Supporting Information

Controllable synthesis of Zn/Cd(II) coordination polymers: dual-emissive luminescent properties, and tailoring emission tendency under varying excitation energy

Kai Xing,[a] Ruiqing Fan,[*a] Song Gao,[a] Xinming Wang,[a] Xi Du,[a] Ping Wang,[a] Ru Fang,[*b] and Yulin Yang[*a]

[a] Department of Chemistry, Harbin Institute of Technology, Harbin 150001, P. R. China

[b] Department of Mathematics, Harbin Institute of Technology, Harbin 150001, P. R. China.

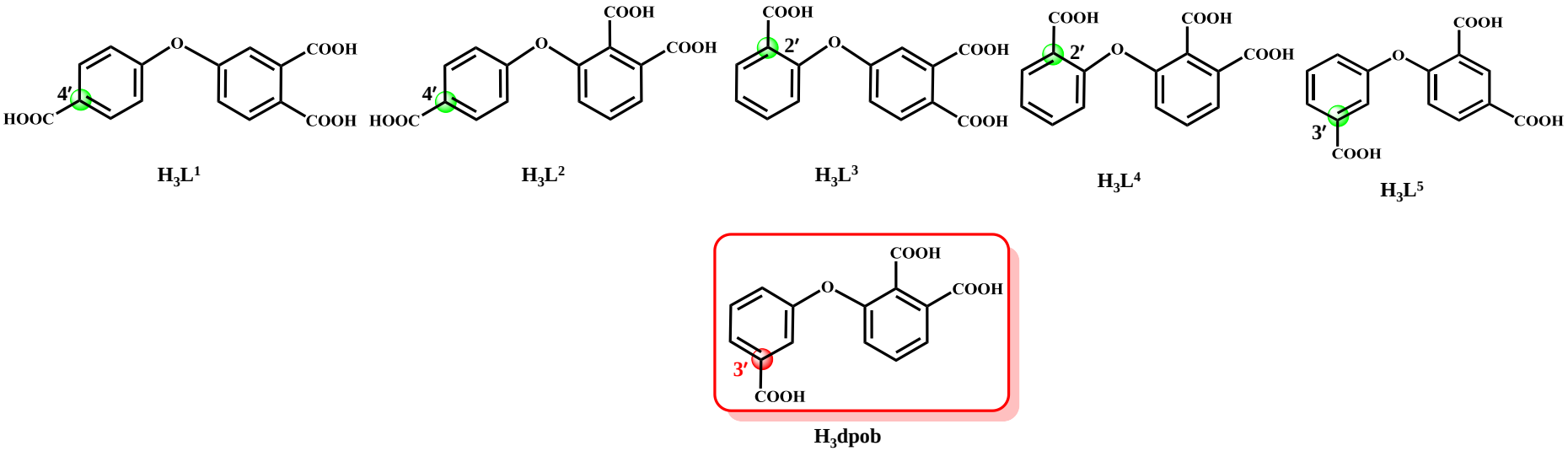


Table S1. The summary of tricarboxylate ligand with different substituent position.

No.	Ligand	Reference	Coordination polymers	Dimension	Property
1	**H_3L^1**	**1**	$[Ag(L^1)(4,4'bpy)]_n$	1D	—
		2	$[Co_{1.5}(L^1)(\mu\text{-}4,4'\text{-}bpy)_2\text{-}(H_2O)_3]_n\cdot(H_2O)_{3n}$	3D	Magnetism
		3	$[Cd_3(L^1)_2(phen)_2(H_2O)_2]_n\cdot\ (H_2O)_{3n}$	3D	Solid state luminescence
		4	$[Zn_2(L^1)_2(dpe)(H_2O)]_n$ndpe	2D	Solid state dual-emission
			$[Zn_4(L^1)_2(dpe)_2(m\text{-}OH)_2]_n$	3D	Solid state dual-emission

		5	$[Zn(L^1)(H_2O)_3]_n$	0D	Solid state luminescence
			$[Zn(L^1)(phen)(H_2O)]_n$	0D	Solid state luminescence
			$[Zn_2(L^1)_2(4,4'\text{-bpy})_3(H_2O)_2]_n \cdot 4nH_2O$	1D	Solid state luminescence
			$[Zn_6(L^1)_4(4,4'\text{-bpy})_2(H_2O)_2]_n$	3D	Solid state luminescence
			$[Zn_3(L^1)_2(bpdb)(H_2O)_2]_n$	3D	Solid state luminescence
			$[Zn_6(L^1)_4(azpy)_2(H_2O)_4]_n$	2D	Solid state luminescence
		6	$[Ni_3(L^1)_2(4,4'\text{-bipy})_4(H_2O)_6] \cdot 6H_2O$	3D	—
2	$\mathbf{H_3L^2}$	**2**	$[Co(HL^2)(\mu\text{-}4,4'\text{-bpy})(H_2O)_3]_n \cdot (4,4'\text{-bpy})_n \cdot (H_2O)_{2n}$	1D	Magnetism
		7	$[Ni_3(L^2)_2(\mu\text{-}4,4'\text{-bpy})_3(H_2O)_2]_n \cdot (4,4'\text{-bpy})_n \cdot (H_2O)_{5n}$	3D	Magnetism
		3	$[Cd_3(L^2)_2(phen)_3]_n \cdot (H_2O)_{2n}$	1D	Solid state luminescence
			$[Cd_3(L^2)_2(2,2'\text{-bpy})_3(H_2O)_2]_n \cdot (H_2O)_{3n}$	3D	Solid state luminescence
			$[Cd_3(L^2)_2(4,4'\text{-bpy})_2]_n \cdot (H_2O)_{4n}$	3D	Solid state luminescence
		8	$[Ag(L^2)(4,4'\text{-bpy})]_n$	1D	Solid state luminescence
		9	$[Zn_3(L^2)_2(4,4'\text{-bpy})_2(H_2O)_4]_n \cdot (H_2O)_{6n}$	3D	Solid state luminescence
			$[Zn_3(HL^2)_2(bix)_2]_n$	2D	Solid state luminescence
		10	$[Cd(HL^2)(\mu\text{-bpp})(H_2O)]_n \cdot (H_2O)_n$ (1), $[Co(H\,L^2)(\mu\text{-bpp})]_n \cdot (H_2O)_n$	2D	—
			$[Ag_2(L^2)_{2/3}(\mu\text{-bpp})]_n$	2D	Magnetism
				2D	—
		11	$[Pb_5(\mu_4\text{-O})(\mu_3\text{-OH})_2(L^2)_2(H_2O)]_n$	3D	Solid state luminescence
		12	$[Zn_3(L^2)_2(tib)_2]_n \cdot (H_2O)_{4.5n}$	3D	Solid state luminescence
			$[Zn_2(HL^2)_2(tib)_2]_n \cdot (H_2O)_n$	3D	Solid state luminescence
			$[Cd_3(L^2)_2(tib)_2(H_2O)_2]_n \cdot (H_2O)_{4n}$	3D	Solid state luminescence
		6	$[Ni(HL^2)(4,4'\text{-bipy})(H_2O)_3] \cdot (4,4'\text{-bipy})\ (H_2O)$	1D	—
			$[Mn_3(L^2)_2(H_2O)(DMF)_2]$		
				1D	Solid state luminescence
		13	$[Co_3(L^2)_2(bpe)_3(H_2O)_4]$	3D	Magnetism

			[Co(μ_2-H_2O)(μ_3-OH)(L^2)(bpe)(H_2O)·$_3$(DMF)$_3$(H_2O)]	3D	Magnetism
			[$Co_3(L^2)_2(bpa)_4$]	3D	Magnetism
3	**H_3L^3**	**2**	[$Co_3(L^3)(HL^3)(OH)(H_2O)_2(\mu$-4,4′-bpy)$_2]_n$ 3·$(H_2O)_{2.5n}$	2D	Magnetism
		3	[$Cd_3(L^3)_2(phen)_2(H_2O)]_n$· $(H_2O)_{2n}$	1D	Solid state luminescence
		9	[$Zn_3(L^3)_2$(4,4′-bpy) $_2]_n$·$(H_2O)_{2n}$	3D	Solid state luminescence
			[$Zn_3(L^3)_2(bix)_3]_n$·$(H_2O)_{7n}$	3D	Solid state luminescence
		12	[$Zn_3(L^3)_2(tib)_2]_n$·$(H_2O)_n$	3D	Solid state luminescence
			[$Cd_3(L^3)_2(tib)_2]_n$·$(H_2O)_{6n}$	3D	Solid state luminescence
4	**H_3L^4**	**2**	[$Co_{1.5}(L^4)(\mu$-4,4′-bpy)$_{1.5}]_n$ 3 (4,4′-bpy)$_{0.5n}$	2D	Magnetism
		7	[$Ni_3(L^4)_2(H_2O)_4(\mu$-4,4′-bpy)$_3]_n$·$(H_2O)_{2n}$	3D	Magnetism
			[$Ni_3(L^4)_2(H_2O)_4(\mu$-4,4′-bpy)$_4]_n$·$(H_2O)_{2n}$	3D	Magnetism
		3	[$Cd_3(L^4)_2(phen)_2]_n$	1D	Solid state luminescence
			[$Cd_3(L^4)_2$(2,2′-bpy)$_2]_n$	1D	Solid state luminescence
		9	[$Zn_3(L^4)_2$-(4,4′-bpy)(H_2O)$_2]_n$·$(H_2O)_{2n}$	2D	Solid state luminescence
			[$Zn_3(L^4)_2(bix)_3]_n$·$(H_2O)_{4n}$	3D	Solid state luminescence
		14	{[$Mn_{1.5}(L^4)$(bpe)$_{1.5}]$·(bpe)$_{0.5}\}_n$	2D	Magnetism
		9	[$Zn_3(L^4)_2(tib)_2]_n$·$(H_2O)_{4n}$	3D	Solid state luminescence
			[$Cd_3(L^4)_2(tib)_2(H_2O)_2]_n$·$(H_2O)_{6n}$	3D	Solid state luminescence

4,4′-bpy = 4,4′-bipyridine; phen = 1,10-phenanthroline; dpe = 1,2-di(4-pyridyl)ethylene; bpdb = 1,4-bis(4-pyridyl)-2,3-diaza-1,3-butadiene; azpy = 4,4′-azopyridine; bix = 1,4-bis(imidazol-1-ylmethyl)benzene; bpp = 1,3-bis(4-pyridyl)propane]; tib = 1,3,5-tris(1-imidazolyl)benzene; bpe = 1,2-bis(4-pyridyl)ethylene; bpa = 1,2-bis(4-pyridyl)ethane;

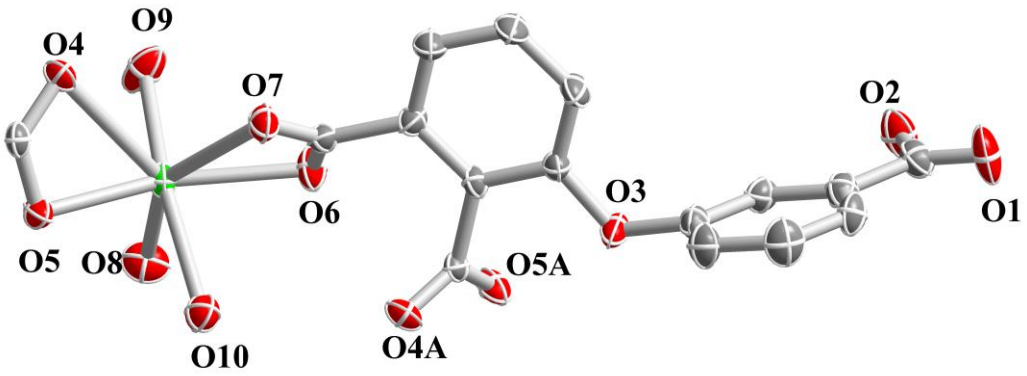


Fig. S1 The structural unit of **1** with labeling scheme and 50% thermal ellipsoids (water molecules and hydrogen atoms are omitted for clarity). Symmetry codes A: *-x, 0.5+y, 0.5-z*.

