	131.4(6)
Odoo	131.5(2)	131.4(3)	132.3(2)	133.1(2)	133.6(2)	133.4(1)	134.2(5)
Odoz	129.3(2)	129.0(3)	128.8(2)	128.1(3)	128.4(2)	129.3(1)	128.8(5)
Odmo	151.1(3)	151.0(3)	150.0(3)	147.9(3)	147.9(3)	149.5(2)	150.3(6)
Odmz	149.3(3)	150.0(4)	151.9(3)	154.7(3)	154.2(3)	153.4(2)	151.8(6)

	Lake Co.	Val Pas- meda/3	Val Pas- meda/6	Val Pas- meda/7	Val Pas meda/8	Monte Somma/1	Monte Somma/6
Oa1o	140.9(3)	138.7(3)	138.7(4)	138.8(3)139.0(2)	139.0(2)	139.4(3)	
Oa1z	138.6(3)	137.7(3)	138.3(4)	137.5(2)137.5(2)	137.3(2)	137.5(2)	
Oa2o	126.4(3)	124.8(3)	123.9(4)	124.7(2)124.1(2)	124.4(2)	124.4(2)	
Oa2z	125.7(3)	124.7(3)	124.9(4)	124.4(2)124.4(2)	124.4(2)	124.9(2)	
Oboo	135.8(3)	133.6(4)	133.4(4)	133.7(3)133.3(2)	133.7(2)	133.0(3)	
Oboz	136.0(3)	133.2(4)	132.7(4)	133.3(3)133.3(2)	133.2(2)	133.6(3)	
Obmo	157.3(4)	156.0(5)	155.2(5)	155.5(3)155.6(3)	156.2(3)	155.0(3)	
Obmz	154.3(3)	153.9(4)	153.1(5)	153.2(3)153.9(2)	153.5(2)	153.7(3)	
Ocoo	131.7(3)	131.8(4)	132.3(4)	132.2(3)132.2(2)	132.3(2)	131.9(3)	
Ocoz	131.2(3)	131.6(3)	131.7(4)	132.1(3)131.6(2)	131.5(2)	132.1(3)	
Ocmo	131.2(3)	130.3(4)	130.1(4)	130.1(3)130.5(2)	130.4(2)	126.0(3)	
Ocmz	130.8(3)	127.9(4)	128.4(4)	128.6(2)128.5(2)	128.1(2)	128.7(3)	
Odoo	133.5(3)	131.6(4)	131.9(4)	131.3(3)131.6(2)	131.7(2)	131.7(2)	
Odoz	130.7(3)	129.4(4)	129.3(4)	129.5(3)129.0(2)	129.4(2)	129.4(3)	
Odmo	150.6(3)	151.7(5)	151.3(5)	152.1(3)152.0(2)	151.3(2)	151.5(3)	
Odmz	152.0(3)	149.9(5)	150.9(6)	150.3(4)150.4(3)	150.5(3)	150.8(3)	

Table 5d (contd): T - O - T bond angles from \bar{I} refinements.

	Monte Somma/7	Monte Somma/8	115082a /1	87975a /1	21704a /1	101377a /1
Oa1o	138.9(3)	138.9(2)	139.2(2)	139.7(3)	140.4(3)	140.0(3)
Oa1z	137.9(3)	137.7(2)	137.5(2)	138.2(3)	138.5(3)	138.9(3)
Oa2o	124.6(3)	124.7(2)	124.9(2)	124.7(3)	125.5(3)	124.9(3)
Oa2z	124.1(3)	124.3(2)	124.2(2)	125.3(3)	124.9(3)	126.3(3)
Oboo	133.2(3)	133.7(3)	133.9(2)	134.1(3)	134.7(3)	135.4(4)
Oboz	133.3(3)	133.1(3)	133.4(2)	134.2(4)	134.8(3)	134.5(4)
Obmo	155.0(4)	155.5(3)	155.8(3)	156.5(4)	155.8(4)	156.2(4)
Obmz	154.1(4)	152.9(3)	153.7(3)	153.0(4)	154.0(4)	155.1(4)
Ocoo	132.7(3)	132.6(3)	132.2(2)	131.6(4)	131.9(3)	131.5(3)
Ocoz	131.8(3)	131.5(3)	131.7(2)	132.4(4)	131.2(3)	131.8(3)
Ocmo	130.3(3)	130.2(3)	130.2(2)	130.8(4)	130.6(3)	131.1(4)
Ocmz	127.8(3)	128.2(3)	128.0(2)	129.0(4)	129.3(3)	130.6(4)
Odoo	131.9(3)	131.4(3)	131.7(2)	132.0(3)	132.7(3)	132.6(3)
Odoz	129.2(3)	129.4(3)	129.3(2)	129.9(3)	130.3(3)	130.4(3)
Odmo	151.7(4)	151.2(3)	151.3(3)	150.6(4)	150.3(4)	150.4(4)
Odmoz	151.3(4)	150.8(4)	150.9(3)	151.3(4)	152.0(4)	150.9(4)