

Supporting Information

Synthesis, crystal structures and luminescent properties of Cd^{II} and Zn^{II} complexes assembled by 4-aminophenyl-hydroxamic acid

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Table S1 Bond lengths [\AA] and angles [$^\circ$] for complex **1**

Cd(1)-O(1)A	2.221(2)	Cd(1)-O(2)	2.318(3)
Cd(1)-O(1)B	2.221(2)	Cd(1)-O(2)B	2.341(3)
Cd(1)-O(2)C	2.318(3)	Cd(1)-O(2)A	2.341(3)
O(1)A-Cd(1)-O(1)B	177.4(4)	O(2)C-Cd(1)-O(2)B	155.22(9)
O(1)A-Cd(1)-O(2)C	98.48(18)	O(2)-Cd(1)-O(2)B	102.34(8)
O(1)B-Cd(1)-O(2)C	83.47(13)	O(1)A-Cd(1)-O(2)A	71.88(13)
O(1)A-Cd(1)-O(2)	83.47(13)	O(1)B-Cd(1)-O(2)A	106.07(18)
O(1)B-Cd(1)-O(2)	98.48(18)	O(2)C-Cd(1)-O(2)A	102.34(8)
O(2)C-Cd(1)-O(2)	83.50(14)	O(2)-Cd(1)-O(2)A	155.22(9)
O(1)A-Cd(1)-O(2)B	106.07(18)	O(2)B-Cd(1)-O(2)A	82.52(14)
O(1)B-Cd(1)-O(2)B	71.88(13)		
Symmetry transformations used to generate equivalent atoms:			
A -x+1,y,z+1/2 B x,-y+1,z+1/2 C -x+1,-y+1,z			

Table S2 Hydrogen bonds for **1** [\AA and $^\circ$]

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
N(2)-H(2B)...O(2)E	0.87	2.05	2.907(4)	167.4
N(2)-H(2B)...N(1)E	0.87	2.58	3.353(4)	149.1
Symmetry transformations used to generate equivalent atoms: E -x+3/2,y+1/2,z+0				

Table S3 Bond lengths [\AA] and angles [$^\circ$] for complex **2**

Zn(1)-O(3)	2.0545(14)	Zn(1)-O(2)	2.1264(13)
Zn(1)-O(1)	2.0838(13)	Zn(1)-O(2)A	2.1337(13)
Zn(1)-O(4)	2.1180(14)	Zn(1)-O(5)	2.1623(13)
O(3)-Zn(1)-O(1)	170.26(6)	O(4)-Zn(1)-O(2)A	172.03(5)
O(3)-Zn(1)-O(4)	78.31(5)	O(2)-Zn(1)-O(2)A	83.06(5)
O(1)-Zn(1)-O(4)	92.12(5)	O(3)-Zn(1)-O(5)	88.88(6)
O(3)-Zn(1)-O(2)	104.53(5)	O(1)-Zn(1)-O(5)	89.76(5)
O(1)-Zn(1)-O(2)	78.11(5)	O(4)-Zn(1)-O(5)	92.31(6)
O(4)-Zn(1)-O(2)	96.66(5)	O(2)-Zn(1)-O(5)	165.12(5)
O(3)-Zn(1)-O(2)A	94.03(5)	O(2)A-Zn(1)-O(5)	89.68(5)
O(1)-Zn(1)-O(2)A	95.60(5)	Zn(1)-O(2)-Zn(1)A	96.94(5)
Symmetry transformations used to generate equivalent atoms: A -x,-y+2,-z			

Table S4 Hydrogen bonds for **2** [\AA and $^\circ$]

