Electronic Supplementary Information (ESI) for

Functional Groups Induced Structure Diversities, Photocatalytic, Magnetic and Luminescence Sensing Properties of Four Cobalt(II) Coordination Polymers Based on 1,3,5-Tris(2-methylimidazol-1-yl)benzene

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Table S1 Crystal data and structure refinement parameters of **1–4**

CP	**1**	**2**	**3**	**4**
Formula	$C_{68}H_{58}Br_4Co_4N_{12}O_{21}$	$C_{17}H_{22}CoN_4O_8$	$C_{112}H_{110}Co_5N_{28}O_{30}$	$C_{52}H_{62}Co_3N_{12}O_{24}S_2$
Formula weight	1934.61	469.31	2622.91	1480.04
Crystal system	Monoclinic	Orthorhombic	Orthorhombic	Monoclinic
Space group	*C*2/*c*	*Ama*2	$Pmn2_1$	*C*2/*c*
a (Å)	32.816(12)	33.563(19)	52.460(7)	19.470(3)
b (Å)	9.466(5)	12.204(4)	7.2110(10)	11.530(15)
c (Å)	33.049(13)	10.119(4)	19.470(3)	29.730(4)
α (°)	90	90	90	90
β (°)	118.73(3)	90	90	107.150(9)
γ (°)	90	90	90	90
V(Å^3)	9002(7)	4145(3)	7365.3(18)	6377(8)
Z	8	8	2	4
D_{calcd} (Mg/m^3)	1.361	1.273	1.166	1.391
μ(mm^{-1})	2.560	0.854	0.621	0.908
Temperature (K)	293(2)	293(2)	173(2)	293(2)
F(000)	3664	1624	2666	2732
R_{int}	0.0651	0.0333	0.0246	0.0674
R_1 [$I > 2\sigma(I)$][a]	0.0338	0.0374	0.0352	0.0803
wR_2 [$I > 2\sigma(I)$][b]	0.0780	0.1016	0.0700	0.1981
Gof	1.044	1.057	1.099	1.174

$R_1 = \Sigma| |F_o|-|F_c| |/\Sigma|F_o|$. $\omega R_2 = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths (Å) and angles (°) for **1–4**

