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Structural variation associated with compositional variation and order-
disorder behavior in anorthite-rich feldspars

R. J. Angel, M. A. Carpenter, L. W. Finger

For deposit: Tables 2, 3, 4, and 5

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Table 2: Positional and thermal parameters from $P\bar{1}$ refinement of Val Pasmaeda.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2652(2)	0.9861(1)	0.0869(1)	0.0033(2)	0.0030(1)	0.0016(1)	-0.0002(1)	0.0009(1)	-0.0008(1)	1.27
Mzoo	0.2683(2)	0.0313(1)	0.5430(1)	0.0030(2)	0.0016(1)	0.0012(1)	0.0006(1)	0.0006(1)	-0.0000(1)	0.86
Moio	0.7735(2)	0.5359(1)	0.5412(1)	0.0028(2)	0.0015(1)	0.0012(1)	0.0005(1)	0.0004(1)	-0.0002(1)	0.85
Mzio	0.7637(2)	0.5051(1)	0.0751(1)	0.0023(2)	0.0031(1)	0.0023(1)	0.0007(1)	0.0003(1)	-0.0015(1)	1.51
T1ooo	0.0090(2)	0.1589(1)	0.1039(1)	0.0020(3)	0.0008(1)	0.0008(1)	-0.0003(1)	0.0005(1)	-0.0000(1)	0.50
T1ooi	0.5066(2)	0.6560(1)	0.6045(1)	0.0029(3)	0.0009(1)	0.0009(1)	-0.0002(1)	0.0007(1)	0.0000(1)	0.60
T1ozo	0.0069(3)	0.1609(1)	0.6111(1)	0.0026(3)	0.0009(1)	0.0009(1)	0.0002(2)	0.0008(2)	0.0002(1)	0.56
T1ozi	0.4988(3)	0.6660(1)	0.1129(1)	0.0034(3)	0.0009(1)	0.0006(1)	0.0001(1)	0.0008(2)	-0.0000(1)	0.57
T1moo	0.9909(2)	0.8153(1)	0.1176(1)	0.0019(3)	0.0011(1)	0.0008(1)	0.0002(1)	0.0006(2)	0.0001(1)	0.56
T1moi	0.5083(3)	0.3146(1)	0.6214(1)	0.0025(3)	0.0008(1)	0.0007(1)	0.0004(2)	0.0004(2)	0.0000(1)	0.53
T1mzo	0.0058(2)	0.8153(1)	0.6132(1)	0.0026(3)	0.0011(1)	0.0005(1)	0.0001(1)	0.0003(1)	0.0000(1)	0.56
T1mzi	0.5050(2)	0.3203(1)	0.1103(1)	0.0030(3)	0.0009(1)	0.0009(1)	0.0004(1)	0.0008(1)	0.0000(1)	0.59
T2ooo	0.6843(2)	0.1132(1)	0.1512(1)	0.0023(3)	0.0009(1)	0.0008(1)	-0.0000(1)	0.0004(2)	-0.0001(1)	0.57
T2ooi	0.1910(3)	0.6111(1)	0.6677(1)	0.0022(3)	0.0008(1)	0.0009(1)	-0.0002(1)	0.0005(2)	0.0001(1)	0.55
T2ozo	0.6817(2)	0.1034(1)	0.6647(1)	0.0020(3)	0.0007(1)	0.0009(1)	0.0002(1)	0.0004(1)	-0.0000(1)	0.53
T2ozi	0.1707(2)	0.6067(1)	0.1491(1)	0.0022(3)	0.0008(1)	0.0010(1)	-0.0002(1)	0.0005(1)	0.0001(1)	0.56
T2moo	0.6739(2)	0.8829(1)	0.1877(1)	0.0027(3)	0.0009(1)	0.0008(1)	0.0001(1)	0.0007(1)	0.0000(1)	0.57
T2moi	0.1761(2)	0.3793(1)	0.6733(1)	0.0023(3)	0.0007(1)	0.0009(1)	0.0002(1)	0.0006(1)	0.0000(1)	0.51
T2mzo	0.6814(3)	0.8716(1)	0.6724(1)	0.0024(3)	0.0007(1)	0.0009(1)	0.0003(1)	0.0005(2)	0.0001(1)	0.54
T2mzi	0.1855(3)	0.3776(1)	0.1816(1)	0.0020(3)	0.0007(1)	0.0009(1)	0.0002(1)	0.0004(2)	0.0001(1)	0.51
Oa1oo	0.0263(6)	0.1246(3)	-0.0043(3)	0.0044(8)	0.0012(3)	0.0009(2)	0.0005(4)	0.0013(4)	0.0002(2)	0.78
Oa1oi	0.4860(6)	0.6236(3)	0.4859(3)	0.0051(9)	0.0014(3)	0.0006(2)	0.0005(4)	0.0008(4)	0.0002(2)	0.81
Oa1zo	0.9811(6)	0.1256(3)	0.4836(3)	0.0044(8)	0.0012(3)	0.0009(2)	0.0005(4)	0.0013(4)	0.0002(2)	0.73
Oa1zi	0.5179(6)	0.6238(3)	0.9965(3)	0.0044(8)	0.0014(3)	0.0009(2)	0.0001(4)	0.0008(4)	0.0002(2)	0.84
Oa2oo	0.5757(6)	0.9906(3)	0.1434(3)	0.0020(8)	0.0006(2)	0.0015(3)	0.0007(3)	0.0002(4)	0.0004(2)	0.69
Oa2oi	0.0721(6)	0.4881(3)	0.6346(3)	0.0026(8)	0.0007(3)	0.0017(3)	-0.0000(4)	0.0009(4)	0.0001(2)	0.70
Oa2zo	0.5723(6)	0.9892(3)	0.6370(3)	0.0025(9)	0.0007(3)	0.0015(3)	0.0004(4)	-0.0000(4)	0.0002(2)	0.79
Oa2zi	0.0716(5)	0.4924(3)	0.1383(3)	0.0029(8)	0.0005(2)	0.0021(3)	-0.0004(3)	0.0016(4)	0.0000(2)	0.71
Obooo	0.8133(5)	0.1016(3)	0.0798(3)	0.0036(7)	0.0013(2)	0.0011(2)	-0.0004(3)	0.0007(4)	-0.0001(2)	0.80
Obooi	0.3331(6)	0.5952(3)	0.6053(3)	0.0033(7)	0.0012(2)	0.0015(3)	-0.0001(3)	0.0015(4)	-0.0001(2)	0.78
Obozo	0.8117(6)	0.0967(3)	0.6057(3)	0.0034(8)	0.0014(2)	0.0010(2)	-0.0012(3)	0.0008(4)	-0.0002(2)	0.78
Obozi	0.2857(6)	0.6034(3)	0.0792(3)	0.0044(8)	0.0014(3)	0.0018(3)	-0.0002(3)	0.0018(4)	-0.0002(2)	0.95
Obmoo	0.8177(6)	0.8549(3)	0.1444(3)	0.0031(8)	0.0027(3)	0.0021(3)	0.0011(4)	0.0017(4)	0.0000(2)	1.18
Obmoi	0.2984(6)	0.3554(3)	0.6111(3)	0.0039(8)	0.0013(2)	0.0012(2)	0.0005(3)	0.0011(4)	0.0001(2)	0.80
Obmzo	0.8105(6)	0.8521(3)	0.6025(3)	0.0027(8)	0.0016(3)	0.0015(3)	0.0003(4)	0.0009(4)	0.0003(2)	0.87
Obmzi	0.3421(6)	0.3577(3)	0.1342(3)	0.0052(8)	0.0022(3)	0.0022(3)	0.0009(4)	0.0020(4)	-0.0002(2)	1.25
Ocooo	0.0151(6)	0.2792(3)	0.1354(3)	0.0061(9)	0.0009(2)	0.0020(3)	-0.0003(4)	0.0020(4)	0.0000(2)	1.02
Ocooi	0.5095(6)	0.7772(3)	0.6350(3)	0.0028(8)	0.0014(2)	0.0016(2)	-0.0003(3)	0.0010(4)	-0.0003(2)	0.87

Ocozo	0.0215(8)	0.2910(4)	0.6485(5)	0.005 (1)	0.0048(3)	0.0023(4)	-0.0003(5)	0.0020(6)	-0.0006(3)	0.79
Ocozi	0.5078(8)	0.7962(4)	0.1495(4)	0.002 (1)	0.0009(3)	0.0019(4)	-0.0002(5)	0.0006(5)	-0.0003(3)	0.84
Ocmoo	-0.0000(8)	0.6801(4)	0.1034(5)	0.004 (1)	0.0006(3)	0.0017(4)	0.0007(5)	0.0009(6)	0.0001(3)	0.84
Ocmoi	0.5148(8)	0.1799(4)	0.6107(5)	0.003 (1)	0.0010(3)	0.0012(4)	-0.0000(5)	0.0004(5)	0.0002(3)	0.77
Ocmzo	0.0093(8)	0.6885(4)	0.6006(4)	0.004 (1)	0.0008(3)	0.0010(3)	0.0001(5)	0.0011(5)	-0.0003(3)	0.64
Ocmzi	0.5075(8)	0.1955(4)	0.0993(5)	0.003 (1)	0.0012(3)	0.0011(4)	0.0007(5)	-0.0007(6)	-0.0005(3)	0.91
Odooo	0.1833(8)	0.1053(5)	0.1910(4)	0.003 (1)	0.0019(4)	0.0003(3)	0.0007(5)	0.0000(5)	0.0000(3)	0.76
Odooi	0.7012(8)	0.6079(4)	0.6800(4)	0.002 (1)	0.0013(4)	0.0012(3)	0.0008(5)	-0.0000(5)	0.0002(3)	0.76
Odozo	0.2136(8)	0.1025(5)	0.6840(4)	0.005 (1)	0.0018(4)	0.0005(3)	0.0003(5)	0.0010(5)	-0.0002(3)	0.81
Odozi	0.6935(8)	0.6043(4)	0.2013(4)	0.005 (1)	0.0012(4)	0.0007(3)	0.0007(5)	0.0007(5)	0.0002(3)	0.81
Odmoo	0.2038(8)	0.8732(4)	0.2108(4)	0.002 (1)	0.0014(3)	0.0010(3)	0.0001(5)	-0.0004(5)	-0.0008(3)	0.83
Odmoi	0.6900(8)	0.3636(5)	0.7317(4)	0.005 (1)	0.0022(4)	0.0011(3)	0.0001(6)	-0.0000(5)	-0.0000(3)	1.24
Odmzo	0.1742(8)	0.8569(4)	0.7183(4)	0.003 (1)	0.0016(4)	0.0007(3)	-0.0002(5)	-0.0013(5)	-0.0003(3)	1.03
Odmzi	0.6992(8)	0.3692(5)	0.1983(4)	0.003 (1)	0.0020(4)	0.0012(3)	0.0004(5)	-0.0004(5)	-0.0002(3)	1.09

