

The various structures of complexes fabricated with transition metal and triazole ligands and inhibiting effect on luminescent xanthine

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Table S1 The selected bond lengths (Å) and angles (°) for the complexes **1-5***

Complex 1					
Cd(1)-O(2)	2.256(3)	Cd(1)-O(3)	2.283(3)	Cd(1)-O(5) ^{#1}	2.287(4)
Cd(1)-O(1)	2.372(4)	Cd(1)-N(1)	2.393(4)	Cd(1)-O(6) ^{#1}	2.614(4)
Cd(1)-O(4)	2.406(3)				
O(2)-Cd(1)-O(3)	168.68(13)	O(2)-Cd(1)-O(5) ^{#1}	91.86(15)	O(3)-Cd(1)-O(5) ^{#1}	97.74(15)
O(2)-Cd(1)-O(1)	81.95(17)	O(3)-Cd(1)-O(1)	87.48(18)	O(5) ^{#1} -Cd(1)-O(1)	127.00(14)
O(2)-Cd(1)-N(1)	90.88(14)	O(3)-Cd(1)-N(1)	84.24(14)	O(5) ^{#1} -Cd(1)-N(1)	147.56(14)
O(1)-Cd(1)-N(1)	85.38(15)	O(2)-Cd(1)-O(4)	102.41(15)	O(3)-Cd(1)-O(4)	85.37(16)
O(5) ^{#1} -Cd(1)-O(4)	78.97(12)	O(1)-Cd(1)-O(4)	153.83(14)	N(1)-Cd(1)-O(4)	68.88(12)
O(2)-Cd(1)-O(6) ^{#1}	95.55(14)	O(3)-Cd(1)-O(6) ^{#1}	85.71(14)	O(5) ^{#1} -Cd(1)-O(6) ^{#1}	52.27(13)
O(1)-Cd(1)-O(6) ^{#1}	75.89(13)	N(1)-Cd(1)-O(6) ^{#1}	159.08(14)	O(4)-Cd(1)-O(6) ^{#1}	128.44(12)
Complex 2					
Co(1)-O(5)	2.109(2)	Co(1)-O(1)	2.117(2)	Co(1)-O(2) ^{#1}	2.1176(18)
Co(1)-O(4)	2.124(2)	Co(1)-O(3)	2.168(2)	Co(1)-N(3)	2.1937(19)
O(5)-Co(1)-O(1)	171.79(6)	O(5)-Co(1)-O(2) ^{#1}	87.71(6)	O(1)-Co(1)-O(2) ^{#1}	98.63(7)
O(5)-Co(1)-O(4)	90.90(6)	O(1)-Co(1)-O(4)	94.39(7)	O(2) ^{#1} -Co(1)-O(4)	89.11(7)
O(5)-Co(1)-O(3)	88.54(6)	O(1)-Co(1)-O(3)	86.63(6)	O(2) ^{#1} -Co(1)-O(3)	86.72(7)
O(4)-Co(1)-O(3)	175.81(5)	O(5)-Co(1)-N(3)	78.36(7)	O(1)-Co(1)-N(3)	95.34(8)
O(2) ^{#1} -Co(1)-N(3)	166.03(5)	O(4)-Co(1)-N(3)	89.99(7)	O(3)-Co(1)-N(3)	93.96(7)
Complex 3					
Zn(1)-O(5) ^{#1}	2.0396(17)	Zn(1)-O(2)	2.0778(17)	Zn(1)-O(4)	2.0838(17)
Zn(1)-O(3)	2.1114(19)	Zn(1)-O(1)	2.157(2)	Zn(1)-N(1)	2.182(2)
O(5) ^{#1} -Zn(1)-O(2)	101.71(7)	O(5) ^{#1} -Zn(1)-O(4)	87.76(7)	O(2)-Zn(1)-O(4)	169.24(7)
O(5) ^{#1} -Zn(1)-O(3)	89.45(7)	O(2)-Zn(1)-O(3)	94.63(8)	O(4)-Zn(1)-O(3)	90.51(7)
O(5) ^{#1} -Zn(1)-O(1)	87.56(8)	O(2)-Zn(1)-O(1)	86.42(8)	O(4)-Zn(1)-O(1)	88.92(7)
O(3)-Zn(1)-O(1)	176.98(7)	O(5) ^{#1} -Zn(1)-N(1)	165.15(7)	O(2)-Zn(1)-N(1)	93.14(7)
O(4)-Zn(1)-N(1)	77.42(7)	O(3)-Zn(1)-N(1)	89.62(8)	O(1)-Zn(1)-N(1)	93.16(8)
Complex 4					
Ni(1)-O(2) ^{#1}	2.0248(9)	Ni(1)-O(5)	2.0526(10)	Ni(1)-O(1)	2.0563(10)
Ni(1)-O(4)	2.0705(11)	Ni(1)-N(3)	2.0879(11)	Ni(1)-O(3)	2.0923(12)
O(2) ^{#1} -Ni(1)-O(5)	86.88(4)	O(2) ^{#1} -Ni(1)-O(1)	98.36(4)	O(5)-Ni(1)-O(1)	173.54(4)
O(2) ^{#1} -Ni(1)-O(4)	88.71(4)	O(5)-Ni(1)-O(4)	89.53(5)	O(1)-Ni(1)-O(4)	94.35(5)
O(2) ^{#1} -Ni(1)-N(3)	166.64(4)	O(5)-Ni(1)-N(3)	79.80(4)	O(1)-Ni(1)-N(3)	95.00(4)
O(4)-Ni(1)-N(3)	90.16(4)	O(2) ^{#1} -Ni(1)-O(3)	87.57(5)	O(5)-Ni(1)-O(3)	89.30(5)
O(1)-Ni(1)-O(3)	87.15(5)	O(4)-Ni(1)-O(3)	176.15(4)	N(3)-Ni(1)-O(3)	93.24(5)
Complex 5					
Cu(1)-O(1) ^{#1}	1.931(2)	Cu(1)-O(1)	1.931(2)	Cu(1)-O(4) ^{#2}	1.994(2)
Cu(1)-O(4) ^{#3}	1.994(2)	Cu(2)-O(1)	1.944(2)	Cu(2)-O(5) ^{#2}	1.953(2)

