Solvent-regulated Assemblies of 1D Lanthanide Coordination Polymers with Tricarboxylate Ligand

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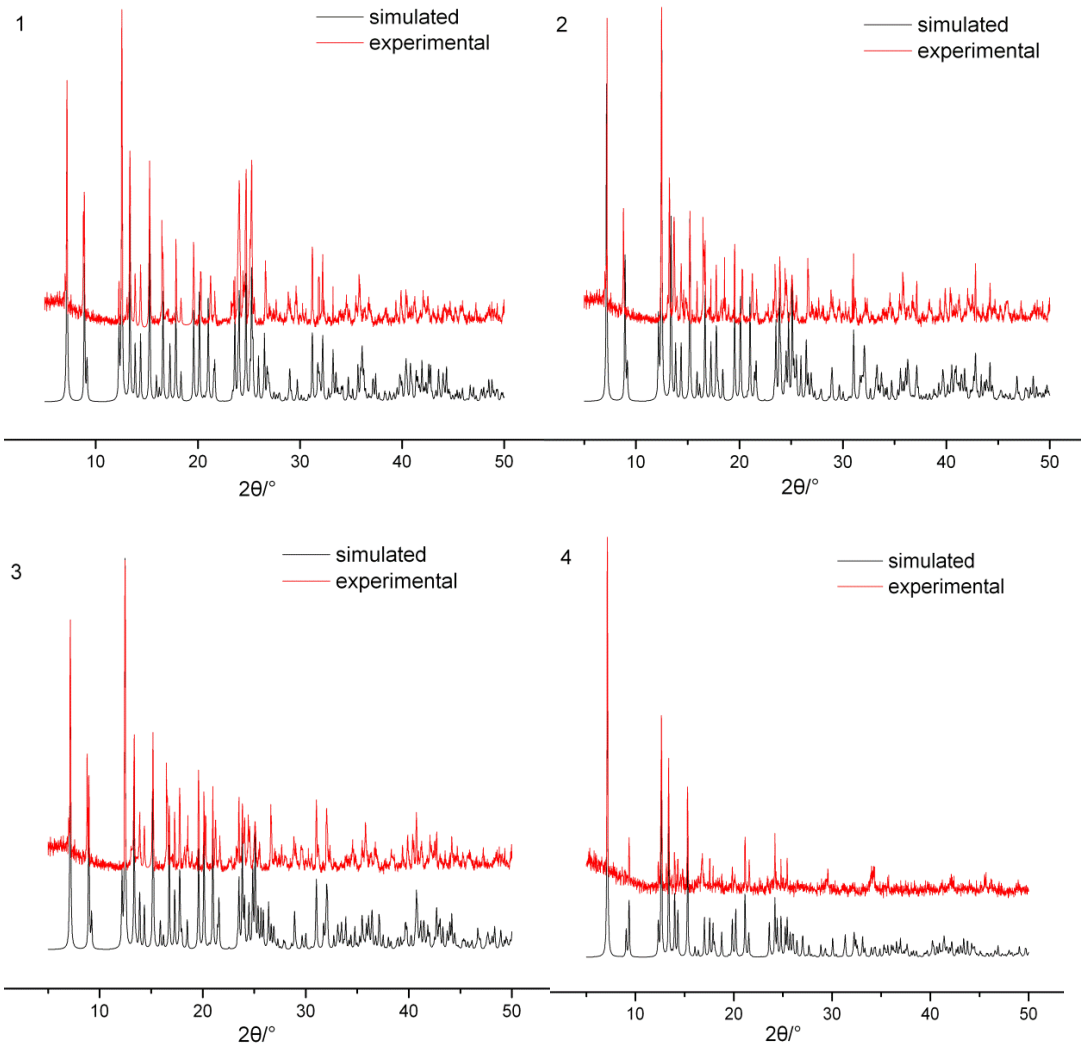