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

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mo ₀₀	0.2659(2)	0.9867(1)	0.0864(1)	0.0026(3)	0.0031(1)	0.0015(1)	-0.0002(1)	0.0007(2)	-0.0008(1)	1.24
Mz ₀₀	0.2683(2)	0.0310(1)	0.5432(1)	0.0027(3)	0.0019(1)	0.0013(1)	0.0008(1)	0.0006(2)	-0.0002(1)	0.93
Mo ₁₀	0.7736(2)	0.5353(1)	0.5421(1)	0.0019(3)	0.0014(1)	0.0012(1)	0.0005(1)	0.0002(1)	-0.0003(1)	0.79
Mz ₁₀	0.7639(2)	0.5073(1)	0.0726(1)	0.0016(3)	0.0041(1)	0.0028(1)	0.0009(2)	-0.0002(2)	-0.0027(1)	1.90
Tl ₀₀₀	0.0094(3)	0.1592(2)	0.1043(2)	0.0024(4)	0.0007(1)	0.0010(1)	0.0002(2)	0.0011(2)	0.0001(1)	0.47
Tl ₀₀₁	0.5064(3)	0.6561(2)	0.6040(2)	0.0021(4)	0.0007(1)	0.0004(1)	-0.0003(2)	0.0002(2)	0.0000(1)	0.43
Tl _{0z0}	0.0069(4)	0.1614(2)	0.6116(2)	0.0020(5)	0.0005(1)	0.0011(1)	-0.0001(2)	0.0013(2)	-0.0001(1)	0.41
Tl _{0z1}	0.4987(4)	0.6658(2)	0.1124(2)	0.0016(5)	0.0010(2)	0.0002(1)	-0.0001(2)	-0.0002(2)	0.0000(1)	0.45
Tl _{1m00}	0.9918(4)	0.8151(2)	0.1177(2)	0.0019(5)	0.0010(2)	0.0005(1)	-0.0000(2)	0.0006(2)	-0.0000(1)	0.46
Tl _{1m01}	0.5073(4)	0.3145(2)	0.6211(2)	0.0019(5)	0.0005(2)	0.0006(2)	0.0004(2)	0.0004(2)	-0.0000(1)	0.38
Tl _{1mz0}	0.0056(3)	0.8156(2)	0.6132(2)	0.0024(5)	0.0009(1)	0.0005(1)	0.0004(2)	0.0005(2)	0.0001(1)	0.47
Tl _{1mz1}	0.5048(3)	0.3200(2)	0.1101(2)	0.0020(4)	0.0006(1)	0.0007(1)	0.0006(2)	0.0005(2)	-0.0000(1)	0.41
T2 ₀₀₀	0.6855(4)	0.1133(2)	0.1521(2)	0.0025(5)	0.0007(1)	0.0008(1)	-0.0000(2)	0.0005(2)	-0.0000(1)	0.51
T2 ₀₀₁	0.1909(3)	0.6113(2)	0.6667(2)	0.0013(5)	0.0007(1)	0.0008(1)	0.0003(2)	0.0004(2)	0.0000(1)	0.40
T2 _{0z0}	0.6817(3)	0.1038(2)	0.6645(2)	0.0018(4)	0.0006(1)	0.0008(1)	-0.0001(2)	0.0002(2)	0.0000(1)	0.48
T2 _{0z1}	0.1710(3)	0.6066(2)	0.1499(2)	0.0010(4)	0.0007(1)	0.0007(1)	-0.0001(2)	0.0003(2)	-0.0001(1)	0.39
T2 _{1m00}	0.6739(3)	0.8831(2)	0.1875(2)	0.0014(4)	0.0006(1)	0.0008(1)	0.0003(2)	0.0007(2)	0.0000(1)	0.39
T2 _{1m01}	0.1768(3)	0.3795(2)	0.6738(2)	0.0015(4)	0.0005(1)	0.0007(1)	0.0003(2)	0.0007(2)	0.0001(1)	0.36
T2 _{1mz0}	0.6813(4)	0.8724(2)	0.6734(2)	0.0022(5)	0.0008(1)	0.0007(1)	0.0003(2)	-0.0000(2)	0.0002(1)	0.55
T2 _{1mz1}	0.1864(4)	0.3773(2)	0.1811(2)	0.0015(4)	0.0007(1)	0.0008(1)	0.0001(2)	0.0007(2)	0.0001(1)	0.40
Oa ₁₀₀	0.0242(9)	0.1242(5)	-0.051(5)	0.005 (1)	0.0013(4)	0.0011(4)	0.0002(5)	0.0015(6)	0.0002(3)	0.84
Oa ₁₀₁	0.4912(8)	0.6251(4)	0.4870(4)	0.002 (1)	0.0015(4)	0.0004(3)	0.0003(5)	0.0003(5)	-0.0001(3)	0.60
Oa _{1z0}	0.9797(8)	0.1252(4)	0.4832(5)	0.005 (1)	0.0007(4)	0.0011(3)	0.0009(5)	0.0012(5)	0.0003(3)	0.68
Oa _{1z1}	0.5176(8)	0.6249(4)	0.9968(4)	0.003 (1)	0.0015(4)	0.0002(3)	-0.0008(5)	0.0005(5)	-0.0003(3)	0.62
Oa ₂₀₀	0.5760(8)	0.9902(4)	0.1426(5)	0.002 (1)	0.0002(3)	0.0012(4)	0.0005(5)	0.0003(6)	0.0004(3)	0.44
Oa ₂₀₁	0.0730(9)	0.4881(5)	0.6345(5)	0.001 (1)	0.0012(4)	0.0014(4)	-0.0006(5)	-0.0003(6)	-0.0002(3)	0.80
Oa _{2z0}	0.5728(8)	0.9893(5)	0.6373(5)	0.002 (1)	0.0003(4)	0.0014(4)	0.0012(5)	0.0004(6)	0.0005(3)	npd
Oa _{2z1}	0.0726(9)	0.4924(5)	0.1391(5)	0.002 (1)	0.0012(4)	0.0018(4)	0.0007(6)	0.0010(6)	0.0000(3)	0.79
Ob ₀₀₀	0.8143(8)	0.1011(4)	0.0803(4)	0.004 (1)	0.0011(3)	0.0013(3)	-0.0003(5)	0.0011(5)	-0.0005(3)	0.75
Ob ₀₀₁	0.3305(8)	0.5964(4)	0.6034(4)	0.005 (1)	0.0009(3)	0.0018(4)	0.0000(5)	0.0026(6)	-0.0002(3)	0.76
Ob _{0z0}	0.8120(7)	0.0975(4)	0.6058(4)	0.002 (1)	0.0010(3)	0.0012(3)	-0.0004(4)	0.0010(5)	-0.0005(3)	0.75
Ob _{0z1}	0.2871(7)	0.6039(4)	0.0811(4)	0.0026(9)	0.0016(4)	0.0016(4)	-0.0008(5)	0.0015(5)	-0.0001(3)	0.84
Ob _{1m00}	0.8171(8)	0.8548(4)	0.1424(5)	0.004 (1)	0.0019(4)	0.0028(4)	-0.0001(5)	0.0034(6)	-0.0003(3)	npd
Ob _{1m01}	0.2984(8)	0.3563(4)	0.6116(4)	0.005 (1)	0.0015(4)	0.0013(3)	0.0004(5)	0.0018(6)	-0.0004(3)	0.93
Ob _{1mz0}	0.8111(8)	0.8523(4)	0.6041(4)	0.002 (1)	0.0017(4)	0.0012(3)	0.0013(5)	0.0014(5)	0.0006(3)	0.67
Ob _{1mz1}	0.3414(8)	0.3582(5)	0.1323(5)	0.005 (1)	0.0023(4)	0.0029(4)	0.0011(5)	0.0027(6)	-0.0002(3)	1.41
Oc ₀₀₀	0.0164(8)	0.2801(4)	0.1368(4)	0.005 (1)	0.0007(3)	0.0016(3)	-0.0001(5)	0.0016(6)	0.0002(3)	0.79
Oc ₀₀₁	0.5084(8)	0.7768(4)	0.6344(4)	0.002 (1)	0.0005(3)	0.0013(3)	-0.0012(4)	0.0002(5)	-0.0008(3)	npd

Ocozo	0.0201(6)	0.2899(3)	0.6477(3)	0.0058(9)	0.0011(2)	0.0019(3)	-0.0002(4)	0.0019(4)	-0.0001(2)	1.03
Ocozi	0.5087(6)	0.7965(3)	0.1499(3)	0.0040(8)	0.0009(2)	0.0016(2)	-0.0003(3)	0.0010(4)	-0.0001(2)	0.85
Ocmoo	0.0000(6)	0.6800(3)	0.1038(3)	0.0020(8)	0.0014(2)	0.0014(3)	0.0003(3)	0.0003(4)	-0.0002(2)	0.82
Ocmoi	0.5168(6)	0.1793(3)	0.6104(3)	0.0043(8)	0.0003(2)	0.0014(3)	-0.0001(3)	0.0004(4)	-0.0001(2)	0.77
Ocmzo	0.0084(6)	0.6885(3)	0.6006(3)	0.0034(8)	0.0011(2)	0.0009(2)	0.0005(3)	0.0005(4)	0.0003(2)	0.72
Ocmzi	0.5071(6)	0.1959(3)	0.0976(3)	0.0046(9)	0.0007(2)	0.0019(3)	0.0003(3)	0.0007(4)	-0.0001(2)	0.99
Odooo	0.1832(6)	0.1062(3)	0.1922(3)	0.0039(8)	0.0017(3)	0.0008(2)	0.0008(3)	0.0004(4)	-0.0000(2)	0.87
Odooi	0.7006(6)	0.6075(3)	0.6783(3)	0.0024(8)	0.0021(3)	0.0011(2)	0.0003(4)	0.0001(4)	0.0000(2)	0.96
Odozo	0.2135(6)	0.1033(3)	0.6835(3)	0.0031(8)	0.0012(2)	0.0009(2)	0.0002(3)	0.0002(4)	-0.0001(2)	0.75
Odozi	0.6894(6)	0.6035(3)	0.2005(3)	0.0036(8)	0.0015(3)	0.0008(2)	0.0006(4)	-0.0000(4)	0.0003(2)	0.86
Odmoo	0.2037(6)	0.8734(3)	0.2098(3)	0.0021(7)	0.0018(3)	0.0006(2)	0.0000(3)	-0.0003(3)	-0.0001(2)	0.79
Odmoi	0.6890(6)	0.3636(3)	0.7327(3)	0.0047(8)	0.0017(3)	0.0012(2)	0.0003(4)	-0.0004(4)	0.0001(2)	1.16
Odmzo	0.1727(6)	0.8564(3)	0.7192(3)	0.0049(9)	0.0019(3)	0.0007(2)	-0.0004(4)	-0.0004(4)	-0.0003(2)	1.11
Odmzi	0.7001(6)	0.3705(3)	0.1968(3)	0.0045(8)	0.0016(3)	0.0007(2)	0.0001(4)	0.0002(4)	-0.0001(2)	0.93

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

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2655(3)	0.9871(2)	0.0856(2)	0.0042(3)	0.0049(2)	0.0023(1)	-0.0002(2)	0.0013(2)	-0.0013(1)	1.93
Mzoo	0.2681(2)	0.0301(1)	0.5445(1)	0.0036(3)	0.0026(1)	0.0017(1)	0.0008(1)	0.0007(2)	-0.0002(1)	1.25
Moio	0.7733(3)	0.5344(2)	0.5431(1)	0.0033(3)	0.0025(1)	0.0018(1)	0.0008(2)	0.0005(2)	-0.0007(1)	1.27
Mzio	0.7654(3)	0.5135(2)	0.0660(2)	0.0018(3)	0.0062(2)	0.0062(2)	0.0012(2)	-0.0002(2)	-0.0054(2)	3.36
T1ooo	0.0089(3)	0.1590(2)	0.1042(2)	0.0025(4)	0.0010(1)	0.0007(1)	-0.0003(2)	0.0008(2)	0.0001(1)	0.51
T1ooi	0.5068(3)	0.6569(2)	0.6044(2)	0.0022(4)	0.0007(1)	0.0007(1)	0.0001(2)	0.0007(2)	0.0001(1)	0.44
T1ozo	0.0053(3)	0.1626(2)	0.6113(2)	0.0027(5)	0.0009(1)	0.0007(1)	-0.0004(2)	0.0011(2)	-0.0001(1)	0.48
T1ozi	0.4996(3)	0.6658(2)	0.1124(2)	0.0019(4)	0.0007(1)	0.0006(1)	0.0002(2)	0.0004(2)	0.0000(1)	0.42
T1moo	0.9938(3)	0.8154(2)	0.1185(2)	0.0026(4)	0.0010(2)	0.0007(1)	0.0008(2)	0.0011(2)	0.0002(1)	0.47
T1moi	0.5061(3)	0.3147(2)	0.6202(2)	0.0025(5)	0.0008(2)	0.0007(1)	0.0004(2)	0.0006(2)	0.0000(1)	0.49
T1mzo	0.0057(3)	0.8162(2)	0.6135(2)	0.0025(4)	0.0008(1)	0.0006(1)	0.0006(2)	0.0006(2)	0.0003(1)	0.48
T1mzi	0.5051(3)	0.3147(2)	0.6202(2)	0.0025(4)	0.0008(1)	0.0006(1)	0.0002(2)	0.0007(2)	-0.0001(1)	0.48
T2ooo	0.6855(3)	0.1130(2)	0.1530(2)	0.0024(4)	0.0006(1)	0.0008(1)	0.0002(2)	0.0005(2)	0.0000(1)	0.49
T2ooi	0.1906(3)	0.6112(2)	0.6647(2)	0.0014(4)	0.0007(1)	0.0011(1)	-0.0000(2)	0.0006(2)	0.0002(1)	0.49
T2ozo	0.6797(3)	0.1046(2)	0.6631(2)	0.0019(4)	0.0008(1)	0.0010(1)	0.0001(2)	0.0006(2)	-0.0001(1)	0.51
T2ozi	0.1733(3)	0.6062(2)	0.1523(2)	0.0020(4)	0.0007(1)	0.0012(1)	-0.0000(2)	0.0007(2)	-0.0001(1)	0.54
T2moo	0.6752(3)	0.8829(2)	0.1864(2)	0.0020(4)	0.0005(1)	0.0007(1)	0.0003(2)	0.0005(2)	0.0000(1)	0.41
T2moi	0.1766(3)	0.3800(2)	0.6759(2)	0.0021(4)	0.0009(1)	0.0012(1)	0.0002(2)	0.0006(2)	0.0002(1)	0.61
T2mzo	0.6814(3)	0.8735(2)	0.6738(2)	0.0024(4)	0.0005(1)	0.0006(1)	0.0003(2)	0.0008(2)	0.0002(1)	0.38
T2mzi	0.1849(4)	0.3761(2)	0.1798(2)	0.0025(5)	0.0010(1)	0.0012(1)	0.0003(2)	0.0011(2)	0.0002(1)	0.62
Oa1oo	0.0222(8)	0.1252(5)	-0.0047(4)	0.006 (1)	0.0017(4)	0.0009(3)	0.0003(5)	0.0017(5)	0.0002(3)	0.90
Oa1oi	0.4939(8)	0.6243(5)	0.4881(4)	0.006 (1)	0.0015(4)	0.0007(3)	0.0014(5)	0.0011(5)	0.0004(3)	0.91
Oa1zo	0.9822(8)	0.1255(4)	0.4838(4)	0.005 (1)	0.0015(4)	0.0009(3)	0.0008(5)	0.0018(5)	0.0003(3)	0.74
Oa1zi	0.5115(8)	0.6241(5)	0.9944(4)	0.007 (1)	0.0013(4)	0.0008(3)	-0.0004(5)	0.0016(5)	0.0001(3)	0.95
Oa2oo	0.5774(8)	0.9910(5)	0.1434(5)	0.003 (1)	0.0012(4)	0.0014(4)	-0.0000(5)	0.0014(6)	0.0001(3)	0.71
Oa2oi	0.0738(8)	0.4890(4)	0.6358(5)	0.004 (1)	0.0002(3)	0.0019(4)	0.0009(5)	0.0008(6)	0.0004(3)	npd
Oa2zo	0.5721(8)	0.9898(4)	0.6373(4)	0.001 (1)	0.0010(4)	0.0012(4)	-0.0001(5)	0.0009(5)	0.0001(3)	0.53
Oa2zi	0.0719(8)	0.4933(4)	0.1375(5)	0.002 (1)	0.0005(4)	0.0018(4)	0.0007(5)	-0.0000(5)	0.0004(3)	0.73
Obooo	0.8156(8)	0.1011(5)	0.0822(5)	0.003 (1)	0.0017(4)	0.0024(4)	0.0002(5)	0.0024(5)	0.0003(3)	1.00
Obooi	0.3281(8)	0.5973(4)	0.6000(5)	0.004 (1)	0.0010(3)	0.0019(4)	-0.0012(5)	0.0020(5)	-0.0005(3)	0.86
Obozo	0.8098(8)	0.0987(4)	0.6037(5)	0.004 (1)	0.0014(4)	0.0023(4)	-0.0002(5)	0.0029(6)	-0.0004(3)	0.93
Obozi	0.2882(8)	0.6029(5)	0.0827(5)	0.004 (1)	0.0013(4)	0.0030(4)	-0.0008(5)	0.0025(6)	-0.0007(3)	1.12
Obmoo	0.8167(8)	0.8553(5)	0.1414(5)	0.005 (1)	0.0021(4)	0.0027(4)	0.0010(5)	0.0019(6)	-0.0005(3)	1.35
Obmoi	0.3003(8)	0.3544(5)	0.6152(5)	0.004 (1)	0.0017(4)	0.0030(4)	0.0002(5)	0.0026(6)	-0.0003(3)	1.19
Obmzo	0.8132(8)	0.8543(5)	0.6058(5)	0.004 (1)	0.0021(4)	0.0018(4)	0.0011(5)	0.0020(5)	0.0012(3)	1.03
Obmzi	0.3342(9)	0.3550(5)	0.1276(6)	0.007 (1)	0.0025(4)	0.0053(5)	0.0012(6)	0.0053(7)	-0.0002(4)	1.88
Ocooo	0.0117(8)	0.2798(4)	0.1360(5)	0.005 (1)	0.0009(3)	0.0017(4)	-0.0004(5)	0.0008(6)	0.0002(3)	1.00
Ocooi	0.5122(8)	0.7777(4)	0.6347(5)	0.004 (1)	0.0005(3)	0.0023(4)	-0.0004(5)	0.0022(5)	-0.0008(3)	0.79

