Supporting Information

Five new 3D transition MOFs based on 1-(3,5-DicarBoxylato benzyl)-3,5-pyrazole dicarboxylic acid displaying the unique luminescent sensing towards Fe^{3+} and magnetic properties

Wei-Ni Liu,‡Wen-Quan Tong,‡ Lu-Lu Ma, Yao Wang, Jiao-Min Wang, Lei Hou* and Yao-Yu Wang*

Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of the Ministry of Education, Shaanxi Key Laboratory of Physico-Inorganic Chemistry, College of Chemistry and Materials Science, Northwest University, Xi'an, Shaanxi 710127, P. R. China. E-mail: wyaoyu@nwu.edu.cn. lhou2009@nwu.edu.cn.

Table S1 Crystal data and structure refinements for **1-5**.

Complexes	**1**	**2**	**3**	**4**	**5**
Formula	$C_{28}H_{20}Zn_3N_4O_{19}$	$C_{14}H_{16}Ba_2N_2O_{15}$	$C_{28}H_{26}Ba_4N_4O_{23}$	$C_{28}H_{24}Cd_3Cl_2N_4O_{20}$	$C_{14}H_{10}Cu_2N_2O_{10}$
M_r	912.65	726.97	1335.89	1144.61	493.34
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic	Orthorhombic
Space group	*Fddd*	$P2_1/n$	*P2/n*	$P2_1/n$	*Fddd*
a (Å)	19.640(2)	9.3811(8)	12.9214(15)	10.880(9)	15.339(3)
b (Å)	22.990(3)	18.3474(17)	10.4575(12)	12.209(9)	30.839(7)
c (Å)	29.085(3)	13.1915(12)	14.1666(16)	14.708(12)	32.070(7)
α (°)	90	90	90	90	90
β (°)	90	105.0625(13)	93.894(2)	107.306(11)	90
γ (°)	90	90	90	90	90
V (Å^3)	13133(2)	2192.5(3)	1909.8(4)	1865(3)	15171(6)
Z	16	4	2	2	32
D_{calc} (g cm^{-3})	1.846	2.202	2.323	2.038	1.728
F(000)	7328	1384	1260	1116	7872
R_{int}	0.0475	0.0271	0.0224	0.0244	0.0607
GOF on F^2	1.050	1.018	1.112	1.080	1.022
$R_1{}^a$ [$I > 2\sigma(I)$]	0.0540	0.0238	0.0234	0.0293	0.0431
$wR_2{}^b$ (all data)	0.1523	0.0569	0.0708	0.0756	0.1119

$^aR_1 = \sum||F_o| - |F_c||/\sum|F_o|$. $^b wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$.

Table S2. Selected bond lengths [Å] and angles [°] for **1-5**.

1(Zn)			
Zn(1)-O(1W)	2.006(5)	Zn(1)-O(1)	2.046(5)
Zn(1)-O(7)#1	2.050(4)	Zn(1)-O(6)#2	2.091(4)
Zn(1)-N(2)#1	2.240(5)	Zn(1)-O(2)	2.334(5)
Zn(2)-O(5)#3	1.923(4)	Zn(2)-O(5)#4	1.923(4)
Zn(2)-O(7)	1.966(4)	Zn(2)-O(7)#5	1.966(4)
N(2)-Zn(1)#1	2.240(5)	O(5)-Zn(2)#6	1.923(4)
O(6)-Zn(1)#2	2.091(4)	O(7)-Zn(1)#1	2.050(4)
O(1W)-Zn(1)-O(1)	151.21(19)	O(1W)-Zn(1)-O(7)#1	104.90(19)
O(1)-Zn(1)-O(7)#1	103.70(18)	O(1W)-Zn(1)-O(6)#2	87.8(2)
O(1)-Zn(1)-O(6)#2	89.1(2)	O(7)#1-Zn(1)-O(6)#2	89.73(18)
O(1W)-Zn(1)-N(2)#1	97.87(19)	O(1)-Zn(1)-N(2)#1	92.19(18)
O(7)#1-Zn(1)-N(2)#1	75.96(15)	O(6)#2-Zn(1)-N(2)#1	165.53(19)
O(1W)-Zn(1)-O(2)	93.48(18)	O(1)-Zn(1)-O(2)	58.63(18)
O(7)#1-Zn(1)-O(2)	160.48(17)	O(6)#2-Zn(1)-O(2)	97.66(19)
N(2)#1-Zn(1)-O(2)	95.30(17)	O(5)#3-Zn(2)-O(5)#4	122.5(3)
O(5)#3-Zn(2)-O(7)	106.83(17)	O(5)#4-Zn(2)-O(7)	102.17(19)
O(5)#3-Zn(2)-O(7)#5	102.17(19)	O(5)#4-Zn(2)-O(7)#5	106.83(17)
O(5)#4-Zn(2)-O(7)#5	106.83(17)	O(7)-Zn(2)-O(7)#5	117.3(3)
Symmetrical codes: #1: -x+1/4, y, -z+1/4; #2: -x+1/2, -y+2, -z+1/2; #3: x-1/4, -y+2, z-1/4; #4: x-1/4, y+1/4, -z+1/2; #5: x, -y+9/4, -z+1/4; #6: x+1/4, y-1/4, -z+1/2.			
2(Ba)			
Ba(1)-O(1)	2.913(2)	Ba(1)-O(1W)	2.868(3)
Ba(1)-O(2)	2.746(2)	Ba(1)-O(2W)	2.913(2)
Ba(1)-O(5)#1	2.687(7)	Ba(1)-O(5A)#1	2.871(7)
Ba(1)-O(6)#1	3.187(2)	Ba(1)-O(6)#2	2.676(2)
Ba(1)-O(6W)	2.785(2)	Ba(1)-O(7)#3	2.787(2)
Ba(2)-O(1)#4	2.7589(19)	Ba(2)-O(2W)	2.984(2)
Ba(2)-O(3)#5	2.793(2)	Ba(2)-O(3W)	2.852(3)
Ba(2)-O(4WA)	2.949(12)	Ba(2)-O(4WB)	2.663(12)
Ba(2)-O(5)#1	2.689(7)	Ba(2)-O(5A)#1	2.698(7)
Ba(2)-O(8)#6	2.727(2)	Ba(2)-N(2)#1	3.068(2)
O(1)-Ba(2)#7	2.7588(18)	O(3)-Ba(2)#8	2.7932(19)
O(5)-Ba(1)#1	2.687(7)	O(5)-Ba(2)#1	2.689(7)
O(5A)-Ba(1)#1	2.871(7)	O(5A)-Ba(2)#1	2.698(7)
O(6)-Ba(1)#1	3.187(2)	O(6)-Ba(1)#9	2.676(2)
O(7)-Ba(1)#10	2.787(2)	O(8)-Ba(2)#11	2.727(2)
N(2)-Ba(2)#1	3.068(2)	O(1)-Ba(1)-O(2W)	80.05(6)
O(1)-Ba(1)-O(6)#1	123.12(6)	O(1W)-Ba(1)-O(1)	77.44(7)
O(1W)-Ba(1)-O(2W)	122.66(8)	O(1W)-Ba(1)-O(5A)#1	160.39(14)
O(1W)-Ba(1)-O(6)#1	139.03(8)	O(2)-Ba(1)-O(1)	45.99(5)
O(2)-Ba(1)-O(1W)	120.79(7)	O(2)-Ba(1)-O(2W)	70.38(7)

