

Table 3: Transition temperatures (in degrees Celsius) for the *Pnma* to *I2mb* phase boundary as determined by the disappearance of the (1 3 1) Bragg-reflection in the powder diffraction patterns.

$x \text{ Al}^{3+}$	T (°C) <i>Pnma</i> $\Rightarrow$ <i>I2mb</i>
0.00	724(4)
0.12	699(4)
0.22	690(4)
0.3	669(4)
0.40	654(5)
0.50	643(5)
0.55	635(5)
0.6	625(5)
0.65	623(5)
0.70	--

Table 4: Linear thermal expansion coefficients  $\alpha$  ( $\cdot 10^{-6}/\text{K}$ ) for samples of the  $\text{Ca}_2\text{Fe}_{2-x}\text{Al}_x\text{O}_5$  solid solution series, determined from the temperature variations of unit cell lengths;  $\alpha = (l_T - l_0)/(l_0 \cdot [T - T_0])$  with  $l_T$  is the unit cell lengths at a temperature  $T$ ,  $l_0$  is the one at  $T_0 = 25^\circ\text{C}$ . The estimated standard deviation is 0.4 - 0.5 for all data.

x (nom.)	<i>a</i>	<i>b</i>	<i>c</i>	<i>Volume</i>	T - range (°C)
0.00	8.8	23.1	9.3	41.35	25 - 420
0.00	8.6	25.7	7.0	41.1	720 - 800
0.40	11.3	20.4	7.4	39.1	25 - 800
0.50	11.9	19.9	6.0	38.1	25 - 800
0.55	11.0	18.8	4.9	34.7	25 - 800
0.60	12.2	21.6	6.0	40.6	25 - 800
0.70	12.5	22.2	5.8	40.8	25 - 800
0.80	12.5	21.5	5.3	40.3	25 - 800
1.00	11.8	20.7	5.1	38.8	25 - 800
1.35	11.1	18.7	4.0	37.0	25 - 800

Table 7: Anisotropic atomic displacement parameters  $U_{ij}$  of selected samples of the  $\text{Ca}_2\text{Fe}_{2-x}\text{Al}_x\text{O}_5$  solid solution series.

