Supplementary Material (ESI) for CrystEngComm

Synthesis, Structure and Luminescent Properties of Coordination Polymers with 1,2-Benzenedicarboxylic and Series of Flexible Dicarboxylate ligands

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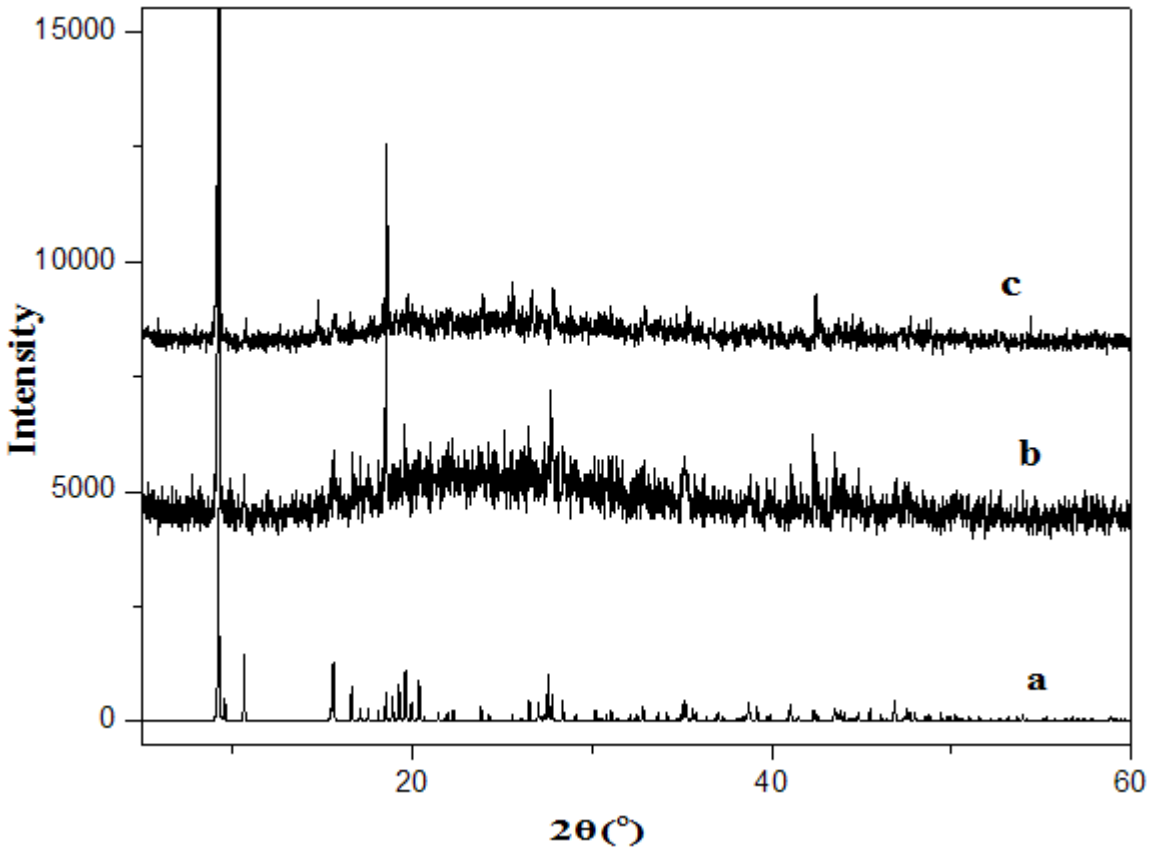


Figure S1 XRD powder patterns of complex **1**: (a) the simulated XPRD pattern calculated from single-crystal structure of complex **1**; (b) experimental XPRD for complex **1**; (c) experimental XPRD for complex **2**.

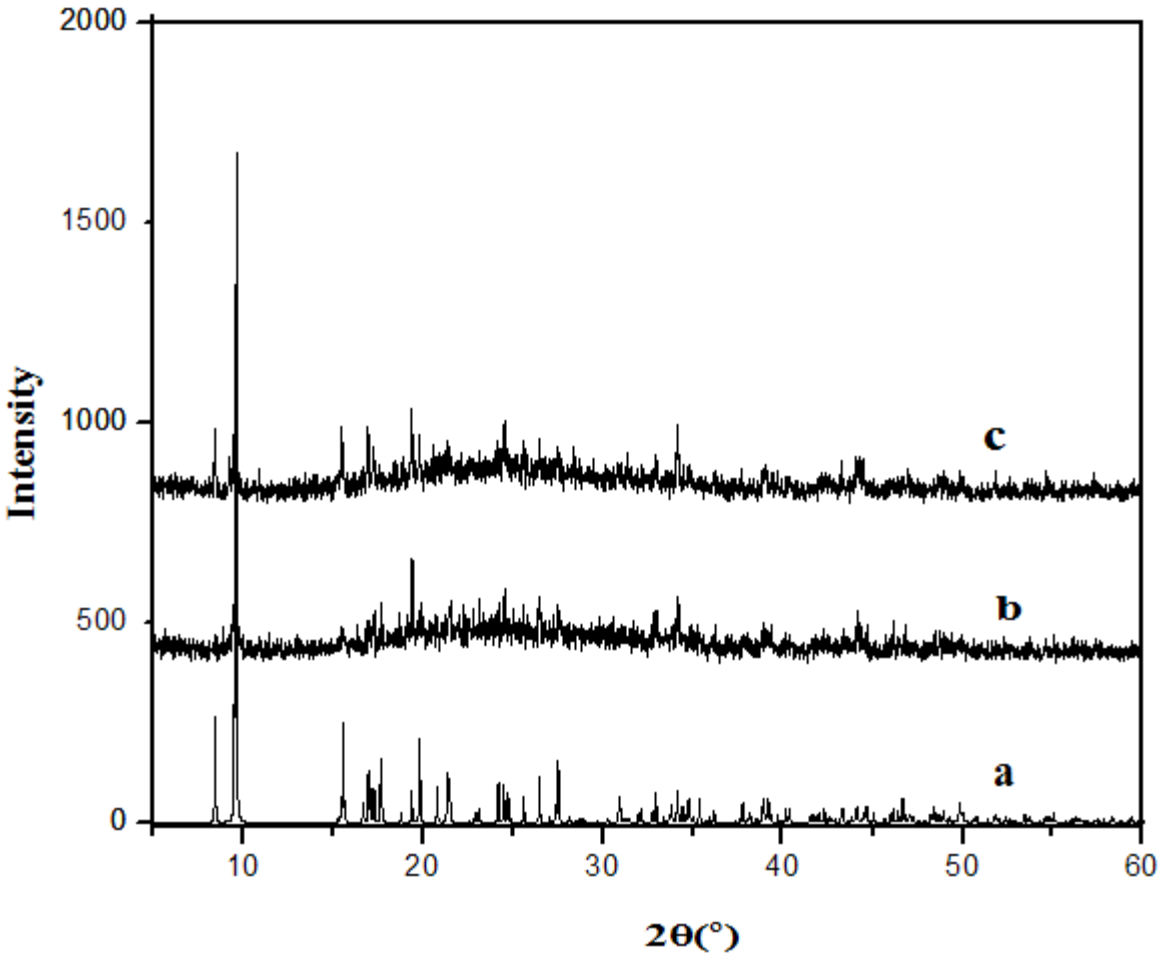


Figure S2 XRD powder patterns of complex **3** and **4**: (a) the simulated XPRD pattern calculated from single-crystal structure of complex **3**; (b) experimental XPRD for complex **3**; (c) experimental XPRD for complex **4**.

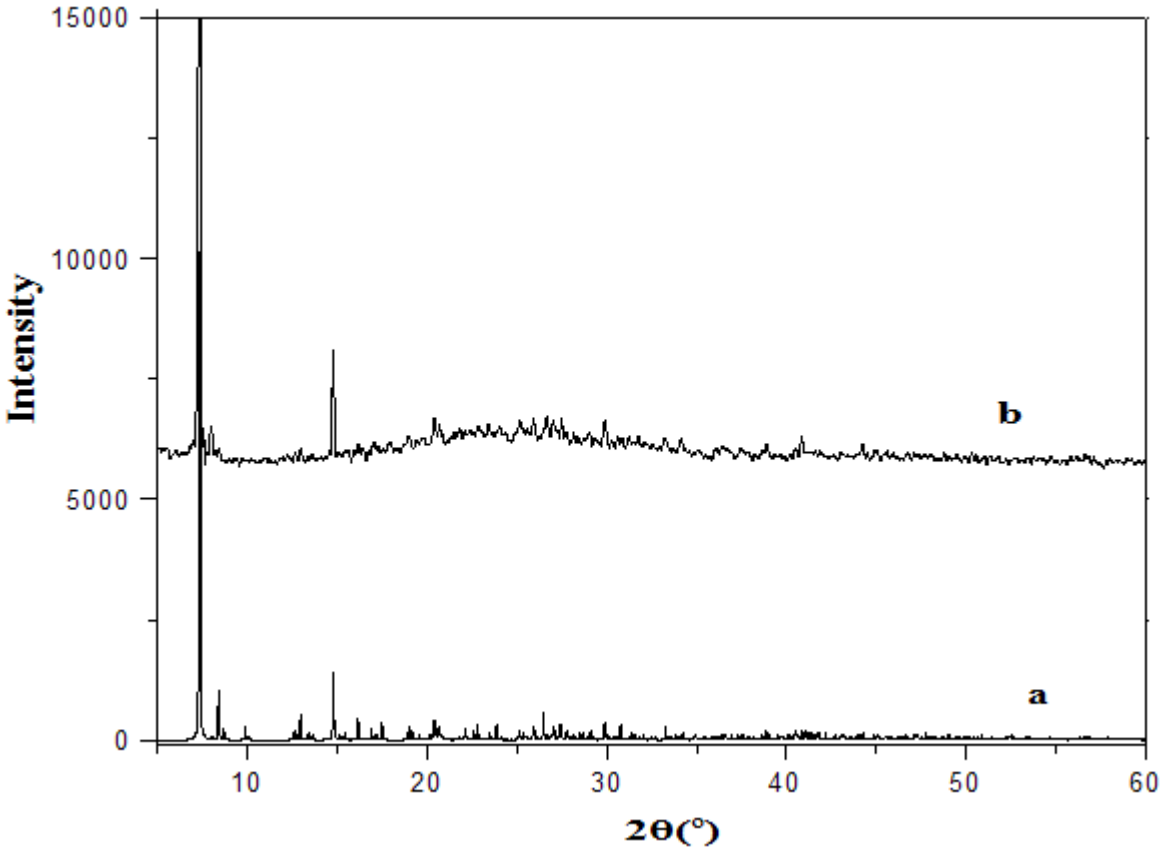


Figure S3 XRD powder patterns of complex **5**: (a) the simulated XPRD pattern calculated from single-crystal structure of complex **5**; (b) experimental XPRD for complex **5**.

