Electronic Supplementary Information

Synthesis, structure, and photoluminescence properties of coordination polymers of 4,4′,4″,4‴-tetrakiscarboxyphenylsilane and 3,5-bis(1′,2′,4′-triazol-1′-yl) pyridine

Jing Sun[a], Tao Zhou[a], Dalong Pan[a], Xinzhu Zhang[a], Yuying Wang[a], Yao-Cheng Shi[a], Huaguang Yu[a,b,*]

[a] *College of Physics Science and Technology, and College of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou 225002, P. R. China*
[b] *School of Chemical and Environmental Engineering, Jianghan University, Wuhan 430056, P. R. China*

[*] Corresponding author. Tel.: +86-514-87975466; fax: +86-514-87975467.
Email address: hgyu@yzu.edu.cn (Huaguang Yu)

Contents

List of Tables

List of Figures

1. Material and methods

Metal nitrates ($M(NO_3)_x \cdot nH_2O$), 3,5-dibromopyridine ($C_5H_3Br_2N$), copper oxide (CuO), 1,2,4-triazole ($C_2H_3N_3$), potassium carbonate (K_2CO_3) and potassium hydroxide (KOH) were purchased from Sinopharm Chemical Reagent Corporation. ^{1}H and $^{13}C\{^1H\}$ nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AVANCE 600 spectrometer. The electrospray ionization mass spectrum (ESI-MS) was collected on a Bruker maXis mass spectrometer. 3,5-Bis(1′,2′,4′-triazol-1′-yl) pyridine (btap) was prepared according to the literature method [1] for the synthesis of 1,3-bis(1′,2′,4′-triazol-1′-yl) benzene with some modifications. The solution of 3,5-dibromopyridine (26.8 g, 113 mmol), 1,2,4-triazole (19.5 g, 283 mmol), copper(II) oxide (2.19 g, 28.3 mmol), potassium carbonate (39.1 g, 283 mmol), and DMSO (150 mL) was heated at 150 °C for 48 h. After cooling to room temperature, the mixture was diluted with 1.5 L CH_2Cl_2, and then filtered through a column of basic alumina. The filtrate was washed with CH_2Cl_2 (500 mL). CH_2Cl_2 was distilled off by rotary evaporation, and a yellow oil liquid was obtained. Saturated NaCl solution was added to it, and a white solid was precipitated. The mixture was filtered through a Buchner funnel, and washed with distilled water for three times. After drying in vacuum an off-white solid was got (19 g, 79 %). ^{1}H NMR (DMSO-d_6, 600.2 MHz): δ 9.5 (s, 2H), 9.2 (d, J = 2.3 Hz, 2H), 8.8 (t, J = 2.2 Hz, 1H), 8.4 (s, 2H). $^{13}C\{^1H\}$ NMR (DMSO-d_6, 150.9 MHz): δ 153.1, 143.4, 139.4, 133.7, 117.8. FT-IR (KBr pellet, cm^{-1}): 3078 (m), 1811 (w), 1596 (m), 1516 (s), 1412 (w), 1340 (w), 1284 (m), 1221 (s), 1133 (s), 982 (m), 886 (m), 790 (w), 663 (m), 471 (w). ESI-MS: m/z = 214.0819 $[M + H]^+$.

2. The crystal structure of compound 1

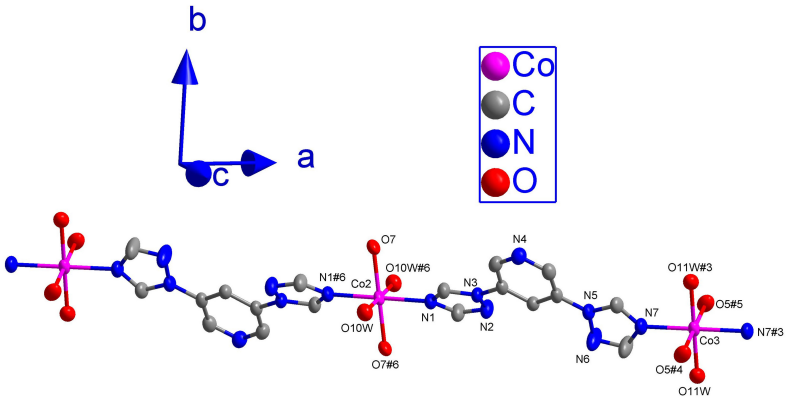

Figure S1: The 1D chain of Co2 and Co3 bridged by btap ligands in compound **1**.

Table S1: Selected bond lengths (Å) for compound **1**

bond	**length (Å)**	**bond**	**length (Å)**
Co1–O8	1.9567(19)	C31–C32	1.384(3)
Co1–O3#1 [1]	1.9298(19)	C31–C35	1.379(4)
Co1–O2#2 [1]	1.992(2)	N4–C35	1.338(3)
Co1–O9	1.961(2)	N4–C34	1.338(3)
Co3–N7	2.161(2)	C16–C17	1.383(4)
Co3–N7#3 [1]	2.161(2)	C16–C15	1.506(4)
Co3–O11	2.151(2)	C16–C21	1.385(4)
Co3–O11#3 [1]	2.151(2)	N5–C37	1.339(3)
Co3–O5#4 [1]	2.0323(18)	N5–N6	1.354(3)
Co3–O5#5 [1]	2.0323(18)	C4–C3	1.376(4)
Co2–O7#6 [1]	2.1060(18)	C28–C27	1.379(4)
Co2–O7	2.1060(18)	O1–C1	1.221(4)
Co2–N1#6 [1]	2.1581(19)	C25–C24	1.389(4)
Co2–N1	2.1581(19)	C29–N1	1.313(3)
Co2–O10	2.098(2)	C12–C13	1.392(4)
Co2–O10#6 [1]	2.098(2)	C18–C17	1.384(4)
Si1–C5	1.865(2)	C7–C6	1.379(4)
Si1–C26	1.873(2)	C7–C2	1.384(4)
Si1–C19	1.862(2)	C10–C9	1.374(4)
Si1–C12	1.870(2)	C37–N7	1.312(3)
C5–C4	1.389(3)	C14–C13	1.386(4)
C5–C6	1.399(4)	C14–C9	1.384(4)
N3–C31	1.430(3)	N1–C30	1.356(3)
N3–C29	1.334(3)	C20–C21	1.369(4)
N3–N2	1.367(3)	C3–C2	1.381(4)
O7–C22	1.250(3)	C2–C1	1.488(4)
C26–C25	1.391(3)	C1–O2	1.282(4)
C26–C27	1.397(4)	O6–C15	1.244(4)
C23–C22	1.504(3)	N2–C30	1.305(3)
C23–C28	1.385(4)	N6–C36	1.310(4)
C23–C24	1.379(4)	O4–C8	1.231(4)
C33–C32	1.384(3)	N7–C36	1.349(4)
C33–N5	1.421(3)	C8–C9	1.501(4)
C33–C34	1.374(4)	C8–O3	1.264(3)
C19–C18	1.391(3)	C15–O5	1.255(4)
C19–C20	1.401(4)	O5–Co3#5 [1]	2.0323(18)
O8–C22	1.263(3)	O3–Co1#7 [1]	1.9298(19)

Continued on next page

Table S1 – continued from previous page

bond	length (Å)	bond	length (Å)
C11–C12	1.398(3)	O2–Co1#8 [1]	1.992(2)
C11–C10	1.385(4)		

[1] #1: – 1/2 + X, 1 – Y, – 1/2 + Z; #2: – 1/2 + X, – 1/2 + Y, + Z;
#3: 3/2 – X, 1/2 – Y, 1 – Z; #4: + X, 1/2 – Y, 1/2 + Z;
#5: 3/2 – X, + Y, 1/2 – Z; #6: 1/2 – X, 1/2 – Y, – Z;
#7: 1/2 + X, 1 – Y, 1/2 + Z; #8: 1/2 + X, 1/2 + Y, + Z.