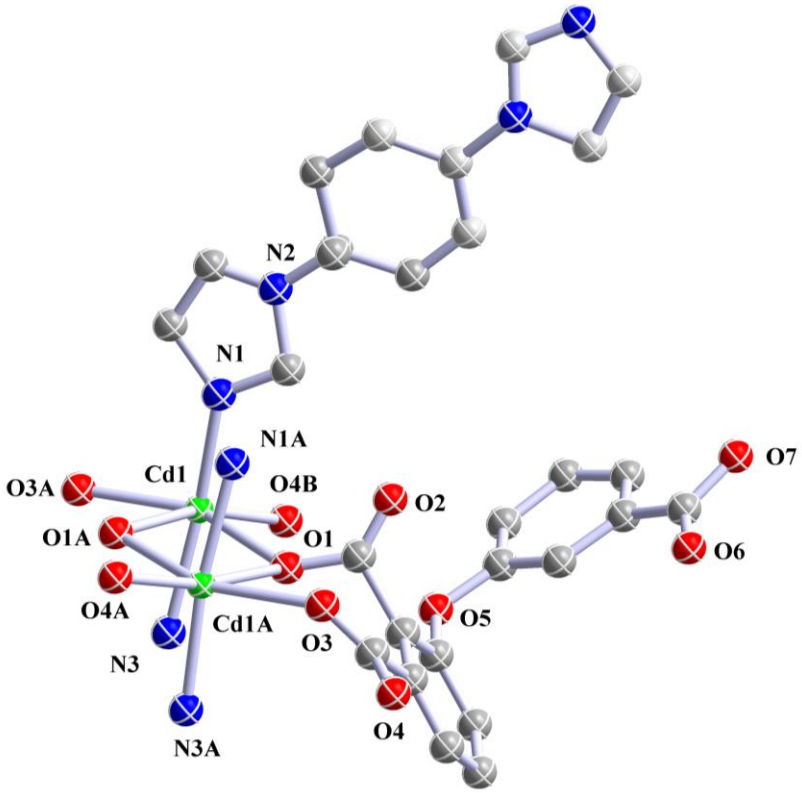


Fig. S2 The structural unit of **2** with labeling scheme and 30% thermal ellipsoids (hydrogen atoms are omitted for clarity). Symmetry codes A: *-x, 1-y, -z*; B: *1+x, y, z*.

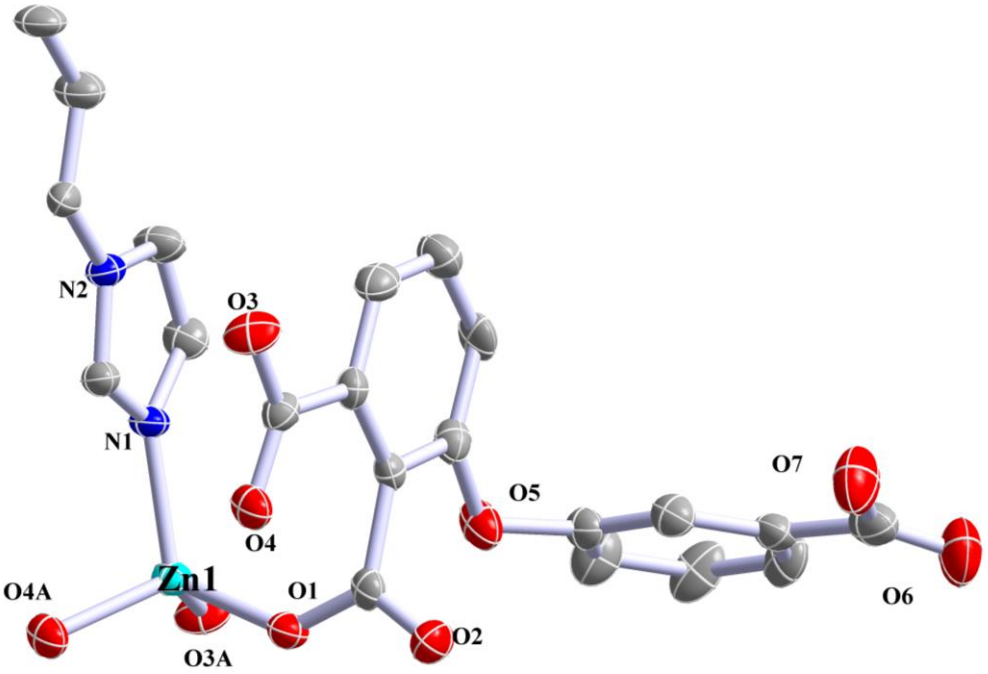
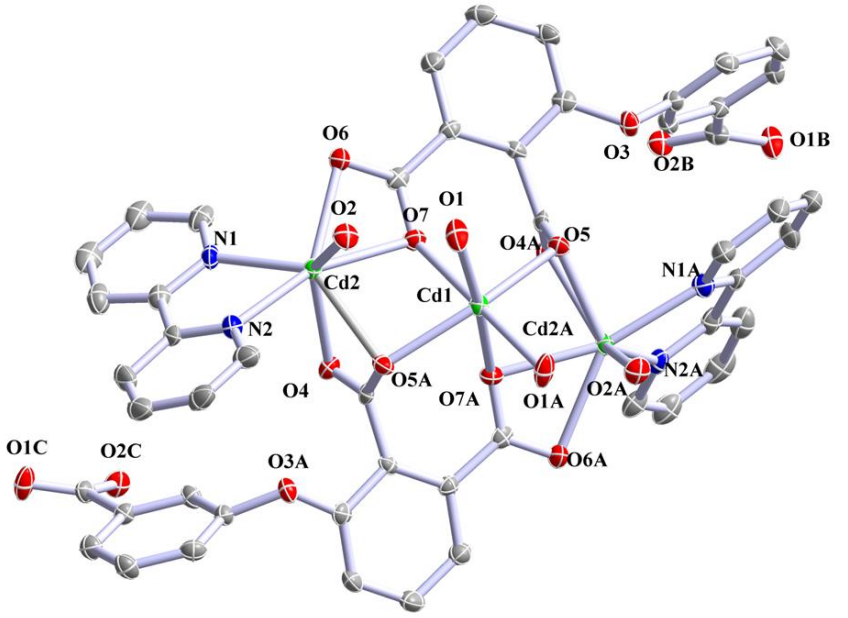
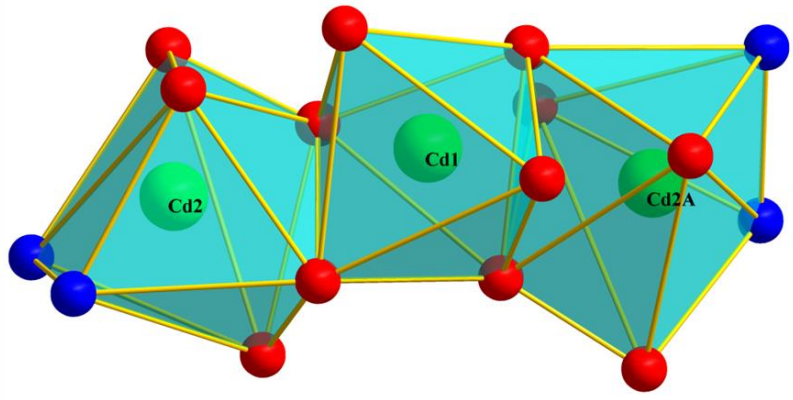


Fig. S3 The structural unit of **3** with labeling scheme and 50% thermal ellipsoids (hydrogen atoms are omitted for clarity). Symmetry codes: O3A *1+x, y, -z*; O4A 1-*x, 1-y, 1-z*.



(a)



(b)

Fig. S4 (a) The structural unit of **4** with labeling scheme and 50% thermal ellipsoids (water molecules and hydrogen atoms are omitted for clarity). Symmetry codes A: *x, -y, -z*; B: *-0.5+x, 0.5+y, z*; C: *-0.5+x, -0.5-y, -z*. (b) Polyhedral representation of the coordination sphere of the Cd^{2+} centre in **4**.