CP **1**							
Co(1)-O(1)	2.394(2)	Co(1)-O(2)	2.0154(18)	Co(1)-N(1)	2.058(2)	Co(1)-O(1)$^{\#1}$	2.394(2)
Co(1)-O(2)$^{\#1}$	2.0155(18)	Co(1)-N(1)$^{\#1}$	2.058(2)	Co(2)-O(3)	2.0636(16)	Co(2)-O(5)	2.0037(16)
Co(2)-O(3)$^{\#2}$	2.0635(16)	Co(2)-O(5)$^{\#2}$	2.0038(16)	Co(2)-O(8)$^{\#3}$	2.1749(17)	Co(2)-O(8)$^{\#4}$	2.1749(17)
Co(3)-O(4)	2.0788(17)	Co(3)-O(6)$^{\#2}$	2.0868(17)	Co(3)-O(8)$^{\#3}$	2.0880(16)	Co(3)-N(4)$^{\#6}$	2.125(2)
Co(3)-N(6)$^{\#5}$	2.072(2)						
O(1)-Co(1)-O(1)$^{\#1}$	94.21(13)	O(2)-Co(1)-O(1)	58.57(8)	O(2)-Co(1)-O(1)$^{\#1}$	91.75(8)	O(2)-Co(1)-O(2)$^{\#1}$	137.73(11)
O(2)-Co(1)-N(1)	116.64(8)	O(2)-Co(1)-N(1)$^{\#1}$	92.87(8)	O(2)$^{\#1}$-Co(1)-O(1)	91.75(8)	O(2)$^{\#1}$-Co(1)-O(1)$^{\#1}$	58.57(8)
O(2)$^{\#1}$-Co(1)-N(1)	92.87(8)	N(1)-Co(1)-O(1)	175.10(7)	N(1)-Co(1)-O(1)$^{\#1}$	86.81(10)	N(1)-Co(1)-N(1)$^{\#1}$	92.57(13)
N(1)$^{\#1}$-Co(1)-O(1)	86.81(10)	N(1)$^{\#1}$-Co(1)-O(1)$^{\#1}$	175.10(7)	O(2)$^{\#1}$-Co(1)-N(1)$^{\#1}$	116.64(8)	O(3)-Co(2)-O(8)$^{\#3}$	90.02(7)
O(3)-Co(2)-O(8)$^{\#4}$	89.98(7)	O(3)$^{\#2}$-Co(2)-O(8)$^{\#3}$	89.98(7)	O(3)$^{\#2}$-Co(2)-O(8)$^{\#4}$	90.02(7)	O(5)-Co(2)-O(3)	84.63(6)
O(5)-Co(2)-O(3)$^{\#2}$	95.37(6)	O(5)-Co(2)-O(8)#3	91.53(6)	O(5)-Co(2)-O(8)$^{\#4}$	88.47(6)	O(5)$^{\#2}$-Co(2)-O(3)	95.37(6)
O(5)$^{\#2}$-Co(2)-O(3)$^{\#2}$	84.63(6)	O(5)$^{\#2}$-Co(2)-O(8)$^{\#3}$	88.47(6)	O(5)$^{\#2}$-Co(2)-O(8)$^{\#4}$	91.53(6)	O(4)-Co(3)-O(6)$^{\#2}$	101.75(7)
O(4)-Co(3)-O(8)$^{\#3}$	86.40(7)	O(4)-Co(3)-N(4)$^{\#6}$	170.29(7)	O(6)$^{\#2}$-Co(3)-O(8)$^{\#3}$	105.46(6)	O(6)$^{\#2}$-Co(3)-N(4)$^{\#6}$	87.85(7)
O(8)$^{\#3}$-Co(3)-N(4)$^{\#6}$	89.64(7)	N(6)$^{\#5}$-Co(3)-O(4)	83.92(7)	N(6)$^{\#5}$-Co(3)-O(6)$^{\#2}$	91.06(7)	N(6)$^{\#5}$-Co(3)-O(8)$^{\#3}$	162.27(7)
N(6)$^{\#5}$-Co(3)-N(4)$^{\#6}$	97.50(8)						
Symmetry codes: #1 -x, y, -z+1/2; #2 -x+1/2, -y+1/2, -z+1/2; #3 -x+1/2, -y+3/2, -z+1/2; #4 x, y-1, z; #5 x+1/2, y+1/2, z+1/2; #6 -x+1/2, -y-1/2, -z+1/2.							
CP **2**							
Co(1)-O(4)	2.011(4)	Co(1)-N(2)	2.031(3)	Co(1)-O(2)$^{\#1}$	2.002(4)	Co(1)-N(1)$^{\#2}$	2.093(3)
O(4)-Co(1)-N(2)	117.94(19)	O(4)-Co(1)-N(1)$^{\#2}$	107.11(17)	N(2)-Co(1)-N(1)$^{\#2}$	115.58(12)	O(2)$^{\#1}$-Co(1)-O(4)	95.05(10)
O(2)$^{\#1}$-Co(1)-N(2)	114.36(19)	O(2)$^{\#1}$-Co(1)-N(1)$^{\#2}$	104.19(17)				
Symmetry codes: #1 x, y, z+1; #2 x, y+1/2, z+1/2.							
CP **3**							
Co(1)-O(1)	2.105(2)	Co(1)-O(2)	2.267(2)	Co(1)-O(6)	2.260(2)	Co(1)-O(7)	2.085(2)
Co(1)-N(2)	2.055(2)	Co(1)-N(6)$^{\#2}$	2.060(3)	Co(2)-O(4)	1.983(2)	Co(2)-O(3)	2.330(2)
Co(2)-N(8)	2.017(3)	Co(2)-N(4)$^{\#3}$	2.081(3)	Co(2)-N(14)$^{\#4}$	2.085(3)	Co(3)-O(8)	2.022(2)
Co(3)-O(8)$^{\#1}$	2.022(2)	Co(3)-N(10)	2.062(4)	Co(3)-N(12)	1.978(4)		
O(1)-Co(1)-O(6)	93.37(8)	O(1)-Co(1)-O(2)	59.89(8)	O(6)-Co(1)-O(2)	85.67(8)	O(7)-Co(1)-O(2)	92.96(8)
O(7)-Co(1)-O(1)	144.52(8)	O(7)-Co(1)-O(6)	59.84(7)	N(2)-Co(1)-O(2)	90.50(9)	N(2)-Co(1)-O(1)	106.22(9)
N(2)-Co(1)-O(6)	154.76(9)	N(2)-Co(1)-O(7)	95.55(9)	N(2)-Co(1)-N(6)$^{\#2}$	103.27(10)	N(6)$^{\#2}$-Co(1)-O(1)	93.47(10)
N(6)$^{\#2}$-Co(1)-O(2)	152.80(9)	N(6)$^{\#2}$-Co(1)-O(6)	90.98(9)	N(6)$^{\#2}$-Co(1)-O(7)	108.63(9)	O(4)-Co(2)-O(3)	60.02(8)
O(4)-Co(2)-N(8)	110.31(10)	O(4)-Co(2)-N(4)$^{\#3}$	122.91(10)	O(4)-Co(2)-N(14)$^{\#4}$	100.99(10)	N(8)-Co(2)-N(4)$^{\#3}$	114.14(11)
N(8)-Co(2)-N(14)$^{\#4}$	104.15(10)	N(8)-Co(2)-O(3)	83.87(9)	N(4)$^{\#3}$-Co(2)-O(3)	91.00(9)	N(4)$^{\#3}$-Co(2)-N(14)$^{\#4}$	100.98(11)
N(14)$^{\#4}$-Co(2)-O(3)	161.01(9)	O(8)-Co(3)-O(8)$^{\#1}$	108.51(12)	O(8)-Co(3)-N(10)	95.77(9)	N(12)-Co(3)-O(8)	104.24(9)
N(12)-Co(3)-N(10)	145.17(16)	N(12)-Co(3)-O(8)$^{\#1}$	104.24(9)	O(8)$^{\#1}$-Co(3)-N(10)	95.77(9)		
Symmetry codes: #1 -x, y, z; #2 -x+1/2, -y, z+1/2; #3 -x+1/2, -y, z-1/2; #4 x, y, z-1.							
CP **4**							
Co(1)-O(2)	1.924(5)	Co(1)-N(1)	1.999(5)	Co(1)-N(3)$^{\#1}$	2.004(5)	Co(1)-N(6)$^{\#2}$	2.014(5)
Co(2)-O(3)	2.194(7)	Co(2)-O(4)	2.117(5)	Co(2)-O(8)	2.043(8)	Co(2)-O(3)$^{\#3}$	2.194(7)
Co(2)-O(4)$^{\#3}$	2.117(5)	Co(2)-O(8)$^{\#3}$	2.043(8)				
O(2)-Co(1)-N(1)	118.2(2)	O(2)-Co(1)-N(3)$^{\#1}$	115.6(2)	O(2)-Co(1)-N(6)$^{\#2}$	103.8(2)	N(1)-Co(1)-N(3)$^{\#1}$	110.8(2)
N(1)-Co(1)-N(6)$^{\#2}$	105.8(2)	N(3)$^{\#1}$-Co(1)-N(6)$^{\#2}$	100.1(2)	O(4)-Co(2)-O(3)	61.3(2)	O(8)-Co(2)-O(3)	89.9(4)
O(4)-Co(2)-O(3)$^{\#3}$	118.7(2)	O(4)$^{\#3}$-Co(2)-O(3)	118.7(2)	O(4)$^{\#3}$-Co(2)-O(3)$^{\#3}$	61.3(2)	O(8)-Co(2)-O(4)	91.8(3)
O(8)-Co(2)-O(3)$^{\#3}$	90.1(4)	O(8)-Co(2)-O(4)$^{\#3}$	88.2(3)	O(8)$^{\#3}$-Co(2)-O(3)	90.1(4)	O(8)$^{\#3}$-Co(2)-O(4)	88.2(3)
O(8)$^{\#3}$-Co(2)-O(3)$^{\#3}$	89.9(4)	O(8)$^{\#3}$-Co(2)-O(4)$^{\#3}$	91.8(3)				
Symmetry codes: #1 x-1/2, -y, z; #2 x, y-1, z; #3 -x+1, -y, -z+1.							