Cu(2)-N(1)	1.987(3)	Cu(2)-O(2)	1.996(2)		
O(1) ^{#1} -Cu(1)-O(1)	179.998(1)	O(1) ^{#1} -Cu(1)-O(4) ^{#2}	88.52(10)	O(1)-Cu(1)-O(4) ^{#2}	91.48(10)
O(1) ^{#1} -Cu(1)-O(4) ^{#3}	91.48(10)	O(1)-Cu(1)-O(4) ^{#3}	88.52(10)	O(4) ^{#2} -Cu(1)-O(4) ^{#3}	179.999(1)
O(1)-Cu(2)-O(5) ^{#2}	93.36(10)	O(1)-Cu(2)-N(1)	96.60(10)	O(5) ^{#2} -Cu(2)-N(1)	170.01(10)
O(1)-Cu(2)-O(2)	166.78(9)	O(5) ^{#2} -Cu(2)-O(2)	88.38(9)	N(1)-Cu(2)-O(2)	81.75(9)
Cu(1)-O(1)-Cu(2)	107.74(11)				

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

Table S2 Bond distances (Å) and angles (°) of hydrogen bonds in Complexes **1-5***

D – H ... A	D (D – H) / Å	D (H ... A) / Å	D (D ... A) / Å	D – H ... A /°
Complex 1				
O(1W)-H(1WB)...O(3W) ^{#4}	0.85	2.07	2.810(7)	145.7
O(1W)-H(1WC)...O(3W) ^{#5}	0.86	2.21	2.856(6)	131.7
O(1)-H(1A)...O(7) ^{#6}	0.85	2.35	2.893(6)	122.5
O(1)-H(1C)...O(1W) ^{#1}	0.85	2.26	3.000(6)	145.8
O(2)-H(2A)...O(4) ^{#7}	0.85	2.15	2.778(5)	130.5
O(2)-H(2C)...O(6) ^{#8}	0.85	2.07	2.748(6)	136.1
O(2W)-H(2WB)...O(5) ^{#9}	0.85	2.14	2.822(6)	137.5
O(2W)-H(2WC)...O(7) ^{#10}	0.85	2.28	2.940(5)	135.3
O(2W)-H(2WC)...O(1) ^{#8}	0.85	2.43	3.187(7)	148.6
C(6)-H(6)...O(3W) ^{#2}	0.93	2.53	3.335(6)	144.5
Complex 2				
O(3)-H(3B)...O(1W)	0.823(10)	2.184(11)	3.003(4)	173(4)
O(3)-H(3E)...O(3W)	0.824(10)	2.03(2)	2.810(6)	157(5)
O(1W)-H(1D)...O(3)	0.830(10)	2.25(2)	3.003(4)	151(5)
O(1W)-H(1E)...O(2W)	0.820(10)	2.081(12)	2.891(5)	169(5)
O(1)-H(1A)...O(7) ^{#4}	0.836(9)	1.960(9)	2.792(3)	174(2)
O(1)-H(1B)...O(5) ^{#1}	0.830(9)	1.975(13)	2.727(2)	150(2)
O(3)-H(3A)...O(6) ^{#5}	0.826(9)	1.934(10)	2.755(3)	172(2)
O(3)-H(3E)...O(3W) ^{#3}	0.824(10)	2.37(2)	3.123(6)	152(3)
O(4)-H(4A)...O(6) ^{#4}	0.822(9)	1.905(9)	2.715(2)	169(2)
O(4)-H(4B)...O(7) ^{#6}	0.822(9)	2.056(10)	2.868(3)	169(2)
O(1W)-H(1C)...O(7) ^{#7}	0.824(10)	2.246(14)	3.049(4)	165(4)
O(2W)-H(2E)...O(2W) ^{#5}	0.819(10)	2.09(2)	2.888(6)	166(6)
O(3W)-H(3F)...O(3) ^{#3}	0.817(10)	2.51(8)	3.123(6)	132(9)
O(3W)-H(3D)...O(4) ^{#1}	0.819(10)	2.18(4)	2.963(6)	159(10)
Complex 3				
O(1)-H(1B)...O(1W) ^{#4}	0.96	2.14	2.914(4)	137.0
O(1)-H(1C)...O(7) ^{#5}	0.96	1.75	2.704(3)	174.5
O(2)-H(2A)...O(4) ^{#1}	0.96	1.91	2.685(2)	135.8

