Supporting Information

Structural characterized homo-trinuclear Zn^{II} and hetero-pentanuclear $[Zn^{II}_4Ln^{III}]$ complexes constructed from a octadentate bis(Salamo)-based ligand: hirshfeld surfaces, fluorescent and catalytic properties

Xiao-Yan Li, Quan-Peng Kang, Chang Liu, Yang Zhang Wen-Kui Dong*

School of Chemical and Biological Engineering, Lanzhou Jiaotong University, Lanzhou, Gansu 730070, PR China

Corresponding authors.
*E-mail: dongwk@126.com. Fax: +86-931-4938703.

* *School of Chemical and Biological Engineering, Lanzhou Jiaotong University, Lanzhou 730070, P. R. China. E-mail:* dongwk@126.com*; Tel: +86 931 4938703*

† CCDC: numbers 1875819-1875824 for complexes **1**–**6**.

Table S1 Selected bond lengths (Å) and angles (°) for complexes **1-6**.

Complex **1**					
Bond	Lengths	Bond	Lengths	Bond	Lengths
N1-Zn6	2.129(4)	N2-Zn6	2.121(4)	N3-Zn4	2.116(4)
N4-Zn4	2.118(4)	N5-Zn1	2.116(4)	N6-Zn1	2.092(4)
N7-Zn2	2.114(4)	N8-Zn2	2.108(4)	O1-Zn6	2.046(3)
O1-Zn5	2.054(3)	O4-Zn6	1.969(3)	O5-Zn6	1.979(4)
O6-Zn5	1.988(4)	O7-Zn5	1.985(3)	O8-Zn4	1.971(4)
O9-Zn4	2.056(3)	O9-Zn5	2.071(3)	O10-Zn4	1.954(3)
O13-Zn5	2.033(3)	O14-Zn1	1.959(3)	O17-Zn1	2.036(3)
O17-Zn3	2.055(3)	O18-Zn3	2.068(3)	O20-Zn1	1.985(3)
O18-Zn2	2.046(3)	O19-Zn3	1.998(3)	O21-Zn3	2.021(3)
O22-Zn2	1.969(3)	O23-Zn3	2.048(3)	O24-Zn2	1.968(3)
Bond	Angles	Bond	Angles	Bond	Angles
N6-Zn1-N5	88.15(15)	N8-Zn2-N7	90.78(16)	O24-Zn2-O18	91.36(13)
O14-Zn1-N5	116.70(15)	O18-Zn2-N7	83.62(14)	O24-Zn2-O22	115.30(15)
O14-Zn1-N6	87.58(15)	O18-Zn2-N8	171.18(14)	O17-Zn3-O18	79.65(11)
O14-Zn1-O17	92.88(13)	O22-Zn2-N7	117.85(16)	O19-Zn3-O17	95.30(13)
