

Lanthanide Metal–Organic Frameworks Based on 4,4'-oxybisbenzoic acid ligand: Synthesis, Structures and Physical Properties

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Supporting Information

- (1) Table of crystal data and structure refinement for 1-6**
- (2) Table of crystal data and structure refinement for 7-8**
- (3) Table of Selected bond lengths (Å) for complexes 1, 2, 5, 6, 7 and 8**
- (4) Figures of the metal- chains and two-dimensional layer structures in 1 and 7**
- (5) TG/DTA curves for 1-8**
- (6) IR of 1-8**

Table S1. Crystal Data and Structure Refinement Summary for compounds 1–6

complex	1	2	3	4	5	6
empirical formula	C ₉₃ H ₇₇ O ₃₇ N ₃ Nd ₄	C ₉₃ H ₇₇ O ₃₇ N ₃ Sm ₄	C ₉₃ H ₇₇ O ₃₇ N ₃ Eu ₄	C ₉₃ H ₇₇ O ₃₇ N ₃ Gd ₄	C ₉₃ H ₇₇ O ₃₇ N ₃ Tb ₄	C ₉₃ H ₇₇ O ₃₇ N ₃ Dy ₄
formula weight	2405.51	2429.99	2436.43	2457.55	2464.27	2478.55
T (K)	296(2)	296(2)	296(2)	296(2)	296(2)	296(2)
crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
space group	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1
a (Å)	14.708(3)	14.604(3)	14.589(2)	14.626(7)	15.089(6)	15.189(3)
b (Å)	15.429(3)	15.309(3)	15.285(2)	15.297(7)	15.275(6)	15.232(2)
c (Å)	23.084(4)	22.870(5)	22.758(3)	23.009(10)	23.654(10)	23.855(4)
<i>a</i> (deg)	84.282(3)	84.603(3)	84.679(3)	84.817(6)	85.902(7)	85.890(3)
<i>β</i> (deg)	82.619(3)	83.640(3)	84.323(3)	83.605(6)	81.506(7)	79.971(3)
<i>γ</i> (deg)	86.756(3)	86.655(3)	86.396(3)	86.488(6)	86.813(8)	86.842(3)
V (Å ³)	5164.1(17)	5053.2(18)	5020.8(12)	5088(4)	5373(4)	5415.7(16)
Z	2	2	2	2	2	2
D calcd (g cm ⁻³)	1.418	1.465	1.479	1.473	1.365	1.363
μ/mm ⁻¹	2.049	2.363	2.537	2.645	2.667	2.793
F (000)	2164	2180	2188	2196	2144	2152
GOF	1.004	0.992	0.986	0.983	1.017	1.005
R1 [I > 2σ(I)] ^a	0.0403	0.0527	0.0652	0.0475	0.0752	0.0562
ωR ₂ (all data) ^b	0.0843	0.1092	0.1246	0.0977	0.1616	0.1221
Data/restraints/para meters	18075 / 2 / 1120	18248 / 1 / 1119	18014 / 6 / 1104	18364 / 1 / 1119	18750 / 5 / 1081	18940 / 0 / 1081
CCDC number	1407369	1407370	1407371	1407372	1407373	1407374

Table S2. Crystal Data and Structure Refinement Summary for compounds 7–8

complex	7	8
empirical formula	C ₉₃ H ₈₁ O ₃₉ N ₃ Tb ₄	C ₉₃ H ₈₁ O ₃₉ N ₃ Dy ₄
formula weight	2500.29	2514.57
T (K)	296(2)	296(2)
crystal system	Triclinic	Triclinic
space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
a (Å)	15.9451(14)	15.970(4)
b (Å)	28.148(3)	28.166(7)
c (Å)	23.416(2)	23.583(6)
<i>a</i> (deg)	90	90
<i>β</i> (deg)	107.837(2)	108.092(3)
<i>γ</i> (deg)	90	90
V (Å ³)	10004.5(16)	10083(4)
Z	4	4
D calcd (g cm ⁻³)	1.515	1.513
<i>μ</i> /mm ⁻¹	2.868	3.004
F (000)	4448	4464
GOF	1.066	1.090
R1 [<i>I</i> > 2σ(<i>I</i>)] ^a	0.0348	0.0476
ωR ₂ (all data) ^b	0.0705	0.1089
Data/restraints/para meters	17607 / 3 / 1118	18257 / 5 / 1113
CCDC number	1407375	1407376

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|, \quad ^b wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum (F_o^2)^2 \}^{1/2}$$

