

# **Synthesis, crystal structure, fluorescence and antimicrobial activity of a series of rare-earth complexes based on indolebutyric acid**

Zhi-Nan Wang,<sup>a</sup> Xue-Ting Xu,<sup>a</sup> Xiao Lv,<sup>b</sup> Feng-Ying Bai,<sup>a\*</sup> Shu-Qing Liu<sup>b\*</sup> and Yong-Heng Xing<sup>a</sup>

<sup>a</sup> College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian, 116029, P. R. China. E-mail: [baifengying2003@163.com](mailto:baifengying2003@163.com)

<sup>b</sup> Department of Biochemistry and Molecular Biology, Dalian Medical University, Dalian, 116044, P. R. China. E-mail: [Lsqsmz@163.com](mailto:Lsqsmz@163.com)

Table S1 the selected bond lengths (Å) and angles (°) of complexes **1-3**  
Table S2 the selected bond lengths (Å) and angles (°) of complexes **4-6**  
Table S3 the selected bond lengths (Å) and angles (°) of complexes **7-10**  
Table S4 Bond distances (Å) and Angles (°) of Hydrogen Bonds in Complexes **1-10\***  
Table S5 Detailed attribution of IR (cm<sup>-1</sup>) for complexes **6, 7, 8** and ligands  
Fig S1-S10 The IR spectra of complexes **1-10**  
Table S6 The UV-vis spectra assignments of complexes **1-10**  
Fig S11-S20 The UV-vis spectra of complexes **1-10**  
Fig S21-S23 Room-temperature solid-state photoluminescence spectrum of complexes **3, 5 and 8**  
Fig S24-S33 The TG curve of complexes **1-10**  
Fig S34-S43 The PXRD spectra of complexes **1-10**  
Fig S44-S63 The structure of complexes **1, 2, 3, 4, 5, 9 and 10**  
Fig S64-S79 The antimicrobial activity of complexes **1-10** against G.S, E.C, P.A and B.S

**Table S1** the selected bond lengths (Å) and angles (°) of complexes **1-3**

Complex 1					
La-O5	2.434(5)	La-O4 <sup>#1</sup>	2.463(5)	La-O6 <sup>#1</sup>	2.484(5)
La-O3	2.562(6)	La-O1	2.585(5)	La-O2	2.603(5)
La-O4	2.666(5)	La-N1	2.708(4)	La-N2	2.727(4)
O5-La-O4 <sup>#1</sup>	74.15(17)	O5-La-O6 <sup>#1</sup>	135.80(16)	O4 <sup>#1</sup> -La-O6 <sup>#1</sup>	74.94(2)
O5-La-O3	78.8(2)	O4 <sup>#1</sup> -La-O3	123.90(17)	O6 <sup>#1</sup> -La-O3	93.3(2)
O5-La-O1	75.78(17)	O4 <sup>#1</sup> -La-O1	75.51(17)	O6 <sup>#1</sup> -La-O1	124.90(17)
O3-La-O1	141.7(2)	O5-La-O2	125.80(17)	O4 <sup>#1</sup> -La-O2	91.46(17)
O6 <sup>#1</sup> -La-O2	85.59(17)	O3-La-O2	143.08(19)	O1-La-O2	50.04(16)
O5-La-O4	69.75(17)	O4 <sup>#1</sup> -La-O4	75.12(17)	O6 <sup>#1</sup> -La-O4	72.31(16)
O3-La-O4	49.43(16)	O1-La-O4	139.47(16)	O2-La-O4	156.39(15)
O5-La-N1	80.77(14)	O4 <sup>#1</sup> -La-N1	140.70(14)	O6 <sup>#1</sup> -La-N1	140.74(14)
O3-La-N1	78.74(16)	O1-La-N1	69.23(14)	O2-La-N1	79.14(14)
O4-La-N1	123.42(13)	O5-La-N2	134.39(15)	O4 <sup>#1</sup> -La-N2	151.46(14)
O6 <sup>#1</sup> -La-N2	80.42(14)	O3-La-N2	71.13(16)	O1-La-N2	108.33(14)
O2-La-N2	72.31(14)	O4-La-N2	110.87(13)	N1-La-N2	60.55(8)
Complex 2					
Pr(1)-O(5)	2.388(3)	Pr(1)-O(4) <sup>#1</sup>	2.422(3)	Pr(1)-O(6) <sup>#1</sup>	2.445(3)
Pr(1)-O(3)	2.521(4)	Pr(1)-O(2)	2.546(3)	Pr(1)-O(1)	2.559(3)
Pr(1)-O(4)	2.627(3)	Pr(1)-N(1)	2.646(4)	Pr(1)-N(2)	2.687(4)
O(5)-Pr(1)-O(4) <sup>#1</sup>	74.44(12)	O(5)-Pr(1)-O(6) <sup>#1</sup>	136.43(11)	O(4) <sup>#1</sup> -Pr(1)-O(6) <sup>#1</sup>	75.25(11)
O(5)-Pr(1)-O(3)	79.33(14)	O(4) <sup>#1</sup> -Pr(1)-O(3)	124.38(11)	O(6) <sup>#1</sup> -Pr(1)-O(3)	92.96(14)
O(5)-Pr(1)-O(2)	75.21(11)	O(4) <sup>#1</sup> -Pr(1)-O(2)	74.99(11)	O(6) <sup>#1</sup> -Pr(1)-O(2)	124.99(12)
O(3)-Pr(1)-O(2)	141.86(14)	O(5)-Pr(1)-O(1)	126.09(12)	O(4) <sup>#1</sup> -Pr(1)-O(1)	91.79(11)
O(6) <sup>#1</sup> -Pr(1)-O(1)	85.23(12)	O(3)-Pr(1)-O(1)	142.11(12)	O(2)-Pr(1)-O(1)	50.93(11)
O(5)-Pr(1)-O(4)	69.90(11)	O(4) <sup>#1</sup> -Pr(1)-O(4)	74.88(11)	O(6) <sup>#1</sup> -Pr(1)-O(4)	72.47(11)
O(3)-Pr(1)-O(4)	50.07(10)	O(2)-Pr(1)-O(4)	138.66(10)	O(1)-Pr(1)-O(4)	156.21(11)
O(5)-Pr(1)-N(1)	80.30(12)	O(4) <sup>#1</sup> -Pr(1)-N(1)	140.64(12)	O(6) <sup>#1</sup> -Pr(1)-N(1)	140.52(12)
O(3)-Pr(1)-N(1)	78.51(13)	O(2)-Pr(1)-N(1)	69.63(13)	O(1)-Pr(1)-N(1)	79.20(13)
O(4)-Pr(1)-N(1)	123.50(12)	O(5)-Pr(1)-N(2)	134.58(12)	O(4) <sup>#1</sup> -Pr(1)-N(2)	150.97(12)
O(6) <sup>#1</sup> -Pr(1)-N(2)	79.44(11)	O(3)-Pr(1)-N(2)	70.49(13)	O(2)-Pr(1)-N(2)	109.42(11)
O(1)-Pr(1)-N(2)	71.99(12)	O(4)-Pr(1)-N(2)	110.73(11)	N(1)-Pr(1)-N(2)	61.30(12)
Complex 3					
Eu(1)-O(6)	2.337(4)	Eu(1)-O(3) <sup>#1</sup>	2.356(3)	Eu(1)-O(5) <sup>#1</sup>	2.393(3)
Eu(1)-O(4)	2.464(6)	Eu(1)-O(1)	2.506(4)	Eu(1)-O(2)	2.507(4)
Eu(1)-N(2)	2.596(4)	Eu(1)-O(3)	2.589(4)	Eu(1)-N(1)	2.628(4)
O(6)-Eu(1)-O(3) <sup>#1</sup>	74.92(12)	O(6)-Eu(1)-O(5) <sup>#1</sup>	136.97(12)	O(3) <sup>#1</sup> -Eu(1)-O(5) <sup>#1</sup>	75.20(12)
O(6)-Eu(1)-O(4)	78.90(14)	O(3) <sup>#1</sup> -Eu(1)-O(4)	124.61(13)	O(5) <sup>#1</sup> -Eu(1)-O(4)	93.58(14)

O(6)-Eu(1)-O(1)	126.88(12)	O(3) <sup>#1</sup> -Eu(1)-O(1)	91.95(13)	O(5) <sup>#1</sup> -Eu(1)-O(1)	84.26(12)
O(4)-Eu(1)-O(1)	141.62(14)	O(6)-Eu(1)-O(2)	75.36(13)	O(3) <sup>#1</sup> -Eu(1)-O(2)	75.01(12)
O(5) <sup>#1</sup> -Eu(1)-O(2)	124.64(12)	O(4)-Eu(1)-O(2)	141.56(14)	O(1)-Eu(1)-O(2)	51.59(12)
O(6)-Eu(1)-N(2)	79.60(13)	O(3) <sup>#1</sup> -Eu(1)-N(2)	140.69(13)	O(5)-Eu(1)-N(2)	140.63(13)
O(4)-Eu(1)-N(2)	77.83(14)	O(1)-Eu(1)-N(2)	79.92(14)	O(2)-Eu(1)-N(2)	69.86(13)
O(6)-Eu(1)-O(3)	70.01(12)	O(3) <sup>#1</sup> -Eu(1)-O(3)	74.24(13)	O(5) <sup>#1</sup> -Eu(1)-O(3)	72.53(12)
O(4)-Eu(1)-O(3)	51.00(12)	O(1)-Eu(1)-O(3)	155.27(12)	O(2)-Eu(1)-O(3)	138.35(12)
N(2)-Eu(1)-O(3)	123.68(13)	O(6)-Eu(1)-N(1)	134.84(13)	O(3) <sup>#1</sup> -Eu(1)-N(1)	150.19(13)
O(5)-Eu(1)-N(1)	78.35(13)	O(4)-Eu(1)-N(1)	70.25(14)	O(1)-Eu(1)-N(1)	71.81(13)
O(2)-Eu(1)-N(1)	110.21(13)	N(2)-Eu(1)-N(1)	62.51(14)	O(3)-Eu(1)-N(1)	110.50(12)

Complex 1: #1 -x,-y+1,-z+2; complex 2: #1 -x+2,-y,-z+1; complex 3: #1: -x+2,-y+1,-z+1

**Table S2** the selected bond lengths (Å) and angles (°) of complexes 4-6

Complex 4					
Gd(1)-O(5)	2.340(7)	Gd(1)-O(4) <sup>#1</sup>	2.347(6)	Gd(1)-O(6) <sup>#1</sup>	2.382(5)
Gd(1)-O(3)	2.465(7)	Gd(1)-O(1)	2.490(6)	Gd(1)-O(2)	2.499(6)
Gd(1)-O(4)	2.581(5)	Gd(1)-N(2)	2.584(6)	Gd(1)-N(1)	2.636(9)
O(5)-Gd(1)-O(4) <sup>#1</sup>	74.7(2)	O(5)-Gd(1)-O(6) <sup>#1</sup>	137.3(2)	O(4) <sup>#1</sup> -Gd(1)-O(6) <sup>#1</sup>	75.2(2)
O(5)-Gd(1)-O(3)	79.1(3)	O(4) <sup>#1</sup> -Gd(1)-O(3)	124.7(2)	O(6) <sup>#1</sup> -Gd(1)-O(3)	94.0(2)
O(5)-Gd(1)-O(1)	126.5(2)	O(4) <sup>#1</sup> -Gd(1)-O(1)	91.9(2)	O(6) <sup>#1</sup> -Gd(1)-O(1)	84.1(2)
O(3)-Gd(1)-O(1)	141.7(3)	O(5)-Gd(1)-O(2)	74.5(2)	O(4) <sup>#1</sup> -Gd(1)-O(2)	74.8(2)
O(6) <sup>#1</sup> -Gd(1)-O(2)	124.7(2)	O(3)-Gd(1)-O(2)	141.1(3)	O(1)-Gd(1)-O(2)	52.0(2)
O(5)-Gd(1)-O(4)	70.5(2)	O(4) <sup>#1</sup> -Gd(1)-O(4)	73.9(2)	O(6) <sup>#1</sup> -Gd(1)-O(4)	72.4(2)
O(3)-Gd(1)-O(4)	51.49(19)	O(1)-Gd(1)-O(4)	154.87(18)	O(2)-Gd(1)-O(4)	137.8(2)
O(5)-Gd(1)-N(2)	78.9(2)	O(4) <sup>#1</sup> -Gd(1)-N(2)	140.1(2)	O(6) <sup>#1</sup> -Gd(1)-N(2)	141.2(3)
O(3)-Gd(1)-N(2)	77.7(2)	O(1)-Gd(1)-N(2)	80.2(2)	O(2)-Gd(1)-N(2)	69.6(2)
O(4)-Gd(1)-N(2)	123.9(2)	O(5)-Gd(1)-N(1)	134.9(2)	O(4) <sup>#1</sup> -Gd(1)-N(1)	150.3(2)
O(6) <sup>#1</sup> -Gd(1)-N(1)	78.0(2)	O(3)-Gd(1)-N(1)	69.7(3)	O(1)-Gd(1)-N(1)	72.7(2)
O(2)-Gd(1)-N(1)	111.3(2)	O(4)-Gd(1)-N(1)	109.9(2)	N(2)-Gd(1)-N(1)	63.5(2)
Complex 5					
Tb(1)-O(6) <sup>#1</sup>	2.324(7)	Tb(1)-O(3) <sup>#1</sup>	2.333(7)	Tb(1)-O(5)	2.353(6)
Tb(1)-O(4)	2.439(8)	Tb(1)-O(1)	2.446(6)	Tb(1)-O(2)	2.491(7)
Tb(1)-N(2)	2.562(8)	Tb(1)-O(3)	2.594(9)	Tb(1)-N(1)	2.596(6)
O(6) <sup>#1</sup> -Tb(1)-O(3) <sup>#1</sup>	75.3(2)	O(6) <sup>#1</sup> -Tb(1)-O(5)	137.9(2)	O(3) <sup>#1</sup> -Tb(1)-O(5)	75.5(2)
O(6) <sup>#1</sup> -Tb(1)-O(4)	79.2(3)	O(3) <sup>#1</sup> -Tb(1)-O(4)	125.6(2)	O(5)-Tb(1)-O(4)	94.1(2)
O(6) <sup>#1</sup> -Tb(1)-O(1)	127.1(2)	O(3) <sup>#1</sup> -Tb(1)-O(1)	91.4(2)	O(5)-Tb(1)-O(1)	83.2(2)
O(4)-Tb(1)-O(1)	141.0(3)	O(6) <sup>#1</sup> -Tb(1)-O(2)	74.8(2)	O(3) <sup>#1</sup> -Tb(1)-O(2)	73.9(2)
O(5)-Tb(1)-O(2)	124.1(2)	O(4)-Tb(1)-O(2)	141.6(2)	O(1)-Tb(1)-O(2)	52.4(2)
O(6) <sup>#1</sup> -Tb(1)-N(2)	79.1(3)	O(3) <sup>#1</sup> -Tb(1)-N(2)	140.0(2)	O(5)-Tb(1)-N(2)	140.5(3)
O(4)-Tb(1)-N(2)	77.9(2)	O(1)-Tb(1)-N(2)	79.9(2)	O(2)-Tb(1)-N(2)	69.9(3)
O(6) <sup>#1</sup> -Tb(1)-O(3)	70.3(2)	O(3) <sup>#1</sup> -Tb(1)-O(3)	74.7(2)	O(5)-Tb(1)-O(3)	73.2(2)
O(4)-Tb(1)-O(3)	51.6(2)	O(1)-Tb(1)-O(3)	154.9(2)	O(2)-Tb(1)-O(3)	137.7(2)
N(2)-Tb(1)-O(3)	124.1(2)	O(6) <sup>#1</sup> -Tb(1)-N(1)	135.3(3)	O(3) <sup>#1</sup> -Tb(1)-N(1)	149.3(2)