Table S3 N-H···O hydrogen bonds in **2**

D-H···A	d(H···A)/Å	d(D···A)/Å	∠(D–H···A)/°
N1-H1AA···O2	2.26	3.013(6)	142
N1-H1AB···O4	2.23	2.980(6)	141

Table S4 Hydrogen bonds in **3**

D-H···A	d(H···A)/Å	d(D···A)/Å	∠(D–H···A)/°
O5-H5B···O2	1.95	2.719(3)	149
O10-H10C···O6	1.93	2.719(3)	154
C23-H23···O14	2.22	3.095(5)	152
C26-H26B···O14	2.47	3.302(5)	142
C31-H31···O13	2.45	3.255(5)	143
C37-H37···O11	2.53	3.179(4)	126
C39-H39···O11	2.40	3.264(4)	151
C52-H52···O8	2.56	3.239(6)	129

Table S5 Hydrogen bonds in **4**

D-H···A	d(H···A)/Å	d(D···A)/Å	∠(D–H···A)/°
O8-H8A···O4	2.48	2.989(13)	115
O8-H8B···O3	2.51	2.997(12)	125
C3-H3···O6	2.46	2.840(13)	105
C9-H9C···O6	2.39	3.262(15)	152
C14-H14···O6	2.23	3.160(11)	174
C23-H23A···O2	2.41	3.262(10)	147

Table S6 Standard deviation and detection limit calculation for Fe^{3+} and $Cr_2O_7^{2-}$ ions in **1**

	Fe^{3+}	$Cr_2O_7^{2-}$
1	513.265040	563.914565
2	513.471239	564.081221
3	513.134660	564.133767
4	513.378433	563.781261
5	513.026512	563.691778
Standard deviation (σ)	0.17943	0.18911
Ksv	1.79×10^4	6.93×10^4
Detection limit (3σ/Ksv)	3.01×10^{-5}	8.19×10^{-6}

Table S7 Standard deviation and detection limit calculation for Fe^{3+} and $Cr_2O_7^{2-}$ ions in **2**

	Fe^{3+}	$Cr_2O_7^{2-}$
1	612.832667	606.678864
2	612.512144	606.831673
3	612.475613	606.412354
4	612.981578	606.521328
5	612.523456	606.971256
Standard deviation (σ)	0.20377	0.20229
Ksv	1.18×10^4	1.36×10^4
Detection limit (3σ/Ksv)	5.18×10^{-5}	4.46×10^{-5}

Table S8 Standard deviation and detection limit calculation for Fe^{3+} and $Cr_2O_7^{2-}$ ions in **3**

	Fe^{3+}	$Cr_2O_7^{2-}$
1	562.047724	553.597770
2	562.178166	553.816231
3	562.423372	553.371456
4	561.945513	553.751585
5	562.321121	553.401584
Standard deviation (σ)	0.19467	0.20037

Ksv	1.51×10^4	3.59×10^4
Detection limit (3σ/Ksv)	3.87×10^{-5}	1.67×10^{-5}

Table S9 Standard deviation and detection limit calculation for Fe^{3+} and $Cr_2O_7^{2-}$ ions in **4**

	Fe^{3+}	$Cr_2O_7^{2-}$
1	476.947351	490.607439
2	476.574783	490.412231
3	476.999332	490.491132
4	477.052179	490.556216
5	476.792177	490.916735
Standard deviation (σ)	0.19304	0.19323
Ksv	1.14×10^4	1.27×10^4
Detection limit (3σ/Ksv)	5.08×10^{-5}	4.56×10^{-5}

Table S10 Comparison of various MOFs sensors for the detection of Fe^{3+} and $Cr_2O_7^{2-}$ ions

