This journal is © The Royal Society of Chemistry 2003

Table TS2 Selected bond distances (Å) and angles (°) in the structure of **1**

Ti(1)-O(2)	1.768(10)	Ti(1)-Co(1)	3.068(4)
Ti(1)-O(5)	1.770(9)	Co(1)-O(6)	1.921(8)
Ti(1)-O(7)	1.966(10)	Co(1)-O(6)#1	1.943(8)
Ti(1)-O(1)	2.005(9)	Co(1)-O(7)	1.952(9)
Ti(1)-O(3)	2.023(10)	Co(1)-O(1)	1.945(9)
Ti(1)-O(4)	2.099(10)	Co(1)-Co(1)#1	2.957(4)
O(2)-Ti(1)-O(5)	97.2(4)	O(1)-Ti(1)-O(3)	89.4(4)
O(2)-Ti(1)-O(7)	97.7(4)	O(2)-Ti(1)-O(4)	86.9(4)
O(5)-Ti(1)-O(7)	100.6(4)	O(5)-Ti(1)-O(4)	171.3(4)
O(2)-Ti(1)-O(1)	169.4(4)	O(6)-Co(1)-O(6)#1	80.2(4)
O(5)-Ti(1)-O(1)	92.6(4)	O(6)-Co(1)-O(7)	127.9(4)
O(7)-Ti(1)-O(1)	76.4(4)	O(6)#1-Co(1)-O(7)	124.1(4)
O(2)-Ti(1)-O(3)	94.6(4)	O(6)-Co(1)-O(1)	125.6(3)
O(5)-Ti(1)-O(3)	90.6(4)	O(6)#1-Co(1)-O(1)	128.2(3)
O(7)-Ti(1)-O(3)	162.2(4)	O(7)-Co(1)-O(1)	78.1(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

This journal is © The Royal Society of Chemistry 2003

Table TS3 Selected bond distances (Å) and angles (°) in the structure of **2**

Co(1)-O(4)	2.009(3)	Co(1)-O(2)	2.064(3)
Co(1)-O(3)	2.037(3)	Co(1)-O(1)	2.151(3)
Co(1)-O(5)	2.042(3)	Co(1)-O(2)#1	2.159(3)
O(4)-Co(1)-O(3)	87.13(11)	O(4)-Co(1)-O(1)	94.06(13)
O(4)-Co(1)-O(5)	90.16(11)	O(3)-Co(1)-O(1)	96.61(12)
O(3)-Co(1)-O(5)	96.00(12)	O(5)-Co(1)-O(1)	166.88(12)
O(4)-Co(1)-O(2)	176.90(11)	O(2)-Co(1)-O(1)	86.84(12)
O(3)-Co(1)-O(2)	89.82(11)	O(4)-Co(1)-O(2)#1	103.03(11)
O(5)-Co(1)-O(2)	89.61(11)	O(3)-Co(1)-O(2)#1	169.57(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z

This journal is © The Royal Society of Chemistry 2003

Table TS4 Selected bond distances (Å) and angles (°) in the structure of **3**

Ta(1)-O(3)	1.88(2)	Co(1)-O(6)#1	1.926(19)
Ta(1)-O(5)	1.902(18)	Co(1)-O(6)	1.934(17)
Ta(1)-O(7)	1.939(19)	Co(1)-O(1)	1.934(17)
Ta(1)-O(2)	1.96(2)	Co(1)-O(2)	1.97(2)
Ta(1)-O(1)	1.99(2)	Co(1)-Co(1)#1	2.963(8)
O(4)-Ta(1)-O(3)	103.8(10)	O(7)-Ta(1)-O(2)	88.9(9)
O(4)-Ta(1)-O(5)	94.0(13)	O(4)-Ta(1)-O(1)	162.5(10)
O(3)-Ta(1)-O(5)	92.7(9)	O(3)-Ta(1)-O(1)	92.9(7)
O(4)-Ta(1)-O(7)	88.2(12)	O(6)#1-Co(1)-O(6)	79.7(8)
O(3)-Ta(1)-O(7)	91.4(10)	O(6)#1-Co(1)-O(1)	125.2(7)
O(5)-Ta(1)-O(7)	174.7(12)	O(6)-Co(1)-O(1)	132.4(9)
O(4)-Ta(1)-O(2)	93.0(11)	O(6)#1-Co(1)-O(2)	129.7(9)
O(3)-Ta(1)-O(2)	163.2(9)	O(6)-Co(1)-O(2)	127.0(9)
O(5)-Ta(1)-O(2)	86.2(9)	O(1)-Co(1)-O(2)	71.5(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