Table S2: Selected angles (°) for compound **1**

angle	(°)	angle	(°)
O8–Co1–O2#1 [1]	101.92(10)	O7–C22–O8	124.2(2)
O8–Co1–O9	105.73(10)	O8–C22–C23	115.5(2)
O3#2–Co1–O8 [1]	109.98(9)	C32–C31–N3	118.4(2)
O3#2–Co1–O2#1 [1]	111.64(10)	C35–C31–N3	121.1(2)
O3#2–Co1–O9 [1]	124.30(10)	C35–C31–C32	120.5(2)
O9–Co1–O2#1 [1]	100.78(9)	C34–N4–C35	117.9(2)
N7#3–Co3–N7 [1]	180.0	C31–C32–C33	116.8(2)
O11#3–Co3–N7 [1]	91.71(8)	C17–C16–C15	120.0(2)
O11#3–Co3–N7#3 [1]	88.29(8)	C17–C16–C21	118.9(2)
O11–Co3–N7	88.29(8)	C21–C16–C15	121.1(3)
O11–Co3–N7#3 [1]	91.71(8)	C37–N5–C33	130.0(2)
O11–Co3–O11#3 [1]	180.0	C37–N5–N6	109.3(2)
O5#4–Co3–N7#3 [1]	90.39(9)	N6–N5–C33	120.6(2)
O5#5–Co3–N7 [1]	90.39(9)	C3–C4–C5	121.8(2)
O5#4–Co3–N7 [1]	89.61(9)	C27–C28–C23	120.2(3)
O5#5–Co3–N7#3 [1]	89.61(9)	C24–C25–C26	121.4(2)
O5#4–Co3–O11#3 [1]	91.03(8)	N1–C29–N3	110.2(2)
O5#4–Co3–O11 [1]	88.97(8)	C11–C12–Si1	121.01(19)
O5#5–Co3–O11#3 [1]	88.97(8)	C13–C12–Si1	121.45(18)
O5#5–Co3–O11 [1]	91.03(8)	C13–C12–C11	117.5(2)
O5#5–Co3–O5#4 [1]	180.0	C17–C18–C19	121.2(3)
O7–Co2–O7#6 [1]	180.0	C6–C7–C2	120.5(3)
O7#6–Co2–N1#6 [1]	93.75(7)	C9–C10–C11	120.3(2)
O7#6–Co2–N1 [1]	86.25(7)	N4–C35–C31	122.0(2)
O7–Co2–N1	93.74(7)	C23–C24–C25	120.0(2)
O7–Co2–N1#6 [1]	86.25(7)	C7–C6–C5	120.9(2)

Continued on next page

Table S2 – continued from previous page

angle	(°)	angle	(°)
N1#6–Co2–N1 [1]	180.0	N7–C37–N5	110.3(2)
O10–Co2–O7#6 [1]	92.73(8)	C9–C14–C13	120.6(3)
O10#6–Co2–O7 [1]	92.73(8)	C14–C13–C12	120.9(2)
O10–Co2–O7	87.27(8)	C29–N1–Co2	129.24(18)
O10#6–Co2–O7#6 [1]	87.27(8)	C29–N1–C30	103.2(2)
O10#6–Co2–N1 [1]	93.95(8)	C30–N1–Co2	127.29(18)
O10–Co2–N1	86.05(8)	C21–C20–C19	121.7(2)
O10#6–Co2–N1#6 [1]	86.06(8)	C4–C3–C2	120.0(2)
O10–Co2–N1#6 [1]	93.95(8)	C7–C2–C1	119.5(3)
O10–Co2–O10#6 [1]	180.0	C3–C2–C7	119.3(2)
C5–Si1–C26	110.96(11)	C3–C2–C1	121.2(3)
C5–Si1–C12	107.79(10)	O1–C1–C2	120.9(3)
C19–Si1–C5	109.92(11)	O1–C1–O2	122.0(3)
C19–Si1–C26	109.03(11)	O2–C1–C2	117.0(3)
C19–Si1–C12	108.04(11)	C30–N2–N3	102.5(2)
C12–Si1–C26	111.04(11)	C36–N6–N5	102.5(2)
C4–C5–Si1	120.20(19)	N4–C34–C33	122.8(2)
C4–C5–C6	117.4(2)	C16–C17–C18	120.5(2)
C6–C5–Si1	122.35(18)	C37–N7–Co3	132.39(18)
C29–N3–C31	130.7(2)	C37–N7–C36	102.8(2)
C29–N3–N2	109.4(2)	C36–N7–Co3	124.6(2)
N2–N3–C31	119.88(19)	O4–C8–C9	120.1(3)
C22–O7–Co2	139.58(17)	O4–C8–O3	124.1(3)
C25–C26–Si1	121.57(19)	O3–C8–C9	115.8(3)
C25–C26–C27	117.4(2)	C10–C9–C14	119.3(2)
C27–C26–Si1	121.03(19)	C10–C9–C8	121.0(2)
C28–C23–C22	118.9(2)	C14–C9–C8	119.7(3)
C24–C23–C22	121.4(2)	N2–C30–N1	114.8(2)
C24–C23–C28	119.5(2)	C28–C27–C26	121.4(2)
C32–C33–N5	119.2(2)	O6–C15–C16	118.3(3)
C34–C33–C32	120.0(2)	O6–C15–O5	125.4(3)
C34–C33–N5	120.9(2)	O5–C15–C16	116.3(3)
C18–C19–Si1	122.94(19)	C20–C21–C16	120.5(3)
C18–C19–C20	117.2(2)	N6–C36–N7	115.0(3)
C20–C19–Si1	119.80(18)	C15–O5–Co3#4 [1]	128.52(18)
C22–O8–Co1	124.55(17)	C8–O3–Co1#7 [1]	117.42(19)
C10–C11–C12	121.4(2)	C1–O2–Co1#8 [1]	108.85(19)
O7–C22–C23	120.3(2)		

Continued on next page

Table S2 – continued from previous page

angle	(°)	**angle**	(°)

[1] #1: – 1/2 + X, – 1/2 + Y, + Z; #2: – 1/2 + X, 1 – Y, – 1/2 + Z;
#3: 3/2 – X, 1/2 – Y, 1 – Z; #4: 3/2 – X, + Y, 1/2 – Z;
#5: + X, 1/2 – Y, 1/2 + Z; #6: 1/2 – X, 1/2 – Y, – Z;
#7: 1/2 + X, 1 – Y, 1/2 + Z; #8: 1/2 + X, 1/2 + Y, + Z.

To get a deeper insight into the frameworks of the three coordination polymers, we have performed the topological analysis using ToposPro software [2] and the concept of the simplified underlying net [3, 4]. The core idea of underlying topology is breaking down a complex structure into its fundamental units without losing its chemical significance [3]. The deconstructive procedure we follow is the method developed by O'Keeffe and Yaghi [3, 4]. Point symbols for nets are used in this work.

3. The crystal structure of compound 2

Table S3: Selected bond lengths (Å) for compound **2**

bond	length (Å)	bond	length (Å)
Co2–O2#1 [1]	2.0571(19)	C25–C24	1.382(4)
Co2–O1#1 [1]	2.3396(19)	C24–C23	1.376(4)
Co2–O3#2 [1]	1.9816(18)	C23–C28	1.369(4)
Co2–O14	2.061(2)	C23–C22	1.494(4)
Co2–O13	2.061(2)	C28–C27	1.381(4)
Co2–O12	2.282(2)	C29–C30	1.489(3)
Co1–O8	2.160(2)	C30–C31	1.377(3)
Co1–O7	2.143(2)	C30–C35	1.381(4)
Co1–O9	2.017(2)	C31–C32	1.383(4)
Co1–O10	2.2322(17)	C32–C33	1.386(4)
Co1–O11	2.155(2)	C33–C34	1.392(4)
Co1–O15#3 [1]	2.029(2)	C34–C35	1.383(4)
Si1–C5	1.878(2)	C36 C37	1.493(4)
Si1–C19	1.869(3)	C37 C42	1.381(4)
Si1–C12	1.864(2)	C37 C38	1.379(4)
Si1–C26	1.865(3)	C42–C41	1.379(4)
Si2–C33	1.875(3)	C41–C40	1.384(4)
Si2–C40	1.864(3)	C40–C39	1.385(4)
Si2–C47	1.872(3)	C39–C38	1.381(4)
Si2–C54	1.912(2)	C43–C44	1.494(4)
O2–Co2#4 [1]	2.0572(19)	C44–C45	1.371(4)
O2–C1	1.267(3)	C44–C49	1.372(5)
O1–Co2#4 [1]	2.3395(19)	C45–C46	1.386(4)
O1–C1	1.238(3)	C46–C47	1.392(4)
O6–C15	1.329(3)	C47–C48	1.386(4)
O5–C15	1.203(3)	C48–C49	1.382(4)
O4–C8	1.231(3)	C50B–C51B	1.493(11)
O3–Co2#5 [1]	1.9818(18)	C50A–C51A	1.534(7)
O3–C8	1.258(3)	C51B–C52B	1.422(11)
O8–C22	1.258(4)	C51B–C56B	1.449(11)
O7–C22	1.245(3)	C52B–C53B	1.376(9)
O10–C29	1.261(3)	C53B–C54	1.500(8)
O11–C29	1.258(3)	C54–C55A	1.3900
O13–C36	1.255(3)	C54–C53A	1.3900
O12–C36	1.262(3)	C54–C55B	1.256(6)
O15–Co1#6 [1]	2.029(2)	C55A–C56A	1.3900