Ocozo	0.0161(8)	0.2926(4)	0.6480(4)	0.005 (1)	0.0008(3)	0.0015(3)	0.0005(5)	0.0012(5)	-.0002(3)	0.88
Ocozi	0.5132(8)	0.7959(4)	0.1494(5)	0.003 (1)	0.0012(3)	0.0021(4)	-.0009(5)	0.0012(5)	-.0002(3)	0.98
Ocmoo	0.0022(8)	0.6816(4)	0.1054(5)	0.004 (1)	0.0011(4)	0.0021(4)	0.0013(5)	0.0009(6)	-.0002(3)	1.04
Ocmoi	0.5132(8)	0.1780(4)	0.6090(4)	0.003 (1)	0.0008(3)	0.0007(3)	0.0004(5)	0.0004(5)	0.0004(3)	0.55
Ocmzo	0.0083(8)	0.6908(4)	0.6005(5)	0.006 (1)	0.0004(3)	0.0017(4)	0.0007(5)	0.0014(6)	-.0001(3)	0.85
Ocmzi	0.5077(8)	0.1932(5)	0.0983(5)	0.005 (1)	0.0016(4)	0.0010(4)	0.0006(5)	0.0005(6)	0.0001(3)	1.02
Odooo	0.1852(8)	0.1057(4)	0.1913(4)	0.003 (1)	0.0012(4)	0.0013(4)	0.0004(5)	-.0001(5)	0.0004(3)	0.87
Odooi	0.6977(8)	0.6073(5)	0.6829(5)	0.005 (1)	0.0018(4)	0.0011(4)	0.0010(5)	0.0002(6)	0.0002(3)	1.09
Odozo	0.2106(8)	0.1029(5)	0.6843(5)	0.003 (1)	0.0019(4)	0.0014(4)	-.0000(5)	0.0007(5)	0.0002(3)	0.95
Odozi	0.6946(8)	0.6038(4)	0.1986(4)	0.006 (1)	0.0013(3)	0.0009(3)	0.0005(5)	0.0003(5)	-.0000(3)	1.00
Odmoo	0.2023(7)	0.8723(4)	0.2108(4)	0.002 (1)	0.0012(3)	0.0011(3)	-.0009(5)	-.0006(5)	-.0005(3)	npd
Odmoi	0.6915(8)	0.3638(5)	0.7292(5)	0.004 (1)	0.0022(4)	0.0018(4)	0.0010(5)	-.0008(5)	0.0000(3)	1.47
Odmzo	0.1762(9)	0.8590(5)	0.7181(5)	0.007 (1)	0.0017(4)	0.0016(4)	-.0001(5)	0.0003(6)	-.0002(3)	1.38
Odmzi	0.6956(9)	0.3664(5)	0.2026(5)	0.006 (1)	0.0024(4)	0.0022(4)	0.0018(6)	-.0007(6)	-.0006(3)	1.79

Table 2: Positional and thermal parameters from $\text{I}\bar{1}$ refinement of Val Paseda.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mo _{oo}	0.2654(2)	0.9859(2)	0.0872(2)	0.0027(3)	0.0028(1)	0.0014(1)	-0.0002(1)	0.0008(2)	-0.0007(1)	1.14
Mz _{oo}	0.2682(3)	0.0303(5)	0.5446(6)	0.0027(3)	0.0017(2)	0.0015(2)	0.0006(1)	0.0004(2)	-0.0003(2)	0.97
Mo _{io}	0.7735(2)	0.5357(1)	0.5415(1)	0.0029(3)	0.0017(1)	0.0012(1)	0.0005(1)	0.0003(1)	-0.0002(1)	0.92
Mz _{io}	0.7633(4)	0.5027(7)	0.0775(8)	0.0026(4)	0.0023(3)	0.0014(3)	0.0006(2)	0.0007(2)	-0.0004(2)	1.03
Tl _{oo}	0.0079(2)	0.1575(1)	0.1041(1)	0.0025(2)	0.0009(1)	0.0009(1)	-0.0003(1)	0.0006(1)	-0.0000(1)	0.58
Tl _{oz}	0.0028(2)	0.1634(1)	0.6120(1)	0.0035(2)	0.0010(1)	0.0008(1)	-0.0001(1)	0.0008(1)	0.0002(1)	0.66
Tl _{mo}	0.9995(2)	0.8149(1)	0.1195(1)	0.0039(2)	0.0010(1)	0.0009(1)	0.0003(1)	0.0009(1)	0.0001(1)	0.67
Tl _{mz}	0.0054(2)	0.8178(1)	0.6117(1)	0.0029(2)	0.0012(1)	0.0008(1)	0.0002(1)	0.0006(1)	-0.0000(1)	0.64
T2 _{oo}	0.6877(2)	0.1121(1)	0.1595(1)	0.0027(2)	0.0009(1)	0.0009(1)	-0.0002(1)	0.0011(1)	-0.0002(1)	0.93
T2 _{oz}	0.6762(2)	0.1051(1)	0.6569(1)	0.0027(2)	0.0008(1)	0.0023(1)	-0.0002(1)	0.0013(1)	-0.0002(1)	0.86
T2 _{mo}	0.6750(2)	0.8811(1)	0.1805(1)	0.0026(2)	0.0009(1)	0.0020(1)	0.0001(1)	0.0005(1)	0.0003(1)	0.89
T2 _{mz}	0.6834(2)	0.8746(1)	0.6770(1)	0.0024(2)	0.0009(1)	0.0013(1)	0.0004(1)	0.0006(1)	0.0004(1)	0.67
Oa _{1o}	0.0061(5)	0.1241(2)	-0.0093(2)	0.0145(8)	0.0014(2)	0.0012(2)	0.0006(3)	0.0034(3)	0.0002(1)	1.46
Oa _{1z}	0.9993(5)	0.1248(2)	0.4901(2)	0.0117(8)	0.0013(2)	0.0018(2)	-0.0001(3)	0.0035(3)	-0.0000(1)	1.34
Oa _{2o}	0.5739(4)	0.9894(2)	0.1389(2)	0.0023(5)	0.0007(2)	0.0020(2)	0.0004(2)	0.0007(3)	0.0004(1)	0.80
Oa _{2z}	0.5718(4)	0.9908(2)	0.6376(2)	0.0029(5)	0.0007(2)	0.0018(2)	-0.0001(2)	0.0008(3)	0.0001(1)	0.78
Ob _{oo}	0.8232(4)	0.0985(2)	0.0926(3)	0.0057(6)	0.0015(2)	0.0051(3)	-0.0013(3)	0.0041(3)	-0.0012(2)	1.70
Ob _{oz}	0.7990(5)	0.0999(2)	0.5927(3)	0.0076(7)	0.0016(2)	0.0054(3)	-0.0017(3)	0.0051(4)	-0.0011(2)	1.82
Ob _{mo}	0.8074(5)	0.8552(3)	0.1269(3)	0.0055(6)	0.0019(2)	0.0086(4)	0.0007(3)	0.0054(4)	0.0001(2)	2.48
Ob _{mz}	0.8254(5)	0.8550(3)	0.6175(3)	0.0094(8)	0.0020(2)	0.0077(3)	0.0016(3)	0.0071(4)	0.0011(2)	2.33
Oc _{oo}	0.0123(4)	0.2782(2)	0.1352(2)	0.0045(6)	0.0013(2)	0.0018(2)	-0.0001(2)	0.0014(3)	-0.0001(1)	0.98
Oc _{oz}	0.0142(4)	0.2932(2)	0.6486(2)	0.0055(6)	0.0012(2)	0.0018(2)	-0.0007(2)	0.0013(3)	0.0000(1)	1.08
Oc _{mo}	0.0081(4)	0.6796(2)	0.1071(2)	0.0045(6)	0.0009(2)	0.0017(2)	0.0002(2)	0.0009(3)	-0.0001(1)	0.93
Oc _{mz}	0.0077(4)	0.6922(2)	0.5992(2)	0.0041(5)	0.0012(2)	0.0016(2)	0.0002(2)	0.0007(3)	-0.0000(1)	0.95
Od _{oo}	0.1920(4)	0.1069(2)	0.1854(3)	0.0050(6)	0.0019(2)	0.0021(2)	0.0008(3)	-0.0012(3)	-0.0002(2)	1.57
Od _{oz}	0.2019(5)	0.1032(2)	0.6919(3)	0.0067(7)	0.0013(2)	0.0026(2)	0.0004(3)	-0.0023(3)	0.0002(2)	1.89
Od _{mo}	0.1970(5)	0.8685(3)	0.2208(3)	0.0045(6)	0.0023(2)	0.0042(3)	0.0009(3)	-0.0026(3)	-0.0015(2)	2.40
Od _{mz}	0.1868(5)	0.8637(3)	0.7077(3)	0.0096(8)	0.0028(2)	0.0040(3)	0.0027(3)	-0.0041(4)	-0.0023(2)	3.15

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

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mo _{oo}	0.2659(3)	0.9861(2)	0.0869(2)	0.0020(4)	0.0029(2)	0.0015(2)	-0.0002(2)	0.0007(2)	-0.0009(1)	1.15
Mz _{oo}	0.2681(4)	0.0304(6)	0.5450(8)	0.0020(3)	0.0017(2)	0.0013(3)	0.0008(2)	0.0001(2)	-0.0003(2)	0.88
Mo _{io}	0.7735(3)	0.5353(2)	0.5422(2)	0.0023(4)	0.0015(1)	0.0013(1)	0.0006(2)	0.0004(2)	-0.0002(1)	0.83
Mz _{io}	0.7637(5)	0.503 (1)	0.077 (1)	0.0026(5)	0.0023(4)	0.0011(4)	0.0006(3)	0.0002(3)	-0.0007(3)	1.03
Tl _{oo}	0.0080(2)	0.1577(1)	0.1042(1)	0.0025(3)	0.0009(1)	0.0007(1)	-0.0000(8)	0.0007(1)	0.0000(1)	0.51
Tl _{oz}	0.0028(2)	0.1635(1)	0.6119(1)	0.0024(2)	0.0009(1)	0.0008(1)	-0.0002(1)	0.0007(1)	-0.0000(1)	0.55
Tl _{mo}	-0.0004(2)	0.8148(1)	0.1194(1)	0.0034(2)	0.0008(1)	0.0007(1)	0.0002(1)	0.0008(1)	-0.0000(1)	0.55
Tl _{mz}	0.0052(2)	0.8178(1)	0.6116(1)	0.0024(3)	0.0009(1)	0.0007(1)	0.0005(1)	0.0005(1)	0.0000(1)	0.52
T2 _{oo}	0.6882(2)	0.1123(1)	0.1595(1)	0.0022(3)	0.0008(1)	0.0019(1)	0.0001(1)	0.0009(1)	-0.0001(1)	0.76
T2 _{oz}	0.6764(2)	0.1052(1)	0.6572(1)	0.0022(3)	0.0007(1)	0.0020(1)	-0.0003(1)	0.0012(1)	-0.0003(1)	0.74
T2 _{mo}	0.6754(2)	0.8813(1)	0.1806(1)	0.0013(2)	0.0007(1)	0.0018(1)	0.0003(1)	0.0005(1)	0.0003(1)	0.74
T2 _{mz}	0.6838(2)	0.8749(1)	0.6772(1)	0.0021(2)	0.0009(1)	0.0011(1)	0.0004(1)	0.0005(1)	0.0003(1)	0.60
Oa _{1o}	0.0071(56)	0.1244(3)	-0.0094(3)	0.0101(9)	0.0015(2)	0.0010(2)	-0.0002(3)	0.0023(3)	-0.0001(2)	1.18
Oa _{1z}	-0.0011(6)	0.1253(3)	0.4902(3)	0.0114(9)	0.0012(2)	0.0018(2)	0.0001(3)	0.0036(4)	-0.0000(2)	1.27
Oa _{2o}	0.5743(5)	0.9893(2)	0.1391(3)	0.0016(7)	0.0009(2)	0.0016(2)	0.0001(3)	0.0003(3)	0.0003(2)	0.72
Oa _{2z}	0.5728(5)	-0.0094(2)	0.6382(3)	0.0020(7)	0.0008(2)	0.0016(2)	0.0008(3)	0.0007(3)	0.0002(1)	0.70
Ob _{oo}	0.8226(6)	0.0988(3)	0.0922(3)	0.0053(7)	0.0010(2)	0.0047(3)	-0.0007(3)	0.0039(4)	-0.0010(2)	1.47
Ob _{oz}	0.7994(6)	0.1005(3)	0.5934(3)	0.0059(8)	0.0016(2)	0.0047(3)	-0.0015(3)	0.0044(4)	-0.0012(2)	1.56
Ob _{mo}	0.8072(6)	0.8555(3)	0.1266(4)	0.0071(9)	0.0018(2)	0.0083(4)	0.0000(4)	0.0065(5)	-0.0009(3)	2.40
Ob _{mz}	0.8247(5)	0.8553(3)	0.6170(3)	0.0081(9)	0.0022(2)	0.0060(4)	0.0022(4)	0.0062(5)	0.0012(2)	1.95
Oc _{oo}	0.0124(5)	0.2783(2)	0.1356(3)	0.0035(7)	0.0008(2)	0.0015(2)	-0.0003(3)	0.0009(3)	-0.0003(1)	0.78
Oc _{oz}	0.0141(5)	0.2935(3)	0.6485(3)	0.0050(7)	0.0008(2)	0.0021(2)	-0.0008(3)	0.0015(3)	-0.0004(2)	1.01
Oc _{mo}	0.0076(5)	0.6800(2)	0.1072(3)	0.0049(7)	0.0008(2)	0.0018(2)	0.0004(2)	0.0012(3)	0.0001(1)	0.93
Oc _{mz}	0.0083(5)	0.6921(2)	0.6001(3)	0.0038(7)	0.0013(2)	0.0012(2)	0.0004(2)	0.0004(3)	-0.0004(1)	0.89
Od _{oo}	0.1919(5)	0.1066(2)	0.1855(3)	0.0038(6)	0.0017(2)	0.0017(2)	0.0012(3)	-0.0013(3)	-0.0000(2)	1.32
Od _{oz}	0.2042(6)	0.1034(3)	0.6926(3)	0.0073(9)	0.0014(2)	0.0023(2)	0.0003(3)	-0.0013(4)	0.0003(2)	1.76
Od _{mo}	0.1973(6)	0.8684(3)	0.2207(3)	0.0040(6)	0.0024(2)	0.0038(3)	0.0007(3)	-0.0019(3)	-0.0016(2)	2.20
Od _{mz}	0.1864(6)	0.8629(3)	0.7083(3)	0.0070(9)	0.0029(3)	0.0035(3)	0.0022(4)	-0.0042(4)	-0.0020(2)	2.81