		BX000 1	BHT005 2	BHT015 1	BHT025 2	BHT030 3	BHT035 1	BHT040 2	bf80i 2	BHT55 1
Ca	$U_{11}$	0.0094(3)	0.0093(2)	0.0089(2)	0.0093(3)	0.0112(3)	0.0109(2)	0.0105(2)	0.0097(3)	0.0096(3)
	$U_{22}$	0.0064(3)	0.0037(2)	0.0051(3)	0.0060(3)	0.0067(3)	0.0055(2)	0.0050(3)	0.0068(3)	0.0032(3)
	$U_{33}$	0.0062(3)	0.0064(2)	0.0063(2)	0.0068(3)	0.0087(2)	0.0074(2)	0.0076(2)	0.0078(3)	0.0064(3)
	$U_{23}$	-0.0002(2)	0.0001(1)	0.0001(1)	0.0006(2)	0.0002(2)	0.0002(1)	0.0001(1)	0.0003(2)	0.0005(1)
	$U_{13}$	0.0014(2)	0.0013(1)	0.0012(1)	0.0010(2)	0.0009(2)	0.0009(1)	0.0011(1)	0.0010(2)	0.0004(2)
M-site	$U_{12}$	-0.0011(2)	-0.0009(1)	-0.0010(1)	-0.0009(2)	-0.0009(2)	-0.0011(1)	-0.0010(1)	-0.0009(2)	-0.0013(2)
	$U_{11}$	0.0027(3)	0.0019(2)	0.0011(3)	0.0020(3)	0.0037(3)	0.0033(2)	0.0028(3)	0.0018(3)	0.0019(3)
	$U_{22}$	0.0091(3)	0.0055(2)	0.0077(3)	0.0096(3)	0.0096(3)	0.0083(2)	0.0083(3)	0.0096(3)	0.0056(3)
	$U_{33}$	0.0029(3)	0.025(2)	0.0019(2)	0.0033(3)	0.0046(2)	0.0028(2)	0.0034(2)	0.0031(3)	0.0020(3)
	$U_{23}$	0.0003(2)	0.0002(1)	0.0001(1)	0.0004(2)	0.0005(2)	0.0003(1)	0.0002(1)	0.0001(2)	-0.0001(2)
T-site	$U_{13}$	-0.0002(2)	-0.0001(1)	0.0001(1)	0.0001(2)	0.0001(2)	0.0000(1)	0.0001(1)	-0.0001(1)	0
	$U_{12}$	0.0006(2)	0.0004(1)	0.0004(1)	0.0003(2)	0.0004(2)	0.0003(1)	0.0004(1)	0.0002(2)	0
	$U_{11}$	0.0049(3)	0.0034(2)	0.0032(2)	0.0029(3)	0.0047(3)	0.0055(2)	0.0049(2)	0.0061(3)	0.0041(3)
	$U_{22}$	0.0043(3)	0.0007(2)	0.0026(2)	0.0027(3)	0.0037(3)	0.0024(2)	0.0023(2)	0.0038(3)	0.0001(3)
	$U_{33}$	0.0047(3)	0.0037(2)	0.0037(2)	0.0037(3)	0.0053(3)	0.0044(2)	0.0043(2)	0.0050(3)	0.0038(3)
	$U_{13}$	-0.0001(2)	0.0002(1)	0.0003(1)	-0.0001(2)	0.0002(2)	0.0003(1)	0.0002(2)	0.0001(2)	-0.0001(2)
O1	$U_{11}$	0.0053(9)	0.0042(5)	0.0040(6)	0.0050(8)	0.0054(7)	0.0066(6)	0.0059(6)	0.0062(9)	0.0044(7)
	$U_{22}$	0.0095(8)	0.0081(5)	0.0094(6)	0.0082(10)	0.0117(8)	0.0102(5)	0.0109(7)	0.0109(8)	0.0082(6)
	$U_{33}$	0.0064(8)	0.0064(6)	0.0056(6)	0.0055(9)	0.0081(7)	0.0063(5)	0.0066(6)	0.0069(7)	0.0056(8)
	$U_{23}$	0.0015(6)	0.0005(3)	0.0004(4)	0.0008(9)	0.0006(6)	0.0004(3)	0.0010(4)	0.0005(6)	0.0005(8)
	$U_{13}$	-0.0018(8)	-0.0022(4)	-0.0025(5)	-0.0027(6)	-0.0029(6)	-0.0019(4)	-0.0035(5)	-0.0017(7)	-0.0015(6)
O2	$U_{12}$	-0.0016(7)	-0.0005(3)	-0.0009(4)	0.0004(8)	-0.0009(6)	-0.0006(4)	-0.0006(4)	-0.0004(6)	-0.0010(5)
	$U_{11}$	0.0126(10)	0.0127(6)	0.0130(7)	0.0122(9)	0.0151(8)	0.0145(6)	0.0139(7)	0.0116(8)	0.0131(9)
	$U_{22}$	0.0056(9)	0.0036(6)	0.0055(8)	0.0071(9)	0.0077(8)	0.0068(6)	0.0070(8)	0.0095(9)	0.0057(9)
	$U_{33}$	0.0070(8)	0.0085(5)	0.0077(6)	0.0084(9)	0.0098(7)	0.0091(4)	0.0096(6)	0.0092(7)	0.0079(10)
	$U_{23}$	0.0007(7)	0.0005(4)	0.0003(5)	0.0009(7)	0.0013(6)	0.0005(4)	0.0009(5)	0.0006(6)	0.0008(5)
O3	$U_{13}$	0.0002(7)	0.0002(4)	0.0008(6)	0.0007(8)	0.0001(6)	0.0007(4)	0.0006(5)	0.0004(6)	0.0013(6)
	$U_{12}$	0.0009(6)	0.0013(4)	0.0011(5)	0.0021(6)	0.0011(6)	0.0013(4)	0.0008(5)	0.0004(6)	0.0001(6)
	$U_{11}$	0.0055(13)	0.0050(7)	0.0058(8)	0.0069(12)	0.0110(11)	0.0111(9)	0.0097(8)	0.0080(13)	0.0098(10)