O14-Zn1-O20	120.51(15)	O22-Zn2-N8	94.13(15)	O19-Zn3-O18	163.17(14)
O17-Zn1-N5	84.56(13)	O22-Zn2-O18	94.51(13)	O19-Zn3-O21	88.50(13)
O17-Zn1-N6	172.06(14)	O24-Zn2-N7	126.84(15)	O19-Zn3-O23	100.67(14)
O20-Zn1-N5	122.79(15)	O24-Zn2-N8	86.53(15)	O21-Zn3-O17	160.39(14)
O20-Zn1-N6	93.60(14)	O10-Zn4-N3	123.44(16)	O13-Zn5-O1	97.23(12)
O20-Zn1-O17	92.99(12)	O10-Zn4-N4	86.61(14)	O13-Zn5-O9	95.15(13)
O21-Zn3-O18	91.20(13)	O10-Zn4-O8	112.59(16)	N2-Zn6-N1	89.08(16)
O21-Zn3-O23	102.65(15)	O10-Zn4-O9	93.57(12)	O1-Zn6-N1	83.97(14)
O23-Zn3-O17	95.55(13)	O1-Zn5-O9	79.32(12)	O1-Zn6-N2	170.56(16)
O23-Zn3-O18	95.82(13)	O6-Zn5-O1	93.50(14)	O4-Zn6-N1	122.03(16)
N3-Zn4-N4	87.12(16)	O6-Zn5-O9	164.11(13)	O4-Zn6-N2	86.92(14)
O8-Zn4-N3	123.96(17)	O6-Zn5-O13	99.83(14)	O4-Zn6-O1	91.35(13)
O8-Zn4-N4	95.49(16)	O7-Zn5-O1	154.48(15)	O4-Zn6-O5	117.40(15)
O8-Zn4-O9	94.44(14)	O7-Zn5-O6	88.62(16)	O5-Zn6-N1	120.57(16)
O9-Zn4-N3	83.74(14)	O7-Zn5-O9	91.92(14)	O5-Zn6-N2	94.77(17)
O9-Zn4-N4	169.17(15)	O7-Zn5-O13	107.47(15)	O5-Zn6-O1	94.26(14)
Complex **2**					
Bond	Lengths	Bond	Lengths	Bond	Lengths
Sm1-O1	2.424(3)	Sm1-O8	2.464(3)	Sm1-O1$^{\#1}$	2.424(3)
Sm1-O4	2.429(3)	Sm1-O8$^{\#1}$	2.464(3)	Sm1-O4$^{\#1}$	2.429(3)
Sm1-O5	2.417(3)	Sm1-O5$^{\#1}$	2.417(3)		
Bond	Angles	Bond	Angles	Bond	Angles
O1-Sm1-O1$^{\#1}$	89.14(15)	O4$^{\#1}$-Sm1-O4	130.00(14)	O5$^{\#1}$-Sm1-O4	145.23(10)
O1-Sm1-O4$^{\#1}$	78.59(11)	O4$^{\#1}$-Sm1-O8$^{\#1}$	127.17(10)	O5-Sm1-O4	64.28(10)
O1$^{\#1}$-Sm1-O4$^{\#1}$	66.15(10)	O4-Sm1-O8	127.17(10)	O5-Sm1-O4$^{\#1}$	145.23(10)
O1$^{\#1}$-Sm1-O4	78.59(10)	O4$^{\#1}$-Sm1-O8	88.09(10)	O5$^{\#1}$-Sm1-O4$^{\#1}$	64.28(10)