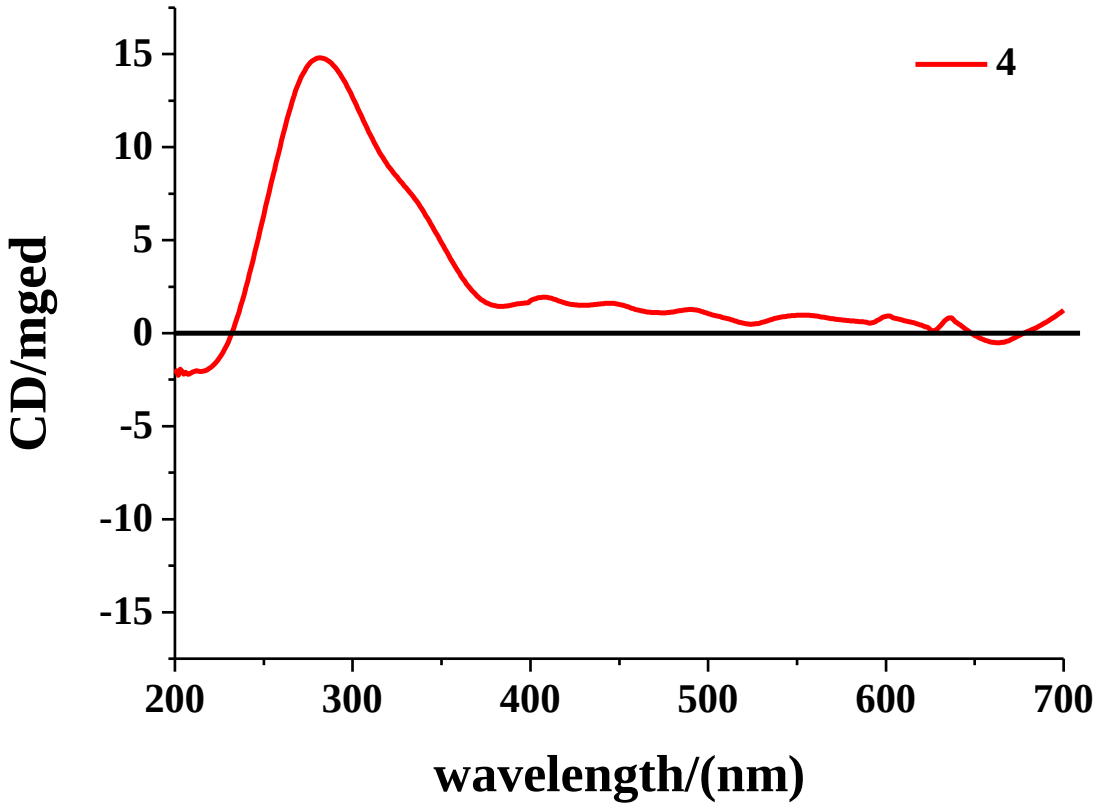
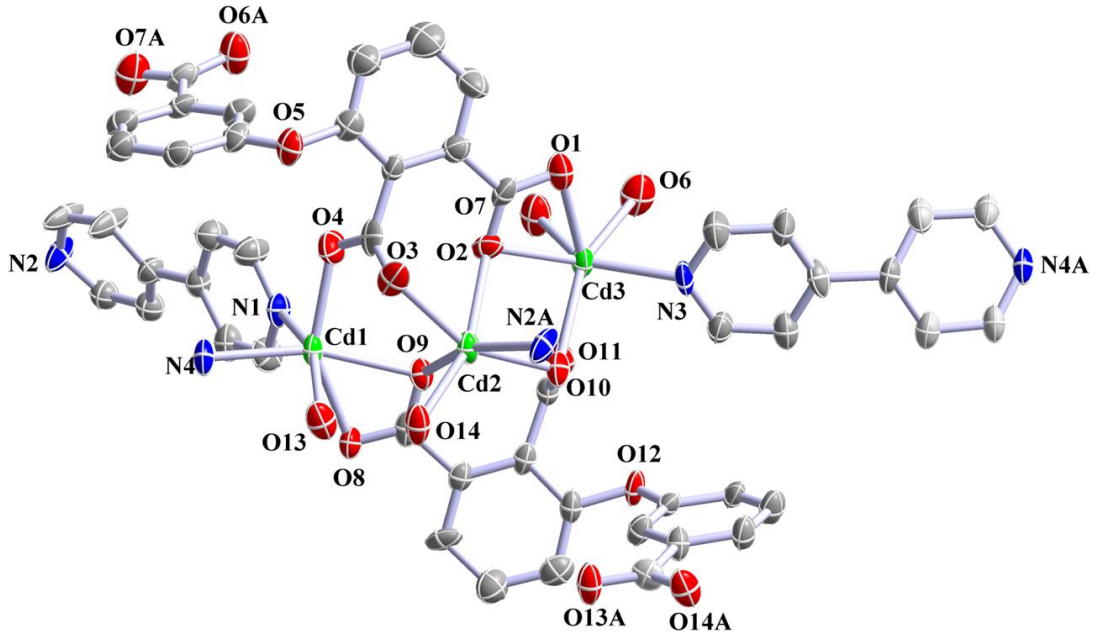
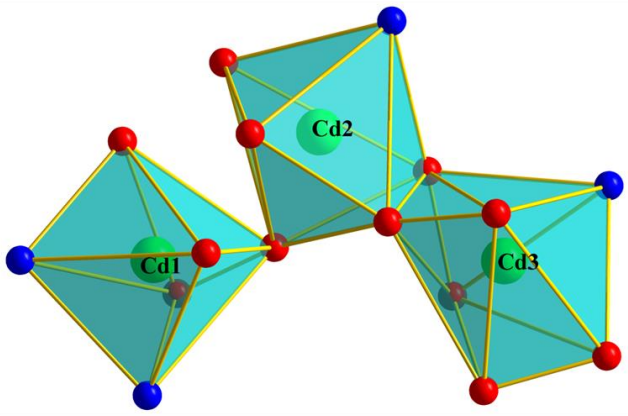


Fig. S5 The solid-state CD spectra of bulk samples of **4**.



(a)



(b)

Fig. S6 (a) The structural unit of **5** with labeling scheme and 50% thermal ellipsoids (water molecules and hydrogen atoms are omitted for clarity). Symmetry codes A: 1-*x, 2-y, 1-z*. (b) Polyhedral representation of the coordination sphere of the Cd^{2+} center in **5**.

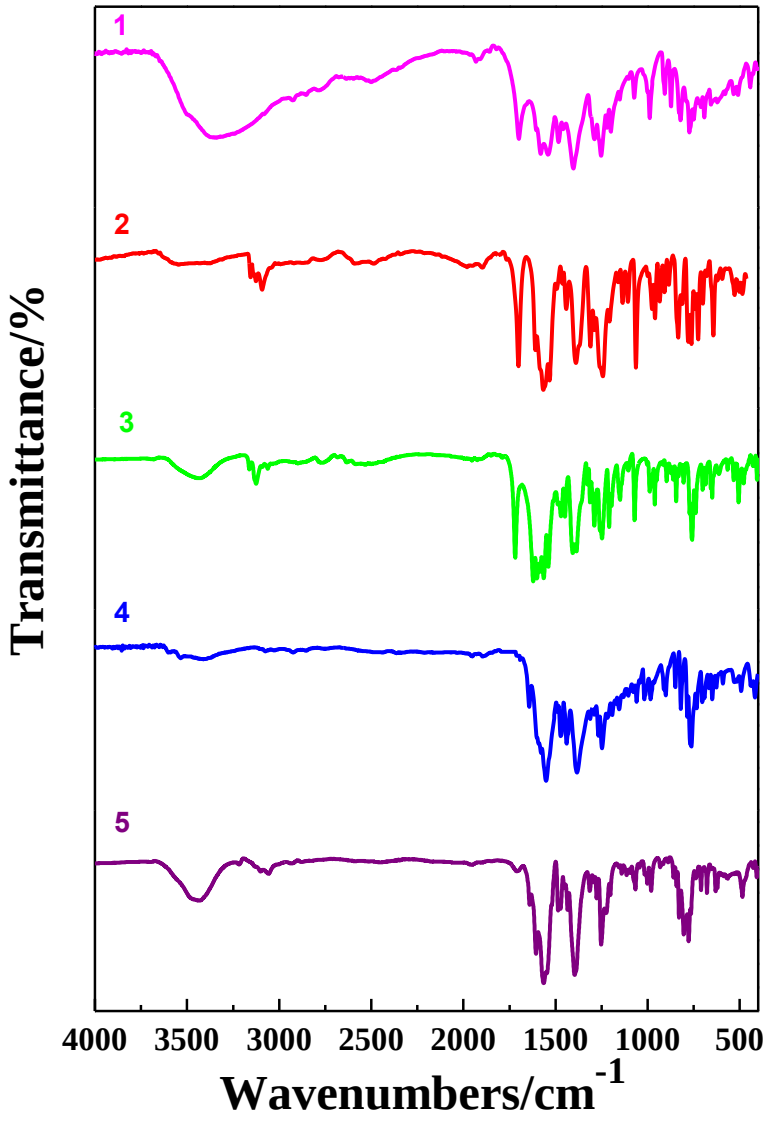


Fig. S7 Infrared spectra of coordination polymers **1**–**5** recorded from a KBr pellet.

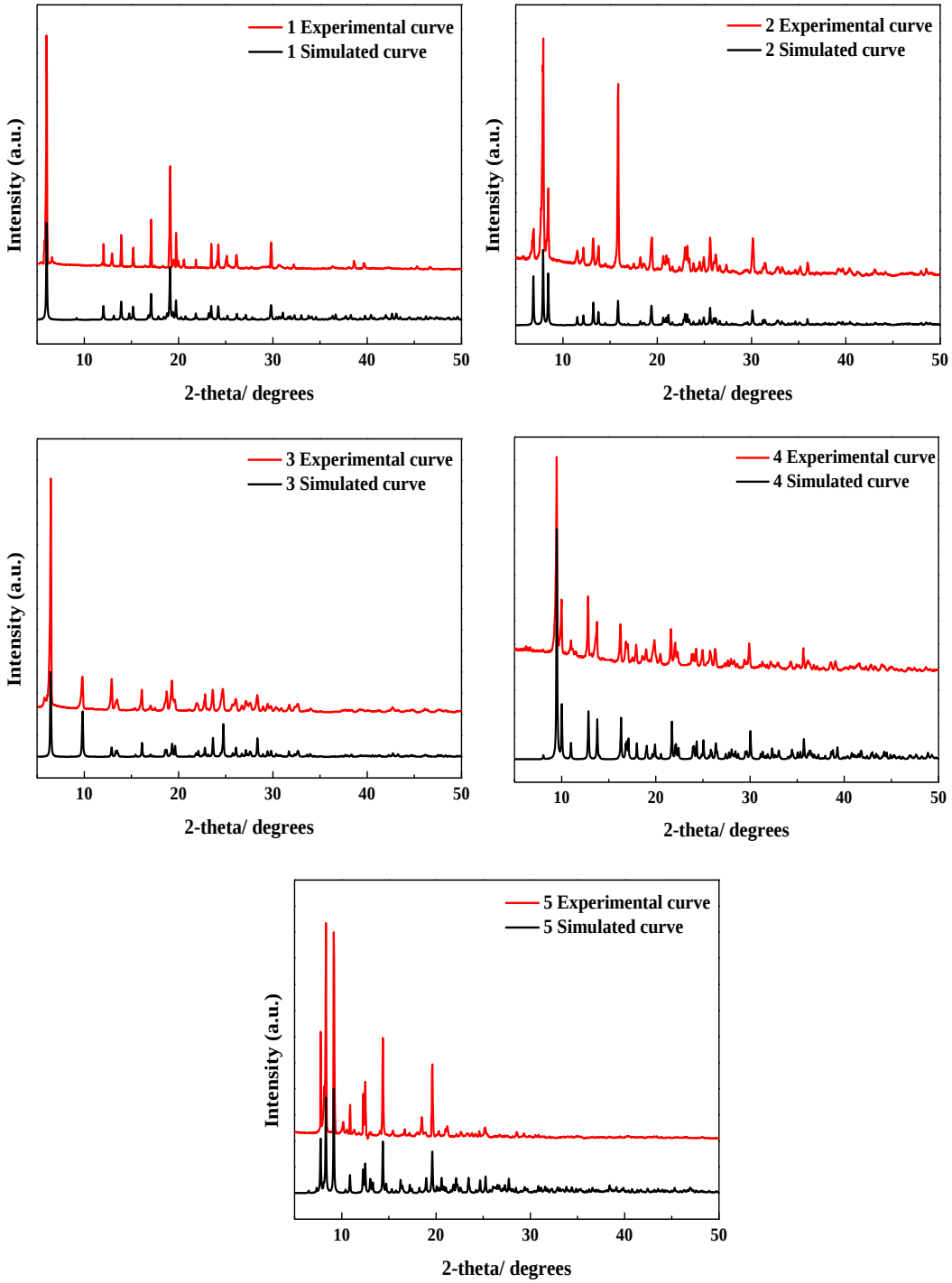


Fig. S8 The PXRD contrast curves of coordination polymers **1**–**5**.

