

Electronic Supplementary Information (ESI) for

Structural Diversity, Magnetic Properties, and Luminescence Sensing of Five 3D Coordination Polymers Derived From Designed 3,5-Di(2',4'-dicarboxylphenyl)benzoic Acid

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Section 1. Preparation of 1-5

Preparation of complex 1. A mixture of H₅DDB (0.10 mmol, 0.045 g), bib (0.30 mmol, 0.072 g), Co(NO₃)₂·6H₂O (0.30 mmol, 0.087 g), NaOH (0.30 mmol, 0.012 g) and 9 mL H₂O in a 25mL Teflon-lined stainless steel vessel was put into an oven at 150 °C for 5 days, and then was cooled to room temperature slowly. Purple block crystals of **1** were obtained with the yield of ca. 57% (based on H₅DDB). Anal. Calcd. for C₄₇H₃₆Co₂N₈O₁₃: C, 54.35; H, 3.49; N, 10.79 (%). Found: C, 54.17; H, 3.61; N, 10.82 (%). IR (cm⁻¹, KBr): 3392 (m), 1676 (m), 1537 (s), 1432 (m), 1369 (s), 1247 (m), 1071 (m), 939 (s), 831 (m), 761 (m), 654 (m).

Preparation of complex 2. A mixture of H₅DDB (0.10 mmol, 0.045 g), bib (0.30 mmol, 0.072 g), Mn(ClO₄)₂·6H₂O (0.30 mmol, 0.108 g), NaOH (0.15 mmol, 0.006 g) and 9 mL H₂O in a 25mL Teflon-lined stainless steel vessel was put into an oven at 150 °C for 5 days, and then was cooled to room temperature slowly. Colorless block crystals of **2** were obtained with the yield of ca. 45% (based on H₅DDB). Anal. Calcd. for C₁₄₀H₉₈Mn₅N₁₆O₄₆: C, 55.77; H, 3.27; N, 7.43. Found: C, 55.91; H, 3.21; N, 7.67. IR (KBr pellet, cm⁻¹): 3396 (s), 1669 (m), 1536 (vs), 1437 (m), 1386 (s), 1249 (m), 1110 (m), 1067 (m), 943 (m), 828 (m), 778 (w), 642 (w).

Preparation of 3-5. a mixture of H₅DDB (0.10 mmol, 0.045 g), bib (0.30 mmol, 0.072 g, for **3**) or bimb (0.30 mmol, 0.077 g for **4&5**), 3CdSO₄·8H₂O (0.10 mmol, 0.077 g), NaOH (0.15 mmol, 0.006 g) and 9 mL H₂O in a 25mL Teflon-lined stainless steel vessel was put into an oven at 150 °C for 5 days, and then was slowly cooled to room temperature with a descent rate of 10 °C/h. Colorless block crystals were obtained with the yield of ca. 43% (based on H₅DDB) for **3**. Anal. Calcd for C₄₁H₂₉Cd₂N₆O₁₂: C, 48.16; H, 2.86; N, 8.22 (%). Found: C, 48.07; H, 2.91; N, 8.19 (%). IR (cm⁻¹, KBr): 3128 (m), 1670 (m), 1607 (s), 1530 (s), 1429 (m), 1376 (s), 1311 (s), 1252 (s), 1116 (m), 1062 (s), 932 (m), 838 (m), 743 (s), 689 (m), 654 (s). The yield is ca. 57% (based on H₅DDB) for **4**. Anal. Calcd for C₃₇H₂₆Cd₂N₄O₁₁: C, 47.92; H, 2.83; N, 6.04 (%). Found: C, 47.91; H, 2.79; N, 6.13 (%). IR (cm⁻¹, KBr): 3392 (m), 1713 (m), 1573 (s), 1445 (m), 1515 (s), 1368 (s), 1236 (m), 1110 (m), 1086 (m), 1032 (m), 939 (s), 823 (m), 775 (m), 792 (m), 694 (m), 654 (m). The yield of **5** is about 61% (based on H₅DDB). Anal. Calcd for C₈₈H₇₁Cd₄N₁₂O₂₅: C, 49.25; H, 3.33; N, 7.83 (%). Found: C, 49.37; H, 3.36; N, 7.93 (%). IR (cm⁻¹, KBr): 3126 (m), 1532 (s), 1428 (m), 1362 (vs), 1174 (w), 1087 (m), 936 (m), 822 (m), 765 (s), 696 (m), 655 (s).

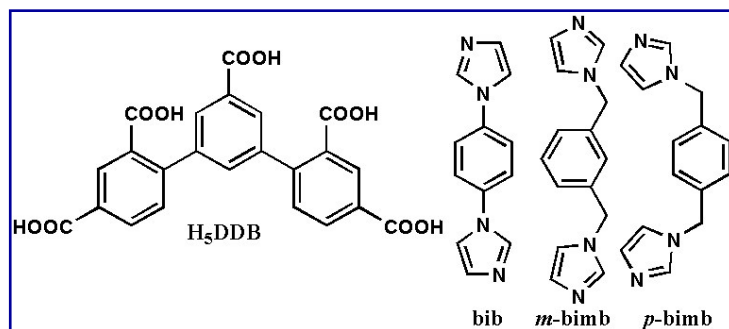


Figure S1. Selected organic ligands in this work.

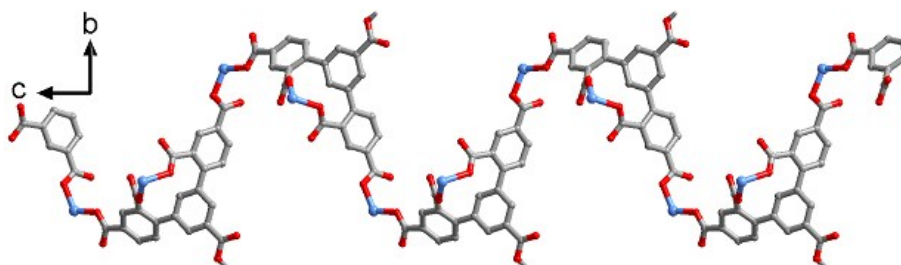


Figure S2. The 1D [Co₂(HDDB)]_n along *a* axis in 1.

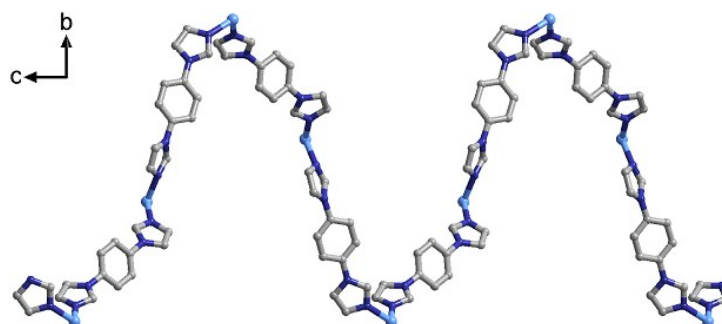


Figure S3. The 1D [Co₂(bib)₂]_n chain along *a* axis in 1.

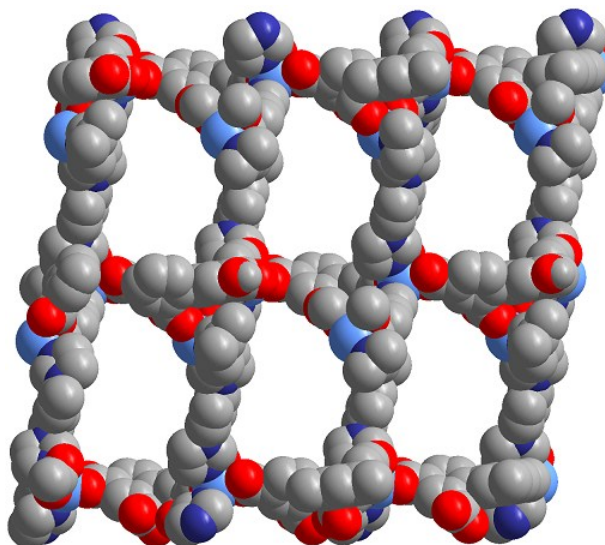


Figure S4. The 3D framework of 1.