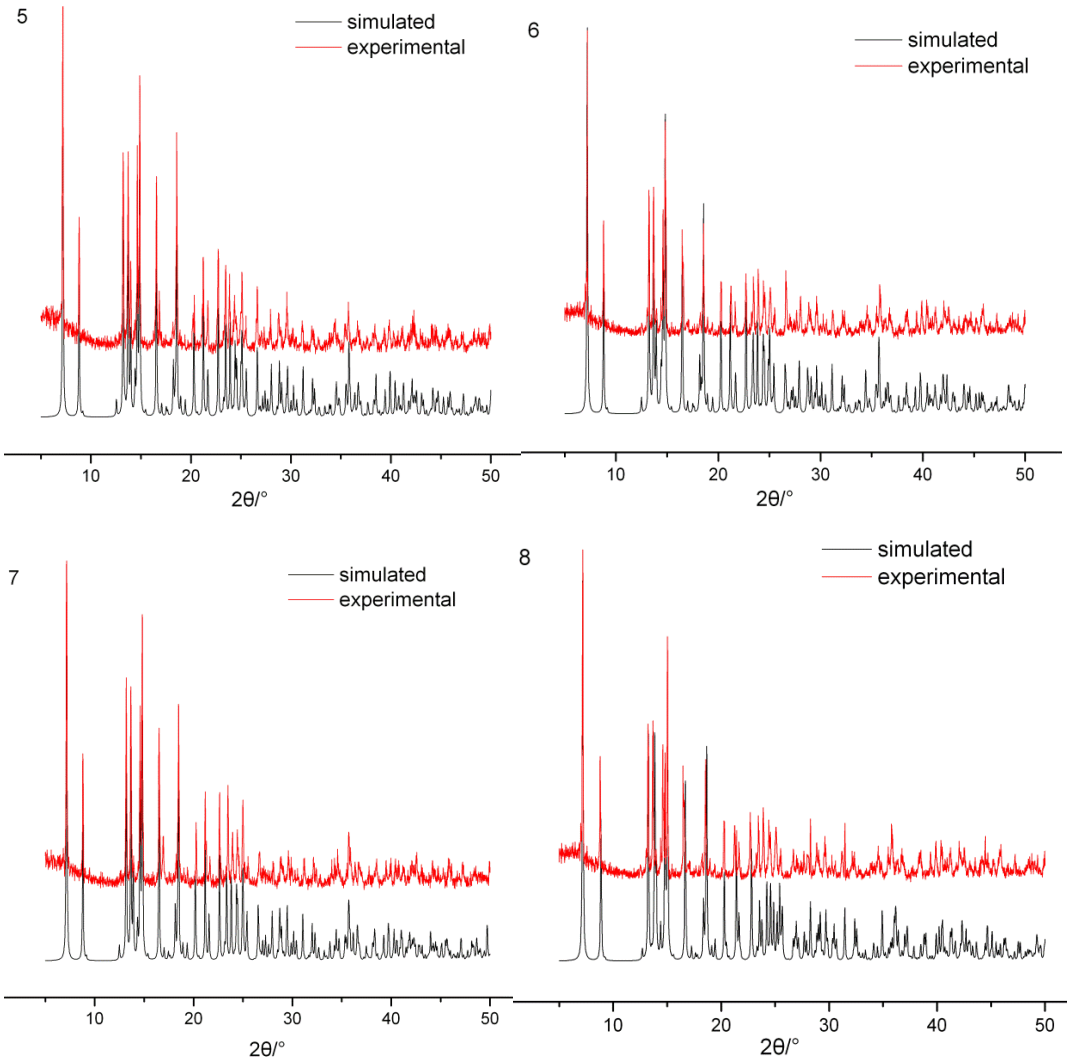

Fig.S1 The simulated and experimental PXRD patterns of **1**-**8**.