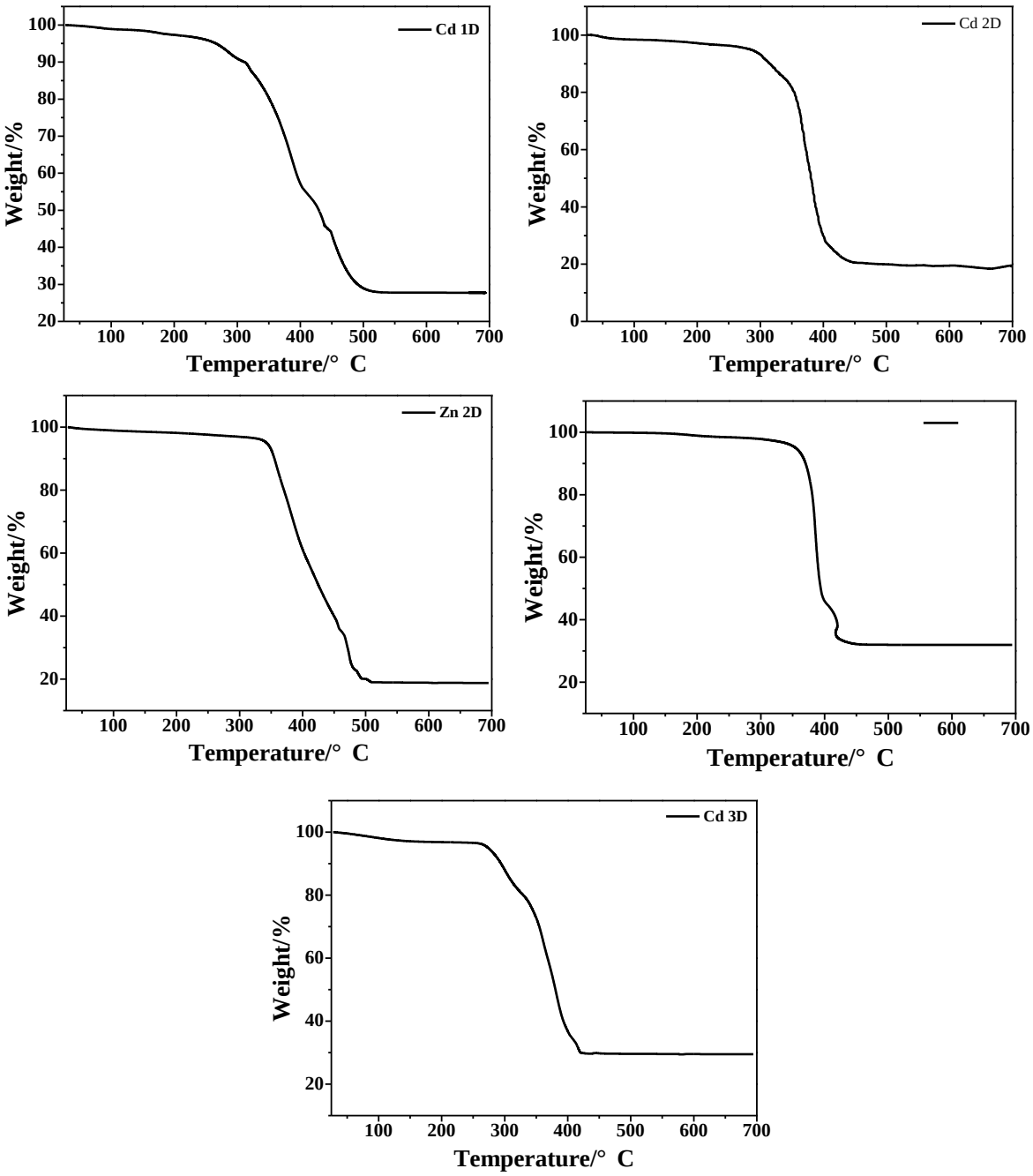


Fig. S9 The TGA curves of coordination polymers **1**–**5**

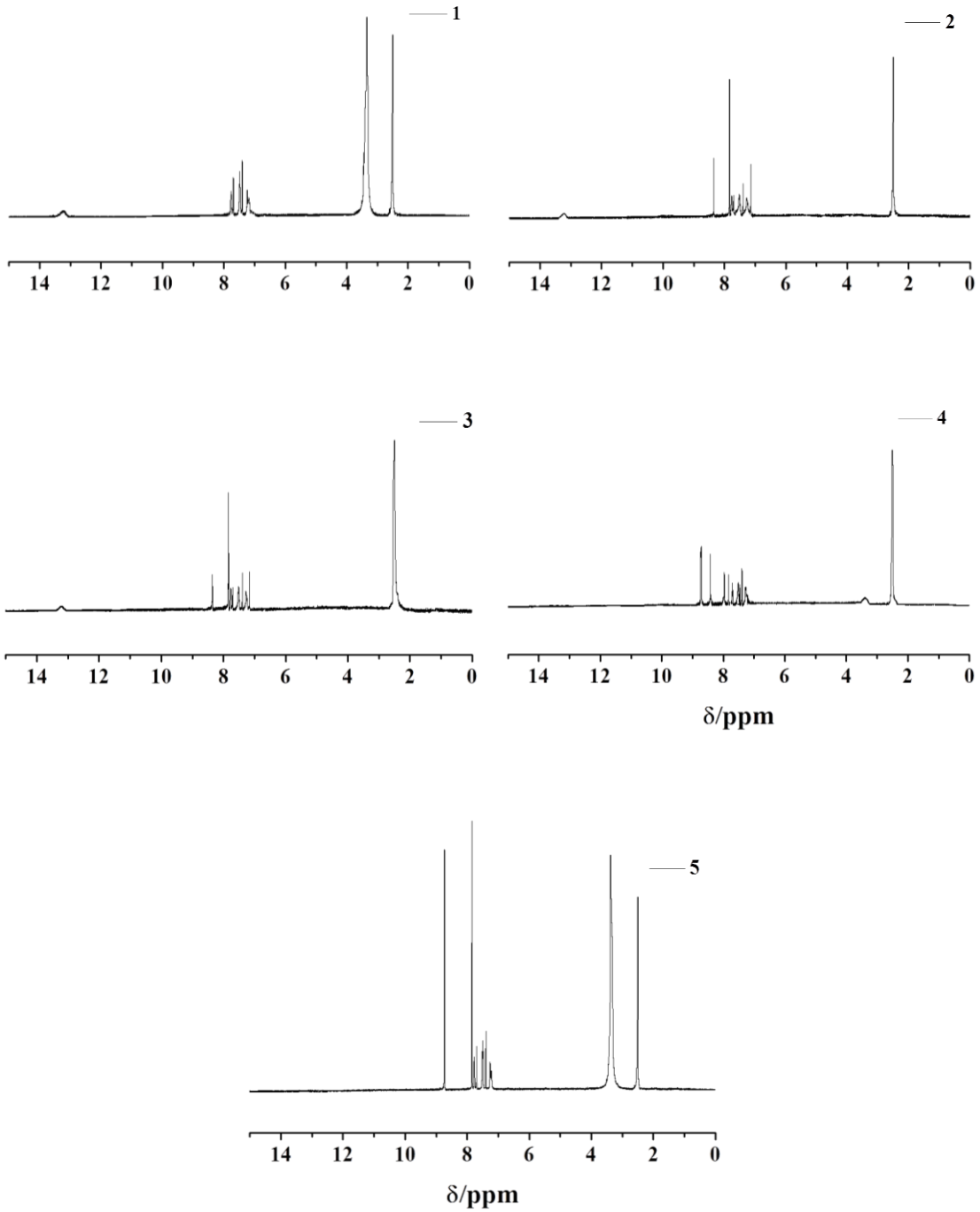


Fig. S10 ^{1}H NMR spectrum of **1–5** in DMSO-d_6.

