

Distances		(1)	(2)	(3)		
[Å]						
Ti-Ti	Ti(1)-Ti(3)	3.0824(11)	Ti(1)-Ti(3)#1	3.1009(9)	Ti(1)-Ti(2)#1	3.1081(11)
	Ti(1)-Ti(2)	3.3574(10)	Ti(1)-Ti(2)#1	3.1185(9)	Ti(1)-Ti(3)#1	3.1093(12)
			Ti(2)-Ti(3)#1	3.1156(9)		
Ti-O	Ti(1)-O(2)	1.755(3)	Ti(1)-O(71)	1.769(3)	Ti(1)-O(71)	1.759(3)
	Ti(1)-O(1)#1	1.902(3)	Ti(1)-O(3)	1.881(3)	Ti(1)-O(1)	1.896(3)
	Ti(1)-O(51)	2.024(3)	Ti(1)-O(1)	1.904(3)	Ti(1)-O(3)	1.899(3)
	Ti(1)-O(11)	2.039(3)	Ti(1)-O(11)	2.035(2)	Ti(1)-O(11)	2.050(3)
	Ti(1)-O(26)	2.044(3)	Ti(1)-O(32)#1	2.071(3)	Ti(1)-O(32)#1	2.066(3)
	Ti(1)-Ti(2)	3.3574(10)	Ti(1)-O(2)#1	2.148(3)	Ti(1)-O(2)#1	2.151(3)
	Ti(2)-O(86)	1.751(4)	Ti(2)-O(91)	1.755(3)	Ti(3)-O(81)	1.766(3)
	Ti(2)-O(2)	1.869(2)	Ti(2)-O(3)	1.896(2)	Ti(3)-O(2)	1.887(3)
	Ti(2)-O(1)	1.906(2)	Ti(2)-O(2)	1.916(3)	Ti(3)-O(1)	1.895(3)
	Ti(2)-O(72)#1	2.056(3)	Ti(2)-O(51)	2.046(3)	Ti(3)-O(12)#1	2.069(3)
	Ti(2)-O(12)	2.072(3)	Ti(2)-O(12)#1	2.073(2)	Ti(3)-O(52)#1	2.074(3)
	Ti(2)-O(32)	2.101(3)	Ti(2)-O(1)#1	2.142(3)	Ti(3)-O(3)#1	2.142(3)
	Ti(3)-O(66)	1.786(3)	Ti(3)-O(81)	1.773(3)	Ti(2)-O(91)	1.769(3)
	Ti(3)-O(46)	1.793(3)	Ti(3)-O(2)	1.880(2)	Ti(2)-O(3)	1.886(3)
	Ti(3)-O(26)	1.978(3)	Ti(3)-O(1)	1.899(3)	Ti(2)-O(2)	1.911(3)
	Ti(3)-O(71)	2.017(3)	Ti(3)-O(31)	2.073(3)	Ti(2)-O(51)	2.043(3)
	Ti(3)-O(1)#1	2.066(2)	Ti(3)-O(52)#1	2.081(3)	Ti(2)-O(31)	2.072(3)
	Ti(3)-O(52)	2.157(3)	Ti(3)-O(3)#1	2.172(3)	Ti(2)-O(1)#1	2.144(3)
Angles		(1)	(2)	(3)		
[°]						
Ti-O-Ti	Ti(1)#1-O(1)-Ti(2)	128.79(13)	O(2)-Ti(1)-O(1)#1	104.53(11)	Ti(3)#1-Ti(2)-Ti(1)#1	68.84(2)
	Ti(1)#1-O(1)-Ti(3)#1	101.84(11)	O(2)-Ti(1)-O(51)	92.97(11)	Ti(3)-O(1)-Ti(1)	135.43(17)
	Ti(2)-O(1)-Ti(3)#1	129.36(14)	O(1)#1-Ti(1)-O(51)	92.98(11)	Ti(3)-O(1)-Ti(2)#1	99.98(13)
	Ti(1)-O(2)-Ti(2)	135.75(14)	O(2)-Ti(1)-O(11)	93.65(11)	Ti(1)-O(1)-Ti(2)#1	100.43(13)
			O(1)#1-Ti(1)-O(11)	90.26(11)	Ti(3)-O(2)-Ti(2)	133.69(16)
			O(51)-Ti(1)-O(11)	171.67(10)	Ti(3)-O(2)-Ti(1)#1	100.50(13)
			O(2)-Ti(1)-O(26)	176.25(12)	Ti(2)-O(2)-Ti(1)#1	99.66(13)
			O(1)#1-Ti(1)-O(26)	79.07(11)	Ti(2)-O(3)-Ti(1)	132.25(16)
			O(51)-Ti(1)-O(26)	85.78(11)	Ti(2)-O(3)-Ti(3)#1	100.33(13)
O-Ti-O	O(2)-Ti(1)-O(1)#1	104.53(11)	O(71)-Ti(1)-O(3)	104.95(12)	O(71)-Ti(1)-O(1)	100.75(14)
	O(2)-Ti(1)-O(51)	92.97(11)	O(71)-Ti(1)-O(1)	100.59(12)	O(71)-Ti(1)-O(3)	99.04(14)
	O(1)#1-Ti(1)-O(51)	92.98(11)	O(3)-Ti(1)-O(1)	101.69(11)	O(1)-Ti(1)-O(3)	102.74(13)
	O(2)-Ti(1)-O(11)	93.65(11)	O(71)-Ti(1)-O(11)	91.56(11)	O(71)-Ti(1)-O(11)	96.10(13)

O(1)#1-Ti(1)-O(11)	90.26(11)	O(3)-Ti(1)-O(11)	157.82(12)	O(1)-Ti(1)-O(11)	157.46(13)
O(51)-Ti(1)-O(11)	171.67(10)	O(1)-Ti(1)-O(11)	89.40(11)	O(3)-Ti(1)-O(11)	89.17(13)
O(2)-Ti(1)-O(26)	176.25(12)	O(71)-Ti(1)-O(32)#1	92.51(12)	O(71)-Ti(1)-O(32)#1	95.21(14)
O(1)#1-Ti(1)-O(26)	79.07(11)	O(3)-Ti(1)-O(32)#1	85.77(11)	O(1)-Ti(1)-O(32)#1	86.55(13)
O(51)-Ti(1)-O(26)	85.78(11)	O(1)-Ti(1)-O(32)#1	162.56(11)	O(3)-Ti(1)-O(32)#1	161.14(13)
O(11)-Ti(1)-O(26)	87.30(10)	O(11)-Ti(1)-O(32)#1	78.70(11)	O(11)-Ti(1)-O(32)#1	77.04(13)
O(2)-Ti(1)-O(31)	91.76(12)	O(3)-Ti(1)-O(2)#1	78.27(10)	O(71)-Ti(1)-O(2)#1	175.77(14)
O(1)#1-Ti(1)-O(31)	163.58(11)	O(1)-Ti(1)-O(2)#1	77.60(11)	O(1)-Ti(1)-O(2)#1	78.00(12)
O(51)-Ti(1)-O(31)	88.14(12)	O(11)-Ti(1)-O(2)#1	85.59(10)	O(3)-Ti(1)-O(2)#1	77.41(12)
O(11)-Ti(1)-O(31)	86.60(11)	O(32)#1-Ti(1)-O(2)#1	88.71(11)	O(11)-Ti(1)-O(2)#1	86.20(11)
O(26)-Ti(1)-O(31)	84.68(11)				