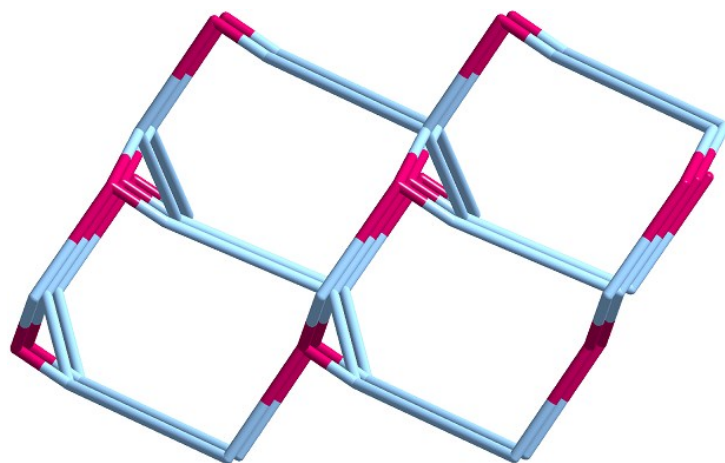


Figure S5. The single 3D (3,4)-c net for **1**.

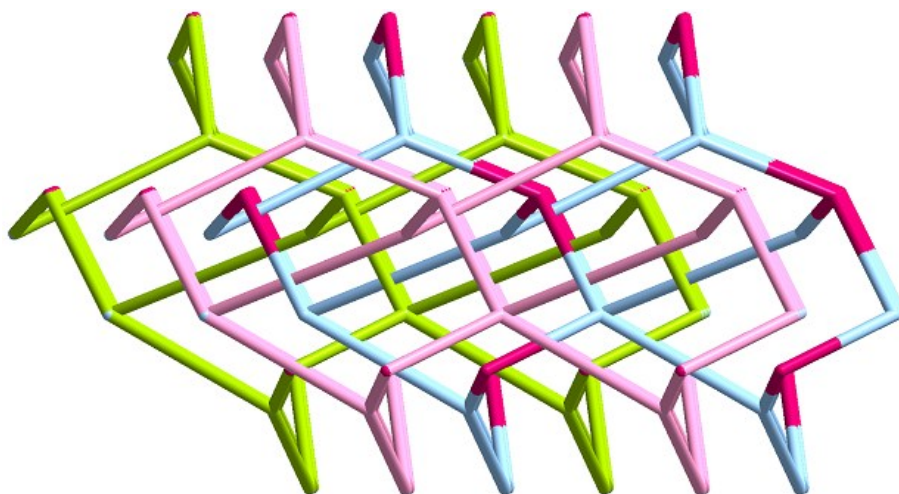


Figure S6. The 3-fold interpenetrated **vtX** nets for **1**.

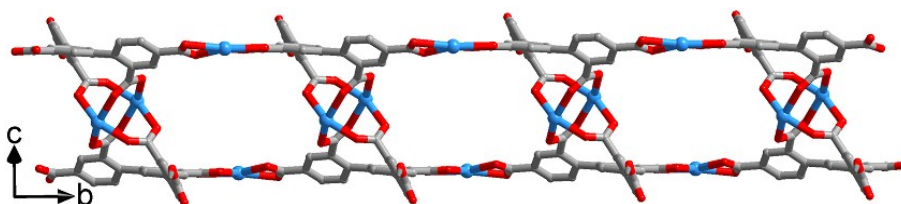


Figure S7. The 1D $[\text{Cd}_2(\text{HDDDB})]_n$ chain along *a* axis in **3**.

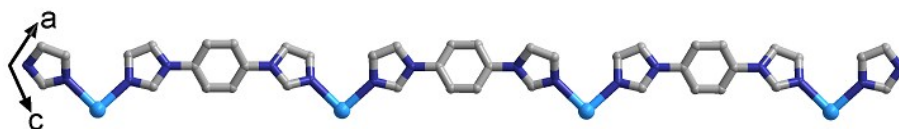


Figure S8. The 1D $\{\text{Cd}(\text{cis-bib})\}_n$ chain along *b* axis in **3**.



Figure S9. The *trans*-bib linked the $\{\text{Cd}_2(\text{COO})_4\}$ SBUs to form a 1D chain along *b* axis in **3**.

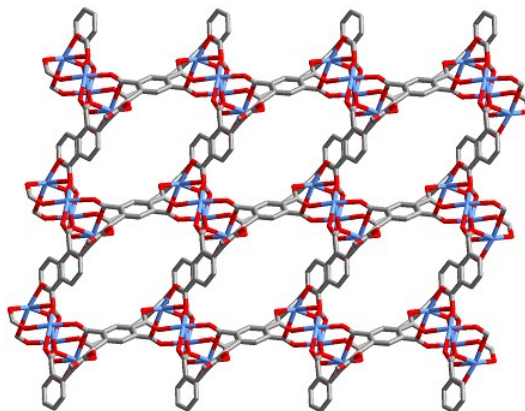


Figure S10. The 2D $[\text{Cd}_2(\text{HDDDB})]_n$ bilayer in **4**.

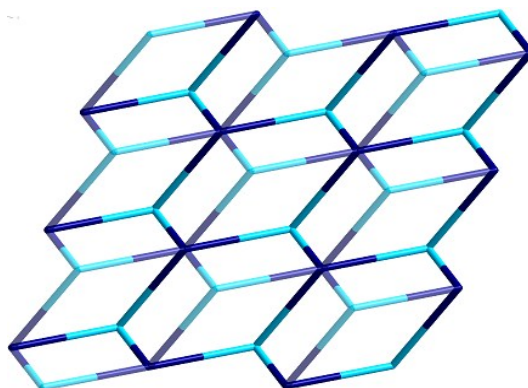


Figure S11. The simplified 3,6-connected $\{4^3\}_2\{4^6.6^6.8^3\}$ -kgm sheet for $[\text{Cd}_2(\text{HDDDB})]_n$ bilayer in **4**.