O(5)-Tb(1)-N(1)	76.9(2)	O(4)-Tb(1)-N(1)	69.4(3)	O(1)-Tb(1)-N(1)	72.2(3)
O(2)-Tb(1)-N(1)	112.0(2)	N(2)-Tb(1)-N(1)	64.1(3)	O(3)-Tb(1)-N(1)	109.6(2)
Complex 6					
Yb-O5	2.253(2)	Yb-O4 <sup>#1</sup>	2.274(2)	Yb-O6 <sup>#1</sup>	2.307(2)
Yb-O3	2.368(2)	Yb-O2	2.411(2)	Yb-O1	2.457(2)
Yb-N1	2.507(3)	Yb-N2	2.562(3)	Yb-O4	2.573(2)
O5-Yb-O4 <sup>#1</sup>	75.53(9)	O5-Yb-O6 <sup>#1</sup>	137.32(8)	O4 <sup>#1</sup> -Yb-O6 <sup>#1</sup>	75.85(8)
O5-Yb-O3	78.98(10)	O4 <sup>#1</sup> -Yb-O3	124.98(8)	O6 <sup>#1</sup> -Yb-O3	92.43(10)
O5-Yb-O2	127.89(8)	O4 <sup>#1</sup> -Yb-O2	91.37(9)	O6 <sup>#1</sup> -Yb-O2	83.63(9)
O3-Yb-O2	141.36(8)	O5-Yb-O1	74.84(8)	O4 <sup>#1</sup> -Yb-O1	74.09(8)
O6 <sup>#1</sup> -Yb-O1	125.48(9)	O3-Yb-O1	141.93(9)	O2-Yb-O1	53.13(8)
O5-Yb-N1	78.45(9)	O4 <sup>#1</sup> -Yb-N1	139.72(9)	O6 <sup>#1</sup> -Yb-N1	141.07(8)
O3-Yb-N1	78.38(9)	O2-Yb-N1	80.93(9)	O1-Yb-N1	69.71(9)
O5-Yb-N2	135.19(9)	O4 <sup>#1</sup> -Yb-N2	149.15(9)	O6 <sup>#1</sup> -Yb-N2	76.64(8)
O3-Yb-N2	69.79(9)	O2-Yb-N2	71.91(9)	O1-Yb-N2	112.02(8)
N1-Yb-N2	64.63(9)	O5-Yb-O4	69.81(8)	O4 <sup>#1</sup> -Yb-O4	73.83(9)
O6 <sup>#1</sup> -Yb-O4	72.22(8)	O3-Yb-O4	51.67(8)	O2-Yb-O4	154.01(8)
O1-Yb-O4	136.88(9)	N1-Yb-O4	124.12(8)	N2-Yb-O4	110.35(8)

Complex 4: #1: -x+1,-y+2,-z+2; complex 5: #1: -x+2,-y+2,-z; complex 6: #1: 1-x, 1-y, 1-z

**Table S3** the selected bond lengths (Å) and angles (°) of complexes **7-10**

Complex 7					
Sm(1)-O(2) <sup>#1</sup>	2.350(4)	Sm(1)-O(4) <sup>#1</sup>	2.372(4)	Sm(1)-O(1)	2.392(4)
Sm(1)-O(3)	2.483(4)	Sm(1)-O(4)	2.588(4)	Sm(1)-N(3)	2.621(5)
Sm(1)-N(2)	2.658(5)	Sm(1)-N(1)	2.665(5)	Sm(1)-N(4)	2.666(5)
O(2) <sup>#1</sup> -Sm(1)-O(4) <sup>#1</sup>	76.47(13)	O(2) <sup>#1</sup> -Sm(1)-O(1)	138.79(13)	O(4) <sup>#1</sup> -Sm(1)-O(1)	74.85(14)
O(2) <sup>#1</sup> -Sm(1)-O(3)	96.35(15)	O(4) <sup>#1</sup> -Sm(1)-O(3)	125.86(14)	O(1)-Sm(1)-O(3)	77.63(14)
O(2) <sup>#1</sup> -Sm(1)-O(4)	71.13(13)	O(4) <sup>#1</sup> -Sm(1)-O(4)	76.77(15)	O(1)-Sm(1)-O(4)	73.93(13)
O(3)-Sm(1)-O(4)	51.00(13)	O(2) <sup>#1</sup> -Sm(1)-N(3)	137.12(14)	O(4) <sup>#1</sup> -Sm(1)-N(3)	141.48(14)
O(1)-Sm(1)-N(3)	81.78(14)	O(3)-Sm(1)-N(3)	76.61(15)	O(4)-Sm(1)-N(3)	125.41(14)
O(2) <sup>#1</sup> -Sm(1)-N(2)	124.03(16)	O(4) <sup>#1</sup> -Sm(1)-N(2)	74.86(15)	O(1)-Sm(1)-N(2)	75.30(15)
O(3)-Sm(1)-N(2)	139.18(15)	O(4)-Sm(1)-N(2)	142.47(14)	N(3)-Sm(1)-N(2)	69.78(16)
O(2) <sup>#1</sup> -Sm(1)-N(1)	74.50(15)	O(4) <sup>#1</sup> -Sm(1)-N(1)	94.09(15)	O(1)-Sm(1)-N(1)	136.23(15)
O(3)-Sm(1)-N(1)	136.29(15)	O(4)-Sm(1)-N(1)	145.61(14)	N(3)-Sm(1)-N(1)	81.98(16)
N(2)-Sm(1)-N(1)	60.96(15)	O(2) <sup>#1</sup> -Sm(1)-N(4)	75.52(14)	O(4) <sup>#1</sup> -Sm(1)-N(4)	149.76(15)
O(1)-Sm(1)-N(4)	135.07(15)	O(3)-Sm(1)-N(4)	68.78(15)	O(4)-Sm(1)-N(4)	104.43(14)
N(3)-Sm(1)-N(4)	62.39(15)	N(2)-Sm(1)-N(4)	112.48(15)	N(1)-Sm(1)-N(4)	67.55(16)
Complex 8					

Eu(1)-O(6) <sup>#1</sup>	2.355(3)	Eu(1)-O(4) <sup>#1</sup>	2.377(3)	Eu(1)-O(5)	2.401(3)
Eu(1)-O(1)	2.441(3)	Eu(1)-O(3)	2.488(3)	Eu(1)-O(2)	2.547(3)
Eu(1)-N(2)	2.618(4)	Eu(1)-O(4)	2.618(3)	Eu(1)-N(1)	2.621(3)
O(6) <sup>#1</sup> -Eu(1)-O(4) <sup>#1</sup>	74.34(9)	O(6) <sup>#1</sup> -Eu(1)-O(5)	136.02(9)	O(4) <sup>#1</sup> -Eu(1)-O(5)	77.34(9)
O(6) <sup>#1</sup> -Eu(1)-O(1)	76.51(10)	O(4) <sup>#1</sup> -Eu(1)-O(1)	81.46(10)	O(5)-Eu(1)-O(1)	131.16(10)
O(6) <sup>#1</sup> -Eu(1)-O(3)	87.58(10)	O(4) <sup>#1</sup> -Eu(1)-O(3)	125.43(9)	O(5)-Eu(1)-O(3)	82.16(10)
O(1)-Eu(1)-O(3)	143.90(10)	O(6) <sup>#1</sup> -Eu(1)-O(2)	125.97(10)	O(4) <sup>#1</sup> -Eu(1)-O(2)	81.27(10)
O(5)-Eu(1)-O(2)	81.03(10)	O(1)-Eu(1)-O(2)	52.37(10)	O(3)-Eu(1)-O(2)	143.88(10)
O(6) <sup>#1</sup> -Eu(1)-N(2)	137.87(10)	O(4) <sup>#1</sup> -Eu(1)-N(2)	147.27(11)	O(5)-Eu(1)-N(2)	78.28(10)
O(1)-Eu(1)-N(2)	98.77(11)	O(3)-Eu(1)-N(2)	71.78(11)	O(2)-Eu(1)-N(2)	73.62(11)
O(6) <sup>#1</sup> -Eu(1)-O(4)	69.31(9)	O(4) <sup>#1</sup> -Eu(1)-O(4)	74.76(10)	O(5)-Eu(1)-O(4)	71.21(9)
O(1)-Eu(1)-O(4)	142.39(10)	O(3)-Eu(1)-O(4)	50.75(9)	O(2)-Eu(1)-O(4)	146.49(9)
N(2)-Eu(1)-O(4)	116.97(10)	O(6) <sup>#1</sup> -Eu(1)-N(1)	76.27(10)	O(4) <sup>#1</sup> -Eu(1)-N(1)	144.03(10)
O(5)-Eu(1)-N(1)	138.58(11)	O(1)-Eu(1)-N(1)	71.86(11)	O(3)-Eu(1)-N(1)	72.97(10)
O(2)-Eu(1)-N(1)	100.01(11)	N(2)-Eu(1)-N(1)	62.84(11)	O(4)-Eu(1)-N(1)	113.16(10)

**Complex 9**

Tb-O6 <sup>#1</sup>	2.326(4)	Tb-O4 <sup>#1</sup>	2.355(4)	Tb-O5	2.372(4)
Tb-O2	2.423(4)	Tb-O3	2.459(4)	Tb-O1	2.522(4)
Tb-N1	2.582(4)	Tb-N2	2.601(4)	Tb-O4	2.616(4)
O6 <sup>#1</sup> -Tb-O4 <sup>#1</sup>	74.57(13)	O6 <sup>#1</sup> -Tb-O5	136.19(12)	O4 <sup>#1</sup> -Tb-O5	77.44(12)
O6 <sup>#1</sup> -Tb-O2	76.72(14)	O4 <sup>#1</sup> -Tb-O2	81.35(13)	O5-Tb-O2	131.00(14)
O6 <sup>#1</sup> -Tb-O3	87.33(14)	O4 <sup>#1</sup> -Tb-O3	125.94(12)	O5-Tb-O3	82.55(13)
O2-Tb-O3	143.54(14)	O6 <sup>#1</sup> -Tb-O1	126.20(14)	O4 <sup>#1</sup> -Tb-O1	80.47(13)
O5-Tb-O1	80.38(14)	O2-Tb-O1	52.65(14)	O3-Tb-O1	144.07(14)
O6 <sup>#1</sup> -Tb-N1	138.27(14)	O4 <sup>#1</sup> -Tb-N1	146.52(14)	O5-Tb-N1	77.98(14)
O2-Tb-N1	98.24(15)	O3-Tb-N1	72.35(14)	O1-Tb-N1	73.28(15)
O6 <sup>#1</sup> -Tb-N2	75.93(13)	O4 <sup>#1</sup> -Tb-N2	143.43(14)	O5-Tb-N2	139.05(14)
O2-Tb-N2	71.19(15)	O3-Tb-N2	73.22(14)	O1-Tb-N2	100.35(14)
N1-Tb-N2	63.56(15)	O6 <sup>#1</sup> -Tb-O4	69.41(12)	O4 <sup>#1</sup> -Tb-O4	74.98(14)
O5-Tb-O4	71.21(12)	O2-Tb-O4	142.64(13)	O3-Tb-O4	51.02(12)
O1-Tb-O4	145.69(12)	N1-Tb-O4	117.41(14)	N2-Tb-O4	113.66(13)

**Complex 10**

Yb-O5	2.256(7)	Yb-O4 <sup>#1</sup>	2.258(6)	Yb-O3	2.293(7)
Yb-O6 <sup>#1</sup>	2.273(6)	Yb-O1	2.417(6)	Yb-O2	2.475(6)
Yb-N2	2.484(9)	Yb-N1	2.541(7)		
O5-Yb-O4 <sup>#1</sup>	81.4(3)	O5-Yb-O3	73.4(2)	O4 <sup>#1</sup> -Yb-O3	126.8(3)
O5-Yb-O6 <sup>#1</sup>	127.2(2)	O4 <sup>#1</sup> -Yb-O6 <sup>#1</sup>	76.2(2)	O3-Yb-O6 <sup>#1</sup>	83.0(3)
O5-Yb-O1	95.0(2)	O4 <sup>#1</sup> -Yb-O1	148.5(2)	O3-Yb-O1	80.9(2)
O6 <sup>#1</sup> -Yb-O1	127.3(2)	O5-Yb-O2	137.5(2)	O4 <sup>#1</sup> -Yb-O2	140.7(3)

O3-Yb-O2	73.8(2)	O6 <sup>#1</sup> -Yb-O2	73.9(2)	O1-Yb-O2	53.5(2)
O5-Yb-N2	137.8(2)	O4 <sup>#1</sup> -Yb-N2	79.1(3)	O3-Yb-N2	146.2(2)
O6 <sup>#1</sup> -Yb-N2	83.3(3)	O1-Yb-N2	83.2(2)	O2-Yb-N2	72.8(2)
O5-Yb-N1	73.9(3)	O4 <sup>#1</sup> -Yb-N1	74.5(2)	O3-Yb-N1	136.7(3)
O6 <sup>#1</sup> -Yb-N1	140.0(3)	O1-Yb-N1	74.5(2)	O2-Yb-N1	115.4(2)
N2-Yb-N1	65.0(3)				

Complex 7: #1 -x,-y,-z+1; complex 8: #1 -x,-y,-z+1; complex 9: #1 1-x, 1-y, 1-z; complex 10: #1 -x+1,-y+1,-z

**Table S4** Bond distances (Å) and Angles (°) of Hydrogen Bonds in Complexes **1-10\***

D-H...A	d (D-H) Å	d (H...A) Å	d (D...A) Å	∠DHA(°)
Complex 1				
N3-H3A...O9 <sup>#2</sup>	0.86	2.19	3.027	164.3
N5-H5A...O1W <sup>#3</sup>	0.86	2.02	2.825(11)	155.8
N7-H7A...O2	0.86	1.95	2.705(8)	146.7
O1W-H1A...O1 <sup>#4</sup>	0.822(10)	2.03(4)	2.816(9)	161(9)
O1W-H1B...O7	0.823(10)	2.31(8)	2.987(15)	140(11)
O10-H10B...O8 <sup>#5</sup>	0.82	2.29	3.02(3)	147.3
C10-H10A...O6 <sup>#6</sup>	0.93	2.59	3.272(10)	130.1
C56-H56A...O7 <sup>#7</sup>	0.93	2.55	3.307(13)	139.3
Complex 2				
O2W-H2WA...O8	0.85	2.25	2.989(10)	144.9
O2W-H2WC...O2 <sup>#2</sup>	0.85	2.05	2.856(5)	157.1
O1W-H1WA...O7 <sup>#3</sup>	0.85	2.33	3.119(15)	155.5
N3-H3A...O9 <sup>#4</sup>	0.86	2.15	2.992(10)	165.0
N4-H4A...N3 <sup>#2</sup>	0.86	2.38	3.199(8)	160.5
N5-H5...O2W <sup>#5</sup>	0.86	2.01	2.809(6)	154.4
N7-H7...O1 <sup>#6</sup>	0.86	1.96	2.714(5)	146.3
C6-H6C...O3 <sup>#6</sup>	0.93	2.56	3.254(6)	131.8
C56-H56A...O8	0.93	2.55	3.298(9)	138.2
Complex 3				
O1W-H1A...O7	0.822(10)	2.220(14)	3.041(10)	176(8)
O2W-H2WB...O8	0.85	2.56	3.133(12)	125.7
N3-H3...O9 <sup>#2</sup>	0.86	2.18	3.024(9)	165.9
N5-H5...O1W <sup>#3</sup>	0.86	2.02	2.829(8)	156.6
N7-H7...O1 <sup>#4</sup>	0.94(6)	1.89(7)	2.722(6)	147(6)
C56-H56A...O7 <sup>#5</sup>	0.93	2.55	3.319(10)	140.5