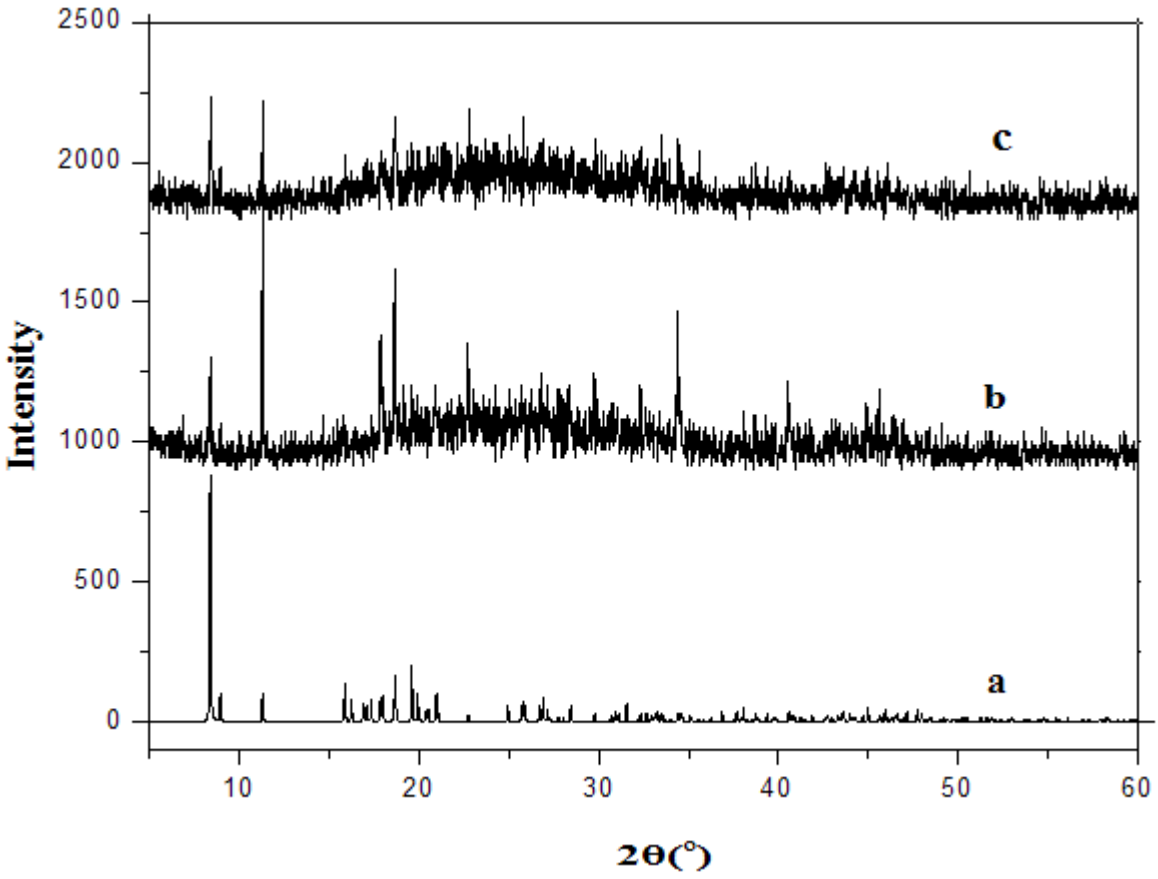


Figure S4 XRD powder patterns of complex **6** and **7**: (a) the simulated XPRD pattern calculated from single-crystal structure of complex **6**; (b) experimental XPRD for complex **6**; (c) experimental XPRD for complex **7**.

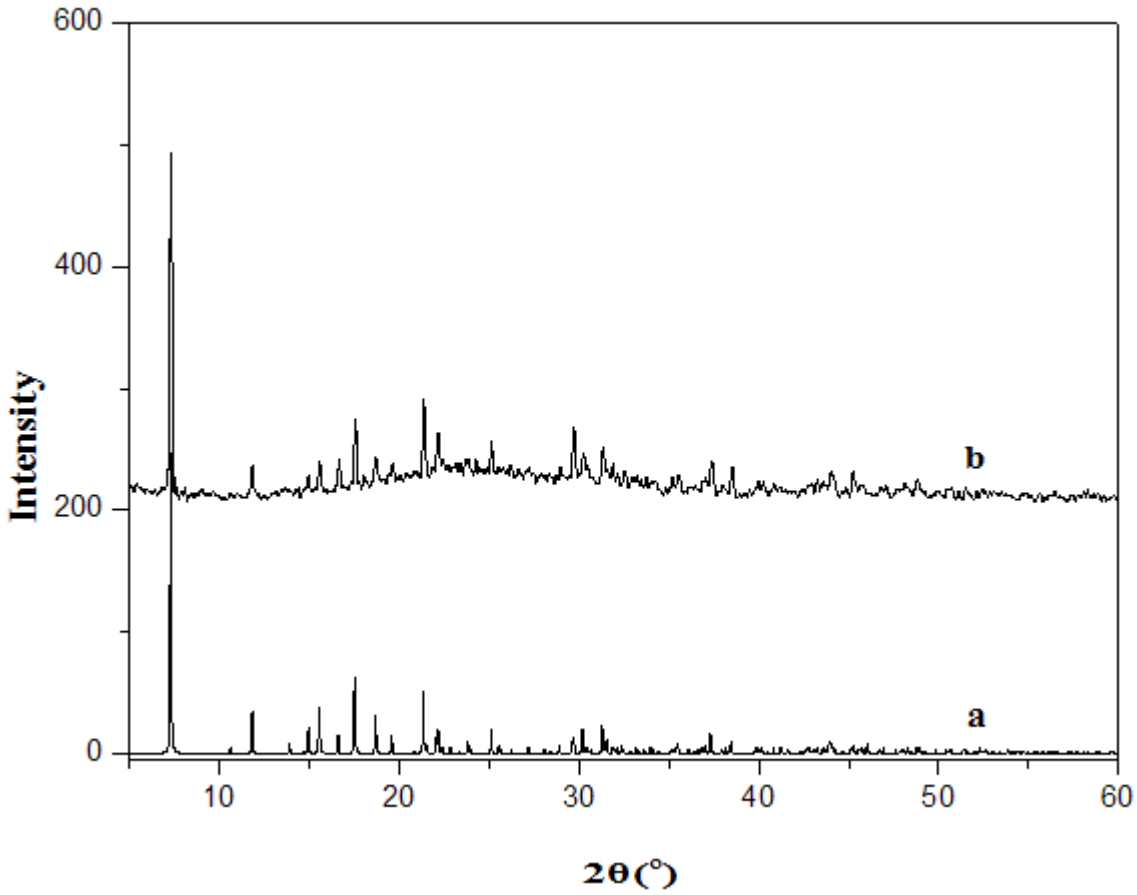


Figure S5 XRD powder patterns complex **8**: (a) the simulated XPRD pattern calculated from single-crystal structure of complex **8**; (b) experimental XPRD for complex **8**.