(3) Figures of the metal- chains and two-dimensional layer structures in 1 and 7

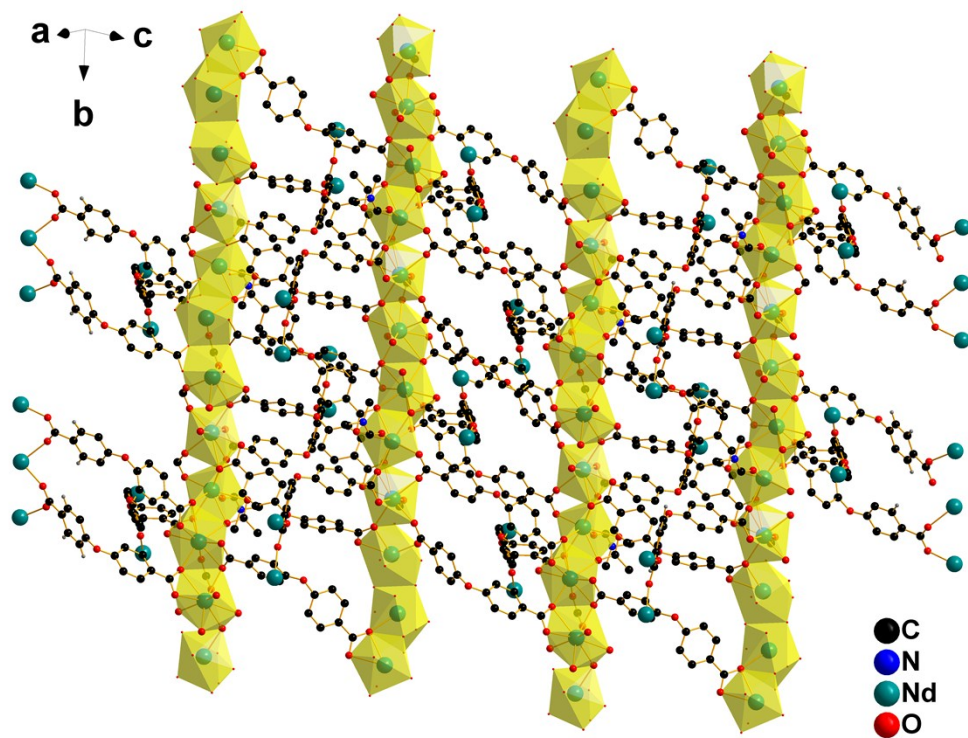


Figure. S1 The metal- chains and two-dimensional layer structures in 1.

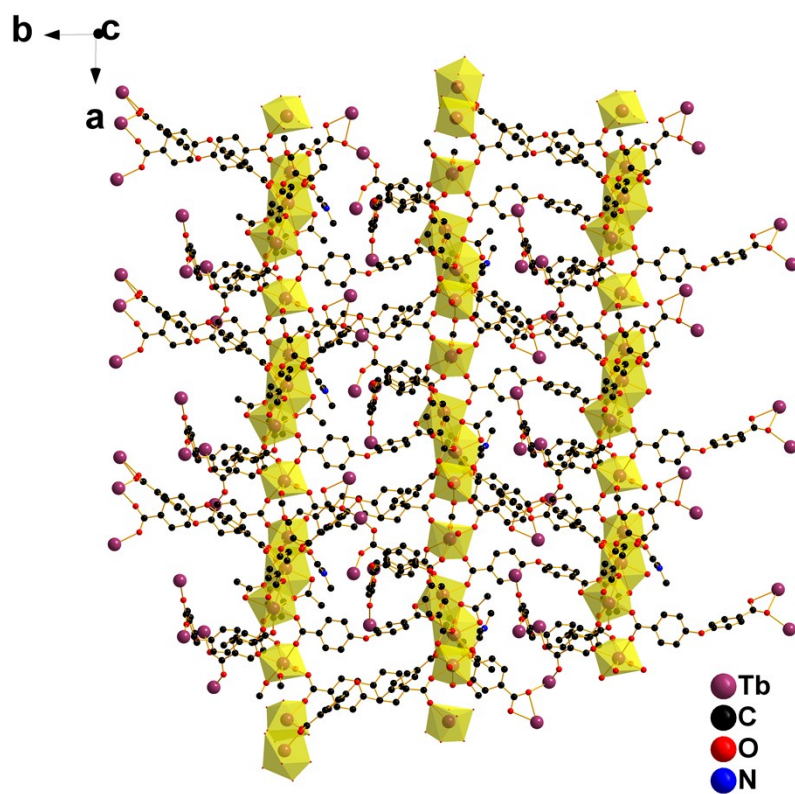


Figure. S2 The metal- chains and two-dimensional layer structures in 7.