This journal is © The Royal Society of Chemistry 2003

Table TS5 Selected bond distances (Å) and angles (°) in the structure of **4**

Ni(1)-O(2)	1.890(14)	Nb(1)-O(10)	1.922(15)
Ni(1)-O(3)	1.933(13)	Nb(1)-O(9)	1.964(15)
Ni(1)-O(1)	1.944(12)	Nb(1)-O(7)	1.955(18)
Ni(1)-O(4)	1.949(13)	Nb(1)-O(8)	1.979(16)
Nb(1)-O(5)	1.717(17)	Nb(1)-O(2)	2.059(14)
Nb(1)-O(6)	1.734(18)	Nb(1)-O(3)	2.059(12)
Nb(1)-O(11)	1.814(14)	Nb(1)-O(4)	2.149(14)
Nb(1)-O(12)	1.830(15)	Nb(1)-O(1)	2.164(13)
O(2)-Ni(1)-O(2)#1	129.2(12)	O(5)-Nb(1)-O(6)	86.3(8)
O(2)-Ni(1)-O(3)#1	176.3(8)	O(5)-Nb(1)-O(11)	138.4(8)
O(2)#1-Ni(1)-O(3)#1	48.3(7)	O(6)-Nb(1)-O(11)	93.7(8)
O(2)-Ni(1)-O(3)	48.3(6)	O(5)-Nb(1)-O(12)	94.8(8)
O(2)#1-Ni(1)-O(3)	176.3(8)	O(6)-Nb(1)-O(12)	137.8(8)
O(3)#1-Ni(1)-O(3)	134.4(9)	O(11)-Nb(1)-O(12)	58.7(8)
O(2)-Ni(1)-O(1)	78.9(6)	O(5)-Nb(1)-O(10)	174.0(7)
O(2)#1-Ni(1)-O(1)	127.8(6)	O(6)-Nb(1)-O(10)	87.7(7)
O(3)#1-Ni(1)-O(1)	100.6(5)	O(11)-Nb(1)-O(10)	42.2(6)
O(3)-Ni(1)-O(1)	55.6(6)	O(12)-Nb(1)-O(10)	89.8(7)
O(3)#1-Ni(1)-O(4)#1	78.9(6)	O(5)-Nb(1)-O(9)	90.4(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

This journal is © The Royal Society of Chemistry 2003

Table TS6 Selected bond distances (Å) and angles (°) in the structure of **5**

Co(1)-O(2)	1.940(4)	Al(1)-O(4)	1.892(5)
Co(1)-O(1)	1.944(4)	Al(1)-O(3)	1.896(4)
Co(1)-Al(1)	2.934(2)	Al(1)-O(6)	1.897(5)
Al(1)-O(1)	1.851(4)	Al(1)-O(5)	1.900(4)
Al(1)-O(2)#1	1.859(4)		
O(2)-Co(1)-O(2)#1	121.9(2)	O(2)#1-Al(1)-O(4)	94.98(19)
O(2)-Co(1)-O(1)	134.53(15)	O(1)-Al(1)-O(3)	95.16(19)
O(2)#1-Co(1)-O(1)	76.67(15)	O(2)#1-Al(1)-O(3)	175.9(2)
O(2)-Co(1)-O(1)#1	76.67(15)	O(4)-Al(1)-O(3)	88.91(18)
O(2)#1-Co(1)-O(1)#1	134.53(15)	O(1)-Al(1)-O(6)	91.81(17)
O(1)-Co(1)-O(1)#1	122.0(2)	O(2)#1-Al(1)-O(6)	91.67(19)
Al(1)-Co(1)-Al(1)#1	179.93(9)	O(4)-Al(1)-O(6)	87.11(19)
O(1)-Al(1)-O(2)#1	80.98(16)	O(3)-Al(1)-O(6)	89.7(2)
O(1)-Al(1)-O(4)	175.8(2)	O(6)-Al(1)-O(5)	175.94(19)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2