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
N(1)-H(1)...N(2)B	0.86	2.27	3.058(2)	152.2
N(2)-H(2A)...O(5)C	0.86	2.27	3.128(2)	174.8
N(2)-H(2B)...O(6)D	0.86	2.24	3.018(3)	149.9
N(4)-H(4A)...O(2)E	0.86	2.20	3.063(3)	175.3
N(4)-H(4B)...O(6)F	0.86	2.35	3.097(3)	145.2
O(5)-H(5A)...O(4)G	0.85	1.85	2.665(2)	160.6
O(5)-H(5B)...O(1)G	0.85	2.00	2.821(2)	161.6
O(6)-H(6A)...O(4)	0.85	1.94	2.782(3)	171.2
C(12)-H(12)...O(3)E	0.93	2.55	3.392(3)	151.0
Symmetry transformations used to generate equivalent atoms:				
A -x,-y+2,-z B -x+1/2,y+1/2,-z-1/2 C x+1/2,-y+3/2,z-1/2				
D x-1/2,-y+3/2,z-1/2 E -x+1/2,y-1/2,-z+1/2				
F x-1/2,-y+3/2,z+1/2 G -x,-y+1,-z				

Table S5 Bond lengths [Å] and angles [°] for complex 3

Zn(1)-O(3)	2.016(2)	Zn(1)-O(5)	2.092(2)
Zn(1)-O(5)A	2.049(2)	Zn(1)-O(1)	2.110(2)
Zn(1)-O(4)B	2.061(2)	Zn(1)-N(2)	2.391(4)
O(3)-Zn(1)-O(5)A	96.59(10)	O(4)B-Zn(1)-O(1)	166.53(10)
O(3)-Zn(1)-O(4)B	92.81(11)	O(5)-Zn(1)-O(1)	76.70(8)
O(5)A-Zn(1)-O(4)B	91.40(11)	O(3)-Zn(1)-N(2)	80.83(13)
O(3)-Zn(1)-O(5)	169.33(10)	O(5)A-Zn(1)-N(2)	172.66(10)
O(5)A-Zn(1)-O(5)	89.59(8)	O(4)B-Zn(1)-N(2)	81.90(12)
O(4)B-Zn(1)-O(5)	95.74(9)	O(5)-Zn(1)-N(2)	94.05(12)
O(3)-Zn(1)-O(1)	93.65(10)	O(1)-Zn(1)-N(2)	87.48(10)
O(5)A-Zn(1)-O(1)	99.58(9)	Zn(1)B-O(5)-Zn(1)	124.23(11)
Symmetry transformations used to generate equivalent atoms:			
A -y+3/4,x+1/4,z+1/4 B y-1/4,-x+3/4,z-1/4 C -x+1/2,-y+1/2,-z-1/2			

Table S6 Hydrogen bonds for 3 [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	∠(DHA)
N(1)-H(1)...O(5)B	0.86	2.20	2.786(3)	124.8
Symmetry transformations used to generate equivalent atoms: B y-1/4,-x+3/4,z-1/4				