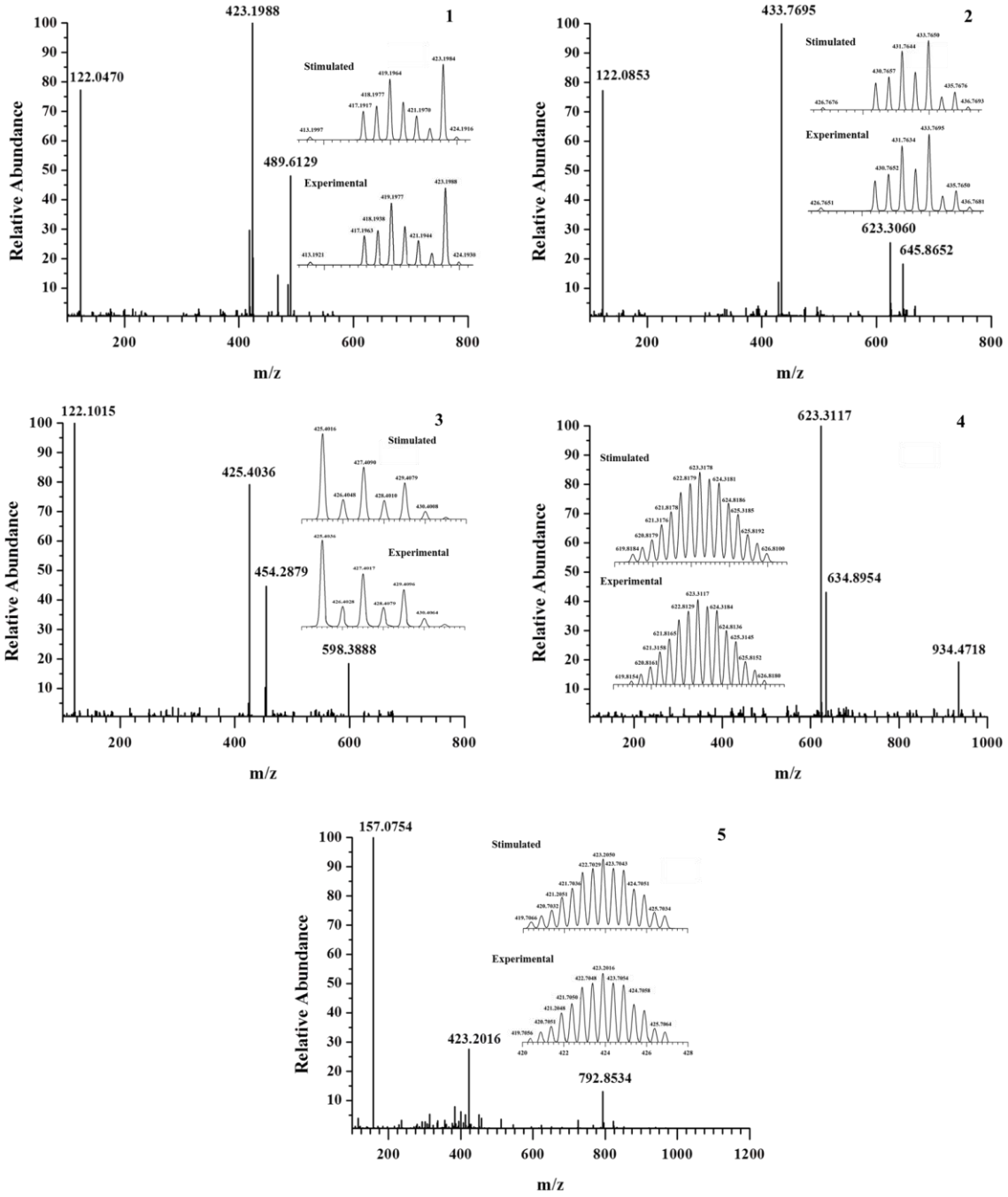


Fig. S11 The ESI-MS spectrum of **1–5.**

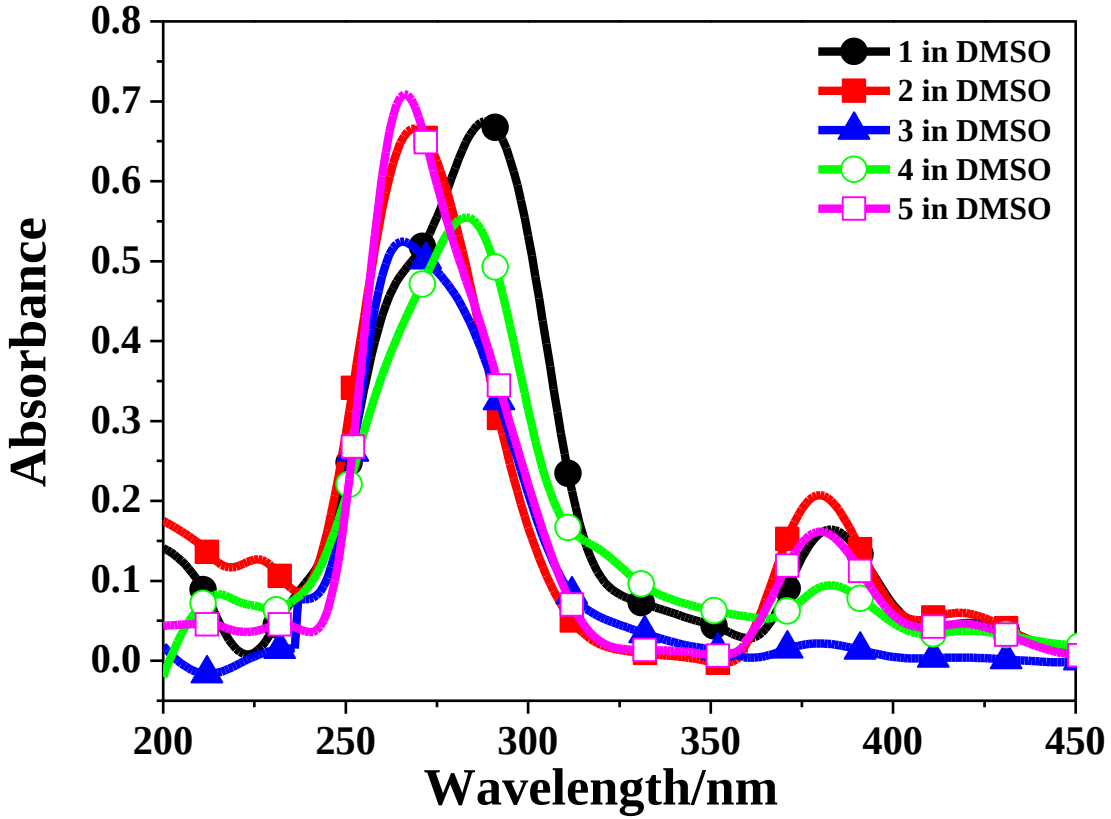


Fig. S12 UV absorption spectra of coordination polymers **1**–**5**

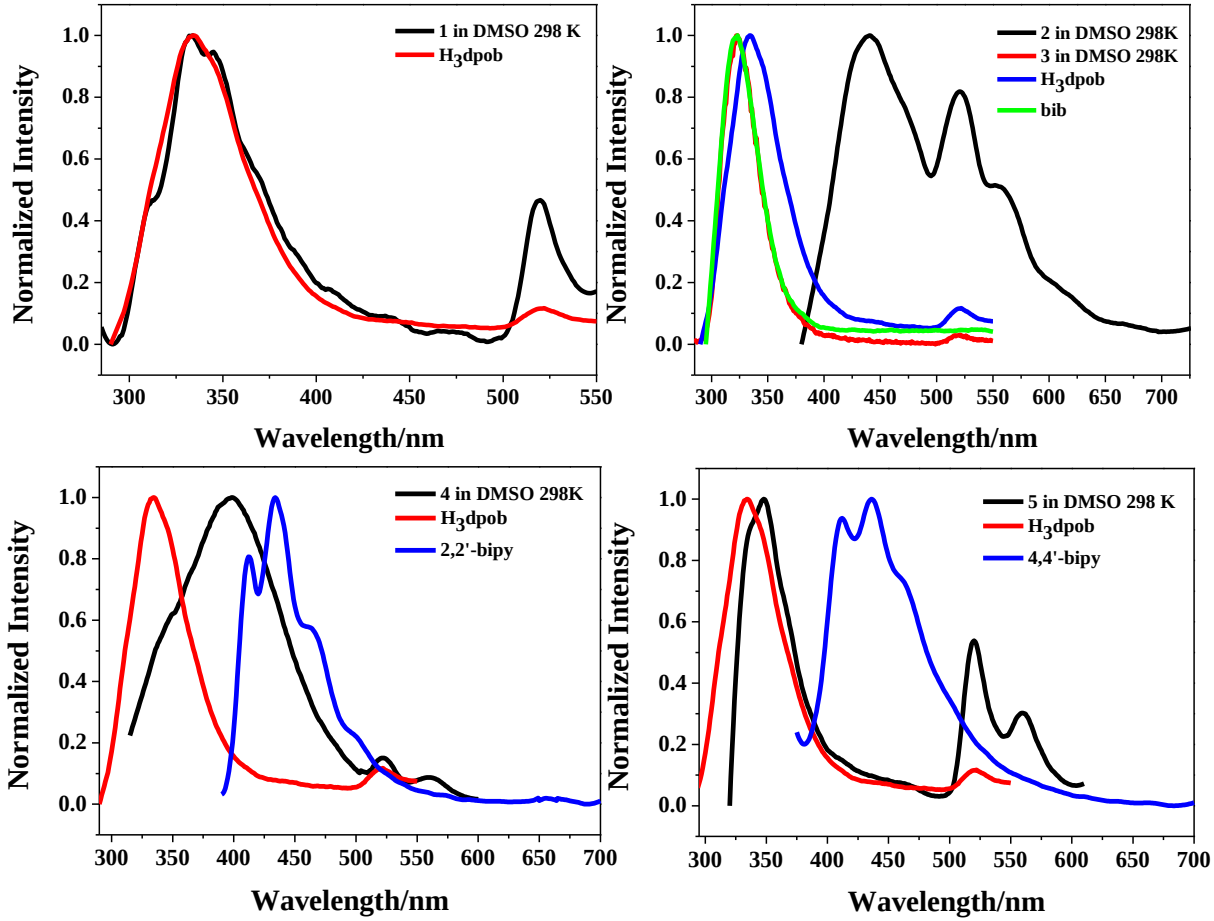


Fig. S13 Normalized emission spectra of coordination polymers **1**–**5** and corresponding ligands in DMSO solution (concentration: (M) ≈ 10^{-5} M) at 298 K

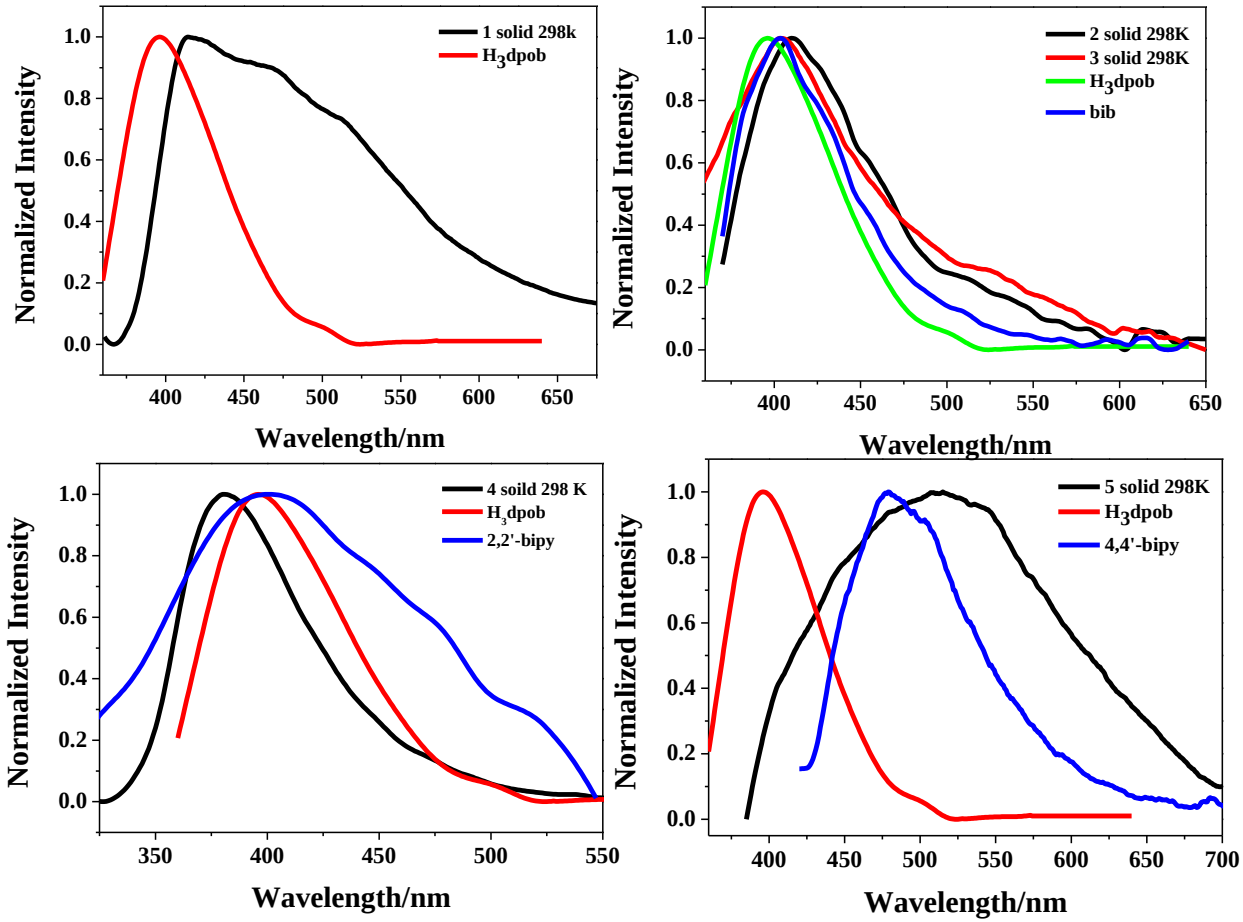


Fig. S14 Normalized emission spectra of coordination polymers **1**–**5** and corresponding ligands in the solid state at room temperature

