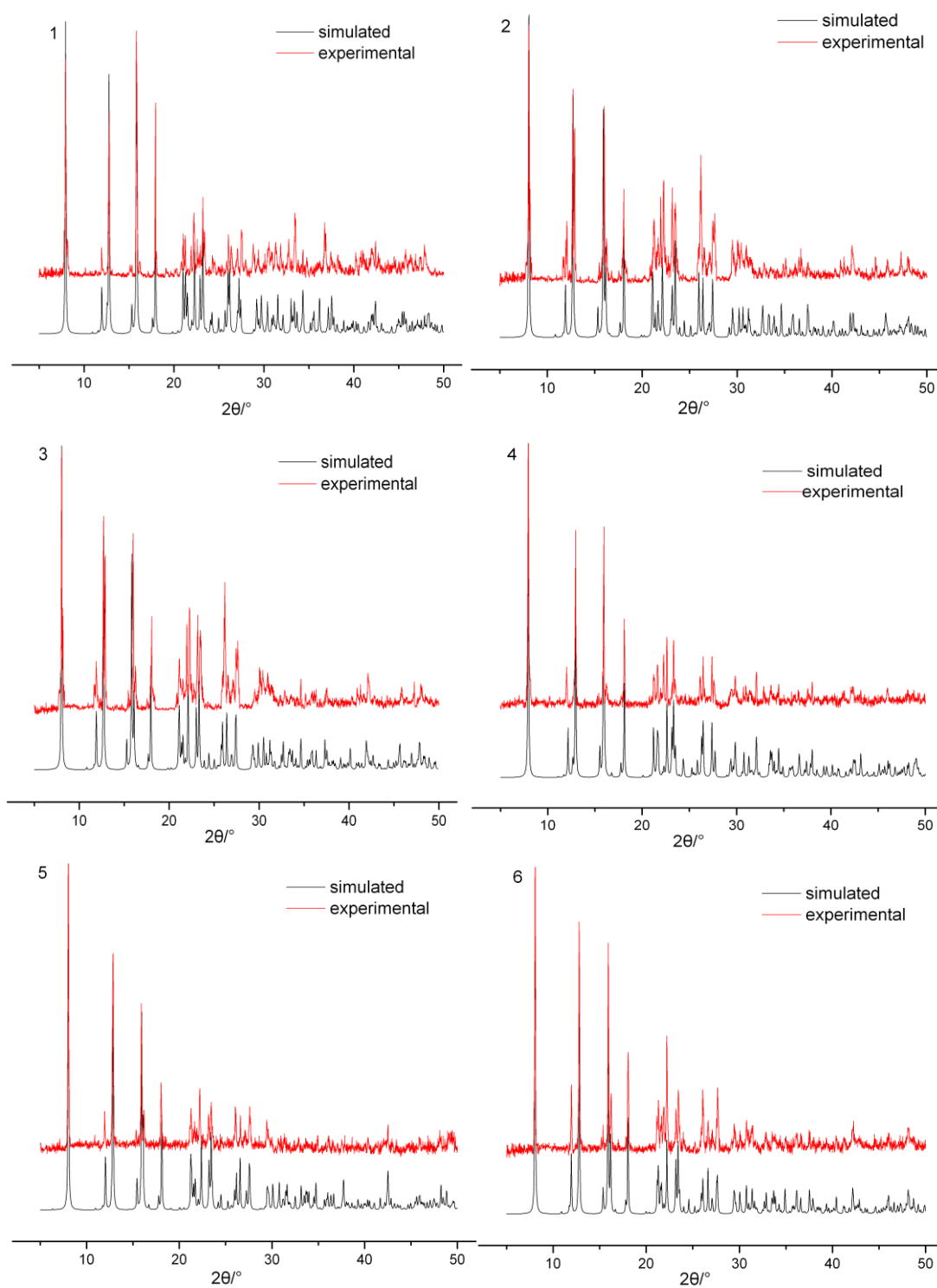


Hydrothermal synthesis, Crystal structure and Properties of Three-Dimensional Co(II)-4f Heterometallic-Organic Frameworks

Shu-Ju Wang, Yan-Wen Tian, Gang Xiong, Li-Xin You, Fu Ding, Mei-yan Guo, En-Jun Gao,
Philippe F. Smet, Dirk Poelman, Lin-Jiu Xiao, Ya-Guang Sun*



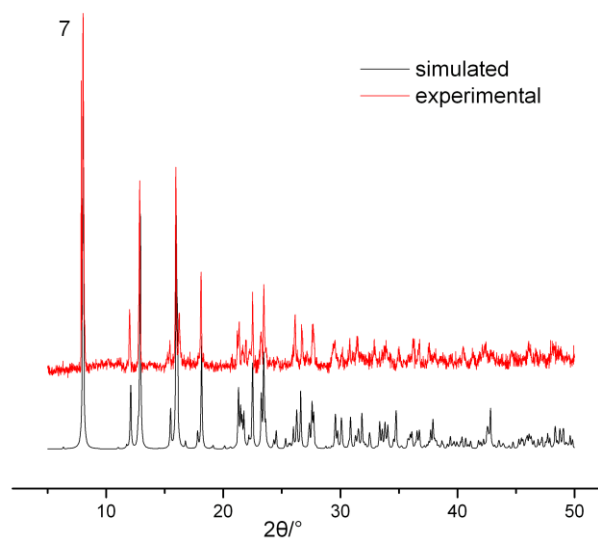


Fig. S1 The simulated and experimental PXRD patterns of **1-7**.