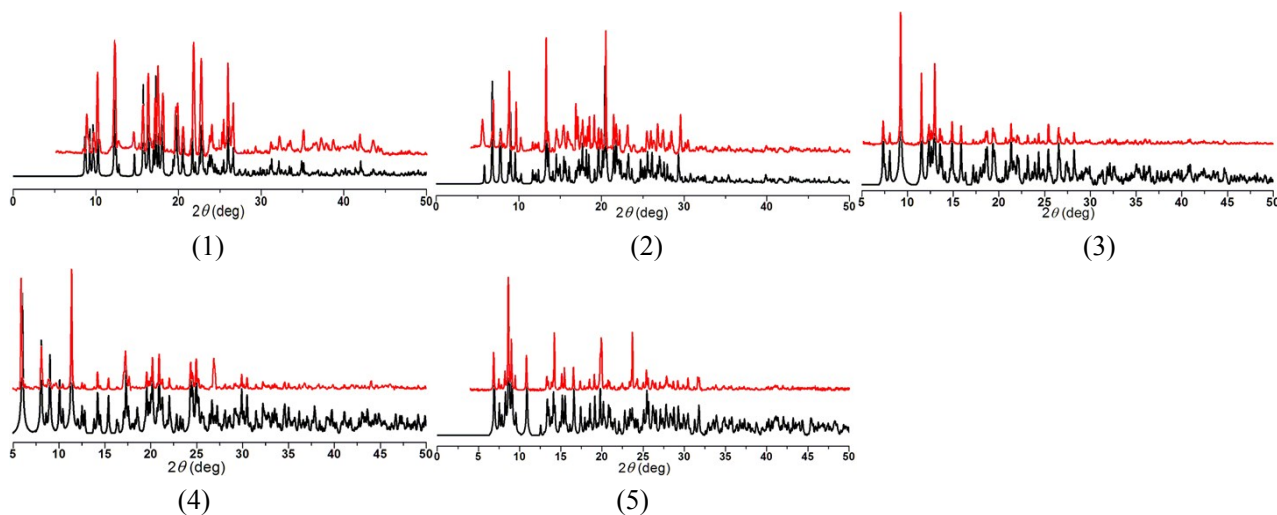


Figure S12. PXRD patterns of **1-5**. Dark: calculated from the X-ray single-crystal data; Red: observed for the as-synthesized solids.

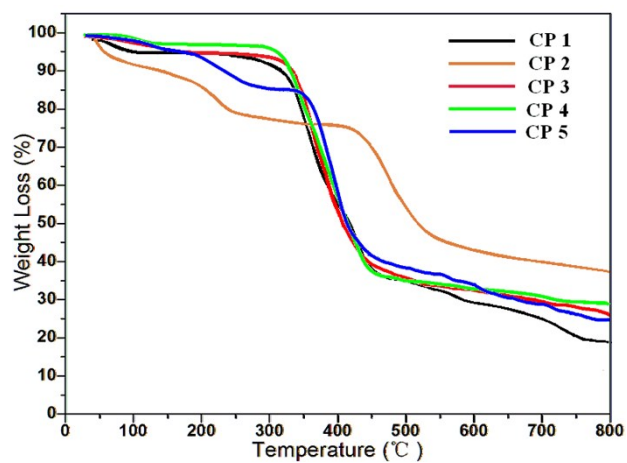


Figure S13. TGA curves for complexes 1-5.

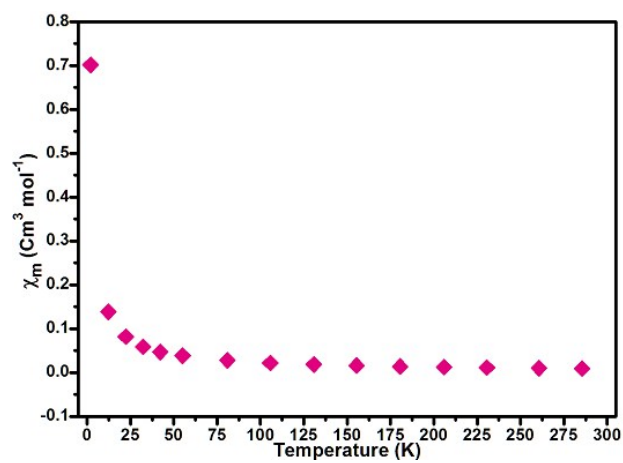


Figure S14. The χ_M -T curve of 1.

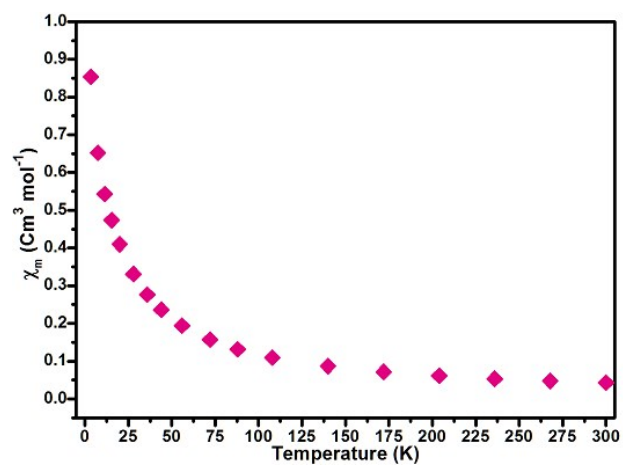


Figure S15. The χ_M -T curve of 2.

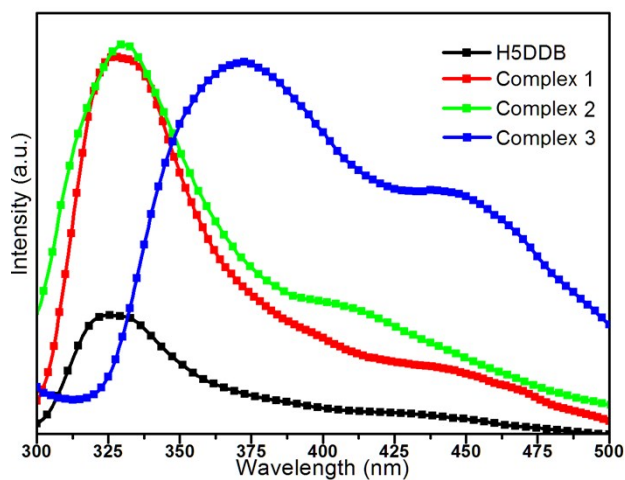


Figure S16. The fluorescence spectrum of free H₅DDB and **3-5**.

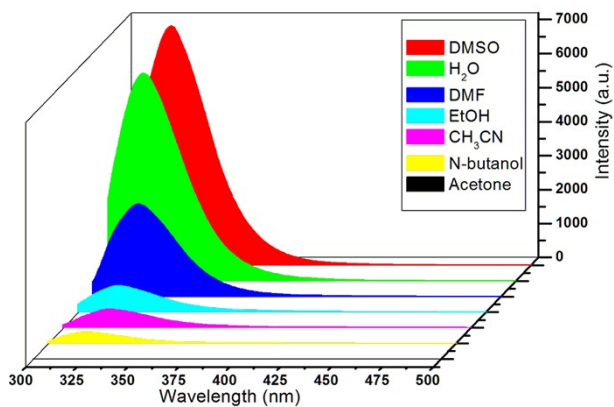


Figure S17. The luminescence intensities of complex **3** after dispersed in different organic solvents.

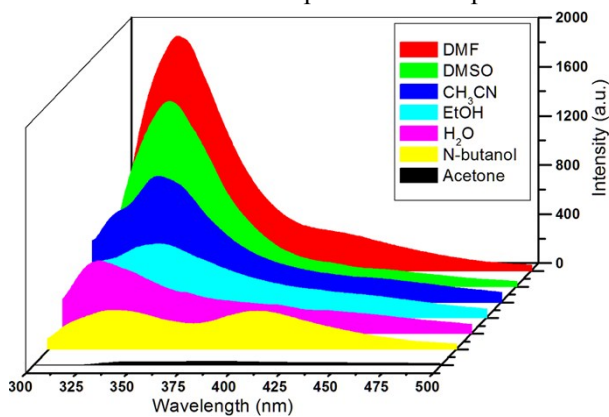


Figure S18. The luminescence intensities of complex **4** after dispersed in different organic solvents.