U <sub>22</sub>	0.0112(13)	0.0060(7)	0.0082(8)	0.0056(14)	0.0076(12)	0.0062(7)	0.0073(9)	0.0094(12)	0.0041(11)
U <sub>33</sub>	0.0055(12)	0.0077(8)	0.0070(7)	0.0091(14)	0.0113(11)	0.0092(7)	0.0091(8)	0.0106(11)	0.0082(14)
U <sub>13</sub>	0.0003(10)	-0.0016(6)	-0.0009(7)	-0.0012(9)	-0.0022(8)	-0.0025(6)	-0.0025(7)	-0.0011(9)	-0.0013(9)

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Table 7 (continued)

		BHT50 2	BHT070 1	BHT120 6	BHT095 2	BHT100 2	BHT110n1	BHT120n2	BHT130 2	BHT140 2
Ca	U11	0.0088(3)	0.0099(3)	0.0097(2)	0.0086(3)	0.0097(3)	0.0086(3)	0.0097(4)	0.0092(3)	0.0093(3)
	U22	0.0044(2)	0.0038(3)	0.0062(2)	0.0056(3)	0.0051(2)	0.0043(3)	0.0069(3)	0.0055(2)	0.0093(2)
	U33	0.0059(2)	0.0061(3)	0.0070(2)	0.0045(2)	0.0059(2)	0.0062(2)	0.0054(3)	0.0075(2)	0.0087(3)
	U23	-0.0049(2)	0.0002(2)	0.0005(1)	0.0003(2)	0.0006(2)	0.0002(2)	0.0004(2)	0.0007(2)	0.0006(2)
	U13	0.0001(2)	0.0007(3)	0.0006(2)	0.0001(3)	-0.0002(2)	0.0001(3)	-0.0004(3)	-0.0003(3)	0.0001(3)
M-site	U12	-0.0013(3)	-0.0014(3)	-0.0010(2)	-0.0012(3)	-0.0013(3)	-0.0015(3)	-0.0013(4)	-0.0007(4)	-0.0008(3)
	U11	0.0008(3)	0.0021(3)	0.0024(2)	0.0013(4)	0.0027(3)	0.0017(3)	0.0014(4)	0.0025(3)	0.0029(4)
	U22	0.0068(3)	0.0063(3)	0.0089(2)	0.0094(3)	0.0084(3)	0.0076(3)	0.0107(4)	0.0088(3)	0.0131(4)
	U33	0.0012(2)	0.0013(3)	0.0027(2)	0.0005(3)	0.0021(2)	0.0017(3)	0.0010(3)	0.0034(3)	0.0052(4)
	U23	0.0003(2)	0.0003(3)	0.0002(1)	0.0001(2)	0.0006(2)	0.0004(2)	0.0003(3)	0.0002(2)	0.0006(3)
T-site	U13	0	0	0	0	0	0	0	0	0
	U12	0	0	0	0	0	0	0	0	0
	U11	0.0030(3)	0.0031(4)	0.0051(3)	0.0030(5)	0.0058(4)	0.0037(5)	0.0035(6)	0.0037(6)	0.0056(6)