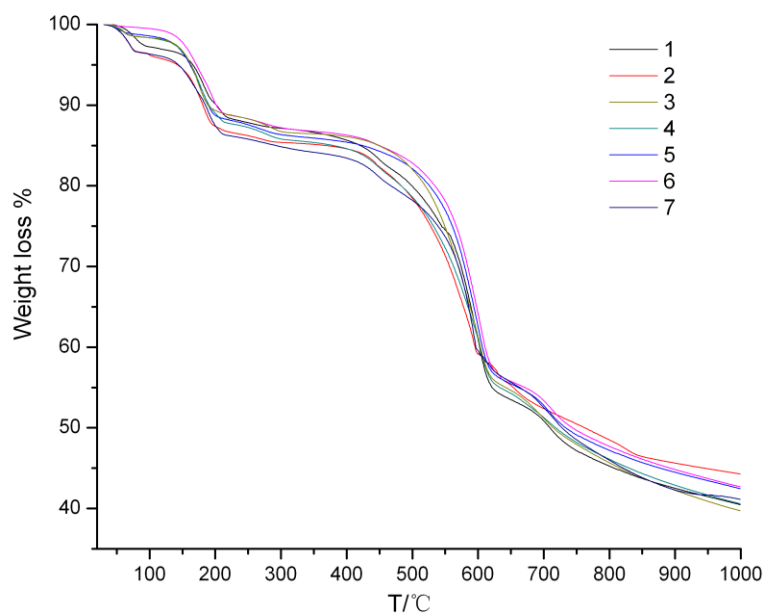


Fig. S2. TGA curves of **1-7**.

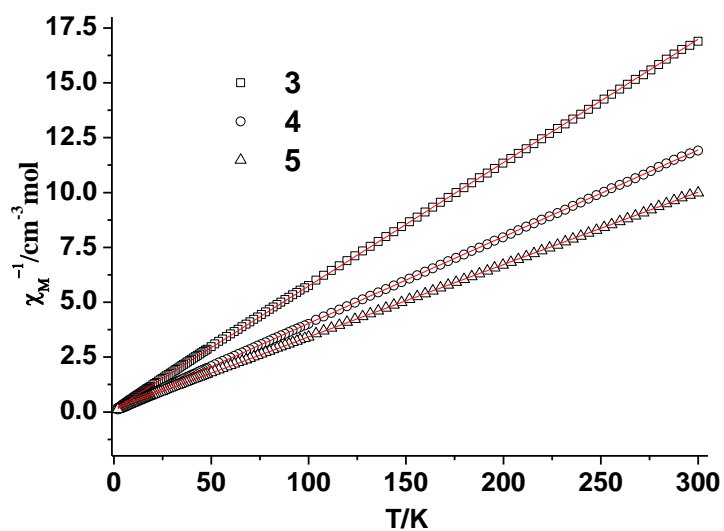


Fig. S3. Temperature vs χ_M^{-1} curves for 3-5. The red solid lines stand for the best fitting.

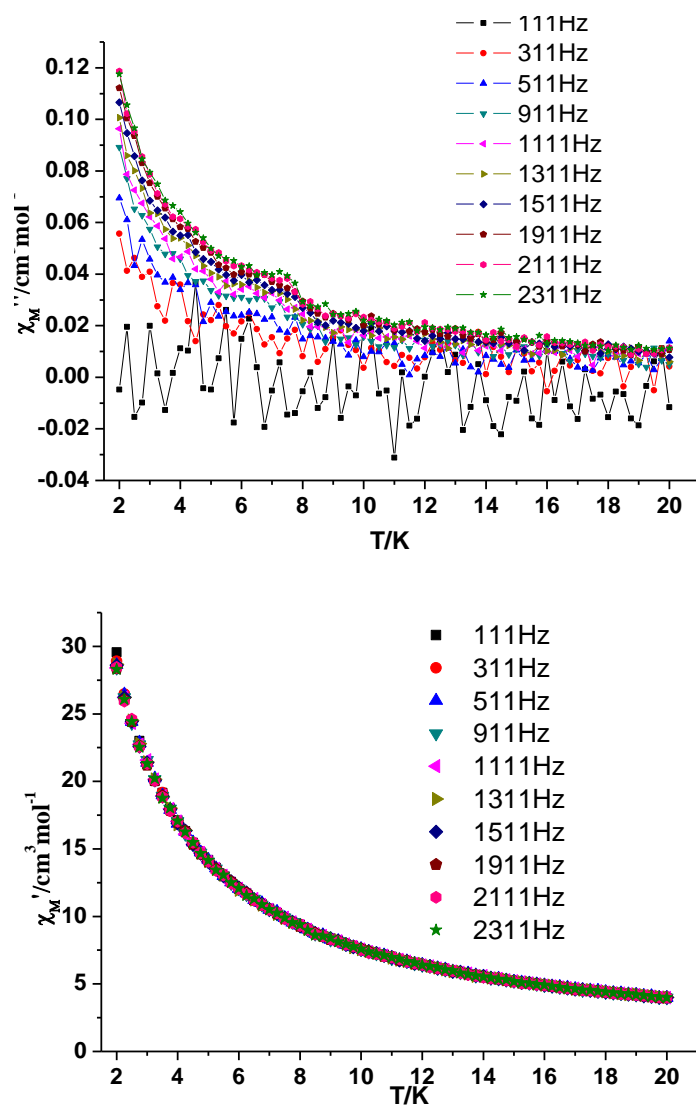


Fig. S4. Temperature dependence of in phase χ_M' and out-of-phase χ_M'' of 4 under zero direct-current (dc) field.

Table S1. Bond lengths [Å] and angles [deg] for **1-7**.