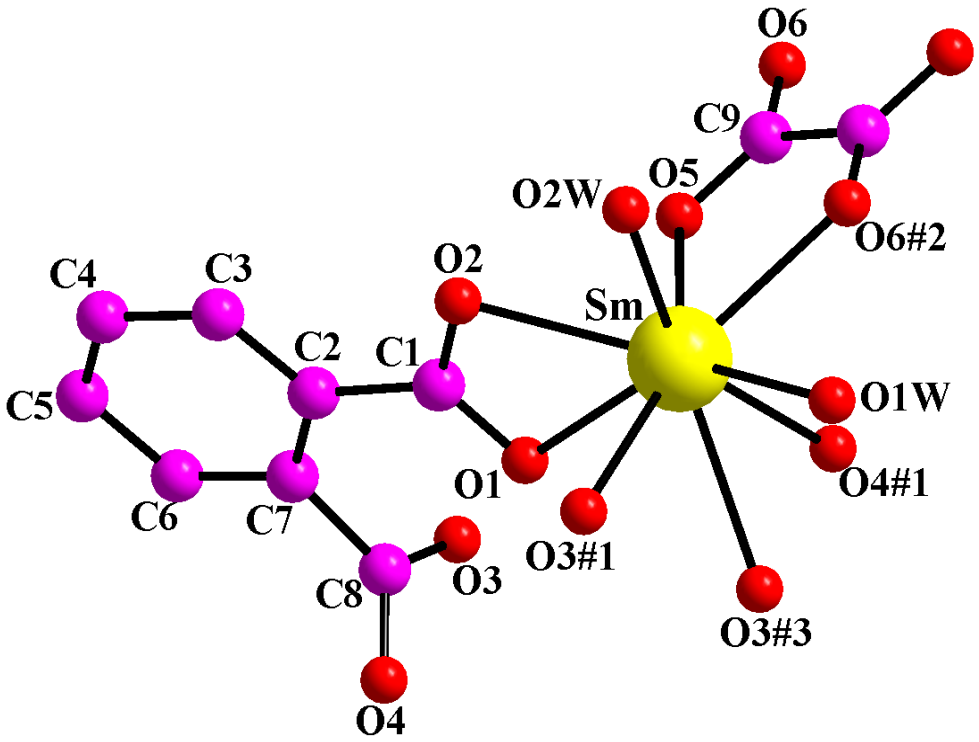
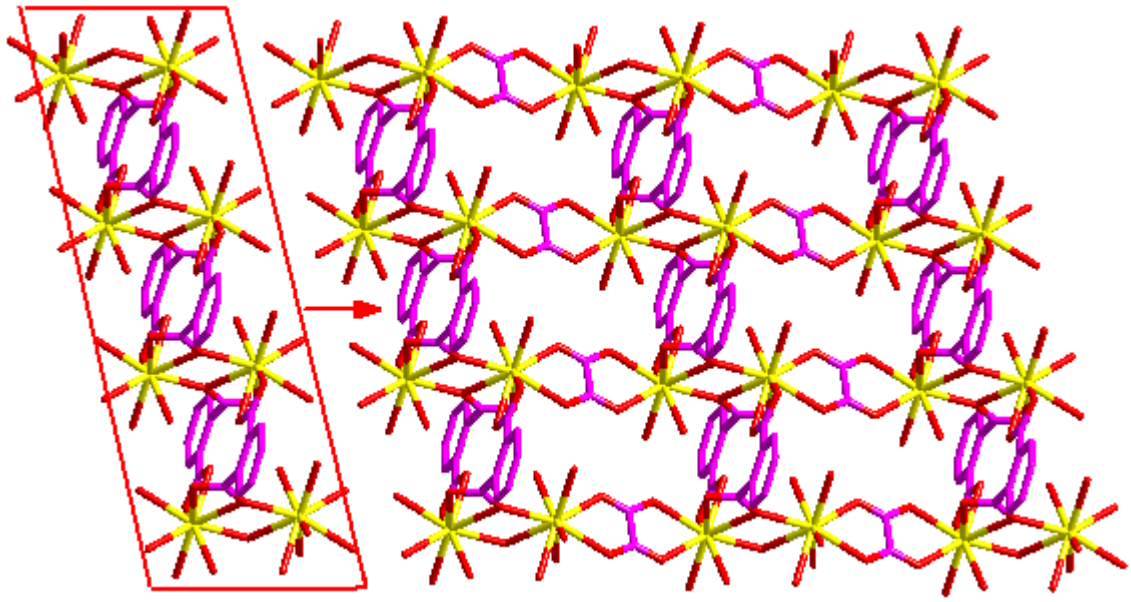


Figure S6 The coordinaton enviroment of Sm in complex **2**. (Symmetry codes follow: #1: x, y−1, z; #2 −x+1, −y, −z; #3 −x+1/2, −y+1/2, −z)



a **b**

Figure S7 a the infinite Sm-phth chain; **b**, 2D network of complex **2**.

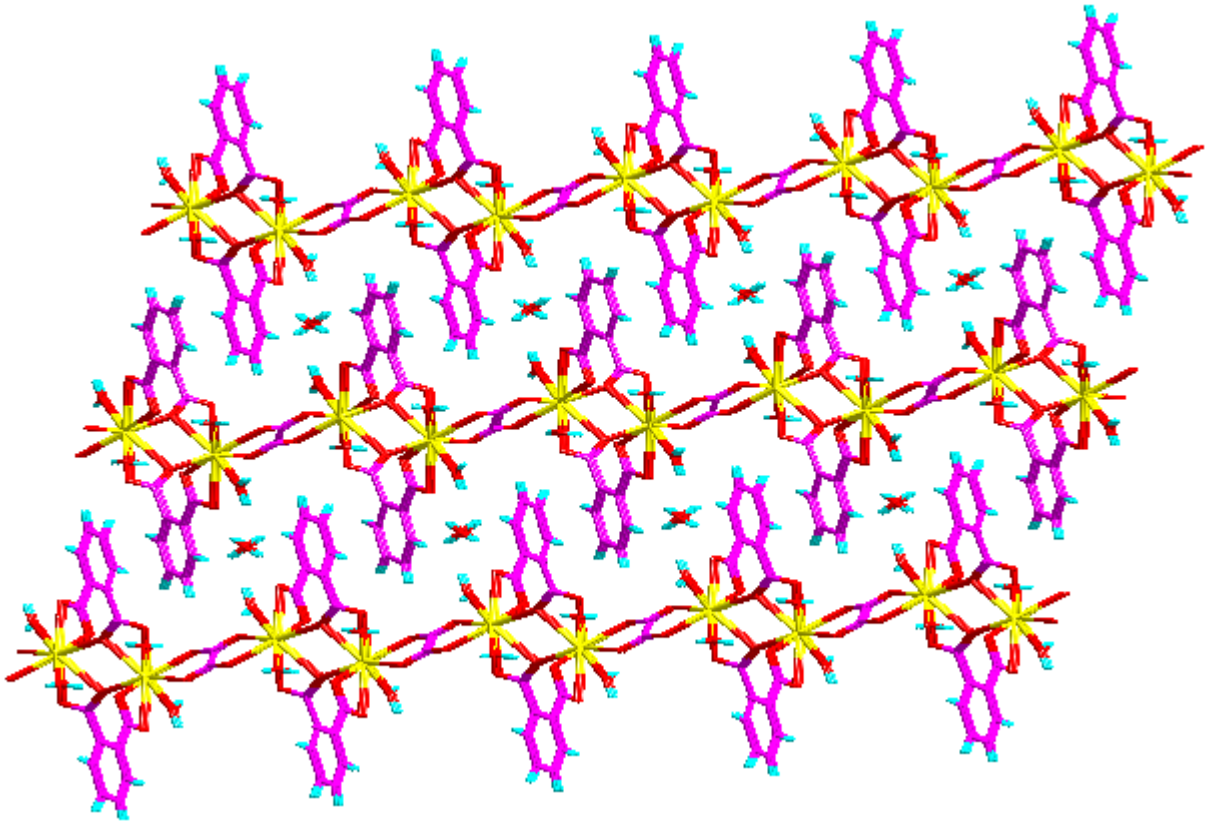


Figure S8. the packing structure of complex **2**.

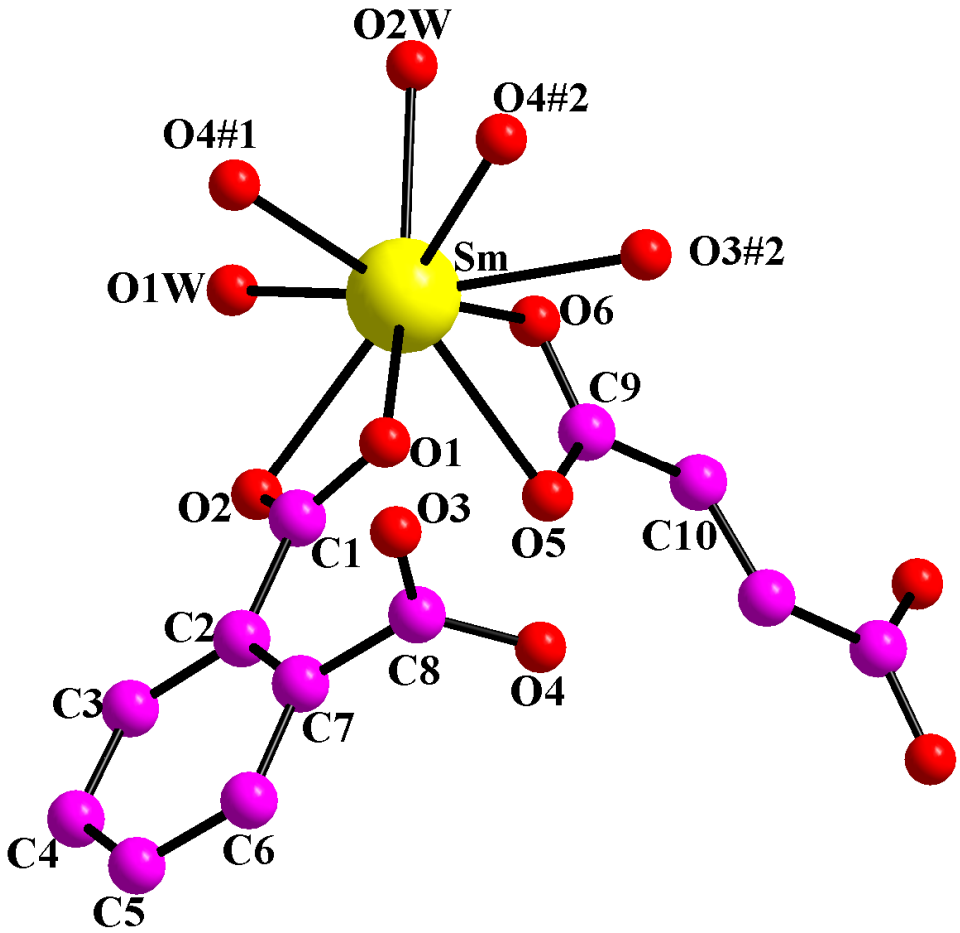
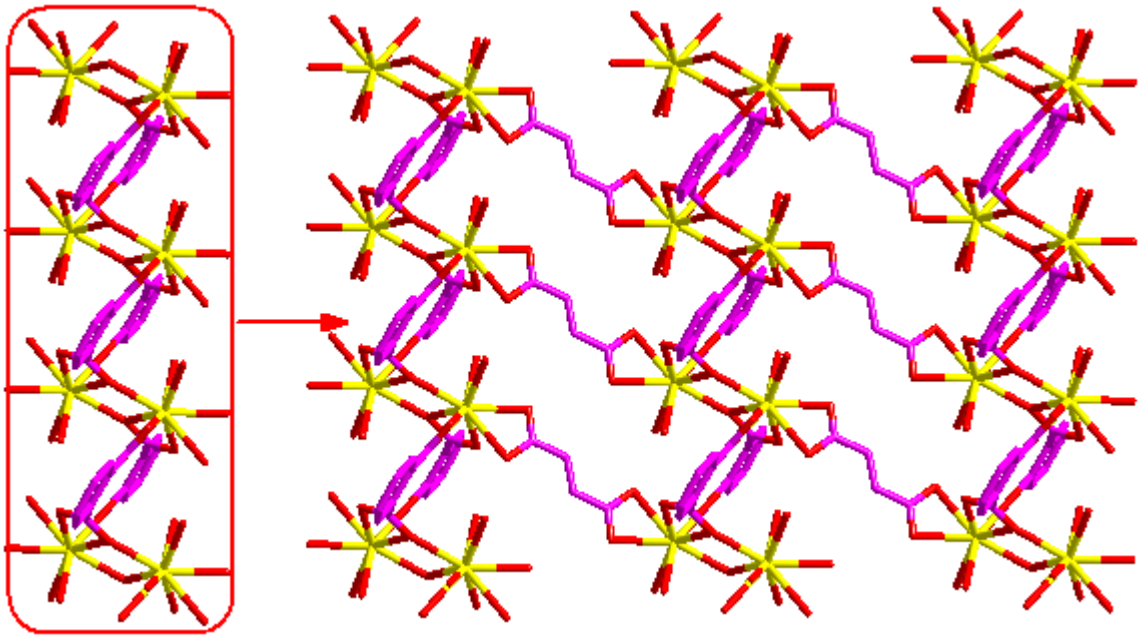