Complex 4				
O1W-H1WA...O7 <sup>#2</sup>	0.85	2.45	3.060(18)	129.1
N3-H3A...O9 <sup>#3</sup>	0.86	2.16	2.995(17)	164.3
N5-H5A...O1W <sup>#4</sup>	0.86	2.02	2.834(15)	158.1
N6-H6...O1 <sup>#5</sup>	0.86	1.98	2.740(12)	146.1
C51-H51A...O7	0.93	2.55	3.32(2)	140.4
Complex 5				
N3-H3A...O7 <sup>#2</sup>	0.86	2.17	3.006(16)	165.5
N5-H5A...O2W	0.86	1.99	2.822(14)	162.3
N7-H7...O1	0.86	2.00	2.745(12)	145.1
C56-H56A...O9	0.93	2.56	3.332(18)	141.1
Complex 6				
N3-H3A...O9 <sup>#2</sup>	0.86	2.18	3.018(7)	165.9
N5-H5A...O1W <sup>#3</sup>	0.86	1.99	2.809(5)	158.5
N7-H7...O2	0.86	1.99	2.733(4)	144.8
C56-H56A...O7 <sup>#4</sup>	0.93	2.53	3.318(7)	142.4
Complex 7				
N5-H5A...O6 <sup>#2</sup>	0.86	2.12	2.965(10)	165.5
N6-H6A...O6 <sup>#3</sup>	0.86	2.12	2.944(10)	159.9
C17-H17A...O3 <sup>#4</sup>	0.93	2.59	3.304(9)	134.3
Complex 8				
N3-H3A...O3 <sup>#2</sup>	0.86	2.05	2.863(5)	158
N4-H4A...O2 <sup>#3</sup>	0.86	2.17	2.983(5)	158
Complex 9				
N3-H3A...O3 <sup>#2</sup>	0.86	2.05	2.857(3)	157
N4-H4A...O1 <sup>#3</sup>	0.86	2.17	2.976(3)	157
Complex 10				
N4-H4A...O2 <sup>#2</sup>	0.86	2.36	3.015(9)	133.6
N5-H5A...O1 <sup>#3</sup>	0.86	2.03	2.828(11)	153.2
C30-H30A...O3 <sup>#4</sup>	0.93	2.46	3.342(11)	159.2

\*Symmetry transformation used to generate equivalent atoms: For complex 1: #2: x, y-1, z #3: x-1, y-1, z+1 #4: 1-x, 1-y, -z #5: 2-x, 1-y, -z #6: -x, 1-y, 1-z #7: 1-x, 2-y, -z; for complex 2: #2: -x+1, -y+1, -z+1 #3: -x+1, -y+1, -z #4: x, y, z+1 #5: x+1, y, z #6: -x+1, -y, -z+1; for complex 3: #2: -x+1, -y+2, -z+2 #3: -x+2, -y+2, -z+1 #4: -x+1, -y+1,



-z+1 #5: 1-x, 2-y, 1-z; for complex **4**: #2: -x+1, -y+1, -z+1 #3: x+1, y, z #4: -x+1, -y+1, -z+2 #5: -x+1, -y+2, -z+1; for complex **5**: #2: -x+1, -y+2, -z+1; for complex **6**: #2: x-1, y+1, z+1 #3: x, y+1, z #4: -x+1, -y, -z+1; for complex **7**: #2: 1+x, y, 1+z #3: x, y, 1+z #4: 1-x, 1-y, 1-z; for complex **8**: #2: 1/2-x, y-1/2, 1/2-z #3: 1/2-x, y+1/2, 3/2-z; for complex **9**: #2: 1/2-x, y-1/2, 1/2-z #3: 1/2-x, y+1/2, 3/2-z; for complex **10**: #2: -x, 1-y, -z #3: 1-x, -y, -z.

**Table S5** Detailed attribution of IR ( $\text{cm}^{-1}$ ) for complexes **6**, **7**, **8** and ligands

complex	<b>6</b>	<b>7</b>	<b>8</b>	IBA	phen
$\nu_{\text{N-H}}$	3407	3406	3416	3393	—
$\nu_{\text{Ar-H}}$	3057	3057	3048	3037	3060
$\nu_{\text{-(CH}_2\text{)-}}$	2930,2869	2929,2869	2947,2826	2911,2874	—
$\nu_{\text{asCOO-}}$	1586	1586	1579	1696	—
$\nu_{\text{sCOO-}}$	1429	1425	1426	1456	—
$\nu_{\text{C=N}}$	1516	1518	1516	1554	1586
$\nu_{\text{C=C}}$	1496	1496	1492	1488	1504
$\nu_{\text{NO}_3^-}$	1385	1385	—	—	—
$\nu_{\text{C-C}}$	1190	1190	1195	1163	1138
$\nu_{\text{C-N}}$	1102	1102	1099	1090	1090
$\nu_{\text{C-O}}$	1029	1030	1031	1031	—
$\delta_{\text{Ar-H}}$	845,746,731	843,746,727	864,773,746	842,763,741	835-739
$\nu_{\text{Ln-O}}$	429	429	421	—	—

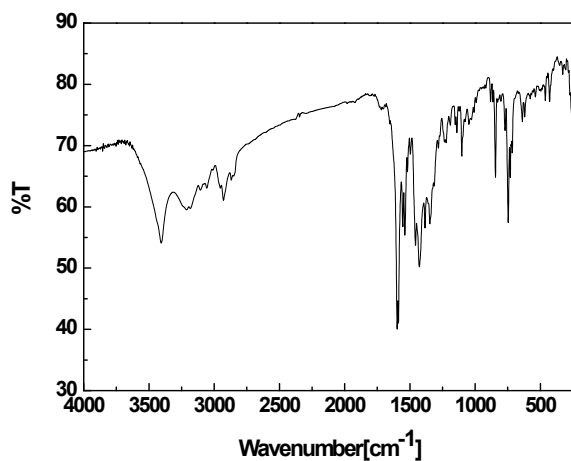


Fig S1 The IR spectrum of complex **1**

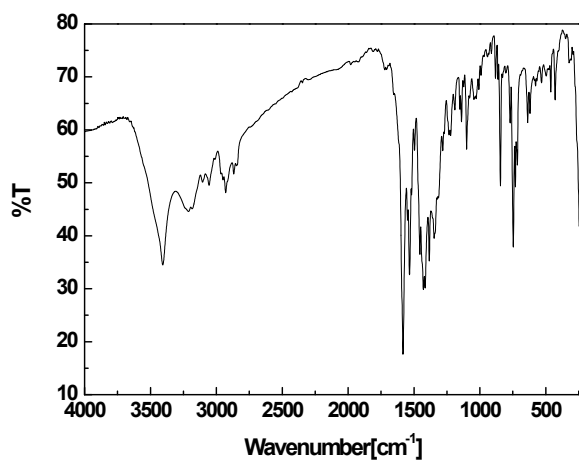


Fig S2 The IR spectrum of complex 2

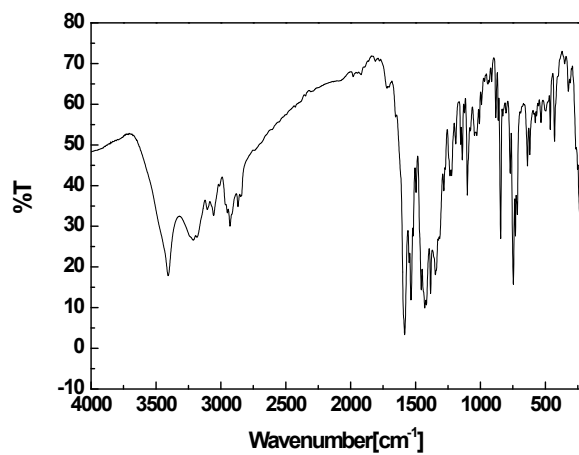


Fig S3 The IR spectrum of complex 3

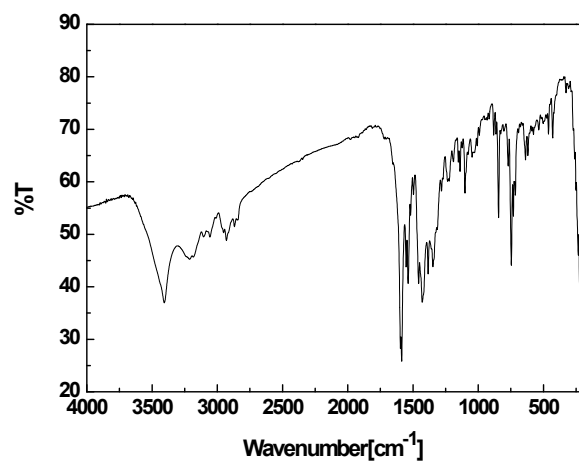


Fig S4 The IR spectrum of complex 4

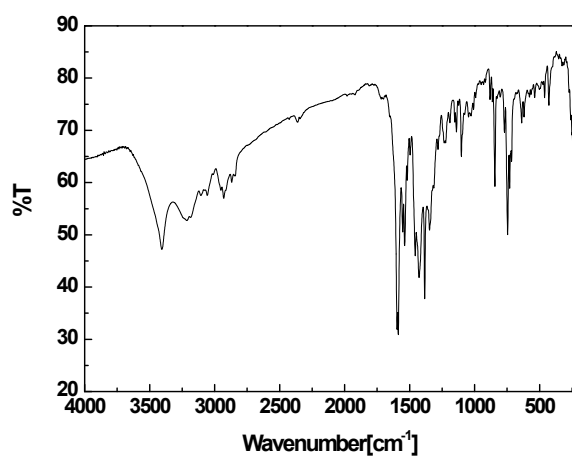


Fig S5 The IR spectrum of complex 5

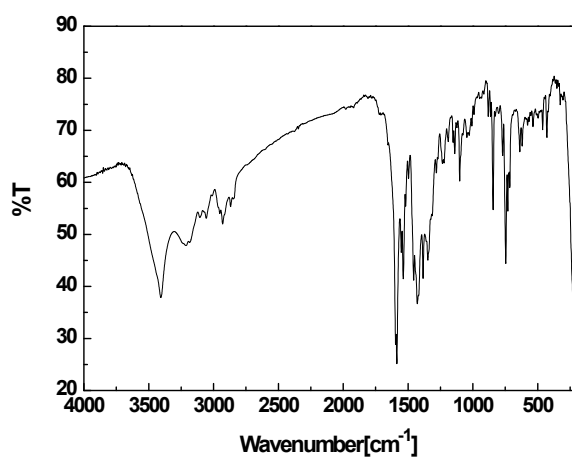


Fig S6 The IR spectrum of complex 6

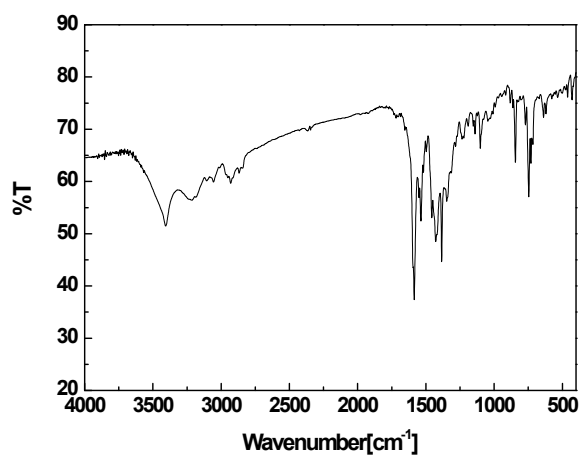


Fig S7 The IR spectrum of complex 7

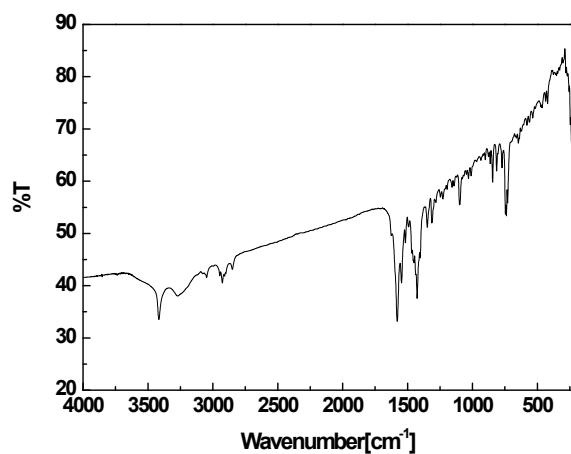


Fig S8 The IR spectrum of complex **8**

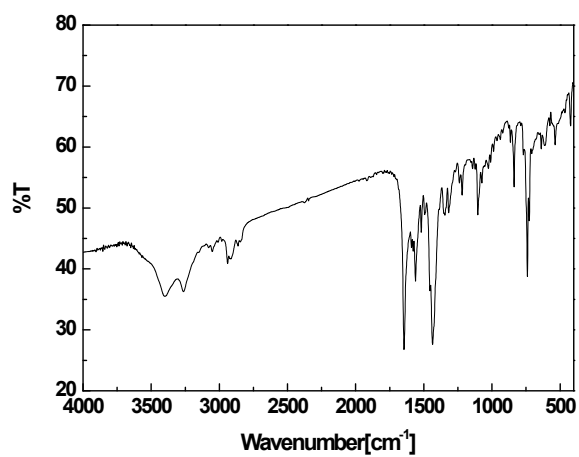


Fig S9 The IR spectrum of complex **9**

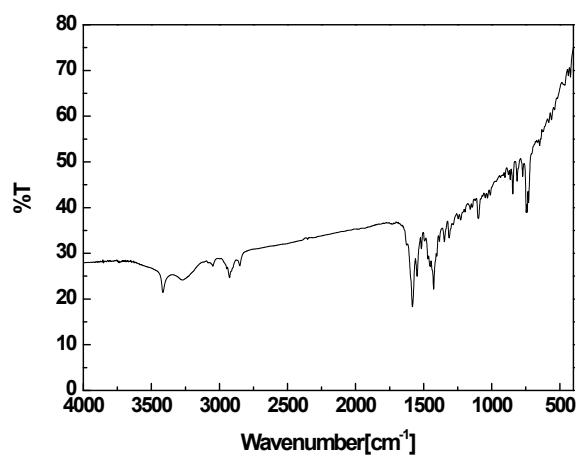
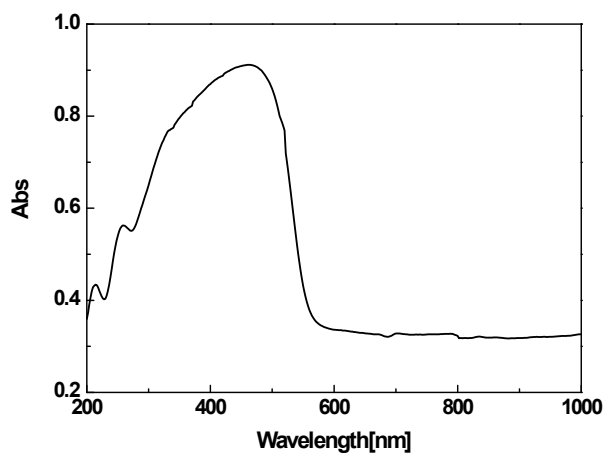