Table S7 Bond lengths [Å] and angles [°] for complex 4

Zn(1)-O(14)A	2.045(4)	Zn(3)-O(10)	2.080(3)
Zn(1)-O(2)	2.076(3)	Zn(3)-O(6)	2.081(3)
Zn(1)-O(3)	2.090(4)	Zn(3)-O(8)	2.107(3)
Zn(1)-O(17)	2.093(5)	Zn(3)-O(11)	2.124(3)
Zn(1)-O(16)A	2.151(4)	Zn(3)-N(4)D	2.186(5)
Zn(1)-N(2)B	2.228(5)	Zn(3)-N(6)	2.197(4)
O(1)-Zn(2)	2.204(4)	Zn(4)-O(15)	2.054(4)
Zn(2)-O(2)	2.020(3)	Zn(4)-O(10)	2.070(3)
Zn(2)-O(6)	2.039(3)	Zn(4)-O(14)	2.088(3)
Zn(2)-O(4)	2.078(4)	Zn(4)-O(12)	2.117(4)
Zn(2)-O(7)	2.102(4)	Zn(4)-O(13)	2.149(4)
Zn(2)-O(5)	2.145(4)	Zn(4)-O(9)	2.177(4)
O(14)A-Zn(1)-O(2)	177.07(16)	O(6)-Zn(3)-O(8)	91.75(13)
O(14)A-Zn(1)-O(3)	88.18(15)	O(10)-Zn(3)-O(11)	91.20(13)
O(2)-Zn(1)-O(3)	94.26(14)	O(6)-Zn(3)-O(11)	87.35(13)
O(14)A-Zn(1)-O(17)	92.77(18)	O(8)-Zn(3)-O(11)	178.85(18)
O(2)-Zn(1)-O(17)	85.60(17)	O(10)-Zn(3)-N(4)D	92.49(15)
O(3)-Zn(1)-O(17)	90.34(19)	O(6)-Zn(3)-N(4)D	87.36(15)
O(14)A-Zn(1)-O(16)A	90.93(14)	O(8)-Zn(3)-N(4)D	93.92(14)
O(2)-Zn(1)-O(16)A	86.69(13)	O(11)-Zn(3)-N(4)D	85.31(15)
O(3)-Zn(1)-O(16)A	177.8(2)	O(10)-Zn(3)-N(6)	87.89(16)
O(17)-Zn(1)-O(16)A	91.71(19)	O(6)-Zn(3)-N(6)	92.24(16)
O(14)A-Zn(1)-N(2)B	94.85(17)	O(8)-Zn(3)-N(6)	87.02(16)
O(2)-Zn(1)-N(2)B	86.65(17)	O(11)-Zn(3)-N(6)	93.75(16)
O(3)-Zn(1)-N(2)B	93.13(16)	N(4)D-Zn(3)-N(6)	179.0(2)
O(17)-Zn(1)-N(2)B	171.7(2)	O(15)-Zn(4)-O(10)	92.31(14)
O(16)A-Zn(1)-N(2)B	84.93(17)	O(15)-Zn(4)-O(14)	97.23(14)
O(2)-Zn(2)-O(6)	166.92(14)	O(10)-Zn(4)-O(14)	165.37(15)
O(2)-Zn(2)-O(4)	93.92(13)	O(15)-Zn(4)-O(12)	90.59(17)
O(6)-Zn(2)-O(4)	94.95(14)	O(10)-Zn(4)-O(12)	95.04(13)
O(2)-Zn(2)-O(7)	94.93(15)	O(14)-Zn(4)-O(12)	95.92(15)
O(6)-Zn(2)-O(7)	94.59(13)	O(15)-Zn(4)-O(13)	173.97(15)
O(4)-Zn(2)-O(7)	90.49(17)	O(10)-Zn(4)-O(13)	93.68(14)
O(2)-Zn(2)-O(5)	90.85(14)	O(14)-Zn(4)-O(13)	76.76(13)
O(6)-Zn(2)-O(5)	79.19(13)	O(12)-Zn(4)-O(13)	89.63(16)

O(4)-Zn(2)-O(5)	92.47(17)	O(15)-Zn(4)-O(9)	92.40(18)
O(7)-Zn(2)-O(5)	173.31(13)	O(10)-Zn(4)-O(9)	75.78(15)
O(2)-Zn(2)-O(1)	77.70(12)	O(14)-Zn(4)-O(9)	92.70(16)
O(6)-Zn(2)-O(1)	93.93(13)	O(12)-Zn(4)-O(9)	170.44(14)
O(4)-Zn(2)-O(1)	170.88(14)	O(13)-Zn(4)-O(9)	88.34(17)
O(7)-Zn(2)-O(1)	86.72(15)	Zn(2)-O(2)-Zn(1)	124.14(17)
O(5)-Zn(2)-O(1)	91.24(15)	Zn(4)-O(10)-Zn(3)	125.20(16)
O(10)-Zn(3)-O(6)	178.55(16)	Zn(2)-O(6)-Zn(3)	125.22(16)
O(10)-Zn(3)-O(8)	89.70(13)	Zn(1)F-O(14)-Zn(4)	124.79(18)
Symmetry transformations used to generate equivalent atoms:			
A x-1/2,y+1/2,z	B x,y+1,z	C x,y-1,z	D x,-y+2,z-1/2
F x+1/2,y-1/2,z	G x,-y+1,z+1/2	H x,-y+1,z-1/2	E x,-y+2,z+1/2