Table S3. Selected bond lengths (Å) for complexes 1, 2, 5, 6, 7 and 8

1		2	
Nd(1)-O(4)#2	2.372(8)	Sm(1)-O(5)#6	2.254(10)
Nd(1)-O(15)#3	2.375(7)	Sm(1)-O(30)#7	2.314(9)
Nd(1)-O(30)#4	2.431(7)	Sm(1)-O(20)#7	2.339(10)
Nd(1)-O(25)#1	2.447(6)	Sm(1)-O(9)#2	2.365(8)
Nd(1)-O(31W)	2.480(8)	Sm(1)-O(6)	2.437(9)
Nd(1)-O(1)	2.501(7)	Sm(1)-O(1)	2.508(10)
Nd(1)-O(6)	2.555(7)	Sm(1)-O(2)	2.648(9)
Nd(1)-O(2)	2.703(6)	Sm(1)-O(7)	2.717(8)
Nd(1)-O(24)#1	2.842(7)	Sm(2)-O(19)#7	2.299(10)
Nd(2)-O(14)#3	2.388(7)	Sm(2)-O(31DMF)	2.368(12)
Nd(2)-O(2)	2.399(6)	Sm(2)-O(2)	2.370(8)
Nd(2)-O(10)#1	2.413(7)	Sm(2)-O(21)	2.392(9)
Nd(2)-O(16)	2.429(7)	Sm(2)-O(16)	2.404(10)
Nd(2)-O(11)	2.514(7)	Sm(2)-O(7)	2.407(9)
Nd(2)-O(6)	2.520(6)	Sm(2)-O(11)	2.509(9)
Nd(2)-O(7)	2.563(7)	Sm(2)-O(12)	2.590(8)
Nd(2)-O(12)	2.609(7)	Sm(3)-O(26)	2.358(8)
Nd(2)-O(17)	2.764(8)	Sm(3)-O(25)#3	2.365(9)
Nd(3)-O(20)#5	2.367(8)	Sm(3)-O(12)	2.397(8)
Nd(3)-O(32DMF)	2.404(9)	Sm(3)-O(17)	2.412(9)
Nd(3)-O(21)	2.425(7)	Sm(3)-O(22)	2.474(8)
Nd(3)-O(26)	2.428(7)	Sm(3)-O(14)#1	2.475(8)
Nd(3)-O(17)	2.440(8)	Sm(3)-O(15)#1	2.526(9)
Nd(3)-O(12)	2.441(7)	Sm(3)-O(21)	2.589(8)
Nd(3)-O(9)#1	2.546(7)	Sm(3)-O(16)	2.725(10)
Nd(3)-O(10)#1	2.598(6)	Sm(4)-O(29)#4	2.356(10)
Nd(4)-O(29)#6	2.286(8)	Sm(4)-O(24)#3	2.372(10)
Nd(4)-O(5)#5	2.339(7)	Sm(4)-O(4)#5	2.407(9)
Nd(4)-O(19)#5	2.381(8)	Sm(4)-O(10)#1	2.415(8)
Nd(4)-O(24)#7	2.399(7)	Sm(4)-O(32W)	2.440(10)
Nd(4)-O(22)	2.476(7)	Sm(4)-O(27)	2.500(9)
Nd(4)-O(27)	2.541(7)	Sm(4)-O(14)#1	2.528(9)
Nd(4)-O(26)	2.635(7)	Sm(4)-O(26)	2.662(8)
Nd(4)-O(21)	2.716(7)	Sm(4)-O(9)#1	2.813(9)

5		6	
Tb(1)-O(27)#9	2.261(18)	Dy(1)-O(5)#2	2.208(13)
Tb(1)-O(6)	2.295(14)	Dy(1)-O(11)	2.253(10)
Tb(1)-O(24)#5	2.305(12)	Dy(1)-O(9)#3	2.255(9)
Tb(1)-O(4)#2	2.315(12)	Dy(1)-O(30)#4	2.276(10)
Tb(1)-O(1)	2.400(14)	Dy(1)-O(6)	2.406(11)
Tb(1)-O(30)#8	2.444(15)	Dy(1)-O(1)	2.428(12)
Tb(1)-O(29)#8	2.593(17)	Dy(1)-O(2)	2.573(13)
Tb(1)-O(2)	2.733(14)	Dy(1)-O(7)	2.693(11)
Tb(2)-O(10)#5	2.296(19)	Dy(2)-O(15)#4	2.257(16)
Tb(2)-O(7)	2.339(16)	Dy(2)-O(12)	2.323(12)
Tb(2)-O(2)	2.354(18)	Dy(2)-O(7)	2.333(11)
Tb(2)-O(11)	2.386(12)	Dy(2)-O(2)	2.346(11)
Tb(2)-O(29)#8	2.390(14)	Dy(2)-O(16)	2.349(10)
Tb(2)-O(31W)	2.41(2)	Dy(2)-O(31W)	2.404(17)
Tb(2)-O(20)#7	2.470(13)	Dy(2)-O(25)#1	2.412(11)
Tb(2)-O(19)#7	2.624(14)	Dy(2)-O(24)#1	2.799(14)
Tb(3)-O(9)#5	2.289(16)	Dy(3)-O(14)#4	2.251(13)
Tb(3)-O(15)#6	2.305(13)	Dy(3)-O(20)#5	2.283(10)
Tb(3)-O(21)	2.341(12)	Dy(3)-O(24)#1	2.298(11)
Tb(3)-O(19)#7	2.368(12)	Dy(3)-O(26)	2.310(11)
Tb(3)-O(12)	2.446(12)	Dy(3)-O(17)	2.382(10)
Tb(3)-O(17)	2.496(12)	Dy(3)-O(21)	2.502(11)
Tb(3)-O(16)	2.528(12)	Dy(3)-O(22)	2.504(10)
Tb(3)-O(11)	2.545(13)	Dy(3)-O(16)	2.584(12)
Tb(4)-O(25)#4	2.312(14)	Dy(4)-O(29)#6	2.274(11)
Tb(4)-O(14)#6	2.334(14)	Dy(4)-O(19)#5	2.324(12)
Tb(4)-O(5)#7	2.363(12)	Dy(4)-O(10)#1	2.325(10)
Tb(4)-O(26)	2.370(13)	Dy(4)-O(32W)	2.344(12)
Tb(4)-O(22)	2.453(14)	Dy(4)-O(4)#7	2.357(10)
Tb(4)-O(17)	2.476(12)	Dy(4)-O(27)	2.402(11)
Tb(4)-O(32W)	2.360(17)	Dy(4)-O(22)	2.444(9)
Tb(4)-O(21)	2.674(12)	Dy(4)-O(26)	2.714(11)