Fig S10 The IR spectrum of complex **10**

**Table S6** The UV-vis spectra assignments of complexes **1-10**

complex	$\lambda$ / nm	$\lambda$ / nm	$\lambda$ / nm	$\lambda$ / nm
<b>1</b>	448(absorption of IBA)	258, 214( $\pi \rightarrow \pi^*$ )		
<b>2</b>	1590( $^3H_4 \rightarrow ^3F_3$ )	1478( $^3H_4 \rightarrow ^3F_4$ )	1104( $^3H_1 \rightarrow ^3G_4$ )	590( $^3H_4 \rightarrow ^3D_2$ )
	462( $^3H_4 \rightarrow ^3P_1$ )	448( $^3H_4 \rightarrow ^3P_2$ )	260, 214( $\pi \rightarrow \pi^*$ )	
<b>3</b>	462(absorption of IBA)	260, 218( $\pi \rightarrow \pi^*$ )		
<b>4</b>	433(absorption of IBA)	293, 217( $\pi \rightarrow \pi^*$ )		
<b>5</b>	458(absorption of IBA)	262, 214( $\pi \rightarrow \pi^*$ )		
<b>6</b>	964( $^2F_{5/2} \rightarrow ^2F_{7/2}$ )	448(absorption of IBA)	260, 214( $\pi \rightarrow \pi^*$ )	
<b>7</b>	1668( $^6H_{5/2} \rightarrow ^6F_{1/2}$ )	1579( $^6H_{5/2} \rightarrow ^6H_{15/2}$ )	1517( $^6H_{5/2} \rightarrow ^6F_{3/2}$ )	1401( $^6H_{5/2} \rightarrow ^6F_{5/2}$ )
	1249( $^6H_{5/2} \rightarrow ^6F_{7/2}$ )	1089( $^6H_{5/2} \rightarrow ^6F_{9/2}$ )	946( $^6H_{5/2} \rightarrow ^6F_{11/2}$ )	427( $^6H_{5/2} \rightarrow ^4F_{7/2}$ )
	309, 264, 216( $\pi \rightarrow \pi^*$ )			
<b>8</b>	350( $\pi \rightarrow \pi^*$ )			
<b>9</b>	460(absorption of IBA)	263, 214( $\pi \rightarrow \pi^*$ )		
<b>10</b>	964( $^2F_{5/2} \rightarrow ^2F_{7/2}$ )	354, 260, 214( $\pi \rightarrow \pi^*$ )		