Table S8 Hydrogen bonds for **4** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	∠(DHA)
N(1)-H(1)...O(16)A	0.86	2.07	2.683(5)	127.6
N(2)-H(2A)...O(2)C	0.86	2.28	2.955(5)	135.7
N(2)-H(2A)...O(18)C	0.86	2.56	3.235(8)	136.6
N(2)-H(2B)...O(12)I	0.86	2.25	3.053(6)	155.9
N(2)-H(2B)...O(14)I	0.86	2.64	3.148(7)	118.9
N(3)-H(3A)...O(11)	0.86	2.17	2.737(5)	123.2
N(4)-H(4A)...O(13)E	0.86	2.06	2.889(6)	160.5
N(4)-H(4A)...O(10)E	0.86	2.61	3.082(5)	115.4
N(4)-H(4B)...O(6)E	0.86	2.20	2.948(6)	145.7
N(5)-H(5A)...O(8)	0.86	2.13	2.745(6)	127.6
N(6)-H(6A)...O(1)	0.86	2.01	2.839(6)	163.1
N(6)-H(3)...O(10)	0.86	2.22	2.969(6)	145.4
N(7)-H(7)...O(3)F	0.86	2.16	2.728(6)	122.9
N(8)-H(8B)...O(18)J	0.86	2.30	3.082(9)	151.4
O(17)-H(17A)...N(8)I	0.85	2.03	2.857(8)	165.4
O(18)-H(18)...O(5)	0.82	2.05	2.848(6)	164.2
O(19)-H(19)...N(6)	0.82	2.51	3.034(14)	123.3
C(38)-H(38A)...O(10)	0.96	2.51	3.427(19)	160.1
C(38)-H(38A)...O(15)	0.96	2.58	3.268(18)	128.3
Symmetry transformations used to generate equivalent atoms: A x-1/2,y+1/2,z B x,y+1,z				
C x,y-1,z	D x,-y+2,z-1/2	E x,-y+2,z+1/2	F x+1/2,y-1/2,z	
G x,-y+1,z+1/2	H x,-y+1,z-1/2	I x-1/2,y-1/2,z	J x+1/2,-y+5/2,z-1/2	

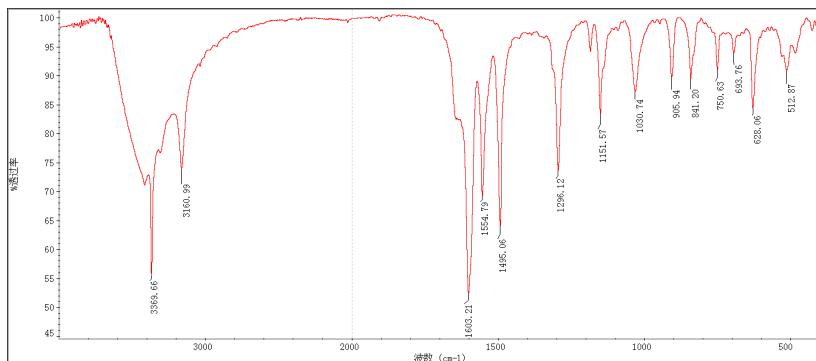


Fig. S1 The IR spectrum of complex 1.

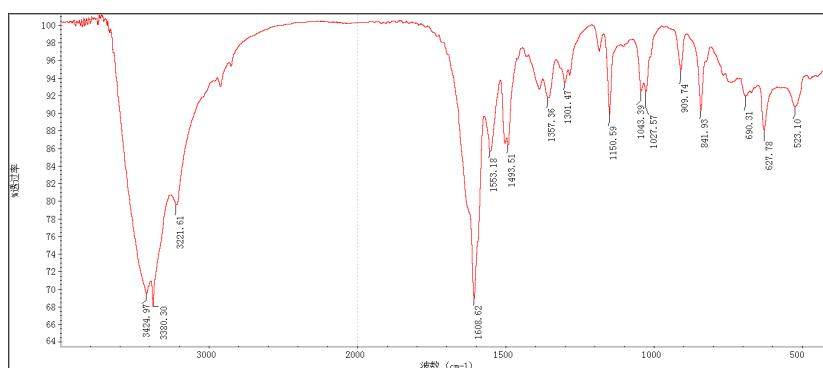


Fig. S2 The IR spectrum of complex 2.

