Electronic Supplementary Information (ESI) for B711447H

R-Isophthalate (R = –H, –NO_2, and –COOH) as modular building blocks for mixed-ligand coordination polymers incorporated with a versatile connector 4-amino-3,5-bis(3-pyridyl)-1,2,4-triazole

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Caption to figures

Fig. S1 (a) Layered network of **1a** showing hydrogen bonds within and between the 1-D coordination arrays. (b) 3-D hydrogen-bonded structure of **1a**.

Fig. S2 3-D hydrogen-bonded network of **1b** viewed along [100], in which the lattice water molecules are omitted for clarity.

Fig. S3 (a) A packing diagram of **2a** showing the interlayer aromatic stacking interactions, in which the lattice water molecules are omitted for clarity. (b) A view of the water tetramer in **2a**, in which the green dashes indicate the H-bonds. (c) A perspective view of the 3-D packing diagram of **2a** along [010], in which the included water tetramers are indicated in red.

Fig. S4 3-D hydrogen-bonded network of **2b** viewed along [001], in which the lattice water molecules are omitted for clarity.

Fig. S5 (a) A packing diagram of **2c** viewed along [100], showing the antiparallel stacking of the coordination layers, in which the lattice water molecules are omitted for clarity. (b) 2-D Cu–Htma honeycomb layer of **2c** constructed by coordinative and hydrogen bonding. (c) A portion view of **2c** displaying all hydrogen-bonding interactions in this structure.

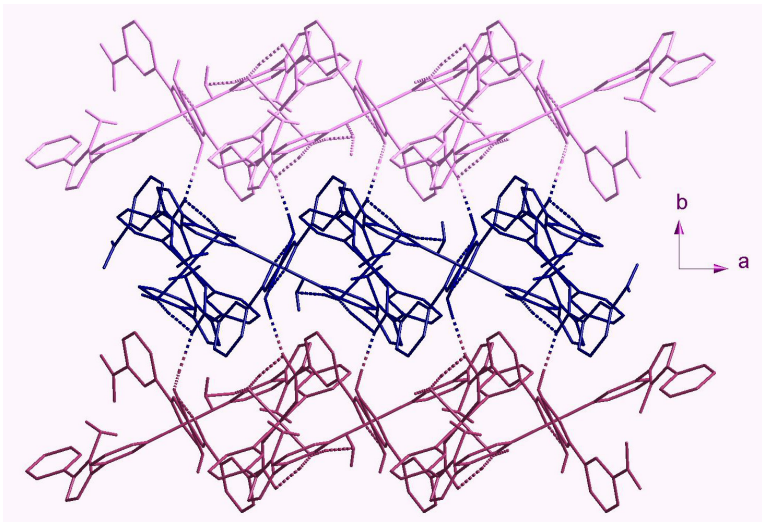
Fig. S6 A portion view of **3a** showing hydrogen bonds between the 1-D coordination frameworks.

Fig. S7 3-D supramolecular network of **3b** showing interlayer hydrogen bonds, in which the lattice water molecules are omitted for clarity.

Fig. S8 TGA curves for compounds **1a**–**1c** (indicated as black, red, and green lines).

Fig. S9 TGA curves for compounds **2a**–**2c** (indicated as black, red, and green lines).

Fig. S10 TGA curves for compounds **3a**–**3c** (indicated as black, red, and green lines).