Figure S9 The coordination environment of Sm in complex **4** (Symmetry codes follow: #1: x, y+1, z; #2: −x+2, −y+1, −z)



a **b**

Figure S10 a, the infinite Sm-phth chain; **b**, 2D network of complex **4**.

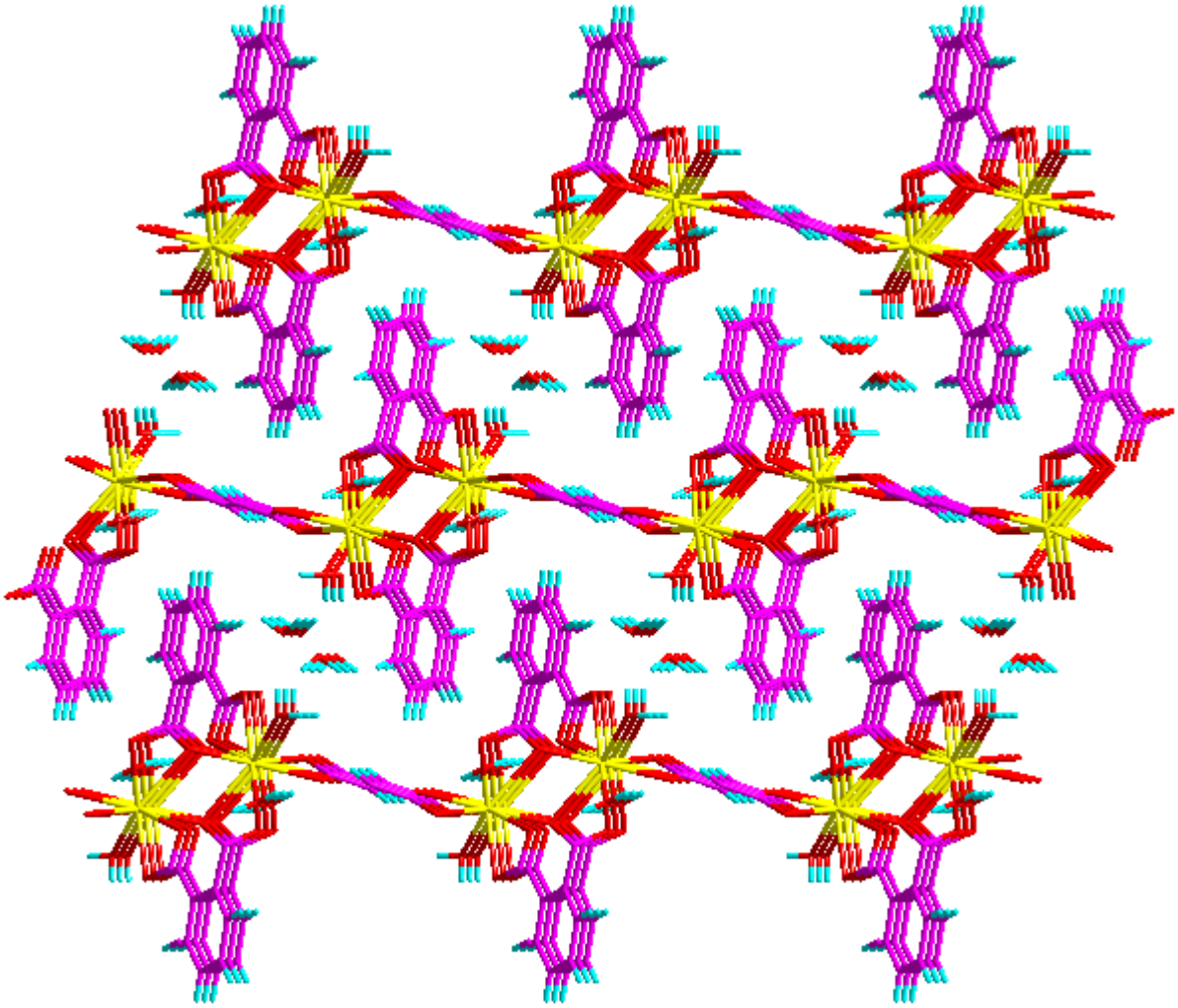


Figure S11. The packing structure of complex **4**.

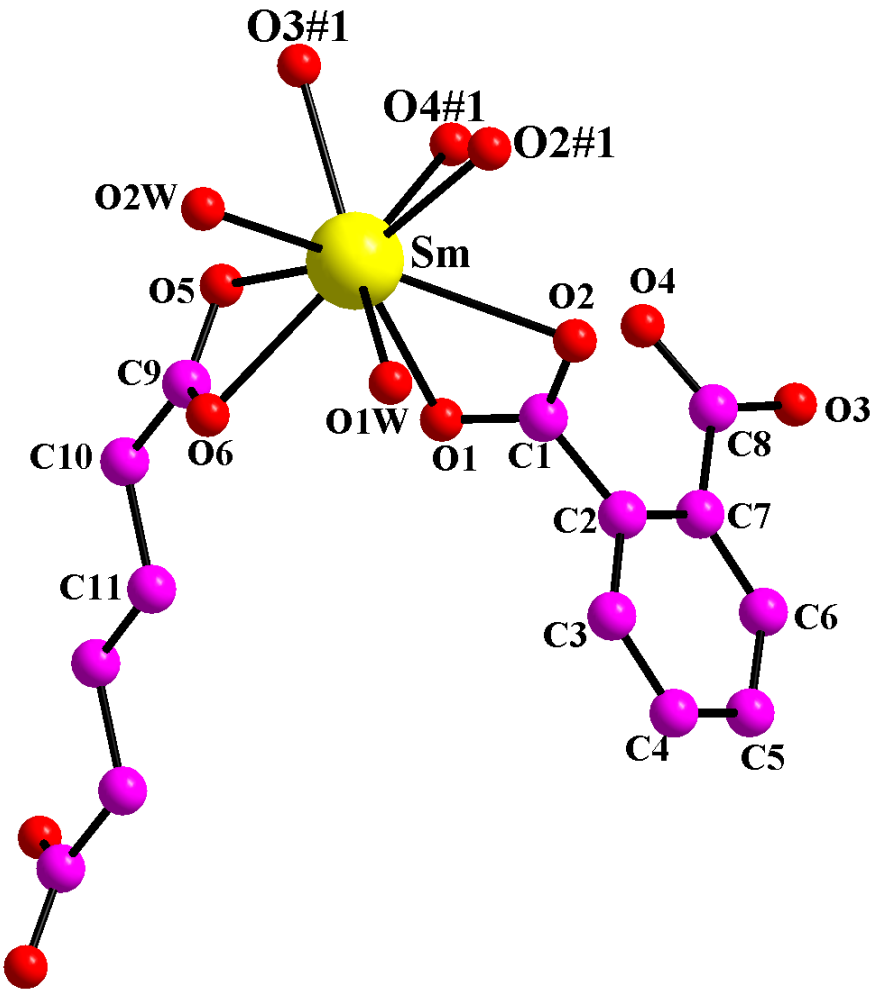
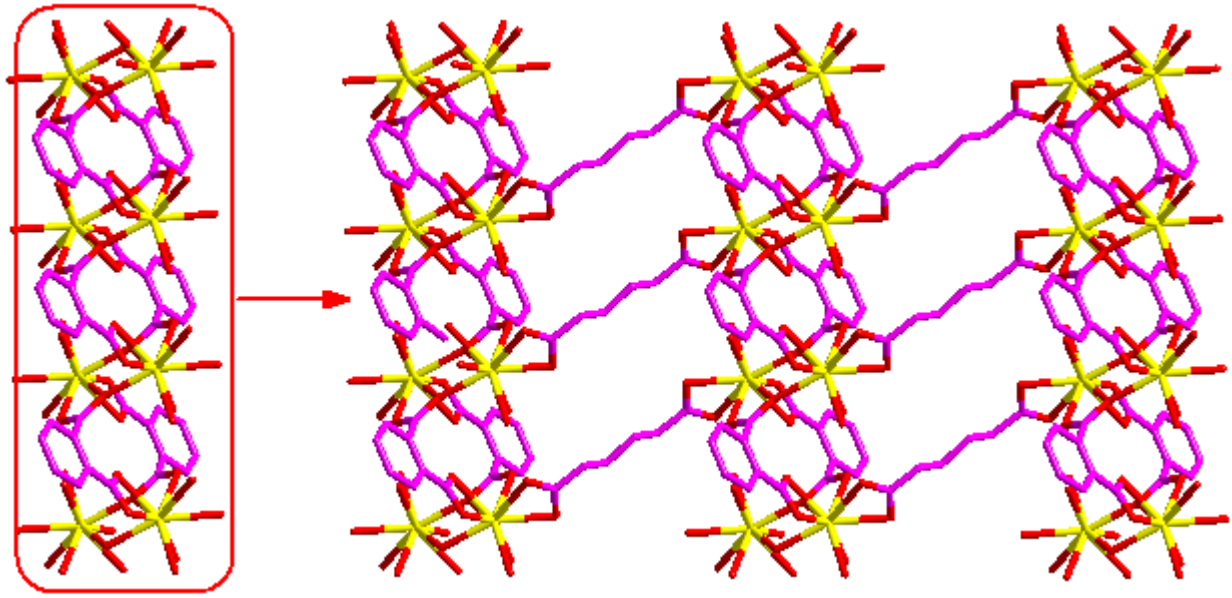