1			
Pr(1)-O(1)	2.393(2)	Pr(1)-O(5)	2.436(2)
Pr(1)-O(6)#1	2.448(4)	Pr(1)-O(9)	2.459(6)
Pr(1)-O(2)#1	2.475(4)	Pr(1)-O(3)#2	2.517(3)
Pr(1)-O(10)	2.561(3)	Pr(1)-O(4)#2	2.679(2)
Pr(1)-O(1)#1	2.840(4)	Co(1)-O(12)	2.094(6)
Co(1)-N(1)	2.110(3)	Co(1)-N(1)#3	2.110(3)
Co(1)-O(11)#3	2.114(3)	Co(1)-O(11)	2.114(3)
Co(1)-O(13)	2.128(6)	O(4)-Pr(1)#4	2.679(2)
O(3)-Pr(1)#4	2.517(3)		
O(1)-Pr(1)-O(5)	81.19(8)	O(1)-Pr(1)-O(6)#1	79.76(8)
O(5)-Pr(1)-O(6)#1	131.48(7)	O(1)-Pr(1)-O(9)	80.86(7)
O(5)-Pr(1)-O(9)	78.66(8)	O(6)#1-Pr(1)-O(9)	140.14(10)
O(1)-Pr(1)-O(2)#1	125.01(7)	O(5)-Pr(1)-O(2)#1	80.44(9)
O(6)#1-Pr(1)-O(2)#1	75.03(14)	O(9)-Pr(1)-O(2)#1	143.33(9)
O(1)-Pr(1)-O(3)#2	135.98(7)	O(5)-Pr(1)-O(3)#2	142.31(6)
O(6)#1-Pr(1)-O(3)#2	73.03(6)	O(9)-Pr(1)-O(3)#2	98.55(7)
O(2)#1-Pr(1)-O(3)#2	80.40(6)	O(1)-Pr(1)-O(10)	148.16(8)
O(5)-Pr(1)-O(10)	74.28(9)	O(6)#1-Pr(1)-O(10)	131.91(7)
O(9)-Pr(1)-O(10)	74.75(9)	O(2)#1-Pr(1)-O(10)	70.74(12)
O(3)#2-Pr(1)-O(10)	68.85(8)	O(1)-Pr(1)-O(4)#2	88.54(8)
O(5)-Pr(1)-O(4)#2	152.50(9)	O(6)#1-Pr(1)-O(4)#2	70.50(11)
O(9)-Pr(1)-O(4)#2	74.53(7)	O(2)#1-Pr(1)-O(4)#2	125.61(7)
O(3)#2-Pr(1)-O(4)#2	50.12(6)	O(10)-Pr(1)-O(4)#2	104.00(9)
O(1)-Pr(1)-O(1)#1	76.47(9)	O(5)-Pr(1)-O(1)#1	65.06(11)
O(6)#1-Pr(1)-O(1)#1	67.24(12)	O(9)-Pr(1)-O(1)#1	139.47(9)
O(2)#1-Pr(1)-O(1)#1	48.81(9)	O(3)#2-Pr(1)-O(1)#1	121.06(10)
O(10)-Pr(1)-O(1)#1	109.89(8)	O(4)#2-Pr(1)-O(1)#1	136.95(6)
O(12)-Co(1)-N(1)	89.71(7)	O(12)-Co(1)-N(1)#3	89.71(7)
N(1)-Co(1)-N(1)#3	179.43(14)	O(12)-Co(1)-O(11)#3	86.83(6)
N(1)-Co(1)-O(11)#3	86.98(8)	N(1)#3-Co(1)-O(11)#3	92.98(8)
O(12)-Co(1)-O(11)	86.83(6)	N(1)-Co(1)-O(11)	92.98(8)
N(1)#3-Co(1)-O(11)	86.98(8)	O(11)#3-Co(1)-O(11)	173.66(13)
O(12)-Co(1)-O(13)	180.000(2)	N(1)-Co(1)-O(13)	90.29(7)
N(1)#3-Co(1)-O(13)	90.29(7)	O(11)#3-Co(1)-O(13)	93.17(6)
O(11)-Co(1)-O(13)	93.17(6)		
#1 -x+1/2,-y+5/2,-z+1	#2 x,-y+2,z+1/2	#3 -x+1,y,-z+3/2	#4 x,-y+2,z-1/2
2			
Eu(1)-O(6')#1	2.331(12)	Eu(1)-O(3)	2.337(3)
Eu(1)-O(5')	2.355(10)	Eu(1)-O(10)	2.399(6)
Eu(1)-O(4)#1	2.421(3)	Eu(1)-O(5)	2.438(11)
Eu(1)-O(6)#1	2.454(12)	Eu(1)-O(9)	2.462(3)