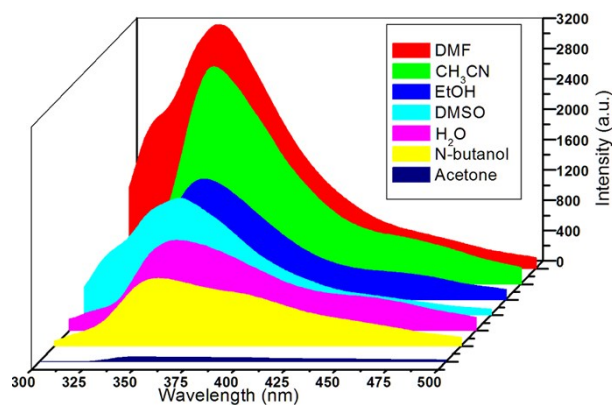


Figure S19. The luminescence intensities of complex **5** after dispersed in different organic solvents.

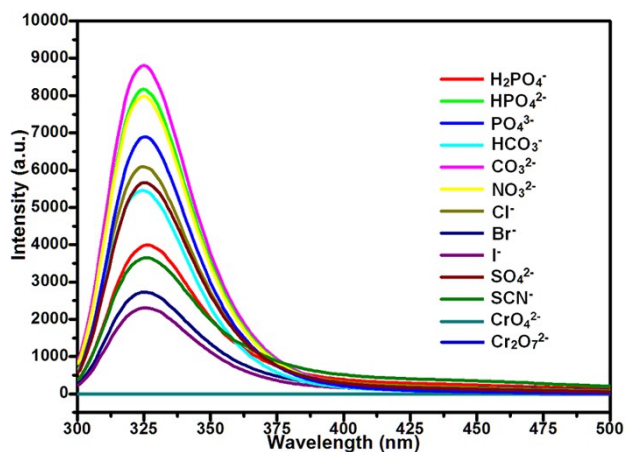


Figure S20. The luminescence intensities of **3** which were dispersed in the aqueous solution of different anions.

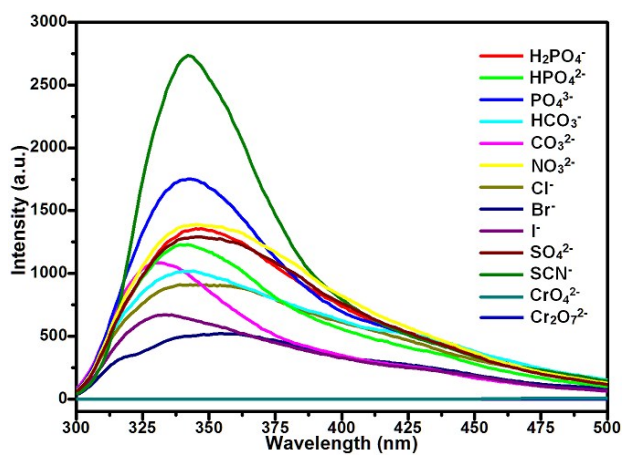


Figure S21. The luminescence intensities of **4** which were dispersed in the aqueous solution of different anions.

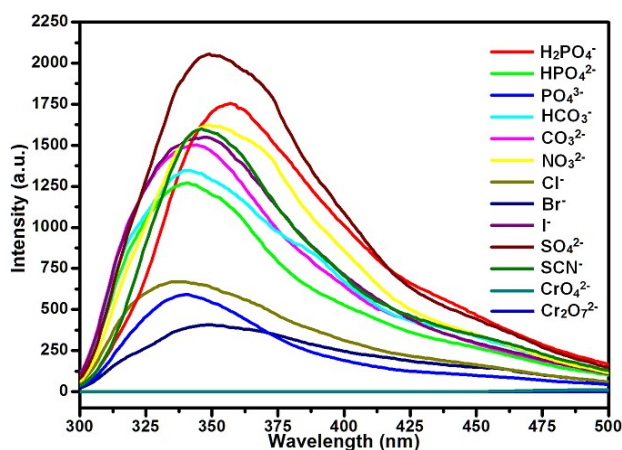


Figure S22. The luminescence intensities of **5** which were dispersed in the aqueous solution of different anions.

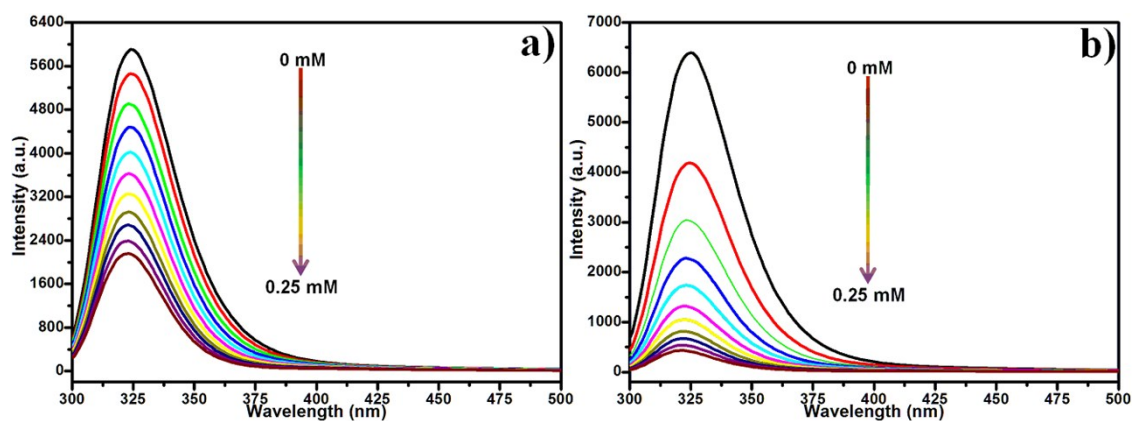


Figure S23. The luminescence intensities of complex **3** with increasing addition of CrO_4^{2-} (a) and $\text{Cr}_2\text{O}_7^{2-}$ (b).

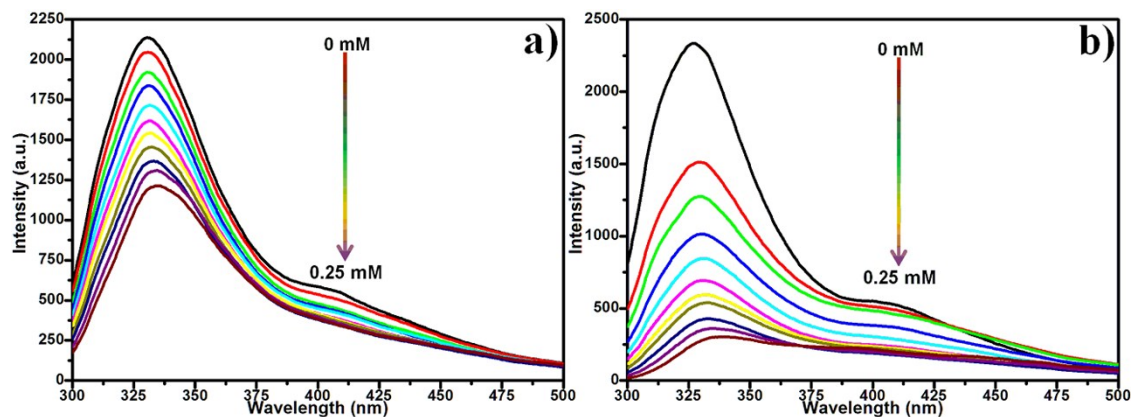


Figure S24. The luminescence intensities of complex **4** with increasing addition of CrO_4^{2-} (a) and $\text{Cr}_2\text{O}_7^{2-}$ (b).