O1-Sm1-O4	66.15(10)	O4-Sm1-O8$^{\#1}$	88.09(10)	O5-Sm1-O5$^{\#1}$	125.42(14)
O1-Sm1-O8$^{\#1}$	89.54(11)	O5-Sm1-O1$^{\#1}$	91.14(10)	O5$^{\#1}$-Sm1-O8	78.92(10)
O1-Sm1-O8	165.94(10)	O5-Sm1-O1	129.30(10)	O5$^{\#1}$-Sm1-O8$^{\#1}$	64.72(10)
O1$^{\#1}$-Sm1-O8	89.54(11)	O5$^{\#1}$-Sm1-O1	91.14(10)	O5-Sm1-O8	64.72(10)
O1$^{\#1}$-Sm1-O8$^{\#1}$	165.94(10)	O5$^{\#1}$-Sm1-O1$^{\#1}$	129.30(10)	O5-Sm1-O8$^{\#1}$	78.92(10)
O8$^{\#1}$-Sm1-O8	95.06(15)				
Complex **3**					
Bond	Lengths	Bond	Lengths	Bond	Lengths
Eu1-O8	2.409(3)	Eu1-O4$^{\#2}$	2.408(3)	Eu1-O1$^{\#2}$	2.450(3)
Eu1-O8$^{\#2}$	2.409(3)	Eu1-O5	2.417(3)	Eu1-O1	2.450(3)
Eu1-O4	2.408(3)	Eu1-O5$^{\#2}$	2.417(3)		
Bond	Angles	Bond	Angles	Bond	Angles
O8-Eu1-O8$^{\#2}$	89.76(16)	O8-Eu1-O5$^{\#2}$	78.67(11)	O5-Eu1-O1$^{\#2}$	87.74(11)
O8-Eu1-O4	129.62(11)	O8$^{\#2}$-Eu1-O5$^{\#2}$	66.13(10)	O5$^{\#2}$-Eu1-O1$^{\#2}$	127.84(10)
O8$^{\#2}$-Eu1-O4	90.70(11)	O4-Eu1-O5$^{\#2}$	144.82(11)	O8-Eu1-O1	165.44(10)
O8-Eu1-O4$^{\#2}$	90.70(11)	O4$^{\#2}$-Eu1-O5$^{\#2}$	64.64(11)	O8$^{\#2}$-Eu1-O1	89.49(11)
O8$^{\#2}$-Eu1-O4$^{\#2}$	129.62(11)	O5-Eu1-O5$^{\#2}$	129.80(15)	O4-Eu1-O1	64.93(11)
O4-Eu1-O4$^{\#2}$	125.40(15)	O8-Eu1-O1$^{\#2}$	89.49(11)	O4$^{\#2}$-Eu1-O1	78.64(11)
O8-Eu1-O5	66.13(10)	O8$^{\#2}$-Eu1-O1$^{\#2}$	165.44(10)	O5-Eu1-O1	127.84(10)
O8$^{\#2}$-Eu1-O5	78.67(11)	O4-Eu1-O1$^{\#2}$	78.64(11)	O5$^{\#2}$-Eu1-O1	87.74(11)
O4-Eu1-O5	64.64(11)	O4$^{\#2}$-Eu1-O1$^{\#2}$	64.93(11)	O1$^{\#2}$-Eu1-O1	94.84(16)
O4$^{\#2}$-Eu1-O5	144.82(11)				
Complex **4**					
Bond	Lengths	Bond	Lengths	Bond	Lengths
Gd1-O4	2.412(5)	Gd1-O5$^{\#3}$	2.408(5)	Gd1-O1$^{\#3}$	2.406(5)
Gd1-O4$^{\#3}$	2.412(5)	Gd1-O8	2.442(5)	Gd1-O1	2.406(5)
Gd1-O5	2.408(5)	Gd1-O8$^{\#3}$	2.442(5)		
Bond	Angles	Bond	Angles	Bond	Angles
O1$^{\#3}$-Gd1-O1	89.9(3)	O1-Gd1-O8$^{\#3}$	89.49(19)	O5-Gd1-O4$^{\#3}$	144.43(19)
O1$^{\#3}$-Gd1-O4$^{\#3}$	65.97(18)	O1$^{\#3}$-Gd1-O8	89.49(19)	O5$^{\#3}$-Gd1-O4$^{\#3}$	64.98(18)
O1$^{\#3}$-Gd1-O4	78.65(19)	O1-Gd1-O8	165.33(18)	O5$^{\#3}$-Gd1-O4	144.43(19)
O1-Gd1-O4	65.96(18)	O4-Gd1-O4$^{\#3}$	129.5(2)	O5-Gd1-O5$^{\#3}$	125.5(3)
O1-Gd1-O4$^{\#3}$	78.66(19)	O4-Gd1-O8$^{\#3}$	87.72(19)	O5$^{\#3}$-Gd1-O8$^{\#3}$	64.83(19)
O1-Gd1-O5	129.83(19)	O4$^{\#3}$-Gd1-O8	87.72(19)	O5$^{\#3}$-Gd1-O8	78.79(19)
O1$^{\#3}$-Gd1-O5	90.41(19)	O4$^{\#3}$-Gd1-O8$^{\#3}$	128.14(18)	O5-Gd1-O8$^{\#3}$	78.79(19)
O1$^{\#3}$-Gd1-O5$^{\#3}$	129.83(19)	O4-Gd1-O8	128.14(18)	O5-Gd1-O8	64.83(19)
O1-Gd1-O5$^{\#3}$	90.41(18)	O5-Gd1-O4	64.98(18)	O8-Gd1-O8$^{\#3}$	94.8(3)
O1$^{\#3}$-Gd1-O8$^{\#3}$	165.33(18)				
Complex **5**					
Bond	Lengths	Bond	Lengths	Bond	Lengths
O14-Tb1	2.378(7)	O13-Tb1	2.350(7)	O1-Tb1	2.446(9)
O4-Tb1	2.384(7)	O5-Tb1	2.386(8)	O8-Tb1	2.470(9)
O9-Tb1	2.420(8)	O12-Tb1	2.360(8)		
Bond	Angles	Bond	Angles	Bond	Angles