O(2)-Ba(1)-O(5A)#1	78.30(14)	O(2)-Ba(1)-O(6)#1	79.20(6)
O(2)-Ba(1)-O(6W)	136.95(7)	O(2)-Ba(1)-O(7)#3	119.80(7)
O(2W)-Ba(1)-O(6)#1	97.07(6)	O(5)#1-Ba(1)-O(1)	133.82(16)
O(5)#1-Ba(1)-O(1W)	146.21(17)	O(5)#1-Ba(1)-O(2)	92.94(16)
O(5)#1-Ba(1)-O(2W)	63.95(16)	O(5)#1-Ba(1)-O(6)#1	42.70(17)
O(5)#1-Ba(1)-O(6W)	81.55(16)	O(5)#1-Ba(1)-O(7)#3	96.08(17)
O(5A)#1-Ba(1)-O(1)	119.23(13)	O(5A)#1-Ba(1)-O(2W)	56.32(14)
O(5A)#1-Ba(1)-O(6)#1	42.57(14)	O(6)#2-Ba(1)-O(1)	75.99(6)
O(6)#2-Ba(1)-O(1W)	80.82(8)	O(6)#2-Ba(1)-O(2)	71.25(7)
O(6)#2-Ba(1)-O(2W)	141.47(7)	O(6)#2-Ba(1)-O(5)#1	115.03(17)
O(6)#2-Ba(1)-O(5A)#1	111.97(15)	O(6)#2-Ba(1)-O(6)#1	72.34(7)
O(6)#2-Ba(1)-O(6W)	72.76(8)	O(6)#2-Ba(1)-O(7)#3	147.08(7)
O(6W)-Ba(1)-O(1)	140.91(8)	O(6W)-Ba(1)-O(1W)	74.94(8)
O(6W)-Ba(1)-O(2W)	138.61(8)	O(6W)-Ba(1)-O(5A)#1	94.20(14)
O(6W)-Ba(1)-O(6)#1	67.93(7)	O(6W)-Ba(1)-O(7)#3	103.25(8)
O(7)#3-Ba(1)-O(1)	90.50(6)	O(7)#3-Ba(1)-O(1W)	66.86(8)
O(7)#3-Ba(1)-O(2W)	61.35(7)	O(7)#3-Ba(1)-O(5A)#1	100.85(15)
O(7)#3-Ba(1)-O(6)#1	137.72(6)	O(1)#4-Ba(2)-O(2W)	89.00(6)
O(1)#4-Ba(2)-O(3)#5	83.45(6)	O(1)#4-Ba(2)-O(3W)	81.23(9)
O(1)#4-Ba(2)-O(4WA)	68.7(2)	O(1)#4-Ba(2)-N(2)#1	158.78(6)
O(2W)-Ba(2)-N(2)#1	112.08(6)	O(3)#5-Ba(2)-O(2W)	143.71(6)
O(3)#5-Ba(2)-O(3W)	138.86(9)	O(3)#5-Ba(2)-O(4WA)	65.6(2)
O(3)#5-Ba(2)-N(2)#1	80.72(6)	O(3W)-Ba(2)-O(2W)	73.91(8)
O(3W)-Ba(2)-O(4WA)	139.3(2)	O(3W)-Ba(2)-N(2)#1	101.70(8)
O(4WA)-Ba(2)-O(2W)	78.6(2)	O(4WA)-Ba(2)-N(2)#1	116.4(2)
O(4WB)-Ba(2)-O(1)#4	79.2(3)	O(4WB)-Ba(2)-O(2W)	71.8(2)
O(4WB)-Ba(2)-O(3)#5	71.9(2)	O(4WB)-Ba(2)-O(3W)	140.5(3)
O(4WB)-Ba(2)-O(5A)#1	99.9(3)	O(4WB)-Ba(2)-O(8)#6	144.3(2)
O(4WB)-Ba(2)-N(2)#1	108.8(3)	O(5)#1-Ba(2)-O(1)#4	138.81(16)
O(5)#1-Ba(2)-O(2W)	62.94(16)	O(5)#1-Ba(2)-O(3)#5	137.04(16)
O(5)#1-Ba(2)-O(3W)	63.02(18)	O(5)#1-Ba(2)-O(4WA)	127.3(2)
O(5)#1-Ba(2)-O(8)#6	95.12(16)	O(5)#1-Ba(2)-N(2)#1	56.52(16)
O(5A)#1-Ba(2)-O(1)#4	143.60(15)	O(5A)#1-Ba(2)-O(2W)	57.17(14)
O(5A)#1-Ba(2)-O(3)#5	131.37(15)	O(5A)#1-Ba(2)-O(3W)	76.90(17)
O(5A)#1-Ba(2)-O(8)#6	108.34(14)	O(5A)#1-Ba(2)-N(2)#1	56.05(15)
O(8)#6-Ba(2)-O(1)#4	90.14(6)	O(8)#6-Ba(2)-O(2W)	142.65(6)
O(8)#6-Ba(2)-O(3)#5	73.04(7)	O(8)#6-Ba(2)-O(3W)	69.07(8)
O(8)#6-Ba(2)-O(4WA)	134.9(2)	O(8)#6-Ba(2)-N(2)#1	71.78(6)
Symmetrical codes: #1: -x+1, -y, -z+2; #2: x-1, y, z; #3: x-1/2, -y+1/2, z+1/2; #4: x+1/2, -y+1/2, z+1/2; #5: x+1, y, z+1; #6: x, y, z+1; #7: x-1/2, -y+1/2, z-1/2; #8: x-1, y, z-1; #9: x+1, y, z; #10: x+1/2, -y+1/2, z-1/2; #11: x, y, z-1.			
3(Ba)			
Ba(3)-O(8)#1	2.726(3)	Ba(3)-O(8)	2.726(3)