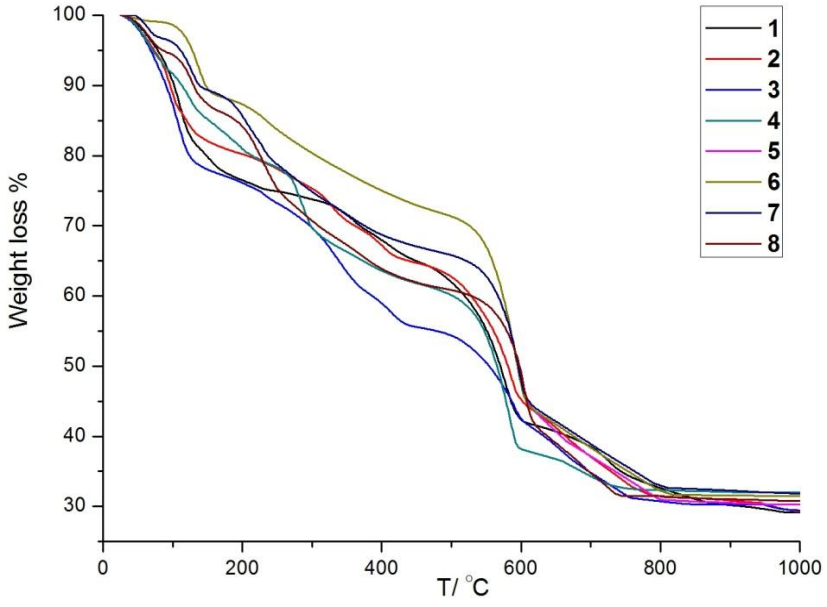

Fig. S2 TGA curves of **1**-**8**.

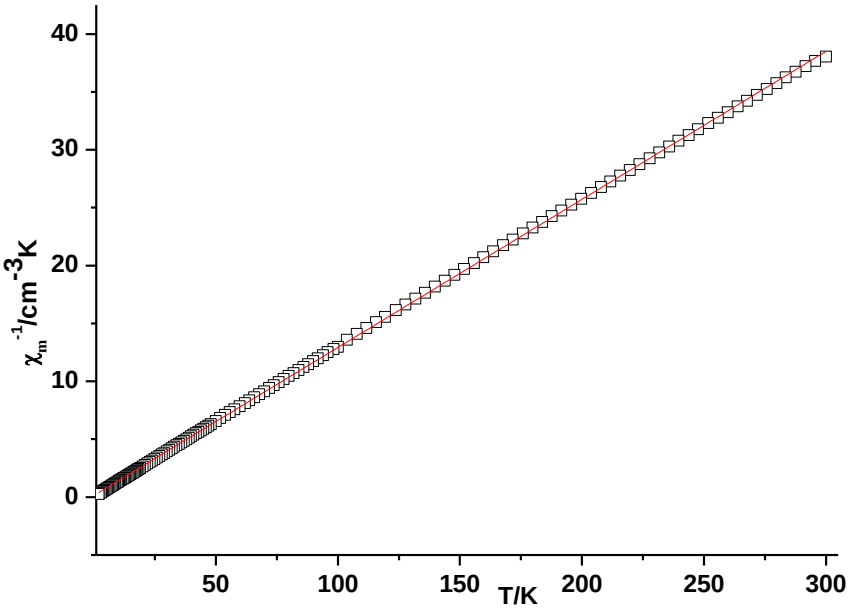

Fig. S3 plot of χ_m^{-1} *vs. T* for compound **6**.

Table S1 Bond lengths [Å] and angles [deg] for **1-8**.