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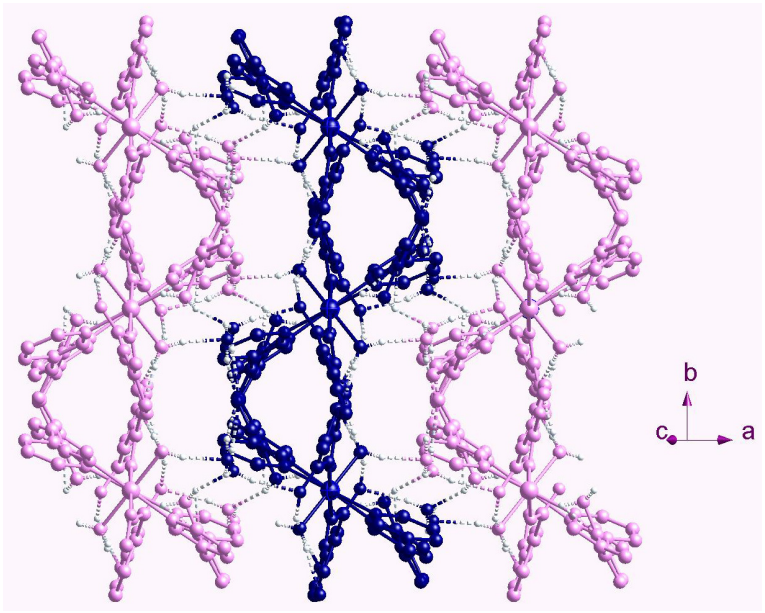
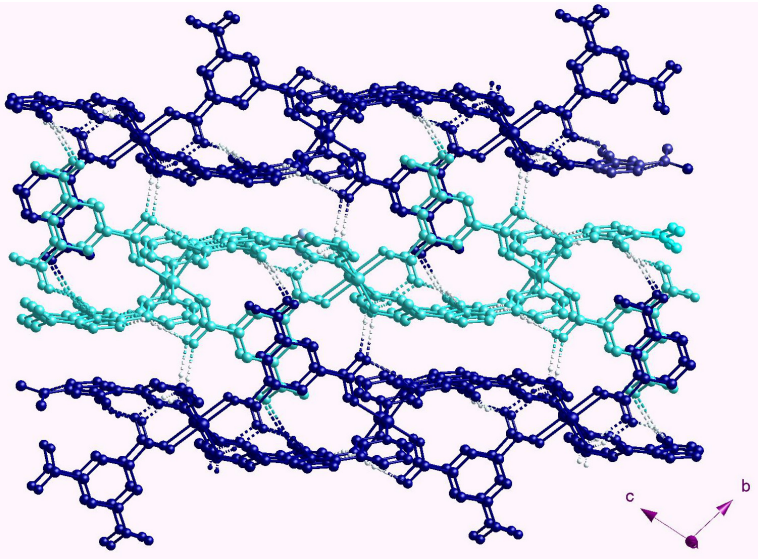


(b)

Fig. S1



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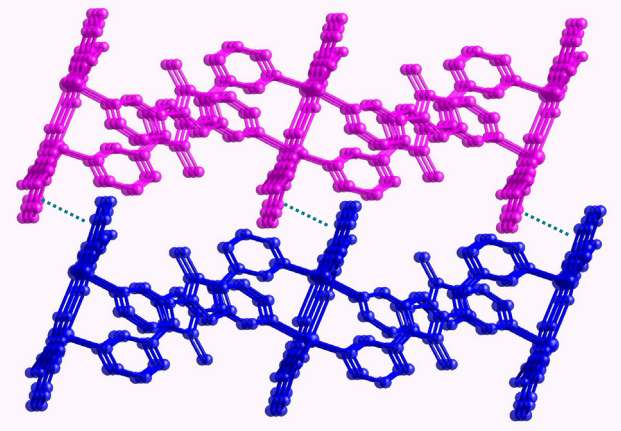

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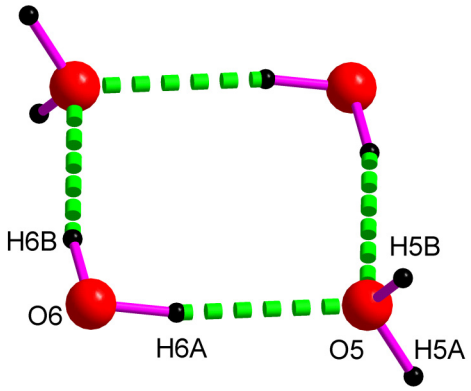

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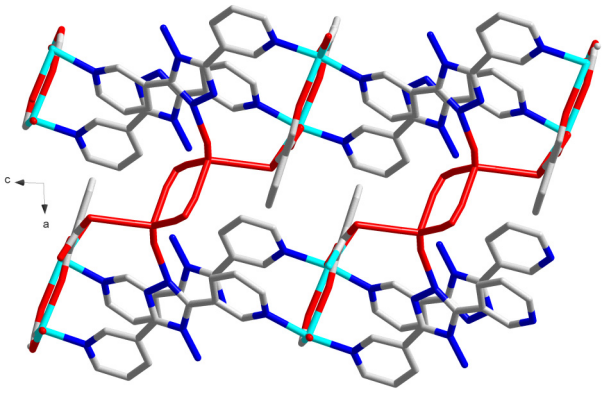