Ba(3)-O(4)#2	2.751(3)	Ba(3)-O(4)#3	2.751(3)
Ba(3)-O(2)#4	2.831(3)	Ba(3)-O(2)#5	2.831(3)
Ba(3)-O(11)	2.753(4)	Ba(3)-O(11)#1	2.753(4)
Ba(2)-O(8)#1	2.845(3)	Ba(2)-O(1)#5	2.868(3)
Ba(2)-O(4)#2	2.882(3)	Ba(2)-O(7)#1	2.932(3)
Ba(2)-O(2)#5	3.106(3)	Ba(2)-O(6)#6	3.190(3)
Ba(2)-O(6)	2.720(3)	Ba(2)-O(3)#2	2.839(3)
Ba(2)-O(5)#6	2.745(3)	Ba(2)-O(12)#7	2.900(5)
Ba(2)-O(10)	3.014(5)	Ba(1)-O(1)#8	2.772(3)
Ba(1)-O(1)#9	2.772(3)	Ba(1)-O(7)#10	2.835(3)
Ba(1)-O(7)#2	2.835(3)	Ba(1)-O(5)	2.592(3)
Ba(1)-O(5)#11	2.592(3)	Ba(1)-O(9)	2.729(7)
O(8)-Ba(3)-O(8)#1	83.00(12)	O(8)-Ba(3)-O(4)#3	72.34(8)
O(8)#1-Ba(3)-O(4)#2	72.34(8)	O(8)-Ba(3)-O(4)#2	85.83(8)
O(8)#1-Ba(3)-O(4)#3	85.83(8)	O(8)-Ba(3)-O(2)#4	65.95(9)
O(8)#1-Ba(3)-O(2)#5	65.95(9)	O(8)-Ba(3)-O(2)#5	147.18(8)
O(8)#1-Ba(3)-O(2)#4	147.18(9)	O(8)#1-Ba(3)-O(11)	119.60(11)
O(8)-Ba(3)-O(11)	136.70(11)	O(8)-Ba(3)-O(11)#1	119.60(11)
O(8)#1-Ba(3)-O(11)#1	136.70(11)	O(4)#2-Ba(3)-O(4)#3	150.92(12)
O(4)#3-Ba(3)-O(2)#4	75.18(9)	O(4)#3-Ba(3)-O(2)#5	113.63(9)
O(4)#2-Ba(3)-O(2)#4	113.63(9)	O(4)#2-Ba(3)-O(2)#5	75.18(9)
O(4)#2-Ba(3)-O(11)	134.32(12)	O(4)#3-Ba(3)-O(11)#1	134.32(12)
O(4)#3-Ba(3)-O(11)	73.19(13)	O(4)#2-Ba(3)-O(11)#1	73.19(13)
O(2)#5-Ba(3)-O(2)#4	146.41(12)	O(11)#1-Ba(3)-O(2)#4	72.14(11)
O(11)#1-Ba(3)-O(2)#5	80.52(11)	O(11)-Ba(3)-O(2)#4	80.52(11)
O(11)-Ba(3)-O(2)#5	72.13(11)	O(11)-Ba(3)-O(11)#1	70.7(2)
O(8)#1-Ba(2)-O(1)#5	74.44(9)	O(8)#1-Ba(2)-O(4)#2	68.74(8)
O(8)#1-Ba(2)-O(7)#1	45.13(8)	O(8)#1-Ba(2)-O(2)#5	60.93(9)
O(8)#1-Ba(2)-O(6)#6	129.96(8)	O(8)#1-Ba(2)-O(12)#7	151.45(15)
O(8)#1-Ba(2)-O(10)	140.27(14)	O(1)#5-Ba(2)-O(4)#2	112.60(8)
O(1)#5-Ba(2)-O(7)#1	64.16(9)	O(1)#5-Ba(2)-O(2)#5	43.57(8)
O(1)#5-Ba(2)-O(6)#6	110.18(8)	O(1)#5-Ba(2)-O(10)	143.55(14)
O(1)#5-Ba(2)-O(12)#7	80.00(15)	O(4)#2-Ba(2)-O(6)#6	136.84(8)
O(4)#2-Ba(2)-O(7)#1	113.07(8)	O(4)#2-Ba(2)-O(2)#5	69.21(8)
O(4)#2-Ba(2)-O(12)#7	111.03(12)	O(4)#2-Ba(2)-O(10)	81.32(13)
O(7)#1-Ba(2)-O(2)#5	84.76(9)	O(7)#1-Ba(2)-O(6)#6	90.37(9)
O(7)#1-Ba(2)-O(10)	143.31(12)	O(2)#5-Ba(2)-O(6)#6	152.13(7)
O(6)-Ba(2)-O(8)#1	74.12(9)	O(6)-Ba(2)-O(1)#5	138.04(10)
O(6)-Ba(2)-O(4)#2	80.43(9)	O(6)-Ba(2)-O(7)#1	73.99(10)
O(6)-Ba(2)-O(2)#5	132.16(9)	O(6)-Ba(2)-O(6)#6	71.68(9)
O(6)-Ba(2)-O(3)#2	111.66(10)	O(6)-Ba(2)-O(5)#6	99.84(10)
O(6)-Ba(2)-O(12)#7	134.42(15)	O(6)-Ba(2)-O(10)	75.69(13)
O(3)#2-Ba(2)-O(8)#1	108.43(10)	O(3)#2-Ba(2)-O(1)#5	104.19(10)