7

0(2)-Tb(1)	2. 233 (7)
0(5)-Tb(1)#1	2. 404 (6)
0(6)-Tb(1)	2. 417 (6)
0(11)-Tb(1)	2. 459 (6)
0(14)-Tb(1)#1	2. 286 (7)
0(29)-Tb(1)#7	2. 341 (6)
0(31W)-Tb(1)	2. 61 (2)
0(33DMF)-Tb(1)	2. 417 (8)
0(4)-Tb(2)#1	2. 423 (6)
0(5)-Tb(2)#1	2. 493 (6)
0(7)-Tb(2)	2. 301 (6)
0(11)-Tb(2)	2. 508 (6)
0(12)-Tb(2)	2. 387 (6)
0(16)-Tb(2)	2. 352 (6)
0(19)-Tb(2)#2	2. 393 (7)
0(20)-Tb(2)#2	2. 612 (6)
0(25)-Tb(2)#3	2. 336 (6)
0(9)-Tb(3)#5	2. 283 (7)
0(16)-Tb(3)	2. 603 (6)
0(17)-Tb(3)	2. 362 (7)
0(20)-Tb(3)#2	2. 358 (6)
0(21)-Tb(3)	2. 328 (6)
0(24)-Tb(3)#3	2. 507 (7)
0(25)-Tb(3)#3	2. 525 (6)
0(26)-Tb(3)	2. 221 (7)
0(1)-Tb(4)#4	2. 272 (7)
0(10)-Tb(4)#5	2. 327 (8)
0(15)-Tb(4)#6	2. 316 (7)
0(22)-Tb(4)	2. 272 (7)
0(27)-Tb(4)	2. 392 (7)
0(30)-Tb(4)#8	2. 267 (8)
0(32W)-Tb(4)	2. 414 (13)

8

Dy(1)-O(2)	2.233(4)
Dy(1)-O(14)#4	2.286(4)
Dy(1)-O(29)#5	2.338(3)
Dy(1)-O(6)	2.402(3)
Dy(1)-O(5)#4	2.404(3)
Dy(1)-O(33DMF)	2.406(4)
Dy(1)-O(11)	2.464(3)
Dy(1)-O(31W)	2.588(11)
Dy(2)-O(7)	2.280(4)
Dy(2)-O(25)#6	2.343(3)
Dy(2)-O(16)	2.351(4)
Dy(2)-O(19)#7	2.390(3)
Dy(2)-O(12)	2.392(3)
Dy(2)-O(4)#4	2.427(3)
Dy(2)-O(5)#4	2.489(3)
Dy(2)-O(11)	2.507(3)
Dy(2)-O(20)#7	2.584(3)
Dy(3)-O(26)	2.212(4)
Dy(3)-O(9)#8	2.278(4)
Dy(3)-O(21)	2.317(4)
Dy(3)-O(17)	2.347(4)
Dy(3)-O(20)#7	2.350(4)
Dy(3)-O(24)#6	2.504(4)
Dy(3)-O(25)#6	2.518(4)
Dy(3)-O(16)	2.608(3)
Dy(4)-O(30)#9	2.253(5)
Dy(4)-O(22)	2.264(3)
Dy(4)-O(1)#10	2.273(4)
Dy(4)-O(15)#3	2.318(4)
Dy(4)-O(10)#8	2.330(4)
Dy(4)-O(27)	2.376(4)
Dy(4)-O(32W)	2.417(7)