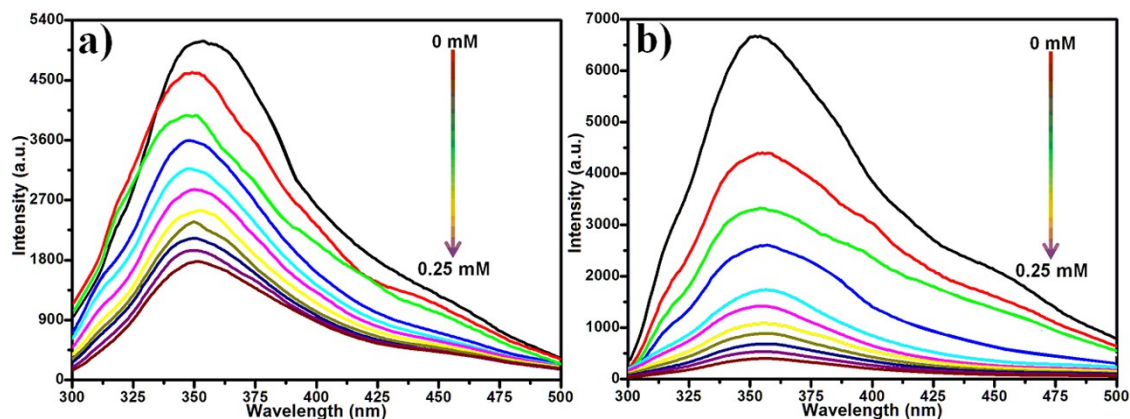


Figure S25. The luminescence intensities of complex **5** with increasing addition of CrO_4^{2-} (a) and $\text{Cr}_2\text{O}_7^{2-}$ (b).

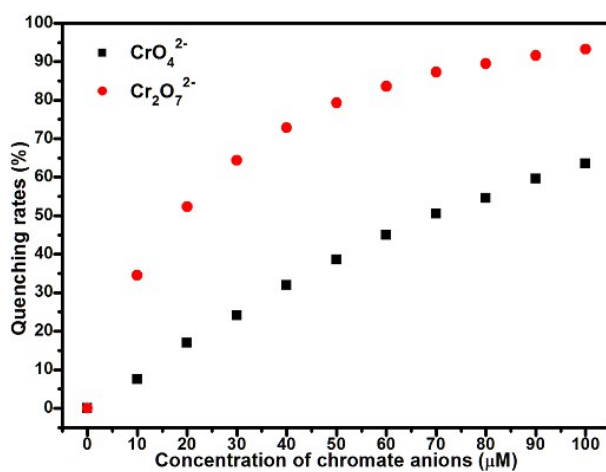


Figure S26 The quenching rates of **3** with different concentrations of chromate anions in aqueous solution.

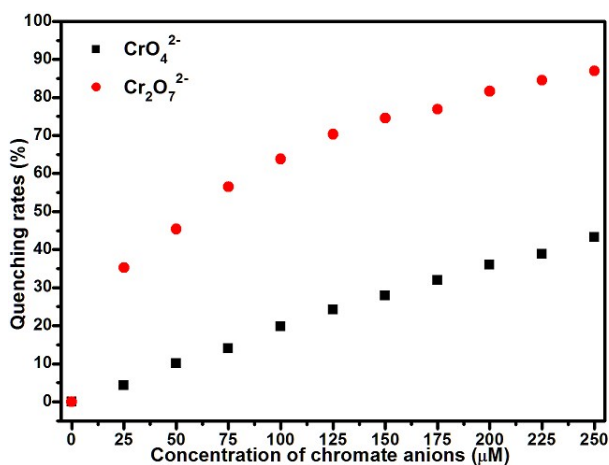


Figure S27 The quenching rates of **4** with different concentrations of chromate anions in aqueous solution.

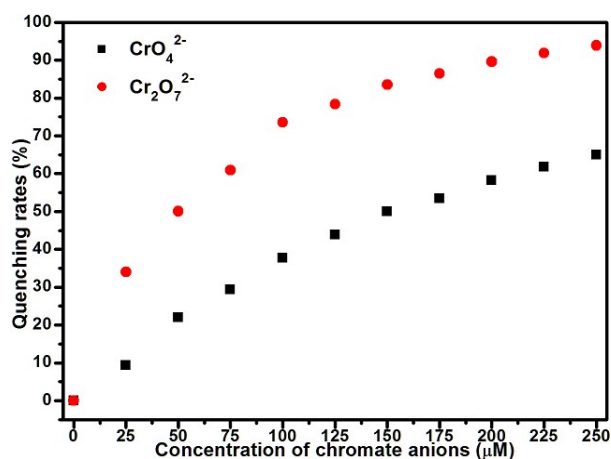


Figure S28 The quenching rates of **5** with different concentrations of chromate anions in aqueous solution.

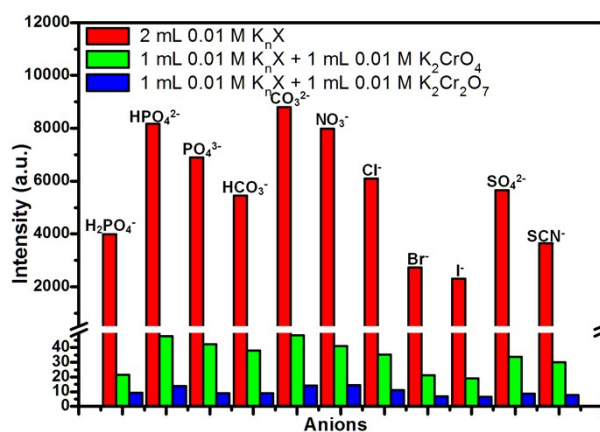


Figure S29 The anti-interferences of **3** in sensing of $CrO_4^{2-}/Cr_2O_7^{2-}$ anions from normal anions in aqueous solution.

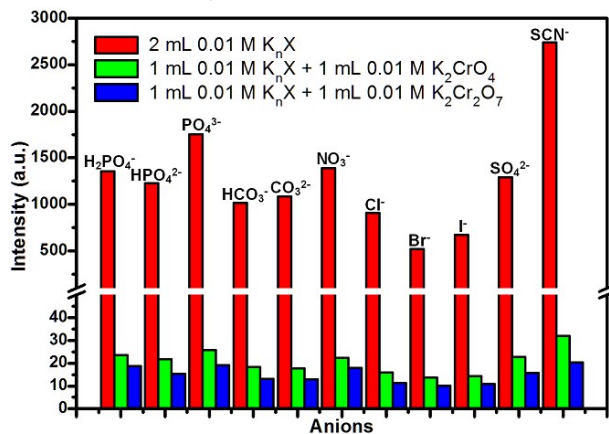


Figure S30 The anti-interferences of **4** in sensing of $CrO_4^{2-}/Cr_2O_7^{2-}$ anions from normal anions in aqueous solution.

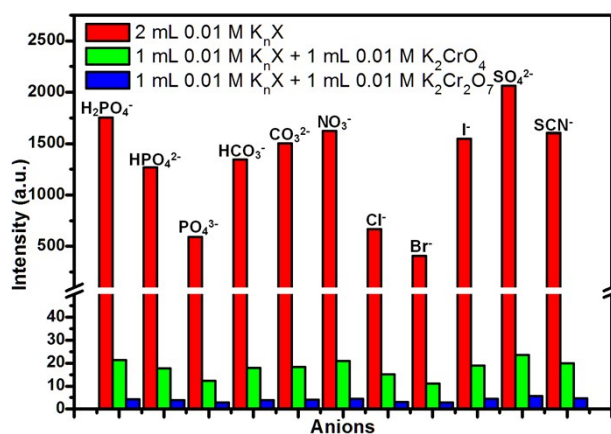


Figure S31 The anti-interferences of **5** in sensing of $\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$ anions from normal anions in aqueous solution.