	U22	0.0009(3)	0.0001(3)	0.0034(3)	0.0034(4)	0.0022(3)	0.0007(4)	0.0037(5)	0.0025(5)	0.0061(5)
	U33	0.0030(2)	0.0016(4)	0.0043(2)	0.0016(4)	0.0029(3)	0.0032(4)	0.0017(5)	0.0031(4)	0.0045(6)
O1	U13	-0.0001(2)	-0.0001(3)	-0.0002(2)	-0.0001(3)	0.0001(3)	-0.0004(3)	-0.0001(4)	-0.0004(4)	-0.0002(5)
	U11	0.0039(8)	0.0061(9)	0.0059(6)	0.0050(10)	0.0062(8)	0.0059(8)	0.0049(10)	0.0060(8)	0.0056(8)
	U22	0.0094(7)	0.0086(11)	0.0105(6)	0.0103(8)	0.0094(7)	0.0069(11)	0.0122(12)	0.0092(9)	0.0122(8)
	U33	0.0048(6)	0.0046(9)	0.0059(5)	0.0033(7)	0.0048(7)	0.0057(7)	0.0046(8)	0.0066(7)	0.0092(9)
	U23	0.0006(9)	0.0019(13)	0.0008(8)	-0.0003(9)	0.0009(9)	-0.0002(12)	-0.0003(14)	-0.0007(14)	0.0012(12)
O2	U13	-0.0015(6)	-0.0029(7)	-0.0028(5)	-0.0014(7)	-0.0019(6)	-0.0010(6)	-0.0016(7)	-0.0011(6)	-0.0004(7)
	U12	-0.0006(5)	-0.0005(8)	-0.0013(6)	-0.0004(8)	-0.0010(6)	-0.0015(9)	-0.0002(10)	0.0002(11)	-0.0001(8)
	U11	0.0099(11)	0.0138(13)	0.0126(9)	0.0099(13)	0.0117(9)	0.0112(12)	0.0097(14)	0.0121(14)	0.0104(12)
	U22	0.0060(8)	0.0056(9)	0.0082(6)	0.0093(9)	0.0081(8)	0.0081(11)	0.0115(10)	0.0082(10)	0.0123(9)
	U33	0.0094(7)	0.0096(11)	0.0096(5)	0.0072(7)	0.0082(7)	0.0091(10)	0.0090(9)	0.0127(8)	0.0125(11)
O3	U23	0.0004(6)	0.0009(7)	0.0013(4)	0.0019(6)	0.0005(6)	0.0014(7)	0.0035(8)	0.0028(7)	0.0023(8)
	U13	0.0005(8)	0.0015(10)	0.0015(7)	-0.0005(8)	0.0013(7)	0.0013(10)	0.0003(12)	0.0026(12)	0.0015(11)
	U12	0.0006(7)	0.0012(7)	0.0012(6)	0.0009(8)	0.0020(7)	0.0017(8)	0.0023(10)	0.0015(9)	0.0012(8)
	U11	0.0099(13)	0.0117(15)	0.0108(10)	0.0108(14)	0.0102(11)	0.0081(13)	0.0087(16)	0.0101(15)	0.0093(13)
	U22	0.0043(12)	0.0060(15)	0.0058(9)	0.0057(12)	0.0065(12)	0.0067(18)	0.0094(17)	0.0053(15)	0.0114(14)