(4) TG/DTA curves for 1-8

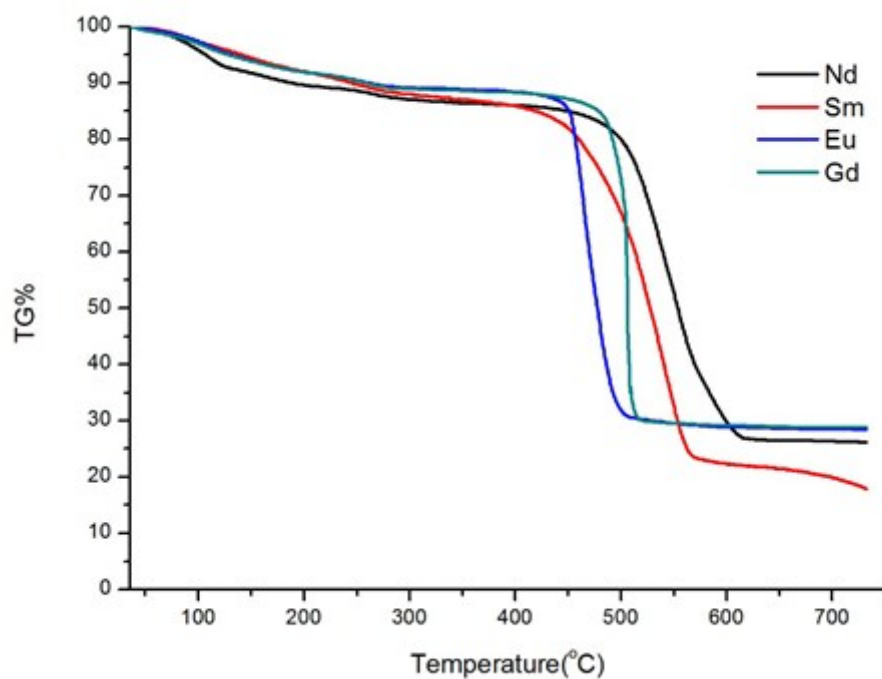


Figure S3.The TGA plots of **1, 2, 3** and **4**

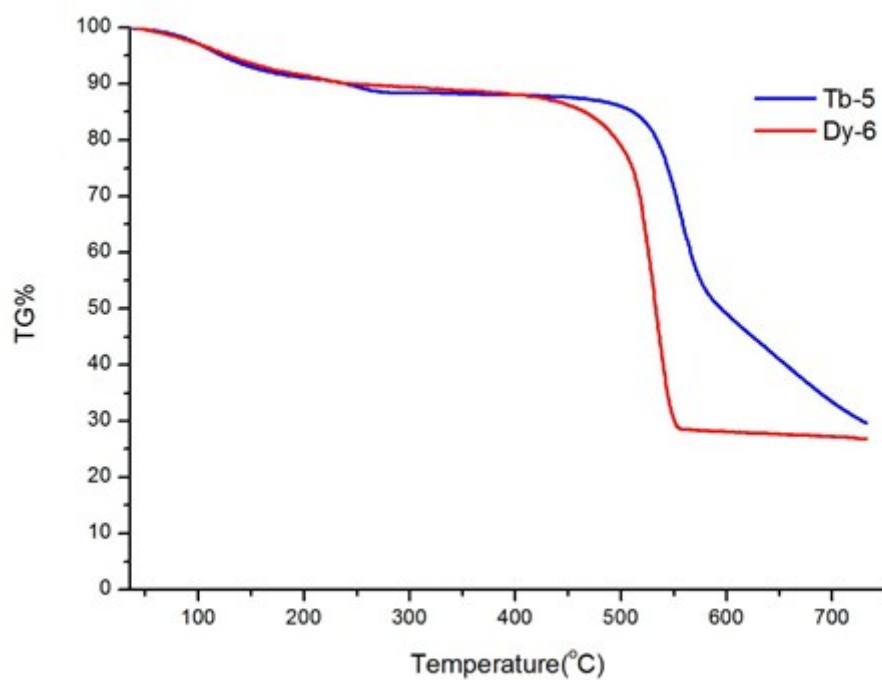


Figure S4.The TGA plots of **5** and **6**

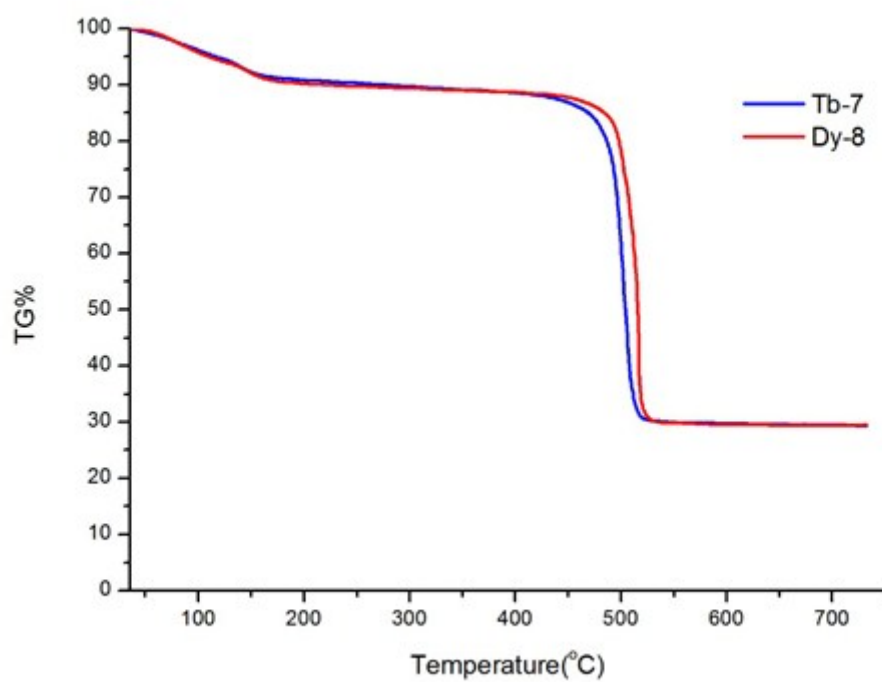