O(2)-H(2B)...O(6) ^{#6}	0.96	1.78	2.733(3)	171.1
O(3)-H(3A)...O(6) ^{#7}	0.96	1.89	2.807(3)	157.7
O(3)-H(3C)...O(7) ^{#6}	0.96	1.78	2.669(2)	153.4
Complex 4				
O(1W)-H(1D)...O(3)	0.832(10)	2.24(4)	2.937(2)	142(6)
O(1W)-H(1D)...O(3W)	0.832(10)	2.61(3)	3.340(6)	147(4)
O(1W)-H(1E)...O(2W)	0.823(10)	1.985(10)	2.804(4)	174(4)
O(3)-H(3B)...O(1W)	0.823(10)	2.132(14)	2.937(2)	166(4)
O(3)-H(3E)...O(3W)	0.825(10)	1.958(17)	2.756(5)	162(4)
O(1)-H(1A)...O(7) ^{#4}	0.823(9)	1.928(9)	2.7466(16)	172.4(19)
O(1)-H(1B)...O(5) ^{#1}	0.828(9)	1.906(11)	2.6674(14)	152.4(19)
O(1W)-H(1C)...O(7) ^{#5}	0.828(10)	2.185(16)	2.966(2)	157(3)
O(2W)-H(2E)...O(2W) ^{#6}	0.819(10)	2.032(19)	2.830(5)	165(4)
O(3)-H(3A)...O(6) ^{#6}	0.823(9)	1.882(9)	2.6990(16)	172(2)
O(3)-H(3E)...O(3W) ^{#3}	0.825(10)	2.35(2)	3.086(5)	149(3)
O(3W)-H(3F)...O(3) ^{#3}	0.817(10)	2.40(5)	3.086(5)	143(7)
O(3W)-H(3D)...O(4) ^{#1}	0.821(10)	2.084(19)	2.897(4)	171(9)
O(4)-H(4A)...O(6) ^{#4}	0.821(9)	1.858(9)	2.6617(15)	165.6(18)
O(4)-H(4B)...O(7) ^{#7}	0.813(9)	2.020(10)	2.8262(15)	171(2)
C(6)-H(6A)...O(1W) ^{#8}	0.93	2.57	3.363(3)	142.8
Complex 5				
O(1W)-H(1WA)...O(2) ^{#5}	0.89(7)	2.06(6)	2.895(4)	155(5)
C(5)-H(5)...O(1W) ^{#6}	0.93	2.46	3.256(5)	143.3

*Symmetry transformation used to generate equivalent atoms for complex1, #1: -x+1/2, -y+2, z+1/2; #2: x, y, z; #4: -x+1, y+1/2, -z+1/2; #5: -x+1/2, -y+1, z-1/2; #6: x, y+1, z; #7: -x, y+1/2, -z+3/2; #8: x-1/2, -y+3/2, -z+1; #9: x, y-1, z; #10: x-1/2, -y+1/2, -z+1; for complex2, #1: -x+1/2, y-1/2, -z+1/2; #3: -x+1/2, -y+1/2, -z+1; #4: -x+1, -y+1, -z; #5: -x+1, y, -z+1/2; #6: x-1/2, y-1/2, z; #7: -x+1, y-1, -z+1/2; for complex3, #1: -x+1/2, y+1/2, -z+1/2; #4: x, y+1, z; #5: -x, y, -z+1/2; #6: -x, -y+2, -z+1; for complex4, #1: -x+1/2, y-1/2, -z+1/2; #3: -x+1/2, -y+1/2, -z+1; #4: -x+1, -y+1, -z; #5: -x+1, y-1, -z+1/2; #6: -x+1, y, -z+1/2; #7: x-1/2, y-1/2, z; #8: x, -y+1, z-1/2; for complex5, #5: -x+1, -y+2, -z+2; #6: x+1, y, z.