Eu(1)-O(2)#2	2.469(3)	Eu(1)-O(10')	2.474(6)
Eu(1)-O(1)#2	2.544(3)	Eu(1)-O(3)#1	2.768(3)
O(1)-Eu(1)#4	2.544(3)	O(2)-Eu(1)#4	2.469(3)
Co(2)-O(12)	2.090(3)	Co(2)-O(12)#3	2.090(3)
Co(2)-O(11)	2.101(4)	Co(2)-O(13)	2.112(4)
Co(2)-N(1)#3	2.117(3)	Co(2)-N(1)	2.117(3)
O(6')#1-Eu(1)-O(3)	83.9(5)	O(6')#1-Eu(1)-O(5')	127.2(8)
O(3)-Eu(1)-O(5')	79.5(3)	O(6')#1-Eu(1)-O(10)	143.6(6)
O(3)-Eu(1)-O(10)	69.99(18)	O(5')-Eu(1)-O(10)	73.5(7)
O(6')#1-Eu(1)-O(4)#1	70.5(6)	O(3)-Eu(1)-O(4)#1	124.57(10)
O(5')-Eu(1)-O(4)#1	78.8(5)	O(10)-Eu(1)-O(4)#1	145.49(17)
O(6')#1-Eu(1)-O(5)	140.0(8)	O(3)-Eu(1)-O(5)	80.9(2)
O(5')-Eu(1)-O(5)	13.19(19)	O(10)-Eu(1)-O(5)	61.4(7)
O(4)#1-Eu(1)-O(5)	88.4(6)	O(6')#1-Eu(1)-O(6)#1	12.5(2)
O(3)-Eu(1)-O(6)#1	73.3(5)	O(5')-Eu(1)-O(6)#1	129.2(7)
O(10)-Eu(1)-O(6)#1	131.3(6)	O(4)#1-Eu(1)-O(6)#1	82.5(6)
O(5)-Eu(1)-O(6)#1	140.6(6)	O(6')#1-Eu(1)-O(9)	132.9(5)
O(3)-Eu(1)-O(9)	143.25(10)	O(5')-Eu(1)-O(9)	76.4(5)
O(10)-Eu(1)-O(9)	76.74(18)	O(4)#1-Eu(1)-O(9)	77.13(11)
O(5)-Eu(1)-O(9)	69.6(4)	O(6)#1-Eu(1)-O(9)	143.1(5)
O(6')#1-Eu(1)-O(2)#2	70.8(4)	O(3)-Eu(1)-O(2)#2	137.69(10)
O(5')-Eu(1)-O(2)#2	142.8(3)	O(10)-Eu(1)-O(2)#2	112.46(18)
O(4)#1-Eu(1)-O(2)#2	78.66(10)	O(5)-Eu(1)-O(2)#2	139.3(3)
O(6)#1-Eu(1)-O(2)#2	76.2(3)	O(9)-Eu(1)-O(2)#2	69.91(11)
O(6')#1-Eu(1)-O(10')	139.6(5)	O(3)-Eu(1)-O(10')	84.61(16)
O(5')-Eu(1)-O(10')	88.2(7)	O(10)-Eu(1)-O(10')	19.35(18)
O(4)#1-Eu(1)-O(10')	144.19(17)	O(5)-Eu(1)-O(10')	75.2(8)
O(6)#1-Eu(1)-O(10')	129.8(5)	O(9)-Eu(1)-O(10')	67.38(16)
O(2)#2-Eu(1)-O(10')	93.13(16)	O(6')#1-Eu(1)-O(1)#2	74.1(4)
O(3)-Eu(1)-O(1)#2	90.25(11)	O(5')-Eu(1)-O(1)#2	154.4(7)
O(10)-Eu(1)-O(1)#2	80.99(17)	O(4)#1-Eu(1)-O(1)#2	125.57(10)
O(5)-Eu(1)-O(1)#2	142.2(7)	O(6)#1-Eu(1)-O(1)#2	68.1(4)
O(9)-Eu(1)-O(1)#2	99.72(11)	O(2)#2-Eu(1)-O(1)#2	50.97(9)
O(10')-Eu(1)-O(1)#2	67.40(15)	O(6')#1-Eu(1)-O(3)#1	67.4(3)
O(3)-Eu(1)-O(3)#1	75.15(10)	O(5')-Eu(1)-O(3)#1	60.0(8)
O(10)-Eu(1)-O(3)#1	125.65(17)	O(4)#1-Eu(1)-O(3)#1	49.85(10)
O(5)-Eu(1)-O(3)#1	73.1(7)	O(6)#1-Eu(1)-O(3)#1	71.8(3)
O(9)-Eu(1)-O(3)#1	114.46(10)	O(2)#2-Eu(1)-O(3)#1	121.41(10)
O(10')-Eu(1)-O(3)#1	144.54(15)	O(1)#2-Eu(1)-O(3)#1	139.81(10)
O(12)-Co(2)-O(12)#3	173.17(15)	O(12)#3-Co(2)-O(11)	86.58(8)
O(12)-Co(2)-O(11)	86.58(8)	O(12)-Co(2)-O(13)	93.42(8)
O(12)#3-Co(2)-O(13)	93.42(8)	O(11)-Co(2)-O(13)	180.000(1)
O(12)-Co(2)-N(1)#3	88.03(11)	O(12)#3-Co(2)-N(1)#3	91.91(11)
O(11)-Co(2)-N(1)#3	89.48(8)	O(13)-Co(2)-N(1)#3	90.52(8)

O(12)-Co(2)-N(1)	91.91(11)	O(12)#3-Co(2)-N(1)	88.03(11)
O(11)-Co(2)-N(1)	89.48(8)	O(13)-Co(2)-N(1)	90.52(8)
N(1)#3-Co(2)-N(1)	178.97(17)		
#1 $-x+3/2, -y-1/2, -z+1$	#2 $x, -y, z-1/2$	#3 $-x+1, y, -z+1/2$	#4 $x, -y, z+1/2$