O1-Tb1-O8	164.6(3)	O12-Tb1-O1	89.9(3)	O13-Tb1-O1	76.6(3)
O4-Tb1-O1	65.3(2)	O12-Tb1-O4	143.2(3)	O13-Tb1-O4	127.3(3)
O4-Tb1-O5	65.9(3)	O12-Tb1-O5	127.1(3)	O13-Tb1-O5	143.3(3)
O4-Tb1-O8	129.9(3)	O12-Tb1-O8	77.5(3)	O13-Tb1-O8	90.1(3)
O4-Tb1-O9	87.3(3)	O12-Tb1-O9	65.5(3)	O13-Tb1-O9	130.0(3)
O5-Tb1-O1	130.6(3)	O12-Tb1-O14	130.4(3)	O13-Tb1-O12	66.2(3)
O5-Tb1-O8	64.8(3)	O14-Tb1-O5	86.4(3)	O13-Tb1-O14	66.2(3)
O5-Tb1-O9	79.5(3)	O14-Tb1-O8	89.5(3)	O14-Tb1-O1	92.0(3)
O9-Tb1-O1	91.2(3)	O14-Tb1-O9	163.8(3)	O14-Tb1-O4	79.7(3)
O9-Tb1-O8	91.6(3)				

Complex **6**

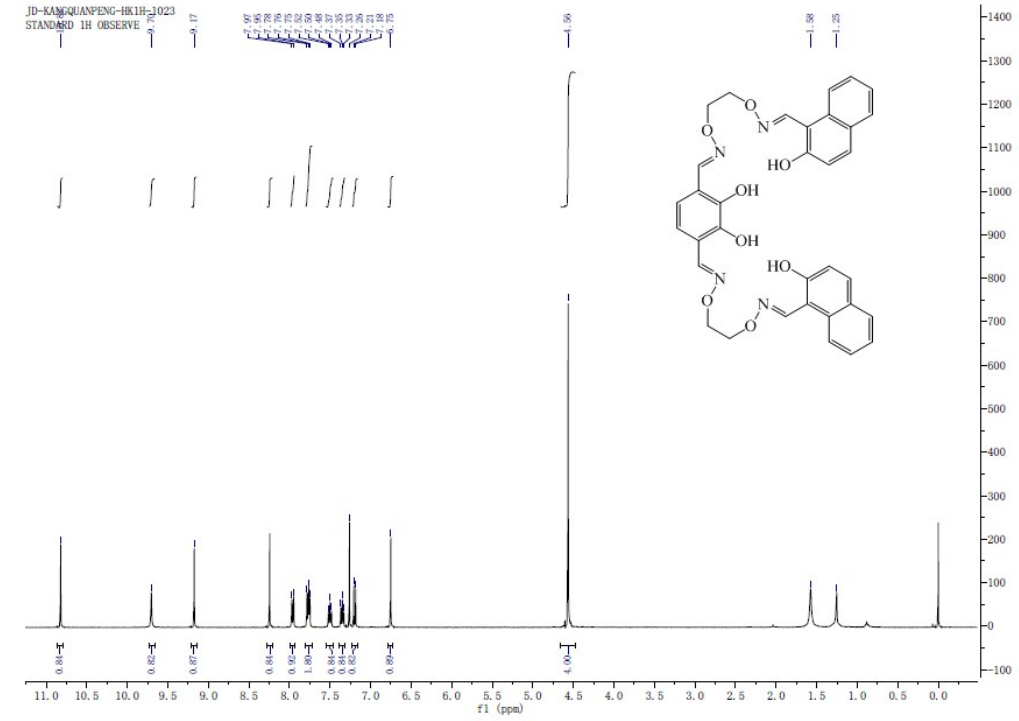
Bond	Lengths	Bond	Lengths	Bond	Lengths
Dy1-O1	2.382(3)	Dy1-O4	2.382(3)	Dy1-O8	2.426(3)
Dy1-O1$^{\#4}$	2.382(3)	Dy1-O5$^{\#4}$	2.374(3)	Dy1-O8$^{\#4}$	2.426(3)
Dy1-O4$^{\#4}$	2.382(3)	Dy1-O5	2.374(3)		
Bond	Angles	Bond	Angles	Bond	Angles
O1-Dy1-O1$^{\#4}$	90.65(15)	O4-Dy1-O1	66.47(11)	O4$^{\#4}$-Dy1-O1	78.43(11)
O1$^{\#4}$-Dy1-O8$^{\#4}$	163.93(11)	O4$^{\#4}$-Dy1-O1$^{\#4}$	66.47(11)	O4-Dy1-O1$^{\#4}$	78.44(11)
O1$^{\#4}$-Dy1-O8	89.32(11)	O5$^{\#4}$-Dy1-O1$^{\#4}$	130.55(11)	O5-Dy1-O4$^{\#4}$	144.27(11)
O1-Dy1-O8$^{\#4}$	89.32(11)	O5-Dy1-O1	130.55(11)	O5-Dy1-O4	65.28(11)
O1-Dy1-O8	163.93(11)	O5-Dy1-O1$^{\#4}$	89.93(11)	O5$^{\#4}$-Dy1-O4	144.27(11)
O4-Dy1-O4$^{\#4}$	129.51(15)	O5$^{\#4}$-Dy1-O1	89.93(11)	O5$^{\#4}$-Dy1-O5	125.04(15)
O4-Dy1-O8	129.12(11)	O5$^{\#4}$-Dy1-O4$^{\#4}$	65.28(11)	O5-Dy1-O8	65.53(11)
O4$^{\#4}$-Dy1-O8$^{\#4}$	129.11(11)	O5$^{\#4}$-Dy1-O8$^{\#4}$	65.53(11)	O5-Dy1-O8$^{\#4}$	77.96(10)
O4$^{\#4}$-Dy1-O8	86.84(11)	O5$^{\#4}$-Dy1-O8	77.96(10)	O8$^{\#4}$-Dy1-O8	95.10(15)
O4-Dy1-O8$^{\#4}$	86.84(11)				