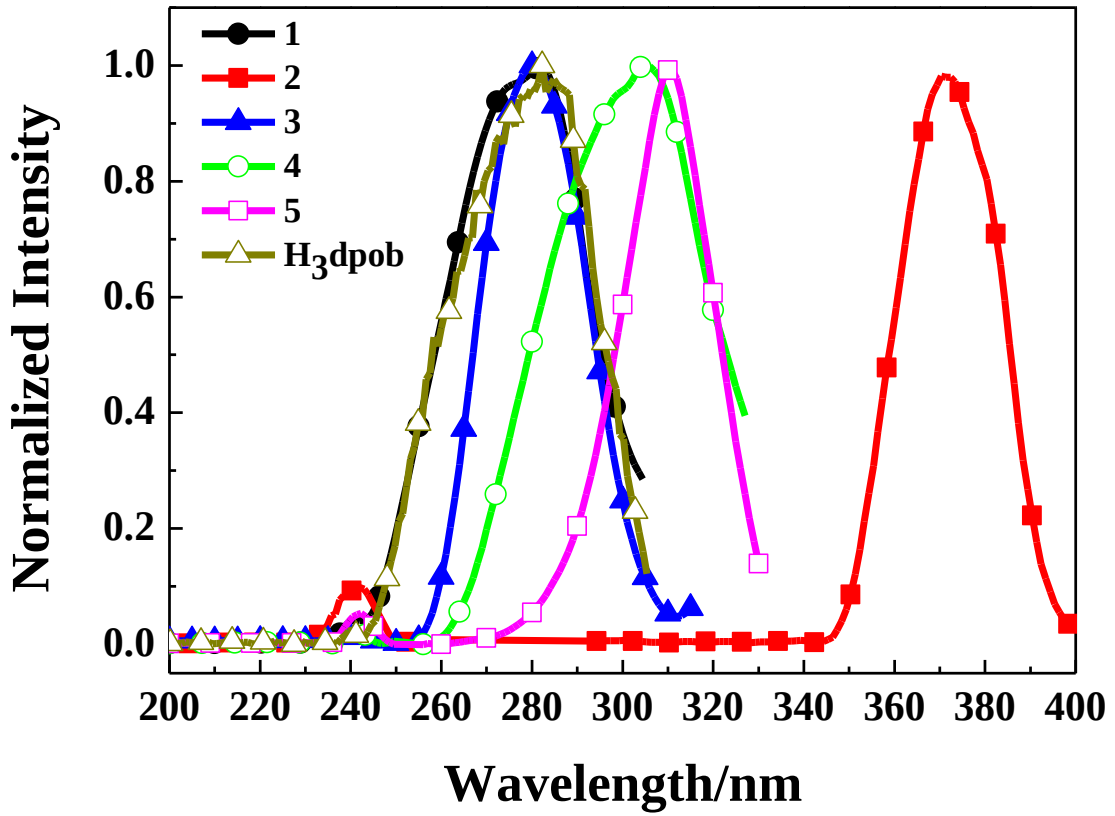


Fig. S15 Normalized excitation spectra of coordination polymers **1**–**5** in DMSO solution (concentration: 10^{-5} M) at 298 K

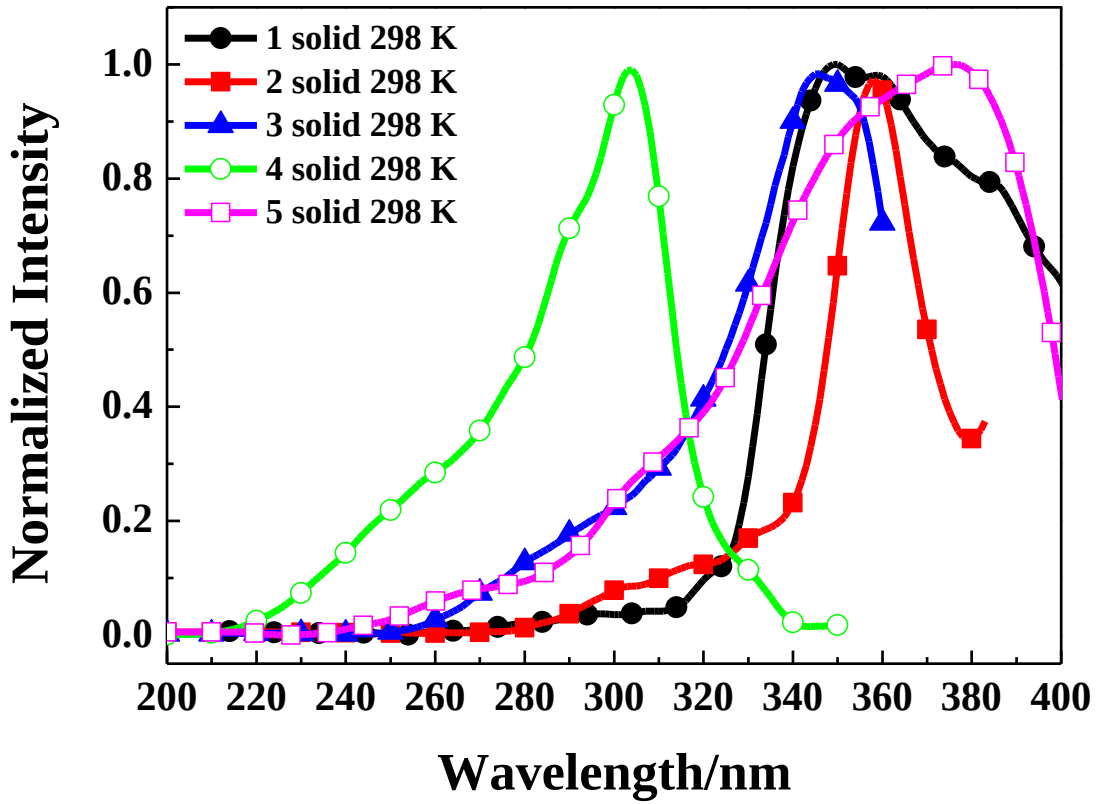


Fig. S16 Normalized excitation spectra of coordination polymers **1**–**5** at 298 K in solid state

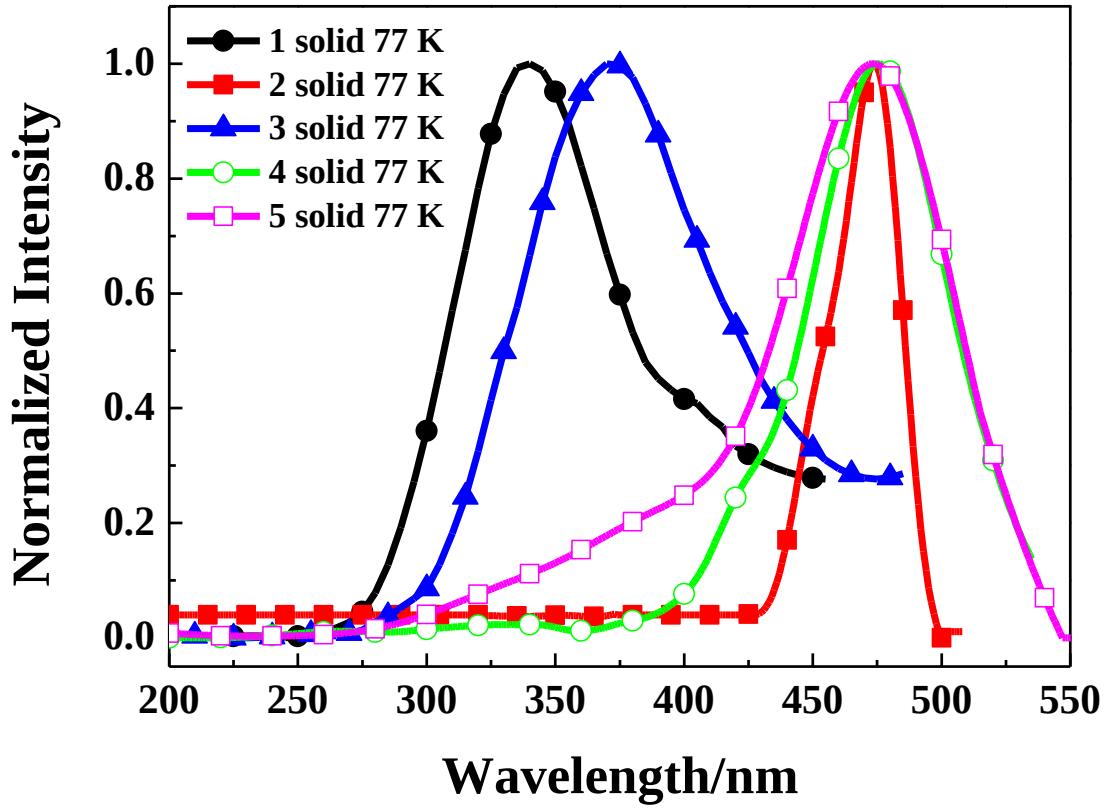


Fig. S17 Normalized excitation spectra of coordination polymers **1**–**5** at 77 K in solid state