U33	0.0072(11)	0.0076(18)	0.0084(9)	0.0045(12)	0.0063(10)	0.0041(14)	0.0065(15)	0.0057(11)	0.0072(16)
U13	-0.0023(9)	-0.0026(11)	-0.0023(8)	-0.0017(10)	-0.0038(9)	-0.0030(9)	-0.0003(12)	0.0011(10)	-0.0009(11)

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Table 8: Selected bond distances (Å) and angles (°) and polyhedral distortion parameters for selected samples of the  $\text{Ca}_2\text{Fe}_{2-x}\text{Al}_x\text{O}_5$  solid solution series.

	bx000_1	BHT005_2	BHT015_1	BHT025_2	BHT030_3	BHT035_1	BHT040_2	bf80i	BHT055_1
<b>Interstitial site</b>									
Ca-O2 (Å)	2.323(2)	2.325(1)	2.325(1)	2.323(2)	2.320(2)	2.320(1)	2.320(1)	2.317(2)	2.320(2)
Ca-O3 (Å)	2.345(1)	2.343(1)	2.343(1)	2.343(1)	2.345(1)	2.345(1)	2.343(1)	2.338(1)	2.342(1)
Ca-O1 (Å)	2.430(2)	2.432(1)	2.439(1)	2.441(1)	2.446(2)	2.451(1)	2.449(1)	2.457(2)	2.452(2)
Ca-O1 (Å)	2.482(2)	2.481(1)	2.479(1)	2.477(1)	2.474(2)	2.473(1)	2.474(1)	2.472(2)	2.482(2)
Ca-O1 (Å)	2.485(2)	2.485(1)	2.487(1)	2.489(1)	2.490(2)	2.494(1)	2.491(1)	2.496(2)	2.547(2)
Ca-O2 (Å)	2.542(2)	2.544(1)	2.549(1)	2.554(1)	2.553(2)	2.559(1)	2.560(1)	2.566(2)	2.571(2)
Ca-O1 (Å)	2.736(2)	2.727(1)	2.710(1)	2.700(1)	2.688(2)	2.679(1)	2.675(1)	2.664(2)	2.580(2)
Ca-O2 (Å)	3.000(2)	2.992(1)	2.981(1)	2.968(1)	2.965(2)	2.955(1)	2.949(1)	2.936(2)	2.926(2)
<Ca-O> (Å)	2.543	2.541	2.539	2.537	2.535	2.535	2.533	2.531	2.528
BLD (%)	6.39	6.29	6.13	6.03	5.92	5.82	5.79	5.67	5.08
<b>Octahedral site</b>									
M-O1 x2 (Å)	1.961(2)	1.960(1)	1.957(1)	1.956(2)	1.955(1)	1.955(1)	1.953(1)	1.952(2)	1.942(2)
M-O1 x2 (Å)	1.969(2)	1.968(1)	1.966(1)	1.963(2)	1.961(1)	1.956(1)	1.958(1)	1.955(2)	1.960(2)
M-O2 x2 (Å)	2.121(2)	2.120(1)	2.126(2)	2.121(2)	2.125(2)	2.127(1)	2.124(2)	2.128(2)	2.125(2)
<M-O> (Å)	2.017	2.016	2.016	2.013	2.014	2.013	2.012	2.012	2.009
<O-O> (Å)	2.835	2.833	2.833	2.829	2.828	2.828	2.826	2.825	2.830
BLD (%)	3.43	3.44	3.63	3.57	3.69	3.79	3.72	3.86	3.85
ELD (%)	2.37	2.36	2.41	2.42	2.47	2.47	2.47	2.48	2.83
O1-M-O1	92.53(3)	92.58(1)	92.61(1)	92.67(2)	92.68(2)	92.70(1)	92.73(2)	92.77(2)	91.87(12)
O1-M-O1	92.53(3)	92.58(1)	92.61(1)	92.67(2)	92.68(2)	92.70(1)	92.73(2)	92.77(2)	93.76(7)
O1-M-O1 x2	87.47(3)	87.58(1)	87.39(1)	87.33(2)	87.32(2)	87.30(1)	87.27(2)	87.23(2)	87.18(2)
O1-M-O2 x2	93.43(7)	93.30(5)	93.33(5)	93.33(7)	93.46(6)	93.36(4)	93.37(5)	93.27(7)	93.86(7)
O1-M-O2 x2	86.57(7)	86.70(5)	86.67(5)	86.67(7)	86.54(6)	86.64(4)	86.63(5)	86.73(7)	86.00(7)
O1-M-O2 x2	90.61(7)	90.69(5)	90.64(5)	90.51(7)	90.51(6)	90.51(4)	90.41(5)	90.40(7)	90.91(6)