		1	
La(1)-O(15)#1	2.413(2)	La(1)-O(7)	2.463(2)
La(1)-O(8)	2.509(2)	La(1)-O(9)	2.5379(2)
La(1)-O(10)#2	2.5585(19)	La(1)-O(13)	2.5782(19)
La(1)-O(5)	2.6344(19)	La(1)-O(11)#2	2.6482(19)
La(1)-O(6)	2.6733(19)		
O(15)#1-La(1)-O(7)	97.67(7)	O(15)#1-La(1)-O(8)	67.31(8)
O(7)-La(1)-O(8)	76.44(7)	O(15)#1-La(1)-O(9)	72.10(7)
O(7)-La(1)-O(9)	71.35(7)	O(8)-La(1)-O(9)	123.15(8)
O(15)#1-La(1)-O(10)#2	83.47(6)	O(7)-La(1)-O(10)#2	149.48(6)
O(8)-La(1)-O(10)#2	75.97(7)	O(9)-La(1)-O(10)#2	136.26(6)
O(15)#1-La(1)-O(13)	75.79(7)	O(7)-La(1)-O(13)	141.37(6)
O(8)-La(1)-O(13)	130.99(7)	O(9)-La(1)-O(13)	70.44(7)
O(10)#2-La(1)-O(13)	68.65(7)	O(15)#1-La(1)-O(5)	141.23(7)
O(7)-La(1)-O(5)	72.45(6)	O(8)-La(1)-O(5)	139.77(7)
O(9)-La(1)-O(5)	69.22(6)	O(10)#2-La(1)-O(5)	124.07(6)
O(13)-La(1)-O(5)	88.91(6)	O(15)#1-La(1)-O(11)#2	130.50(7)
O(7)-La(1)-O(11)#2	130.53(6)	O(8)-La(1)-O(11)#2	108.93(7)
O(9)-La(1)-O(11)#2	127.69(6)	O(10)#2-La(1)-O(11)#2	50.04(6)
O(13)-La(1)-O(11)#2	72.28(6)	O(5)-La(1)-O(11)#2	74.75(6)
O(15)#1-La(1)-O(6)	135.02(7)	O(7)-La(1)-O(6)	71.53(6)
O(8)-La(1)-O(6)	67.71(7)	O(9)-La(1)-O(6)	136.47(6)
O(10)#2-La(1)-O(6)	86.08(6)	O(13)-La(1)-O(6)	138.63(6)
O(5)-La(1)-O(6)	78.56(7)	O(11)#2-La(1)-O(6)	66.41(6)

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

2

Pr(1)-O(3)#1	2.372(3)	Pr(1)-O(4)#2	2.420(3)
Pr(1)-O(10)	2.494(4)	Pr(1)-O(11)	2.511(3)
Pr(1)-O(2)	2.523(3)	Pr(1)-O(9)	2.533(3)
Pr(1)-O(8)	2.566(3)	Pr(1)-O(1)	2.608(3)
Pr(1)-O(7)	2.641(3)		
O(3)#1-Pr(1)-O(4)#2	96.87(11)	O(3)#1-Pr(1)-O(10)	67.93(12)
O(4)#2-Pr(1)-O(10)	75.99(12)	O(3)#1-Pr(1)-O(11)	73.11(12)
O(4)#2-Pr(1)-O(11)	73.01(11)	O(10)-Pr(1)-O(11)	125.92(14)
O(3)#1-Pr(1)-O(2)	83.75(10)	O(4)#2-Pr(1)-O(2)	148.91(11)
O(10)-Pr(1)-O(2)	75.53(12)	O(11)-Pr(1)-O(2)	135.40(10)
O(3)#1-Pr(1)-O(9)	77.02(12)	O(4)#2-Pr(1)-O(9)	141.82(11)
O(10)-Pr(1)-O(9)	131.95(11)	O(11)-Pr(1)-O(9)	69.14(11)
O(2)-Pr(1)-O(9)	68.77(11)	O(3)#1-Pr(1)-O(8)	142.13(12)
O(4)#2-Pr(1)-O(8)	73.79(11)	O(10)-Pr(1)-O(8)	139.28(11)
O(11)-Pr(1)-O(8)	69.05(11)	O(2)-Pr(1)-O(8)	123.09(10)
O(9)-Pr(1)-O(8)	88.06(11)	O(3)#1-Pr(1)-O(1)	131.55(10)
O(4)#2-Pr(1)-O(1)	130.11(10)	O(10)-Pr(1)-O(1)	108.08(12)
O(11)-Pr(1)-O(1)	125.83(11)	O(2)-Pr(1)-O(1)	50.61(9)
O(9)-Pr(1)-O(1)	72.20(10)	O(8)-Pr(1)-O(1)	73.22(10)
O(3)#1-Pr(1)-O(7)	135.47(12)	O(4)#2-Pr(1)-O(7)	71.35(11)
O(10)-Pr(1)-O(7)	67.55(12)	O(11)-Pr(1)-O(7)	136.26(11)
O(2)-Pr(1)-O(7)	86.41(11)	O(9)-Pr(1)-O(7)	137.69(11)
O(8)-Pr(1)-O(7)	77.27(12)	O(1)-Pr(1)-O(7)	65.61(10)