	Analyte	MOFs-based fluorescent Materials	Quenching constant (K_{SV}, M^{-1})	Detection Limits (DL)	Media	Ref
1	Fe^{3+}	$[Mg_2(APDA)_2(H_2O)_3]\cdot 5DMA\cdot 5H_2O$	2.06×10^4	152 ppb	DMF	38
2		$\{Eu_2L_3(DMF)\}\cdot 2DMF$	4×10^4	6.62 μM	H_2O	39
3		$[Ag(CIP^-)]$	7.1×10^3	1.2×10^{-6} M	H_2O	40
4		$[Zn(ACA)_4]\cdot CB[6]\cdot[NH_2(CH_3)_2]\cdot 8H_2O$	1.088×10^4	9.5×10^{-7} M	H_2O	41
5		$\{[Eu_2(L)_2(H_2O)_2]\cdot 5H_2O\cdot 6DMAC\}_n$	5941 M	10^{-5} mM	H_2O	42
1	$Cr_2O_7^{2-}$	$[H_2N(CH_3)_2]_2[Zn_2L(HPO_3)_2]$	4.44×10^4	1.09×10^{-3} mM	H_2O	43
2		$[Tb(ppda)(bdc)_{0.5}(C_2H_5OH)(H_2O)]_n$	4.03×10^3	5.0×10^{-5} M	DMF	44
3		$\{[(CH_3)_2NH_2]_2\ [Zn_5\ (TDA)_4TZ)_4]$ □4DMF$\}_n$	6.77×10^3	7.48 μmol L^{-1}	H_2O	45
4		$[Cd_3(cpota)_2(phen)_3]_n\cdot 5nH_2O$	1.21×10^4	3.70×10^{-7} M	H_2O	46
5		$[Zn(NH_2\text{-}bdc)(4,4'\text{-}bpy)]$	7.62×10^3	1.30 μM	H_2O	47
6		$\{[Cd_2L_2(H_2O)_4]\cdot H_2O\}_n$	1.25×10^4	3.7 μM	H_2O	48
7		$\{[Zn_2L_2(H_2O)_4]\cdot H_2O\}_n$	1.77×10^4	2.6 μM	H_2O	

H_2APDA= 4,4′-(4-aminopyridine-3,5-diyl)dibenzoic acid;

L=(6-[1-(4-carboxyphenyl)-1H-1,2,3-triazol-4-yl]nicotinic acid;

HCIP = 4-(4-carboxylphenyl)-2,6-di(4-imidazol-1-yl)phenyl)pyridine;

CB[6]=cucurbit[6]uril, HACA = anthracene-9-carboxylic acid;

H_3L = 4,4'-(((5-carboxy-1,3-phenylene)bis(azanediyl))bis(carbonyl)) dibenzoic acid, DMAC = N,N'-dimethylacetamide

H_2L=2′,3′,5′,6′-tetramethyl-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylic acid;

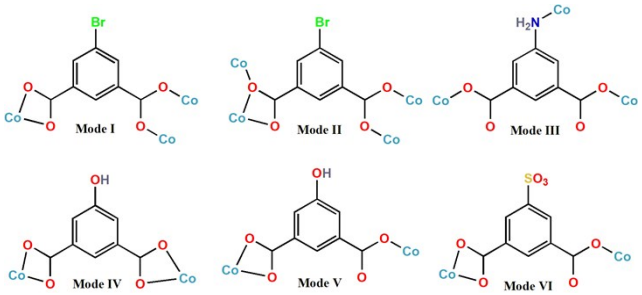
H_2ppda=4-(pyridin-3-yloxy)-phthalic acid, H_2bdc=terephthalic acid;

H_2TDA = thiophene-2,5-dicarboxylic acid, HTZ = 1H-1,2,4-Triazole;

H_3cpota = 2-(4-carboxyphenoxy)terephthalic acid, phen = 1,10-phenanthroline;

NH_2-H_2bdc = 2-amino-1,4-benzenedicarboxylic acid, 4,4'-bpy = 4,4'-bipyridine;

H_2L = 5-(1H-1,2,4-triazol-1-yl)isophthalic acid).



