

Table 4. M-O bond distances (Å), M2-O1-M2 angle (°), polyhedral volumes (Å³), octahedral angle variance (OAV in °) and quadratic elongation (OQE) of the M1 and M2 octahedra at each pressure point.

P (GPa)	0.0001(1)	0.70(7)	2.15(8)	3.82(5)	6.36(5)	7.27(9)	8.48(5)	9.97(19)	11.63(7)	12.62(5)	13.98(10)	16.09(7)	17.06(5)
M1-O3(x2)	2.048(12)	2.045(8)	2.046(8)	2.025(8)	2.022(8)	2.021(9)	2.008(8)	2.012(9)	2.005(9)	1.992(9)	1.999(9)	1.992(9)	1.992(10)
M1-O2(x4)	2.069(4)	2.067(3)	2.064(4)	2.057(3)	2.047(3)	2.047(4)	2.041(3)	2.037(3)	2.031(4)	2.027(4)	2.021(3)	2.017(4)	2.013(4)
<M1-O>	2.062(7)	2.060(2)	2.058(2)	2.046(2)	2.038(2)	2.036(3)	2.030(2)	2.029(2)	2.023(2)	2.015(3)	2.014(2)	2.009(3)	2.006(3)
V _{M1}	11.653(66)	11.616(40)	11.584(45)	11.380(40)	11.275(47)	11.211(47)	11.130(39)	11.103(42)	11.002(47)	10.873(46)	10.863(42)	10.784(46)	10.744(49)
OAV _{M1}	0.00438	0.00470	0.00387	0.00684	0.00546	0.00771	0.00727	0.00534	0.00589	0.00746	0.00476	0.00554	0.00482
OQE M1	1.0019	1.0022	1.0017	1.0024	1.0016	1.0021	1.0016	1.0015	1.0018	1.0017	1.0014	1.0014	1.0012
M2-O1	1.956(5)	1.942(5)	1.939(4)	1.937(5)	1.929(5)	1.919(5)	1.925(5)	1.911(6)	1.909(5)	1.906(5)	1.908(5)	1.895(5)	1.896(5)
M2-O3(x2)	2.032(3)	2.035(3)	2.028(3)	2.028(2)	2.026(3)	2.017(3)	2.014(2)	2.010(3)	2.012(3)	2.002(3)	2.007(3)	2.000(3)	2.000(3)

M2-O2(x2)	2.059(6)	2.061(4)	2.052(5)	2.051(4)	2.040(5)	2.040(5)	2.035(4)	2.034(5)	2.032(5)	2.030(5)	2.027(5)	2.023(5)	2.020(6)
M2-O2	2.228(14)	2.219(10)	2.227(11)	2.192(10)	2.194(11)	2.185(15)	2.190(11)	2.191(11)	2.161(12)	2.169(13)	2.160(11)	2.153(13)	2.153(13)
<M2-O>	2.061(3)	2.059(2)	2.054(2)	2.048(2)	2.043(3)	2.036(3)	2.035(2)	2.032(2)	2.026(3)	2.023(3)	2.023(2)	2.016(3)	2.015(3)
M2-O1-M2	120.72(27)	120.29(25)	120.25(24)	119.80(24)	120.5(26)	119.75(28)	119.69(24)	119.76(27)	119.87(27)	119.17(27)	119.74(28)	119.41(27)	119.33(28)
V _{M2}	11.491(66)	11.435(42)	11.372(46)	11.257(42)	11.172(48)	11.074(54)	11.064(41)	10.995(47)	10.919(46)	10.862(49)	10.853(46)	10.754(49)	10.742(52)
OAV _{M2}	0.02703	0.02662	0.02799	0.02462	0.02476	0.02553	0.02528	0.02704	0.02403	0.02627	0.02412	0.02516	0.02457
OQE M2	1.0122	1.0132	1.0127	1.0129	1.0126	1.0126	1.0122	1.0129	1.0118	1.0127	1.0120	1.0117	1.0114
M3-O1(x2)	2.059(4)	2.057(3)	2.051(3)	2.045(3)	2.043(3)	2.039(4)	2.031(3)	2.028(3)	2.030(3)	2.017(3)	2.015(4)	2.013(3)	2.008(4)
M3-O3(x4)	2.221(7)	2.209(5)	2.201(5)	2.194(5)	2.172(5)	2.177(6)	2.171(5)	2.162(5)	2.149(6)	2.152(6)	2.139(6)	2.131(6)	2.125(6)
<M3-O>	2.167(3)	2.159(2)	2.151(2)	2.144(2)	2.129(2)	2.131(2)	2.124(2)	2.117(2)	2.109(2)	2.107(2)	2.098(2)	2.092(2)	2.086(2)
V _{M3}	9.57(99)	9.44(93)	9.34(90)	9.25(93)	9.08(91)	9.07(91)	9.00(91)	8.90(85)	8.78(89)	8.77(88)	8.65(88)	8.55(86)	8.47(83)