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1, y, -z+1/2; $^{\#2}$ -x+1, y, -z+1/2; $^{\#3}$ -x+1, y, -z+1/2; $^{\#4}$ -x+1, y, -z+3/2.

Table S2 Hydrogen bonding interactions [Å °] for complexes **1-6**.

D–H···A	d(D–H)	d(H–A)	d(D–A)	∠D–X–A	Sum
Complex **1**					
O13–H13D···O4	0.84	1.94	2.738(5)	157	
O13–H13C···O10	1.03	1.69	2.662(5)	155	
O23–H23B···O24	0.84	1.88	2.676(5)	158	
O23–H23A···O14	0.94	1.86	2.748(5)	157	
C12–H12B···O5	0.99	2.29	3.228(7)	157	
C23–H23C···O8	0.99	2.42	3.301(9)	147	
C50–H50B···O20	0.99	2.38	3.233(6)	144	
C16–H16···O16	0.95	2.49	3.413(6)	164	1-x,1-y,1-z
C51–H51A···O10	0.99	2.56	3.505(6)	160	
C54–H54···O12	0.95	2.58	3.439(6)	150	
C78–H78A···O25	0.99	2.51	3.418(14)	152	1+x,y,z
Complex **2**					
C13–H13A···O11	0.99	2.52	3.503(8)	173	
O13–H13D···O21	0.87	2.11	2.42(3)	101	
C24–H24···O7	0.95	2.42	2.877(6)	109	1-x,y,1/2-z
C33–H33···O10	0.95	2.51	3.454(6)	173	1-x,y,1/2-z
C36–H36C···O9	0.98	2.32	3.260(2)	160	1-x,y,1/2-z
C23–H23A···O11	0.99	2.49	3.088(7)	118	-1/2+x,-1/2+y,z
Complex **3**					
C2–H2···O11	0.95	2.50	3.440(6)	172	1-x,y,1/2-z
C5–H5···O2	0.95	2.43	2.877(9)	108	1-x,y,1/2-z
C6–H6B···O9	0.99	2.47	3.066(8)	119	-1/2+x,1/2+y,z
C16–H16B···O9	0.99	2.53	3.509(9)	172	
C16–H16B···N4	0.99	2.51	3.509(9)	100	
C21–H21···O18	0.95	2.54	3.46(2)	165	1/2+x,-1/2+y,z
C30A–H30F···O10	0.98	2.25	3.19(2)	161	1-x,y,1/2-z
Complex **4**					
C8–H8···O19	0.95	2.48	3.400(3)	165	-1/2+x,1/2+y,z
C11–H11···O2	0.95	2.59	2.977(12)	105	1-x,y,3/2-z
C13–H13B···O12	0.99	2.53	3.515(14)	171	1-x,y,1/2-z
C23–H23B···O12	0.99	2.45	3.062(13)	119	-1/2+x,-1/2+y,z
C24–H24···O7	0.95	2.40	2.885(13)	111	1-x,y,3/2-z
C29–H29···O10	0.95	2.48	3.12(2)	124	1-x,y,3/2-z
Complex **5**					
C2–H2···O13	0.95	2.55	3.220(14)	128	
C2–H2···O20	0.95	2.42	3.244(17)	144	
C22–H22A···O26	0.99	2.53	3.432(16)	151	
C33–H33···O12	0.95	2.50	3.244(14)	136	
C33–H33···O17	0.95	2.56	3.317(16)	137	
C45–H45···O2	0.95	2.47	3.092(16)	123	