Figure S12 The coordination environment of Sm in complex **7**. (Symmetry codes follow: #1: −x+2, −y+2, −z+1)



a **b**

Figure S13 a the infinite Sm-phth chain; **b**, 2D network of complex **7**.

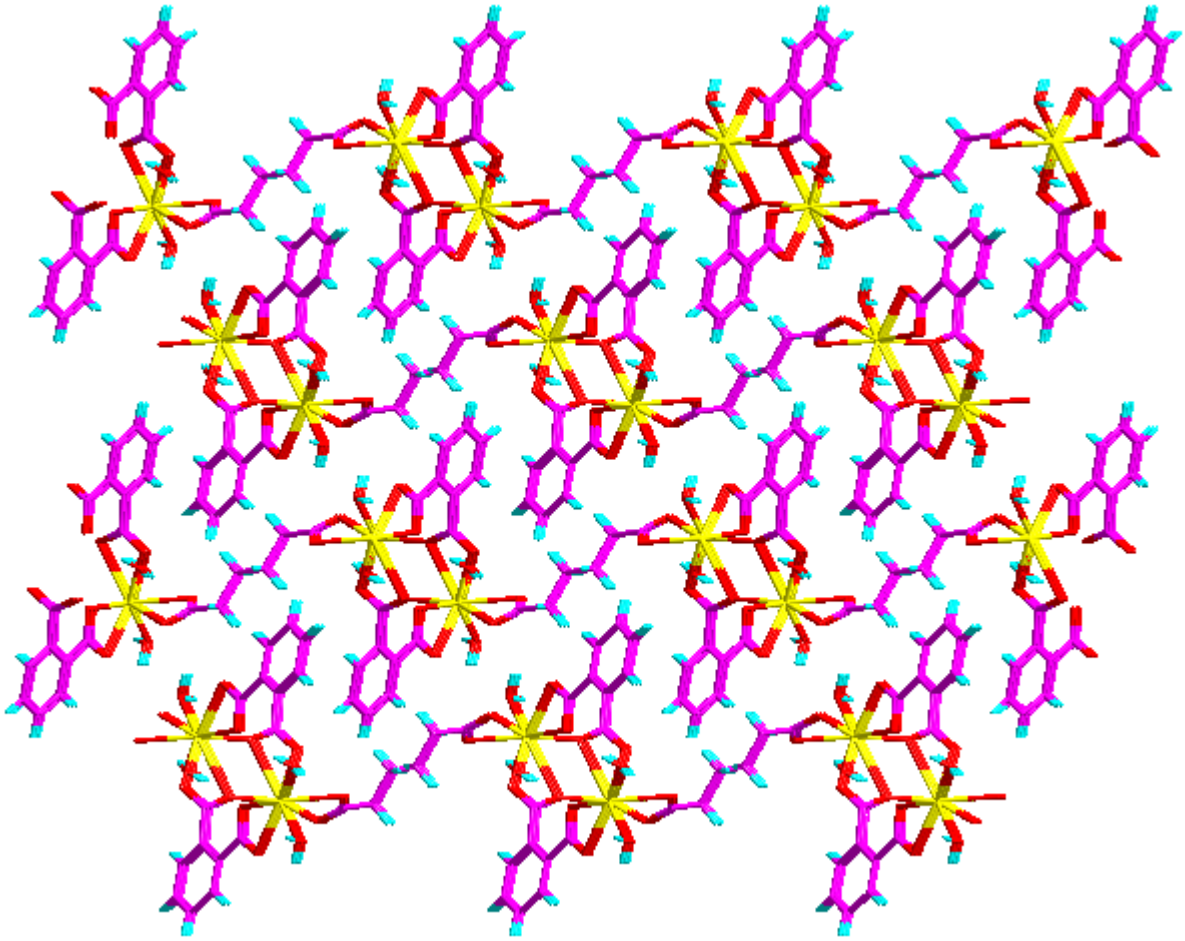


Figure S14. The packing structure of complex **7**

Table S1. Selected Angles (º) for Complex **1**

O2W–Tb1–O1	74.60(12)	O2W–Tb1–O1W	76.83(13)	O1–Tb1–O1W	84.52(13)
O2W–Tb1–O6$^{\#1}$	67.87(12)	O1–Tb1–O6$^{\#1}$	139.93(12)	O1W–Tb1–O6$^{\#1}$	73.97(13)
O2W–Tb1–O5	133.44(12)	O1–Tb1–O5	151.94(12)	O1W–Tb1–O5	99.63(14)
O6$^{\#1}$–Tb1–O5	66.66(12)	O2W–Tb1–O3$^{\#2}$	141.74(13)	O1–Tb1–O3$^{\#2}$	80.43(12)
O1W–Tb1–O3$^{\#2}$	72.29(13)	O6$^{\#1}$–Tb1–O3$^{\#2}$	122.30(12)	O5–Tb1–O3$^{\#2}$	74.60(12)
O2W–Tb1–O2$^{\#3}$	86.77(13)	O1–Tb1–O2$^{\#3}$	114.64(12)	O1W–Tb1–O2$^{\#3}$	150.64(13)
O6$^{\#1}$–Tb1–O2$^{\#3}$	77.35(12)	O5–Tb1–O2$^{\#3}$	74.21(12)	O3$^{\#2}$–Tb1–O2$^{\#3}$	130.43(12)
O2W–Tb1–O4$^{\#2}$	143.38(12)	O1–Tb1–O4$^{\#2}$	78.34(12)	O1W–Tb1–O4$^{\#2}$	124.67(12)
O6$^{\#1}$–Tb1–O4$^{\#2}$	141.58(12)	O5–Tb1–O4$^{\#2}$	76.55(11)	O3$^{\#2}$–Tb1–O4$^{\#2}$	53.23(12)
O2$^{\#3}$–Tb1–O4$^{\#2}$	82.52(12)	O2W–Tb1–O1$^{\#3}$	70.13(12)	O1–Tb1–O1$^{\#3}$	63.47(13)
O1W–Tb1–O1$^{\#3}$	138.64(12)	O6$^{\#1}$–Tb1–O1$^{\#3}$	113.68(11)	O5–Tb1–O1$^{\#3}$	121.07(12)
O3$^{\#2}$–Tb1–O1$^{\#3}$	122.69(11)	O2$^{\#3}$–Tb1–O1$^{\#3}$	51.31(11)	O4$^{\#2}$–Tb1–O1$^{\#3}$	75.92(11)

Symmetry transformations used to generate equivalent atoms: #1 −x+1, −y+2, −z #2 x, y+1, z #3−x+1/2, -y+3/2, −z for **1**

Table S2. Selected Angles (º) for Complex **3**

$O3^{\#1}$–Eu–O1W	78.64(16)	$O3^{\#1}$–Eu–O2W	84.92(18)	O1W–Eu–O2W	75.3(2)
$O3^{\#1}$–Eu–O5	151.85(14)	O1W–Eu–O5	76.67(17)	O2W-Eu–O5	75.9(2)
$O3^{\#1}$–Eu–O2	83.48(15)	O1W–Eu–O2	144.14(16)	O2W–Eu–O2	72.3(2)
O5–Eu–O2	109.41(17)	$O3^{\#1}$–Eu–O1	76.24(14)	O1W–Eu–O1	146.55(16)
O2W–Eu–O1	123.5(2)	O5–Eu–O1	131.66(14)	O2–Eu–O1	53.08(14)
$O3^{\#1}$–Eu-$O4^{\#2}$	116.57(15)	O1W–Eu–$O4^{\#2}$	84.67(16)	O2W–Eu–$O4^{\#2}$	147.2(2)
O5–Eu–$O4^{\#2}$	74.34(16)	O2–Eu–$O4^{\#2}$	131.19(15)	O1–Eu–$O4^{\#2}$	87.13(14)
$O3^{\#1}$–Eu–O6	153.85(14)	O1W–Eu–O6	127.47(16)	O2W–Eu–O6	101.94(19)
O5–Eu–O6	52.78(14)	O2–Eu–O6	74.89(16)	O1–Eu–O6	79.03(14)
$O4^{\#2}$–Eu–O6	70.16(15)	$O3^{\#1}$–Eu–$O3^{\#2}$	65.71(16)	O1W–Eu–$O3^{\#2}$	72.12(15)
O2W–Eu–$O3^{\#2}$	139.49(18)	O5–Eu–$O3^{\#2}$	118.02(16)	O2–Eu–$O3^{\#2}$	127.13(14)
O1–Eu–$O3^{\#2}$	77.56(13)	$O4^{\#2}$–Eu–$O3^{\#2}$	50.92(14)	O6–Eu–$O3^{\#2}$	116.83(14)

Symmetry transformations used to generate equivalent atoms: #1 x, y+1, z,
#2 −x+2,−y+1,−z for **3**.