Fig S11 The UV-vis spectrum of complex **1**

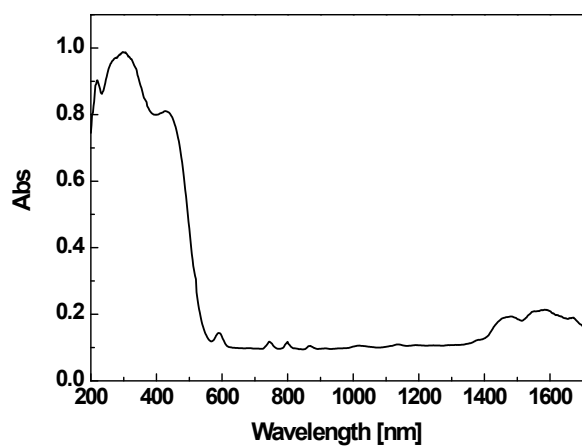


Fig S12 The UV-vis spectrum of complex 2

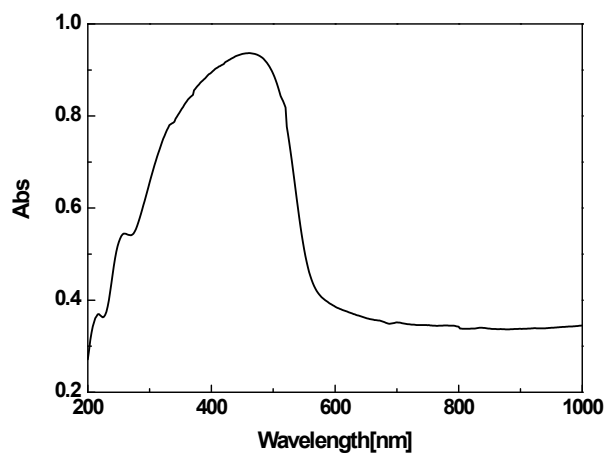


Fig S13 The UV-vis spectrum of complex 3

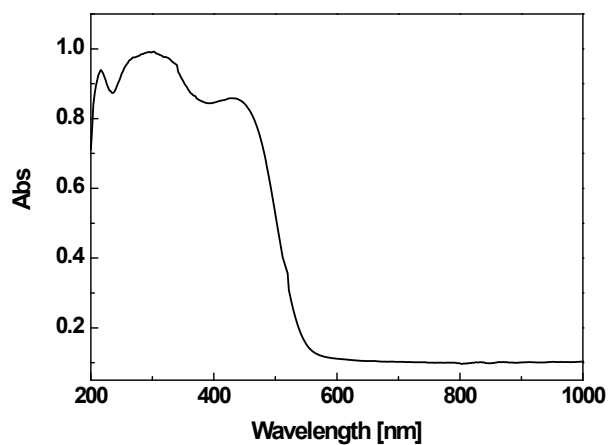


Fig S14 The UV-vis spectrum of complex 4

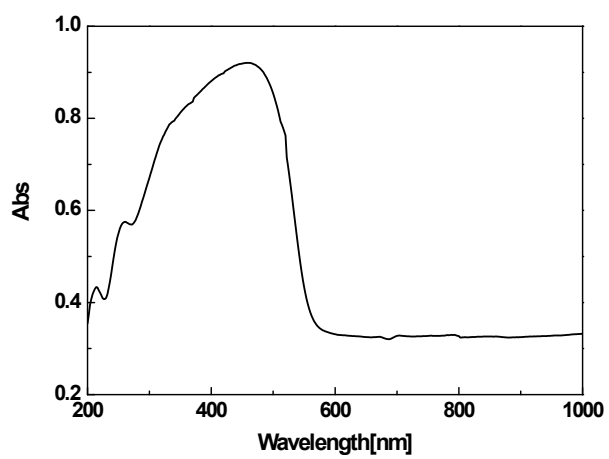


Fig S15 The UV-vis spectrum of complex 5

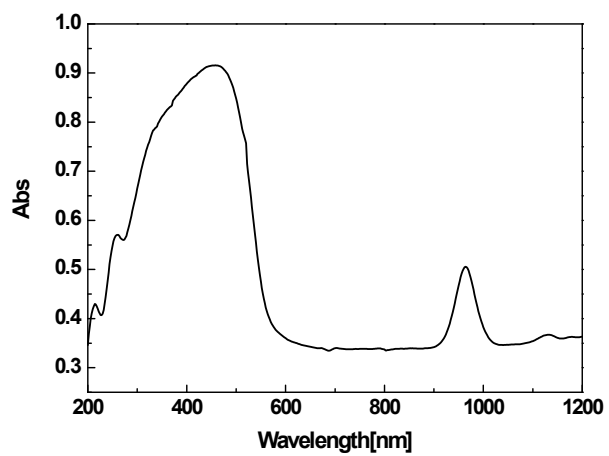


Fig S16 The UV-vis spectrum of complex 6

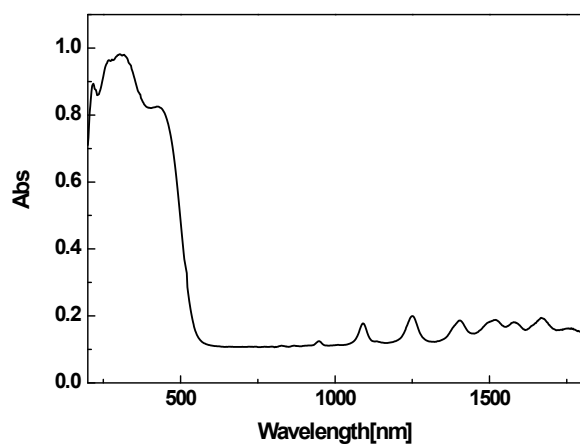


Fig S17 The UV-vis spectrum of complex 7

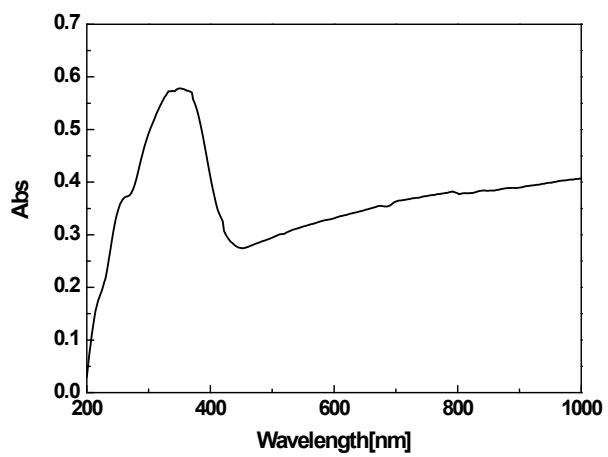


Fig S18 The UV-vis spectrum of complex 8

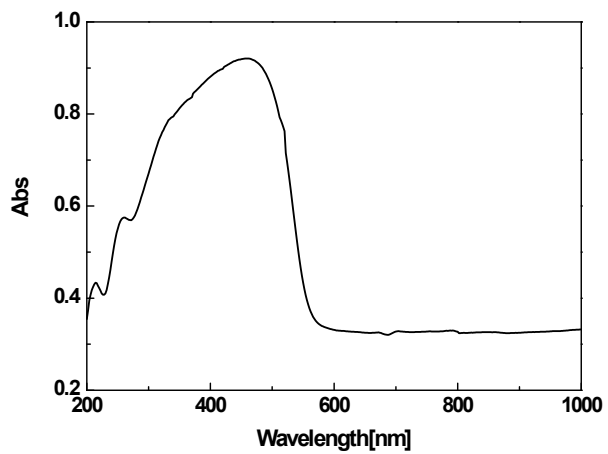


Fig S19 The UV-vis spectrum of complex 9

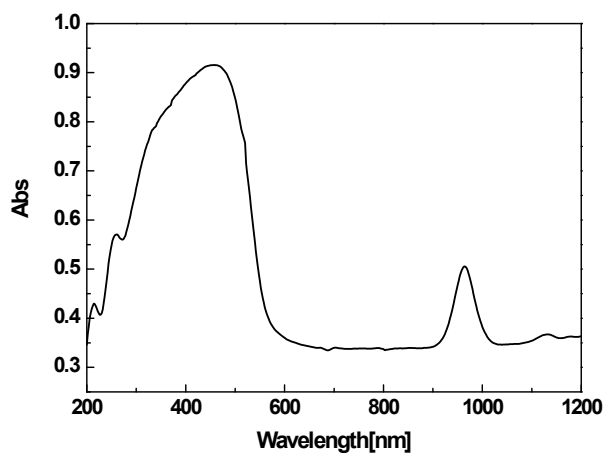


Fig S20 The UV-vis spectrum of complex 10



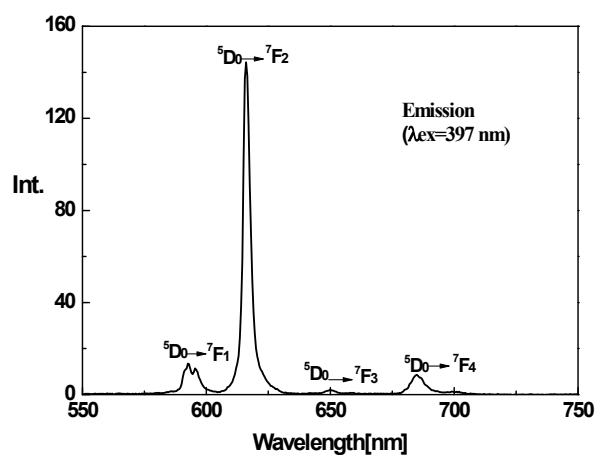


Fig. S21 Room-temperature solid-state photoluminescence spectrum of complex 3

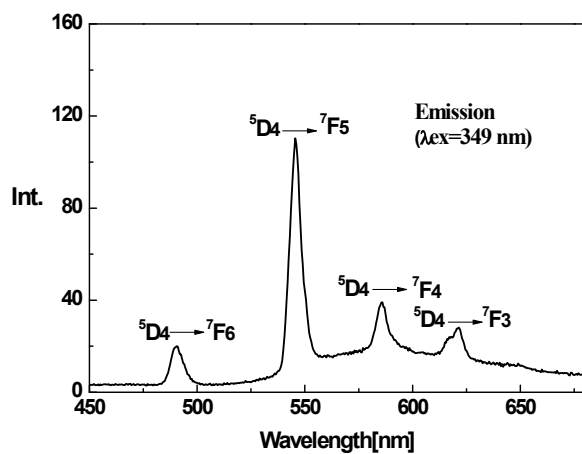


Fig. S22 Room-temperature solid-state photoluminescence spectrum of complex 5

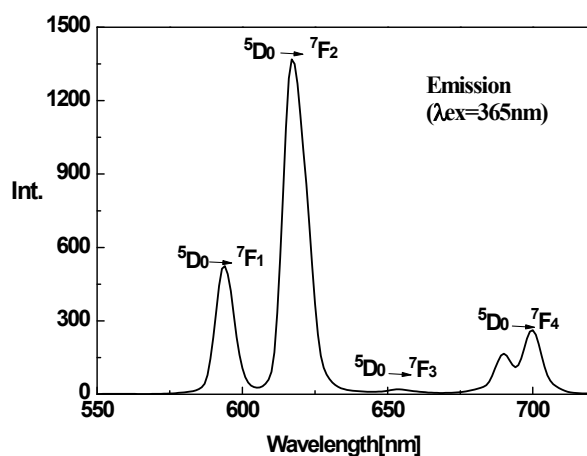


Fig. S23 Room-temperature solid-state photoluminescence spectrum of complex 8

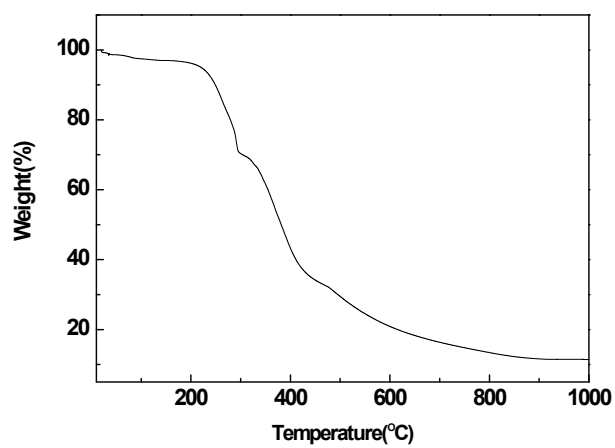


Fig S24 The TG curve of complex 1

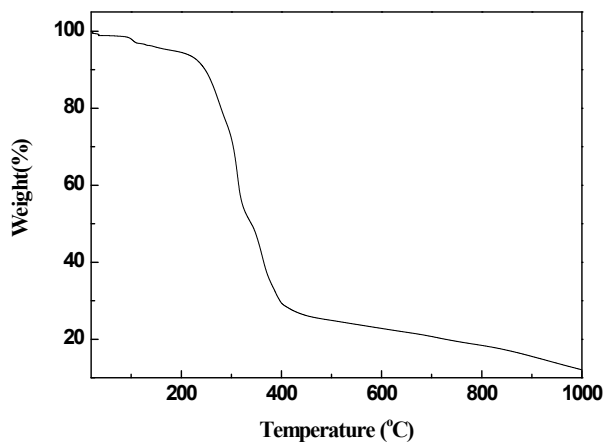


Fig S25 The TG curve of complex 2

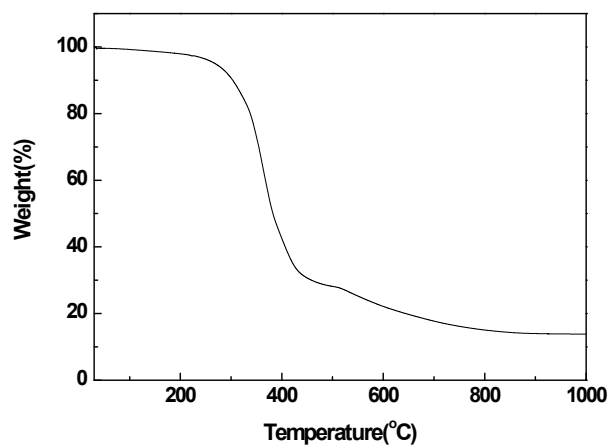


Fig S26 The TG curve of complex 3

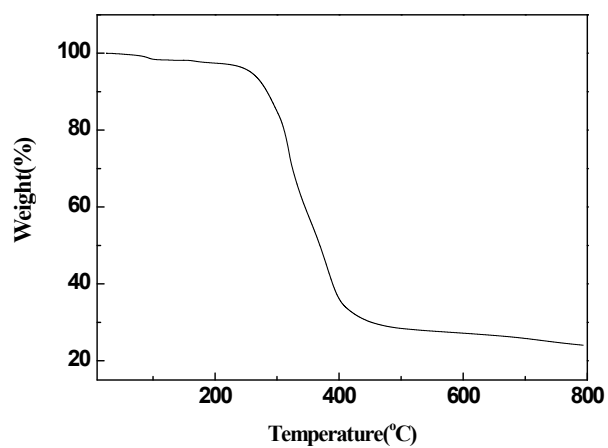


Fig S27 The TG curve of complex 4

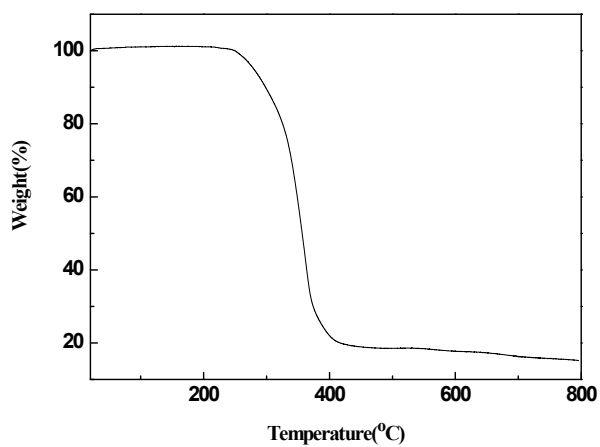


Fig S28 The TG curve of complex 5

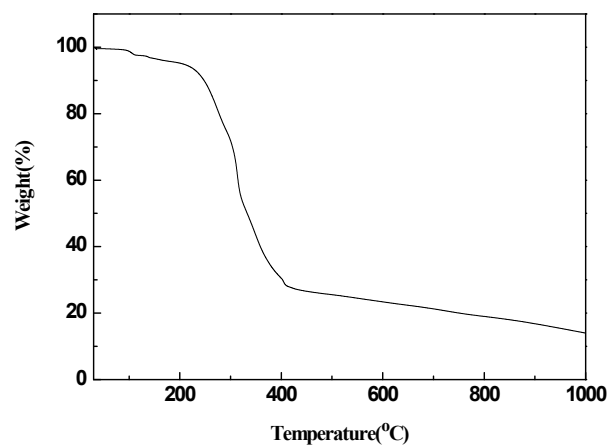


Fig S29 The TG curve of complex 6

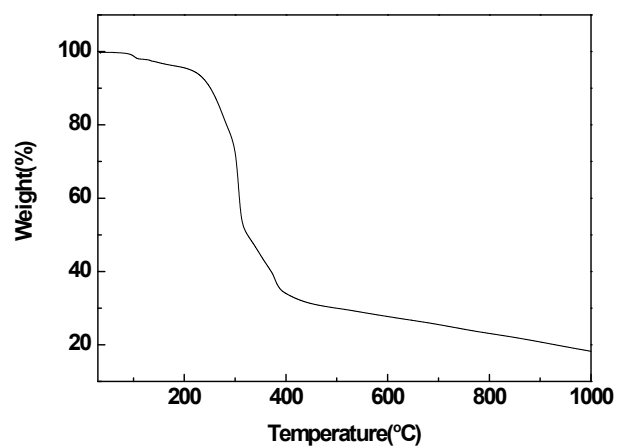


Fig S30 The TG curve of complex 7

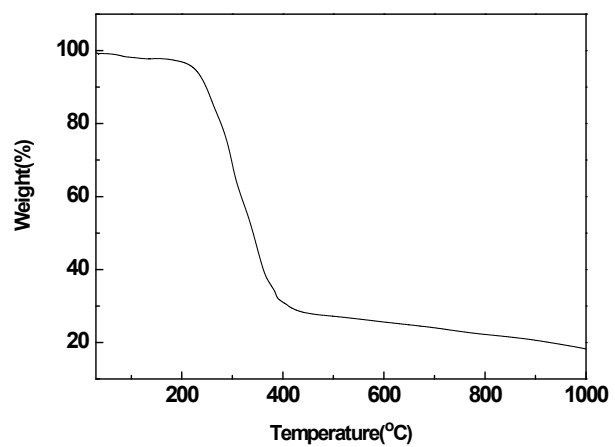


Fig S31 The TG curve of complex 8

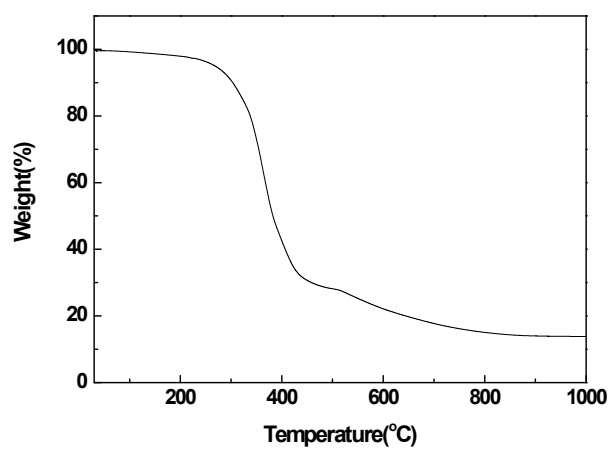


Fig S32 The TG curve of complex 9

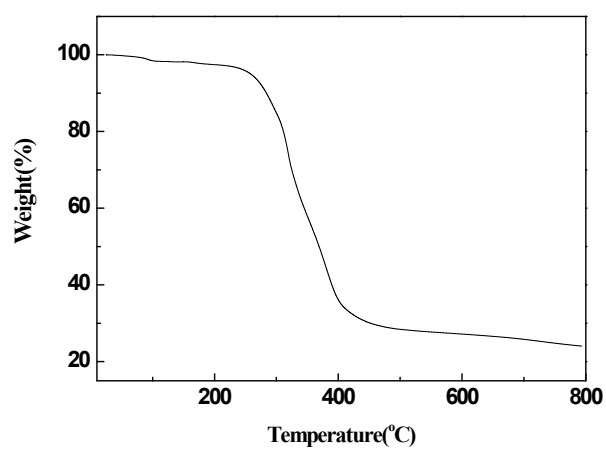


Fig S33 The TG curve of complex 10

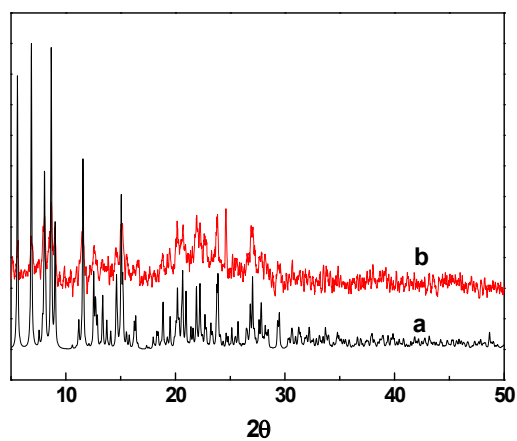


Fig S34 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 1

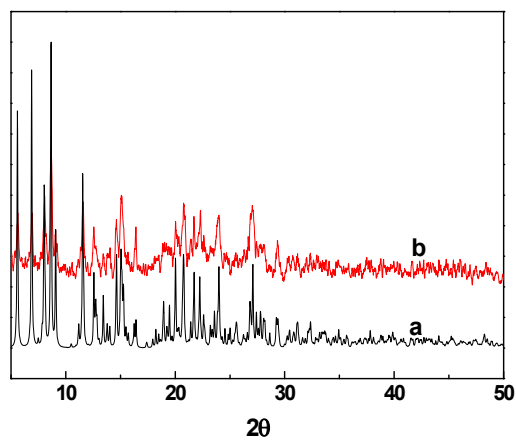


Fig S35 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 2

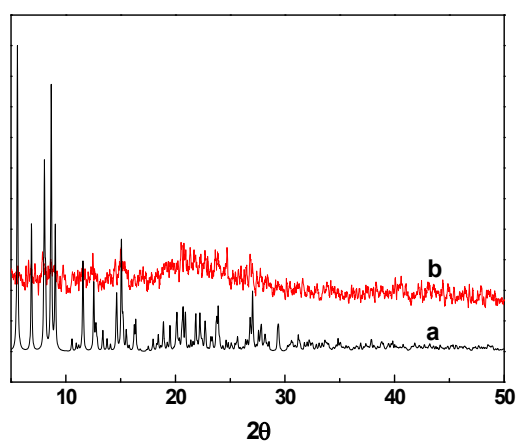


Fig S36 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 3

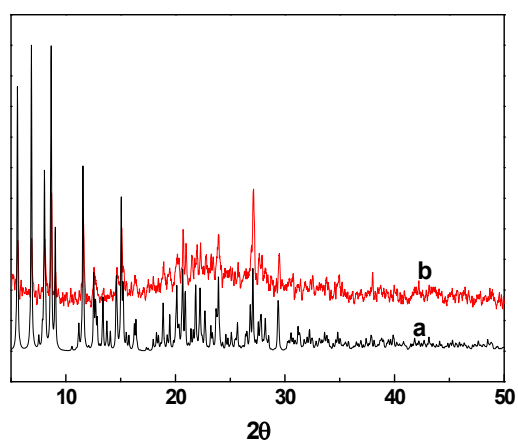


Fig S37 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 4

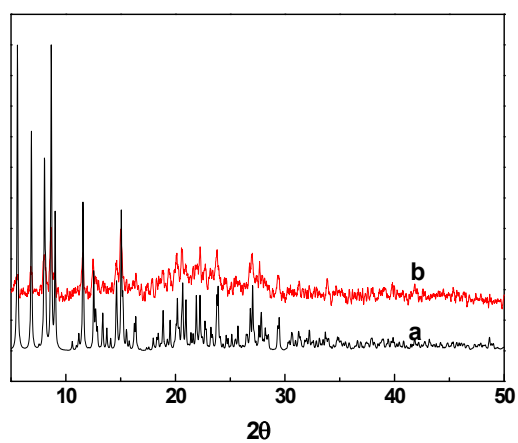


Fig S38 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 5

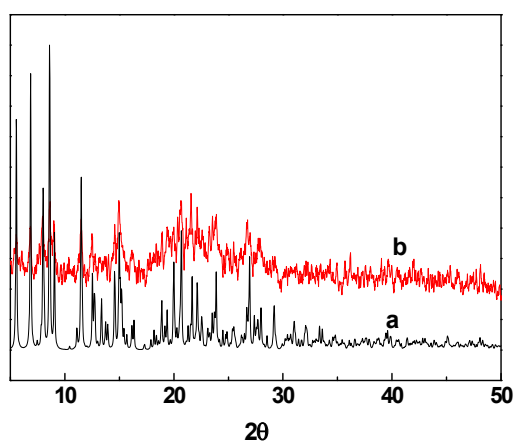


Fig S39 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 6

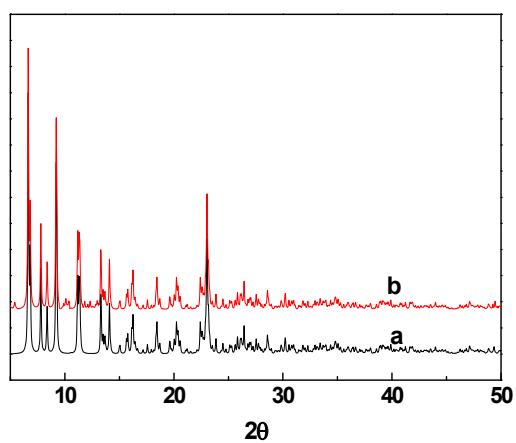


Fig S40 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 7

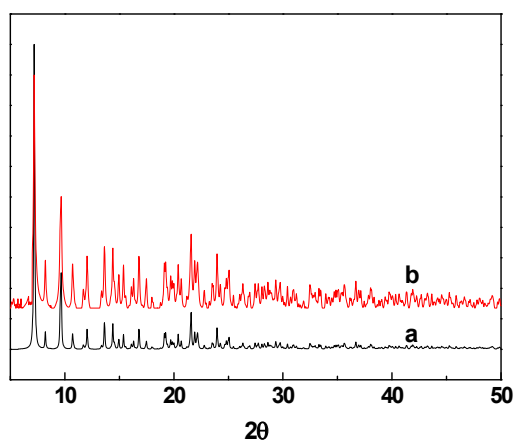


Fig S41 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 8

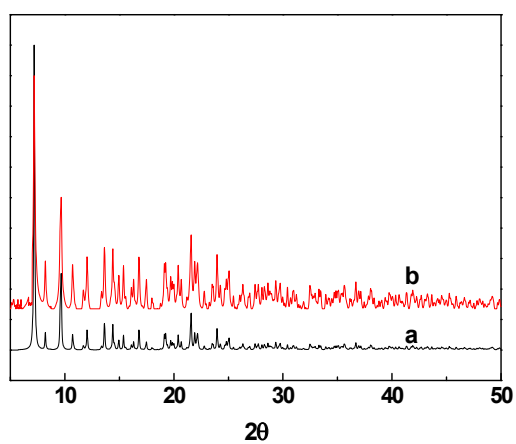


Fig S42 The simulated PXR D pattern (a) and measured PXR D spectrum (b) of complex 9

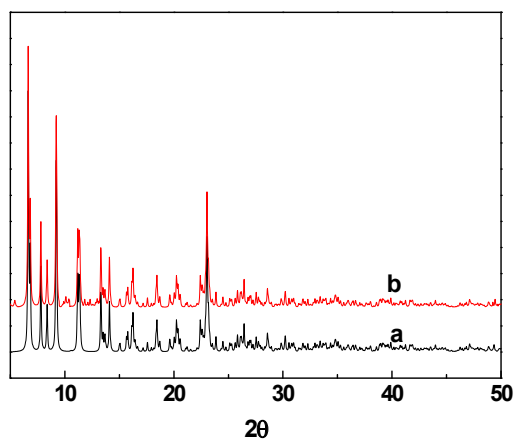


Fig S43 The simulated PXR D pattern (a) and measured PXR D spectrum (b) of complex 10