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

3

Nd(1)-O(13)#1	2.339(6)	Nd(1)-O(15)#2	2.421(6)
Nd(1)-O(28)	2.505(8)	Nd(1)-O(9)	2.509(6)
Nd(1)-O(6)	2.514(5)	Nd(1)-O(3)	2.516(5)
Nd(1)-O(21)	2.517(6)	Nd(1)-O(12)	2.572(6)
Nd(1)-O(26)	2.619(7)		
O(13)#1-Nd(1)-O(15)#2	96.9(2)	O(13)#1-Nd(1)-O(28)	67.8(3)
O(15)#2-Nd(1)-O(28)	74.6(2)	O(13)#1-Nd(1)-O(9)	74.3(2)
O(15)#2-Nd(1)-O(9)	73.9(2)	O(28)-Nd(1)-O(9)	126.3(3)
O(13)#1-Nd(1)-O(6)	78.0(2)	O(15)#2-Nd(1)-O(6)	143.3(2)
O(28)-Nd(1)-O(6)	132.7(2)	O(9)-Nd(1)-O(6)	69.8(2)
O(13)#1-Nd(1)-O(3)	82.6(2)	O(15)#2-Nd(1)-O(3)	147.8(2)
O(28)-Nd(1)-O(3)	75.6(2)	O(9)-Nd(1)-O(3)	135.3(2)
O(6)-Nd(1)-O(3)	68.3(2)	O(13)#1-Nd(1)-O(21)	143.8(2)
O(15)#2-Nd(1)-O(21)	74.4(2)	O(28)-Nd(1)-O(21)	137.9(3)
O(9)-Nd(1)-O(21)	69.5(2)	O(6)-Nd(1)-O(21)	88.3(2)
O(3)-Nd(1)-O(21)	123.33(19)	O(13)#1-Nd(1)-O(12)	131.7(2)
O(15)#2-Nd(1)-O(12)	128.9(2)	O(28)-Nd(1)-O(12)	106.4(3)

O(9)-Nd(1)-O(12)	127.3(2)	O(6)-Nd(1)-O(12)	73.2(2)
O(3)-Nd(1)-O(12)	51.07(18)	O(21)-Nd(1)-O(12)	73.2(2)
O(13)#1-Nd(1)-O(26)	133.5(3)	O(15)#2-Nd(1)-O(26)	70.2(2)
O(28)-Nd(1)-O(26)	65.7(3)	O(9)-Nd(1)-O(26)	136.3(2)
O(6)-Nd(1)-O(26)	137.9(2)	O(3)-Nd(1)-O(26)	86.8(2)
O(21)-Nd(1)-O(26)	77.4(3)	O(12)-Nd(1)-O(26)	64.8(2)