C47–H47A···O22	0.99	2.36	3.281(15)	155	
C56–H56A···O18	0.99	2.50	3.273(18)	134	
C56–H56A···N3	0.99	2.62	2.955(17)	100	
C57–H57A···N4	0.99	2.32	2.759(17)	106	
C58–H58···O7	0.95	2.56	3.022(14)	110	
C69–H69A···O8	0.99	2.47	3.13(2)	124	
O27–H27A···O23	0.90	2.30	3.097(18)	148	
O26–H26B···O19	0.88	2.04	2.732(14)	135	-x,1-y,1-z
C39–H39···O17	0.95	2.42	3.331(18)	162	1+x,y,z
C46–H46B···O22	0.99	2.54	3.466(16)	156	1-x,1-y,2-z
C55–H55···O25	0.95	2.52	3.418(18)	158	-1+x,y,z
Complex **6**					
C8–H8···O19	0.93	2.47	3.392(2)	169	-1/2+x,1/2+y,z
C11–H11···O2	0.93	2.54	2.946(6)	107	1-x,y,3/2-z
C13–H13B···O12	0.97	2.56	3.523(9)	172	
C24–H24···O7	0.93	2.42	2.874(7)	110	1-x,y,3/2-z
C29–H29···O10	0.93	2.52	3.443(6)	171	1-x,y,3/2-z
C23–H23B···O12	0.97	2.47	3.061(8)	119	-1/2+x,-1/2+y,z



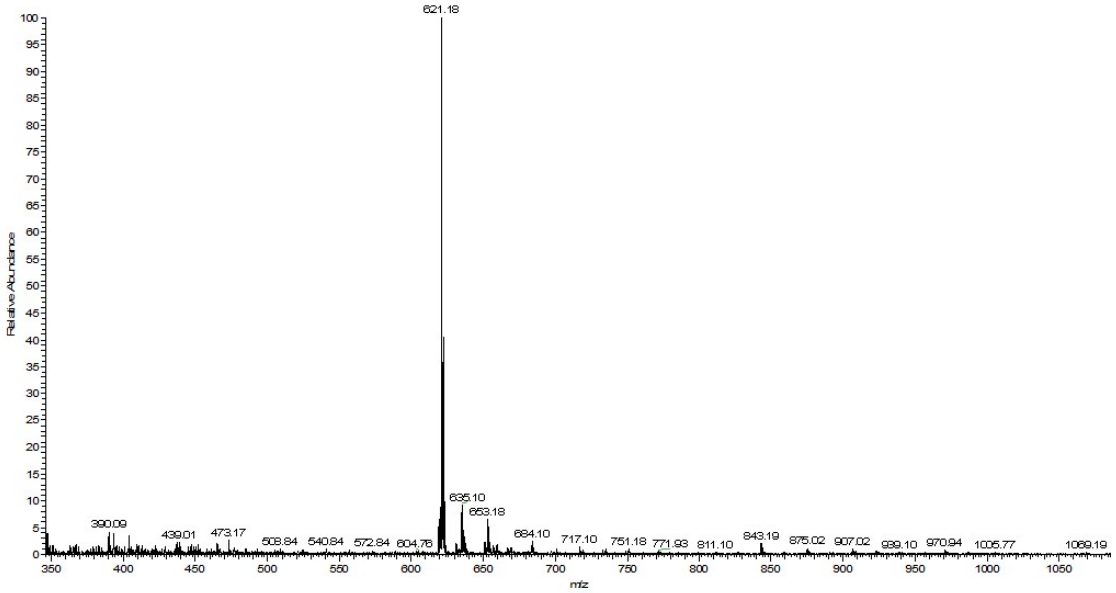


Fig. S1 ^{1}H NMR and MS of H_4L.