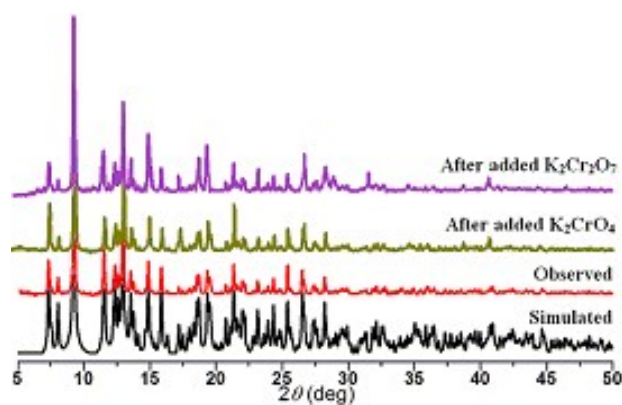


Figure S32. The PXRD pattern of **3** after immersing in analytes.

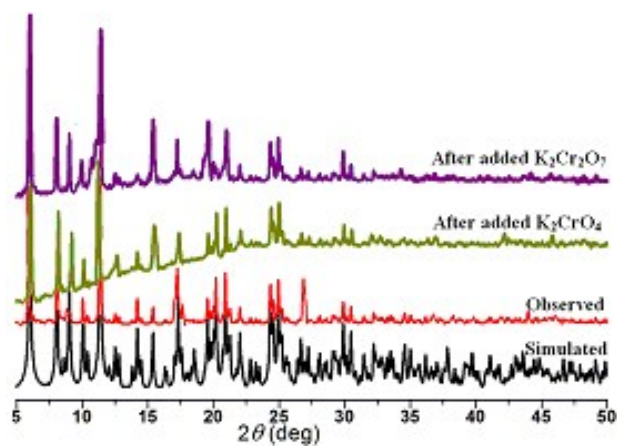


Figure S33. The PXRD pattern of **4** after immersing in analytes.

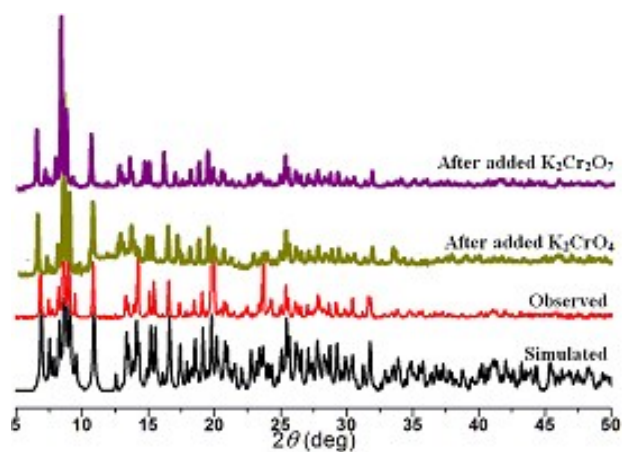


Figure S34. The PXRD pattern of **5** after immersing in analytes.

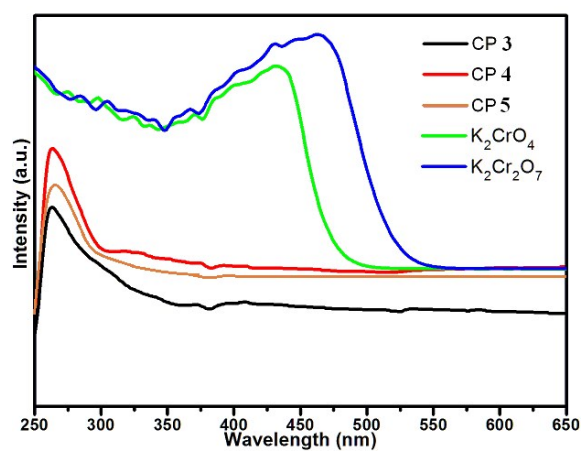


Figure S35. The UV-Vis spectrum of chromate anions and CP **3-5**.

Table S1 Crystal data for 1–5

Compound	1	2	3	4	5
Empirical formula	C ₄₇ H ₃₆ Co ₂ N ₈ O ₁₃	C ₁₄₀ H ₉₈ Mn ₅ N ₁₆ O ₄₆	C ₁₆₄ H ₁₂₈ Cd ₈ N ₂₄ O ₅₄	C ₃₇ H ₂₆ Cd ₂ N ₄ O ₁₁	C ₈₈ H ₇₁ Cd ₄ N ₁₂ O ₂₅
Formula weight	1038.70	3015.04	4198.10	927.42	2146.17
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	<i>Cc</i>	<i>P2₁/n</i>	<i>I2/a</i>	<i>P2₁/c</i>	<i>P</i> -1
<i>a</i> (Å)	12.0843(6)	13.928(5)	25.7978(13)	11.0510(4)	13.2168(5)
<i>b</i> (Å)	19.0920(9)	22.935(8)	14.0191(5)	29.4197(11)	13.4274(5)
<i>c</i> (Å)	20.1439(10)	21.219(6)	26.2388(9)	10.4787(4)	13.7151(5)
α (°)	90	90	90	90	74.3210(10)
β (°)	91.114(2)	107.49(2)	114.875(3)	97.2150(10)	70.0860(10)
γ (°)	90	90	90	90	61.7430(10)
<i>V</i> (Å ³)	4646.6(4)	6465(4)	8609.2(6)	3379.8(2)	1998.20(13)
<i>Z</i>	4	2	2	4	1
<i>D</i> _{calcd} (Mg/m ³)	1.485	1.549	1.619	1.823	1.784
μ (mm ⁻¹)	0.789	0.575	1.060	1.330	1.142
<i>T</i> (K)	296(2)	293(2)	296(2)	295(2)	293(2)
<i>F</i> (000)	2128	3086	4192	1840	1075
<i>R</i> _{int}	0.0883	0.0527	0.0677	0.0855	0.0514
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)] ^a	<i>R</i> ₁ = 0.0656, <i>R</i> ₂ = 0.1122	<i>R</i> ₁ = 0.0634, <i>R</i> ₂ = 0.1741	<i>R</i> ₁ = 0.0587, <i>R</i> ₂ = 0.1533	<i>R</i> ₁ = 0.0398, <i>wR</i> ₂ = 0.0844	<i>R</i> ₁ = 0.0300, <i>wR</i> ₂ = 0.0729
<i>R</i> indices (all data) ^a	<i>R</i> ₁ = 0.1127, <i>wR</i> ₂ = 0.1294	<i>R</i> ₁ = 0.1070, <i>wR</i> ₂ = 0.2025	<i>R</i> ₁ = 0.0827, <i>wR</i> ₂ = 0.1667	<i>R</i> ₁ = 0.0652, <i>wR</i> ₂ = 0.0927	<i>R</i> ₁ = 0.0342, <i>wR</i> ₂ = 0.0751
Gof	1.090	1.032	1.041	1.020	0.999

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|, wR_2 = [\sum w(F_o^2 - F_c^2)^2] / \sum w(F_o^2)^2]^{1/2}$$

Table S2 Selected bond lengths (Å) and angles (°) for 1-5.