Figure S5.The TGA plots of **7** and **8**

(5) IR of 1-8

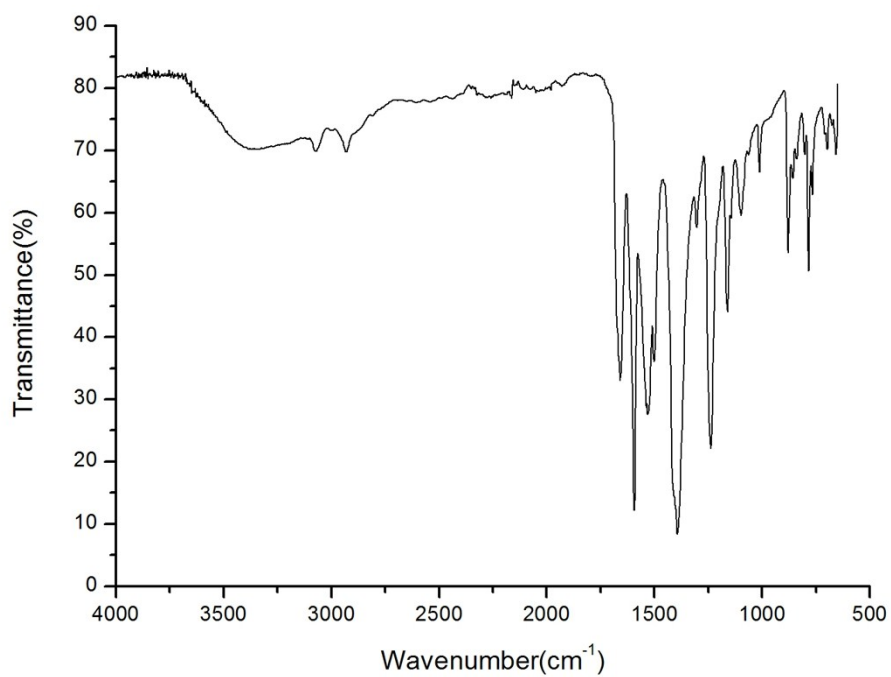


Figure S6.IR spectrum of complex **1**

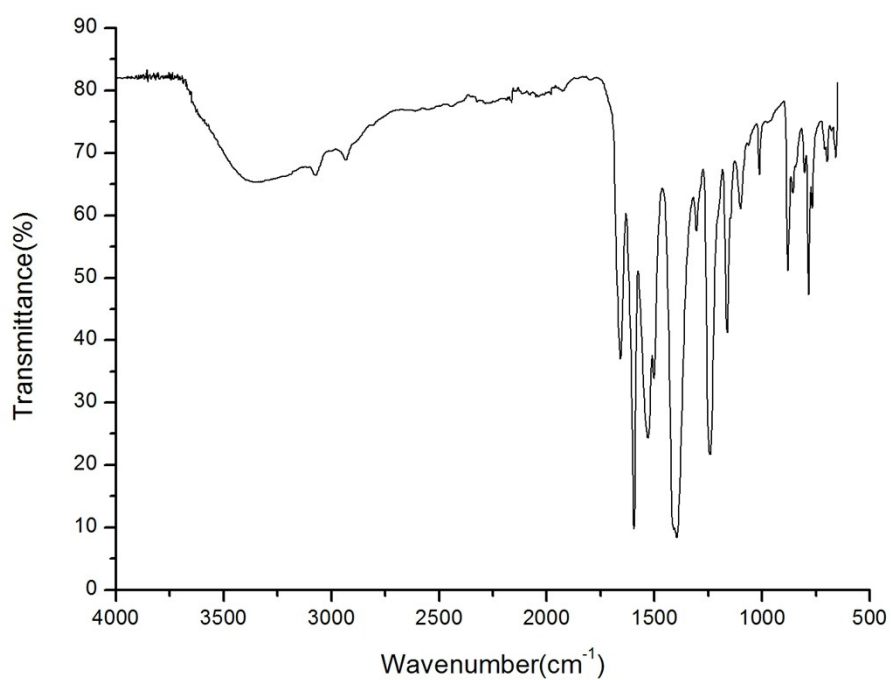


Figure S7. IR spectrum of complex **2**