Continued on next page

Table S3 – continued from previous page

bond	length (Å)	bond	length (Å)
O15–C43	1.238(4)	C56A–C51A	1.3900
O16–C43	1.241(5)	C51A–C52A	1.3900
O18B–C50B	1.192(10)	C52A–C53A	1.3900
O17A–C50A	1.240(10)	C55B–C56B	1.330(7)
O17B–C50B	1.355(15)	Co3–O19	2.066(2)
O18A–C50A	1.250(14)	Co3–O20	2.070(3)
C1–C2	1.487(3)	Co3–O21	2.0397(19)
C2–C7	1.360(4)	Co3–O22	2.100(2)
C2–C3	1.353(4)	Co3–N6	2.202(2)
C7–C6	1.386(4)	Co3–N1#3 [1]	2.203(2)
C6–C5	1.361(4)	N6–C64	1.308(3)
C5–C4	1.368(4)	N6–C65	1.345(4)
C4–C3	1.384(4)	N7–N5	1.354(3)
C15–C16	1.482(4)	N7–C65	1.312(4)
C16–C17	1.382(4)	N5–C64	1.342(3)
C16–C21	1.366(4)	N5–C62	1.420(3)
C17–C18	1.379(4)	N4–C60	1.333(3)
C18–C19	1.393(4)	N4–C61	1.333(3)
C19–C20	1.385(4)	N2–N3	1.358(3)
C20–C21	1.381(4)	N2–C59	1.422(3)
C8–C9	1.494(3)	N2–C58	1.339(3)
C9–C10	1.371(3)	N3–C57	1.313(3)
C9–C14	1.373(4)	N1–Co3#6 [1]	2.203(2)
C10–C11	1.388(3)	N1–C57	1.352(4)
C11–C12	1.383(3)	N1–C58	1.311(3)
C12–C13	1.387(3)	C62–C63	1.384(3)
C13–C14	1.379(4)	C62–C61	1.381(4)
C26–C25	1.378(4)	C63–C59	1.384(3)
C26–C27	1.384(4)	C59–C60	1.377(4)

[1] #1: – 1 + X, – 1 + Y, + Z; #2: – 1/2 + X, – 1/2 – Y, – 1/2 + Z; #3: 1/2 + X, – 1/2 – Y, – 1/2 + Z; #4: 1 + X, 1 + Y, + Z; #5: 1/2 + X, – 1/2 – Y, 1/2 + Z; #6: – 1/2 + X, – 1/2 – Y, 1/2 + Z.

Table S4: Selected angles (°) for compound **2**

angle	(°)	angle	(°)
O2#1–Co2–O1#1 [1]	58.60(7)	O11–C29–C30	120.7(2)

Continued on next page

Table S4 – continued from previous page

angle	(°)	angle	(°)
O2#1–Co2–O14 [1]	99.28(9)	C31–C30–C29	120.0(2)
O2#1–Co2–O13 [1]	147.03(9)	C31–C30–C35	119.2(2)
O2#1–Co2–O12 [1]	95.78(8)	C35–C30–C29	120.8(2)
O3#2–Co2–O2#1 [1]	104.71(8)	C30–C31–C32	120.5(2)
O3#2–Co2–O1#1 [1]	161.44(8)	C31–C32–C33	121.4(2)
O3#2–Co2–O14 [1]	92.09(8)	C32–C33–Si2	122.15(19)
O3#2–Co2–O13 [1]	100.57(9)	C32–C33–C34	117.2(2)
O3#2–Co2–O12 [1]	97.20(8)	C34–C33–Si2	120.6(2)
O14–Co2–O1#1 [1]	83.52(8)	C35–C34–C33	121.7(3)
O14–Co2–O13	100.60(9)	C30–C35–C34	120.0(2)
O14–Co2–O12	159.69(8)	O13–C36–O12	120.0(3)
O13–Co2–O1#1 [1]	97.97(8)	O13–C36–C37	119.4(2)
O13–Co2–O12	59.99(8)	O12–C36–C37	120.6(3)
O12–Co2–O1#1 [1]	92.87(8)	C42–C37–C36	119.7(3)
O8–Co1–O10	86.35(8)	C38–C37–C36	121.9(2)
O7–Co1–O8	60.48(8)	C38–C37–C42	118.4(3)
O7–Co1–O10	107.61(9)	C41–C42–C37	120.5(3)
O7–Co1–O11	156.57(9)	C42–C41–C40	121.8(3)
O9–Co1–O8	155.85(13)	C41–C40–Si2	118.4(2)
O9–Co1–O7	101.63(12)	C41–C40–C39	117.2(2)
O9–Co1–O10	84.10(9)	C39–C40–Si2	123.9(2)
O9–Co1–O11	96.43(11)	C38–C39–C40	121.3(3)
O9–Co1–O15#3 [1]	112.18(12)	C37–C38–C39	120.8(3)
O11–Co1–O8	97.66(8)	O15–C43–O16	121.6(3)
O11–Co1–O10	59.37(7)	O15–C43–C44	118.5(3)
O15#3–Co1–O8 [1]	87.03(10)	O16–C43–C44	119.9(3)
O15#3–Co1–O7 [1]	95.55(10)	C45–C44–C43	121.6(3)
O15#3–Co1–O10 [1]	148.61(9)	C45–C44–C49	119.4(3)
O15#3–Co1–O11 [1]	91.26(8)	C49–C44–C43	118.9(3)
C19–Si1–C5	111.49(12)	C44–C45–C46	119.9(3)
C12–Si1–C5	105.61(11)	C45–C46–C47	122.0(3)
C12–Si1–C19	109.21(11)	C46–C47–Si2	123.4(2)
C12–Si1–C26	110.45(11)	C48–C47–Si2	120.0(2)
C26–Si1–C5	111.27(11)	C48–C47–C46	116.5(2)
C26–Si1–C19	108.77(11)	C49–C48–C47	121.8(3)
C33–Si2–C54	108.60(12)	C44–C49–C48	120.4(3)
C40–Si2–C33	108.08(11)	O18B–C50B–O17B	121.3(10)
C40–Si2–C47	107.71(12)	O18B–C50B–C51B	125.5(11)

Continued on next page

Table S4 – continued from previous page

angle	(°)	angle	(°)
C40–Si2–C54	114.26(13)	O17B–C50B–C51B	112.9(8)
C47–Si2–C33	110.51(12)	O17A–C50A–O18A	123.7(9)
C47–Si2–C54	107.67(12)	O17A–C50A–C51A	123.8(8)
C1–O2–Co2#4 [1]	97.02(16)	O18A–C50A–C51A	112.5(8)
C1–O1–Co2#4 [1]	84.73(15)	C52B–C51B–C50B	117.4(7)
C8–O3–Co2#5 [1]	127.43(18)	C52B–C51B–C56B	119.4(6)
C22–O8–Co1	89.09(17)	C56B–C51B–C50B	122.2(8)
C22–O7–Co1	90.26(18)	C53B–C52B–C51B	118.2(6)
C29–O10–Co1	88.85(14)	C52B–C53B–C54	117.0(6)
C29–O11–Co1	92.47(16)	C53B–C54–Si2	110.4(3)
C36–O13–Co2	95.11(17)	C55A–C54–Si2	113.39(19)
C36–O12–Co2	84.85(17)	C55A–C54–C53A	120.0
C43–O15–Co1#6 [1]	112.4(2)	C53A–C54–Si2	126.12(19)
O2–C1–C2	118.4(2)	C55B–C54–Si2	125.3(4)
O1–C1 O2	119.6(2)	C55B–C54–C53B	122.0(4)
O1–C1–C2	121.9(2)	C54–C55A–C56A	120.0
C7–C2–C1	121.2(2)	C51A–C56A–C55A	120.0
C3–C2–C1	120.9(2)	C56A–C51A–C50A	117.7(5)
C3–C2–C7	117.9(3)	C56A–C51A–C52A	120.0
C2–C7–C6	121.1(3)	C52A–C51A–C50A	122.1(5)
C5–C6–C7	121.9(3)	C53A–C52A–C51A	120.0
C6–C5–Si1	123.4(2)	C52A–C53A–C54	120.0
C6–C5–C4	116.0(2)	C54–C55B–C56B	123.2(7)
C4–C5–Si1	120.7(2)	C55B–C56B–C51B	118.0(7)
C5–C4–C3	122.6(3)	O19–Co3–O20	87.82(12)
C2–C3–C4	120.5(3)	O19–Co3–O22	90.20(10)
O6–C15–C16	113.5(2)	O19–Co3–N6	90.10(8)
O5–C15–O6	122.5(3)	O19–Co3–N1#3 [1]	94.49(9)
O5–C15–C16	124.0(3)	O20–Co3–O22	176.42(10)
C17–C16–C15	119.0(2)	O20–Co3–N6	93.49(10)
C21–C16–C15	121.9(2)	O20–Co3–N1#3 [1]	89.29(10)
C21–C16–C17	119.0(3)	O21–Co3–O19	173.97(8)
C18–C17–C16	120.5(2)	O21–Co3–O20	92.22(11)
C17–C18–C19	121.7(2)	O21–Co3–O22	90.06(8)
C18–C19–Si1	122.75(19)	O21–Co3–N6	83.88(8)
C20–C19–Si1	120.9(2)	O21–Co3–N1#3 [1]	91.54(8)
C20–C19–C18	116.1(2)	O22–Co3–N6	89.50(8)
C21–C20–C19	122.6(3)	O22–Co3–N1#3 [1]	87.88(8)