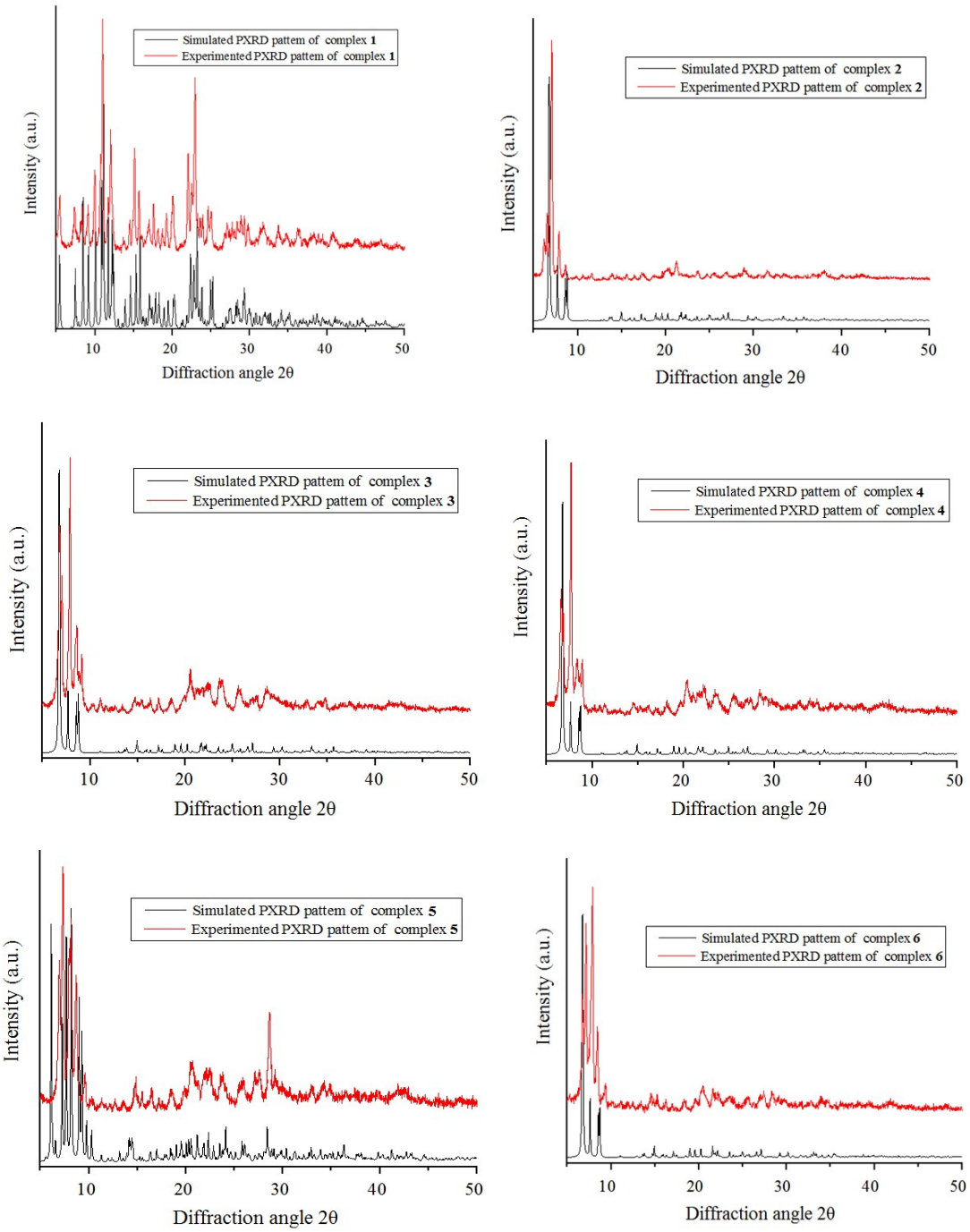


Fig. S2 PXRD patterns for the complexes **1–6**.