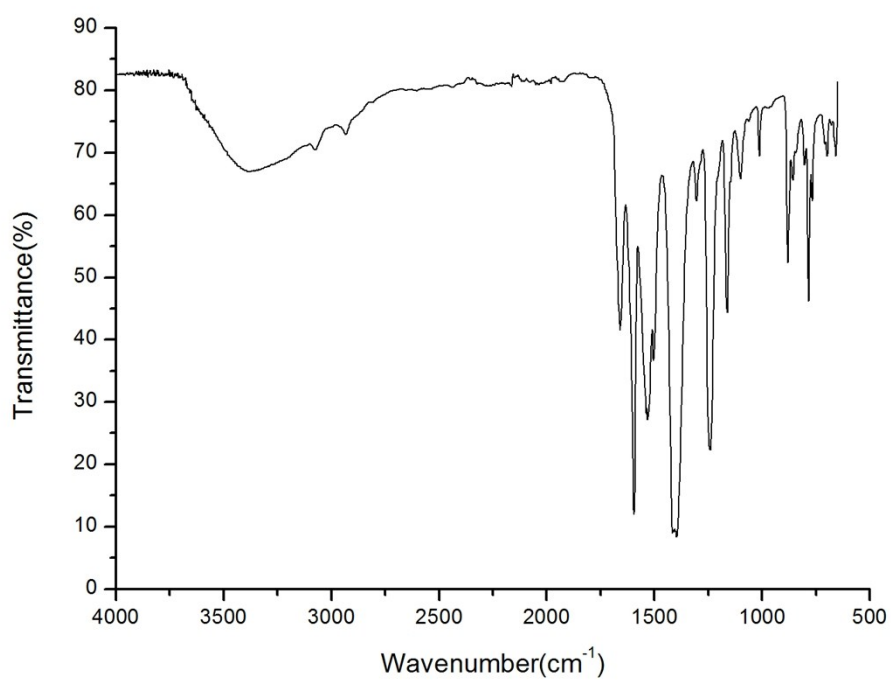


Figure S8. IR spectrum of complex **3**

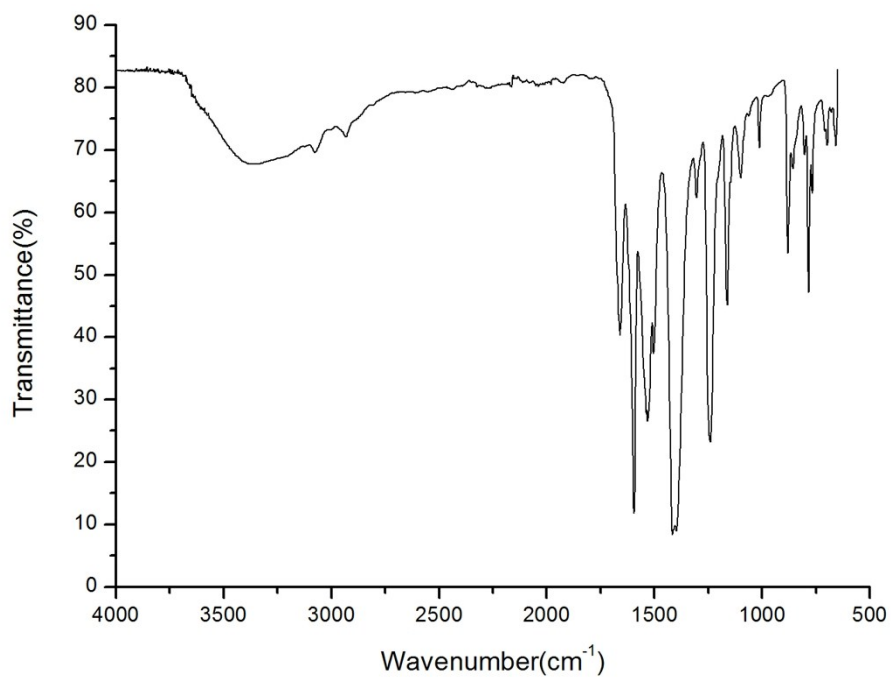


Figure S9.IR spectrum of complex 4

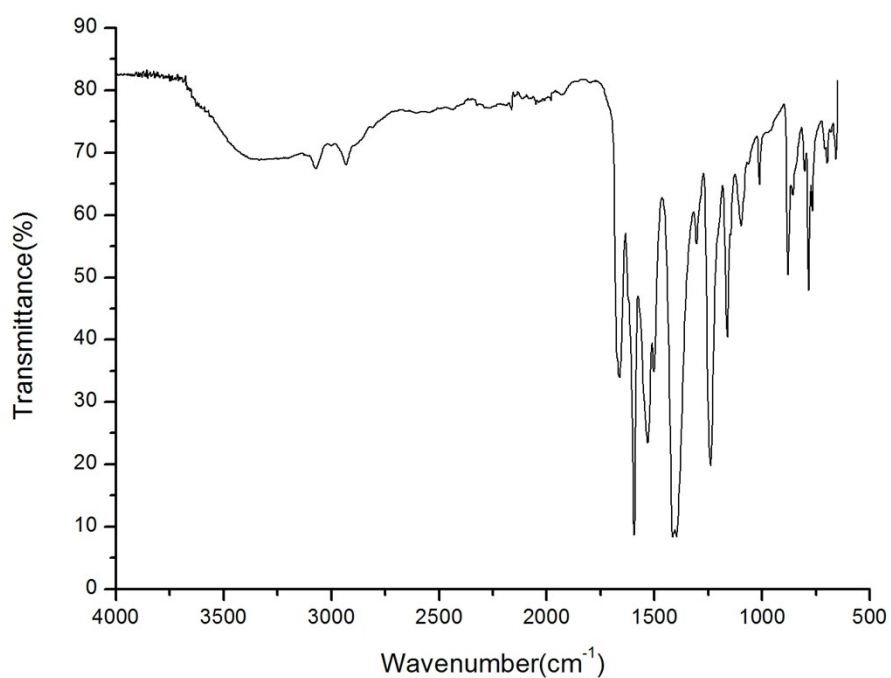


Figure S10.IR spectrum of complex 5