Continued on next page

Table S4 – continued from previous page

angle	(°)	angle	(°)
C16–C21–C20	120.1(3)	N6–Co3–N1#3 [1]	174.72(9)
O4–C8–O3	126.1(2)	C64–N6–Co3	128.58(18)
O4–C8–C9	117.3(2)	C64–N6–C65	102.7(2)
O3–C8–C9	116.6(2)	C65–N6–Co3	128.31(18)
C10–C9–C8	122.0(2)	C65–N7–N5	101.7(2)
C10–C9–C14	119.1(2)	N7–N5–C62	120.6(2)
C14–C9–C8	118.9(2)	C64–N5–N7	109.7(2)
C9–C10–C11	120.4(2)	C64–N5–C62	129.7(2)
C12–C11–C10	121.2(2)	C60–N4–C61	119.0(2)
C11–C12–Si1	123.73(18)	N3–N2–C59	121.0(2)
C11–C12–C13	117.4(2)	C58–N2–N3	109.3(2)
C13–C12–Si1	118.80(18)	C58–N2–C59	129.7(2)
C14–C13–C12	121.3(2)	C57–N3–N2	102.4(2)
C9–C14–C13	120.6(2)	C57–N1–Co3#6 [1]	127.69(18)
C25–C26–Si1	121.9(2)	C58–N1–Co3#6 [1]	129.4(2)
C25–C26–C27	116.9(3)	C58–N1–C57	102.8(2)
C27–C26–Si1	121.1(2)	N6–C64–N5	110.2(2)
C26–C25–C24	121.7(3)	N7–C65–N6	115.7(3)
C23–C24–C25	120.6(3)	C63–C62–N5	119.9(2)
C24–C23–C22	121.3(3)	C61–C62–N5	119.9(2)
C28–C23–C24	118.4(3)	C61–C62–C63	120.2(2)
C28–C23–C22	120.3(2)	C59–C63–C62	117.0(2)
C23–C28–C27	120.8(3)	C63–C59–N2	120.6(2)
C28–C27–C26	121.6(3)	C60–C59–N2	119.3(2)
O8–C22–C23	119.0(3)	C60–C59–C63	120.2(2)
O7–C22–O8	120.0(3)	N4–C60–C59	121.9(2)
O7–C22–C23	121.0(3)	N4–C61–C62	121.7(2)
O10–C29–C30	120.0(2)	N3–C57–N1	115.0(3)
O11–C29–O10	119.3(2)	N1–C58–N2	110.5(3)

[1] #1: – 1 + X, – 1 + Y, + Z; #2: – 1/2 + X, – 1/2 – Y, – 1/2 + Z; #3: 1/2 + X, – 1/2 – Y, – 1/2 + Z; #4: 1 + X, 1 + Y, + Z; #5: 1/2 + X, – 1/2 – Y, 1/2 + Z; #6: – 1/2 + X, – 1/2 – Y, 1/2 + Z.

Table S5: Hydrogen bonding interactions between the 3D motif and the 1D motif in the structures of compound **2**

Donor$\cdots$acceptor	Hydrogen bond length (Å)
O6–H$\cdots$N4	2.735
O19–H$\cdots$O11	2.768
O22–H$\cdots$O8	2.928
O21–H$\cdots$O2	2.712
O21–H$\cdots$O4	2.567
O22–H$\cdots$O12	2.738

4. The crystal structure of compound 3

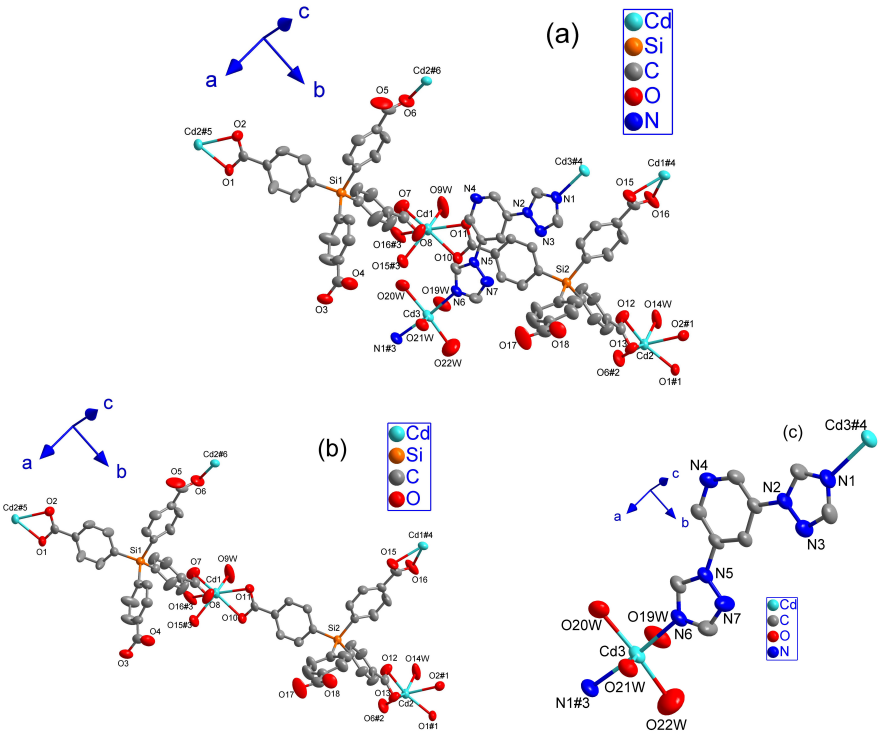

Figure S2: (a) Coordination environments (at 50 % probability level) of Cd(II)1, Cd(II)2 and Cd(II)3 centers in compound **3**. The hydrogen atoms and crystal water molecules are omitted for clarity. Symmetry codes for the generated atoms: #1: – 1 + X, 1 + Y, + Z; #2: – 1/2 + X, – 1/2 – Y, – 1/2 + Z; #3: 1/2 + X, – 1/2 – Y, – 1/2 + Z; #4: – 1/2 + X, – 1/2 – Y, 1/2 + Z; #5: 1 + X, – 1 + Y, + Z; #6: 1/2 + X, – 1/2 – Y, 1/2 + Z. (b) The coordination environment of L1 ligands of the 3D motif in compound **3**. (c) The 1D cationic motif in compound **3**.

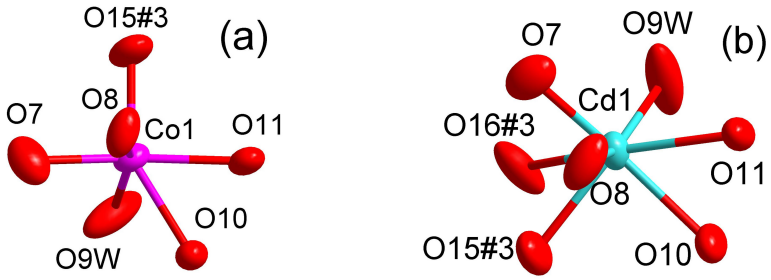

Figure S3: Coordination environments of (a) Co1 in compound **2** and (b) Cd1 in compound **3**.