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

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mo _{oo}	0.2658(2)	0.9859(2)	0.0865(2)	0.0036(3)	0.0038(2)	0.0019(1)	-0.0002(2)	0.0013(2)	-0.0011(1)	1.50
Mz _{oo}	0.2681(3)	0.0301(4)	0.5459(5)	0.0033(2)	0.0020(1)	0.0016(2)	0.0007(1)	0.0007(1)	-0.0003(1)	1.08
Mo _{io}	0.7737(2)	0.5350(2)	0.5429(2)	0.0034(3)	0.0020(1)	0.0015(1)	0.0009(1)	0.0007(2)	-0.0003(1)	1.06
Mz _{io}	0.7636(5)	0.502 (1)	0.077 (1)	0.0029(5)	0.0025(4)	0.0017(4)	0.0006(3)	0.0010(3)	-0.0006(3)	1.13
Tl _{oo}	0.0078(1)	0.1580(1)	0.1042(1)	0.0027(2)	0.0010(1)	0.0008(1)	-0.0001(1)	0.0008(1)	0.0001(1)	0.58
Tl _{oz}	0.0025(2)	0.1642(1)	0.6119(1)	0.0028(2)	0.0010(1)	0.0008(1)	-0.0002(1)	0.0008(1)	-0.0000(1)	0.57
Tl _{mo}	-0.0001(2)	0.8151(1)	0.1194(1)	0.0038(2)	0.0010(1)	0.0008(1)	0.0005(1)	0.0011(1)	0.0001(1)	0.62
Tl _{mz}	0.0054(1)	0.8176(1)	0.6120(1)	0.0029(2)	0.0010(1)	0.0008(1)	0.0005(1)	0.0007(1)	0.0001(1)	0.58
T2 _{oo}	0.6879(2)	0.1120(1)	0.1588(1)	0.0025(2)	0.0008(1)	0.0019(1)	0.0001(1)	0.0010(1)	0.0000(1)	0.76
T2 _{oz}	0.6765(1)	0.1054(1)	0.6577(1)	0.0026(2)	0.0009(1)	0.0018(1)	-0.0000(1)	0.0012(1)	-0.0002(1)	0.76
T2 _{mo}	0.6760(1)	0.8815(1)	0.1813(1)	0.0025(2)	0.0009(1)	0.0017(1)	0.0003(1)	0.0006(1)	0.0003(1)	0.76
T2 _{mz}	0.6831(2)	0.8748(1)	0.6766(1)	0.0029(2)	0.0009(1)	0.0012(1)	0.0004(1)	0.0011(1)	0.0003(1)	0.64
Oa _{1o}	0.0076(4)	0.1247(2)	-0.0087(2)	0.0110(7)	0.0018(2)	0.0011(2)	0.0009(3)	0.0027(3)	0.0002(1)	1.31
Oa _{1z}	-0.0035(4)	0.1248(2)	0.4893(2)	0.0115(7)	0.0015(2)	0.0016(2)	0.0002(3)	0.0036(3)	0.0001(1)	1.31
Oa _{2o}	0.5756(4)	0.9901(2)	0.1396(2)	0.0035(5)	0.0010(1)	0.0018(2)	0.0004(2)	0.0012(2)	0.0003(1)	0.85
Oa _{2z}	0.5717(3)	0.9910(2)	0.6376(2)	0.0019(4)	0.0009(1)	0.0016(2)	0.0002(2)	0.0007(2)	0.0002(1)	0.70
Ob _{oo}	0.8216(4)	0.0994(2)	0.0910(3)	0.0052(5)	0.0015(2)	0.0043(2)	-0.0009(2)	0.0038(3)	-0.0007(2)	1.47
Ob _{oz}	0.7994(4)	0.1006(2)	0.5936(3)	0.0071(6)	0.0015(2)	0.0051(2)	-0.0008(2)	0.0053(3)	-0.0009(2)	1.65
Ob _{mo}	0.8088(4)	0.8549(2)	0.1282(3)	0.0061(6)	0.0021(2)	0.0074(3)	0.0005(3)	0.0052(4)	-0.0005(2)	2.29
Ob _{mz}	0.8224(4)	0.8550(2)	0.6153(3)	0.0083(6)	0.0024(2)	0.0062(3)	0.0013(3)	0.0062(4)	0.0007(2)	2.06
Oc _{oo}	0.0120(4)	0.2787(2)	0.1353(2)	0.0051(5)	0.0009(1)	0.0021(2)	-0.0004(2)	0.0018(3)	-0.0004(1)	0.99
Oc _{oz}	0.0144(4)	0.2941(2)	0.6484(2)	0.0045(5)	0.0013(2)	0.0019(2)	-0.0004(2)	0.0014(2)	-0.0001(1)	1.02
Oc _{mo}	0.0076(4)	0.6799(2)	0.1073(2)	0.0047(5)	0.0010(1)	0.0016(2)	0.0008(2)	0.0011(2)	0.0002(1)	0.92
Oc _{mz}	0.0078(4)	0.6920(2)	0.5995(2)	0.0059(5)	0.0012(2)	0.0015(2)	0.0005(2)	0.0010(3)	-0.0000(1)	1.04
Od _{oo}	0.1910(4)	0.1065(2)	0.1869(2)	0.0046(5)	0.0017(2)	0.0019(2)	0.0007(2)	-0.0004(3)	0.0002(1)	1.34
Od _{oz}	0.2029(4)	0.1035(2)	0.6915(2)	0.0063(6)	0.0016(2)	0.0024(2)	0.0005(2)	-0.0010(3)	0.0003(1)	1.66
Od _{mo}	0.1976(4)	0.8685(2)	0.2193(3)	0.0040(5)	0.0022(2)	0.0033(2)	0.0007(3)	-0.0018(3)	-0.0010(2)	2.01
Od _{mz}	0.1854(5)	0.8625(3)	0.7105(3)	0.0088(7)	0.0027(2)	0.0036(2)	0.0018(3)	-0.0020(3)	-0.0013(2)	2.64

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

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M _{ooo}	0.2667(3)	0.9850(3)	0.0869(2)	0.0031(5)	0.0048(2)	0.0027(1)	-0.0013(2)	0.0011(2)	-0.0019(2)	1.97
M _{zoo}	0.2674(3)	0.0298(5)	0.5465(6)	0.0028(3)	0.0019(2)	0.0017(2)	0.0005(1)	0.0004(2)	-0.0003(2)	1.07
M _{oio}	0.7743(4)	0.5345(3)	0.5446(3)	0.0046(6)	0.0020(2)	0.0020(2)	0.0007(2)	0.0007(3)	-0.0007(2)	1.29
M _{zio}	0.765 (1)	0.500 (2)	0.078 (2)	0.004 (1)	0.0034(8)	0.0016(7)	0.0003(6)	0.0010(6)	-0.0008(7)	1.49
T _{1oo}	0.0075(2)	0.1582(1)	0.1041(1)	0.0027(3)	0.0010(1)	0.0008(1)	-0.0004(1)	0.0005(1)	0.0000(1)	0.62
T _{1oz}	0.0022(2)	0.1645(1)	0.6112(1)	0.0036(3)	0.0010(1)	0.0009(1)	-0.0001(1)	0.0008(1)	0.0001(1)	0.66
T _{1mo}	-0.0004(2)	0.8155(1)	0.1190(1)	0.0034(3)	0.0010(1)	0.0010(1)	0.0000(1)	0.0008(1)	-0.0000(1)	0.69
T _{1mz}	0.0054(2)	0.8174(1)	0.6121(1)	0.0034(3)	0.0011(1)	0.0009(1)	0.0003(1)	0.0006(1)	0.0001(1)	0.69
T _{2oo}	0.6875(2)	0.1117(1)	0.1576(1)	0.0032(3)	0.0009(1)	0.0015(1)	0.0001(1)	0.0005(1)	0.0001(1)	0.82
T _{2oz}	0.6777(2)	0.1057(1)	0.6588(1)	0.0027(3)	0.0007(1)	0.0017(1)	-0.0002(1)	0.0008(1)	-0.0001(1)	0.76
T _{2mo}	0.6770(2)	0.8815(1)	0.1820(1)	0.0026(3)	0.0006(1)	0.0015(1)	0.0000(1)	0.0004(1)	0.0002(1)	0.70
T _{2mz}	0.6830(2)	0.8750(1)	0.6758(1)	0.0032(3)	0.0009(1)	0.0014(1)	0.0002(1)	0.0009(1)	0.0002(1)	0.74
O _{a1o}	0.0108(5)	0.1251(3)	-0.0079(3)	0.0083(8)	0.0019(2)	0.0011(2)	-0.0002(3)	0.0017(3)	-0.0000(2)	1.22
O _{a1z}	0.9929(5)	0.1263(3)	0.4884(3)	0.0093(9)	0.0016(2)	0.0017(2)	0.0008(3)	0.0027(4)	0.0002(2)	1.26
O _{a2o}	0.5774(4)	0.9901(2)	0.1402(3)	0.0037(7)	0.0011(2)	0.0018(2)	0.0003(3)	0.0005(3)	0.0002(2)	0.97
O _{a2z}	0.5728(5)	0.9908(2)	0.6372(3)	0.0028(7)	0.0005(2)	0.0021(2)	-0.0002(3)	0.0007(3)	0.0002(2)	0.84
O _{boo}	0.8193(5)	0.1006(3)	0.0899(3)	0.0044(8)	0.0015(2)	0.0034(3)	-0.0013(3)	0.0028(4)	-0.0007(2)	1.29
O _{boz}	0.8016(5)	0.1011(3)	0.5962(3)	0.0056(8)	0.0013(2)	0.0042(3)	-0.0001(3)	0.0039(4)	-0.0005(2)	1.40
O _{bmo}	0.8104(6)	0.8552(3)	0.1294(4)	0.0076(9)	0.0022(2)	0.0062(3)	-0.0001(3)	0.0053(5)	-0.0005(2)	2.13
O _{bmoz}	0.8204(5)	0.8556(3)	0.6133(3)	0.0065(8)	0.0019(2)	0.0046(3)	0.0009(3)	0.0039(4)	0.0003(2)	1.70
O _{coo}	0.0124(5)	0.2791(3)	0.1356(3)	0.0044(7)	0.0011(2)	0.0023(2)	-0.0006(3)	0.0011(3)	-0.0002(2)	1.11
O _{coz}	0.0145(5)	0.2944(3)	0.6480(3)	0.0051(7)	0.0011(2)	0.0023(2)	-0.0008(2)	0.0018(3)	-0.0004(2)	1.09
O _{cmo}	0.0091(5)	0.6805(3)	0.1080(3)	0.0052(7)	0.0010(2)	0.0019(2)	0.0004(3)	0.0010(3)	0.0003(2)	1.06
O _{cmz}	0.0086(5)	0.6914(3)	0.5996(3)	0.0067(8)	0.0010(2)	0.0016(2)	0.0002(3)	0.0008(3)	-0.0001(2)	1.15
O _{doo}	0.1893(5)	0.1061(3)	0.1878(3)	0.0042(7)	0.0020(2)	0.0014(2)	-0.0000(3)	-0.0007(3)	-0.0000(2)	1.29
O _{doz}	0.2038(6)	0.1038(3)	0.6902(3)	0.0074(8)	0.0013(3)	0.0025(2)	0.0003(3)	-0.0001(4)	0.0003(2)	1.63
O _{dmo}	0.2002(5)	0.8687(3)	0.2181(3)	0.0050(8)	0.0018(2)	0.0030(3)	-0.0002(3)	-0.0014(4)	-0.0010(2)	1.86
O _{dmoz}	0.1820(6)	0.8620(3)	0.7125(3)	0.0082(9)	0.0024(3)	0.0027(3)	-0.0000(4)	-0.0017(4)	-0.0010(2)	2.23