Table S2. Luminescence data for coordination polymers **1**–**5**

Coordination polymers	Absorption (nm) ε/dm^{3}cm^{-1}mol^{-1}	Excitation (λ, nm)	Emission (λ_{max}, nm)	CIE (x, y)	Lifetime (μs)					Quantum yields(Φ)[b]	Conditions[a]
					τ_1 (μs)	A_1%	τ_2 (μs)	A_2%	<τ> (μs)		
1	288 (72670), 383 (16420)	275	334, 520	0.15, 0.48	0.88	81.15%	7.27	18.85%	5.08	0.089	DMSO, 298K
	—	350	414	0.23, 0.26	1.16	62.43%	8.74	37.57%	7.37	—	Solid State, 298K
	—	340	475	0.19, 0.29	0.97	57.44%	8.78	42.56%	7.77	—	Solid State, 77K
2	268 (65654), 380 (20710)	370	441, 521, 563 *sh*	0.21, 0.27	1.04	73.06%	8.50	26.40%	6.60	0.123	DMSO, 298K
	—	360	410	0.18, 0.14	1.16	64.70%	9.06	35.30%	7.56	—	Solid State, 298K
	—	475	560	0.45, 0.53	0.92	35.36%	9.17	64.64%	8.74	—	Solid State, 77K
3	264 (55663), 381 (2170)	275	323, 519	0.15, 0.34	0.98	84.31%	7.79	15.69%	5.04	0.095	DMSO, 298K
	—	345	403	0.19, 0.18	0.97	84.76%	8.77	15.24%	5.80	—	Solid State, 298K
	—	370	530	0.32, 0.45	1.09	55.74%	8.73	44.26%	7.69	—	Solid State, 77K
4	283 (57679), 384 (9450)	305	394, 522, 559 *sh*	0.17, 0.12	1.04	73.06%	8.50	26.40%	6.60	0.092	DMSO, 298K
	—	305	380	0.18, 0.13	1.16	64.70%	9.06	35.30%	7.56	—	Solid State, 298K
	—	475	587	0.52, 0.47	1.23	52.12%	9.94	47.88%	8.91	—	Solid State, 77K
5	263 (76340), 379 (16170)	310	384, 520, 560 *sh*	0.26, 0.53	1.05	80.28%	8.66	19.72%	6.15	0.090	DMSO, 298K
	—	375	515	0.29, 0.36	1.12	63.71%	9.10	36.29%	7.68	—	Solid State, 298K
	—	470	590	0.49, 0.49	1.15	55.94%	11.06	44.06%	9.90	—	Solid State, 77K
H_3dpob	—	280	334, 520	0.15, 0.28	1.06	85.51%	7.69	14.49%	4.79	0.026	DMSO, 298K
	—	350	396	0.24, 0.10	1.02	57.57%	10.72	42.43%	9.61	—	Solid State, 298K
bib	—	285	323	0.14, 0.25	1.10	87.68%	11.11	12.32%	6.97	0.022	DMSO, 298K
	—	360	404	0.17, 0.09	1.11	54.90%	9.75	45.10%	8.70	—	Solid State, 298K
2,2’ –bipy	—	380	412 *sh*, 434, 466 *sh*	0.16, 0.29	1.12	63.55%	9.74	36.45%	8.30	0.012	DMSO, 298K
	—	340	403	0.14, 0.10	1.09	62.38%	9.17	37.62%	7.84	—	Solid State, 298K
4,4’–bipy	—	365	412 *sh*, 436, 462*sh*	0.17, 0.12	1.10	68.90%	8.79	31.10%	7.12	0.015	DMSO, 298K
	—	350	479	0.21, 0.32	1.14	54.69%	9.56	45.31%	8.50	—	Solid State, 298K

a Concentration in DMSO solution: (M) = 1×10^{-5} M.

b Determined using quinine sulfate in 0.1 M sulphuric acid ((M) = 1×10^{-5} M, $\Phi_s = 0.546$)

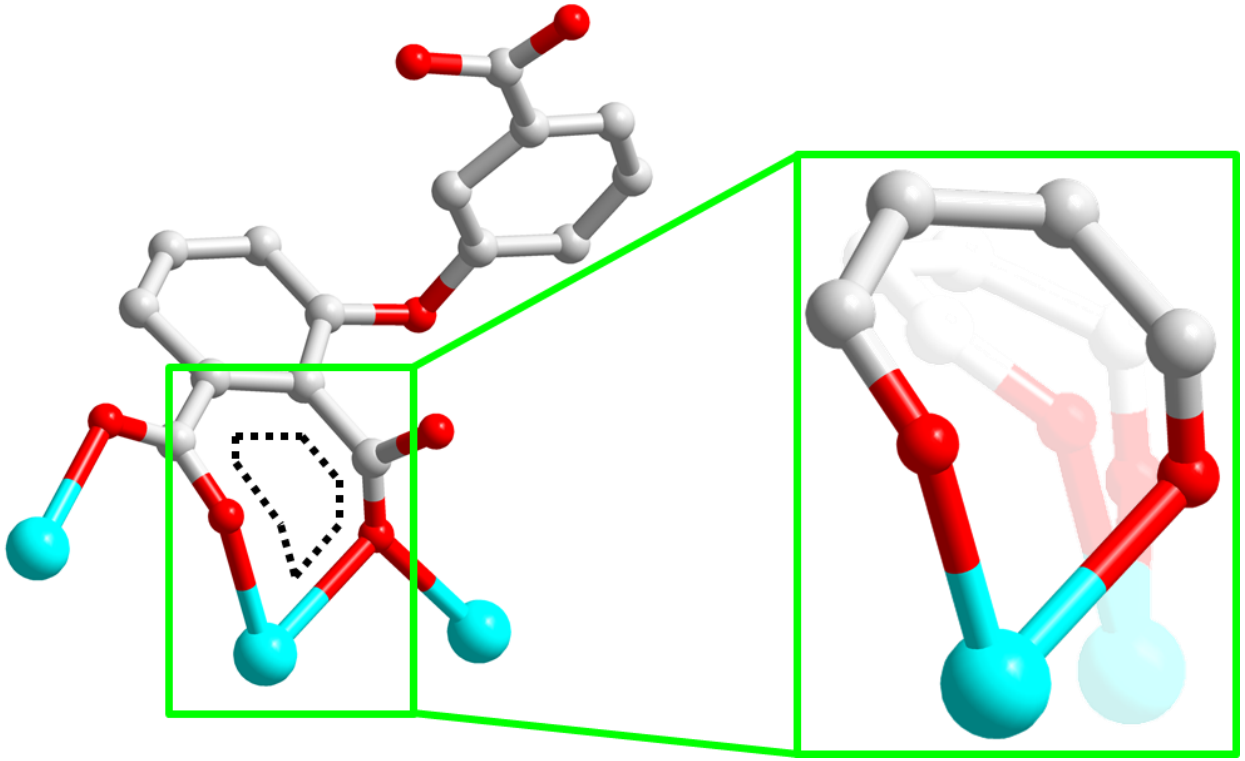


Fig. S18 The seven-atom chair-like circle structure in coordination polymers **2.**

Table S3. Integrated intensity data for coordination polymers **2** and **3** via varying excitation in DMSO.

Coordination polymers	Excitation (λ, nm)	Integrated intensity of HE	Normalized integrated intensity of HE (%)	Integrated intensity of LE	Normalized integrated intensity of LE (%)
2	330	219335.538	100	531374.164	100
	340	198596.005	90.54	306955.548	57.77
	350	161313.702	73.55	224282.648	42.21
	360	152244.224	69.55	185143.074	34.84
	370	138396.079	63.10	117711.591	22.15
3	280	205773.502	100	8553.118	10.18
	290	164773.413	80.08	16744.368	19.94
	300	78768.108	38.28	33062.330	39.37
	310	47897.531	23.28	59842.029	71.26
	320	37276.268	18.12	83980.425	100

Table S4. Luminescence data for coordination polymers **2** and **3** via varying excitation in DMSO.

Coordination polymers	Excitation (λ, nm)	Emission (λ_{max}, nm)	Intensity	CIE (x, y)
2	330	438,521	1590, 9518	0.30, 0.50
	340	439,519	1814, 5370	0.28, 0.42
	350	438,519	1860, 3776	0.26, 0.38
	360	442,517	2032, 3120	0.24, 0.34
	370	440,521	1975, 1691	0.22, 0.27
3	280	325,521	4521,231	0.16, 0.36
	290	326,519	3359, 364	0.19, 0.42
	300	330,519	1317, 650	0.24, 0.47
	310	335,519	823, 1106	0.28, 0.49
	320	336,519	618, 1471	0.29, 0.48

Table S5. Hydrogen-bond (Å, deg) for coordination polymers **1**–**3**.

Coordination polymers	D-H···A	d(H..A)	<DHA	d(D..A)
1	O2-H2···O5[x, -y+1/2, z-1/2]	1.797	176.56	2.616
	O8-H8B···O4 [-x+1/2, y+1/2, z]	2.240	143.88	2.969
2	O6-H6···O4 [-x, -y+2, -z+1]	1.815	167.10	2.620
3	O7-H7···O4 [-x+1, -y, -z]	1.859	159.69	2.644

Table S6.

Selected bond distance (Å) and angles (˚) in coordination polymers **1**.

1					
Cd(1)-O(9)	2.273(3)	Cd(1)-O(5)	2.287(3)	Cd(1)-O(8)	2.290(3)
Cd(1)-O(10)	2.369(3)	Cd(1)-O(7)	2.384(3)	Cd(1)-O(6)	2.385(3)
Cd(1)-O(4)	2.607(3)	Cd(1)-C(12)	2.714(4)		
O(9)-Cd(1)-O(5)	110.10(11)	O(9)-Cd(1)-O(8)	83.64(13)	O(5)-Cd(1)-O(8)	98.62(11)
O(9)-Cd(1)-O(10)	162.01(12)	O(5)-Cd(1)-O(10)	81.57(11)	O(8)-Cd(1)-O(10)	81.01(12)
O(9)-Cd(1)-O(7)	102.62(13)	O(5)-Cd(1)-O(7)	111.09(11)	O(8)-Cd(1)-O(7)	144.74(11)
O(10)-Cd(1)-O(7)	84.90(11)	O(9)-Cd(1)-O(6)	88.38(12)	O(5)-Cd(1)-O(6)	159.87(10)
O(8)-Cd(1)-O(6)	91.10(11)	O(10)-Cd(1)-O(6)	82.61(11)	O(7)-Cd(1)-O(6)	54.97(10)
O(9)-Cd(1)-O(4)	74.70(11)	O(5)-Cd(1)-O(4)	52.58(9)	O(8)-Cd(1)-O(4)	131.72(11)
O(10)-Cd(1)-O(4)	122.84(10)	O(7)-Cd(1)-O(4)	82.78(9)	O(6)-Cd(1)-O(4)	129.87(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z+1/2 #2 -x,y-1/2,-z+1/2

Selected bond distance (Å) and angles (˚) in coordination polymers **2**.