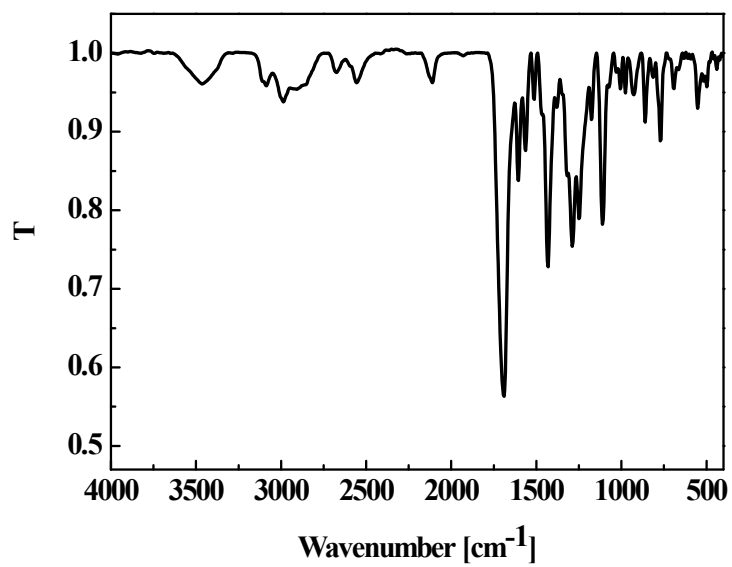


Fig. S1 The IR spectrum of H₂L

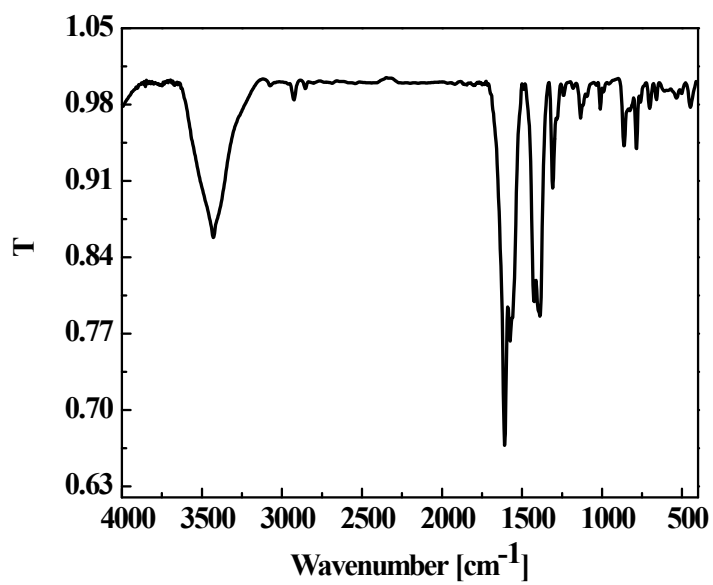


Fig. S2 The IR spectrum of complex 1

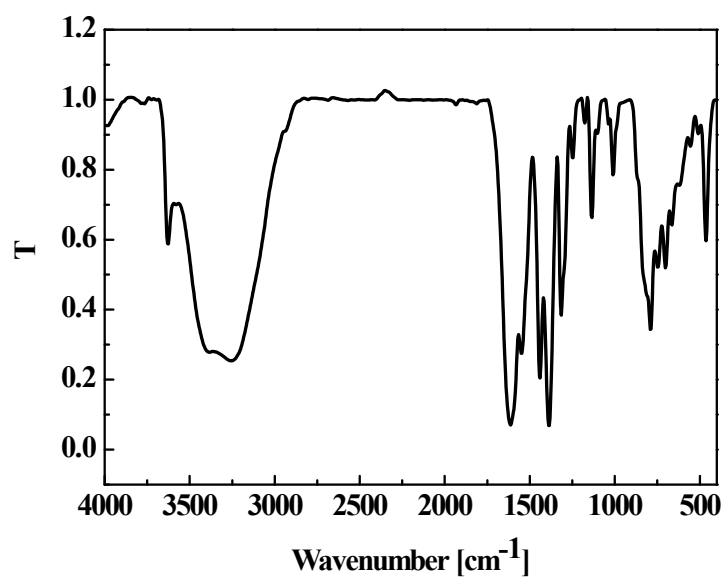


Fig. S3 The IR spectrum of complex 2

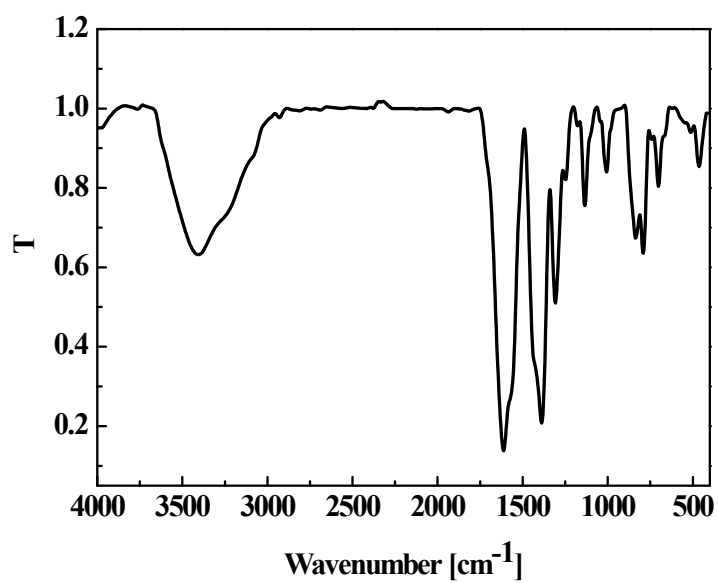


Fig. S4 The IR spectrum of complex 3

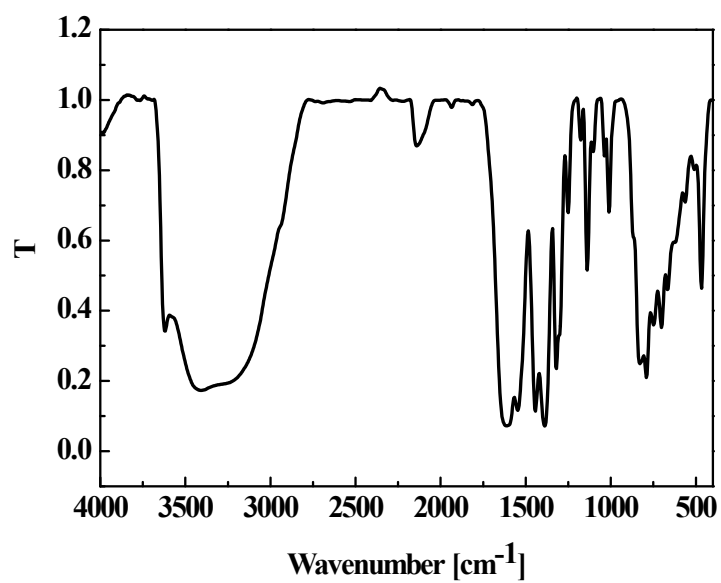


Fig. S5 The IR spectrum of complex 4