#1 -x,-y,-z; #2 x,-y,z-1/2; #3 x,-y,z+1/2; #4 -x+1/2,-y+3/2,-z

4

Sm(1)-O(2)#1	2.294(5)	Sm(1)-O(1)	2.338(5)
Sm(1)-O(8)	2.448(5)	Sm(1)-O(11)	2.458(5)
Sm(1)-O(7)	2.468(7)	Sm(1)-O(9)	2.469 (5)
Sm(1)-O(3)#2	2.477(4)	Sm(1)-O(4)#2	2.520(5)
Sm(1)-O(10)	2.658(9)		
O(2)#1-Sm(1)-O(1)	96.54(18)	O(2)#1-Sm(1)-O(8)	75.26(19)
O(1)-Sm(1)-O(8)	74.63(17)	O(2)#1-Sm(1)-O(11)	79.51(19)
O(1)-Sm(1)-O(11)	144.12(18)	O(8)-Sm(1)-O(11)	69.86(16)
O(2)#1-Sm(1)-O(7)	68.9(2)	O(1)-Sm(1)-O(7)	73.6(2)
O(8)-Sm(1)-O(7)	128.2(3)	O(11)-Sm(1)-O(7)	134.4(2)
O(2)#1-Sm(1)-O(9)	146.4(2)	O(1)-Sm(1)-O(9)	75.3(2)
O(8)-Sm(1)-O(9)	71.13(18)	O(11)-Sm(1)-O(9)	88.4(2)
O(7)-Sm(1)-O(9)	135.3(2)	O(2)#1-Sm(1)-O(3)#2	82.85(17)
O(1)-Sm(1)-O(3)#2	146.73(18)	O(8)-Sm(1)-O(3)#2	135.86(16)
O(11)-Sm(1)-O(3)#2	68.73(18)	O(7)-Sm(1)-O(3)#2	75.2(2)
O(9)-Sm(1)-O(3)#2	121.75(17)	O(2)#1-Sm(1)-O(4)#2	133.52(16)
O(1)-Sm(1)-O(4)#2	125.80(17)	O(8)-Sm(1)-O(4)#2	129.27(19)
O(11)-Sm(1)-O(4)#2	76.01(18)	O(7)-Sm(1)-O(4)#2	102.5(3)
O(9)-Sm(1)-O(4)#2	71.52(18)	O(3)#2-Sm(1)-O(4)#2	51.57(15)
O(2)#1-Sm(1)-O(10)	132.2(3)	O(1)-Sm(1)-O(10)	69.0(2)
O(8)-Sm(1)-O(10)	135.8(2)	O(11)-Sm(1)-O(10)	138.0(2)
O(7)-Sm(1)-O(10)	63.3(3)	O(9)-Sm(1)-O(10)	76.0(3)
O(3)#2-Sm(1)-O(10)	86.7(2)	O(4)#2-Sm(1)-O(10)	62.2(2)

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

5

Eu(1)-O(3)#1	2.291(4)	Eu(1)-O(5)#2	2.359(4)
Eu(1)-O(7)	2.405(4)	Eu(1)-O(8)	2.421(4)
Eu(1)-O(9)	2.419(4)	Eu(1)-O(10)	2.435(4)
Eu(1)-O(2)	2.470(4)	Eu(1)-O(1)	2.478(4)
O(3)#1-Eu(1)-O(5)#2	118.52(16)	O(3)#1-Eu(1)-O(7)	143.60(18)
O(5)#2-Eu(1)-O(7)	76.18(16)	O(3)#1-Eu(1)-O(9)	73.81(19)
O(5)#2-Eu(1)-O(9)	74.12(15)	O(7)-Eu(1)-O(9)	141.31(18)
O(3)#1-Eu(1)-O(8)	75.73(16)	O(5)#2-Eu(1)-O(8)	80.42(15
O(7)-Eu(1)-O(8)	74.41(16)	O(9)-Eu(1)-O(8)	123.39(19)
O(3)#1-Eu(1)-O(10)	79.31(17)	O(5)#2-Eu(1)-O(10)	148.62(15)
O(7)-Eu(1)-O(10)	75.27(16)	O(9)-Eu(1)-O(10)	137.26(15)