(c)

Fig. S3

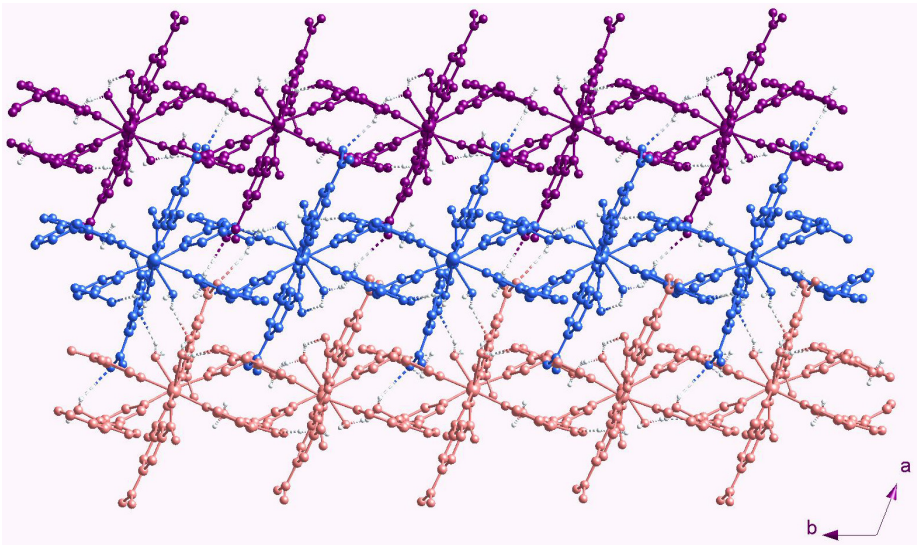
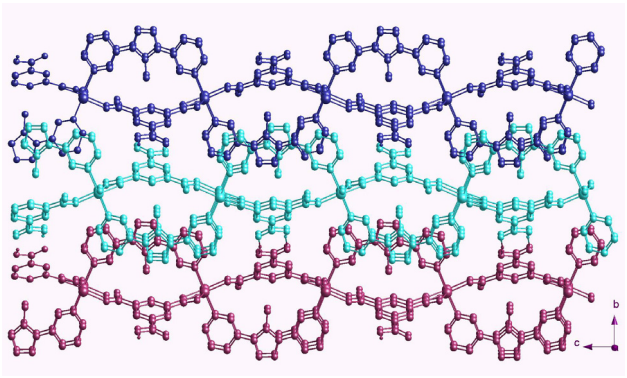


Fig. S4



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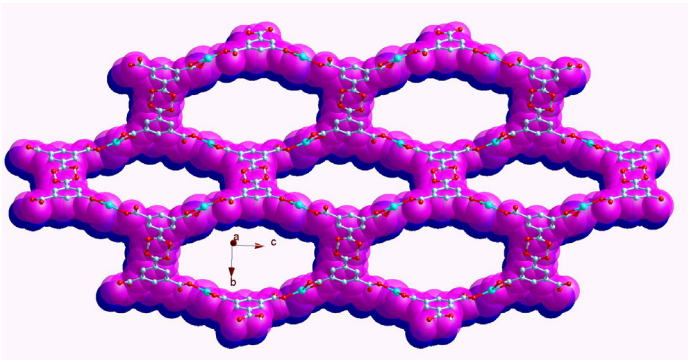

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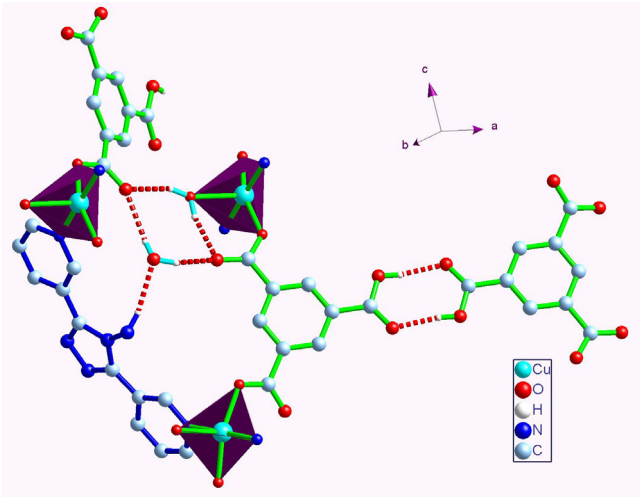