O1-M-O2 x2 OAV	89.39(7) 6.74	89.31(5) 6.41	89.65(5) 6.61	89.49(7) 6.72	89.49(6) 7.06	89.49(4) 6.85	89.59(5) 6.90	89.60(7) 6.74	89.31(6) 7.94
<b>Tetrahedral site</b>									
T-O2 x2 (Å)	1.843(2)	1.835(1)	1.822(2)	1.821(2)	1.815(2)	1.807(1)	1.806(2)	1.795(2)	1.795(2)
T-O3 (Å)	1.912(3)	1.908(2)	1.898(2)	1.895(2)	1.886(2)	1.879(1)	1.879(2)	1.872(2)	1.870(3)
T-O3 (Å)	1.914(2)	1.911(2)	1.905(2)	1.895(2)	1.892(2)	1.887(2)	1.882(2)	1.883(3)	1.876(2)
<T-O> (Å)	1.878	1.872	1.862	1.858	1.852	1.845	1.843	1.836	1.834
<O-O> (Å)	3.058	3.049	3.033	3.026	3.017	3.006	3.002	2.992	2.988
BLD	1.86	1.99	2.14	2.00	2.00	2.06	2.02	2.25	2.13
ELD	1.86	1.84	1.73	1.80	1.74	1.73	1.75	1.75	1.77
O2-T-O2	122.39(12)	122.48(8)	122.14(9)	122.28(10)	121.89(11)	121.86(7)	121.90(9)	121.91(12)	121.74(11)
O2-T-O3 x2	106.39(7)	107.40(4)	107.42(5)	107.27(7)	107.40(6)	107.30(4)	107.24(5)	106.97(7)	106.99(6)
O2-T-O3 x2	107.47(7)	106.39(4)	106.52(5)	106.55(7)	106.61(5)	106.69(4)	106.71(5)	106.97(6)	106.94(6)
O3-T-O3	105.62(7)	105.65(4)	105.75(5)	105.88(7)	105.92(6)	106.02(4)	106.09(5)	106.08(7)	106.34(7)
<O-T-O>	109.29	109.29	109.30	109.30	109.31	109.31	109.32	109.31	109.32
TAV	39.58	41.26	39.01	39.87	37.47	37.22	37.46	37.20	36.41

Table 8 (continued)

	BHT050 2	BHT070 1	BHT120 6	BHT095 2	BHT100 2	BHT110n1	BHT120n2	BHT130 2	BHT140 2
<b>Interstitial site</b>									
Ca-O2 (Å)	2.320(2)	2.318(2)	2.313(1)	2.313(2)	2.312(2)	2.316(2)	2.313(2)	2.309(2)	2.313(2)
Ca-O3 (Å)	2.345(1)	2.342(2)	2.342(1)	2.343(2)	2.344(1)	2.347(2)	2.339(2)	2.344(2)	2.339(2)
Ca-O1 (Å)	2.456(2)	2.450(3)	2.451(2)	2.452(2)	2.452(2)	2.444(3)	2.451(3)	2.446(3)	2.440(3)
Ca-O1 (Å)	2.483(2)	2.481(3)	2.478(2)	2.478(2)	2.473(2)	2.472(3)	2.465(3)	2.460(3)	2.461(2)
Ca-O1 (Å)	2.549(2)	2.541(2)	2.536(2)	2.532(2)	2.531(2)	2.525(2)	2.524(3)	2.513(3)	2.504(2)
Ca-O2 (Å)	2.577(2)	2.571(2)	2.566(2)	2.561(2)	2.555(2)	2.555(2)	2.542(3)	2.532(3)	2.527(2)
Ca-O1 (Å)	2.578(2)	2.575(3)	2.570(2)	2.574(3)	2.574(2)	2.576(2)	2.571(3)	2.567(3)	2.568(2)
Ca-O2 (Å)	2.921(2)	2.916(2)	2.902(2)	2.892(3)	2.889(2)	2.878(2)	2.869(3)	2.857(3)	2.845(2)
<Ca-O> (Å)	2.529	2.524	2.520	2.518	2.516	2.514	2.509	2.504	2.500
BLD	5.05	5.01	4.91	4.83	4.81	4.75	4.67	4.54	4.46