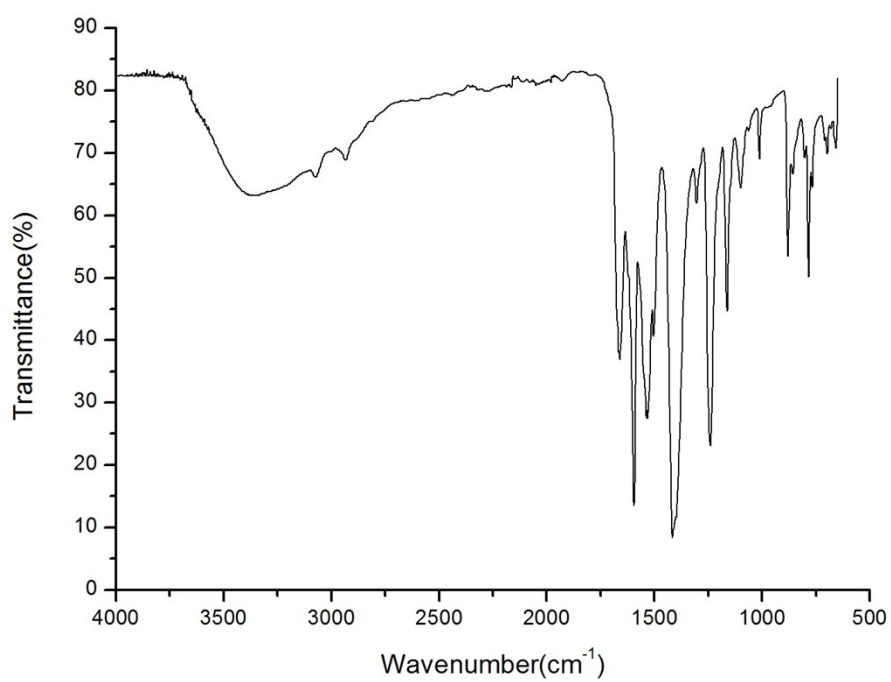


Figure S11. IR spectrum of complex 6

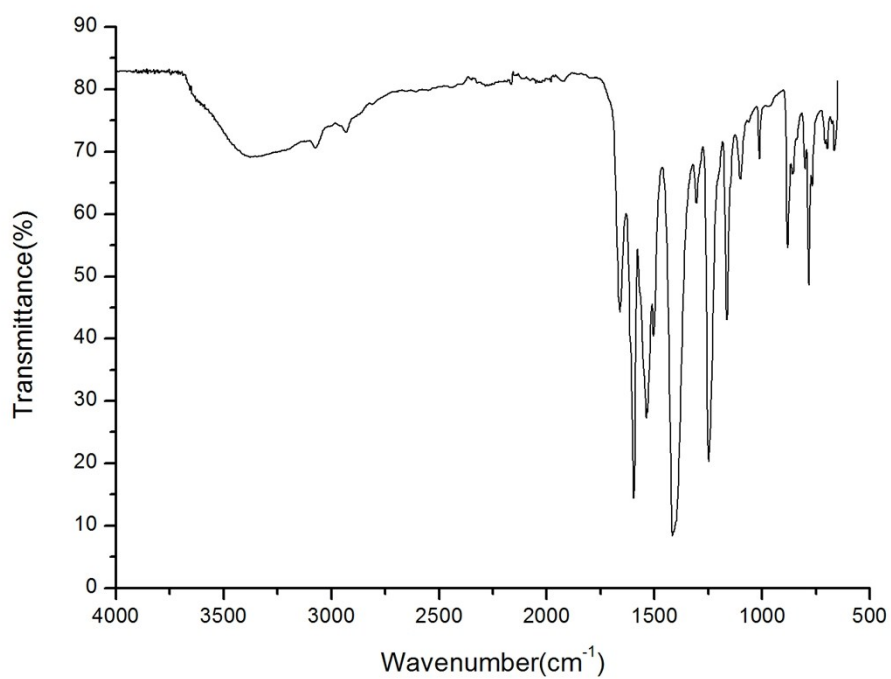


Figure S12. IR spectrum of complex 7

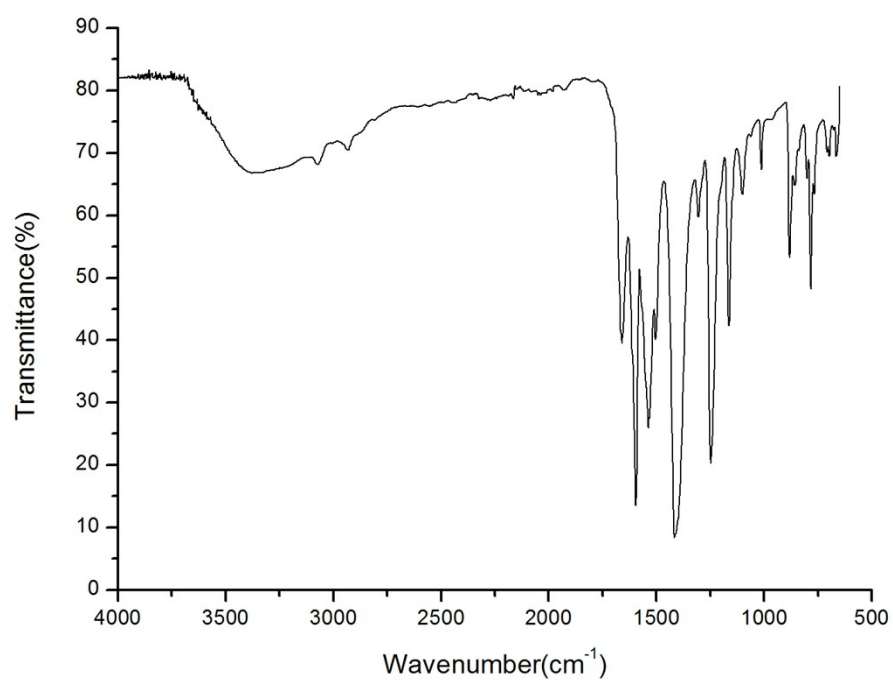


Figure S13.IR spectrum of complex **8**