2					
Cd(1)-N(3)	2.247(4)	Cd(1)-O(4)#1	2.269(4)	Cd(1)-N(1)	2.287(4)
Cd(1)-O(3)#2	2.315(3)	Cd(1)-O(1)	2.336(3)	Cd(1)-O(1)#2	2.497(3)
N(3)-Cd(1)-O(4)#1	101.50(15)	N(3)-Cd(1)-N(1)	173.81(13)	O(4)#1-Cd(1)-N(1)	84.17(15)
N(3)-Cd(1)-O(3)#2	95.09(13)	O(4)#1-Cd(1)-O(3)#2	110.29(13)	N(1)-Cd(1)-O(3)#2	80.50(13)
N(3)-Cd(1)-O(1)	96.60(13)	O(4)#1-Cd(1)-O(1)	90.37(12)	N(1)-Cd(1)-O(1)	85.75(13)
O(3)#2-Cd(1)-O(1)	153.65(12)	N(3)-Cd(1)-O(1)#2	89.18(13)	O(4)#1-Cd(1)-O(1)#2	166.30(12)
N(1)-Cd(1)-O(1)#2	85.59(13)	O(3)#2-Cd(1)-O(1)#2	76.84(11)	O(1)-Cd(1)-O(1)#2	79.79(11)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 -x,-y+1,-z #3 x-1,y,z #4 x,y,z+1 #5 x,y,z-1

Selected bond distance (Å) and angles (˚) in coordination polymers **3**.

3					
Zn(1)-O(3)	1.916(3)	Zn(1)-O(1)	1.931(3)	Zn(1)-O(4)	1.963(3)
Zn(1)-N(1)	1.977(3)				
O(3)-Zn(1)-O(1)	108.22(14)	O(3)-Zn(1)-O(4)	122.78(14)	O(1)-Zn(1)-O(4)	101.37(14)
O(3)-Zn(1)-N(1)	107.68(15)	O(1)-Zn(1)-N(1)	114.17(14)	O(4)-Zn(1)-N(1)	102.81(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x+1,-y+1,-z+1 #3 -x+2,-y+2,-z+1

Selected bond distance (Å) and angles (˚) in coordination polymers **4**.

4					
Cd(1)-O(1)	2.196(4)	Cd(1)-O(1)#1	2.196(4)	Cd(1)-O(5)#1	2.274(3)
Cd(1)-O(5)	2.274(3)	Cd(1)-O(7)	2.347(3)	Cd(1)-O(7)#1	2.347(3)
Cd(2)-O(2)	2.300(3)	Cd(2)-N(2)	2.316(4)	Cd(2)-N(1)	2.331(4)
Cd(2)-O(7)	2.363(3)	Cd(2)-O(6)	2.438(4)	Cd(2)-O(5)#1	2.439(4)
Cd(2)-O(4)	2.479(4)				
O(1)-Cd(1)-O(1)#1	95.7(2)	O(1)-Cd(1)-O(5)#1	98.54(13)	O(1)#1-Cd(1)-O(5)#1	99.72(14)
O(1)-Cd(1)-O(5)	99.72(14)	O(1)#1-Cd(1)-O(5)	98.54(13)	O(5)#1-Cd(1)-O(5)	152.65(18)
O(1)-Cd(1)-O(7)	90.00(14)	O(1)#1-Cd(1)-O(7)	173.96(14)	O(5)#1-Cd(1)-O(7)	81.25(12)
O(5)-Cd(1)-O(7)	78.56(12)	O(1)-Cd(1)-O(7)#1	173.96(14)	O(1)#1-Cd(1)-O(7)#1	90.00(14)
O(5)#1-Cd(1)-O(7)#1	78.56(12)	O(5)-Cd(1)-O(7)#1	81.25(12)	O(7)-Cd(1)-O(7)#1	84.34(17)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y,-z #2 x-1/2,y+1/2,z #3 x+1/2,y-1/2,z

Selected bond distance (Å) and angles (˚) in coordination polymers **5**.

5					
Cd(1)-O(3)	2.232(7)	Cd(1)-O(13)	2.289(6)	Cd(1)-N(4)	2.330(8)
Cd(1)-N(1)	2.340(8)	Cd(1)-O(9)	2.354(6)	Cd(1)-O(8)	2.451(6)
Cd(2)-O(14)	2.220(6)	Cd(2)-O(4)	2.232(7)	Cd(2)-N(2)#1	2.252(9)
Cd(2)-O(9)	2.278(6)	Cd(2)-O(11)	2.307(6)	Cd(2)-O(2)	2.444(6)
Cd(3)-N(3)	2.280(8)	Cd(3)-O(7)	2.308(7)	Cd(3)-O(10)	2.331(6)
Cd(3)-O(2)	2.361(6)	Cd(3)-O(1)	2.410(7)	Cd(3)-O(6)	2.448(7)
Cd(3)-O(11)	2.594(6)				
O(3)-Cd(1)-O(13)	114.4(3)	O(3)-Cd(1)-N(4)	100.6(3)	O(13)-Cd(1)-N(4)	82.5(3)
O(3)-Cd(1)-N(1)	86.6(3)	O(13)-Cd(1)-N(1)	157.3(3)	N(4)-Cd(1)-N(1)	85.4(3)
O(3)-Cd(1)-O(9)	95.1(2)	O(13)-Cd(1)-O(9)	85.9(2)	N(4)-Cd(1)-O(9)	163.3(2)
N(1)-Cd(1)-O(9)	101.3(2)	O(3)-Cd(1)-O(8)	145.7(2)	O(13)-Cd(1)-O(8)	81.9(2)
N(4)-Cd(1)-O(8)	111.8(3)	N(1)-Cd(1)-O(8)	85.0(3)	O(9)-Cd(1)-O(8)	54.4(2)
O(14)-Cd(2)-O(4)	88.4(2)	O(14)-Cd(2)-N(2)#1	88.3(3)	O(4)-Cd(2)-N(2)#1	103.9(3)
O(14)-Cd(2)-O(9)	93.4(2)	O(4)-Cd(2)-O(9)	97.4(3)	N(2)#1-Cd(2)-O(9)	158.7(3)
O(14)-Cd(2)-O(11)	121.4(2)	O(4)-Cd(2)-O(11)	150.0(2)	N(2)#1-Cd(2)-O(11)	81.3(3)
O(9)-Cd(2)-O(11)	79.7(2)	O(14)-Cd(2)-O(2)	160.5(2)	O(4)-Cd(2)-O(2)	73.7(2)
N(2)#1-Cd(2)-O(2)	103.2(3)	O(9)-Cd(2)-O(2)	81.5(2)	O(11)-Cd(2)-O(2)	76.3(2)
N(3)-Cd(3)-O(7)	136.5(3)	N(3)-Cd(3)-O(10)	101.8(3)	O(7)-Cd(3)-O(10)	85.8(3)
N(3)-Cd(3)-O(2)	128.3(3)	O(7)-Cd(3)-O(2)	91.3(2)	O(10)-Cd(3)-O(2)	99.6(2)
N(3)-Cd(3)-O(1)	95.8(3)	O(7)-Cd(3)-O(1)	94.2(3)	O(10)-Cd(3)-O(1)	154.3(2)
O(2)-Cd(3)-O(1)	54.8(2)	N(3)-Cd(3)-O(6)	82.8(3)	O(7)-Cd(3)-O(6)	54.4(2)
O(10)-Cd(3)-O(6)	107.6(2)	O(2)-Cd(3)-O(6)	133.0(2)	O(1)-Cd(3)-O(6)	92.9(3)
N(3)-Cd(3)-O(11)	84.0(2)	O(7)-Cd(3)-O(11)	130.4(2)	O(10)-Cd(3)-O(11)	53.1(2)
O(2)-Cd(3)-O(11)	72.6(2)	O(1)-Cd(3)-O(11)	111.3(2)	O(6)-Cd(3)-O(11)	153.4(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 -x+1,-y+1,-z #3 -x+1,-y+2,-z+1 #4 x-1,y,z-1 #5 x+1,y,z+1

#6 x,y,z+1

References

1. Q. R. Wu, X. L. Chen, H. M. Hu, T. Qin, F. Fu, B. Zhang, X. L. Wu, M. L. Yang, G. L. Xue and L. F. Xu, *Inorg. Chem. Commun.*, 2008, **11**, 28-32.
2. H. L. Wang, D. P. Zhang, D. F. Sun, Y. T. Chen, L. F. Zhang, L. J. Tian, J. Z. Jiang and Z. H. Ni, *Cryst. Growth Des.*, 2009, **9**, 5273-5282.
3. H. L. Wang, K. Wang, D. F. Sun, Z. H. Ni and J. Z. Jiang, *CrystEngComm*, 2011, **13**, 279-286.
4. S. Q. Zhang, F. L. Jiang, Y. Bu, M. Y. Wu, J. Ma, X. C. Shan, K. C. Xiong and M. C. Hong, *CrystEngComm*, 2012, **14**, 6394-6396.
5. S. Q. Zhang, F. L. Jiang, M. Y. Wu, J. Ma, Y. Bu and M. C. Hong, *Cryst. Growth Des.*, 2012, **12**, 1452-1463.
6. Z. Jin, H. Y. Zhao, X. J. Zhao, X. D. Yao and G. S. Zhu, *Inorg. Chem. Commun.*, 2014, **46**, 329-334.
7. H. L. Wang, D. P. Zhang, D. F. Sun, Y. T. Chen, K. Wang, Z. H. Ni, L. J. Tian and J. Z. Jiang, *CrystEngComm*, 2010, **12**, 1096-1102.
8. J. Chen, L. Hou, Y. N. Zhang, L. Cui, Q. Z. Shi and Y. Y. Wang, *Inorg. Chem. Commun.*, 2012, **24**, 73-76.
9. W. Yang, C. M. Wang, Q. Ma, X. N. Feng, H. L. Wang and J. Z. Jiang, *Cryst. Growth Des.*, 2013, **13**, 4695-4704.
10. J. Chen, G. P. Yang, W. H. Huang, L. Y. Pang, C. P. Zhang, Y. Y. Wang and Q. Z. Shi, *Inorganica Chimica Acta*, 2013, **400**, 7-12.
11. J. Chen, L. Hou, W. H. Huang, W. P. Wu, C. P. Zhang, Y. Y. Wang and Q. Z. Shi, *Inorg. Chem. Commun.*, 2013, **36**, 14-17.
12. W. Yang, C. M. Wang, Q. Ma, C. X. Liu, H. L. Wang and J. Z. Jiang, *CrystEngComm*, 2014, **16**, 4554-4561.
13. L. Cui, G. P. Yang, W. P. Wu, H. H. Miao, Q. Z. Shi and Y. Y. Wang, *Dalton Trans*, 2014, **43**, 5823-5830.
14. X. Chen, Y. Y. Wang, B. Liu, B. Yin, P. Liu and Q. Z. Shi, *Dalton Trans*, 2013, **42**, 7092-7100.