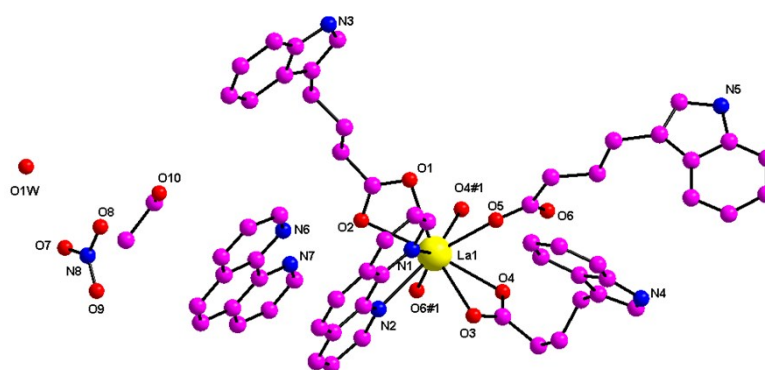


Fig S44 The unit structure of complex 1(symmetry codes: #1 -x,-y+1,-z+2)



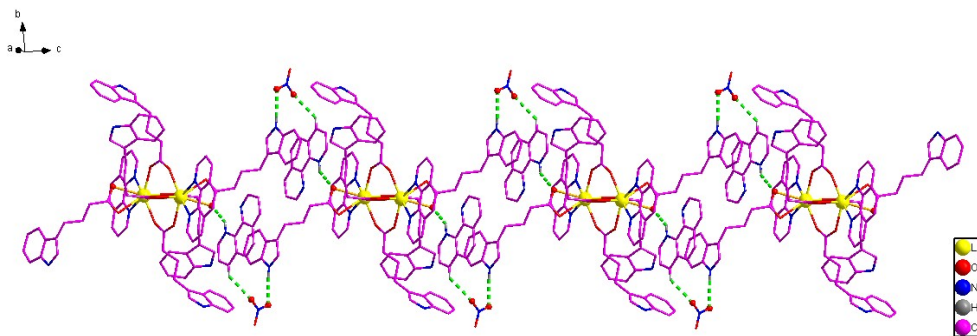


Fig S45 The 1D chain structure connected by hydrogen bonds of complex 1

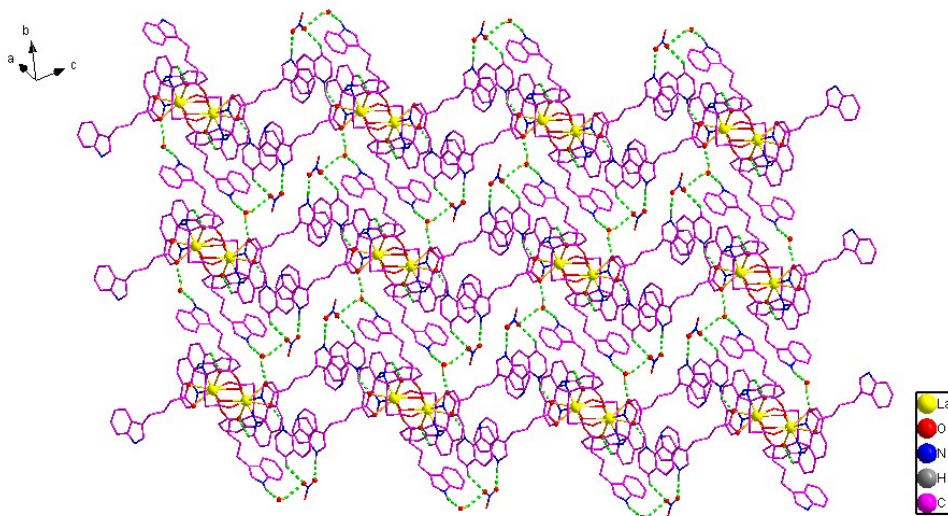


Fig S46 The 2D sheet structure connected by hydrogen bonds of complex 1

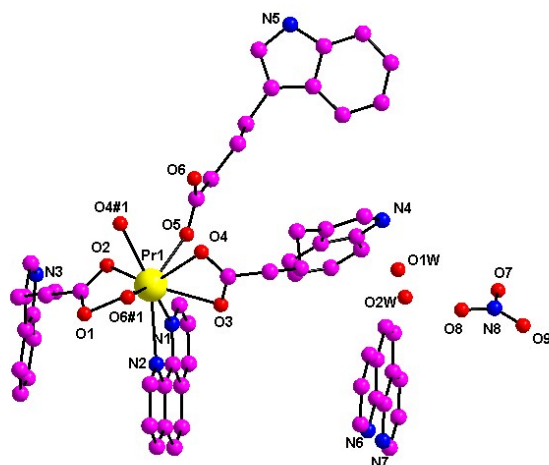


Fig S47 The unit structure of complex 2(symmetry codes: #1 -x+2,-y,-z+1)

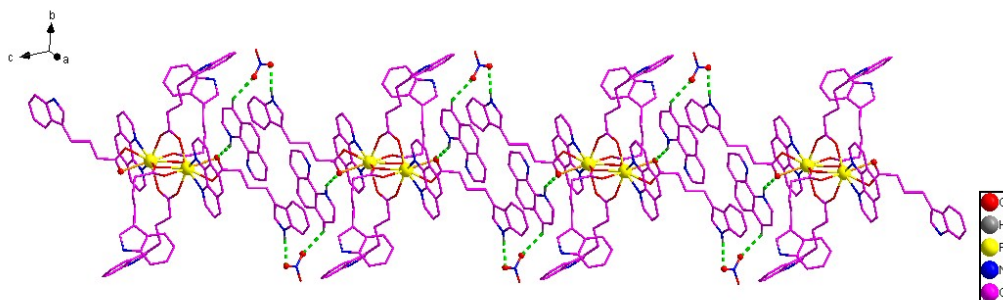


Fig S48 The 1D chain structure connected by hydrogen bonds of complex 2

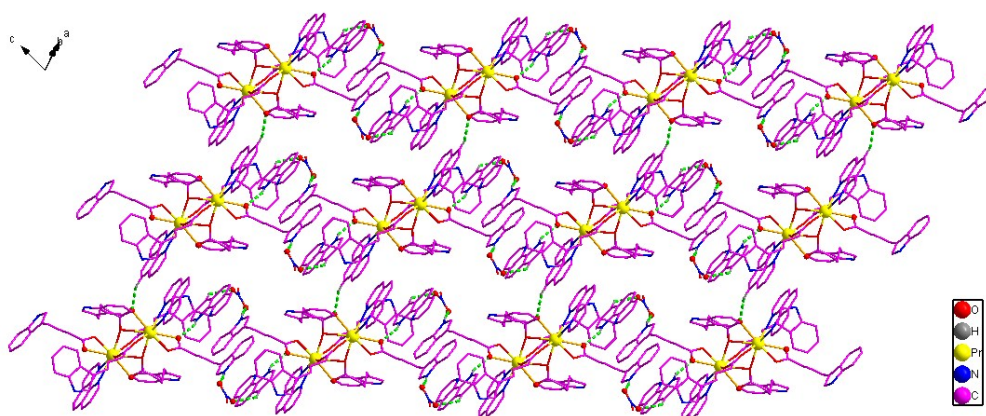


Fig S49 The 2D sheet structure connected by hydrogen bonds of complex 2

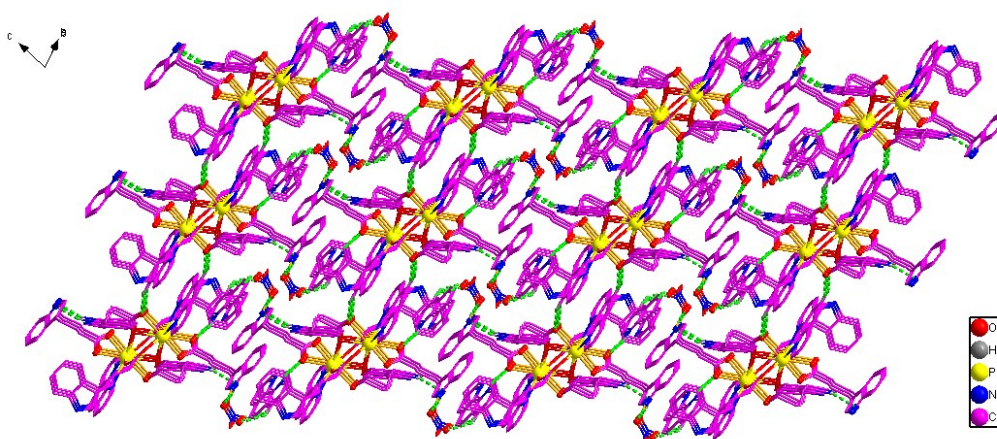


Fig S50 The 3D network structure connected by hydrogen bonds of complex 2

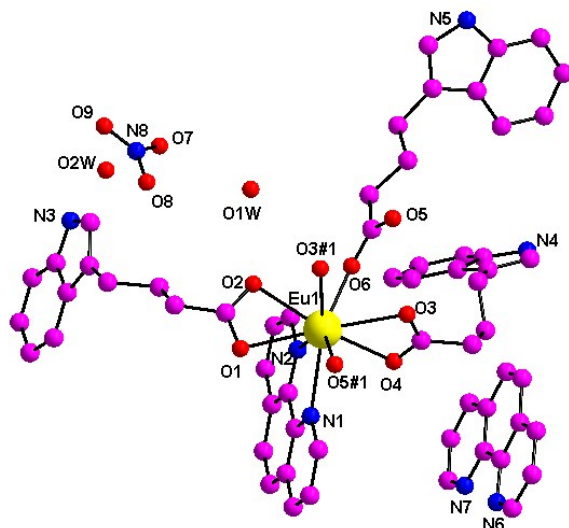


Fig S51 The unit structure of complex **3** (symmetry codes: #1:  $-x+2, -y+1, -z+1$ )

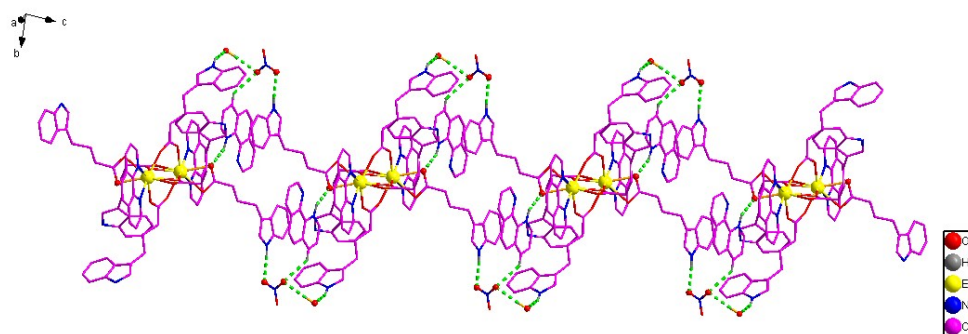


Fig S52 The 1D chain structure connected by hydrogen bonds of complex **3**

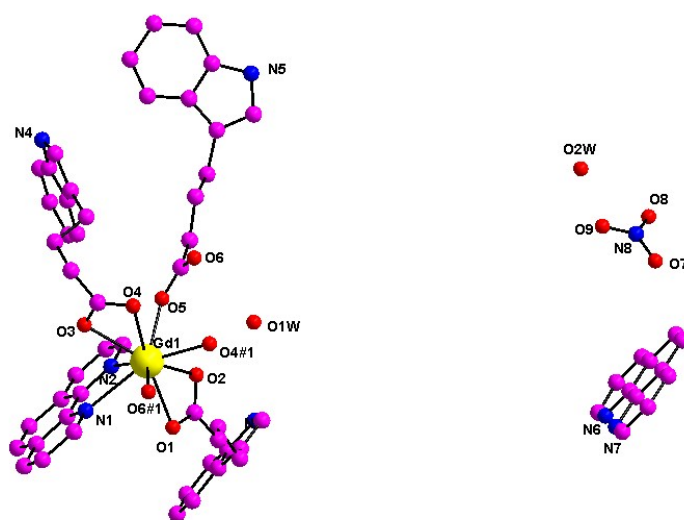


Fig S53 The unit structure of complex **4** (symmetry codes: #1:  $2-x, 2-y, -z$ )

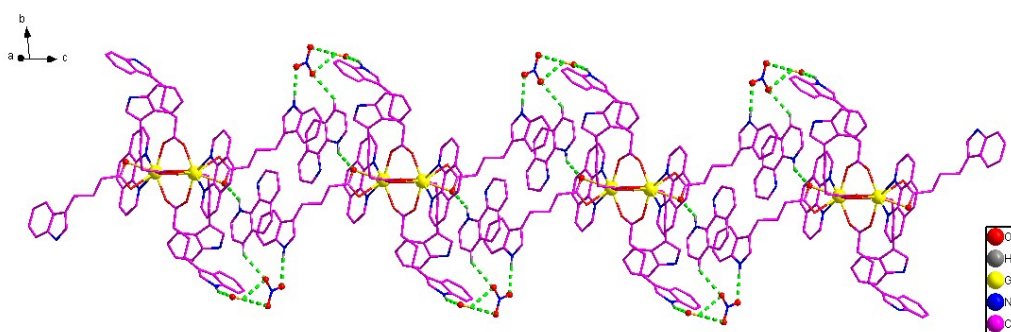


Fig S54 The 1D chain structure connected by hydrogen bonds of complex 4

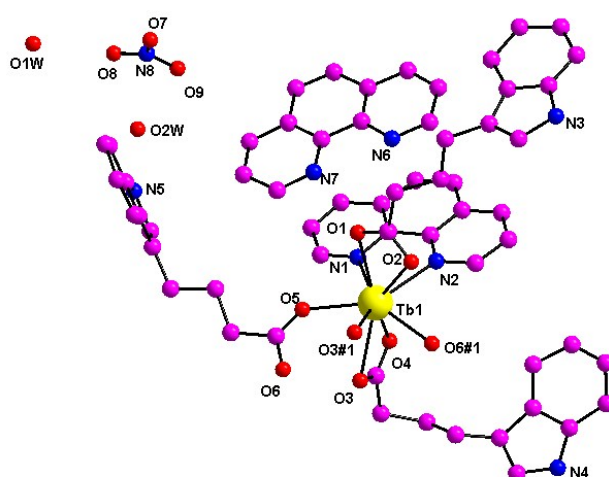


Fig S55 The unit structure of complex 5 (symmetry codes: #1: 1-x, 1-y, 1-z)