O(8)-Eu(1)-O(10)	79.63(15)	O(3)#1-Eu(1)-O(2)	131.48(14)
O(5)#2-Eu(1)-O(2)	97.84(15)	O(7)-Eu(1)-O(2)	72.03(15)
O(9)-Eu(1)-O(2)	88.02(18)	O(8)-Eu(1)-O(2)	145.77(16)
O(10)-Eu(1)-O(2)	85.52(15)	O(3)#1-Eu(1)-O(1)	79.04(14)
O(5)#2-Eu(1)-O(1)	136.73(14)	O(7)-Eu(1)-O(1)	114.21(14)
O(9)-Eu(1)-O(1)	74.10(15)	O(8)-Eu(1)-O(1)	142.39(14)
O(10)-Eu(1)-O(1)	68.55(14)	O(2)-Eu(1)-O(1)	52.58(13)

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

6

Gd(1)-O(5)#1	2.280(4)	Gd(1)-O(1)	2.360(4)
Gd(1)-O(10)	2.396(4)	Gd(1)-O(8)	2.413(4)
Gd(1)-O(9)	2.417(4)	Gd(1)-O(7)	2.432(4)
Gd(1)-O(3)#2	2.466(4)	Gd(1)-O(4)#2	2.482(3)
O(5)#1-Gd(1)-O(1)	118.11(16)	O(5)#1-Gd(1)-O(10)	143.94(17)
O(1)-Gd(1)-O(10)	76.36(15)	O(5)#1-Gd(1)-O(8)	75.55(15)
O(1)-Gd(1)-O(8)	80.41(14)	O(10)-Gd(1)-O(8)	74.84(15)
O(5)#1-Gd(1)-O(9)	73.52(18)	O(1)-Gd(1)-O(9)	73.99(14)
O(10)-Gd(1)-O(9)	141.26(16)	O(8)-Gd(1)-O(9)	123.08(17)
O(5)#1-Gd(1)-O(7)	79.94(17)	O(1)-Gd(1)-O(7)	148.69(15)
O(10)-Gd(1)-O(7)	75.07(15)	O(8)-Gd(1)-O(7)	80.01(14)
O(9)-Gd(1)-O(7)	137.32(14)	O(5)#1-Gd(1)-O(3)#2	131.68(14)
O(1)-Gd(1)-O(3)#2	97.74(14)	O(10)-Gd(1)-O(3)#2	71.84(15)
O(8)-Gd(1)-O(3)#2	146.05(15)	O(9)-Gd(1)-O(3)#2	88.00(16)
O(7)-Gd(1)-O(3)#2	85.33(14)	O(5)#1-Gd(1)-O(4)#2	79.09(14)
O(1)-Gd(1)-O(4)#2	136.59(13)	O(10)-Gd(1)-O(4)#2	114.21(13)
O(8)-Gd(1)-O(4)#2	142.45(13)	O(9)-Gd(1)-O(4)#2	73.96(13)
O(7)-Gd(1)-O(4)#2	68.56(13)	O(3)#2-Gd(1)-O(4)#2	52.76(12)