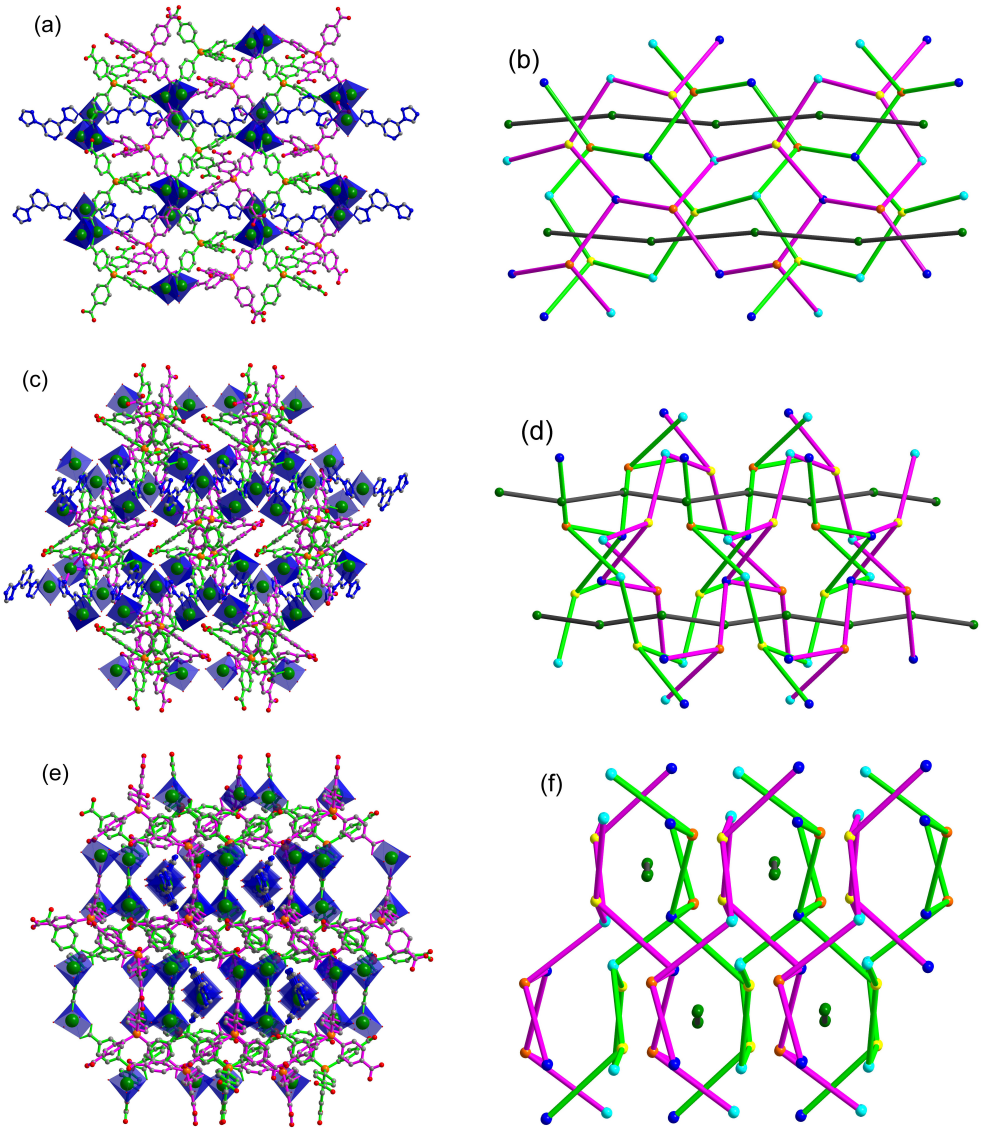

Figure S4: (a) (c) and (e) Perspective view of the 3D network in compound **3**. (b) (d) and (f) Schematic view of the 3D 3-connected framework with the $(10^3)_4$ topology in compound **3**. Color code: yellow ball, 3-connected $Htcps^{3-}$ (Htcps-1) node; light yellow ball, 3-connected $Htcps^{3-}$ (Htcps-2) node; blue ball, 3-connected Cd1 node; light green ball, 3-connected Cd2 node; blackish green ball, 2-connected Cd3 node.

Table S6: Selected bond lengths (Å) for compound **3**

bond	**length (Å)**	**bond**	**length (Å)**
Cd2–O13	2.423(3)	C37–C42	1.371(6)
Cd2–O12	2.282(3)	C37–C38	1.397(6)
Cd2–O2#1 [1]	2.456(3)	C40–C41	1.396(6)
Cd2–O1#1 [1]	2.280(3)	C40–C39	1.368(6)
Cd2–O3#2 [1]	2.192(3)	C41–C42	1.367(6)
Cd2–O14	2.283(3)	C38–C39	1.378(6)
Cd1–O10	2.375(3)	C44–C49	1.357(6)
Cd1–O11	2.397(3)	C44–C45	1.365(6)
Cd1–O16#3 [1]	2.447(3)	C44–C43	1.506(5)
Cd1–O15#3 [1]	2.315(3)	C49–C48	1.387(6)
Cd1–O8	2.418(3)	C45–C46	1.391(6)
Cd1–O7	2.281(3)	C13–C14	1.380(6)
Cd1–O9	2.250(3)	C9–C10	1.354(6)
Si1–C5	1.884(4)	C9–C14	1.368(6)
Si1–C19	1.871(4)	C9–C8	1.496(6)
Si1–C12	1.873(4)	C11–C10	1.377(6)
Si1–C26	1.863(4)	N1–Cd3#4 [1]	2.362(3)
Si2–C33	1.880(4)	N1–C57	1.345(6)
Si2–C47	1.881(4)	N1–C58	1.308(6)
Si2–C40	1.868(4)	O16–Cd1#4 [1]	2.447(3)
Si2–C54	1.895(3)	O16–C43	1.253(6)
C33–C34	1.378(6)	C43–Cd1#4 [1]	2.732(4)
C33–C32	1.390(6)	C43–O15	1.251(6)
O10–C29	1.260(5)	O15–Cd1#4 [1]	2.315(3)
O11–C29	1.249(5)	C23 C28	1.375(6)
C29–C30	1.488(6)	C23–C24	1.370(6)
C30–C31	1.385(6)	C23–C22	1.492(6)
C30–C35	1.371(5)	C2–C3	1.332(7)
C34–C35	1.382(6)	C2–C7	1.357(6)
C32–C31	1.374(6)	C2–C1	1.489(6)
Cd3–N6	2.373(3)	C24–C25	1.363(7)
Cd3–N1#3 [1]	2.362(3)	C3–C4	1.399(7)
Cd3–O21	2.274(3)	C7–C6	1.390(7)
Cd3–O20	2.269(3)	O2–Cd2#5 [1]	2.456(3)
Cd3–O19	2.265(4)	O2–C1	1.244(5)
Cd3–O22	2.253(5)	C1–Cd2#5 [1]	2.727(4)
C47–C46	1.379(6)	C1–O1	1.266(5)

Continued on next page

Table S6 – continued from previous page

bond	length (Å)	bond	length (Å)
C47–C48	1.382(6)	C16–C17	1.375(6)
C5–C6	1.352(7)	C16–C21	1.374(7)
C5–C4	1.342(6)	C16–C15	1.476(6)
C19–C18	1.365(6)	C20–C21	1.380(7)
C19–C20	1.373(6)	O1–Cd2#5 [1]	2.280(3)
C12–C13	1.391(6)	O6–C15	1.349(5)
C12–C11	1.378(6)	O8–C22	1.241(5)
C26–C27	1.388(6)	O7–C22	1.243(5)
C26–C25	1.377(6)	O5–C15	1.202(5)
N5–C64	1.334(5)	O4–C8	1.226(7)
N5–N7	1.356(5)	C8–O3	1.268(7)
N5–C62	1.433(5)	O3–Cd2#6 [1]	2.192(3)
C64–N6	1.303(5)	C51B–C52B	1.3900
N7–C65	1.303(5)	C51B–C56B	1.3900
N6–C65	1.337(6)	C51B–C50B	1.579(11)
C27–C28	1.376(6)	C52B–C53B	1.3900
C18–C17	1.392(6)	C53B–C54	1.3900
C63–C62	1.386(5)	C54–C55B	1.3900
C63–C59	1.393(5)	C54–C53A	1.376(5)
C61–C62	1.383(6)	C54–C55A	1.402(5)
C61–N4	1.339(5)	C55B–C56B	1.3900
N3–N2	1.351(5)	C50B–O17B	1.176(11)
N3–C57	1.311(5)	C50B–O18B	1.304(17)
N2–C59	1.421(5)	C52A–C53A	1.388(5)
N2–C58	1.336(5)	C52A–C51A	1.388(5)
C59–C60	1.375(6)	C55A–C56A	1.393(5)
N4–C60	1.329(5)	C56A–C51A	1.387(5)
O13–C36	1.267(5)	C51A–C50A	1.455(15)
O12–C36	1.262(5)	C50A–O17A	1.26(2)
C36–C37	1.482(5)	C50A–O18A	1.217(14)

[1] #1: – 1 + X, 1 + Y, + Z; #2: – 1/2 + X, – 1/2 – Y, – 1/2 + Z; #3: 1/2 + X, – 1/2 – Y, – 1/2 + Z; #4: – 1/2 + X, – 1/2 – Y, 1/2 + Z; #5: 1 + X, – 1 + Y, + Z; #6: 1/2 + X, – 1/2 – Y, 1/2 + Z.