Table S3. Selected Angles (º) for Complex **5**

O15−Pr1−O12$^{\#1}$	137.09(11)	O15−Pr1−O13	72.58(11)	O12$^{\#1}$−Pr1−O13	132.97(11)
O15−Pr1−O9$^{\#1}$	130.37(11)	O15−Pr1−O7$^{\#2}$	133.19(12)	O2−Pr1−O7$^{\#2}$	139.78(11)
O12$^{\#1}$−Pr1−O8$^{\#2}$	130.41(11)	O9$^{\#1}$−Pr1−O8$^{\#2}$	110.35(11)	O2−Pr1−O8$^{\#2}$	153.63(11)
O13−Pr1−O1	122.77(11)	O9$^{\#1}$−Pr1−O1	115.82(11)	O7#2−Pr1−O1	155.37(11)
O8$^{\#2}$−Pr1−O1	133.83(10)	O15−Pr1−O12	113.07(10)	O13−Pr1−O12	144.11(11)
O9$^{\#1}$−Pr1−O12	116.53(10)	O2−Pr1−O12	133.03(11)	O12$^{\#1}$−Pr1−O11	100.81(11)
O13−Pr1−O11	126.21(11)	O9$^{\#1}$−Pr1−O11	163.89(10)	O2−Pr1−O11	115.71(10)
O4$^{\#3}$-Pr2-O5$^{\#2}$	132.09(13)	O4$^{\#3}$-Pr2-O17$^{\#4}$	84.05(13)	O17$^{\#4}$−Pr2−O6	137.34(12)
O5$^{\#2}$−Pr2−O10$^{\#1}$	143.69(12)	O17$^{\#4}$−Pr2−O10$^{\#1}$	142.34(12)	O4$^{\#3}$−Pr2−O13	133.53(12)
O6−Pr2−O13	126.70(11)	O4$^{\#3}$−Pr2−O9$^{\#1}$	126.07(12)	O17$^{\#4}$−Pr2−O9$^{\#1}$	145.29(11)
O5$^{\#2}$−Pr2−O14	123.57(11)	O6−Pr2−O14	148.53(12)	O10#1−Pr2−O1W$^{\#3}$	128.53(11)
O13−Pr2−O1W$^{\#3}$	145.28(12)	O9$^{\#1}$−Pr2−O1W$^{\#3}$	132.00(10)	O14−Pr2−O1W$^{\#3}$	136.24(10)
O15−Pr3−O3	102.05(12)	O11−Pr3−O3	140.03(11)	O15−Pr3−O16$^{\#5}$	125.56(11)
O11−Pr3−O16$^{\#5}$	139.35(11)	O11−Pr3−O16	128.40(11)	O16$^{\#5}$−Pr3−O1	144.69(11)
O16−Pr3−O1	108.83(11)	O3−Pr3−O3W	144.75(11)	O1−Pr3−O3W	139.32(11)
O16−Pr3−O3W	73.06(12)	O1−Pr3−O3W	139.32(11)	O15−Pr3−O2W	134.52(13)
O16−Pr3−O2W	126.39(12)	O1−Pr3−O2W	124.77(12)	O15−Pr3−O1W	127.60(11)

Symmetry transformations used to generate equivalent atoms: #1 −x+1,−y,−z+1; #2 −x+2, −y, −z+1; #3 x+1, y, z; #4 −x+2, −y+1, −z+1; #5 −x+1,−y+1,−z+1; for **5**

Table S4. Selected Angles (º) for Complex **6**

O2W−Eu1−O1	144.80(18)	O1W−Eu1−O1	76.63(17)	O2−Eu1−O1	53.63(15)
$O3^{\#1}$−Eu1−O5	152.25(16)	O2W−Eu1−O5	131.33(18)	O1W−Eu1−O5	94.74(18)
O2-Eu1-O5	79.29(16)	O1-Eu1-O5	72.84(16)	$O3^{\#1}$-Eu1-$O4^{\#2}$	114.94(15)
O2W-Eu1-$O4^{\#2}$	85.39(17)	O1W-Eu1-$O4^{\#2}$	145.80(18)	O2-Eu1-$O4^{\#2}$	81.69(15)
O1-Eu1-O4#2	128.99(16)	O5-Eu1-O4#2	76.09(16)	$O3^{\#1}$-Eu1-O6	153.90(16)
O2W-Eu1-O6	79.01(18)	O1W-Eu1-O6	77.65(19)	O2-Eu1-O6	128.26(15)
O1-Eu1-O6	116.10(16)	O5-Eu1-O6	52.46(16)	$O4^{\#2}$-Eu1-O6	70.64(15)
$O3^{\#1}$-Eu1-$O3^{\#2}$	65.35(17)	O2W-Eu1-$O3^{\#2}$	69.96(16)	O1W-Eu1-$O3^{\#2}$	141.00(17)
O2-Eu1-$O3^{\#2}$	74.65(14)	O1-Eu1-$O3^{\#2}$	123.44(15)	O5-Eu1-$O3^{\#2}$	122.06(16)
$O4^{\#2}$-Eu1-$O3^{\#2}$	49.75(14)	O6-Eu1-$O3^{\#2}$	113.15(15)		

Symmetry transformations used to generate equivalent atoms: #1 x,y−1,z
#2 −x+2,−y+1,−z+1.

Table S5. Selected Angles (º) for Complex **8**

O2W−Pr1−O8$^{\#1}$	133.3(3)	O5−Pr1−O8$^{\#1}$	151.4(3)	O2W−Pr1−O3$^{\#2}$	142.2(3)
O3$^{\#2}$−Pr1−O10	125.1(2)	O2W−Pr1−O9	123.9(3)	O5−Pr1−O1W	141.2(3)
O3$^{\#2}$−Pr1−O1W	138.0(2)	O9−Pr1−O1W	114.8(3)	O8$^{\#1}$−Pr1−O2	117.09(19)
O10−Pr1−O2	151.2(2)	O9−Pr1−O2	139.6(2)	O1W−Pr1−O2	105.6(2)
O5−Pr1−O1	123.3(2)	O10−Pr1−O1	142.5(2)	O9−Pr1−O1	147.9(2)
O4$^{\#2}$−Pr2−O12$^{\#3}$	129.1(3)	O4$^{\#2}$−Pr2−O3W	139.3(3)	O1−Pr2−O3W	145.8(3)
O12$^{\#3}$−Pr2−O4W	107.9(3)	O1−Pr2−O4W	145.1(3)	O1−Pr2−O7$^{\#1}$	116.31(19)
O4$^{\#2}$−Pr2−O6$^{\#4}$	137.5(2)	O11$^{\#3}$−Pr2−O6$^{\#4}$	132.1(2)	O4W−Pr2−O6$^{\#4}$	132.4(3)
O11$^{\#3}$−Pr2−O8$^{\#1}$	142.5(2)	O4W−Pr2−O8$^{\#1}$	107.9(2)		

Symmetry transformations used to generate equivalent atoms: #1 x,y+1,z #2 x+1,y,z #3 x-1,y+1,z-1 for **8**.