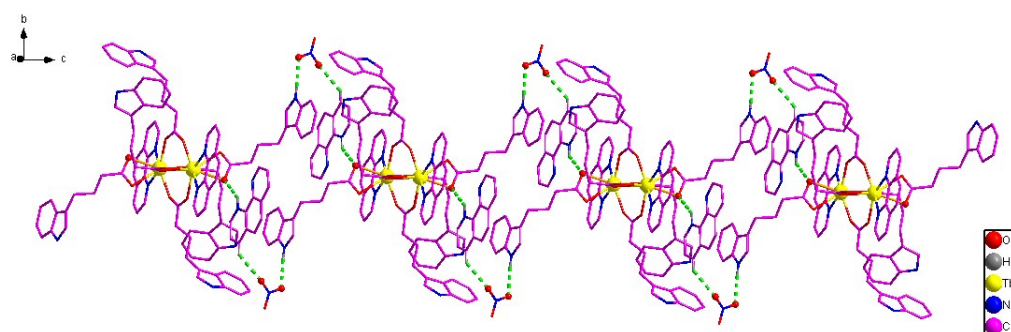


Fig S56 The 1D chain structure connected by hydrogen bonds of complex 5



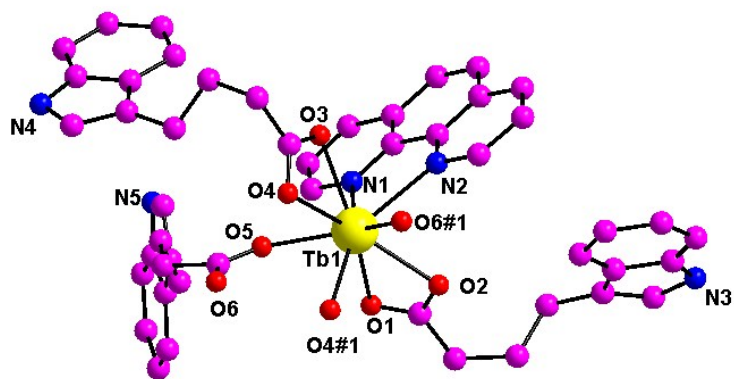


Fig S57 The unit structure of complex **9** (symmetry codes: #1: 1-x, 1-y, 1-z)

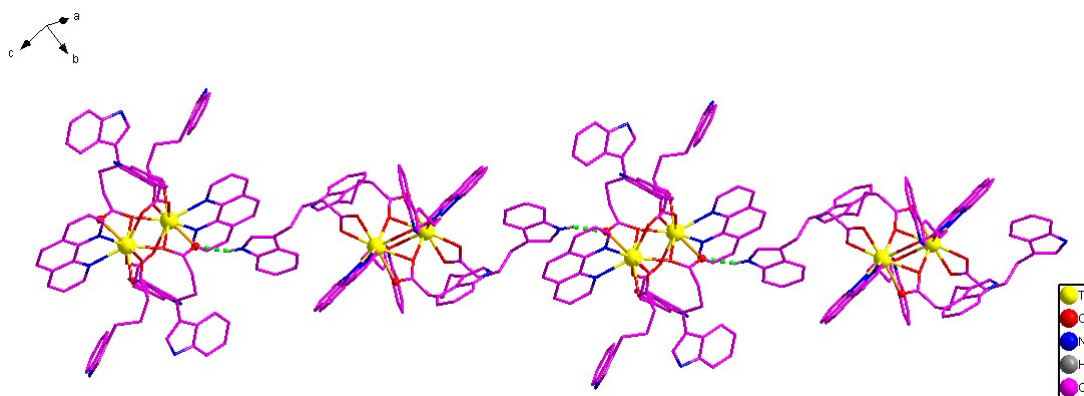


Fig S58 The 1D chain structure connected by hydrogen bonds of complex **9**

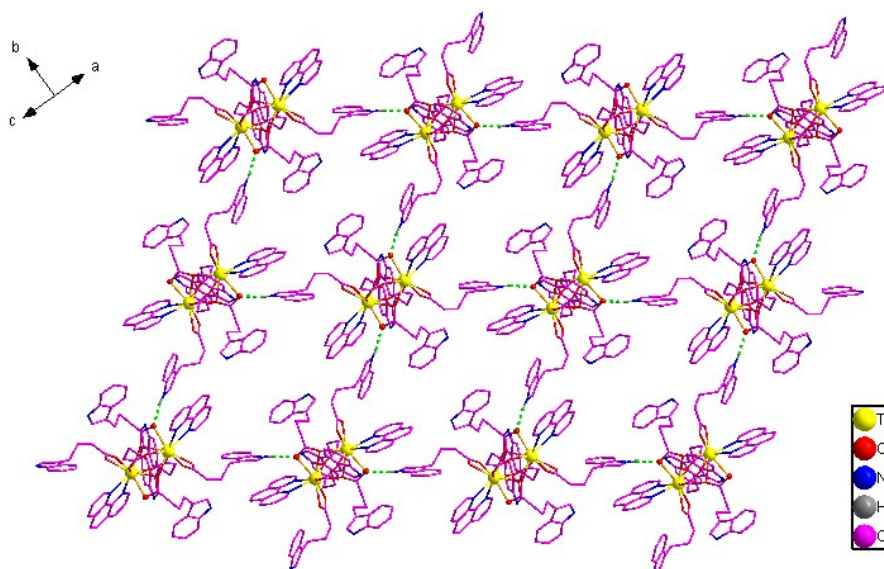


Fig S59 The 2D sheet structure connected by hydrogen bonds of complex **9**

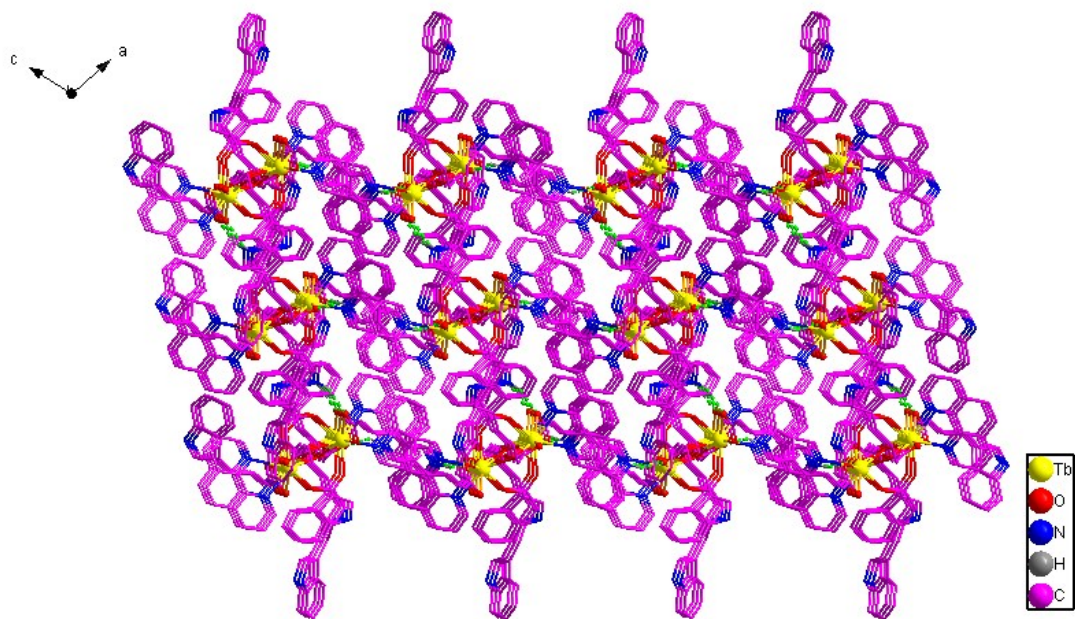


Fig S60 The 3D network structure connected by hydrogen bonds of complex 9

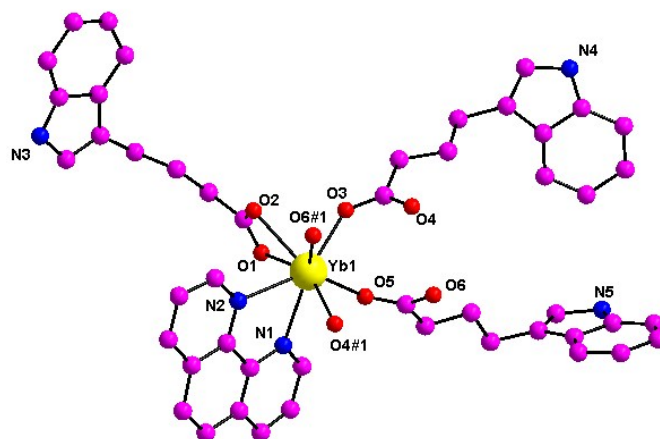


Fig S61 The unit structure of complex 10(symmetry codes: #1: 1-x, 1-y, -z)

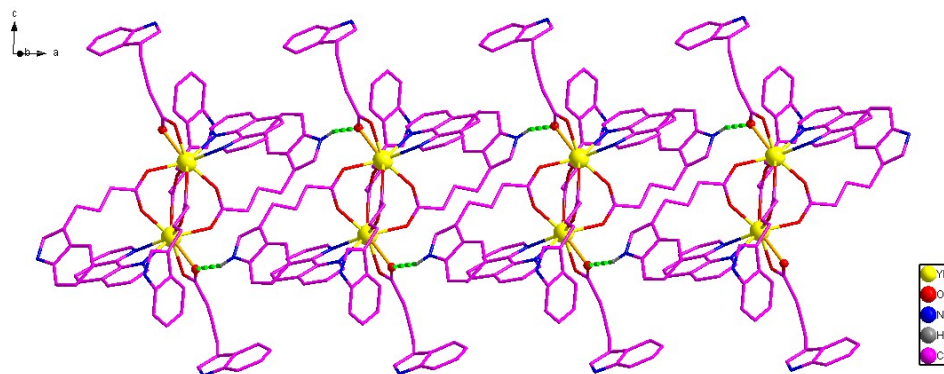


Fig S62 The 1D chain structure connected by hydrogen bonds of complex 10

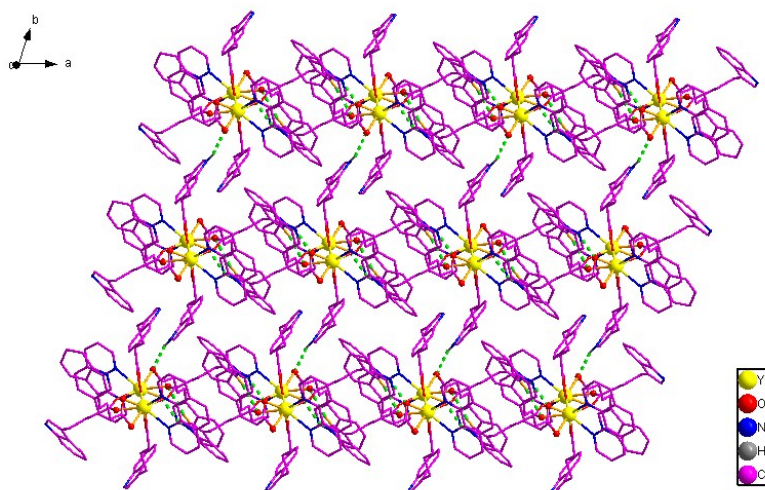


Fig S63 The 2D sheet structure connected by hydrogen bonds of complex **10**

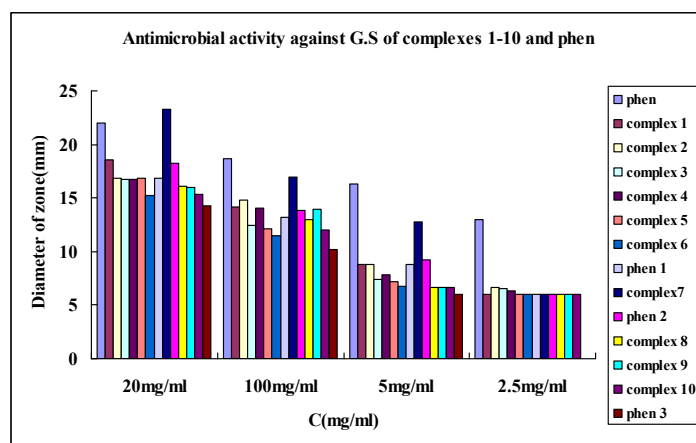


Fig S64 Antimicrobial activity against G. S of complexes 1-10 and phen (**phen 1**: 6.15 mg/ml, 3.08 mg/ml, 1.54 mg/ml, 0.77 mg/ml; **phen 2**: 7.34 mg/ml, 3.67 mg/ml, 1.84 mg/ml, 0.92 mg/ml; **phen 3**: 3.83 mg/ml, 1.92 mg/ml, 0.96 mg/ml, 0.48 mg/ml)

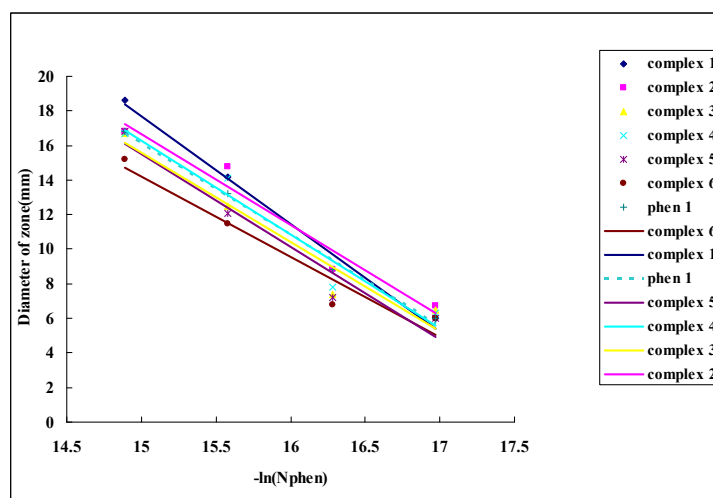


Fig S65 The associations of the diameters of the inhibition zones with relative amounts of phen against G. S

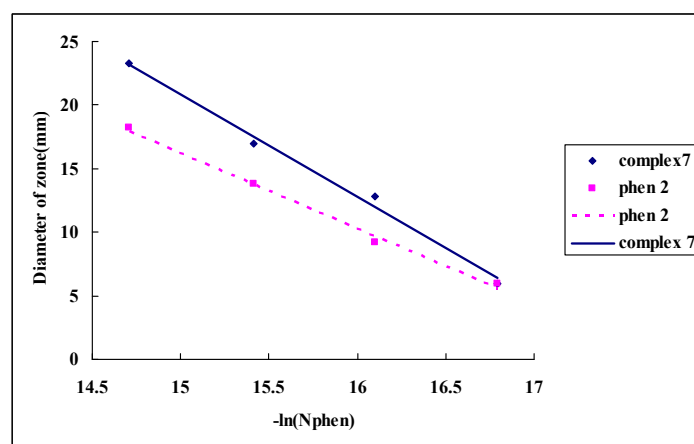


Fig S66 The associations of the diameters of the inhibition zones with relative amounts of phen against G. S

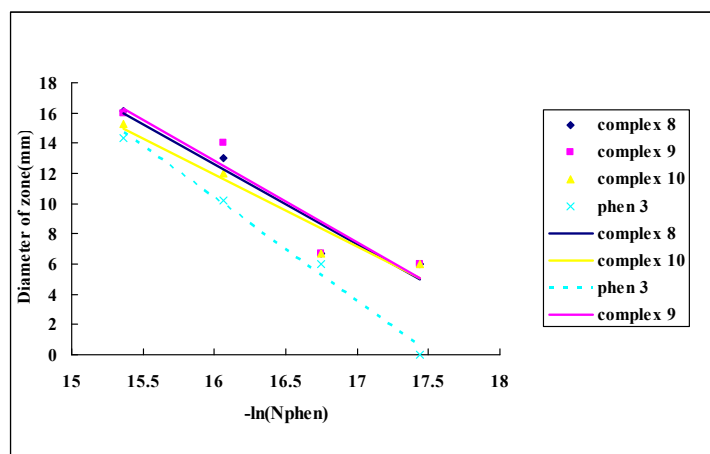


Fig S67 The associations of the diameters of the inhibition zones with relative amounts of phen against G. S