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

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M _{ooo}	0.2673(3)	0.9853(3)	0.0865(2)	0.0045(4)	0.0050(2)	0.0025(2)	-0.0009(2)	0.0016(2)	-0.0019(2)	2.03
M _{zoo}	0.2674(3)	0.0294(3)	0.5468(5)	0.0036(3)	0.0022(2)	0.0015(2)	0.0009(1)	0.0004(1)	-0.0004(1)	1.16
M _{oio}	0.7747(4)	0.5345(3)	0.5450(3)	0.0035(5)	0.0025(2)	0.0019(2)	0.0007(2)	0.0007(2)	-0.0005(2)	1.29
M _{zio}	0.764 (1)	0.498 (2)	0.079 (2)	0.006 (1)	0.0059(9)	0.0019(8)	0.0003(6)	0.0012(5)	-0.0008(7)	2.20
T _{1oo}	0.0074(2)	0.1586(1)	0.1043(1)	0.0037(2)	0.0012(1)	0.0009(1)	-0.0004(1)	0.0009(1)	0.0000(1)	0.70
T _{1oz}	0.0028(2)	0.1648(1)	0.6112(1)	0.0029(2)	0.0011(1)	0.0009(1)	-0.0002(1)	0.0007(1)	-0.0001(1)	0.64
T _{1mo}	-0.0005(2)	0.8156(1)	0.1189(1)	0.0039(3)	0.0012(1)	0.0009(1)	0.0004(1)	0.0009(1)	0.0000(1)	0.73
T _{1mz}	0.0054(2)	0.8174(1)	0.6123(1)	0.0033(2)	0.0012(1)	0.0007(1)	0.0004(1)	0.0007(1)	-0.0000(1)	0.66
T _{2oo}	0.6878(2)	0.1118(1)	0.1573(1)	0.0036(3)	0.0009(1)	0.0014(1)	-0.0001(1)	0.0008(1)	0.0000(1)	0.78
T _{2oz}	0.6780(2)	0.1060(1)	0.6589(1)	0.0031(2)	0.0010(1)	0.0015(1)	-0.0001(1)	0.0009(1)	-0.0001(1)	0.78
T _{2mo}	0.6774(2)	0.8817(1)	0.1820(1)	0.0033(2)	0.0009(1)	0.0015(1)	0.0001(1)	0.0006(1)	0.0002(1)	0.79
T _{2mz}	0.6832(2)	0.8751(1)	0.6756(1)	0.0047(3)	0.0015(1)	0.0018(1)	0.0001(1)	0.0013(1)	0.0002(1)	1.07
O _{a1o}	0.0113(5)	0.1263(3)	-0.0075(3)	0.0091(8)	0.0020(2)	0.0012(2)	-0.0005(3)	0.0020(3)	0.0001(2)	1.31
O _{a1z}	-0.0077(5)	0.1265(3)	0.4878(3)	0.0105(8)	0.0022(2)	0.0013(2)	0.0007(3)	0.0026(3)	0.0004(2)	1.41
O _{a2o}	0.5772(4)	0.9899(2)	0.1402(2)	0.0042(6)	0.0010(2)	0.0018(2)	0.0005(3)	0.0010(3)	0.0003(2)	0.94
O _{a2z}	0.5735(4)	0.9918(2)	0.6373(2)	0.0023(6)	0.0012(2)	0.0018(2)	-0.0002(3)	0.0006(3)	0.0002(2)	0.87
O _{boo}	0.8193(5)	0.1009(3)	0.0903(3)	0.0054(7)	0.0020(2)	0.0031(2)	-0.0010(3)	0.0027(3)	-0.0006(2)	1.39
O _{boz}	0.8022(5)	0.1021(2)	0.5960(3)	0.0051(7)	0.0015(2)	0.0039(3)	-0.0007(3)	0.0032(4)	-0.0005(2)	1.41
O _{bmo}	0.8118(5)	0.8551(3)	0.1304(3)	0.0073(7)	0.0022(2)	0.0060(3)	0.0002(3)	0.0050(4)	-0.0006(2)	2.06
O _{bmoz}	0.8202(5)	0.8549(3)	0.6128(3)	0.0054(7)	0.0025(2)	0.0045(3)	0.0009(3)	0.0038(4)	-0.0000(2)	1.72
O _{coo}	0.0115(5)	0.2800(2)	0.1352(3)	0.0059(7)	0.0014(2)	0.0021(2)	-0.0010(3)	0.0017(3)	-0.0005(2)	1.19
O _{coz}	0.0155(5)	0.2950(2)	0.6479(3)	0.0053(6)	0.0013(2)	0.0023(2)	-0.0006(3)	0.0015(3)	-0.0002(2)	1.18
O _{cmo}	0.0091(4)	0.6807(3)	0.1082(3)	0.0046(6)	0.0020(2)	0.0014(2)	0.0001(3)	0.0005(3)	-0.0003(2)	1.16
O _{cmz}	0.0094(5)	0.6914(3)	0.6005(3)	0.0072(7)	0.0014(2)	0.0020(2)	0.0012(3)	0.0014(3)	0.0000(2)	1.30
O _{doo}	0.1900(5)	0.1068(3)	0.1882(3)	0.0058(7)	0.0020(2)	0.0014(2)	0.0005(3)	-0.0001(3)	0.0002(2)	1.36
O _{doz}	0.2046(5)	0.1047(3)	0.6905(3)	0.0066(7)	0.0016(2)	0.0017(2)	0.0003(3)	-0.0005(3)	0.0001(2)	1.48
O _{dmo}	0.1993(5)	0.8691(3)	0.2178(3)	0.0060(7)	0.0021(2)	0.0025(2)	0.0002(3)	-0.0012(3)	-0.0007(2)	1.86
O _{dmoz}	0.1836(5)	0.8615(3)	0.7129(3)	0.0078(8)	0.0022(2)	0.0026(2)	0.0004(3)	-0.0014(3)	-0.0008(2)	2.08

Table 2: Positional and thermal parameters from $\bar{I}\bar{I}$ refinement of 101377a.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M _{oo}	0.2677(2)	0.9836(2)	0.0862(2)	0.0051(3)	0.0069(2)	0.0033(1)	-0.0017(2)	0.0021(2)	-0.0027(1)	2.68
M _{zo}	0.2683(3)	0.0297(2)	0.5469(4)	0.0037(2)	0.0025(1)	0.0015(1)	0.0008(1)	0.0005(1)	-0.0005(1)	1.24
M _{io}	0.7753(2)	0.5339(2)	0.5460(2)	0.0042(3)	0.0026(1)	0.0022(1)	0.0010(1)	0.0008(1)	-0.0005(1)	1.45
M _{zi}	0.7640(6)	0.498 (2)	0.077 (1)	0.0040(5)	0.0085(8)	0.0029(4)	-0.0003(4)	0.0012(3)	-0.0027(6)	2.92
T _{1oo}	0.0077(1)	0.1596(1)	0.1045(1)	0.0036(1)	0.0014(1)	0.0010(1)	-0.0004(1)	0.0008(1)	0.0000(1)	0.78
T _{1oz}	0.0034(1)	0.1650(1)	0.6109(1)	0.0036(2)	0.0012(1)	0.0010(1)	-0.0002(1)	0.0009(1)	0.0001(1)	0.74
T _{1mo}	0.0001(1)	0.8155(1)	0.1186(1)	0.0038(2)	0.0014(1)	0.0009(1)	0.0006(1)	0.0008(1)	0.0001(1)	0.76
T _{1mz}	0.0052(1)	0.8173(1)	0.6128(1)	0.0040(1)	0.0015(1)	0.0010(1)	0.0006(1)	0.0009(1)	0.0000(1)	0.82
T _{2oo}	0.6880(1)	0.1116(1)	0.1579(1)	0.0029(2)	0.0011(1)	0.0014(1)	0.0000(1)	0.0006(1)	0.0001(1)	0.80
T _{2oz}	0.6789(1)	0.1063(1)	0.6587(1)	0.0034(1)	0.0010(1)	0.0016(1)	0.0000(1)	0.0008(1)	-0.0001(1)	0.85
T _{2mo}	0.6777(1)	0.8815(1)	0.1812(1)	0.0035(1)	0.0010(1)	0.0015(1)	0.0003(1)	0.0007(1)	0.0002(1)	0.84
T _{2mz}	0.6834(1)	0.8757(1)	0.6766(1)	0.0034(2)	0.0010(1)	0.0014(1)	0.0002(1)	0.0009(1)	0.0002(1)	0.78
O _{a1o}	0.0092(3)	0.1277(2)	-0.0083(2)	0.0101(5)	0.0023(1)	0.0015(1)	0.0004(2)	0.0025(2)	0.0001(1)	1.47
O _{a1z}	0.9956(3)	0.1269(2)	0.4885(2)	0.0105(5)	0.0025(1)	0.0016(1)	0.0009(2)	0.0026(2)	0.0003(1)	1.54
O _{a2o}	0.5788(3)	0.9908(2)	0.1399(2)	0.0040(4)	0.0014(1)	0.0021(1)	0.0004(2)	0.0011(2)	0.0004(1)	1.08
O _{a2z}	0.5750(3)	0.9914(2)	0.6377(2)	0.0035(4)	0.0012(1)	0.0020(1)	-0.0003(2)	0.0007(2)	0.0001(1)	1.04
O _{boo}	0.8194(3)	0.1019(2)	0.0915(2)	0.0060(4)	0.0018(1)	0.0031(1)	-0.0008(2)	0.0027(2)	-0.0003(1)	1.42
O _{boz}	0.8031(3)	0.1025(2)	0.5955(2)	0.0058(4)	0.0019(1)	0.0036(2)	-0.0007(2)	0.0032(2)	-0.0004(1)	1.50
O _{bmo}	0.8108(3)	0.8542(2)	0.1282(2)	0.0076(5)	0.0025(1)	0.0052(2)	0.0004(2)	0.0045(3)	-0.0006(1)	2.03
O _{b mz}	0.8199(3)	0.8544(2)	0.6153(2)	0.0066(5)	0.0029(1)	0.0044(2)	0.0009(2)	0.0038(2)	-0.0000(1)	1.91
O _{coo}	0.0129(3)	0.2817(2)	0.1362(2)	0.0065(4)	0.0018(1)	0.0026(1)	-0.0004(2)	0.0020(2)	-0.0001(1)	1.39
O _{coz}	0.0144(3)	0.2944(2)	0.6468(2)	0.0054(4)	0.0017(1)	0.0026(1)	-0.0006(2)	0.0015(2)	-0.0000(1)	1.36
O _{cmo}	0.0100(3)	0.6816(2)	0.1084(2)	0.0054(4)	0.0019(1)	0.0019(1)	0.0009(2)	0.0007(2)	-0.0000(1)	1.32
O _{cmz}	0.0100(3)	0.6914(2)	0.6014(2)	0.0078(4)	0.0018(1)	0.0019(1)	0.0013(2)	0.0010(2)	-0.0001(1)	1.45
O _{do}	0.1910(3)	0.1072(2)	0.1885(2)	0.0056(4)	0.0022(1)	0.0016(1)	0.0005(2)	-0.0001(2)	0.0002(1)	1.42
O _{doz}	0.2030(3)	0.1045(2)	0.6914(2)	0.0059(4)	0.0020(1)	0.0018(1)	0.0003(2)	-0.0002(2)	0.0001(1)	1.47
O _{dmo}	0.1967(3)	0.8680(2)	0.2180(2)	0.0060(4)	0.0024(1)	0.0024(1)	0.0003(2)	-0.0009(2)	-0.0007(1)	1.85
O _{d mz}	0.1844(3)	0.8624(2)	0.7129(2)	0.0073(5)	0.0029(2)	0.0027(2)	0.0006(2)	-0.010(2)	-0.0007(1)	2.16

Table 2: Positional and thermal parameters from $\bar{1}\bar{1}$ refinement of Crystal Bay.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2691(9)	0.981 (1)	0.0877(8)	0.004 (1)	0.0064(7)	0.0037(5)	-0.0020(6)	0.0024(6)	-0.0026(6)	2.50
Mzoo	0.268 (1)	0.030 (1)	0.546 (2)	0.002 (1)	0.0025(6)	0.0007(5)	0.0015(4)	-0.0010(5)	-0.0001(3)	npd
Moio	0.775 (1)	0.5331(8)	0.5472(8)	0.008 (1)	0.0032(6)	0.0037(6)	-0.0001(6)	0.0023(7)	-0.0013(4)	2.16
Mzio	0.765 (2)	0.502 (6)	0.073 (4)	0.009 (2)	0.010 (3)	0.004 (2)	0.002 (1)	0.000 (1)	-0.003 (2)	4.03
T1oo	0.0074(5)	0.1593(2)	0.1043(3)	0.0047(6)	0.0014(2)	0.0013(2)	-0.0003(2)	0.0012(3)	-0.0007(1)	0.94
T1oz	0.0036(5)	0.1662(2)	0.6109(3)	0.0037(6)	0.0015(2)	0.0006(2)	-0.0003(3)	0.0007(3)	0.0006(1)	0.71
T1mo	0.0001(5)	0.8163(2)	0.1181(3)	0.0042(7)	0.0012(2)	0.0007(2)	0.0006(3)	0.0009(3)	0.0003(1)	0.68
T1mz	0.0059(5)	0.8167(2)	0.6130(3)	0.0040(7)	0.0021(2)	0.0015(2)	0.0004(3)	0.00009(3)	-0.0003(2)	1.10
T2oo	0.6889(5)	0.1113(2)	0.1590(3)	0.0030(7)	0.0008(2)	0.0019(2)	0.0006(3)	0.0012(3)	0.0004(2)	0.77
T2oz	0.6792(5)	0.1062(2)	0.6580(2)	0.0037(6)	0.0018(2)	0.0014(2)	-0.0007(3)	0.0004(3)	-0.0006(2)	1.06
T2mo	0.6791(5)	0.8810(3)	0.1811(3)	0.0027(6)	0.0016(2)	0.0022(2)	-0.0002(3)	0.0013(3)	0.0001(2)	0.99
T2mz	0.6828(5)	0.8763(2)	0.6768(3)	0.0052(7)	0.0010(2)	0.0008(2)	0.0007(3)	0.0006(3)	0.0003(1)	0.80
Oa1o	0.007 (1)	0.1279(6)	-0.085(6)	0.012 (2)	0.0017(5)	0.0008(5)	0.0004(7)	0.0015(6)	0.0001(4)	1.50
Oa1z	-0.002 (1)	0.1283(7)	0.4885(7)	0.009 (2)	0.0044(7)	0.0026(6)	0.0011(9)	0.0035(9)	0.0003(5)	2.00
Oa2o	0.580 (1)	-0.0094(5)	0.1399(6)	0.002 (2)	0.0012(4)	0.0020(5)	0.0011(6)	-0.0001(7)	0.0003(4)	1.00
Oa2z	0.577 (1)	-0.0079(6)	0.6379(6)	0.007 (2)	0.0020(5)	0.0022(6)	-0.0013(7)	0.0024(9)	0.0001(4)	1.37
Oboo	0.820 (1)	0.1029(6)	0.0916(7)	0.008 (2)	0.0020(5)	0.0041(6)	-0.0010(7)	0.0045(9)	-0.0006(4)	1.65
Oboz	0.803 (1)	0.1029(6)	0.5966(7)	0.005 (1)	0.0018(4)	0.0031(5)	-0.0006(6)	0.0024(8)	-0.0001(4)	1.38
Obmo	0.815 (1)	0.8528(6)	0.1291(8)	0.010 (2)	0.0022(5)	0.0065(8)	-0.0019(8)	0.005 (1)	-0.0019(5)	2.53
Obmz	0.816 (1)	0.8545(6)	0.6166(7)	0.007 (2)	0.0034(5)	0.0036(5)	0.0023(8)	0.0033(8)	0.0010(4)	1.83
Ocoo	0.014 (1)	0.2842(6)	0.1367(7)	0.007 (2)	0.0028(5)	0.0027(5)	0.0001(7)	0.0029(9)	-0.0001(4)	1.61
Ocoz	0.014 (1)	0.2938(6)	0.6457(6)	0.006 (2)	0.0021(5)	0.0024(5)	-0.0010(7)	0.0012(8)	0.0006(4)	1.49
Ocmo	0.012 (1)	0.6810(6)	0.1091(7)	0.006 (2)	0.0017(4)	0.0023(5)	0.0004(6)	0.0006(7)	0.0001(4)	1.43
Ocmz	0.013 (1)	0.6930(6)	0.6023(6)	0.007 (2)	0.0022(4)	0.0013(4)	0.0018(6)	0.0011(7)	0.0001(3)	1.30
Odoo	0.192 (1)	0.1078(6)	0.1892(6)	0.006 (2)	0.0027(5)	0.0009(5)	-0.0004(7)	-0.0008(8)	0.0001(4)	1.50
Odoz	0.204 (1)	0.1054(6)	0.6916(7)	0.007 (2)	0.0020(5)	0.0029(6)	0.0001(7)	0.0011(9)	-0.0003(4)	1.69
Odmo	0.193 (1)	0.8688(6)	0.2174(7)	0.008 (2)	0.0035(6)	0.0023(6)	0.0005(9)	-0.0005(9)	0.0003(5)	2.16
Odmz	0.188 (1)	0.8636(6)	0.7134(7)	0.006 (2)	0.0020(5)	0.0027(6)	-0.0001(7)	-0.0016(9)	-0.0013(4)	1.97