**Octahedral site**

M-O1 x2 (Å)	1.945(2)	1.938(3)	1.936(2)	1.933(3)	1.936(2)	1.929(3)	1.926(4)	1.915(3)	1.916(3)
M-O1 x2 (Å)	1.958(2)	1.958(3)	1.951(2)	1.949(3)	1.942(2)	1.943(3)	1.937(4)	1.934(3)	1.923(3)
M-O2 x2 (Å)	2.125(2)	2.124(2)	2.123(1)	2.120(3)	2.120(2)	2.123(2)	2.114(2)	2.113(2)	2.110(2)
<M-O> (Å)	2.009	2.007	2.003	2.001	1.999	1.998	1.992	1.987	1.983
<O-O> (Å)	2.822	2.826	2.821	2.817	2.815	2.811	2.807	2.799	2.790
BLD (%)	3.84	3.90	3.98	3.98	4.02	4.16	4.07	4.22	4.27
ELD (%)	2.86	2.84	2.84	2.82	2.83	2.74	2.82	2.83	2.72

O1-M-O1 (°)	91.71(13)	92.03(18)	91.93(12)	91.94(15)	91.73(13)	92.03(17)	91.50(21)	91.69(20)	91.89(17)
O1-M-O1 (°)	93.86(6)	93.64(18)	93.80(12)	93.77(15)	93.96(13)	93.71(17)	94.14(21)	93.85(20)	93.55(17)
O1-M-O1 x2 (°)	87.21(2)	87.17(3)	87.14(2)	87.15(2)	87.16(2)	87.13(2)	87.18(2)	87.23(2)	87.28(2)
O1-M-O2 x2 (°)	93.81(6)	93.90(8)	93.77(5)	93.70(7)	93.72(6)	93.43(8)	93.47(9)	93.57(8)	93.49(8)
O1-M-O2 x2 (°)	86.06(7)	85.97(8)	86.11(5)	86.17(8)	86.16(6)	86.49(8)	86.39(10)	86.28(8)	86.42(8)
O1-M-O2 x2 (°)	90.78(6)	90.81(8)	90.71(5)	90.55(7)	90.50(6)	90.55(8)	90.48(9)	90.41(8)	90.30(8)
O1-M-O2 x2 (°)	89.44(7)	89.39(9)	89.49(5)	89.65(8)	89.71(7)	89.59(8)	89.76(10)	89.81(8)	89.85(8)
OAV (°)	8.67	8.11	7.64	7.39	7.27	6.71	6.47	6.78	6.56

**Tetrahedral site**

T-O2 x2 (Å)	1.795(2)	1.787(2)	1.777(1)	1.774(3)	1.771(2)	1.758(2)	1.758(2)	1.753(2)	1.748(2)
T-O3 (Å)	1.869(2)	1.856(3)	1.846(2)	1.840(2)	1.835(2)	1.828(3)	1.823(3)	1.806(3)	1.802(3)
T-O3 (Å)	1.874(3)	1.872(3)	1.853(2)	1.845(2)	1.840(2)	1.829(3)	1.826(4)	1.815(3)	1.810(3)
<T-O> (Å)	1.833	1.826	1.813	1.808	1.804	1.793	1.791	1.782	1.777
<O-O> (Å)	2.987	2.975	2.954	2.947	2.940	2.922	2.919	2.903	2.895
BLD (%)	2.09	2.11	2.00	1.89	1.84	1.97	1.86	1.61	1.63
ELD (%)	1.81	1.75	1.78	1.86	1.84	1.93	1.99	2.04	2.16

O2-T-O2 (°)	121.94(11)	121.68(15)	121.62(9)	121.73(12)	121.63(11)	121.81(14)	122.12(16)	122.22(14)	122.67(15)
O2-T-O3 x2 (°)	106.96(6)	107.02(8)	107.04(5)	106.87(8)	107.03(7)	106.91(8)	106.78(9)	106.82(9)	106.52(9)
O2-T-O3 x2 (°)	106.86(6)	106.97(8)	106.88(5)	106.89(7)	106.79(6)	106.73(7)	106.67(9)	106.52(8)	106.50(8)
O3-T-O3 (°)	106.34(7)	106.26(9)	106.52(6)	106.76(8)	106.75(7)	106.96(8)	107.04(10)	107.13(9)	107.35(9)
<O-T-O> (°)	109.32	109.32	109.33	109.34	109.34	109.34	109.34	109.34	109.34
TAV (°)	37.71	35.97	35.91	36.76	36.26	37.58	39.60	40.54	43.62