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

7

Tb(1)-O(6)#1	2.283(3)	Tb(1)-O(3)#2	2.341(3)
Tb(1)-O(7)	2.392(3)	Tb(1)-O(9)	2.406(3)
Tb(1)-O(8)	2.420(3)	Tb(1)-O(2)	2.463(3)
Tb(1)-O(1)	2.470(3)	O(3)-Tb(1)#2	2.341(3)
O(6)#1-Tb(1)-O(3)#2	118.71(13)	O(6)#1-Tb(1)-O(7)	143.60(14)
O(3)#2-Tb(1)-O(7)	76.19(12)	O(6)#1-Tb(1)-O(9)	74.24(15)
O(3)#2-Tb(1)-O(9)	74.08(11)	O(7)-Tb(1)-O(9)	140.98(13)
O(6)#1-Tb(1)-O(10)	75.06(13)	O(3)#2-Tb(1)-O(10)	80.44(12)
O(7)-Tb(1)-O(10)	75.33(13)	O(9)-Tb(1)-O(10)	122.97(15)
O(6)#1-Tb(1)-O(8)	79.28(14)	O(3)#2-Tb(1)-O(8)	148.60(12)
O(7)-Tb(1)-O(8)	75.19(12)	O(9)-Tb(1)-O(8)	137.31(11)
O(10)-Tb(1)-O(8)	80.08(12)	O(6)#1-Tb(1)-O(2)	131.81(11)
O(3)#2-Tb(1)-O(2)	97.20(11)	O(7)-Tb(1)-O(2)	71.81(11)
O(9)-Tb(1)-O(2)	87.42(14)	O(10)-Tb(1)-O(2)	146.61(12)
O(8)-Tb(1)-O(2)	85.93(12)	O(6)#1-Tb(1)-O(1)	78.95(11)

O(3)#2-Tb(1)-O(1)	136.29(11)	O(7)-Tb(1)-O(1)	114.39(11)
O(9)-Tb(1)-O(1)	73.48(11)	O(10)-Tb(1)-O(1)	142.62(11)
O(8)-Tb(1)-O(1)	68.97(11)	O(2)-Tb(1)-O(1)	53.00(9)
#1 -x+1,-y,-z+2; #2 -x,-y,-z+2			

8

Dy(2)-O(3)#1	2.271(2)	Dy(2)-O(6)#2	2.3322(19)
Dy(2)-O(10)	2.3662(19)	Dy(2)-O(8)	2.3755(18)
Dy(2)-O(9)	2.3757(18)	Dy(2)-O(7)	2.3935(18)
Dy(2)-O(1)	2.4428(19)	Dy(2)-O(2)	2.4450(18)
O(3)#1-Dy(2)-O(6)#2	119.73(7)	O(3)#1-Dy(2)-O(10)	142.94(7)
O(6)#2-Dy(2)-O(10)	76.09(7)	O(3)#1-Dy(2)-O(8)	74.30(7)
O(6)#2-Dy(2)-O(8)	80.76(6)	O(10)-Dy(2)-O(8)	76.01(7)
O(3)#1-Dy(2)-O(9)	74.01(7)	O(6)#2-Dy(2)-O(9)	74.14(6)
O(10)-Dy(2)-O(9)	141.84(6)	O(8)-Dy(2)-O(9)	121.30(8)
O(3)#1-Dy(2)-O(7)	78.58(7)	O(6)#2-Dy(2)-O(7)	148.70(6)
O(10)-Dy(2)-O(7)	75.12(6)	O(8)-Dy(2)-O(7)	80.61(7)
O(9)-Dy(2)-O(7)	137.16(6)	O(3)#1-Dy(2)-O(1)	132.56(7)
O(6)#2-Dy(2)-O(1)	95.99(7)	O(10)-Dy(2)-O(1)	71.18(7)
O(8)-Dy(2)-O(1)	146.80(6)	O(9)-Dy(2)-O(1)	88.72(7)
O(7)-Dy(2)-O(1)	86.19(7)	O(3)#1-Dy(2)-O(2)	79.20(7)
O(6)#2-Dy(2)-O(2)	135.78(6)	O(10)-Dy(2)-O(2)	113.99(6)
O(8-Dy(2)-O(2)	142.82(6)	O(9)-Dy(2)-O(2)	74.12(6)
O(7)-Dy(2)-O(2)	68.82(7)	O(1)-Dy(2)-O(2)	53.46(6)
#1 -x,-y+1,-z; #2 -x+1,-y+1,-z			