Scheme S1 The coordination modes of functional H_2IPA in **1-4**

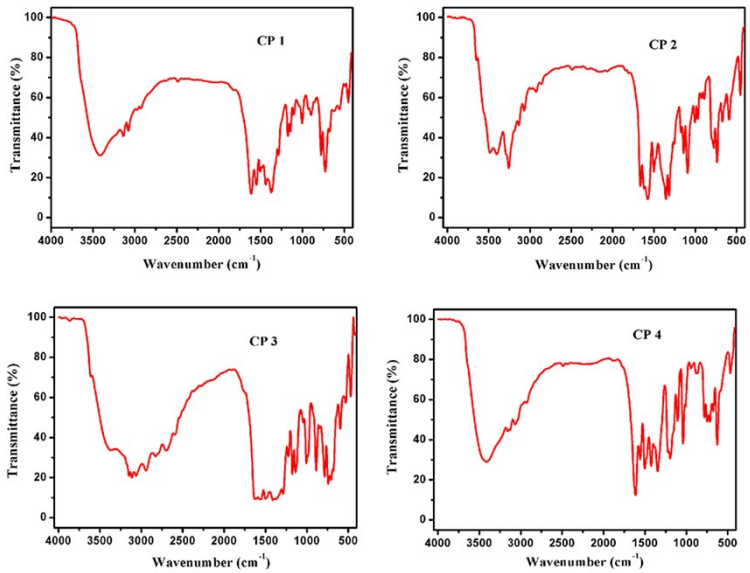


Fig. S1 The IR spectra of **1-4**

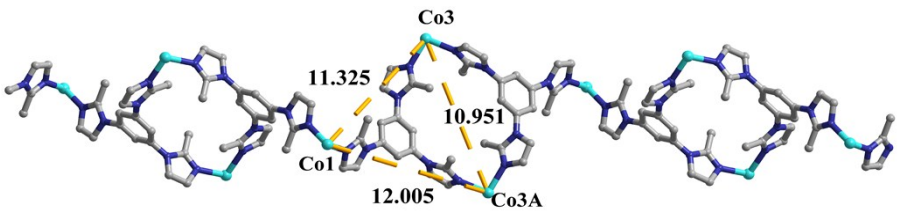


Fig. S2 The 1D $[Co_3(timb)_2]_n$ polymeric loop chain in **1**

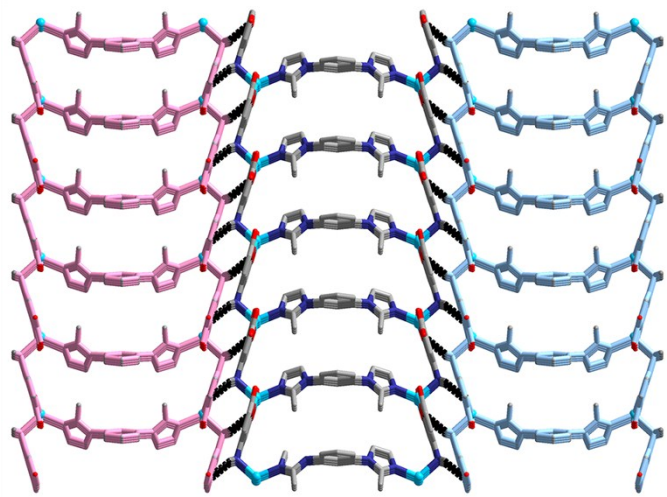


Fig. S3 The 3D supramolecular structure of **2**

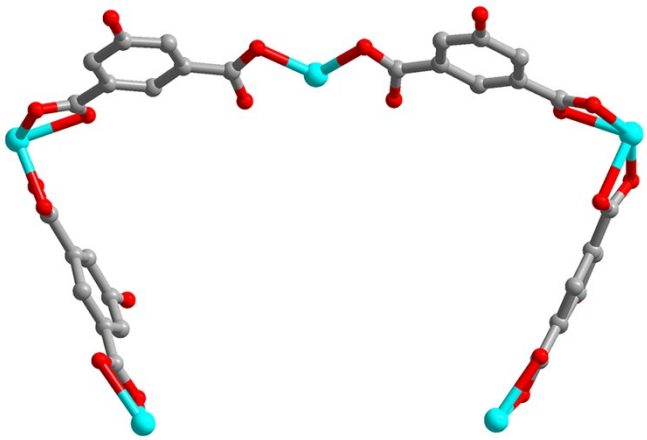


Fig. S4 The crab shape $[Co_5(OH\text{-}IPA)_4]$ motif in **3**

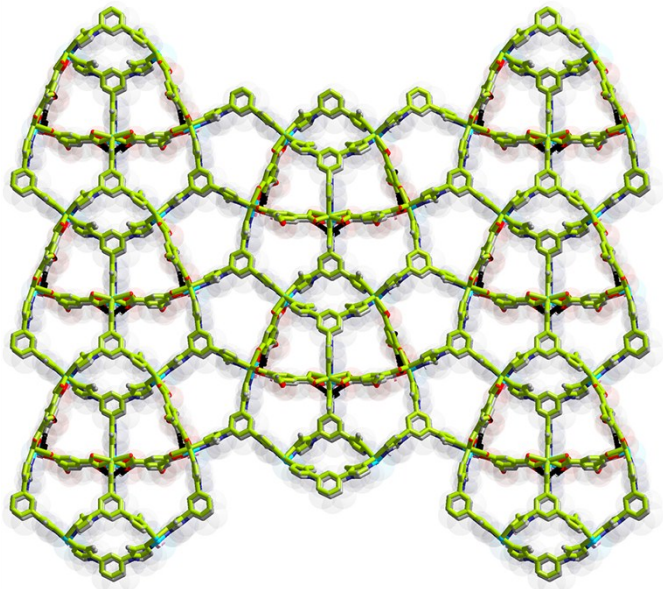


Fig. S5 The 3D supramolecular structure of **3**

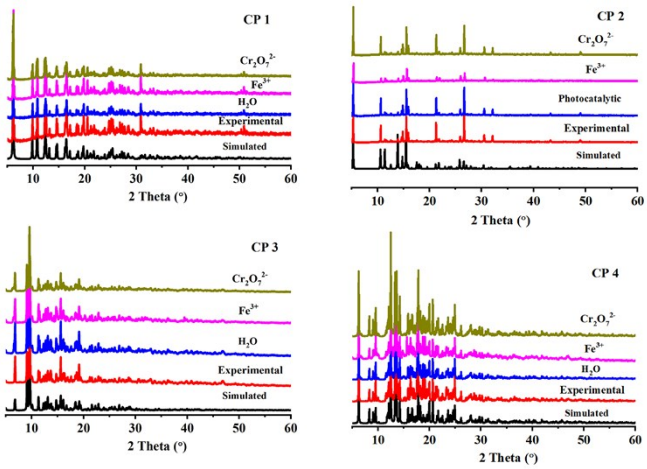