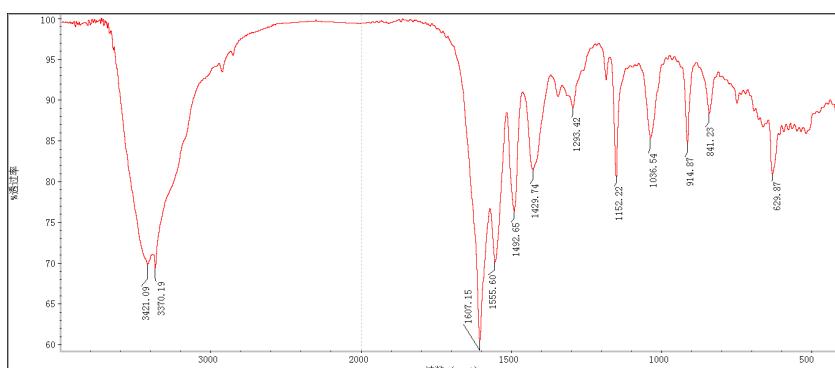


Fig. S3 The IR spectrum of complex 3.

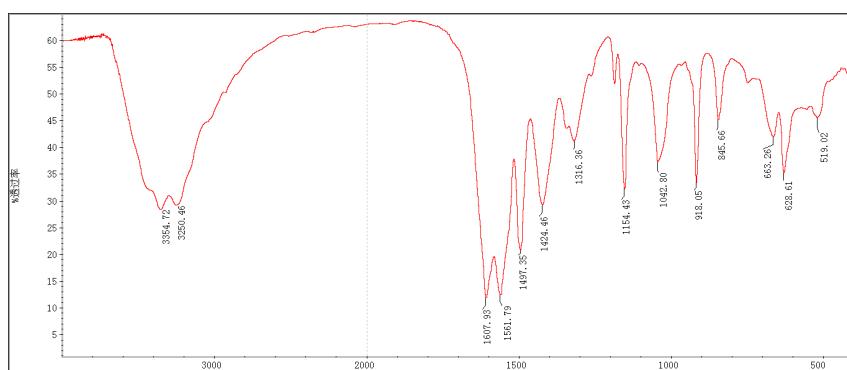


Fig. S4 The IR spectrum of complex 4.