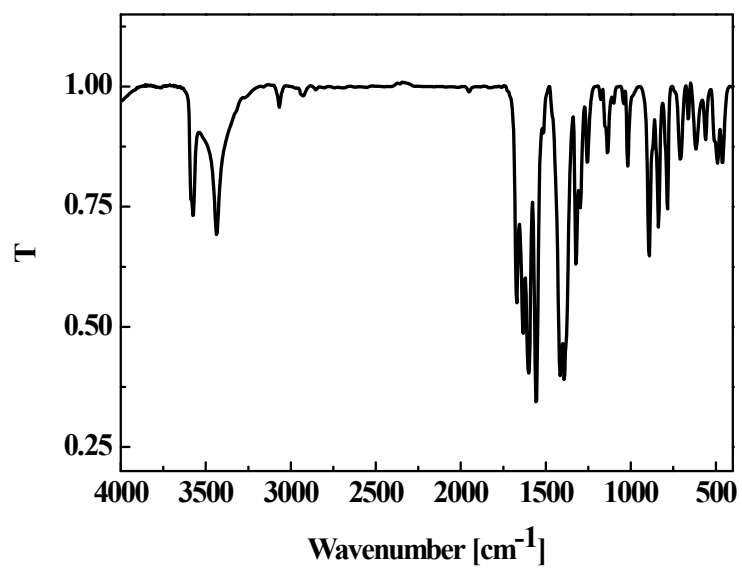


Fig. S6 The IR spectrum of complex 5

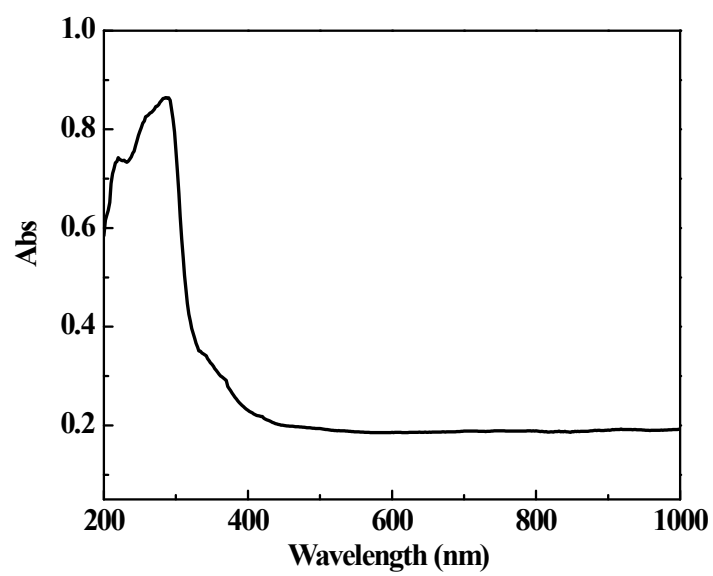


Fig. S7 The UV-vis spectrum of H₂L

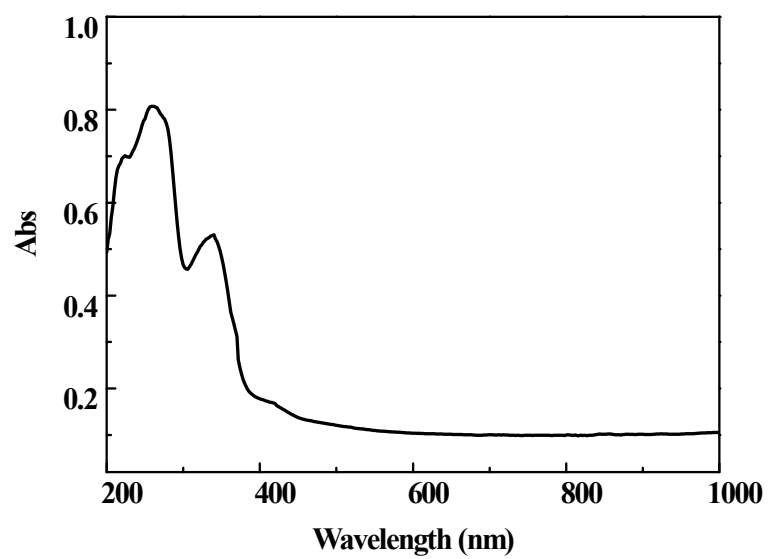


Fig. S8 The UV-vis spectrum of complex 1

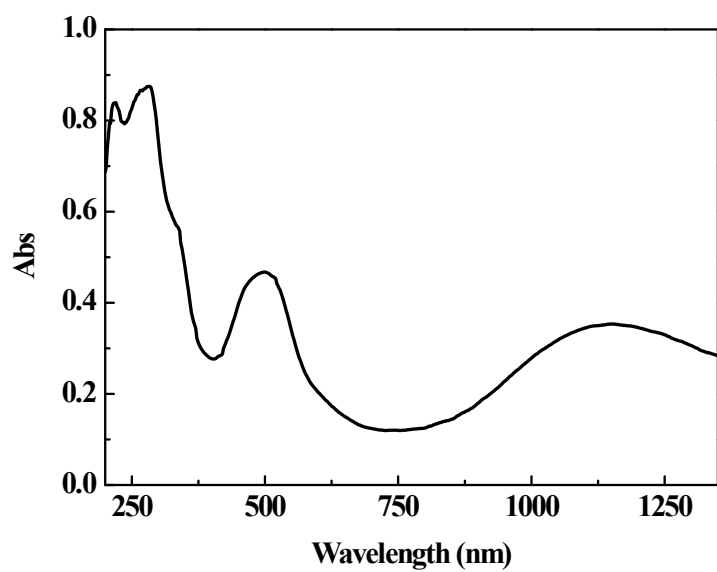


Fig. S9 The UV-vis spectrum of complex 2

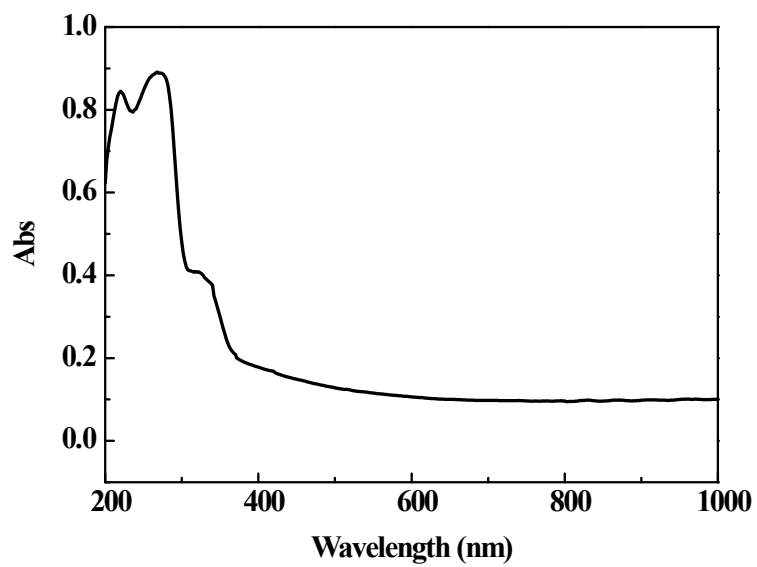