Table S7: Selected angles (°) for compound **3**

angle	(°)	**angle**	(°)
O13–Cd2–O2#1 [1]	87.45(11)	C60–C59–C63	120.0(3)
O12–Cd2–O13	55.74(10)	C60–C59–N2	120.3(3)
O12–Cd2–O2#1 [1]	100.87(12)	C60–N4–C61	119.1(4)
O12–Cd2–O14	94.76(14)	N4–C60–C59	122.4(4)
O1#1–Cd2–O13 [1]	99.86(11)	C36–O13–Cd2	88.2(2)
O1#1–Cd2–O12 [1]	148.59(12)	C36–O12–Cd2	94.8(3)
O1#1–Cd2–O2#1 [1]	54.61(11)	O13–C36–C37	120.6(4)
O1#1–Cd2–O14 [1]	99.48(13)	O12–C36–O13	121.2(4)
O3#2–Cd2–O13 [1]	113.04(14)	O12–C36–C37	118.2(4)
O3#2–Cd2–O12 [1]	101.58(13)	C42–C37–C36	120.6(4)
O3#2–Cd2–O2#1 [1]	155.68(13)	C42–C37–C38	117.9(4)
O3#2–Cd2–O11 [1]	106.77(14)	C38–C37–C36	121.5(4)
O3#2–Cd2–O14 [1]	87.88(16)	C41–C40–Si2	117.9(3)
O14–Cd2–O13	145.68(14)	C39–C40–Si2	124.6(3)
O14–Cd2–O2#1 [1]	81.04(11)	C39–C40–C41	117.2(4)
O10–Cd1–O11	54.41(10)	C42–C41–C40	121.1(4)
O10–Cd1–O16#3 [1]	114.78(13)	C41–C42–C37	121.6(4)
O10–Cd1–O8	95.04(11)	C39–C38–C37	120.0(4)
O11–Cd1–O16#3 [1]	156.44(12)	C49–C44–C45	119.2(4)
O11–Cd1–O8	80.71(12)	C49–C44–C43	121.2(4)
O15#3–Cd1–O10 [1]	84.56(11)	C45–C44–C43	119.5(4)
O15#3–Cd1–O11 [1]	133.98(11)	C44–C49–C48	120.6(4)
O15#3–Cd1–O16#3 [1]	54.40(11)	C44–C45–C46	120.1(4)
O15#3–Cd1–O8 [1]	83.56(14)	C47–C46–C45	121.9(4)
O8–Cd1–O16#3 [1]	122.61(12)	C14–C13–C12	121.0(4)
O7–Cd1–O10	149.43(11)	C10–C9–C14	119.1(4)
O7–Cd1–O11	109.94(12)	C10–C9–C8	121.7(5)
O7–Cd1–O16#3 [1]	88.71(14)	C14–C9–C8	119.1(5)
O7–Cd1–O15#3 [1]	94.98(13)	C10–C11–C12	120.3(4)
O7–Cd1–O8	54.70(11)	C57–N1–Cd3#4 [1]	129.0(3)
O9–Cd1–O10	97.32(15)	C58–N1–Cd3#4 [1]	127.8(3)
O9–Cd1–O11	80.95(12)	C58–N1–C57	102.6(4)
O9–Cd1–O16#3 [1]	80.02(13)	N3–C57–N1	115.0(4)
O9–Cd1–O15#3 [1]	129.18(17)	N1–C58–N2	110.8(4)
O9–Cd1–O8	145.86(19)	C9–C10–C11	121.7(4)
O9–Cd1–O7	106.25(17)	C43–O16–Cd1#4 [1]	89.1(3)
C19–Si1–C5	111.22(19)	C44–C43–Cd1#4 [1]	173.2(3)

Continued on next page

Table S7 – continued from previous page

angle	(°)	angle	(°)
C19–Si1–C12	110.95(18)	O16–C43–Cd1#4 [1]	63.6(2)
C12–Si1–C5	106.67(17)	O16–C43–C44	120.2(4)
C26–Si1–C5	111.05(18)	O15–C43–Cd1#4 [1]	57.5(2)
C26–Si1–C19	108.05(18)	O15–C43–C44	118.7(4)
C26–Si1–C12	108.89(18)	O15–C43–O16	121.0(4)
C33–Si2–C47	109.73(18)	C47–C48–C49	121.7(4)
C33–Si2–C54	107.23(17)	C43–O15–Cd1#4 [1]	95.4(3)
C47–Si2–C54	110.33(16)	C40–C39–C38	122.2(4)
C40–Si2–C33	108.17(17)	C28–C23–C22	121.7(4)
C40–Si2–C47	108.15(17)	C24–C23–C28	117.4(4)
C40–Si2–C54	113.19(18)	C24–C23–C22	120.9(4)
C34–C33–Si2	122.9(3)	C3–C2–C7	118.5(4)
C34–C33–C32	116.8(4)	C3–C2–C1	121.7(4)
C32–C33–Si2	120.3(3)	C7–C2–C1	119.7(4)
C29–O10–Cd1	92.8(3)	C23–C28–C27	121.1(4)
C29–O11–Cd1	92.0(2)	C25–C24–C23	121.6(5)
O10–C29–C30	119.9(4)	C2–C3–C4	121.4(4)
O11–C29–O10	120.8(4)	C2–C7–C6	118.9(5)
O11–C29–C30	119.3(3)	C24–C25–C26	121.9(4)
C31–C30–C29	121.2(4)	C5–C6–C7	123.8(5)
C35–C30–C29	120.1(4)	C5–C4–C3	121.7(5)
C35–C30–C31	118.6(4)	C1–O2–Cd2#5 [1]	88.7(2)
C33–C34–C35	121.9(4)	C2–C1–Cd2#5 [1]	173.8(3)
C31–C32–C33	121.8(4)	O2–C1–Cd2#5 [1]	64.2(2)
C32–C31–C30	120.4(4)	O2–C1–C2	121.2(4)
C30–C35–C34	120.5(4)	O2–C1–O1	120.4(4)
N1#3–Cd3–N6 [1]	172.16(13)	O1–C1–Cd2#5 [1]	56.2(2)
O21–Cd3–N6	79.73(12)	O1–C1–C2	118.4(4)
O21–Cd3–N1#3 [1]	94.79(13)	C17–C16–C15	119.3(4)
O20–Cd3–N6	88.71(12)	C21–C16–C17	118.2(4)
O20–Cd3–N1#3 [1]	85.97(13)	C21–C16–C15	122.4(4)
O20–Cd3–O21	93.04(12)	C16–C17–C18	120.5(4)
O19–Cd3–N6	88.38(13)	C19–C20–C21	123.2(5)
O19–Cd3–N1#3 [1]	97.47(14)	C16–C21–C20	119.8(5)
O19–Cd3–O21	167.30(13)	C1–O1–Cd2#5 [1]	96.3(3)
O19–Cd3–O20	91.11(14)	C22–O8–Cd1	88.7(3)
O22–Cd3–N6	97.55(17)	C22–O7–Cd1	95.1(3)
O22–Cd3–N1#3 [1]	88.10(18)	O6–C15–C16	113.8(4)

Continued on next page

Table S7 – continued from previous page

angle	(°)	angle	(°)
O22–Cd3–O21	91.07(18)	O5–C15–C16	123.8(4)
O22–Cd3–O20	173.04(18)	O5–C15–O6	122.4(4)
O22–Cd3–O19	86.1(2)	O8–C22–C23	119.0(4)
C46–C47–Si2	122.0(3)	O8–C22–O7	121.0(4)
C46–C47–C48	116.5(4)	O7–C22–C23	120.0(4)
C48–C47–Si2	121.5(3)	C9–C14–C13	120.2(4)
C6–C5–Si1	121.5(3)	O4–C8–C9	120.6(5)
C4–C5–Si1	122.8(3)	O4–C8–O3	123.4(5)
C4–C5–C6	115.7(4)	O3–C8–C9	116.0(5)
C18–C19–Si1	124.2(3)	C8–O3–Cd2#6 [1]	108.6(4)
C18–C19–C20	116.1(4)	C52B–C51B–C56B	120.0
C20–C19–Si1	119.4(3)	C52B–C51B–C50B	122.5(5)
C13–C12–Si1	119.9(3)	C56B–C51B–C50B	117.2(5)
C11–C12–Si1	122.2(3)	C51B–C52B–C53B	120.0
C11–C12–C13	117.7(4)	C52B–C53B–C54	120.0
C27–C26–Si1	122.1(3)	C53B–C54–Si2	116.6(2)
C25–C26–Si1	121.3(3)	C53B–C54–C55B	120.0
C25–C26–C27	116.4(4)	C55B–C54–Si2	122.0(2)
C64–N5–N7	109.7(3)	C53A–C54–Si2	125.7(5)
C64–N5–C62	130.4(4)	C53A–C54–C55A	115.4(6)
N7–N5–C62	119.8(3)	C55A–C54–Si2	116.2(4)
N6–C64–N5	109.6(4)	C54–C55B–C56B	120.0
C65–N7–N5	102.0(4)	C55B–C56B–C51B	120.0
C64–N6–Cd3	129.6(3)	O17B–C50B–C51B	118.1(10)
C64–N6–C65	103.7(4)	O17B–C50B–O18B	126.3(12)
C65–N6–Cd3	126.4(3)	O18B–C50B–C51B	115.6(10)
C28–C27–C26	121.4(4)	C53A–C52A–C51A	124.4(10)
C19–C18–C17	122.1(4)	C54–C53A–C52A	119.0(8)
C62–C63–C59	116.7(4)	C56A–C55A–C54	126.3(8)
N4–C61–C62	121.3(4)	C51A–C56A–C55A	116.4(9)
C63–C62–N5	119.1(4)	C52A–C51A–C50A	121.8(9)
C61–C62–N5	120.4(3)	C56A–C51A–C52A	117.9(10)
C61–C62–C63	120.6(3)	C56A–C51A–C50A	119.7(9)
C57–N3–N2	102.6(4)	O17A–C50A–C51A	115.0(12)
N3–N2–C59	121.1(3)	O18A–C50A–C51A	121.7(11)
C58–N2–N3	109.0(3)	O18A–C50A–O17A	122.8(12)
C58–N2–C59	129.8(4)	N7–C65–N6	115.0(4)
C63–C59–N2	119.7(4)		

Continued on next page

Table S7 – continued from previous page

angle	(°)	**angle**	(°)

[1] #1: – 1 + X, 1 + Y, + Z; #2: – 1/2 + X, – 1/2 – Y, – 1/2 + Z; #3: 1/2 + X, – 1/2 – Y, – 1/2 + Z; #4: – 1/2 + X, – 1/2 – Y, 1/2 + Z; #5: 1 + X, – 1 + Y, + Z; #6: 1/2 + X, – 1/2 – Y, 1/2 + Z.