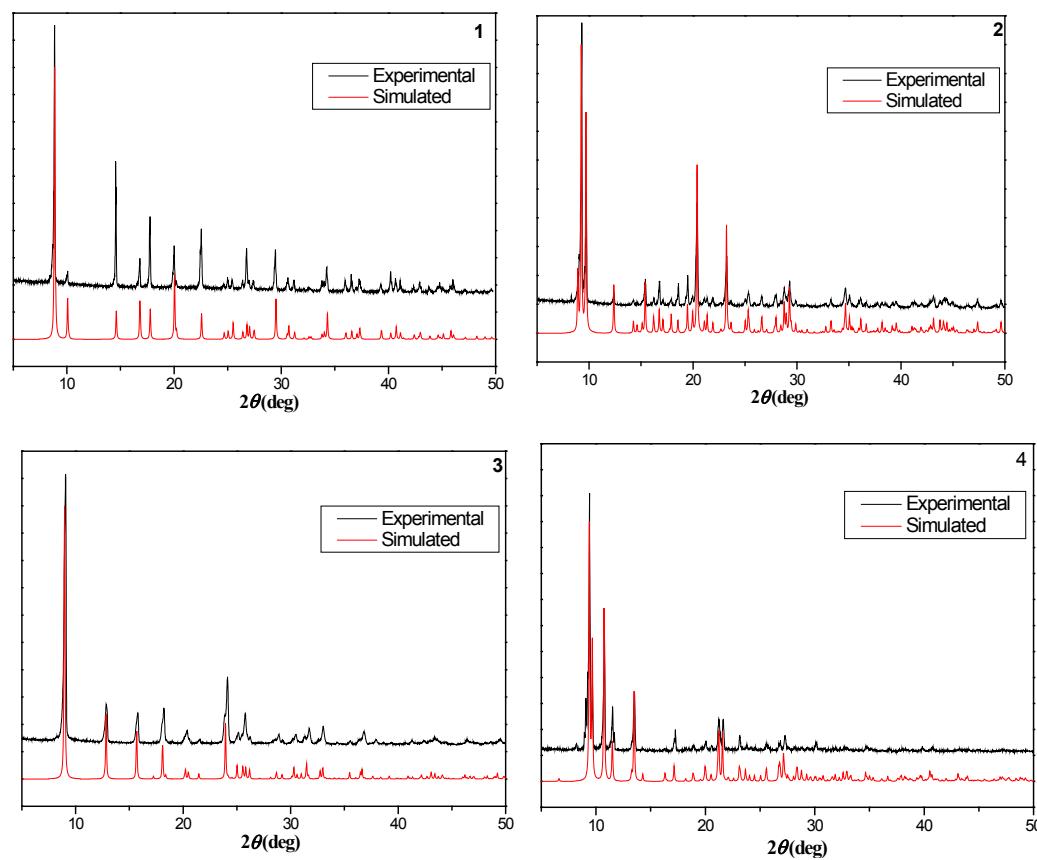


Fig. S5 The XRD patterns of complexes 1-4.

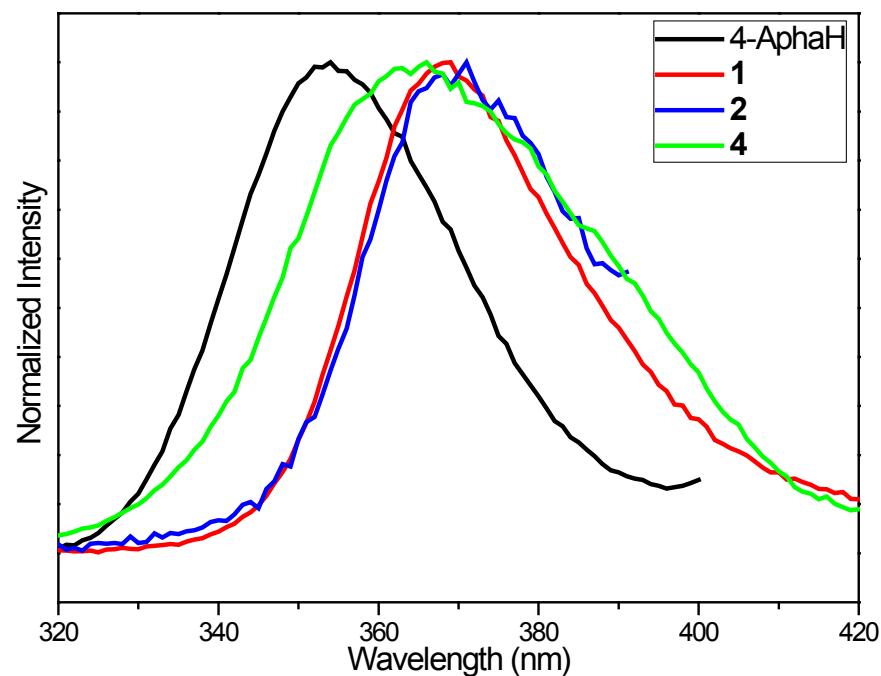


Fig. S6 The excitation spectra of 4-AphaH, 1, 2 and 4.