Complex 1							
Co(1)-O(7)	2.080(5)	Co(1)-N(4) ^{#1}	2.135(6)	Co(2)-O(12)	1.923(6)	Co(2)-N(1)	1.996(7)
Co(1)-O(1)	2.087(5)	Co(1)-O(4)	2.158(6)	Co(2)-O(9) ^{#2}	1.933(5)	Co(2)-N(5) ^{#3}	2.035(7)
Co(1)-N(8)	2.095(6)	Co(1)-O(11)	2.196(5)	O(7)-Co(1)-O(11)	172.0(2)	O(12)-Co(2)-N(1)	117.6(3)
O(7)-Co(1)-O(1)	88.0(2)	N(8)-Co(1)-N(4) ^{#1}	91.3(3)	O(1)-Co(1)-O(11)	85.2(2)	O(9) ^{#2} -Co(2)-N(1)	112.4(3)
O(7)-Co(1)-N(8)	97.6(2)	O(7)-Co(1)-O(4)	92.5(2)	N(8)-Co(1)-O(11)	86.5(2)	O(12)-Co(2)-N(5) ^{#3}	109.0(3)
O(1)-Co(1)-N(8)	88.4(2)	O(1)-Co(1)-O(4)	90.7(2)	N(4) ^{#1} -Co(1)-O(11)	95.6(2)	O(9) ^{#2} -Co(2)-N(5) ^{#3}	101.6(3)
O(7)-Co(1)-N(4) ^{#1}	91.2(2)	N(8)-Co(1)-O(4)	169.8(2)	O(4)-Co(1)-O(11)	83.3(2)	N(1)-Co(2)-N(5) ^{#3}	99.9(3)
O(1)-Co(1)-N(4) ^{#1}	179.1(2)	N(4) ^{#1} -Co(1)-O(4)	89.8(2)	O(12)-Co(2)-O(9) ^{#2}	113.9(3)		
Symmetry codes: #1 x+3/2, y+1/2, z; #2 x-1/2, -y+3/2, z+1/2; #3 x-1/2, -y+1/2, z+1/2.							
Complex 2							
Mn(1)-O(17)	2.106(2)	Mn(1)-N(7)	2.352(8)	Mn(2)-O(18) ^{#1}	2.223(2)	Mn(3)-O(12) ^{#3}	2.168(3)
Mn(1)-O(6)	2.117(3)	Mn(1)-O(22)	2.463(3)	Mn(2)-O(5)	2.239(3)	Mn(3)-O(20)	2.184(3)
Mn(1)-O(16)	2.150(3)	Mn(2)-O(22) ^{#1}	2.192(2)	Mn(2)-O(5) ^{#1}	2.239(3)	Mn(3)-O(19)	2.346(3)
Mn(1)-O(4)	2.155(2)	Mn(2)-O(22)	2.192(2)	Mn(3)-O(2) ^{#1}	2.105(3)	Mn(3)-O(21)	2.430(5)
Mn(1)-O(24)	2.201(8)	Mn(2)-O(18)	2.223(2)	Mn(3)-O(1) ^{#2}	2.133(3)	O(17)-Mn(1)-O(6)	89.55(11)
O(17)-Mn(1)-O(16)	91.18(11)	O(17)-Mn(1)-O(22)	90.28(9)	O(22) ^{#1} -Mn(2)-O(5)	91.38(10)	O(2) ^{#1} -Mn(3)-O(20)	153.53(10)
O(6)-Mn(1)-O(16)	179.02(9)	O(6)-Mn(1)-O(22)	94.13(9)	O(22)-Mn(2)-O(5)	88.62(10)	O(1) ^{#2} -Mn(3)-O(20)	95.84(11)
O(17)-Mn(1)-O(4)	175.66(9)	O(16)-Mn(1)-O(22)	86.52(9)	O(12) ^{#3} -Mn(3)-O(20)	92.23(11)	O(18)-Mn(2)-O(5)	96.73(11)
O(6)-Mn(1)-O(4)	90.28(10)	O(4)-Mn(1)-O(22)	85.41(8)	O(12) ^{#3} -Mn(3)-O(19)	91.07(10)	O(2) ^{#1} -Mn(3)-O(19)	95.33(9)
O(16)-Mn(1)-O(4)	89.05(10)	O(24)-Mn(1)-O(22)	166.7(3)	O(22) ^{#1} -Mn(2)-O(5) ^{#1}	88.62(10)	O(1) ^{#2} -Mn(3)-O(19)	153.97(10)
O(17)-Mn(1)-O(24)	83.7(2)	N(7)-Mn(1)-O(22)	166.5(2)	O(22)-Mn(2)-O(5) ^{#1}	91.38(10)	O(5)-Mn(2)-O(5) ^{#1}	180.0
O(6)-Mn(1)-O(24)	97.7(3)	O(22) ^{#1} -Mn(2)-O(22)	180.0	O(18)-Mn(2)-O(5) ^{#1}	83.27(11)	O(20)-Mn(3)-O(19)	58.35(9)
O(16)-Mn(1)-O(24)	81.8(3)	O(22) ^{#1} -Mn(2)-O(18)	90.89(9)	O(18) ^{#1} -Mn(2)-O(5) ^{#1}	96.73(11)	O(2) ^{#1} -Mn(3)-O(21)	87.39(12)
O(4)-Mn(1)-O(24)	100.6(2)	O(22)-Mn(2)-O(18)	89.11(9)	O(12) ^{#3} -Mn(3)-O(21)	173.68(13)	O(1) ^{#2} -Mn(3)-O(21)	88.55(14)
O(17)-Mn(1)-N(7)	102.5(2)	O(22) ^{#1} -Mn(2)-O(18) ^{#1}	89.11(9)	O(2) ^{#1} -Mn(3)-O(1) ^{#2}	110.59(11)	O(18) ^{#1} -Mn(2)-O(5)	83.27(11)
O(6)-Mn(1)-N(7)	90.1(2)	O(22)-Mn(2)-O(18) ^{#1}	90.89(9)	O(2) ^{#1} -Mn(3)-O(12) ^{#3}	90.96(11)	O(20)-Mn(3)-O(21)	91.95(12)
O(16)-Mn(1)-N(7)	89.1(2)	O(18)-Mn(2)-O(18) ^{#1}	180.0	O(1) ^{#2} -Mn(3)-O(12) ^{#3}	86.32(11)	O(19)-Mn(3)-O(21)	95.16(14)
O(4)-Mn(1)-N(7)	81.79(19)						
Symmetry codes: #1 -x+1, -y, -z+1; #2 x, y, z+1; #3 x+1/2, -y+1/2, z+1/2.							
Complex 3							
Cd(1)-N(4)	2.301(5)	Cd(1)-O(11)	2.364(4)	Cd(1)-O(9)	2.499(4)	Cd(2)-O(4) ^{#3}	2.202(5)
Cd(1)-N(1) ^{#1}	2.335(5)	Cd(1)-O(7) ^{#2}	2.366(4)	Cd(2)-N(5)	2.162(5)	Cd(2)-O(3)	2.218(4)
Cd(1)-O(10)	2.357(4)	Cd(1)-O(8) ^{#2}	2.486(4)	Cd(2)-O(5)	2.189(4)	Cd(2)-O(6) ^{#3}	2.315(4)
N(4)-Cd(1)-N(1) ^{#1}	94.59(18)	O(10)-Cd(1)-O(7) ^{#2}	79.31(14)	N(1) ^{#1} -Cd(1)-O(9)	93.25(16)	N(5)-Cd(2)-O(3)	100.5(2)
N(5)-Cd(2)-O(4) ^{#3}	100.1(2)	O(11)-Cd(1)-O(7) ^{#2}	89.04(18)	N(1) ^{#1} -Cd(1)-O(7) ^{#2}	86.0(2)	O(5)-Cd(2)-O(3)	86.49(19)