Table S8: Hydrogen bonding interactions between the 3D motif and the 1D motif in the structures of compound **3**

Donor$\cdots$acceptor	Hydrogen bond length (Å)
O6–H$\cdots$N4	2.740
O19–H$\cdots$O10	2.782
O21–H$\cdots$O1	2.679
O21–H$\cdots$O4	2.672
O20–H$\cdots$O15	2.853

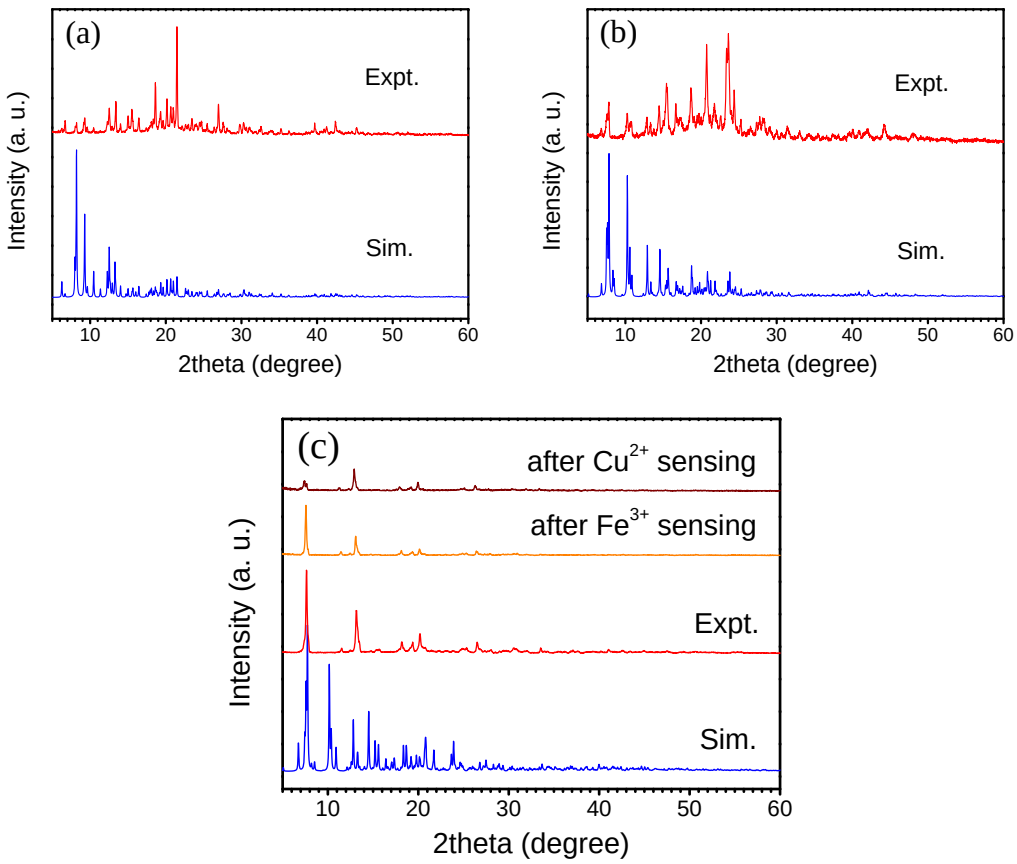

Figure S5: Experimental powder X-ray diffraction patterns versus simulated powder patterns for compounds (a) **1**, (b) **2** and (c) **3**.

5. PXRD, IR and TG

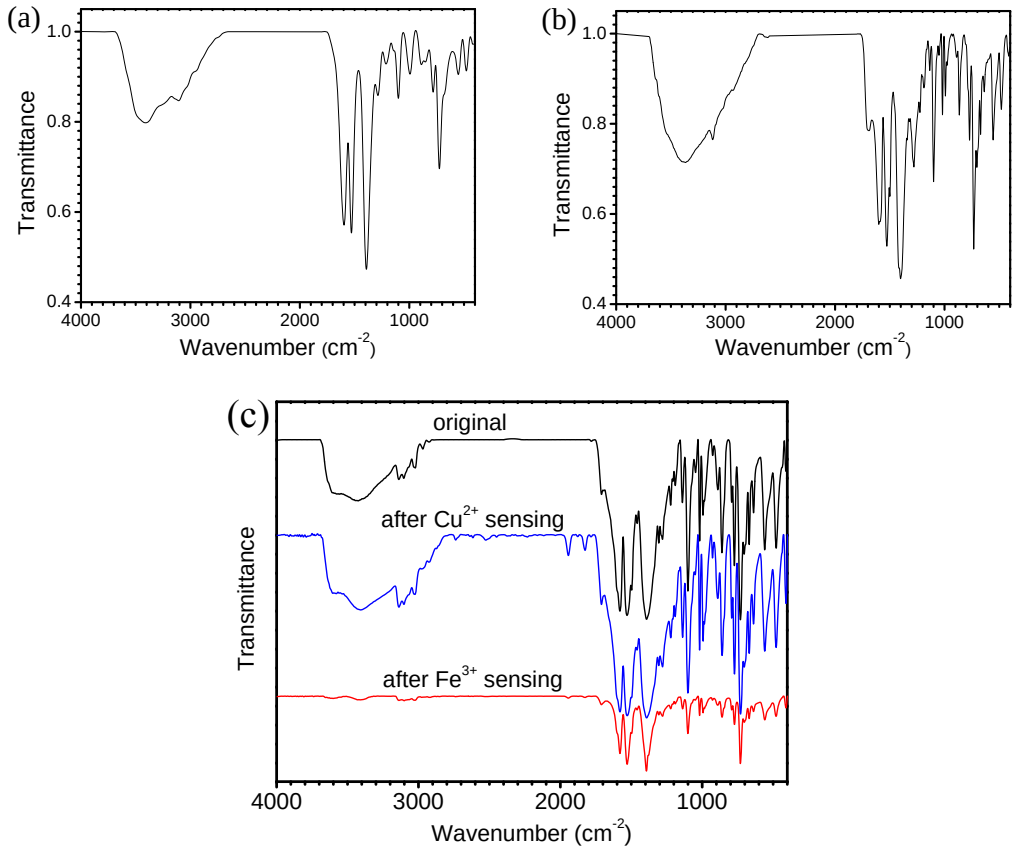

Figure S6: FT-IR spectra of compounds (a) **1**, (b) **2** and (c) **3**.