3

O(4)-Gd(1)#1	2.313(4)	O(4)-Gd(1)#2	2.829(4)
O(3)-Gd(1)#2	2.395(4)	Gd(1)-O(4)#3	2.313(4)
Gd(1)-O(5)	2.359(4)	Gd(1)-O(8)#4	2.373(4)
Gd(1)-O(3)#5	2.395(4)	Gd(1)-O(13)	2.414(4)
Gd(1)-O(12)	2.473(4)	Gd(1)-O(2)	2.475(3)
Gd(1)-O(1)	2.559(4)	Gd(1)-O(4)#5	2.829(4)
Co-O(9)	2.082(4)	Co-O(9)#6	2.082(4)
Co-O(10)	2.097(6)	Co-N(1)#6	2.112(4)
Co-N(1)	2.112(4)	Co-O(11)	2.133(7)
O(4)#3-Gd(1)-O(5)	77.75(14)	O(4)#3-Gd(1)-O(8)#4	80.71(13)
O(5)-Gd(1)-O(8)#4	133.20(13)	O(4)#3-Gd(1)-O(3)#5	124.49(13)
O(5)-Gd(1)-O(3)#5	77.27(14)	O(8)#4-Gd(1)-O(3)#5	81.74(13)
O(4)#3-Gd(1)-O(13)	78.45(15)	O(5)-Gd(1)-O(13)	136.76(15)
O(8)#4-Gd(1)-O(13)	76.68(14)	O(3)#5-Gd(1)-O(13)	145.31(14)
O(4)#3-Gd(1)-O(12)	145.46(14)	O(5)-Gd(1)-O(12)	136.69(14)
O(8)#4-Gd(1)-O(12)	75.02(13)	O(3)#5-Gd(1)-O(12)	76.03(14)
O(13)-Gd(1)-O(12)	72.35(15)	O(4)#3-Gd(1)-O(2)	137.65(12)
O(5)-Gd(1)-O(2)	73.82(13)	O(8)#4-Gd(1)-O(2)	141.22(13)
O(3)#5-Gd(1)-O(2)	78.66(12)	O(13)-Gd(1)-O(2)	101.90(15)
O(12)-Gd(1)-O(2)	67.94(13)	O(4)#3-Gd(1)-O(1)	90.32(13)
O(5)-Gd(1)-O(1)	71.39(14)	O(8)#4-Gd(1)-O(1)	149.73(14)
O(3)#5-Gd(1)-O(1)	126.03(13)	O(13)-Gd(1)-O(1)	73.20(14)
O(12)-Gd(1)-O(1)	98.37(14)	O(2)-Gd(1)-O(1)	51.14(13)
O(4)#3-Gd(1)-O(4)#5	75.48(14)	O(5)-Gd(1)-O(4)#5	68.66(12)
O(8)#4-Gd(1)-O(4)#5	65.91(12)	O(3)#5-Gd(1)-O(4)#5	49.32(11)
O(13)-Gd(1)-O(4)#5	137.04(14)	O(12)-Gd(1)-O(4)#5	114.87(12)
O(2)-Gd(1)-O(4)#5	120.36(12)	O(1)-Gd(1)-O(4)#5	139.55(13)
O(9)-Co-O(9)#6	172.9(2)	O(9)-Co-O(10)	86.45(12)
O(9)#6-Co-O(10)	86.45(12)	O(9)-Co-N(1)#6	87.55(17)
O(9)#6-Co-N(1)#6	92.46(17)	O(10)-Co-N(1)#6	90.11(14)
O(9)-Co-N(1)	92.46(17)	O(9)#6-Co-N(1)	87.55(17)
O(10)-Co-N(1)	90.11(14)	N(1)#6-Co-N(1)	179.8(3)
O(9)-Co-O(11)	93.55(12)	O(9)#6-Co-O(11)	93.55(12)
O(10)-Co-O(11)	180.000(1)	N(1)#6-Co-O(11)	89.89(14)
N(1)-Co-O(11)	89.89(14)		
#1 $x, -y, z-1/2$	#2 $-x+3/2, y-1/2, -z+3/2$	#3 $x, -y, z+1/2$	#4 $-x+3/2, -y+1/2, -z+2$
#5 $-x+3/2, y+1/2, -z+3/2$	#6 $-x+1, y, -z+1/2$		

4

Tb(1)-O(4)	2.291(2)	Tb(1)-O(6)#1	2.349(2)
------------	----------	--------------	----------