O(3)#2-Ba(2)-O(4)#2	45.32(9)	O(3)#2-Ba(2)-O(7)#1	151.99(10)
O(3)#2-Ba(2)-O(2)#5	71.21(11)	O(3)#2-Ba(2)-O(6)#6	117.59(11)
O(3)#2-Ba(2)-O(12)#7	65.72(12)	O(3)#2-Ba(2)-O(10)	60.76(13)
O(5)#6-Ba(2)-O(8)#1	112.20(9)	O(5)#6-Ba(2)-O(1)#5	67.81(9)
O(5)#6-Ba(2)-O(4)#2	179.05(9)	O(5)#6-Ba(2)-O(7)#1	67.87(9)
O(5)#6-Ba(2)-O(2)#5	111.13(8)	O(5)#6-Ba(2)-O(6)#6	42.64(8)
O(5)#6-Ba(2)-O(3)#2	133.84(10)	O(5)#6-Ba(2)-O(12)#7	68.13(13)
O(5)#6-Ba(2)-O(10)	97.86(13)	O(12)#7-Ba(2)-O(7)#1	130.96(12)
O(12)#7-Ba(2)-O(2)#5	91.67(14)	O(12)#7-Ba(2)-O(6)#6	71.03(13)
O(12)#7-Ba(2)-O(10)	63.58(17)	O(10)-Ba(2)-O(2)#5	131.49(12)
O(10)-Ba(2)-O(6)#6	60.53(12)	O(1)#8-Ba(1)-O(1)#9	86.03(12)
O(1)#8-Ba(1)-O(7)#10	148.90(9)	O(1)#8-Ba(1)-O(7)#2	66.65(9)
O(1)#9-Ba(1)-O(7)#10	66.65(9)	O(1)#9-Ba(1)-O(7)#2	148.90(9)
O(7)#10-Ba(1)-O(7)#2	143.33(12)	O(5)-Ba(1)-O(1)#9	71.37(10)
O(5)#11-Ba(1)-O(1)#8	71.37(10)	O(5)-Ba(1)-O(1)#8	114.97(10)
O(5)#11-Ba(1)-O(1)#9	114.97(10)	O(5)#11-Ba(1)-O(7)#2	71.39(9)
O(5)#11-Ba(1)-O(7)#10	105.96(9)	O(5)-Ba(1)-O(7)#10	71.39(9)
O(5)-Ba(1)-O(7)#2	105.96(9)	O(5)-Ba(1)-O(5)#11	171.95(16)
O(5)#11-Ba(1)-O(9)	85.98(8)	O(5)-Ba(1)-O(9)	85.97(8)
O(9)-Ba(1)-O(1)#9	136.98(6)	O(9)-Ba(1)-O(1)#8	136.98(6)
O(9)-Ba(1)-O(7)#10	71.67(6)	O(9)-Ba(1)-O(7)#2	71.67(6)
Symmetrical codes: #1: -x+1/2, y, -z+1/2; #2: -x+1, -y+1, -z+1; #3: x-1/2, -y+1, z-1/2; #4: x, y-1, z; #5: -x+1/2, y-1, -z+1/2; #6: -x, -y+1, -z+1; #7: x-1, y-1, z; #8: -x+1, -y+2, -z+1; #9: x-1/2, -y+2, z+1/2; #10: x-1/2, -y+1, z+1/2; #11: -x+1/2, y, -z+3/2; #12: x+1/2, -y+1, z+1/2; #13: -x+1/2, y+1, -z+1/2; #14: x, y+1, z; #15: x+1, y+1, z.			
4(Cd)			
Cd(1)-O(1)#1	2.309(2)	Cd(1)-O(1)	2.420(2)
Cd(1)-O(3)#2	2.280(2)	Cd(1)-O(7)#3	2.369(2)
Cd(1)-N(1)	2.428(3)	Cd(2)-O(4)#2	2.326(2)
Cd(2)-O(4)#5	2.326(2)	Cd(2)-O(9)#4	2.335(3)
Cd(2)-O(9)	2.335(3)	O(1)#1-Cd(1)-O(1)	73.60(8)
O(1)#1-Cd(1)-O(7)#3	90.76(10)	O(1)-Cd(1)-N(1)	69.36(7)
O(1)#1-Cd(1)-N(1)	142.65(7)	O(3)#2-Cd(1)-O(1)	79.65(8)
O(3)#2-Cd(1)-O(1)#1	90.16(10)	O(3)#2-Cd(1)-O(7)#3	170.34(8)
O(3)#2-Cd(1)-N(1)	87.86(9)	O(7)#3-Cd(1)-O(1)	91.39(9)
O(7)#3-Cd(1)-N(1)	85.58(9)	O(4)#5-Cd(2)-O(4)#2	180.00(10)
O(4)#5-Cd(2)-O(9)#4	89.23(11)	O(4)#2-Cd(2)-O(9)	89.23(11)
O(4)#2-Cd(2)-O(9)#4	90.77(11)	O(4)#5-Cd(2)-O(9)	90.77(11)
Symmetrical codes: #1: -x+1, -y+1, -z; #2: -x+3/2, y+1/2, -z+1/2; #3: -x+1, -y, -z; #4: -x+2, -y+1, -z; #5: x+1/2, -y+1/2, z-1/2; #6: -x+3/2, y-1/2, -z+1/2.			
5(Cu)			
Cu(1)-O(2)#1	1.942(3)	Cu(1)-O(1)	1.955(3)
Cu(1)-O(7)#2	1.964(3)	Cu(1)-O(8)#3	1.969(3)

Cu(1)-O(10)	2.112(3)	Cu(2)-O(4)	1.895(3)
Cu(2)-O(5)#4	1.937(3)	Cu(2)-O(9)	1.948(3)
Cu(2)-N(2)#4	2.029(3)	O(5)-Cu(2)#4	1.937(3)
O(2)-Cu(1)#1	1.942(3)	O(8)-Cu(1)#5	1.969(3)
N(2)-Cu(2)#4	2.029(3)	O(7)-Cu(1)#2	1.964(3)
O(2)#1-Cu(1)-O(1)	167.74(13)	O(2)#1-Cu(1)-O(7)#2	89.31(17)
O(1)-Cu(1)-O(7)#2	89.31(18)	O(2)#1-Cu(1)-O(8)#3	89.42(16)
O(1)-Cu(1)-O(8)#3	89.38(16)	O(7)#2-Cu(1)-O(8)#3	167.95(12)
O(2)#1-Cu(1)-O(10)	100.29(14)	O(1)-Cu(1)-O(10)	91.96(14)
O(7)#2-Cu(1)-O(10)	98.81(13)	O(8)#3-Cu(1)-O(10)	93.20(13)
O(4)-Cu(2)-O(5)#4	176.24(12)	O(4)-Cu(2)-O(9)	94.48(11)
O(5)#4-Cu(2)-O(9)	84.61(11)	O(4)-Cu(2)-N(2)#4	98.25(12)
O(5)#4-Cu(2)-N(2)#4	81.92(12)	O(9)-Cu(2)-N(2)#4	162.65(12)
Symmetrical codes: #1: -x+1, -y+3/2, -z+1/2; #2: -x+5/4, -y+5/4, z; #3: x-1/4, y+1/4, -z+1/2; #4: -x+3/4, y, -z+3/4; #5: x+1/4, y-1/4, -z+1/2.			

Table S3 Standard Deviation (δ) calculation for the detection of Fe^{3+} for **1**(Zn).

Test	Fluorescence intensity (nm)
1	5506.319
2	5507.293
3	5507.033
4	5506.435
5	5506.632
6	5507.155
7	5506.914
8	5507.332
9	5507.139
10	5507.265
average	5506.952
Standard deviation (δ)	0.367

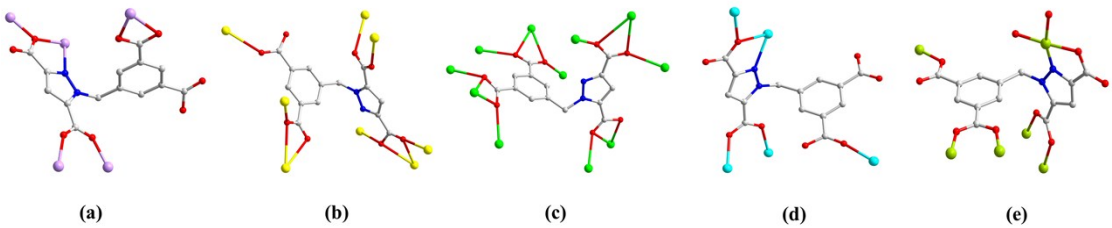

Fig. S1 Coordination modes of H_4L in **1-5**.