(c)

Fig. S5

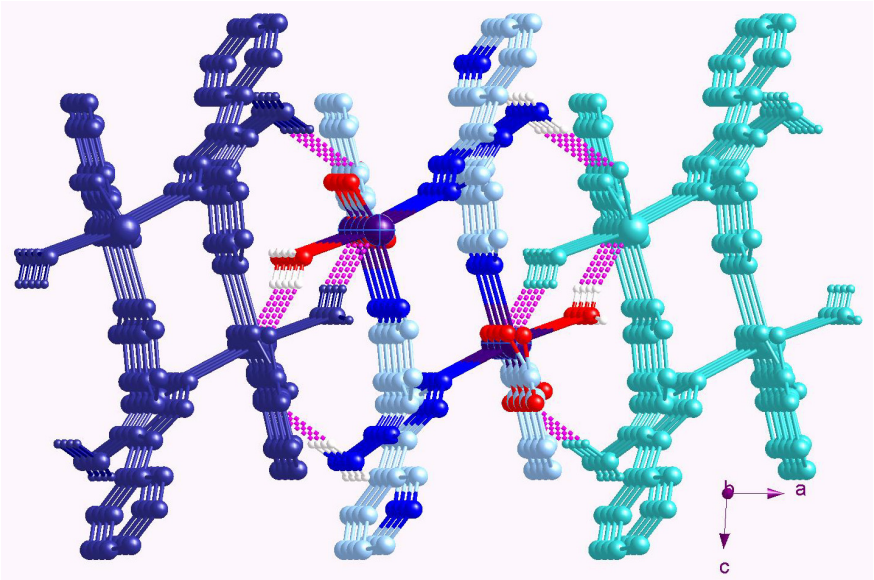

Fig. S6

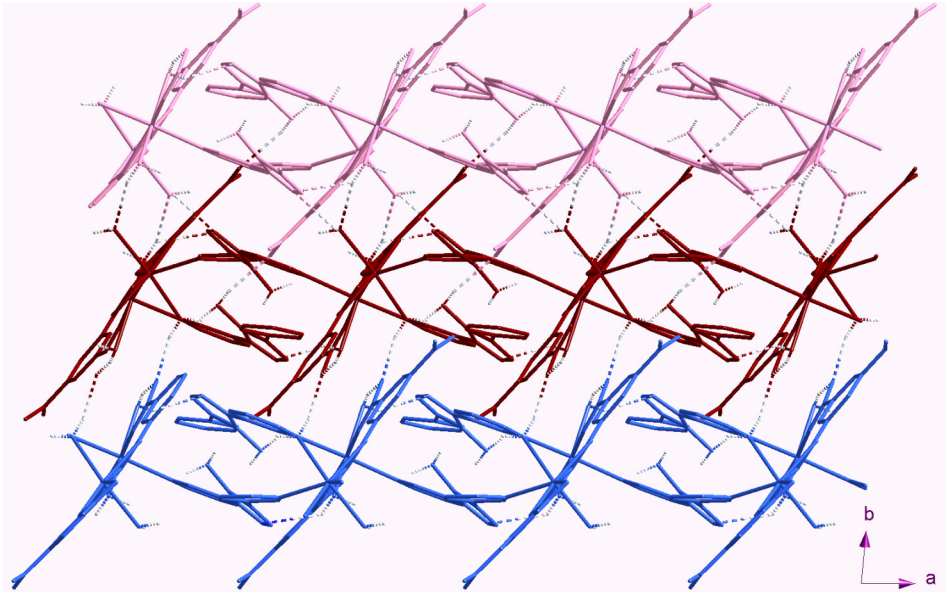

Fig. S7

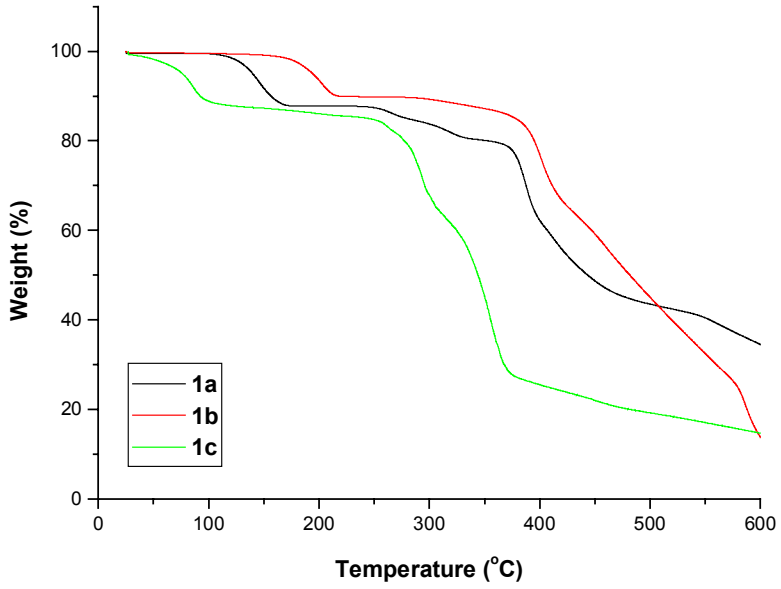
Weight (%)
Temperature (°C)
1a
1b
1c
0
20
40
60
80
100
0
100
200
300
400
500
600

Fig. S8