Fig. S10 The UV-vis spectrum of complex 3

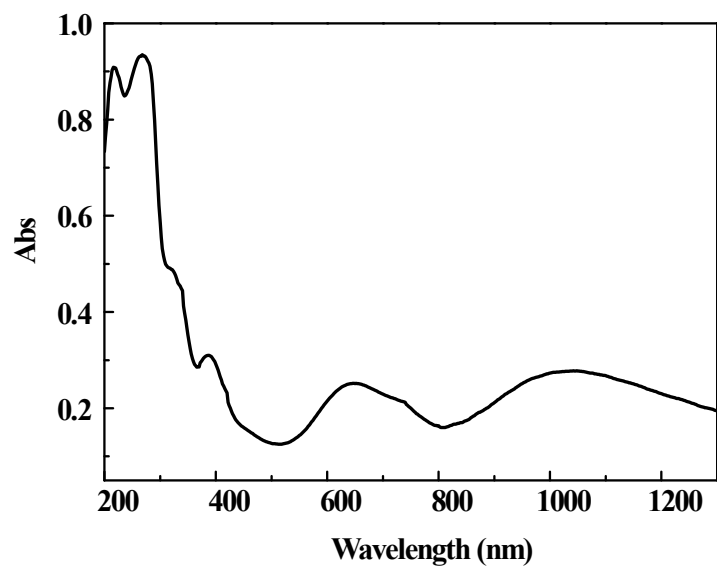


Fig. S11 The UV-vis spectrum of complex 4

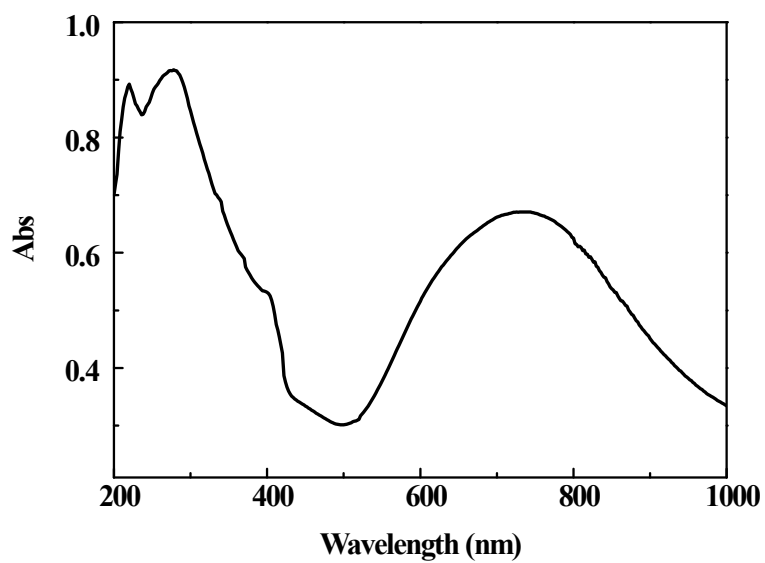


Fig. S12 The UV-vis spectrum of complex 5

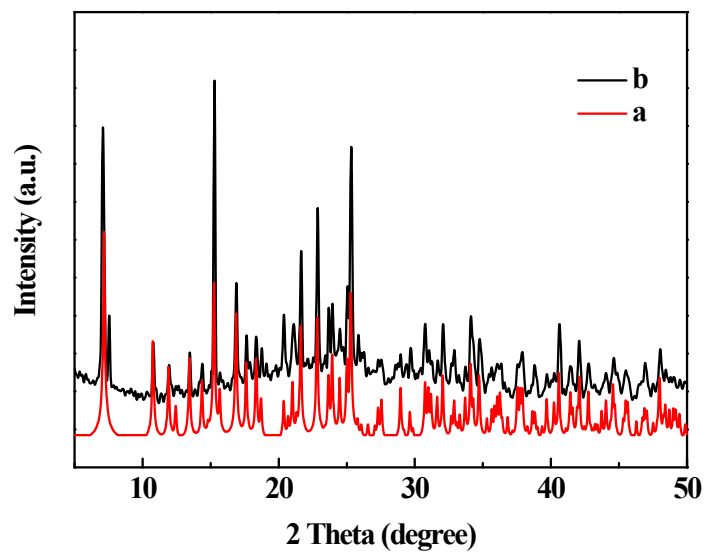


Fig. S13 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 1

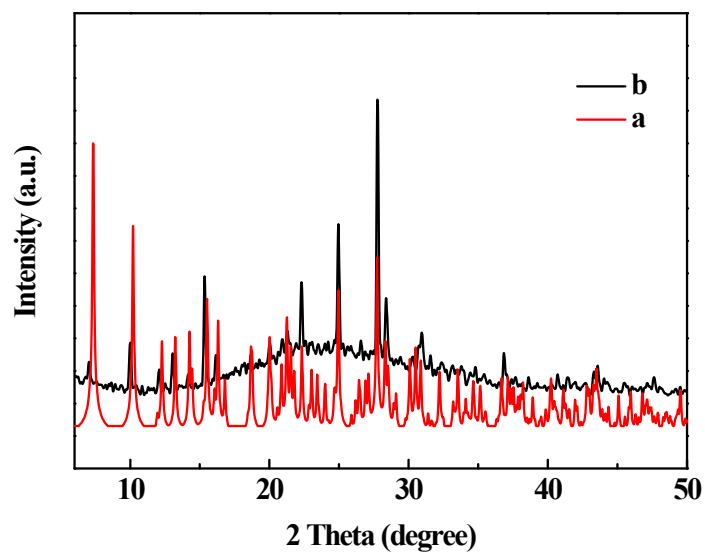