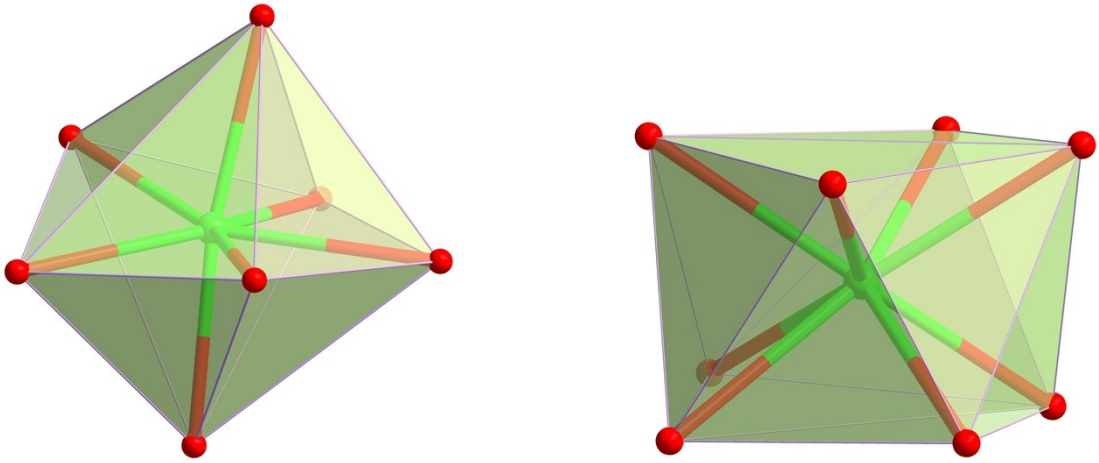

Fig. S2 Coordination arrangement of $Ba^{2+}1$ (a) and $Ba^{2+}3$ (b) ions could be described as a distorted pentagonal bipyramid and distorted prismaid coordination geometry respectively.

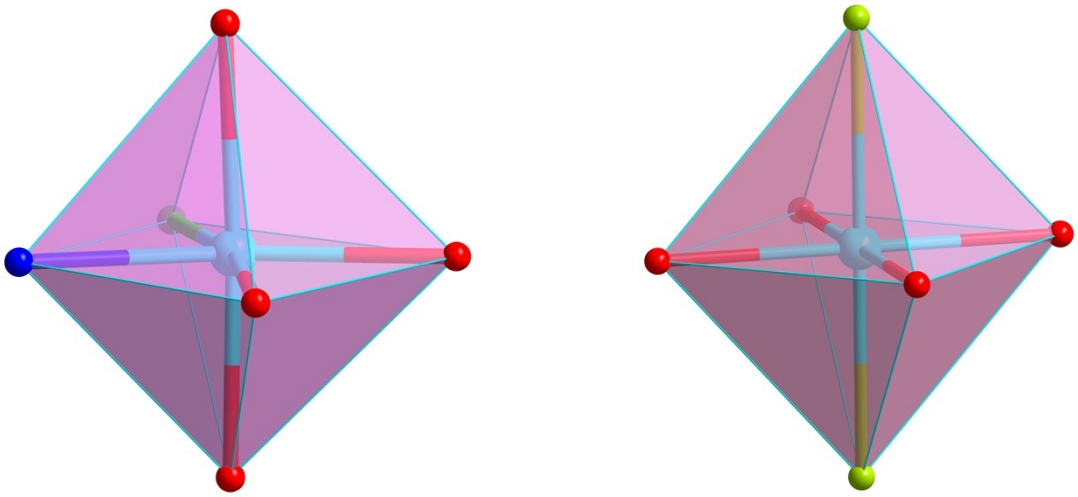

Fig. S3 Coordination arrangement of $Cd^{2+}1$ (a) and $Cd^{2+}2$ (b) ions could be described as a distorted quadrilateral bipyramid and quadrilateral bipyramid coordination geometry respectively.

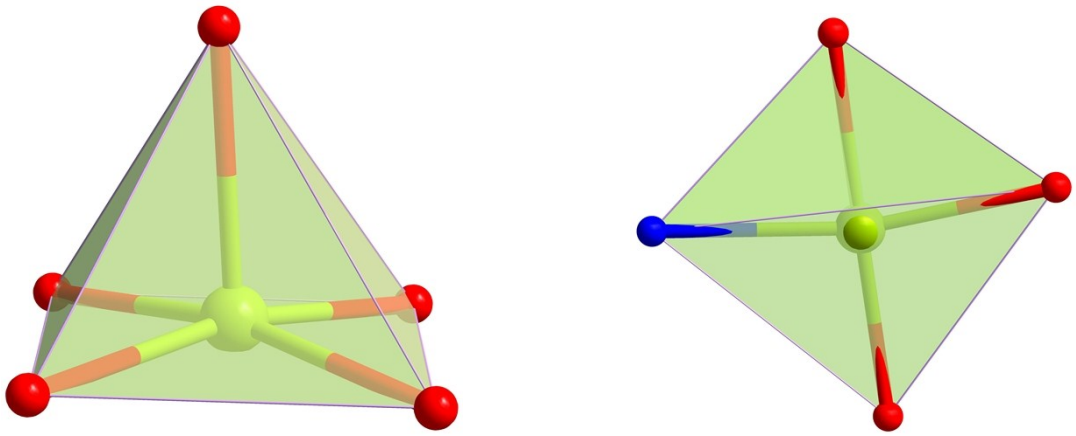

Fig. S4 Coordination arrangement of $Cu^{2+}1$ (a) and $Cu^{2+}2$ (b) ions could be described as a distorted pentagonal pyramid and distorted quadrilateral coordination geometry respectively.