N(1) ^{#1} -Cd(1)-O(10)	98.01(18)	N(4)-Cd(1)-O(8) ^{#2}	84.62(14)	N(4)-Cd(1)-O(7) ^{#2}	137.38(15)	O(4) ^{#3} -Cd(2)-O(3)	156.5(2)
N(4)-Cd(1)-O(11)	85.88(16)	N(1) ^{#1} -Cd(1)-O(8) ^{#2}	92.32(17)	O(7) ^{#2} -Cd(1)-O(9)	132.40(14)	N(5)-Cd(2)-O(6) ^{#3}	90.92(19)
O(11)-Cd(1)-O(9)	93.50(14)	O(10)-Cd(1)-O(8) ^{#2}	130.13(13)	O(8) ^{#2} -Cd(1)-O(9)	172.67(13)	O(5)-Cd(2)-O(6) ^{#3}	158.05(16)
O(10)-Cd(1)-O(11)	85.63(16)	O(11)-Cd(1)-O(8) ^{#2}	81.00(16)	N(5)-Cd(2)-O(5)	110.40(19)	O(4) ^{#3} -Cd(2)-O(6) ^{#3}	84.00(17)
O(10)-Cd(1)-O(9)	53.61(12)	O(7) ^{#2} -Cd(1)-O(8) ^{#2}	52.82(14)	N(1) ^{#1} -Cd(1)-O(11)	173.24(17)	O(3)-Cd(2)-O(6) ^{#3}	84.47(19)
N(4)-Cd(1)-O(9)	90.18(14)	N(4)-Cd(1)-O(10)	142.07(15)	O(5)-Cd(2)-O(4) ^{#3}	96.84(19)		
Symmetry codes: #1 x, -y+1/2, z-1/2; #2 x, y-1, z; #3 -x+3/2, -y+3/2, -z+1/2.							
Complex 4							
Cd(1)-O(2) ^{#1}	2.232(3)	Cd(1)-O(10)	2.307(2)	Cd(2)-N(1) ^{#4}	2.259(3)	Cd(2)-O(10)	2.349(2)
Cd(1)-O(8) ^{#2}	2.259(3)	Cd(1)-O(4)	2.330(2)	Cd(2)-O(1) ^{#5}	2.281(3)	Cd(2)-O(9)	2.444(3)
Cd(1)-N(4)	2.276(3)	Cd(2)-O(7) ^{#3}	2.251(3)	Cd(2)-O(3)	2.292(2)	O(2) ^{#1} -Cd(1)-O(8) ^{#2}	100.79(11)
O(2) ^{#1} -Cd(1)-N(4)	88.02(11)	O(8) ^{#2} -Cd(1)-O(4)	168.78(10)	O(7) ^{#3} -Cd(2)-O(3)	96.11(10)	O(3)-Cd(2)-O(10)	87.84(8)
O(8) ^{#2} -Cd(1)-N(4)	86.74(10)	O(2) ^{#1} -Cd(1)-O(10)	160.48(9)	N(1) ^{#4} -Cd(2)-O(3)	91.15(11)	O(7) ^{#3} -Cd(2)-O(9)	171.20(9)
N(4)-Cd(1)-O(4)	97.03(10)	N(4)-Cd(1)-O(10)	107.02(9)	O(1) ^{#5} -Cd(2)-O(3)	173.71(10)	N(1) ^{#4} -Cd(2)-O(9)	85.11(10)
O(8) ^{#2} -Cd(1)-O(10)	92.60(9)	O(7) ^{#3} -Cd(2)-N(1) ^{#4}	100.50(11)	O(7) ^{#3} -Cd(2)-O(10)	119.93(9)	O(1) ^{#5} -Cd(2)-O(9)	88.46(10)
O(10)-Cd(1)-O(4)	76.20(9)	O(7) ^{#3} -Cd(2)-O(1) ^{#5}	84.33(11)	N(1) ^{#4} -Cd(2)-O(10)	139.44(10)	O(3)-Cd(2)-O(9)	90.51(9)
O(2) ^{#1} -Cd(1)-O(4)	89.92(10)	N(1) ^{#4} -Cd(2)-O(1) ^{#5}	94.94(12)	O(1) ^{#5} -Cd(2)-O(10)	86.52(10)	O(10)-Cd(2)-O(9)	54.37(8)
Symmetry codes: #1 -x+1, -y+1, -z+1; #2 -x, -y+1, -z+2; #3 x, y, z-1; #4 x-1, -y+3/2, z-1/2; #5 x-1, y, z.							
Complex 5							
Cd(1)-N(4)	2.26(3)	Cd(1)-O(6)	2.48(3)	Cd(2)-N(1) ^{#3}	2.25(3)	Cd(2)-O(3) ^{#5}	2.37(2)
Cd(1)-O(7)	2.30(3)	Cd(1)-O(8)	2.49(3)	Cd(2)-O(1)	2.33(3)	Cd(2)-O(4) ^{#5}	2.41(2)
Cd(1)-O(4) ^{#1}	2.34(2)	Cd(1)-O(10) ^{#2}	2.57(3)	Cd(2)-O(9) ^{#4}	2.35(3)	Cd(2)-O(2)	2.41(3)
Cd(1)-O(5)	2.43(3)	O(5)-Cd(1)-O(6)	53.0(10)	O(5)-Cd(1)-O(10) ^{#2}	157.1(10)	N(1) ^{#3} -Cd(2)-O(4) ^{#5}	140.3(10)
N(4)-Cd(1)-O(7)	162.3(11)	N(4)-Cd(1)-O(8)	108.7(11)	O(6)-Cd(1)-O(10) ^{#2}	149.9(10)	O(1)-Cd(2)-O(4) ^{#5}	82.0(9)
N(4)-Cd(1)-O(4) ^{#1}	99.2(10)	O(7)-Cd(1)-O(8)	54.3(9)	O(8)-Cd(1)-O(10) ^{#2}	80.7(10)	O(9) ^{#4} -Cd(2)-O(4) ^{#5}	89.1(9)
O(7)-Cd(1)-O(4) ^{#1}	98.1(9)	O(4) ^{#1} -Cd(1)-O(8)	140.5(9)	N(1) ^{#3} -Cd(2)-O(1)	135.1(11)	O(3) ^{#5} -Cd(2)-O(4) ^{#5}	54.8(8)
N(4)-Cd(1)-O(5)	106.2(11)	O(5)-Cd(1)-O(8)	115.2(10)	N(1) ^{#3} -Cd(2)-O(9) ^{#4}	81.4(11)	N(1) ^{#3} -Cd(2)-O(2)	94.8(11)
O(7)-Cd(1)-O(5)	80.2(10)	O(6)-Cd(1)-O(8)	78.8(10)	O(1)-Cd(2)-O(9) ^{#4}	122.4(10)	O(1) ^{#5} -Cd(2)-O(2)	55.1(9)
O(4) ^{#1} -Cd(1)-O(5)	81.7(9)	N(4)-Cd(1)-O(10) ^{#2}	82.2(10)	N(1) ^{#3} -Cd(2)-O(3) ^{#5}	97.7(10)	O(9) ^{#4} -Cd(2)-O(2)	85.4(9)
N(4)-Cd(1)-O(6)	83.9(11)	O(7)-Cd(1)-O(10) ^{#2}	98.3(9)	O(1)-Cd(2)-O(3) ^{#5}	100.0(9)	O(3) ^{#5} -Cd(2)-O(2)	152.8(9)
O(7)-Cd(1)-O(6)	87.2(10)	O(4) ^{#1} -Cd(1)-O(10) ^{#2}	75.9(9)	O(9) ^{#4} -Cd(2)-O(3) ^{#5}	120.2(9)	O(4) ^{#5} -Cd(2)-O(2)	122.8(9)
O(4) ^{#1} -Cd(1)-O(6)	132.9(9)						
Symmetry codes: #1 -x+1, -y, -z+2; #2 -x+1, -y+1, -z+1; #3 x+1, y, z+1; #4 x, y, z+1; #5 x, y+1, z.							