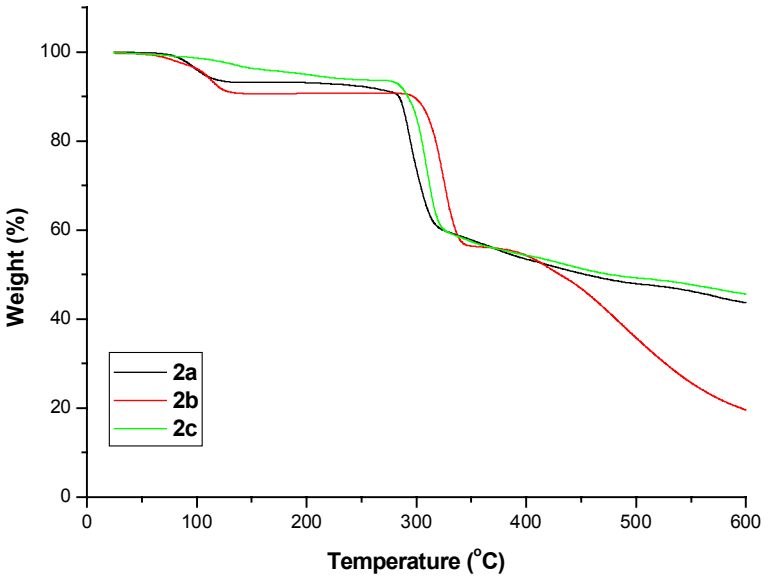
Weight (%)
Temperature (°C)
2a
2b
2c
0
20
40
60
80
100
0
100
200
300
400
500
600

Fig. S9

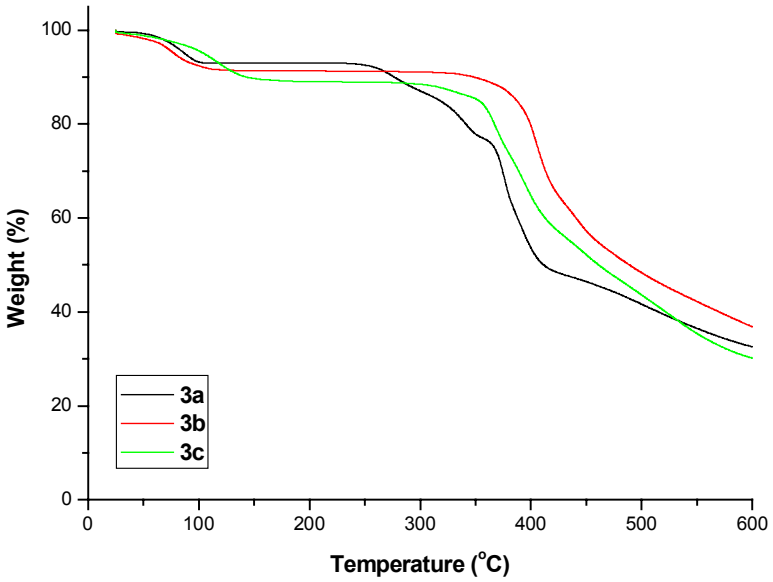
Weight (%)
Temperature (°C)
3a
3b
3c
0
20
40
60
80
100
0
100
200
300
400
500
600