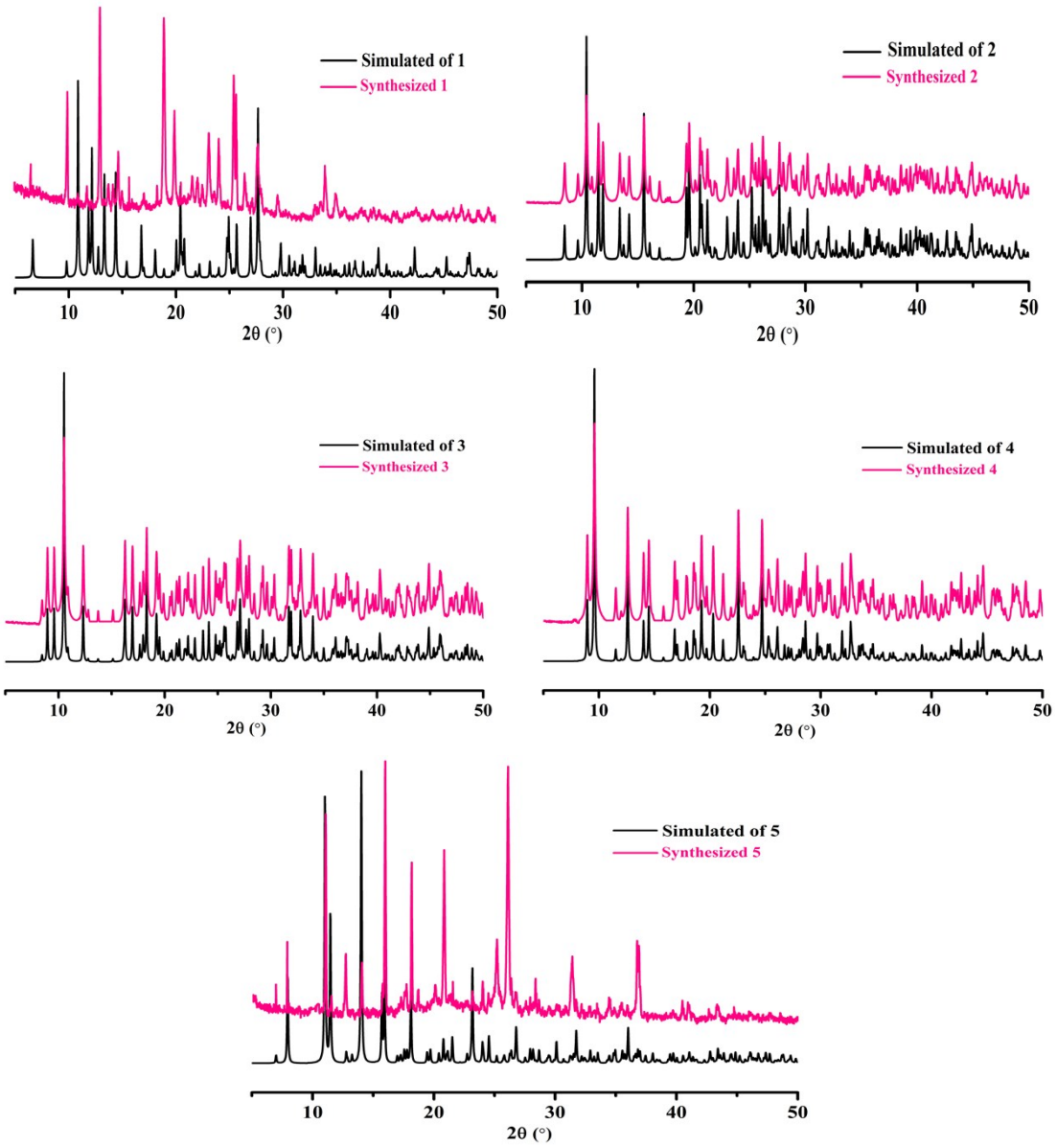

Fig. S5 PXRD patterns of complex **1-5** simulated from the X-ray single-crystal data and as-synthesized products.

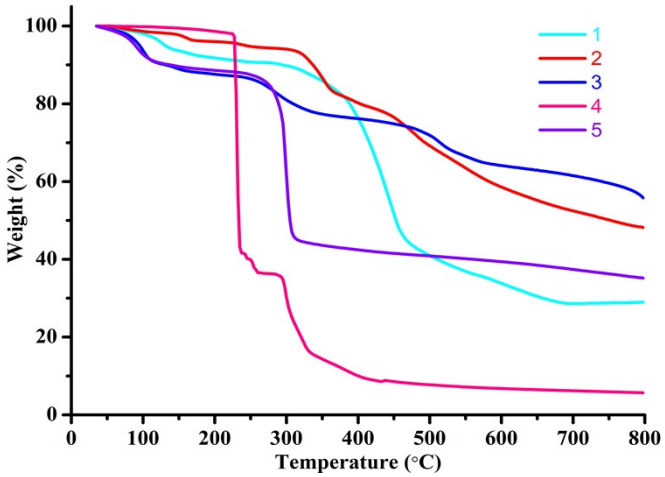

Fig. S6 The TGA curve of complex **1-5**.