Tb(1)-O(5)	2.349(2)	Tb(1)-O(9)	2.355(2)
Tb(1)-O(3)	2.363(2)	Tb(1)-O(1)	2.432(2)
Tb(1)-O(10)	2.478(2)	Tb(1)-O(2)	2.620(2)
Tb(1)-O(4)#1	2.887(2)	Co-O(13)	2.091(3)
Co-N(1)#2	2.109(3)	Co-N(1)	2.109(3)
Co-O(12)#2	2.113(2)	Co-O(12)	2.113(2)
Co-O(11)	2.122(4)		
O(4)-Tb(1)-O(6)#1	81.26(8)	O(4)-Tb(1)-O(5)	80.37(8)
O(6)#1-Tb(1)-O(5)	130.54(8)	O(4)-Tb(1)-O(9)	80.63(8)
O(6)#1-Tb(1)-O(9)	79.95(8)	O(5)-Tb(1)-O(9)	140.27(9)
O(4)-Tb(1)-O(3)	125.02(8)	O(6)#1-Tb(1)-O(3)	79.11(8)
O(5)-Tb(1)-O(3)	74.93(9)	O(9)-Tb(1)-O(3)	143.28(9)
O(4)-Tb(1)-O(1)	135.88(8)	O(6)#1-Tb(1)-O(1)	142.36(8)
O(5)-Tb(1)-O(1)	73.10(8)	O(9)-Tb(1)-O(1)	97.91(8)
O(3)-Tb(1)-O(1)	81.22(8)	O(4)-Tb(1)-O(10)	146.79(8)
O(6)#1-Tb(1)-O(10)	74.26(8)	O(5)-Tb(1)-O(10)	132.76(8)
O(9)-Tb(1)-O(10)	73.37(8)	O(3)-Tb(1)-O(10)	72.09(8)
O(1)-Tb(1)-O(10)	69.26(7)	O(4)-Tb(1)-O(2)	87.07(8)
O(6)#1-Tb(1)-O(2)	152.69(8)	O(5)-Tb(1)-O(2)	70.67(8)
O(9)-Tb(1)-O(2)	73.82(8)	O(3)-Tb(1)-O(2)	127.21(8)
O(1)-Tb(1)-O(2)	51.25(7)	O(10)-Tb(1)-O(2)	104.68(8)
O(4)-Tb(1)-O(4)#1	76.48(8)	O(6)#1-Tb(1)-O(4)#1	64.38(7)
O(5)-Tb(1)-O(4)#1	66.80(8)	O(9)-Tb(1)-O(4)#1	139.85(8)
O(3)-Tb(1)-O(4)#1	48.72(7)	O(1)-Tb(1)-O(4)#1	121.43(7)
O(10)-Tb(1)-O(4)#1	111.21(7)	O(2)-Tb(1)-O(4)#1	136.27(7)
O(13)-Co-N(1)#2	89.85(8)	O(13)-Co-N(1)	89.85(8)
N(1)#2-Co-N(1)	179.70(17)	O(13)-Co-O(12)#2	86.93(7)
N(1)#2-Co-O(12)#2	93.20(10)	N(1)-Co-O(12)#2	86.78(10)
O(13)-Co-O(12)	86.93(7)	N(1)#2-Co-O(12)	86.78(10)
N(1)-Co-O(12)	93.20(10)	O(12)#2-Co-O(12)	173.86(13)
O(13)-Co-O(11)	180.0	N(1)#2-Co-O(11)	90.15(8)
N(1)-Co-O(11)	90.15(8)	O(12)#2-Co-O(11)	93.07(7)
O(12)-Co-O(11)	93.07(7)		
#1 -x+1/2,-y+1/2,-z+1	#2 -x,y,-z-1/2	#3 -x+1/2,y-1/2,-z+1/2	#4 -x+1/2,y+1/2,-z+1/2

5

Co(1)-O(13)	2.093(5)	Co(1)-O(12)	2.100(3)
Co(1)-O(12)#1	2.100(3)	Co(1)-N(1)	2.108(4)
Co(1)-N(1)#1	2.108(4)	Co(1)-O(11)	2.147(5)
Dy(1)-O(2)	2.286(3)	Dy(1)-O(7)#2	2.328(3)
Dy(1)-O(5)	2.332(3)	Dy(1)-O(1)#2	2.353(3)
Dy(1)-O(10)	2.400(3)	Dy(1)-O(9)	2.442(3)
Dy(1)-O(3)	2.451(3)	Dy(1)-O(4)	2.525(3)
Dy(1)-O(2)#2	2.838(3)		
O(13)-Co(1)-O(12)	87.05(9)	O(13)-Co(1)-O(12)#1	87.05(9)

O(12)-Co(1)-O(12)#1	174.10(18)	O(13)-Co(1)-N(1)	90.31(11)
O(12)-Co(1)-N(1)	87.90(14)	O(12)#1-Co(1)-N(1)	92.13(14)
O(13)-Co(1)-N(1)#1	90.31(11)	O(12)-Co(1)-N(1)#1	92.13(14)
O(12)#1-Co(1)-N(1)#1	87.90(14)	N(1)-Co(1)-N(1)#1	179.4(2)
O(13)-Co(1)-O(11)	180.000(1)	O(12)-Co(1)-O(11)	92.95(9)
O(12)#1-Co(1)-O(11)	92.95(9)	N(1)-Co(1)-O(11)	89.69(11)
N(1)#1-Co(1)-O(11)	89.69(11)	O(2)-Dy(1)-O(7)#2	77.89(12)
O(2)-Dy(1)-O(5)	80.78(11)	O(7)#2-Dy(1)-O(5)	133.27(12)
O(2)-Dy(1)-O(1)#2	123.99(11)	O(7)#2-Dy(1)-O(1)#2	77.21(13)
O(5)-Dy(1)-O(1)#2	81.28(12)	O(2)-Dy(1)-O(10)	77.37(14)
O(7)#2-Dy(1)-O(10)	136.91(13)	O(5)-Dy(1)-O(10)	75.80(14)
O(1)#2-Dy(1)-O(10)	145.56(13)	O(2)-Dy(1)-O(9)	145.07(11)
O(7)#2-Dy(1)-O(9)	136.94(12)	O(5)-Dy(1)-O(9)	74.68(11)
O(1)#2-Dy(1)-O(9)	76.56(11)	O(10)-Dy(1)-O(9)	72.82(13)
O(2)-Dy(1)-O(3)	137.81(11)	O(7)#2-Dy(1)-O(3)	73.33(12)
O(5)-Dy(1)-O(3)	141.10(11)	O(1)#2-Dy(1)-O(3)	78.64(11)
O(10)-Dy(1)-O(3)	103.86(14)	O(9)-Dy(1)-O(3)	68.44(11)
O(2)-Dy(1)-O(4)	90.17(11)	O(7)#2-Dy(1)-O(4)	71.36(12)
O(5)-Dy(1)-O(4)	149.70(12)	O(1)#2-Dy(1)-O(4)	126.64(11)
O(10)-Dy(1)-O(4)	74.01(13)	O(9)-Dy(1)-O(4)	98.60(12)
O(3)-Dy(1)-O(4)	51.74(11)	O(2)-Dy(1)-O(2)#2	75.32(11)
O(7)#2-Dy(1)-O(2)#2	68.81(11)	O(5)-Dy(1)-O(2)#2	65.75(10)
O(1)#2-Dy(1)-O(2)#2	48.96(10)	O(10)-Dy(1)-O(2)#2	135.55(13)
O(9)-Dy(1)-O(2)#2	114.96(11)	O(3)-Dy(1)-O(2)#2	119.93(10)
O(4)-Dy(1)-O(2)#2	139.60(11)		
#1 -x+1,y,-z+1/2	#2 -x+3/2,-y+3/2,-z+2	#3 x,-y+1,z-1/2	#4 x,-y+1,z+1/2