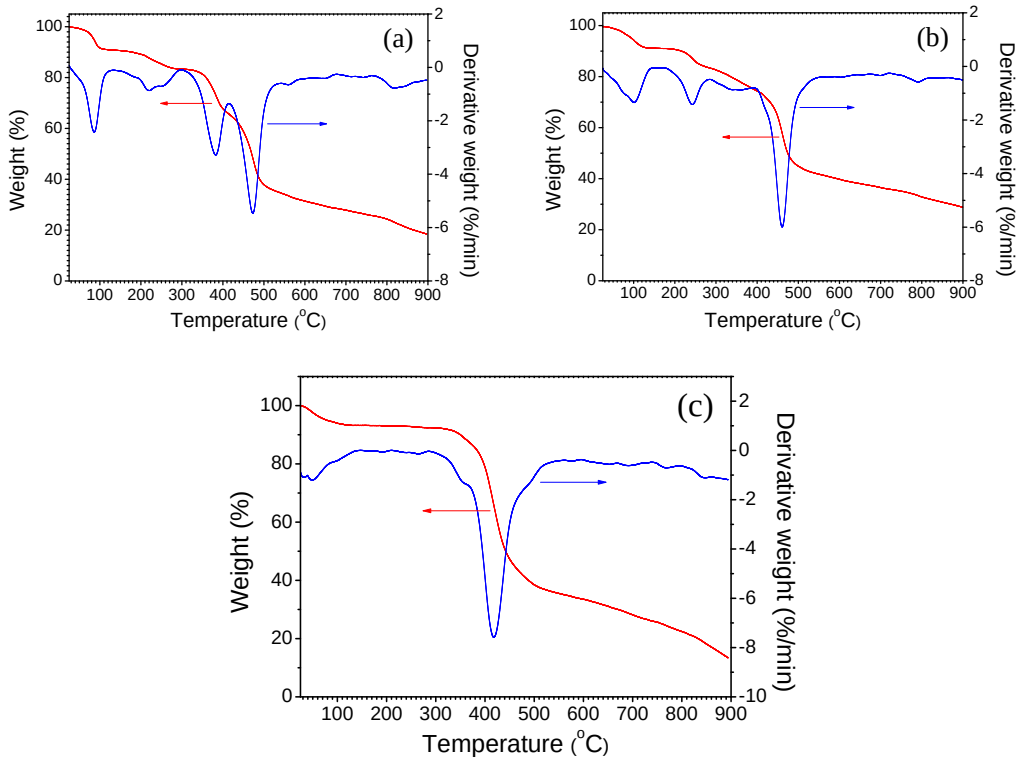

Figure S7: TG-DTG curves of compounds (a) **1**, (b) **2** and (c) **3**.

6. The photoluminescence properties of compound 3

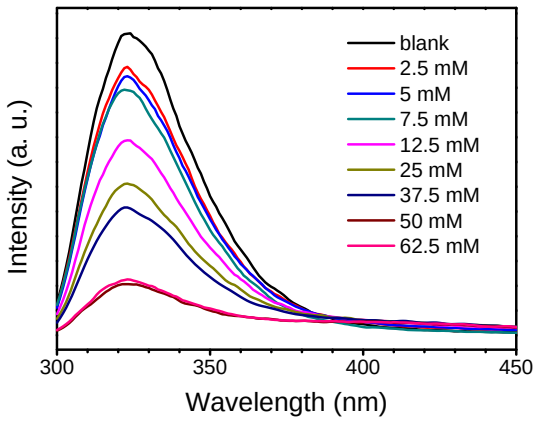

Figure S8: Luminescence responses of compound **3** toward different concentrations of acetone in deionized water (λ_{ex} = 290 nm).

Table S9: ICP-AES analysis results for **3**–$Fe(NO_3)_3$ and **3**–$Cu(NO_3)_2$

Samples	Amount of Fe or Cu	Amount of Cd
3–$Fe(NO_3)_3$	33.5 ppm (Fe)	877 ppm
3–$Cu(NO_3)_2$	18.1 ppm (Cu)	977 ppm

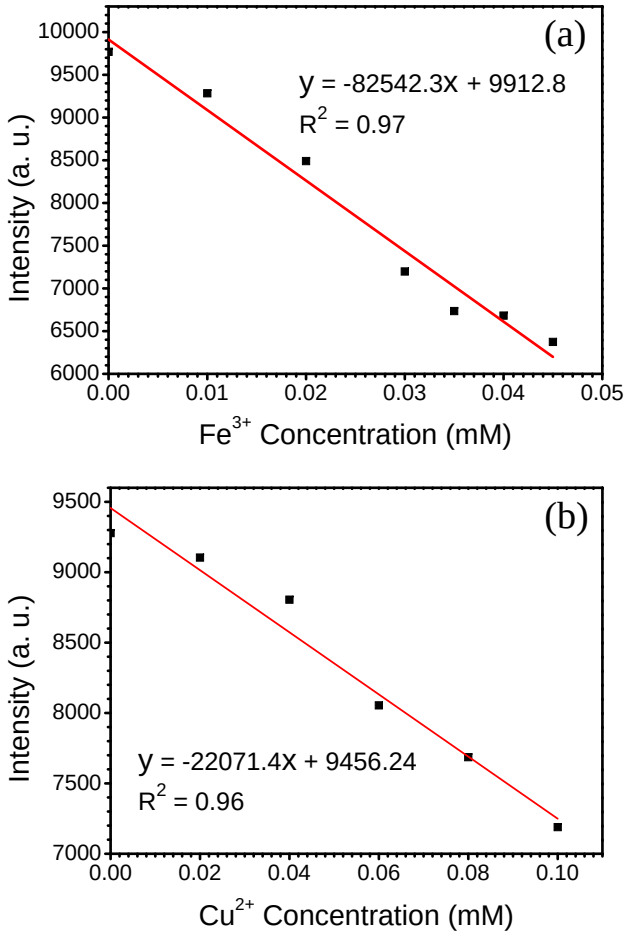

Figure S9: Linear region of fluorescence intensity of **3** in water upon addition of (a) Fe^{3+} (0 – 0.05 mM) and (b) Cu^{2+} (0 – 0.1 mM) in water at λ_{ex} = 290 nm.

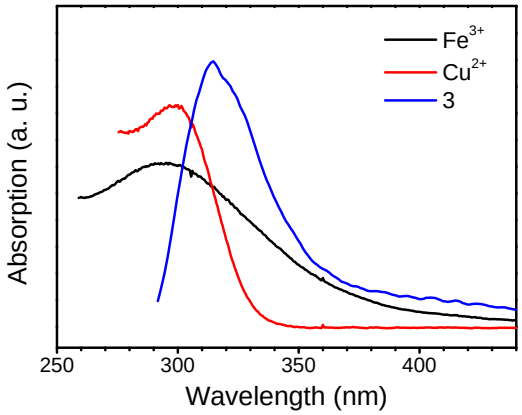

Figure S10: UV-Vis adsorption spectra of deionized water suspensions containing Fe^{3+}, Cu^{2+} metal ions (10^{-3} M) and the emission spectrum of compound **3** (8 mg) dispersed in deionized water (100 mL).

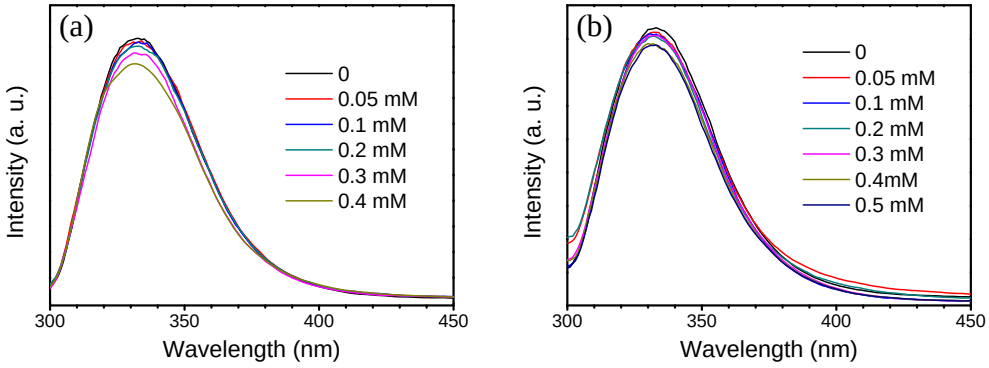

Figure S11: Luminescence responses of compound **3** towards different concentrations of (a) $Cr_2O_7^{2-}$ and (b) MnO_4^- in deionized water (λ_{ex} = 290 nm).

References

[1] W. D. Clark, G. E. Tyson, T. K. Hollis, H. U. Valle, E. J. Valente, A. G. Oliver, M. P. Dukes, Toward molecular rotors: tetra-*N*-heterocyclic carbene Ag(I)-halide cubane-type clusters, Dalton Trans. 42 (2013) 7338–7344. doi:10.1039/C3DT32862G.
URL http://dx.doi.org/10.1039/C3DT32862G

[2] V. A. Blatov, A. P. Shevchenko, D. M. Proserpio, Applied topological analysis of crystal structures with the program package ToposPro, Cryst. Growth Des. 14 (7) (2014) 3576–3586. arXiv:http://dx.doi.org/10.1021/cg500498k, doi:10.1021/cg500498k.
URL http://dx.doi.org/10.1021/cg500498k

[3] M. O'Keeffe, O. M. Yaghi, Deconstructing the crystal structures of metal–organic frameworks and related materials into their underlying nets, Chem. Rev. 112 (2) (2012) 675–702. arXiv:http://dx.doi.org/10.1021/cr200205j, doi:10.1021/cr200205j.
URL http://dx.doi.org/10.1021/cr200205j

[4] M. Li, D. Li, M. O'Keeffe, O. M. Yaghi, Topological analysis of metal–organic frameworks with polytopic linkers and/or multiple building units and the minimal transitivity principle, Chem. Rev. 114 (2) (2014) 1343–1370. arXiv:http://dx.doi.org/10.1021/cr400392k, doi:10.1021/cr400392k.
URL http://dx.doi.org/10.1021/cr400392k