Table S6. Selected Bond Lengths (Å) and Angles (º) for Complex **2**

Complex **2**

Sm–O1W	2.412(2)	Sm–O3$^{\#1}$	2.414(2)	Sm–O2W	2.438(2)
Sm–O6$^{\#2}$	2.445(2)	Sm–O5	2.474(2)	Sm–O2	2.477(2)
Sm–O4$^{\#3}$	2.498(2)	Sm–O1	2.499(2)	Sm–O3$^{\#3}$	2.606(2)
O1W–Sm–O3$^{\#1}$	74.63(7)	O1W–Sm–O2W	76.46(8)	O3$^{\#1}$–Sm–O2W	84.32(7)
O1W–Sm–O6$^{\#2}$	67.77(7)	O3$^{\#1}$–Sm–O6$^{\#2}$	139.94(7)	O2W–Sm–O6$^{\#2}$	74.15(8)
O1W–Sm–O5	132.53(7)	O3$^{\#1}$–Sm–O5	152.81(7)	O2W–Sm–O5	99.67(8)
O6$^{\#2}$–Sm–O5	65.80(7)	O1W–Sm–O2	142.05(8)	O3$^{\#1}$–Sm–O2	80.64(7)
O2W–Sm–O2	72.81(7)	O6$^{\#2}$–Sm–O2	122.44(7)	O5–Sm–O2	75.03(8)
O1W–Sm–O4$^{\#3}$	87.01(7)	O3$^{\#1}$–Sm–O4$^{\#3}$	114.59(7)	O2W–Sm–O4$^{\#3}$	150.80(7)
O6$^{\#2}$–Sm–O4$^{\#3}$	77.37(8)	O5–Sm–O4$^{\#3}$	73.97(7)	O2–Sm–O4$^{\#3}$	129.88(7)
O1W–Sm–O1	143.69(7)	O3$^{\#1}$–Sm–O1	78.16(7)	O2W–Sm–O1	124.27(7)
O6$^{\#2}$–Sm–O1	141.77(7)	O5–Sm–O1	77.46(7)	O2–Sm–O1	52.42(7)
O4$^{\#3}$–Sm–O1	82.88(7)	O1W–Sm–O3$^{\#3}$	70.54(7)	O3$^{\#1}$–Sm–O3$^{\#3}$	63.88(8)
O2W–Sm-O3$^{\#3}$	138.81(7)	O6$^{\#2}$–Sm–O3$^{\#3}$	113.43(7)	O5–Sm–O3$^{\#3}$	120.71(7)
O2–Sm–O3$^{\#3}$	122.59(7)	O4$^{\#3}$–Sm–O3$^{\#3}$	50.84(6)	O1–Sm–O3$^{\#3}$	76.11(7)

Symmetry transformations used to generate equivalent atoms: #1 x,y−1,z
#2 −x+1,−y,−z #3 −x+1/2,−y+1/2,−z.

Table S7. Selected Bond Lengths (Å) and Angles (º) for Complex **4**

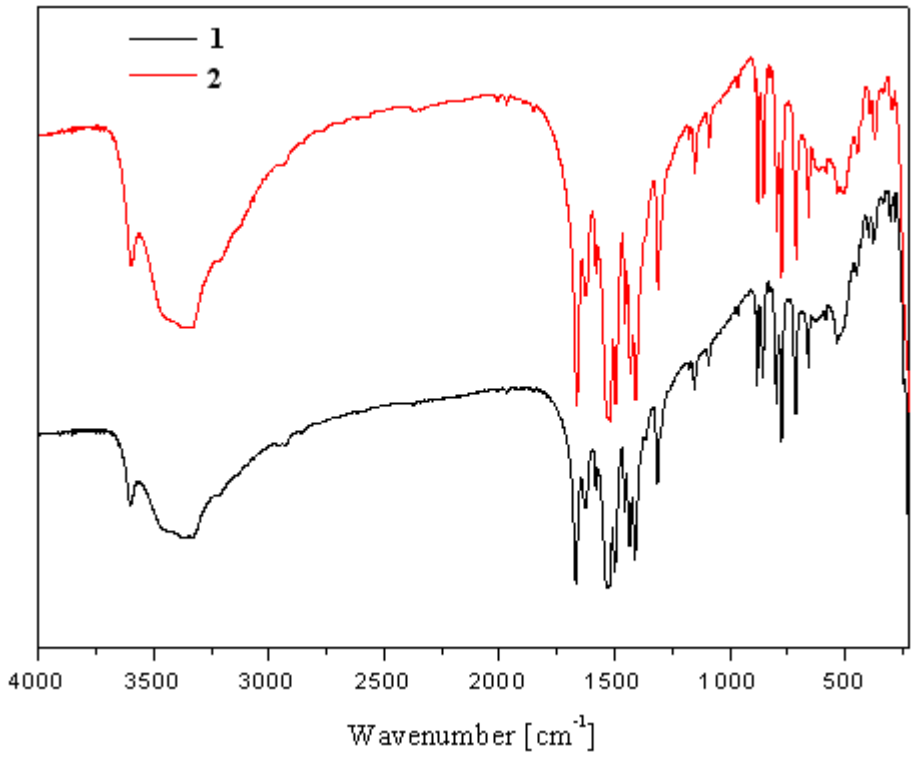
Sm1–O4$^{\#1}$	2.395(6)	Sm1–O2W	2.410(7)	Sm1–O1W	2.422(7)
Sm1–O6	2.440(6)	Sm1–O2	2.453(6)	Sm1–O1	2.493(6)
Sm1–O3$^{\#2}$	2.504(6)	Sm1–O5	2.534(6)	Sm1–O4$^{\#2}$	2.593(6)
Sm1–O4$^{\#1}$	2.395(6)	Sm1–O2W	2.410(7)	Sm1–O1W	2.422(7)
O4$^{\#1}$–Sm1–O2W	78.4(2)	O4$^{\#1}$–Sm1–O1	84.8(2)	O2W–Sm1–O1W	75.4(2)
O4$^{\#1}$–Sm1–O6	152.3(2)	O2W–Sm1–O6	77.2(2)	O1W–Sm1–O6	76.5(2)
O4$^{\#1}$–Sm1–O2	83.3(2)	O2W–Sm1–O2	144.1(2)	O1W–Sm1–O2	72.3(2)
O6–Sm1–O2	109.5(2)	O4$^{\#1}$–Sm1–O1	76.0(2)	O2W–Sm1–O1	146.4(2)
O1W–Sm1–O1	122.9(2)	O6–Sm1–O1	131.5(2)	O2–Sm1–O1	52.55(19)
O4$^{\#1}$–Sm1–O3$^{\#2}$	116.4(2)	O2W–Sm1–O3$^{\#}$	85.0(2)	O1W–Sm1–O3$^{\#2}$	147.7(2)
O6–Sm1–O3$^{\#2}$	74.3(2)	O2–Sm1–O3#2	130.9(2)	O1–Sm1–O3$^{\#2}$	87.3(2)
O4$^{\#1}$–Sm1–O5	153.8(2)	O2W–Sm1–O5	127.7(2)	O1W–Sm1–O5	101.9(2)
O6–Sm1–O5	52.3(2)	O2–Sm1–O5	74.9(2)	O1–Sm1–O5	79.28(19)
O3$^{\#2}$–Sm1–O5	70.3(2)	O4$^{\#1}$–Sm1–O4$^{\#2}$	65.8(2)	O2W–Sm1–O4$^{\#2}$	72.0(2)
O1W–Sm1–O4$^{\#2}$	139.5(2)	O6–Sm1–O4$^{\#2}$	117.9(2)	O2–Sm1–O4$^{\#2}$	127.0(2)
O1–Sm1–O4$^{\#2}$	77.84(18)	O3$^{\#2}$–Sm1–O4$^{\#2}$	50.75(19)	O5–Sm1–O4$^{\#2}$	116.9(2)

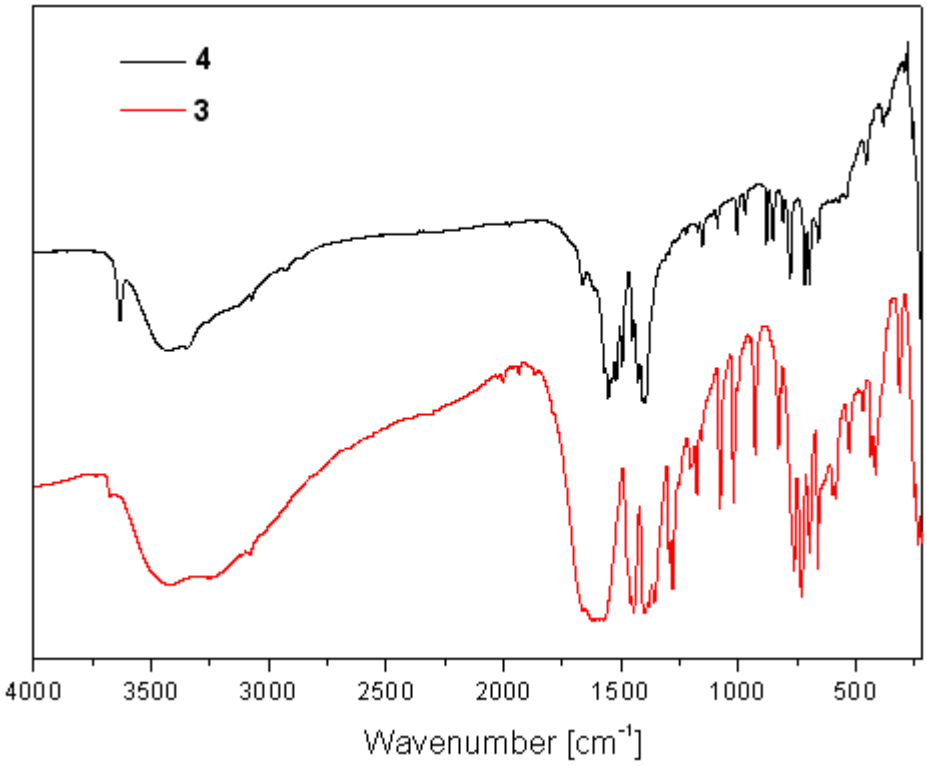
Symmetry transformations used to generate equivalent atoms: #1 x, y+1, z
#2 −x+2,−y+1,-z