6

O(2)-Ho(1)#1	2.344(2)	O(1)-Ho(1)#2	2.270(2)
O(1)-Ho(1)#1	2.855(2)	Co(2)-O(13)	2.084(4)
Co(2)-O(11)	2.099(2)	Co(2)-O(11)#3	2.099(2)
Co(2)-N(1)#3	2.103(3)	Co(2)-N(1)	2.103(3)
Co(2)-O(12)	2.148(4)	Ho(1)-O(1)#4	2.270(2)
Ho(1)-O(5)	2.316(2)	Ho(1)-O(6)#5	2.326(2)
Ho(1)-O(2)#6	2.344(2)	Ho(1)-O(10)	2.386(3)
Ho(1)-O(9)	2.426(3)	Ho(1)-O(3)	2.443(2)
Ho(1)-O(4)	2.517(3)	Ho(1)-O(1)#6	2.855(2)
O(13)-Co(2)-O(11)	86.79(7)	O(13)-Co(2)-O(11)#3	86.79(7)
O(11)-Co(2)-O(11)#3	173.59(15)	O(13)-Co(2)-N(1)#3	90.34(9)
O(11)-Co(2)-N(1)#3	87.65(10)	O(11)#3-Co(2)-N(1)#3	92.39(10)
O(13)-Co(2)-N(1)	90.34(9)	O(11)-Co(2)-N(1)	92.39(10)
O(11)#3-Co(2)-N(1)	87.65(10)	N(1)#3-Co(2)-N(1)	179.32(18)
O(13)-Co(2)-O(12)	180.000(1)	O(11)-Co(2)-O(12)	93.21(7)
O(11)#3-Co(2)-O(12)	93.21(7)	N(1)#3-Co(2)-O(12)	89.66(9)
N(1)-Co(2)-O(12)	89.66(9)	O(1)#4-Ho(1)-O(5)	78.01(9)

O(1)#4-Ho(1)-O(6)#5	80.68(8)	O(5)-Ho(1)-O(6)#5	133.04(9)
O(1)#4-Ho(1)-O(2)#6	124.01(9)	O(5)-Ho(1)-O(2)#6	77.35(10)
O(6)#5-Ho(1)-O(2)#6	80.92(9)	O(1)#4-Ho(1)-O(10)	77.41(11)
O(5)-Ho(1)-O(10)	136.47(11)	O(6)#5-Ho(1)-O(10)	76.68(11)
O(2)#6-Ho(1)-O(10)	145.79(10)	O(1)#4-Ho(1)-O(9)	144.99(9)
O(5)-Ho(1)-O(9)	136.90(10)	O(6)#5-Ho(1)-O(9)	74.87(9)
O(2)#6-Ho(1)-O(9)	76.53(10)	O(10)-Ho(1)-O(9)	72.87(11)
O(1)#4-Ho(1)-O(3)	137.75(8)	O(5)-Ho(1)-O(3)	73.18(9)
O(6)#5-Ho(1)-O(3)	141.28(8)	O(2)#6-Ho(1)-O(3)	78.80(9)
O(10)-Ho(1)-O(3)	103.39(12)	O(9)-Ho(1)-O(3)	68.53(9)
O(1)#4-Ho(1)-O(4)	89.97(9)	O(5)-Ho(1)-O(4)	71.65(10)
O(6)#5-Ho(1)-O(4)	149.53(10)	O(2)#6-Ho(1)-O(4)	127.21(8)
O(10)-Ho(1)-O(4)	72.98(11)	O(9)-Ho(1)-O(4)	98.53(10)
O(3)-Ho(1)-O(4)	52.00(8)	O(1)#4-Ho(1)-O(1)#6	75.30(8)
O(5)-Ho(1)-O(1)#6	68.73(8)	O(6)#5-Ho(1)-O(1)#6	65.57(8)
O(2)#6-Ho(1)-O(1)#6	48.96(8)	O(10)-Ho(1)-O(1)#6	136.16(11)
O(9)-Ho(1)-O(1)#6	115.11(9)	O(3)-Ho(1)-O(1)#6	119.88(8)
O(4)-Ho(1)-O(1)#6	139.74(9)		
#1 -x+3/2,y-1/2,-z+3/2	#2 x,-y+1,z-1/2	#3 -x+1,y,-z+1/2	#4 x,-y+1,z+1/2
#5 -x+3/2,-y+3/2,-z+2	#6 -x+3/2,y+1/2,-z+3/2		