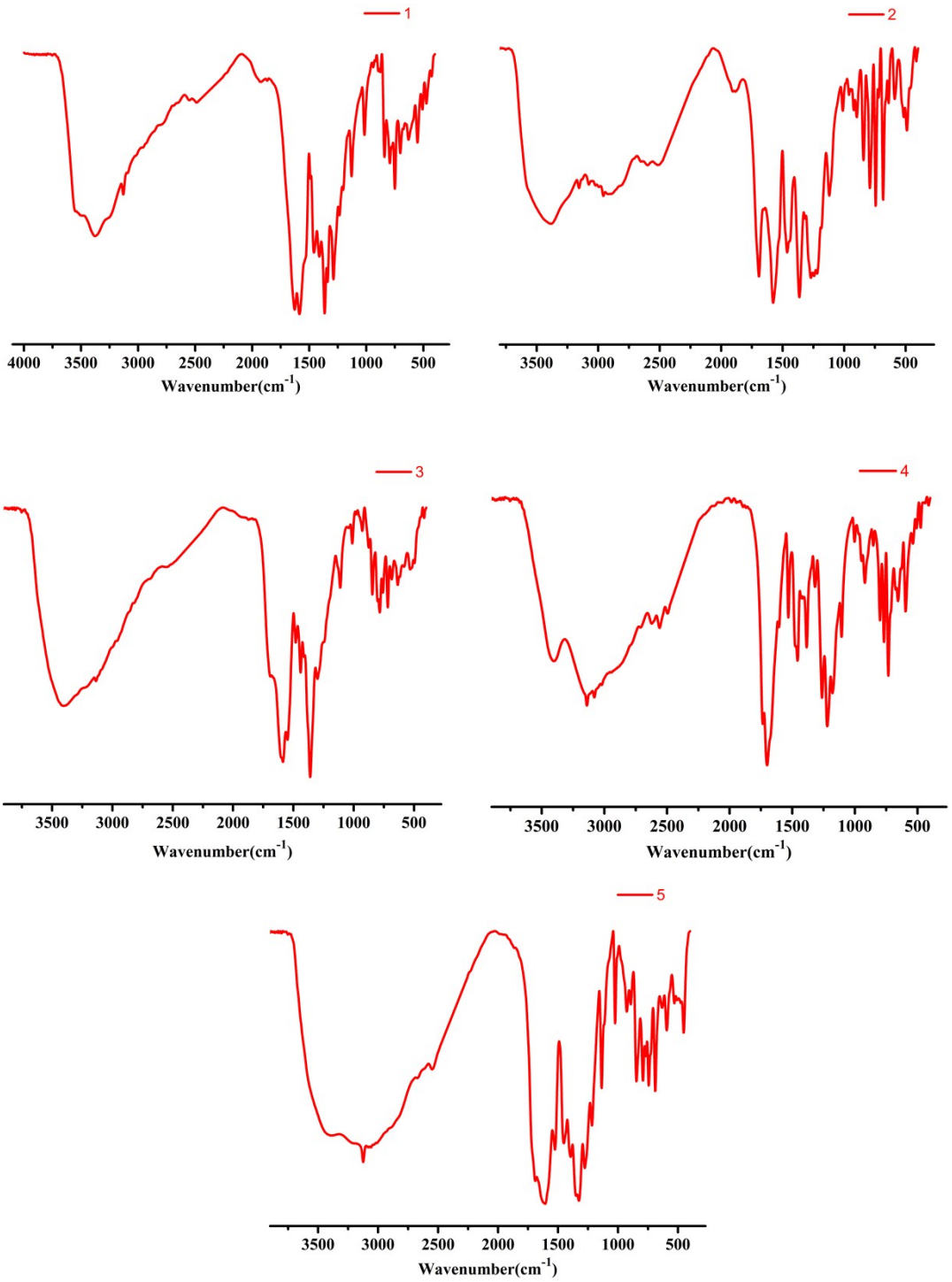

Fig. S7 The FT-IR spectra of complex **1-5**.

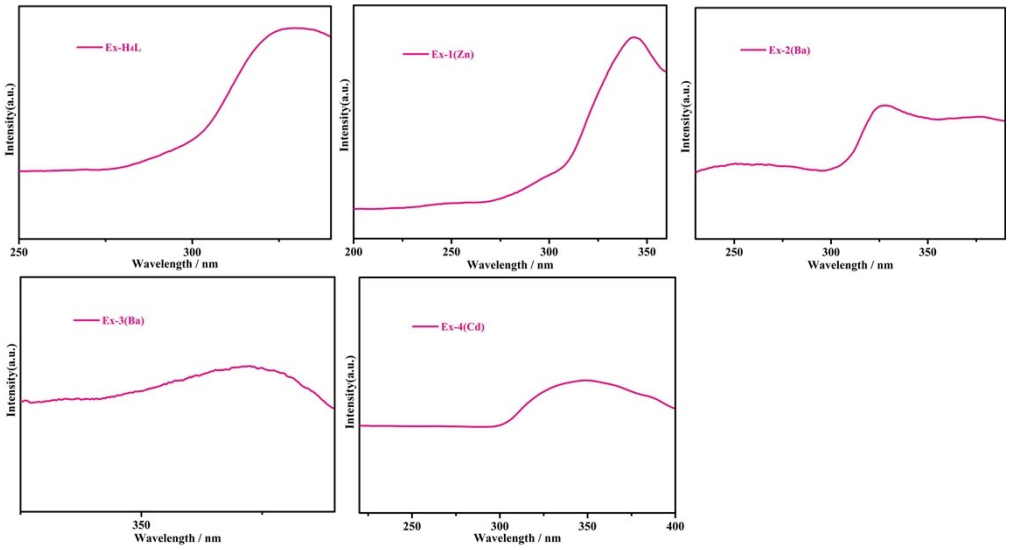

Fig. S8 Solid-state excitation spectra of H_4L ligands and MOFs **1–4**.

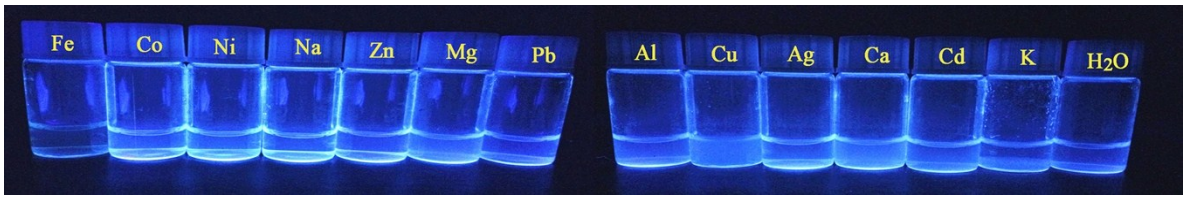

Fig. S9 Pictures of different M^{n+}@**1**(Zn) solutions.

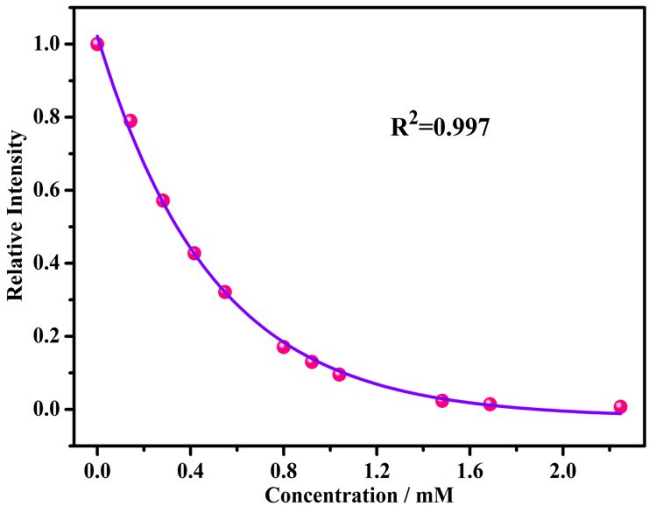

Fig. S10 The linear correlation for the plot of I_0/I vs concentration of Fe^{3+} ions in low concentration range.