Fig. S14 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 2

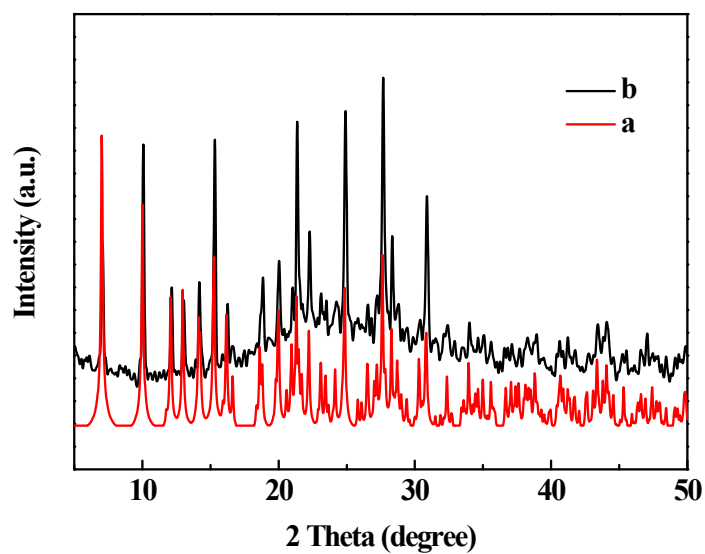


Fig. S15 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 3

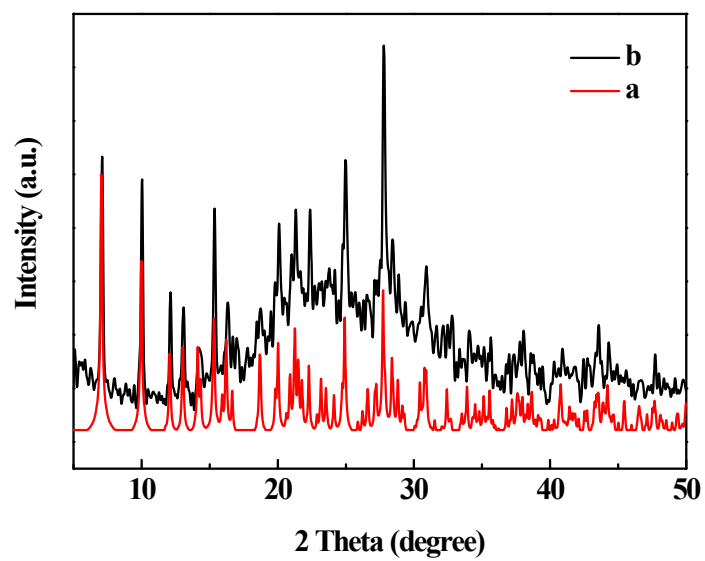


Fig. S16 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 4

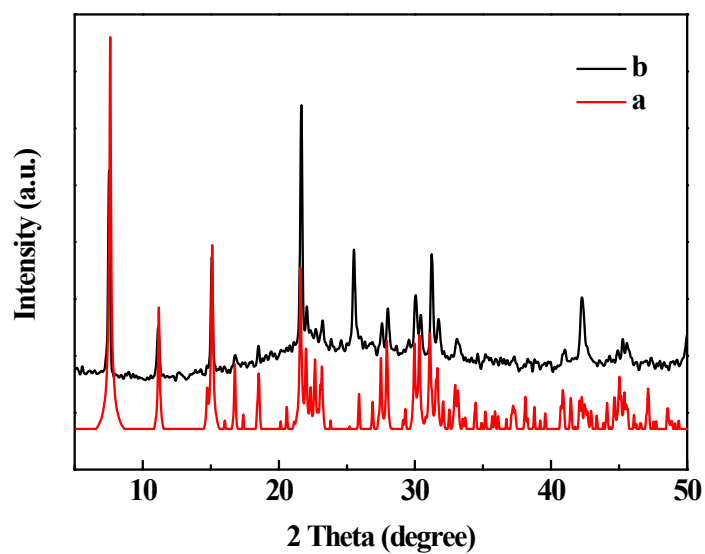


Fig. S17 The simulated PXRD pattern (a) and measured PXRD spectrum (b) of complex 5