Table 2: Positional and thermal parameters from $\text{I}\bar{1}$ refinement of Lake County.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2675(5)	0.9834(7)	0.0849(5)	0.0046(7)	0.0083(6)	0.0037(4)	-0.0026(4)	0.0021(4)	-0.0036(4)	3.08
Mzoo	0.2691(4)	0.0291(5)	0.5487(5)	0.0038(4)	0.0031(2)	0.0021(2)	0.0011(2)	0.0003(2)	-0.0007(2)	1.56
Moio	0.7747(5)	0.5329(4)	0.5463(4)	0.0057(6)	0.0033(3)	0.0027(2)	0.0016(3)	0.0012(3)	-0.0007(2)	1.83
Mzio	0.7649(9)	0.489 (2)	0.081 (1)	0.007 (1)	0.009 (1)	0.0036(6)	0.0003(7)	0.0024(6)	-0.0017(8)	3.33
T1oo	0.0076(2)	0.1607(1)	0.1053(1)	0.0037(3)	0.0014(1)	0.0013(1)	-0.0004(1)	0.0010(1)	-0.0000(1)	0.84
T1oz	0.0043(2)	0.1649(1)	0.6098(1)	0.0041(3)	0.0016(1)	0.0010(1)	-0.0002(1)	0.0008(1)	0.0001(1)	0.87
T1mo	0.0011(2)	0.8156(1)	0.1180(1)	0.0047(3)	0.0016(1)	0.0011(1)	0.0008(1)	0.0012(2)	0.0001(1)	0.91
T1mz	0.0046(2)	0.8170(1)	0.6133(1)	0.0035(3)	0.0017(1)	0.0011(1)	0.0008(1)	0.0007(1)	0.0001(1)	0.88
T2oo	0.6878(2)	0.1109(1)	0.1585(1)	0.0039(3)	0.0012(1)	0.0016(1)	0.0001(1)	0.0009(1)	0.0001(1)	0.92
T2oz	0.6811(2)	0.1068(1)	0.6587(1)	0.0036(3)	0.0013(1)	0.0015(1)	0.00019(1)	0.0009(1)	-0.0000(1)	0.91
T2mo	0.6787(2)	0.8808(1)	0.1802(1)	0.0033(3)	0.0013(1)	0.0014(1)	0.0001(1)	0.0007(1)	0.0002(1)	0.87
T2mz	0.6829(2)	0.8764(1)	0.6774(1)	0.0039(3)	0.0012(1)	0.0015(1)	0.0004(1)	0.0012(2)	0.0003(1)	0.86
Oa1o	0.0072(6)	0.1287(3)	-0.0089(3)	0.0091(9)	0.0028(3)	0.0013(2)	0.0007(4)	0.0017(4)	0.0002(2)	1.53
Oa1z	0.9982(6)	0.1279(3)	0.4889(3)	0.011 (1)	0.0032(3)	0.0019(3)	0.0010(4)	0.0028(5)	0.0006(2)	1.78
Oa2o	0.5802(5)	0.9912(3)	0.1397(3)	0.0049(8)	0.0014(2)	0.0021(3)	0.0008(3)	0.0013(4)	0.0005(2)	1.10
Oa2z	0.5776(5)	0.9914(3)	0.6387(3)	0.0043(8)	0.0015(2)	0.0025(3)	-0.0006(3)	0.0011(4)	0.0002(2)	1.23
Oboo	0.8190(6)	0.1028(3)	0.0930(3)	0.0066(8)	0.0020(2)	0.0033(3)	-0.0007(3)	0.0027(4)	-0.0001(2)	1.57
Oboz	0.8056(6)	0.1034(3)	0.5952(3)	0.0076(8)	0.0019(2)	0.0042(3)	-0.0005(3)	0.0038(4)	-0.0003(2)	1.72
Obmo	0.8108(6)	0.8536(3)	0.1256(4)	0.0090(9)	0.0024(3)	0.0056(4)	0.0003(4)	0.0046(5)	-0.0006(2)	2.22
Obmz	0.8195(6)	0.8537(3)	0.6179(4)	0.0067(8)	0.0038(3)	0.0051(3)	0.0011(4)	0.0038(5)	0.0000(3)	2.29
Ocoo	0.0133(6)	0.2837(3)	0.1371(3)	0.0085(9)	0.0021(2)	0.0029(3)	-0.0006(4)	0.0029(4)	-0.0000(2)	1.62
Ocoz	0.0156(6)	0.2945(3)	0.6454(3)	0.0056(8)	0.0022(2)	0.0028(3)	-0.0006(3)	0.0014(4)	0.0001(2)	1.53
Ocmo	0.0112(6)	0.6825(3)	0.1083(3)	0.0050(8)	0.0027(3)	0.0024(3)	0.0011(3)	0.0010(4)	0.0002(2)	1.55
Ocmz	0.0121(6)	0.6905(3)	0.6028(3)	0.0086(9)	0.0020(2)	0.0021(3)	0.0011(4)	0.0012(4)	-0.0004(2)	1.62
Odoo	0.1937(6)	0.1086(3)	0.1892(3)	0.0063(9)	0.0026(3)	0.0018(2)	0.0000(4)	0.0008(4)	0.0001(2)	1.51
Odoz	0.2008(6)	0.1049(3)	0.6924(3)	0.0080(9)	0.0020(2)	0.0020(2)	0.0008(4)	0.0003(4)	0.0002(2)	1.62
Odmo	0.1934(6)	0.8676(3)	0.2177(3)	0.0075(9)	0.0027(3)	0.0030(3)	0.0008(4)	-0.0000(4)	-0.0001(2)	2.07
Odmz	0.1869(6)	0.8640(3)	0.7133(3)	0.0069(9)	0.0035(3)	0.0019(3)	0.0005(4)	-0.0008(4)	-0.0007(2)	2.03

Table 2: Positional and thermal parameters from $\bar{I}\bar{1}$ refinement of Val Paseda/3.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M _{ooo}	0.2672(5)	0.9855(5)	0.0872(4)	0.0030(7)	0.0047(3)	0.0021(3)	-0.0008(3)	0.0013(3)	-0.0016(3)	1.72
M _{zoo}	0.2689(5)	0.0308(9)	0.546 (1)	0.0025(5)	0.0018(3)	0.0018(4)	0.0003(2)	0.0004(3)	-0.0004(3)	1.05
M _{oio}	0.7740(4)	0.5354(3)	0.5431(3)	0.0031(5)	0.0023(2)	0.0014(2)	0.0012(2)	0.0004(2)	-0.0003(2)	1.10
M _{zio}	0.7633(9)	0.502 (2)	0.077 (2)	0.0026(9)	0.0034(8)	0.0019(7)	0.0006(5)	0.0004(5)	-0.0008(7)	1.45
T _{1oo}	0.0080(3)	0.1576(2)	0.1043(2)	0.0029(4)	0.0011(1)	0.0008(1)	-0.0001(2)	0.0006(2)	-0.0000(1)	0.63
T _{1oz}	0.0028(3)	0.1637(2)	0.6121(2)	0.0025(4)	0.0012(1)	0.0009(1)	-0.0001(2)	0.0007(2)	0.0000(1)	0.64
T _{1mo}	0.9998(3)	0.8148(2)	0.1196(2)	0.0038(4)	0.0011(1)	0.0011(1)	0.0006(2)	0.0012(2)	0.0002(1)	0.72
T _{1mz}	0.0043(3)	0.8175(1)	0.6118(2)	0.0027(4)	0.0010(1)	0.0007(1)	0.0005(2)	0.0003(2)	-0.0000(1)	0.61
T _{2oo}	0.6877(3)	0.1127(2)	0.1594(2)	0.0028(4)	0.0009(1)	0.0017(1)	0.0001(2)	0.0007(2)	-0.0000(1)	0.82
T _{2oz}	0.6764(3)	0.1052(2)	0.6573(2)	0.0025(4)	0.0008(1)	0.0018(1)	-0.0000(2)	0.0010(2)	-0.0002(1)	0.77
T _{2mo}	0.6755(3)	0.8814(2)	0.1809(2)	0.0019(4)	0.0009(1)	0.0016(1)	0.0004(2)	0.0002(2)	0.0002(1)	0.75
T _{2mz}	0.6832(3)	0.8749(2)	0.6774(2)	0.0031(4)	0.0010(1)	0.0014(1)	0.0004(2)	0.0009(2)	0.0004(1)	0.74
O _{a1o}	0.0062(8)	0.1246(4)	-0.0091(4)	0.012 (1)	0.0018(3)	0.0016(3)	0.0010(5)	0.0035(6)	-0.0001(3)	1.41
O _{a1z}	0.9998(8)	0.1259(4)	0.4903(4)	0.012 (1)	0.0019(3)	0.0010(3)	0.0007(5)	0.0026(6)	0.0004(3)	1.38
O _{a2o}	0.5745(7)	0.9895(4)	0.1400(4)	0.0022(9)	0.0010(3)	0.0020(3)	-0.0002(4)	0.0008(5)	0.0000(2)	0.84
O _{a2z}	0.5733(7)	0.9916(4)	0.6379(4)	0.0026(9)	0.0007(3)	0.0021(3)	0.0003(4)	0.0004(5)	0.0002(2)	0.89
O _{boo}	0.8211(8)	0.0990(4)	0.0919(5)	0.005 (1)	0.0015(3)	0.0044(4)	-0.0004(4)	0.0033(6)	-0.0006(3)	1.50
O _{boz}	0.7992(8)	0.1005(4)	0.5925(5)	0.005 (1)	0.0010(3)	0.0049(4)	-0.0010(4)	0.0041(6)	-0.0009(3)	1.50
O _{bmo}	0.8079(9)	0.8563(4)	0.1259(5)	0.007 (1)	0.0019(3)	0.0071(6)	0.0003(5)	0.0051(7)	-0.0005(3)	2.26
O _{bmoz}	0.8235(8)	0.8556(4)	0.6171(5)	0.008 (1)	0.0023(3)	0.0056(5)	0.0018(5)	0.0055(7)	0.0005(3)	1.91
O _{coo}	0.0129(8)	0.2791(4)	0.1368(4)	0.0043(9)	0.0018(3)	0.0020(3)	0.0001(4)	0.0016(5)	-0.0001(3)	1.11
O _{coz}	0.0150(7)	0.2928(4)	0.6491(4)	0.0048(9)	0.0009(3)	0.0022(3)	-0.0004(4)	0.0015(5)	-0.0004(2)	1.03
O _{cmo}	0.0071(8)	0.6799(4)	0.1066(4)	0.004 (1)	0.0017(3)	0.0015(3)	0.0012(4)	0.0000(5)	0.0003(3)	1.13
O _{cmz}	0.0053(8)	0.6911(4)	0.5995(4)	0.0035(9)	0.0013(3)	0.0017(3)	0.0004(4)	0.0007(5)	-0.0003(2)	0.97
O _{do}	0.1916(8)	0.1060(4)	0.1858(4)	0.004 (1)	0.0014(3)	0.0020(3)	0.0004(4)	-0.0007(5)	0.0003(3)	1.28
O _{doz}	0.2019(8)	0.1027(4)	0.6925(4)	0.005 (1)	0.0022(3)	0.0018(3)	0.0007(5)	-0.0015(5)	-0.0004(3)	1.66
O _{dmo}	0.1964(9)	0.8680(4)	0.2209(5)	0.004 (1)	0.0023(3)	0.0038(4)	0.0010(5)	-0.0027(6)	-0.0016(3)	2.32
O _{dmoz}	0.1863(9)	0.8627(4)	0.7084(5)	0.010 (1)	0.0020(3)	0.0040(4)	0.0017(6)	-0.0021(6)	-0.0011(3)	2.71