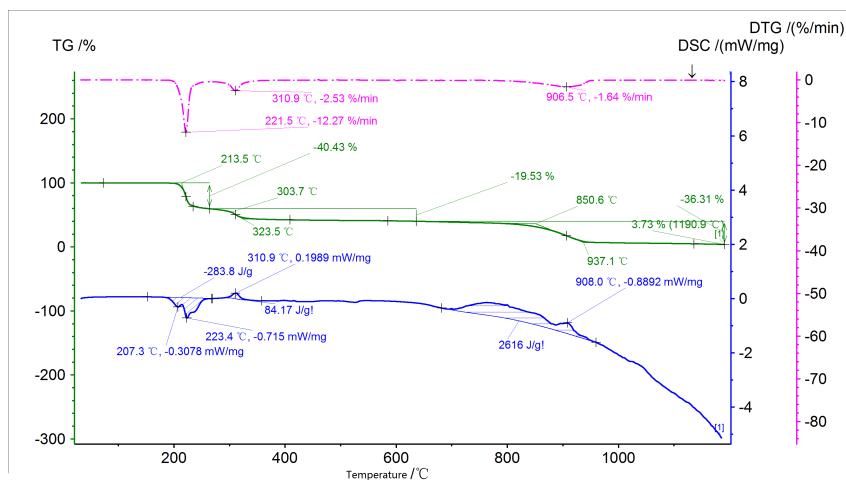


Fig. S7 TGA curve of complex 1.

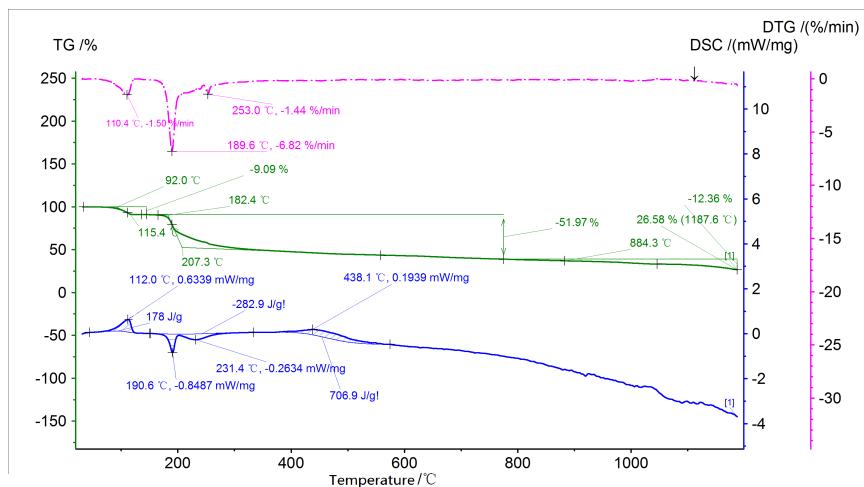


Fig. S8 TGA curve of complex 2.

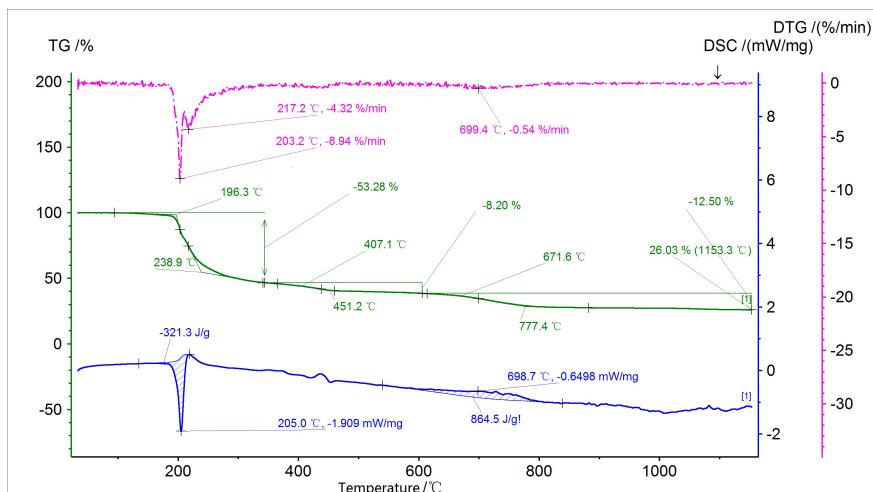


Fig. S9 TGA curve of complex 3.