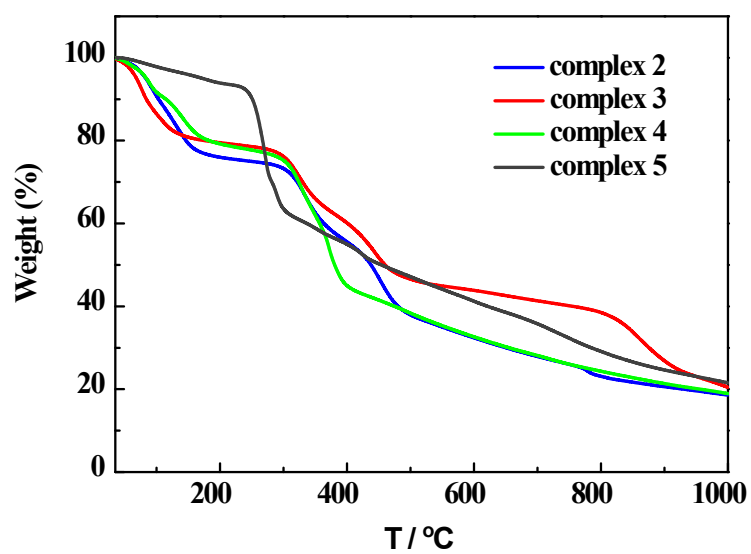


Fig. S18 The TG curve of complexes 2-5

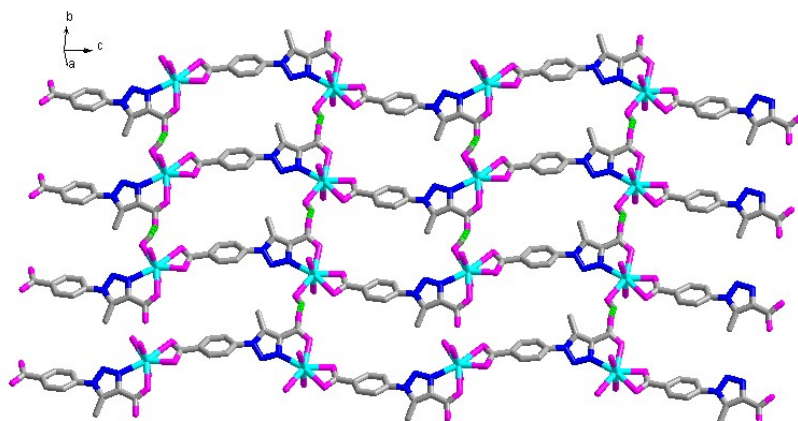


Fig. S19 The 2D chain structure connected by hydrogen bonds of complex **1**

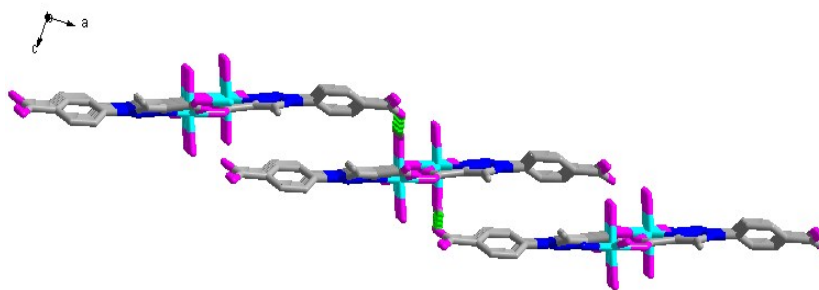


Fig. S20 The 2D chain structure connected by hydrogen bonds of complex **4**

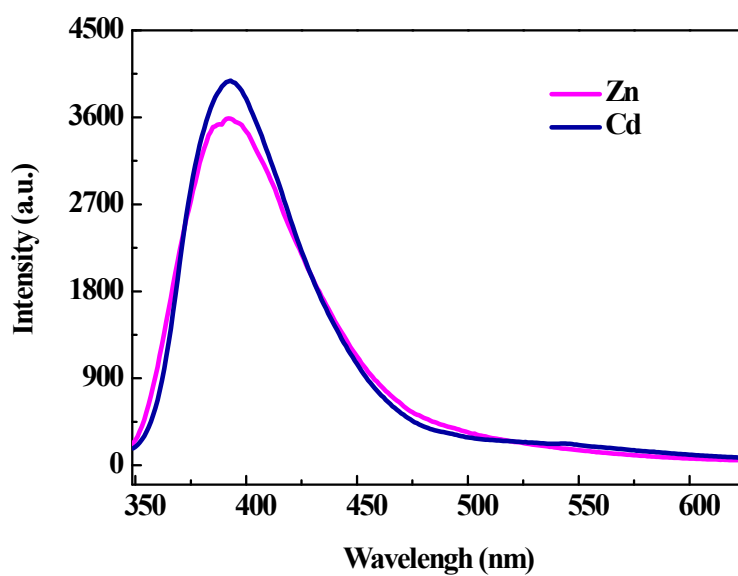


Fig. S21 The solid-state photoluminescence spectra of **1** and **3** at room temperature.

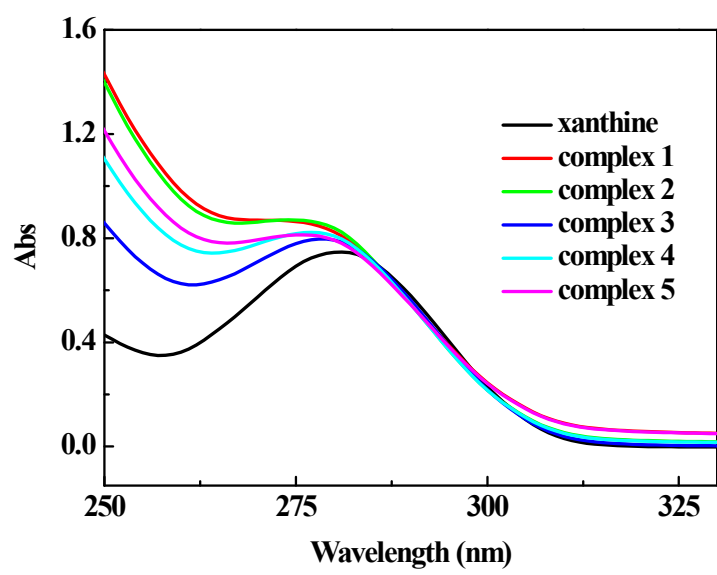


Fig. S22 The UV-vis spectra of xanthine solution and complexes **1a-5a**