Fig S6 PXRD patterns of **1-4**

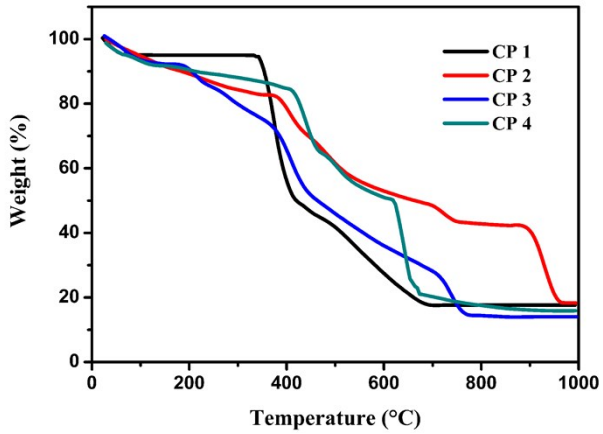


Fig S7 TGA curves for **1**−**4**

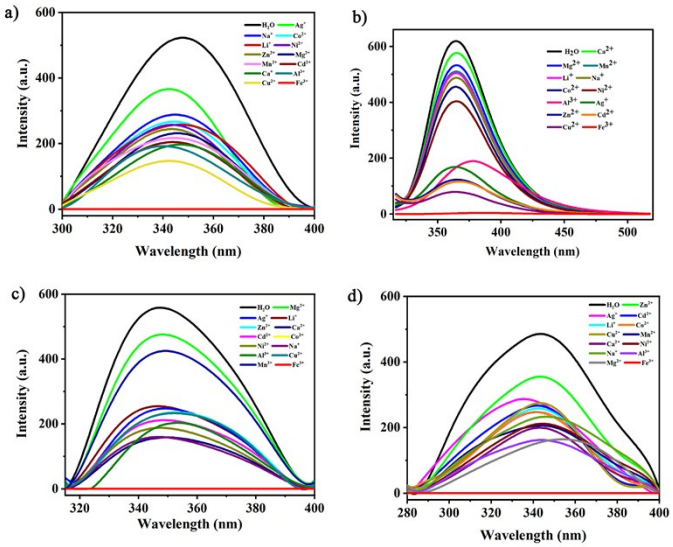


Fig S8 Fluorescence response of **1**(a)**, 2**(b)**, 3**(c) and **4**(d) toward different metal cations in H_2O solution

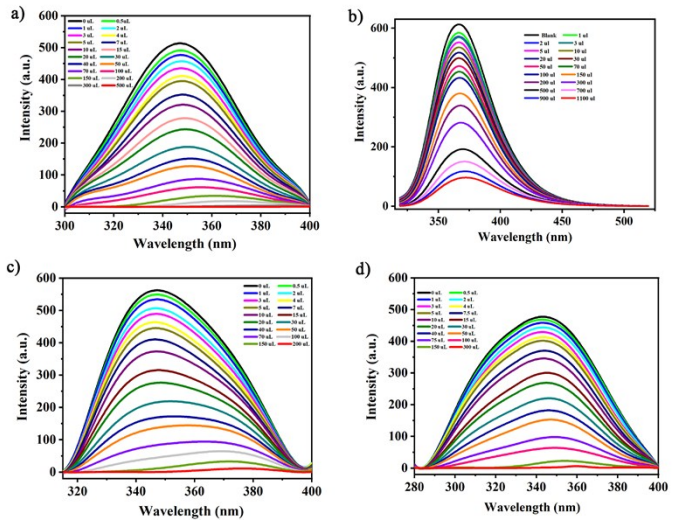


Fig S9 Variation of luminescence intensities of **1**(a)**, 2**(b)**, 3**(c) and **4**(d) titrated with $Fe(NO_3)_3$

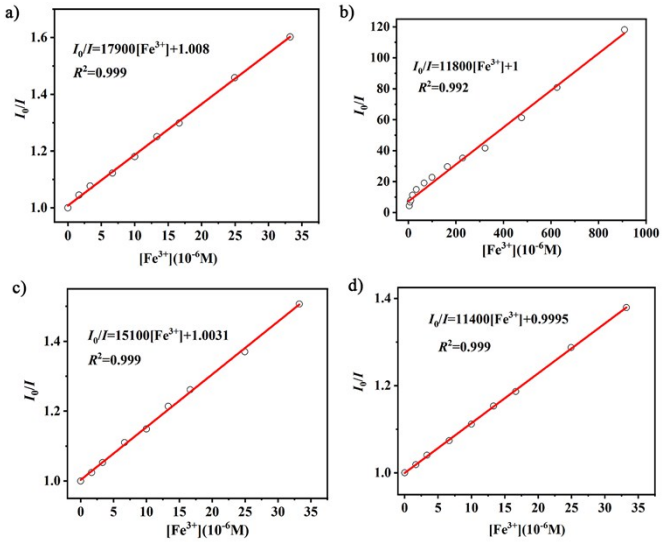


Fig S10 Stern−Volmer plots of Fe^{3+} in **1**(a)**, 2**(b)**, 3**(c) and **4**(d)