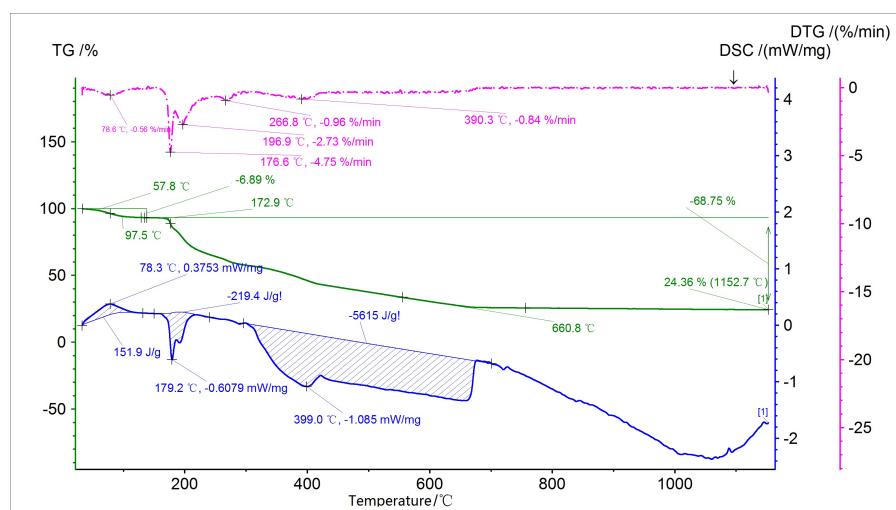


Fig. S10 TGA curve of complex 4.

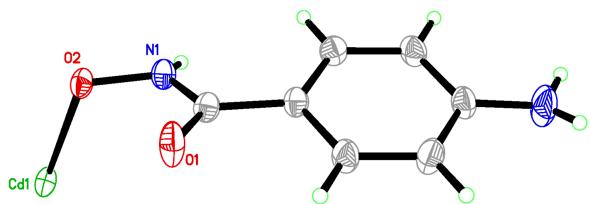


Fig. S11 ORTEP figure of the asymmetric unit in 1.

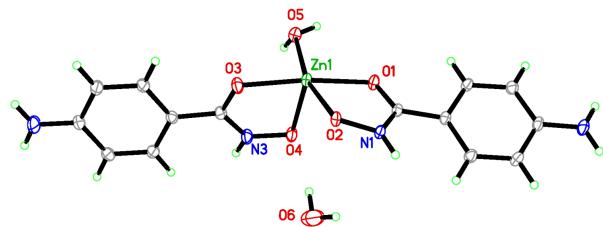


Fig. S12 ORTEP figure of asymmetric unit in 2.

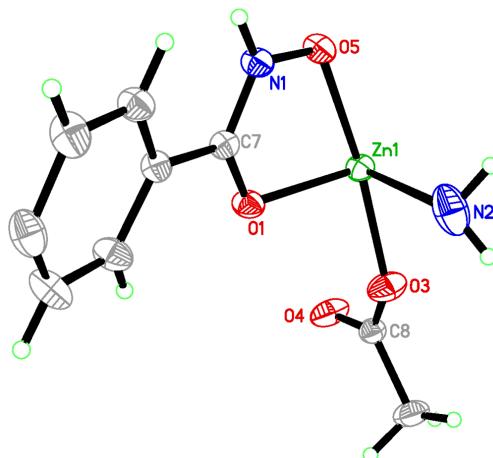


Fig. S13 ORTEP figure of asymmetric unit in 3.

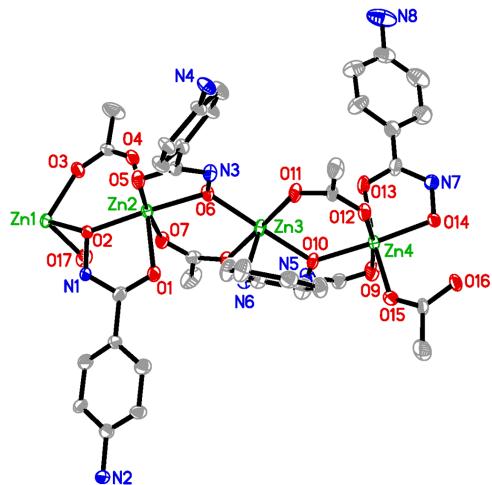


Fig. S14 ORTEP figure of asymmetric unit in **4**.