This journal is © The Royal Society of Chemistry 2003

Table TS7 Selected bond distances (Å) and angles (°) in the structure of **7**

Mg(1)-O(3)	1.935(2)	Al(1)-O(3)	1.862(3)
Mg(1)-Al(1)	2.9043(16)	Al(1)-O(1)	1.896(3)
		Al(1)-O(2)	1.900(3)
O(3)-Mg(1)-O(3)#1	78.37(14)	O(3)#1-Al(1)-O(3)	82.10(15)
O(3)-Mg(1)-O(3)#2	133.51(14)	O(3)-Al(1)-O(1)#1	95.19(11)
O(3)#1-Mg(1)-O(3)#2	120.87(14)	O(3)#1-Al(1)-O(1)	95.19(11)
O(3)-Mg(1)-O(3)#3	120.87(14)	O(3)-Al(1)-O(1)	176.91(11)
O(3)#1-Mg(1)-O(3)#3	133.52(14)	O(1)#1-Al(1)-O(1)	87.56(16)
O(3)#2-Mg(1)-O(3)#3	78.37(14)	O(3)#1-Al(1)-O(2)	91.48(11)
Al(1)-Mg(1)-Al(1)#2	180.0	O(3)-Al(1)-O(2)	91.87(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x+0,-y+1/2,z #2 -x,y,-z+3/2 #3 x+0,-y+1/2,-z+3/2

This journal is © The Royal Society of Chemistry 2003

Table TS8 Selected bond distances (Å) and angles (°) in the structure of **8**

Zn(1)-O(8)	1.946(5)	Al(1)-O(6)	1.866(6)
Zn(1)-O(7)	1.949(5)	Al(1)-O(2)	1.879(8)
Zn(1)-O(6)	1.954(6)	Al(1)-O(5)	1.872(7)
Zn(1)-O(5)	1.959(6)	Al(1)-O(1)	1.901(7)
Zn(1)-Zn(1)#1	2.934(2)	Al(1)-O(3)	1.906(7)
Zn(1)-Al(1)	2.942(3)	Al(1)-O(4)	1.906(7)
O(8)-Zn(1)-O(7)	82.2(3)	O(6)-Al(1)-O(5)	81.7(3)
O(8)-Zn(1)-O(6)	122.9(2)	O(2)-Al(1)-O(5)	175.7(3)
O(7)-Zn(1)-O(6)	129.75(19)	O(6)-Al(1)-O(1)	93.7(3)
O(8)-Zn(1)-O(5)	129.0(2)	O(2)-Al(1)-O(1)	90.3(3)
O(7)-Zn(1)-O(5)	122.7(2)	O(5)-Al(1)-O(1)	90.6(3)
O(6)-Zn(1)-O(5)	77.3(3)	O(6)-Al(1)-O(3)	176.3(3)
Zn(1)#1-Zn(1)-Al(1)	179.71(8)	O(2)-Al(1)-O(3)	89.6(3)
O(6)-Al(1)-O(2)	94.1(3)	O(5)-Al(1)-O(3)	94.7(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2 #2 -x+1,y,-z+1/2

This journal is © The Royal Society of Chemistry 2003

Table TS9 Selected bond distances (Å) and angles (°) in the structure of **9**

Ni(1)-O(2)	1.982(9)	Ni(1)-O(1)	2.051(7)
Ni(1)-O(3)	1.997(8)	Ni(1)-O(1)#1	2.136(8)
Ni(1)-O(8)	2.022(7)	Ni(1)-O(6)	2.146(10)
O(2)-Ni(1)-O(3)	86.2(3)	O(3)-Ni(1)-O(1)#1	101.7(3)
O(2)-Ni(1)-O(8)	94.7(3)	O(8)-Ni(1)-O(1)#1	87.2(3)
O(3)-Ni(1)-O(8)	90.6(3)	O(1)-Ni(1)-O(1)#1	79.9(3)
O(2)-Ni(1)-O(1)	92.2(3)	O(2)-Ni(1)-O(6)	97.2(4)
O(3)-Ni(1)-O(1)	178.2(3)	O(3)-Ni(1)-O(6)	93.8(4)
O(8)-Ni(1)-O(1)	90.2(3)	O(8)-Ni(1)-O(6)	167.6(4)
O(2)-Ni(1)-O(1)#1	171.8(3)	O(1)-Ni(1)-O(6)	85.7(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z