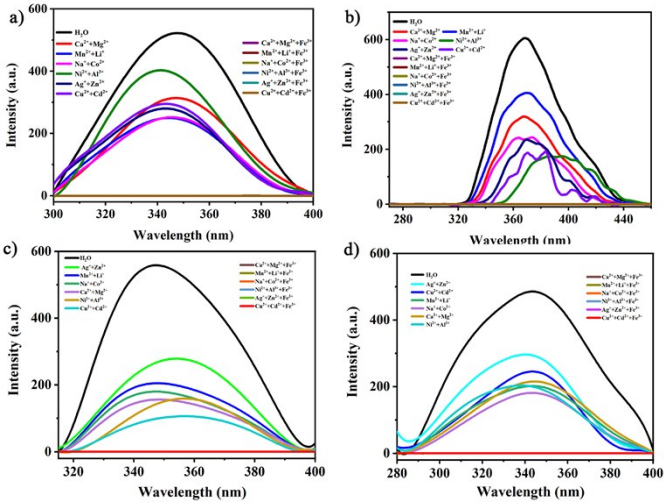


Fig S11 Emission spectra of **1**(a)**, 2**(b)**, 3**(c) and **4**(d) with different mixed cations solution added Fe^{3+} ions (10^{-2} M)

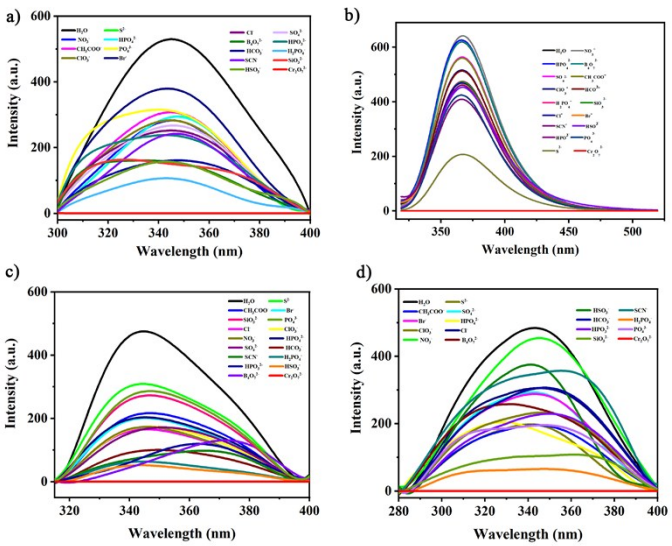


Fig S12 Fluorescence response of **1**(a)**, 2**(b)**, 3**(c) and **4**(d) toward different anions in H_2O solution

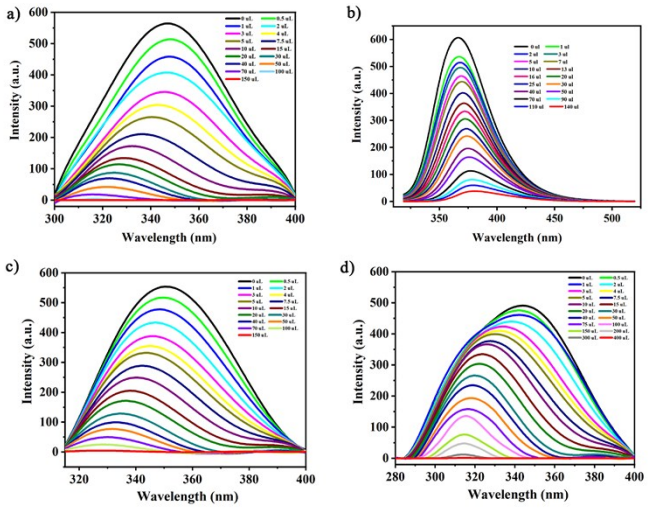


Fig S13 Variation of luminescence intensities of **1**(a)**, 2**(b)**, 3**(c) and **4**(d) titrated with $Na_2Cr_2O_7$

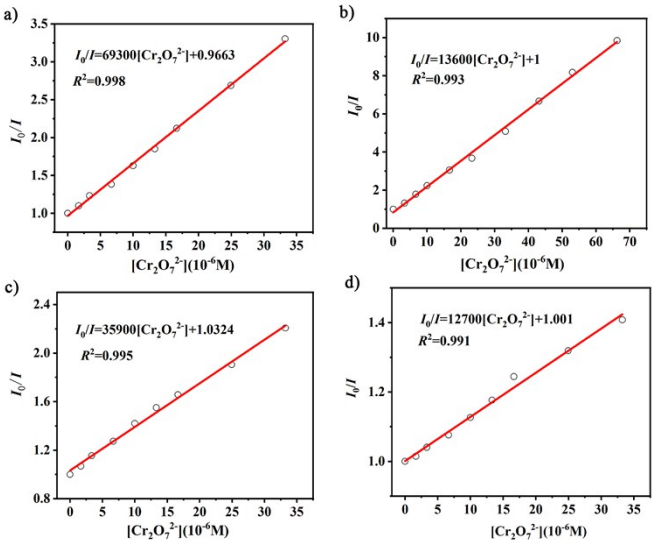


Fig S14 Stern−Volmer plots of $Cr_2O_7^{2-}$ in **1**(a)**, 2**(b)**, 3**(c) and **4**(d)