7

Er(1)-O(9)	2.295(3)	Er(1)-O(1)	2.301(3)
Er(1)-O(7)	2.311(3)	Er(1)-O(13)	2.335(3)
Er(1)-O(17)	2.352(3)	Er(1)-O(18)	2.376(3)
Er(1)-O(6)	2.378(3)	Er(1)-O(5)	2.458(3)
Er(2)-O(8)	2.226(3)	Er(2)-O(10)	2.302(3)
Er(2)-O(19)	2.341(3)	Er(2)-O(14)	2.350(3)
Er(2)-O(2)	2.351(3)	Er(2)-O(3)#1	2.364(3)
Er(2)-O(20)	2.433(3)	Er(2)-O(1)	2.672(3)
Er(2)-O(4)#1	2.786(3)	Co(1)-O(24)	2.053(3)
Co(1)-O(23)	2.103(3)	Co(1)-N(2)	2.109(4)
Co(1)-N(4)#2	2.112(4)	Co(1)-O(21)	2.140(3)
Co(1)-O(22)	2.141(3)	O(3)-Er(2)#3	2.364(3)
O(4)-Er(2)#3	2.786(3)		
O(9)-Er(1)-O(1)	72.08(11)	O(9)-Er(1)-O(7)	79.93(11)
O(1)-Er(1)-O(7)	116.26(10)	O(9)-Er(1)-O(13)	130.89(10)
O(1)-Er(1)-O(13)	80.12(11)	O(7)-Er(1)-O(13)	77.23(11)
O(9)-Er(1)-O(17)	141.26(11)	O(1)-Er(1)-O(17)	146.21(10)
O(7)-Er(1)-O(17)	82.86(11)	O(13)-Er(1)-O(17)	77.40(11)
O(9)-Er(1)-O(18)	133.22(12)	O(1)-Er(1)-O(18)	75.71(10)
O(7)-Er(1)-O(18)	145.87(12)	O(13)-Er(1)-O(18)	73.57(11)
O(17)-Er(1)-O(18)	73.93(11)	O(9)-Er(1)-O(6)	75.04(11)
O(1)-Er(1)-O(6)	97.90(11)	O(7)-Er(1)-O(6)	128.33(10)
O(13)-Er(1)-O(6)	149.90(10)	O(17)-Er(1)-O(6)	89.34(11)

O(18)-Er(1)-O(6)	76.84(11)	O(9)-Er(1)-O(5)	72.52(10)
O(1)-Er(1)-O(5)	139.32(11)	O(7)-Er(1)-O(5)	76.03(11)
O(13)-Er(1)-O(5)	139.62(10)	O(17)-Er(1)-O(5)	69.73(11)
O(18)-Er(1)-O(5)	116.99(10)	O(6)-Er(1)-O(5)	53.62(10)
O(8)-Er(2)-O(10)	79.71(11)	O(8)-Er(2)-O(19)	79.95(11)
O(10)-Er(2)-O(19)	80.40(11)	O(8)-Er(2)-O(14)	83.44(11)
O(10)-Er(2)-O(14)	135.89(10)	O(19)-Er(2)-O(14)	135.90(11)
O(8)-Er(2)-O(2)	131.32(11)	O(10)-Er(2)-O(2)	85.22(11)
O(19)-Er(2)-O(2)	142.33(11)	O(14)-Er(2)-O(2)	76.03(11)
O(8)-Er(2)-O(3)#1	130.57(11)	O(10)-Er(2)-O(3)#1	144.49(10)
O(19)-Er(2)-O(3)#1	86.91(11)	O(14)-Er(2)-O(3)#1	73.68(10)
O(2)-Er(2)-O(3)#1	84.97(10)	O(8)-Er(2)-O(20)	144.00(11)
O(10)-Er(2)-O(20)	74.08(11)	O(19)-Er(2)-O(20)	71.78(10)
O(14)-Er(2)-O(20)	132.51(10)	O(2)-Er(2)-O(20)	70.83(10)
O(3)#1-Er(2)-O(20)	70.46(11)	O(8)-Er(2)-O(1)	80.05(10)
O(10)-Er(2)-O(1)	69.33(9)	O(19)-Er(2)-O(1)	146.14(10)
O(14)-Er(2)-O(1)	67.74(10)	O(2)-Er(2)-O(1)	51.37(10)
O(3)#1-Er(2)-O(1)	126.67(9)	O(20)-Er(2)-O(1)	112.14(10)
O(8)-Er(2)-O(4)#1	81.11(10)	O(10)-Er(2)-O(4)#1	146.57(9)
O(19)-Er(2)-O(4)#1	69.45(10)	O(14)-Er(2)-O(4)#1	67.77(10)
O(2)-Er(2)-O(4)#1	127.67(10)	O(3)#1-Er(2)-O(4)#1	49.82(10)
O(20)-Er(2)-O(4)#1	108.25(10)	O(1)-Er(2)-O(4)#1	133.16(9)
O(24)-Co(1)-O(23)	85.70(13)	O(24)-Co(1)-N(2)	92.65(14)
O(23)-Co(1)-N(2)	93.13(13)	O(24)-Co(1)-N(4)#2	87.15(14)
O(23)-Co(1)-N(4)#2	87.42(13)	N(2)-Co(1)-N(4)#2	179.39(16)
O(24)-Co(1)-O(21)	172.47(12)	O(23)-Co(1)-O(21)	86.79(12)
N(2)-Co(1)-O(21)	87.17(14)	N(4)#2-Co(1)-O(21)	93.11(14)
O(24)-Co(1)-O(22)	97.58(12)	O(23)-Co(1)-O(22)	175.08(13)
N(2)-Co(1)-O(22)	90.39(13)	N(4)#2-Co(1)-O(22)	89.07(13)
O(21)-Co(1)-O(22)	89.95(12)		
#1 -x+2,y-1/2,-z+1/2	#2 -x+1,-y+1,-z+1	#3 -x+2,y+1/2,-z+1/2	#4 -x+1,y+1/2,-z+1/2
#5 -x+1,y-1/2,-z+1/2			