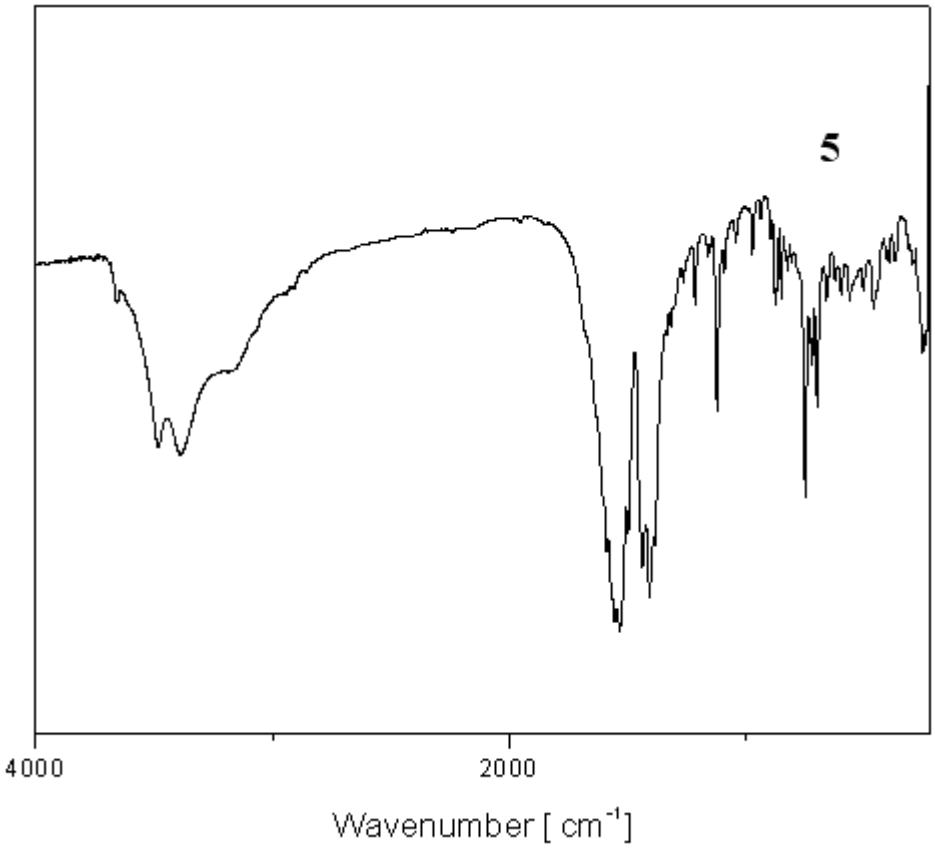
Table S8. Selected Bond Lengths (Å) and Angles (º) for Complex **7**

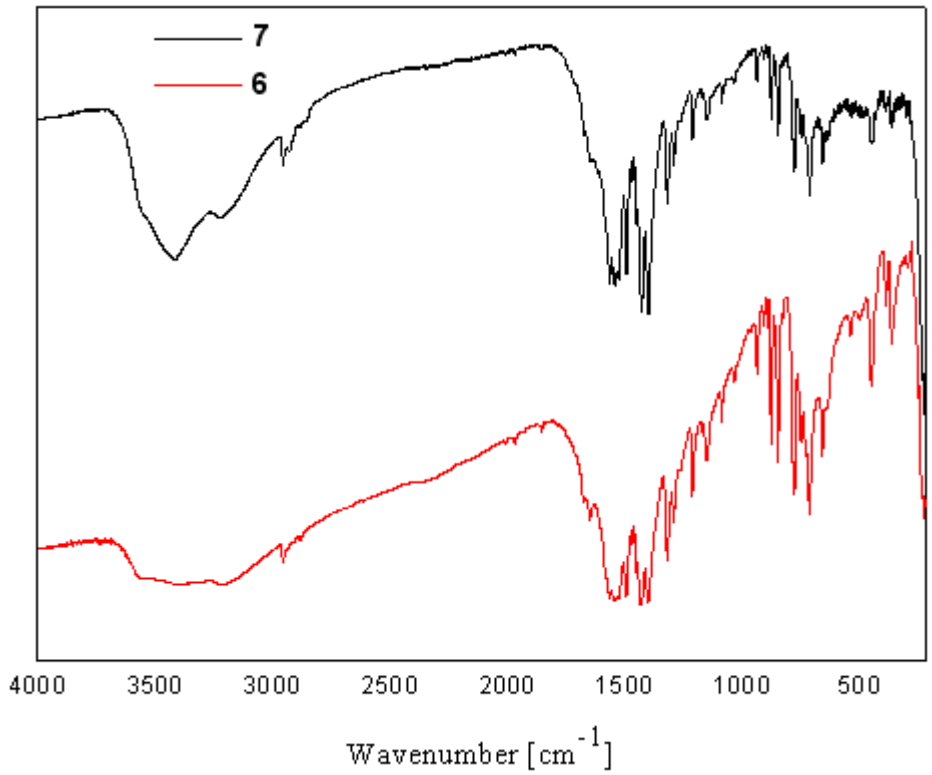
Sm1–O2$^{\#1}$	2.394(8)	Sm1–O2W	2.427(9)	Sm1–O1W	2.434(10)
Sm1–O4$^{\#2}$	2.446(9)	Sm1–O3$^{\#2}$	2.461(9)	Sm1–O5	2.464(9)
Sm1–O1	2.471(8)	Sm1–O6	2.485(10)	Sm1–O2	2.703(9)
O2$^{\#1}$–Sm1–O2W	89.4(3)	O2$^{\#1}$–Sm1–O1W	77.1(3)	O2W–Sm1–O1W	75.6(3)
O2$^{\#1}$–Sm1–O$^{\#2}$	77.4(3)	O2W–Sm1–O4$^{\#2}$	130.1(3)	O1W–Sm1–O4$^{\#2}$	143.2(3)
O2$^{\#1}$–Sm1–O3$^{\#2}$	80.4(3)	O2W–Sm1–O3$^{\#2}$	77.1(3)	O1W–Sm1–O3$^{\#2}$	144.5(4)
O4$^{\#2}$–Sm1–O3$^{\#2}$	53.5(3)	O2$^{\#1}$–Sm1–O5	151.9(3)	O2W–Sm1–O5	94.3(3)
O1W–Sm1–O5	130.8(4)	O4$^{\#2}$–Sm1–O5	79.0(3)	O3$^{\#2}$–Sm1–O5	73.3(3)
O2$^{\#1}$–Sm1–O1	115.1(3)	O2W–Sm1–O1	145.1(3)	O1W–Sm1–O1	85.6(3)
O4$^{\#2}$–Sm1–O1	81.6(3)	O3$^{\#2}$–Sm1–O1	129.1(3)	O5–Sm1–O1	76.0(3)
O2$^{\#1}$–Sm1–O6	154.0(3)	O2W–Sm1–O6	76.3(3)	O1W–Sm1–O6	78.3(3)
O2$^{\#1}$–Sm1–O2W	89.4(3)	O2$^{\#1}$–Sm1–O1W	77.1(3)	O2W–Sm1–O1W	75.6(3)
O2$^{\#1}$–Sm1–O$^{\#2}$	77.4(3)	O2W–Sm1–O4$^{\#2}$	130.1(3)	O1W–Sm1–O4$^{\#2}$	143.2(3)
O2$^{\#1}$–Sm1–O3$^{\#2}$	80.4(3)	O2W–Sm1–O3$^{\#2}$	77.1(3)	O1W–Sm1–O3$^{\#2}$	144.5(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+2,-z+1 #2 -x+2,-y+1,-z+1









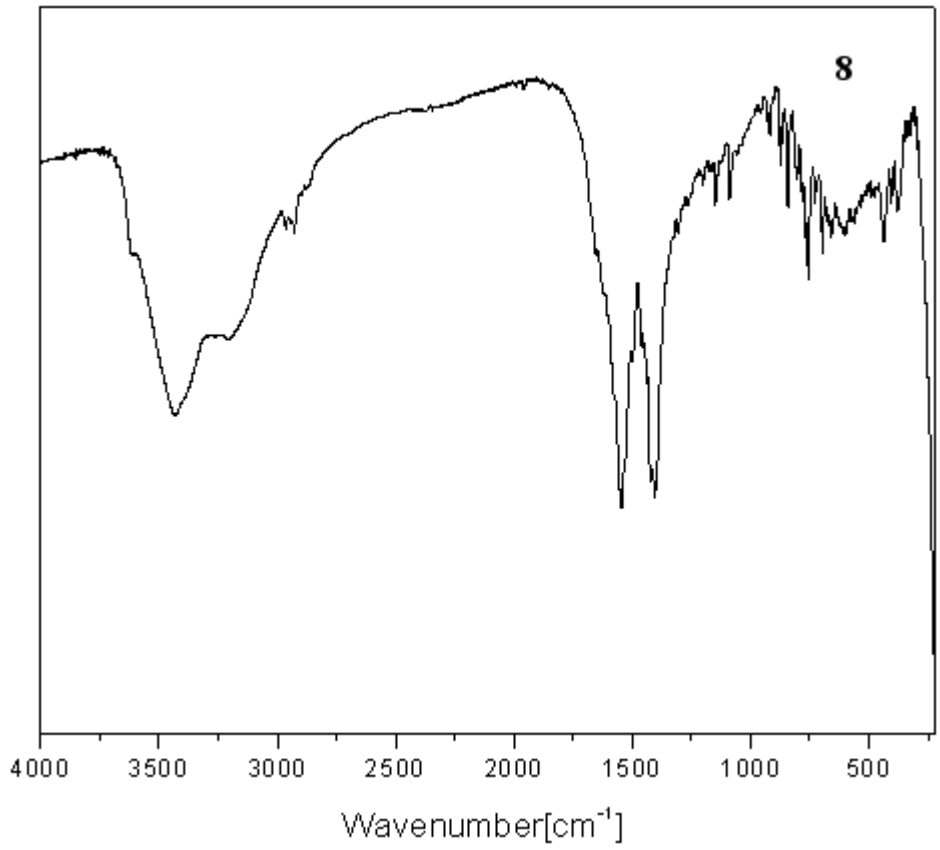


Figure S15. The infrared spectra of complexes **1-8**