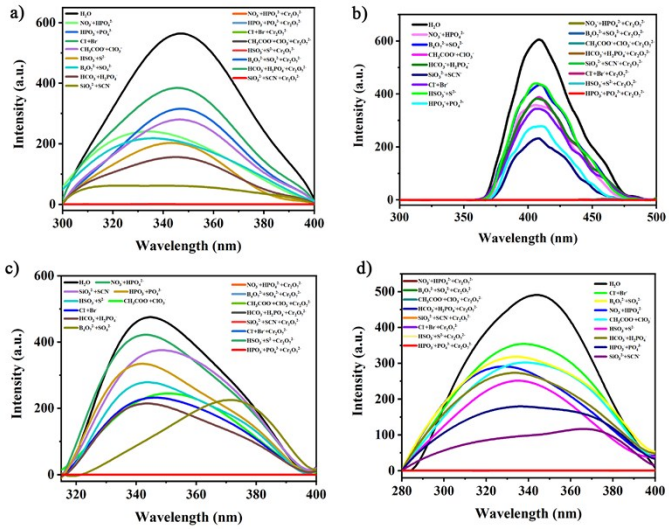


Fig S15 Emission spectra of **1**(a)**, 2**(b)**, 3**(c) and **4**(d) with different mixed cations solution added $Cr_2O_7^{2-}$ ions (10^{-2} M)

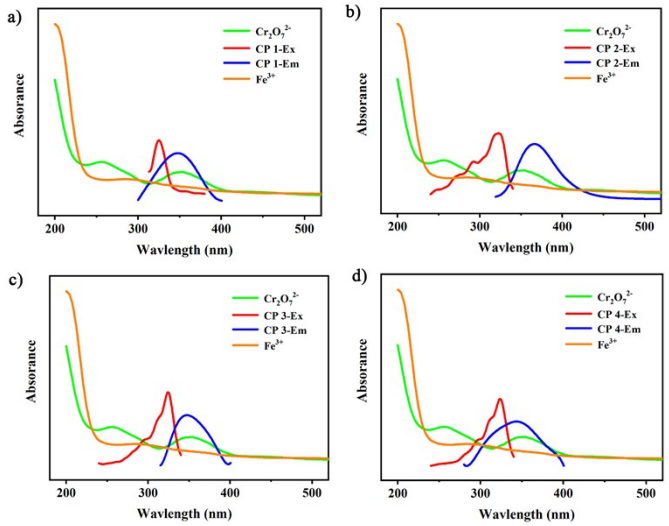


Fig. **S16** UV-vis spectra of Fe^{3+} (blue) and $Cr_2O_7^{2-}$ (magenta) in H_2O solutions, and the excitation and emission spectra of **1**(a)**, 2**(b)**, 3**(c) and **4**(d)

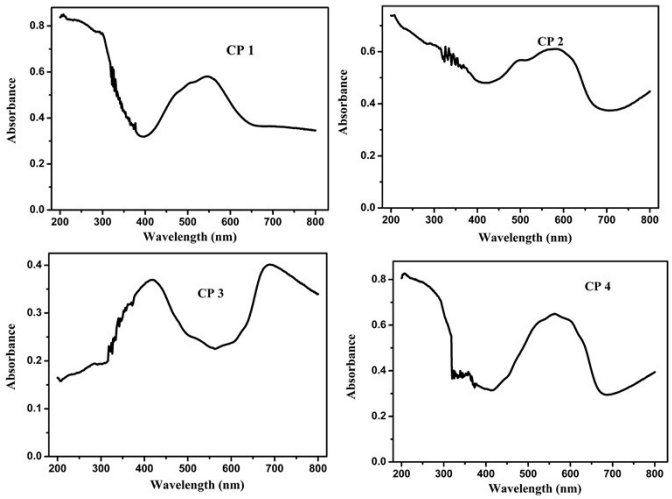


Fig S17 The solid state diffuse-reflectance spectra for the **1-4**

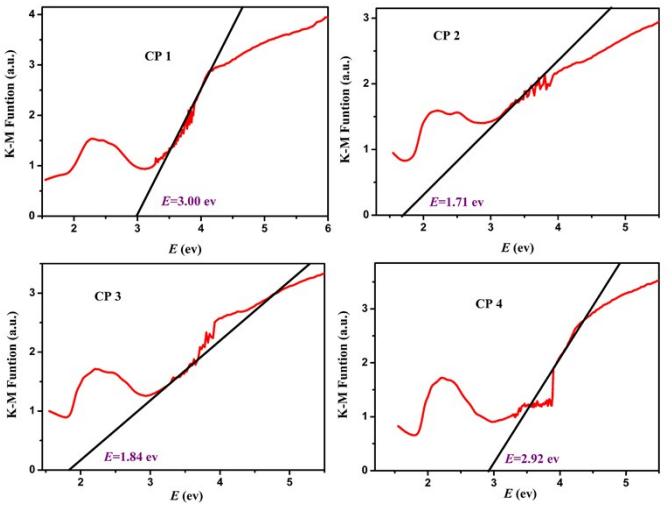


Fig S18 Kubelka–Munk-transformed diffuse reflectance spectra of **1-4**

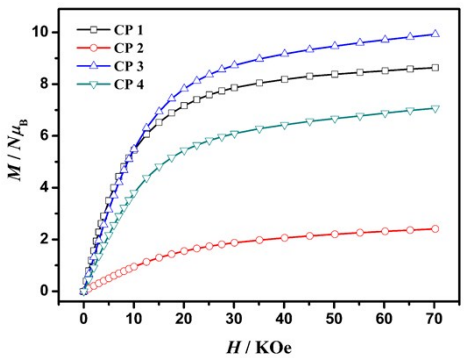


Fig. S19 M vs. H plots at 1.8 K for **1-4**.