Table 2: Positional and thermal parameters from $\bar{1}\bar{1}$ refinement of Val Pasmaeda/6.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2662(7)	0.9852(7)	0.0859(5)	0.0030(9)	0.0070(6)	0.0019(3)	-0.0012(5)	0.0005(4)	-0.0021(4)	2.32
Mzoo	0.271 (1)	0.0307(8)	0.547 (1)	0.0009(8)	0.0021(4)	0.0020(4)	0.0003(3)	0.0001(3)	-0.0005(3)	1.07
Moio	0.7742(5)	0.5361(3)	0.5438(3)	0.0051(6)	0.0021(2)	0.0013(2)	0.0010(3)	0.0007(3)	-0.0003(2)	1.19
Mzio	0.763 (1)	0.501 (4)	0.075 (4)	0.006 (1)	0.007 (2)	0.005 (1)	-0.0007(9)	0.0029(9)	-0.004 (1)	2.92
T1oo	0.0072(3)	0.1582(2)	0.1045(2)	0.0026(4)	0.0013(1)	0.0007(1)	-0.0003(2)	0.0004(2)	0.0000(1)	0.65
T1oz	0.0027(4)	0.1638(2)	0.6118(2)	0.0044(5)	0.0012(1)	0.0009(2)	-0.0004(2)	0.0012(2)	-0.0001(1)	0.75
T1mo	0.0004(4)	0.8152(2)	0.1195(2)	0.0036(5)	0.0014(1)	0.0006(1)	0.0002(2)	0.0005(2)	-0.0001(1)	0.71
T1mz	0.0033(4)	0.8170(2)	0.6121(2)	0.0034(5)	0.0012(1)	0.0010(1)	0.0006(2)	0.0006(2)	0.0001(1)	0.74
T2oo	0.6882(4)	0.1124(2)	0.1601(2)	0.0019(5)	0.0011(1)	0.0016(2)	0.0001(2)	0.0002(2)	0.0001(1)	0.82
T2oz	0.6767(4)	0.1061(2)	0.6571(2)	0.0038(4)	0.0008(1)	0.0017(1)	-0.0001(2)	0.0011(2)	-0.0002(1)	0.85
T2mo	0.6766(3)	0.8812(2)	0.1810(2)	0.0026(4)	0.0008(1)	0.0015(1)	0.0003(2)	0.0007(2)	0.0002(1)	0.72
T2mz	0.6825(4)	0.8755(2)	0.6778(2)	0.0033(5)	0.0012(1)	0.0012(1)	0.0003(2)	0.0008(2)	0.0002(1)	0.77
Oa1o	0.0068(9)	0.1248(5)	-0.0098(4)	0.008 (1)	0.0024(4)	0.0005(3)	0.0015(6)	0.0013(6)	0.0003(3)	1.17
Oa1z	0.0002(9)	0.1269(5)	0.4904(5)	0.012 (2)	0.0018(3)	0.0021(4)	-0.0001(6)	0.0035(7)	0.0001(3)	1.52
Oa2o	0.5738(9)	0.9885(4)	0.1396(5)	0.006 (1)	0.0007(3)	0.0016(4)	-0.0002(5)	0.0009(6)	0.0001(3)	0.96
Oa2z	0.5735(8)	0.9919(4)	0.6379(5)	0.001 (1)	0.0011(3)	0.0018(4)	0.0006(5)	0.0001(6)	0.0002(3)	0.81
Oboo	0.8203(9)	0.0989(4)	0.0923(5)	0.004 (1)	0.0013(3)	0.0036(4)	-0.0015(5)	0.0025(6)	-0.0003(3)	1.31
Oboz	0.7992(9)	0.1007(5)	0.5917(5)	0.007 (1)	0.0017(4)	0.0043(5)	-0.0009(5)	0.0039(7)	-0.0007(3)	1.63
Obmo	0.8078(9)	0.8568(5)	0.1252(6)	0.008 (1)	0.0023(4)	0.0055(6)	0.0004(6)	0.0046(8)	-0.0002(4)	2.10
Obmz	0.8206(9)	0.8553(5)	0.6165(6)	0.007 (1)	0.0021(4)	0.0055(5)	0.0009(6)	0.0048(7)	-0.0000(4)	1.92
Ocoo	0.0132(9)	0.2801(5)	0.1369(5)	0.006 (1)	0.0018(3)	0.0022(4)	-0.0008(5)	0.0017(6)	0.0001(3)	1.29
Ocoz	0.0161(9)	0.2924(5)	0.6497(5)	0.005 (1)	0.0015(3)	0.0019(4)	-0.0002(5)	0.0013(5)	-0.0004(3)	1.13
Ocmo	0.0070(9)	0.6808(5)	0.1069(5)	0.005 (1)	0.0018(4)	0.0020(4)	0.0010(5)	0.0007(6)	-0.0004(3)	1.24
Ocmz	0.0065(9)	0.6901(5)	0.6012(5)	0.005 (1)	0.0019(4)	0.0015(4)	0.0007(5)	0.0004(6)	-0.0003(3)	1.21
Odoo	0.1915(9)	0.1063(5)	0.1858(5)	0.007 (1)	0.0023(4)	0.0023(4)	0.0010(6)	0.0010(6)	0.0001(3)	1.61
Odoz	0.2006(9)	0.1026(5)	0.6919(5)	0.003 (1)	0.0018(4)	0.0012(3)	-0.0002(5)	-0.0016(5)	0.0001(3)	1.23
Odmo	0.1965(9)	0.8674(5)	0.2203(5)	0.005 (1)	0.0023(4)	0.0036(5)	0.0003(6)	-0.0018(6)	-0.0006(4)	2.20
Odmz	0.1860(9)	0.8631(5)	0.7101(5)	0.007 (2)	0.0028(4)	0.0028(4)	0.0019(6)	-0.0023(6)	-0.0013(3)	2.35

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

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mo _{oo}	0.2663(4)	0.9851(4)	0.0863(3)	0.0029(5)	0.0060(3)	0.0023(2)	-.0013(3)	0.0012(3)	-.0024(2)	2.12
Mz _{oo}	0.2688(3)	0.0294(5)	0.5480(7)	0.0025(3)	0.0025(2)	0.0021(3)	0.0007(2)	0.0003(2)	-.0009(2)	1.30
Mo _{io}	0.7741(3)	0.5357(2)	0.5435(2)	0.0043(4)	0.0022(1)	0.0015(1)	0.0007(2)	0.0006(2)	-.0001(1)	1.19
Mz _{io}	0.7631(8)	0.498 (1)	0.080 (1)	0.0044(9)	0.0046(7)	0.0013(5)	-.0007(5)	0.0011(4)	-.0008(5)	1.65
Tl _{oo}	0.0071(2)	0.1582(1)	0.1034(1)	0.0028(3)	0.0013(1)	0.0009(1)	-.0004(1)	0.0006(1)	0.0000(1)	0.70
Tl _{oz}	0.0030(2)	0.1635(1)	0.6118(1)	0.0033(3)	0.0012(1)	0.0010(1)	-.0004(1)	0.0009(1)	0.0000(1)	0.69
Tl _{mo}	0.9996(2)	0.8147(1)	0.1191(1)	0.0038(3)	0.0011(1)	0.0009(1)	0.0004(1)	0.0009(1)	0.0001(1)	0.71
Tl _{mz}	0.0041(2)	0.8173(1)	0.6122(1)	0.0034(3)	0.0012(1)	0.0008(1)	0.0004(1)	0.0006(1)	-.0000(1)	0.71
T2 _{oo}	0.6876(2)	0.1124(1)	0.1598(1)	0.0028(3)	0.0009(1)	0.0016(1)	-.0000(1)	0.0006(1)	-.0000(1)	0.80
T2 _{oz}	0.6766(2)	0.1058(1)	0.6574(1)	0.0028(3)	0.0010(1)	0.0018(1)	-.0001(1)	0.0010(1)	-.0001(1)	0.83
T2 _{mo}	0.6762(2)	0.8814(1)	0.1809(1)	0.0029(3)	0.0010(1)	0.0016(1)	0.0002(1)	0.0005(1)	0.0003(1)	0.83
T2 _{mz}	0.6831(2)	0.8755(1)	0.6778(1)	0.0026(3)	0.0011(1)	0.0014(1)	0.0002(1)	0.0008(1)	0.0002(1)	0.72
Oa _{1o}	0.0069(6)	0.1252(3)	-.0097(3)	0.0106(9)	0.0020(2)	0.0011(2)	0.0005(4)	0.0022(4)	0.0001(2)	1.39
Oa _{1z}	0.0002(5)	0.1257(3)	0.4901(3)	0.0096(9)	0.0015(2)	0.0017(2)	0.0003(3)	0.0025(4)	0.0003(2)	1.30
Oa _{2o}	0.5750(5)	0.9897(3)	0.1395(3)	0.0024(6)	0.0009(2)	0.0016(2)	0.0000(3)	0.0002(3)	0.0003(2)	0.81
Oa _{2z}	0.5727(5)	0.9905(3)	0.6378(3)	0.0037(7)	0.0010(2)	0.0023(3)	0.0003(3)	0.0013(4)	0.0003(2)	0.98
Ob _{oo}	0.8218(5)	0.0990(3)	0.0924(3)	0.0060(7)	0.0016(2)	0.0034(3)	-.0012(3)	0.0032(4)	-.0006(2)	1.39
Ob _{oz}	0.7987(5)	0.1011(3)	0.5922(3)	0.0047(7)	0.0015(2)	0.0042(3)	-.0010(3)	0.0033(4)	-.0004(2)	1.46
Ob _{mo}	0.8068(8)	0.8564(3)	0.1253(4)	0.0060(8)	0.0021(2)	0.0067(4)	0.0000(4)	0.0052(5)	-.0005(2)	2.13
Ob _{mz}	0.8220(8)	0.8555(3)	0.6166(4)	0.0076(8)	0.0023(2)	0.0054(3)	0.0009(4)	0.0050(5)	-.0000(2)	1.94
Oc _{oo}	0.0124(5)	0.2788(3)	0.1368(3)	0.0056(7)	0.0012(2)	0.0023(2)	-.0004(3)	0.0020(4)	-.0000(2)	1.14
Oc _{oz}	0.0166(5)	0.2930(3)	0.6490(3)	0.0043(7)	0.0013(2)	0.0021(2)	-.0006(3)	0.0010(3)	-.0000(2)	1.10
Oc _{mo}	0.0065(5)	0.6801(3)	0.1074(3)	0.0059(8)	0.0014(2)	0.0015(2)	0.0001(3)	0.0008(3)	-.0001(2)	1.14
Oc _{mz}	0.0067(5)	0.6910(3)	0.6005(3)	0.0034(7)	0.0016(2)	0.0018(2)	0.0007(3)	0.0007(3)	-.0001(2)	1.05
Od _{oo}	0.1931(5)	0.1060(3)	0.1862(3)	0.0047(8)	0.0017(2)	0.0022(2)	0.0010(3)	0.0001(4)	0.0003(2)	1.37
Od _{oz}	0.2004(6)	0.1023(3)	0.6921(3)	0.0073(8)	0.0017(2)	0.0017(2)	0.0003(4)	-.0007(4)	0.0001(2)	1.58
Od _{mo}	0.1954(8)	0.8671(3)	0.2204(3)	0.0046(8)	0.0024(3)	0.0032(3)	0.0004(4)	-.0018(4)	-.0008(2)	2.07
Od _{mz}	0.1866(6)	0.8622(3)	0.7091(4)	0.0080(9)	0.0028(3)	0.0034(3)	0.0010(4)	-.0015(4)	-.0011(2)	2.45

Table 2: Positional and thermal parameters from \bar{I} refinement of Val Paseda/8.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2664(3)	0.9857(3)	0.0864(2)	0.0028(4)	0.0049(3)	0.0021(2)	-0.0010(2)	0.0010(2)	-0.0018(2)	1.81
Mzoo	0.2691(5)	0.0306(5)	0.5459(8)	0.0022(3)	0.0020(2)	0.0015(2)	0.0005(2)	0.0005(2)	-0.0004(2)	0.99
Moio	0.7740(2)	0.5358(2)	0.5433(2)	0.0035(3)	0.0018(1)	0.0014(1)	0.0007(1)	0.0004(1)	-0.0003(1)	1.07
Mzio	0.7635(6)	0.503 (2)	0.076 (2)	0.0028(5)	0.0051(7)	0.0028(6)	0.0002(4)	0.0009(3)	-0.0020(6)	2.06
T1oo	0.0073(2)	0.1579(1)	0.1043(1)	0.0026(2)	0.0011(1)	0.0008(1)	-0.0004(1)	0.0007(1)	-0.0000(1)	0.61
T1oz	0.0030(1)	0.1637(1)	0.6118(1)	0.0030(3)	0.0010(8)	0.0008(8)	-0.0003(1)	0.0006(1)	0.0000(1)	0.63
T1mo	0.9996(2)	0.8148(1)	0.1193(1)	0.0035(3)	0.0010(1)	0.0007(1)	0.0002(1)	0.0007(1)	0.0000(1)	0.63
T1mz	0.0042(2)	0.8174(1)	0.6119(1)	0.0026(2)	0.0012(1)	0.0008(1)	0.0005(1)	0.0006(1)	-0.0000(1)	0.64
T2oo	0.6878(2)	0.1123(1)	0.1597(1)	0.0023(2)	0.0011(1)	0.0016(1)	-0.0001(1)	0.0007(1)	-0.0001(1)	0.78
T2oz	0.6764(2)	0.1056(1)	0.6572(1)	0.0027(2)	0.0009(1)	0.0019(1)	-0.0001(1)	0.0009(1)	-0.0002(1)	0.81
T2mo	0.6756(2)	0.8815(1)	0.1806(1)	0.0027(2)	0.0009(1)	0.0016(1)	0.0001(1)	0.0006(1)	0.0002(1)	0.76
T2mz	0.6830(2)	0.8753(1)	0.6776(1)	0.0020(2)	0.0009(1)	0.0014(1)	0.0002(1)	0.0006(1)	0.0003(1)	0.65
Oa1o	0.0068(5)	0.1251(2)	-0.0090(3)	0.0084(7)	0.0017(2)	0.0013(2)	0.0002(3)	0.0017(3)	0.0000(2)	1.23
Oa1z	0.9988(5)	0.1258(2)	0.4896(3)	0.0112(8)	0.0016(2)	0.0013(2)	0.0004(3)	0.0030(4)	0.0001(2)	1.27
Oa2o	0.5735(4)	0.9895(2)	0.1390(2)	0.0026(6)	0.0011(2)	0.0017(2)	-0.0001(2)	0.0008(3)	0.0002(1)	0.80
Oa2z	0.5725(4)	0.9905(2)	0.6383(2)	0.0022(6)	0.0009(2)	0.0020(2)	0.0002(2)	0.0006(3)	0.0002(1)	0.83
Oboo	0.8208(5)	0.0988(2)	0.0917(3)	0.0046(6)	0.0014(2)	0.0034(2)	-0.0011(3)	0.0027(3)	-0.0007(2)	1.30
Oboz	0.7988(5)	0.1007(3)	0.5925(3)	0.0050(7)	0.0017(2)	0.0046(3)	-0.0011(3)	0.0039(4)	-0.0006(2)	1.57
Obmo	0.8066(5)	0.8562(3)	0.1253(3)	0.0050(7)	0.0019(2)	0.0065(3)	0.0000(3)	0.0040(4)	-0.0008(2)	2.07
Obmz	0.8228(5)	0.8558(3)	0.6173(3)	0.0068(7)	0.0025(2)	0.0058(3)	0.0013(3)	0.0048(4)	0.0003(2)	2.06
Ocoo	0.0128(5)	0.2790(2)	0.1369(3)	0.0045(6)	0.0015(2)	0.0020(2)	-0.0004(3)	0.0016(3)	0.0001(2)	1.04
Ocoz	0.0159(5)	0.2930(2)	0.6496(3)	0.0038(6)	0.0012(2)	0.0024(2)	-0.0006(3)	0.0012(3)	-0.0002(2)	1.09
Ocmo	0.0074(4)	0.6799(2)	0.1076(3)	0.0032(6)	0.0012(2)	0.0019(2)	0.0006(3)	0.0005(3)	0.0002(2)	0.99
Ocmz	0.0067(5)	0.6910(3)	0.5997(3)	0.0047(6)	0.0013(2)	0.0016(2)	0.0007(3)	0.0005(3)	-0.0001(2)	1.07
Odoo	0.1917(5)	0.1064(3)	0.1855(3)	0.0040(6)	0.0018(2)	0.0016(2)	0.0005(3)	-0.0006(3)	0.0002(2)	1.26
Odoz	0.2024(5)	0.1025(3)	0.6920(3)	0.0055(7)	0.0019(2)	0.0018(2)	0.0004(3)	-0.0010(3)	0.0003(2)	1.51
Odmo	0.1957(5)	0.8677(3)	0.2208(3)	0.0056(7)	0.0022(2)	0.0034(3)	0.0001(3)	-0.0016(4)	-0.0013(2)	2.15
Odmoz	0.1871(6)	0.8620(3)	0.7093(3)	0.0079(8)	0.0029(3)	0.0029(3)	0.0015(3)	-0.0024(4)	-0.0009(2)	2.47