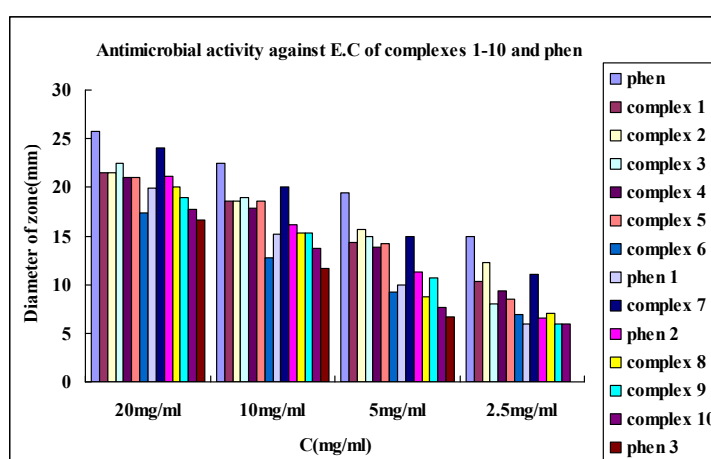


Fig S68 Antimicrobial activity against E. C of complexes 1-10 and phen (**phen 1**: 6.15 mg/ml, 3.08 mg/ml, 1.54 mg/ml, 0.77 mg/ml; **phen 2**: 7.34 mg/ml, 3.67 mg/ml, 1.84 mg/ml, 0.92 mg/ml; **phen 3**: 3.83 mg/ml, 1.92 mg/ml, 0.96 mg/ml, 0.48 mg/ml)



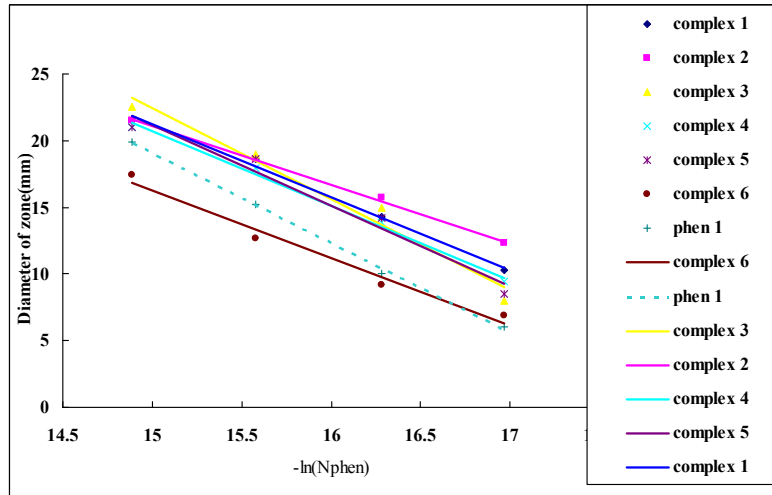


Fig S69 The associations of the diameters of the inhibition zones with relative amounts of phen against E. C

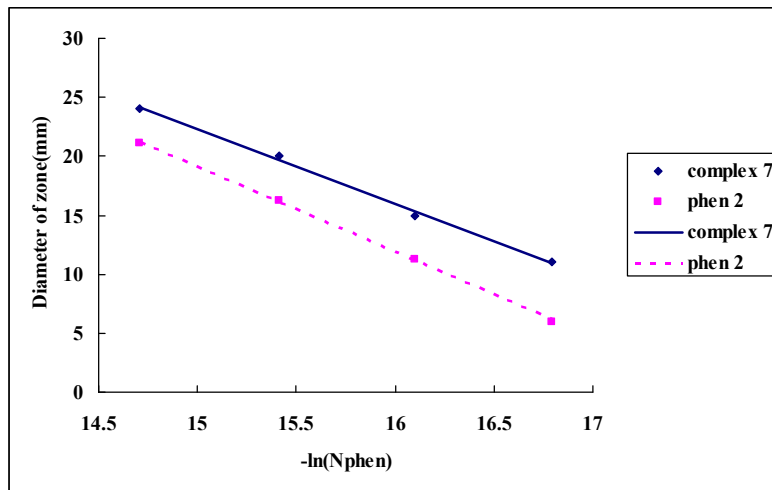


Fig S70 The associations of the diameters of the inhibition zones with relative amounts of phen against E. C

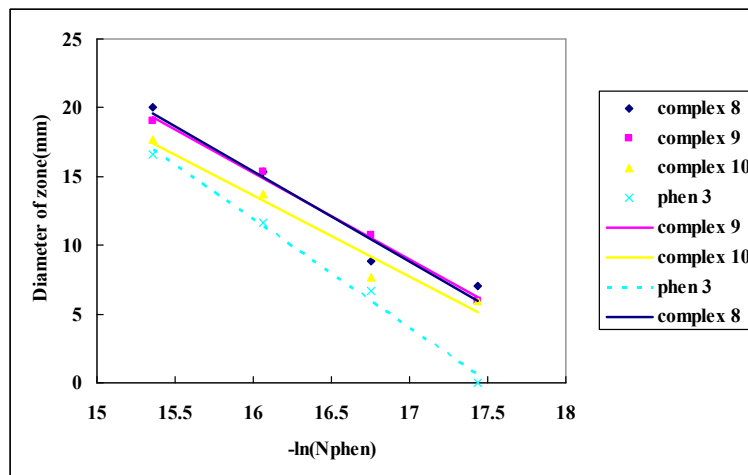


Fig S71 The associations of the diameters of the inhibition zones with relative amounts of phen against E. C

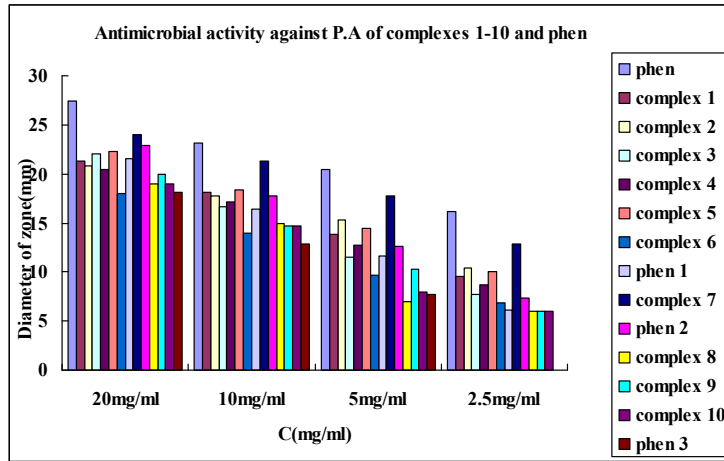


Fig S72 Antimicrobial activity against P.A. of complexes 1-10 and phen (**phen 1**: 6.15 mg/ml, 3.08 mg/ml, 1.54 mg/ml, 0.77 mg/ml; **phen 2**: 7.34 mg/ml, 3.67 mg/ml, 1.84 mg/ml, 0.92 mg/ml; **phen 3**: 3.83 mg/ml, 1.92 mg/ml, 0.96 mg/ml, 0.48 mg/ml)

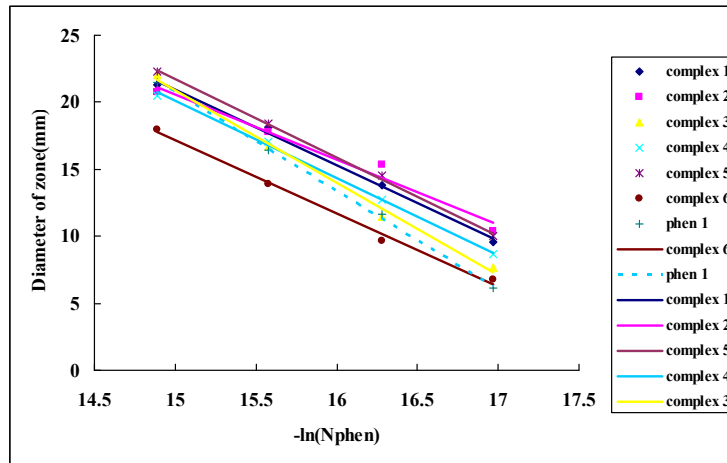


Fig S73 The associations of the diameters of the inhibition zones with relative amounts of phen against P. A

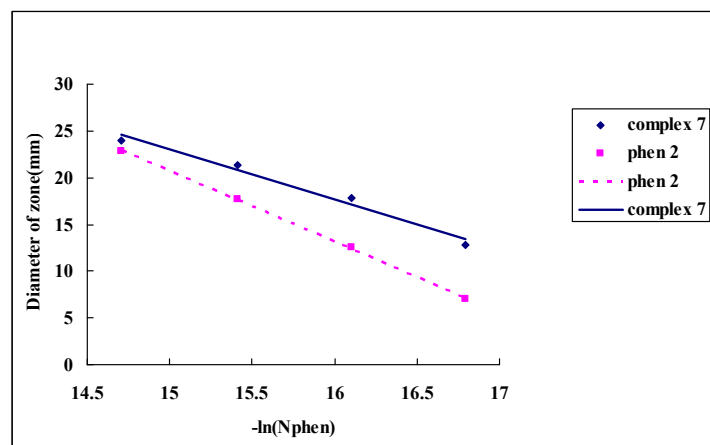


Fig S74 The associations of the diameters of the inhibition zones with relative amounts of phen against P. A

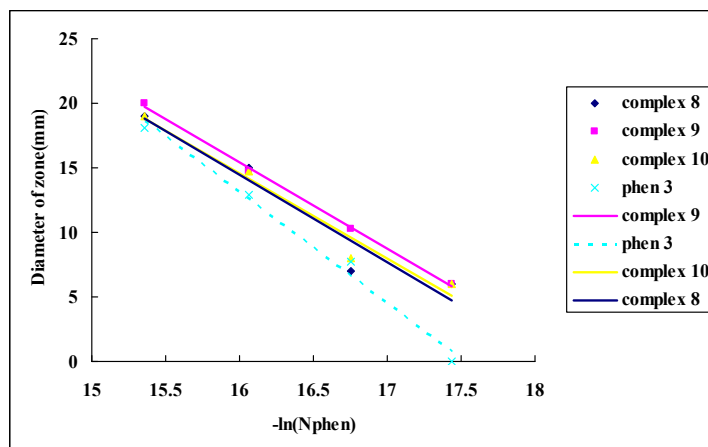


Fig S75 The associations of the diameters of the inhibition zones with relative amounts of phen against P. A

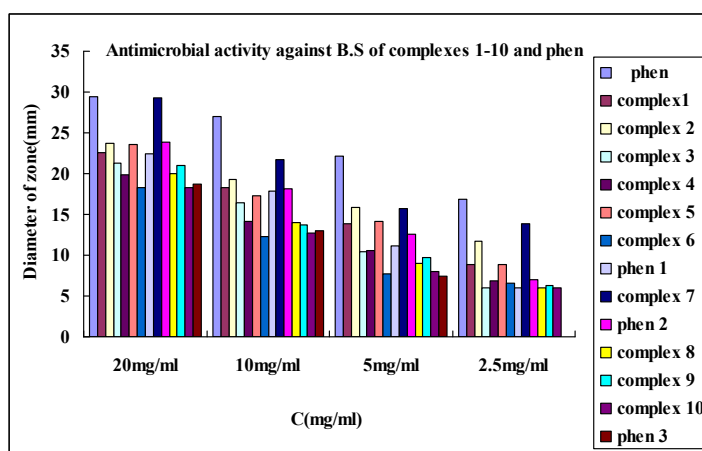


Fig S76 Antimicrobial activity against B.S of complexes 1-10 and phen (**phen 1**: 6.15 mg/ml, 3.08 mg/ml, 1.54 mg/ml, 0.77 mg/ml; **phen 2**: 7.34 mg/ml, 3.67 mg/ml, 1.84 mg/ml, 0.92 mg/ml; **phen 3**: 3.83 mg/ml, 1.92 mg/ml, 0.96 mg/ml, 0.48 mg/ml)

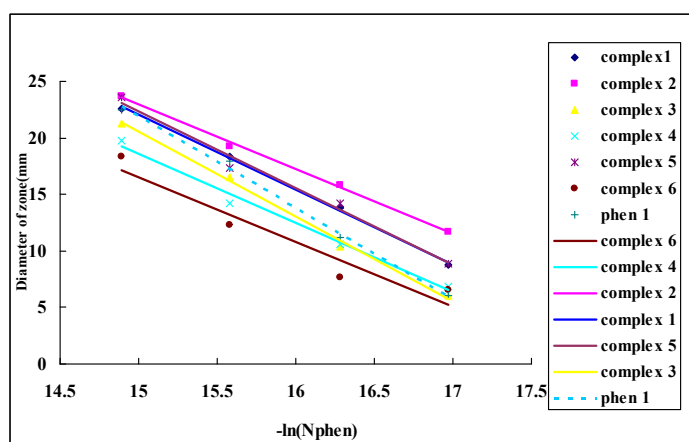


Fig S77 The associations of the diameters of the inhibition zones with relative amounts of phen against B. S

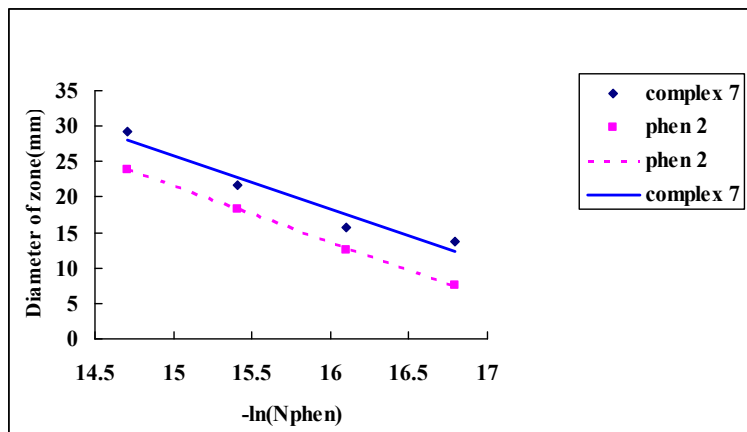


Fig S78 The associations of the diameters of the inhibition zones with relative amounts of phen against B. S

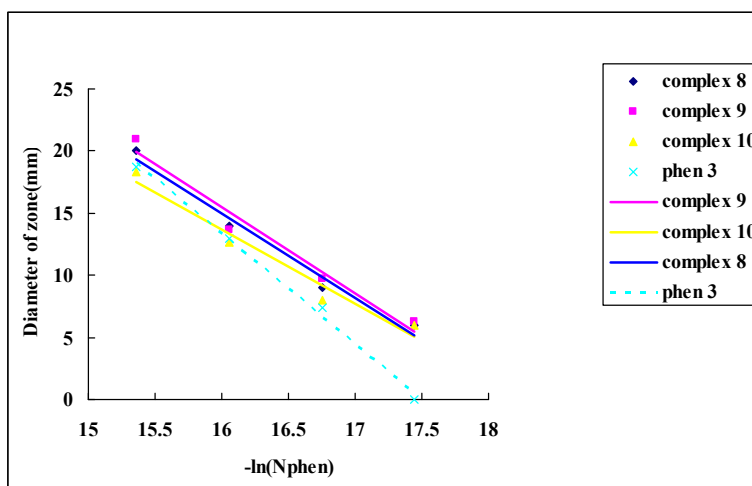


Fig S79 The associations of the diameters of the inhibition zones with relative amounts of phen against B. S