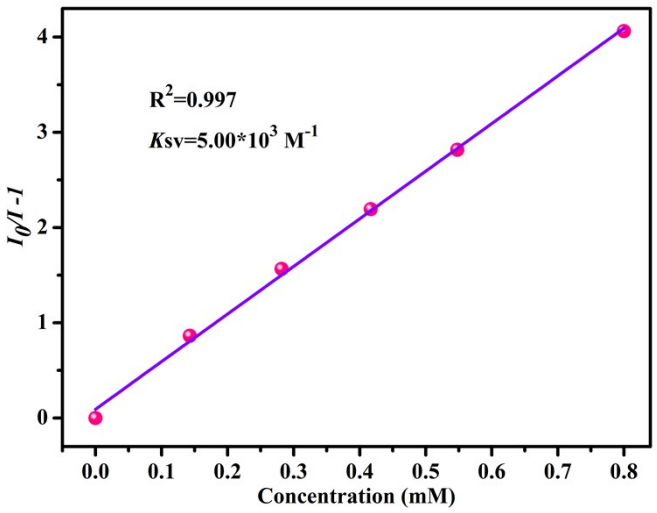

Fig. S11 Quenching efficiency defined by the Stern–Volmer relationship for Fe^{3+} ions.

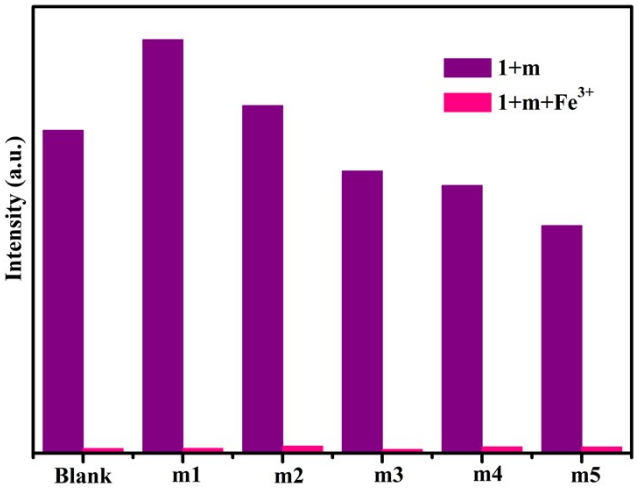

Fig. S12 Luminescence intensity at 407 nm of **1**(Zn) dispersed in water with addition of different mixed ions (10^{-2}M) mixed solution added Fe^{3+} ions (10^{-2} M) (m1: K^{+}/Cd^{2+}; m2: $Ca^{2+}/Ag^{+}/Cd^{2+}$; m3: $Al^{3+}/Pb^{2+}/Cu^{2+}$; m4: $Na^{+}/Co^{2+}/Zn^{2+}$; m5:Mg^{2+}/Ni^{2+}).

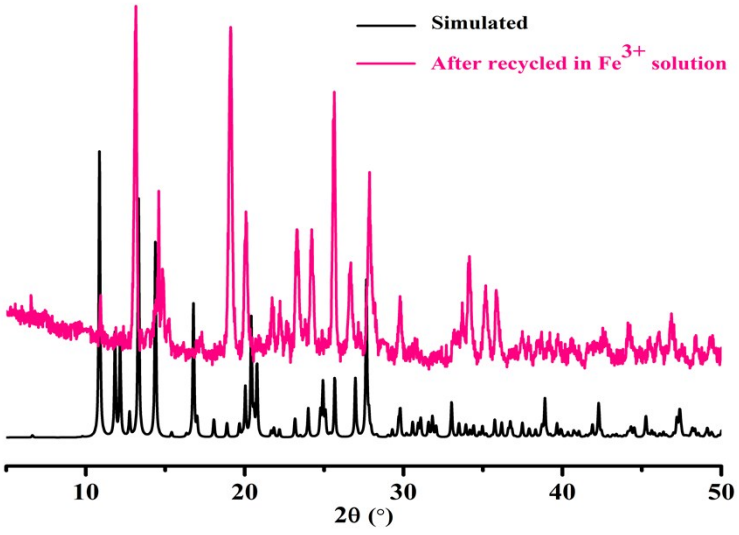

Fig. S13 The PXRD patterns of **1**(Zn) treated by Fe^{3+} aqueous solutions.

Sample	Concentration of Zn^{2+} (ug/mL)
Blank sample (H_2O)	0.0206
Initial solution after immersing in H_2O	0.0318
Final solution after recycle sensing experiment for Fe^{3+}	0.0296

Fig. S14 ICP experiments of **1**(Zn) after immersing in different solution.

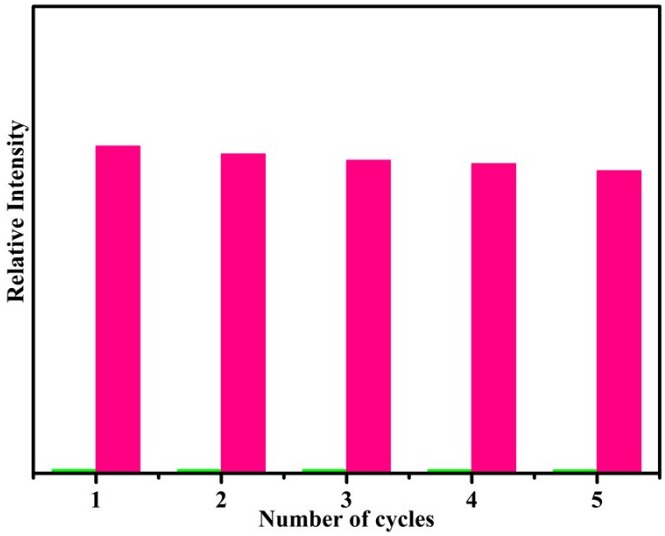

Fig. S15 Luminescent intensity at 407 nm of **1**(Zn) after five recycles in Fe^{3+} solutions (10^{-2} M).

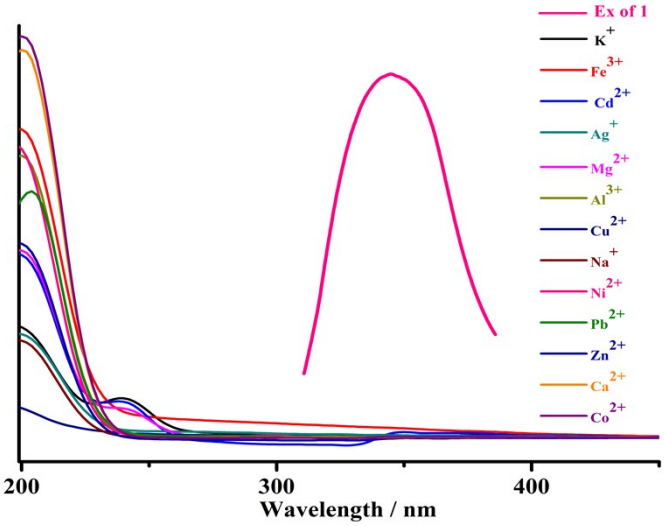

Fig. S16 UV-Vis adsorption spectrum of $M(NO_3)_n$ aqueous solution and the excitation spectrum of **1**(Zn).