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

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	0.2659(3)	0.9860(2)	0.0862(2)	0.0024(3)	0.0040(2)	0.0019(1)	-0.0007(2)	0.0010(2)	-0.0014(1)	1.52
Mzoo	0.2681(3)	0.0292(4)	0.5471(5)	0.0026(2)	0.0022(2)	0.0018(2)	0.0007(1)	0.0005(1)	-0.0007(1)	1.15
Moio	0.7740(2)	0.5353(1)	0.5430(1)	0.0027(3)	0.0017(1)	0.0015(1)	0.0006(1)	0.0006(1)	-0.0003(1)	0.95
Mzio	0.7639(5)	0.501 (1)	0.079 (1)	0.0025(5)	0.0030(4)	0.0011(3)	0.0000(3)	0.0009(3)	-0.0005(3)	1.10
T1oo	0.0076(1)	0.1580(1)	0.1043(1)	0.0023(2)	0.0011(1)	0.0008(5)	-0.0004(8)	0.0006(1)	-0.0000(1)	0.58
T1oz	0.0027(2)	0.1636(1)	0.6119(1)	0.0032(2)	0.0009(1)	0.0009(1)	-0.0004(1)	0.0008(1)	0.0000(1)	0.62
T1mo	0.0000(2)	0.8150(1)	0.1195(1)	0.0037(2)	0.0009(1)	0.0009(1)	0.0002(1)	0.0010(1)	0.0000(1)	0.63
T1mz	0.0046(1)	0.8174(1)	0.6118(1)	0.0024(2)	0.0011(5)	0.0008(1)	0.0004(1)	0.0006(1)	0.0000(1)	0.58
T2oo	0.6877(2)	0.1124(1)	0.1597(1)	0.0025(2)	0.0008(1)	0.0018(1)	-0.0002(1)	0.0009(1)	-0.0001(1)	0.76
T2oz	0.6767(1)	0.1056(1)	0.6574(1)	0.0024(2)	0.0007(1)	0.0019(1)	-0.0002(1)	0.0011(1)	-0.0002(1)	0.76
T2mo	0.6760(1)	0.8816(1)	0.1808(1)	0.0021(2)	0.0008(1)	0.0016(1)	0.0000(1)	0.0004(1)	0.0002(1)	0.72
T2mz	0.6831(2)	0.8751(1)	0.6773(1)	0.0026(2)	0.0008(1)	0.0013(1)	0.0003(1)	0.0009(1)	0.0003(1)	0.64
Oa1o	0.0073(4)	0.1251(2)	-0.0090(2)	0.0099(6)	0.0017(2)	0.0013(2)	0.0001(2)	0.0023(3)	-0.0001(1)	1.28
Oa1z	0.9984(4)	0.1254(2)	0.4899(2)	0.0114(7)	0.0015(2)	0.0016(2)	0.0004(2)	0.0033(3)	0.0004(1)	1.30
Oa2o	0.5743(3)	0.9896(2)	0.1391(2)	0.0021(5)	0.0008(1)	0.0019(2)	-0.0002(2)	0.0007(2)	0.0002(1)	0.78
Oa2z	0.5727(3)	0.9906(2)	0.6381(2)	0.0021(5)	0.0010(1)	0.0017(2)	0.0000(2)	0.0005(2)	0.0002(1)	0.79
Oboo	0.8217(4)	0.0993(2)	0.0919(2)	0.0048(5)	0.0013(2)	0.0039(2)	-0.0014(2)	0.0031(3)	-0.0007(1)	1.38
Oboz	0.7984(4)	0.1007(2)	0.5924(2)	0.0058(5)	0.0014(2)	0.0050(2)	-0.0014(2)	0.0045(3)	-0.0009(2)	1.59
Obmo	0.8079(4)	0.8562(2)	0.1261(3)	0.0065(6)	0.0018(2)	0.0071(3)	0.0001(3)	0.0053(4)	-0.0006(2)	2.19
Obmz	0.8231(4)	0.8558(2)	0.6166(3)	0.0082(6)	0.0020(2)	0.0058(3)	0.0012(3)	0.0058(3)	0.0005(2)	1.95
Ocoo	0.0129(4)	0.2789(2)	0.1360(2)	0.0044(5)	0.0014(2)	0.0019(2)	-0.0007(2)	0.0014(2)	-0.0003(1)	1.05
Ocoz	0.0152(4)	0.2933(2)	0.6490(2)	0.0051(5)	0.0012(1)	0.0020(2)	-0.0004(2)	0.0014(2)	-0.0002(1)	1.09
Ocmo	0.0078(4)	0.6797(2)	0.1073(2)	0.0048(5)	0.0010(1)	0.0018(2)	0.0006(2)	0.0011(2)	-0.0000(1)	0.98
Ocmz	0.0058(4)	0.6912(2)	0.5997(2)	0.0035(5)	0.0012(1)	0.0015(2)	0.0004(2)	0.0002(2)	-0.0003(1)	0.95
Odoe	0.1920(4)	0.1062(2)	0.1863(2)	0.0043(5)	0.0018(2)	0.0017(2)	0.0005(2)	-0.0004(2)	-0.0000(1)	1.30
Odoz	0.2020(4)	0.1032(2)	0.6921(2)	0.0060(6)	0.0013(2)	0.0023(2)	0.0003(2)	-0.0010(3)	0.0002(1)	1.57
Odmo	0.1970(4)	0.8679(2)	0.2207(2)	0.0047(6)	0.0023(2)	0.0037(2)	0.0007(3)	-0.0012(3)	-0.0012(2)	2.09
Odmoz	0.1860(4)	0.8623(2)	0.7088(2)	0.0074(6)	0.0025(2)	0.0031(2)	0.0013(3)	-0.0027(3)	-0.0014(2)	2.44

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}
Mooo	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
Mzoo	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
Moio	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
Mzio	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
T1oo	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
T1oz	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
T1mo	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
T1mz	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
T2oo	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
T2oz	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
T2mo	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
T2mz	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
Oa1o	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
Oa1z	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
Oa2o	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
Oa2z	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
Oboo	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
Oboz	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
Obmo	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
Obmz	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
Ocoo	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
Ocoz	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
Ocmo	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
Ocmz	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
Odoo	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
Odoz	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
Odmo	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
Odmz	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 $\text{I}\bar{1}$ refinement of Monte Somma/7.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mo _{oo}	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
Mz _{oo}	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
Mo _{io}	0.7742(3)	0.5353(2)	0.5436(2)	0.0033(4)	0.0018(2)	0.0010(2)	0.0006(2)	0.0006(2)	-0.0003(1)	1.14
Mz _{io}	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
Tl _{oo}	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
Tl _{oz}	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
Tl _{mo}	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
Tl _{mz}	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
T2 _{oo}	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
T2 _{oz}	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
T2 _{mo}	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
T2 _{mz}	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
Oa _{1o}	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
Oa _{1z}	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
Oa _{2o}	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
Oa _{2z}	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
Ob _{oo}	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
Ob _{oz}	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
Ob _{mo}	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
Ob _{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
Oc _{oo}	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
Oc _{oz}	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
Oc _{mo}	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
Oc _{mz}	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
Od _{oo}	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
Od _{oz}	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
Od _{mo}	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
Od _{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
T1oo	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
T1oz	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
T1mo	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
T1mz	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 $\text{I}\bar{\text{I}}$ refinement of 115082a/1.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
Mooo	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
Mzoo	0.2685(4)	0.0305(6)	0.5462(9)	0.0033(3)	0.0020(2)	0.0014(3)	0.0009(2)	0.0007(2)	-0.00027(2)	1.03
Moio	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
Mzio	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
T1oo	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
T1oz	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
T1mo	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
T1mz	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
T2oo	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
T2oz	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
T2mo	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
T2mz	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
Oa1o	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
Oa1z	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
Oa2o	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
Oa2z	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
Oboo	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
Oboz	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
Obmo	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
Obmz	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
Ocoo	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
Ocoz	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
Ocmo	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
Ocmz	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
Odoo	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
Odoz	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
Odmo	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
Odmz	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 $\bar{I}\bar{1}$ refinement of 87975a/1.

Site	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B_{eq}
M _{oo}	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 _{zo}	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 _{io}	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 _{zi}	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 _{boo}	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 _{b mz}	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 _{coo}	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 _{d mz}	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 $\text{I}\bar{1}$ 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)	0.0076(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
T1oo	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
T1oz	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
T1mo	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
T1mz	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	0.5778(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
Odoz	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 (supplement). M site occupancies from $\bar{I}\bar{I}$ refinements.

	Val Pasmeda	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		Monte		115082a	
	Pasmeda		Somma			
	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{I} refinements.

	Val Pasmeda	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
T1mo - 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)
Odmo	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)
Odmo	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 $\bar{I}\bar{I}$ 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
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 $\bar{I}\bar{1}$ 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)
Odoe	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)
Odoe	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
Mooo - Oa1oo	2.620(4)	2.624(6)	2.629(6)
Oa1oo	2.512(4)	2.506(6)	2.501(6)
Oa2oo	2.303(4)	2.301(6)	2.310(6)
Obooo	2.371(4)	2.369(6)	2.381(6)
Odoe	2.395(4)	2.378(6)	2.377(6)
Odmoe	2.528(4)	2.556(6)	2.583(6)
Ave.	2.455	2.456	2.464
Moio - Oa1oi	2.453(4)	2.433(6)	2.409(6)
Oa1oi	2.806(4)	2.838(6)	2.832(6)
Oa2oi	2.328(4)	2.332(7)	2.327(6)
Obioi	2.428(4)	2.424(6)	2.401(6)
Obmoe	2.493(4)	2.508(6)	2.581(6)
Ocmzo	2.549(4)	2.561(6)	2.590(6)
Odooi	2.412(4)	2.424(6)	2.465(6)
Ave.	2.496	2.503	2.515
Mzoo - Oa1zo	2.492(4)	2.500(6)	2.495(6)
Oa1zo	2.728(4)	2.717(6)	2.720(6)
Oa2zo	2.343(4)	2.346(6)	2.332(6)
Obozo	2.441(4)	2.447(6)	2.443(6)
Obmzo	2.479(4)	2.498(5)	2.519(6)
Ocmoe	2.570(4)	2.569(6)	2.554(6)
Odozo	2.371(4)	2.371(5)	2.377(6)
Ave.	2.489	2.493	2.490
Mzio - Oa1zi	2.445(4)	2.434(6)	2.407(6)
Oa1zi	2.586(4)	2.614(6)	2.641(6)
Oa2zi	2.287(4)	2.294(7)	2.283(6)
Obozi	2.401(4)	2.410(6)	2.386(6)
Ocmoe	2.826(4)	2.801(6)	2.738(6)
Odozi	2.422(4)	2.432(6)	2.440(6)
Odmzi	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} 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)
Odmoe	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)
Odmz	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(8)	2.363(6)	2.359(6)
Odmoe	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 Pasmcda		Monte Somma		115082a	
	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)
Odoz	123.9(3)	134.5(3)	123.6(4)	134.5(4)	124.2(4)	133.1(4)
Odmo	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 Pasmaeda</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)
T1m oi	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)
T2o oi	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)
T2m oi	108.9(3)	105.6(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 $\bar{I}1$ 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>						
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)	103.8(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 Paseda/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 Paseda/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 Paseda/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 Paseda/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)

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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)	99.6(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)	105.6(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} 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)
Odo	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)	
Odo	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)
Odoz	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)