Fig. S10

Table S1 Selective bond lengths (Å) and angles (°) for complexes **1a**–**1c**

		1a	
Co1–O1	2.067(1)	Co1–O6	2.130(1)
Co1–N1	2.163(1)	Co2–O4	2.098(1)
Co2–N6	2.117(1)	Co2–O5	2.144(1)
O1–Co1–O6	90.34(5)	O1–Co1–N1	90.29(5)
O6–Co1–N1	91.21(5)	O4–Co2–N6	89.87(5)
O4–Co2–O5	90.06(5)	N6–Co2–O5	86.37(5)
		1b	
Co1–O8	2.070(1)	Co1–O4	2.105(2)
Co1–N6A	2.186(2)	Co2–O1	2.034(2)
Co2–O7	2.140(2)	Co2–N1	2.143(2)
O8–Co1–O4	91.28(6)	O8–Co1–N6A	89.19(6)
O4–Co1–N6A	92.59(6)	O1–Co2–O7	91.07(5)
O1–Co2–N1	90.26(6)	O7–Co2–N1	96.54(6)
		1c	
Co1–O8	2.090(1)	Co1–O7	2.091(1)
Co1–N1	2.168(2)		
O8–Co1–O7	89.33(5)	O8–Co1–N1	87.51(6)
O7–Co1–N1	90.89(6)		

Symmetry code for **1b**: A $x + 1$, y, z.

Table S2 Selective bond lengths (Å) and angles (°) for complexes **2a**–**2c**

2a

Cu1–O4A	1.934(1)	Cu1–N6B	2.026(2)
Cu1–O1	2.027(1)	Cu1–N1	2.038(2)
Cu1–O3C	2.279(2)	Cu1–O2	2.545(2)
O4A–Cu1–N6B	92.05(7)	O4A–Cu1–O1	150.27(7)
N6B–Cu1–O1	87.87(7)	O4A–Cu1–N1	93.30(7)
N6B–Cu1–N1	170.72(7)	O1–Cu1–N1	91.23(7)
O4A–Cu1–O3C	120.49(6)	N6B–Cu1–O3C	86.13(7)
O1–Cu1–O3C	89.18(6)	N1–Cu1–O3C	84.63(7)
O4A–Cu1–O2	95.01(7)	N6B–Cu1–O2	102.93(7)
O1–Cu1–O2	56.24(7)	N1–Cu1–O2	84.18(7)
O2–Cu1–O3C	143.25(6)		

2b

Cu1–O1	1.959(3)	Cu1–O7	1.961(4)
Cu1–N1	2.051(4)	Cu1–N7	2.056(4)
Cu1–O25	2.254(3)	Cu2–O22A	1.960(3)
Cu2–O13	1.965(3)	Cu2–N12	2.034(4)
Cu2–N6B	2.038(4)	Cu2–O28	2.284(4)
Cu3–O19	1.957(4)	Cu3–O18C	1.978(4)
Cu3–N19	2.048(4)	Cu3–N18	2.066(4)
Cu3–O26	2.361(4)	Cu3–O27	2.415(4)
Cu4–O9	1.953(3)	Cu4–O6D	1.971(3)
Cu4–N13	2.013(4)	Cu4–N24B	2.020(4)
Cu4–O29	2.492(3)		

O1–Cu1–O7	174.58(16)	O1–Cu1–N1	92.01(15)
O7–Cu1–N1	89.97(15)	O1–Cu1–N7	89.51(15)
O7–Cu1–N7	89.31(15)	N1–Cu1–N7	171.04(17)
O1–Cu1–O25	88.84(14)	O7–Cu1–O25	85.97(15)
N1–Cu1–O25	94.51(15)	N7–Cu1–O25	94.34(15)
O22A–Cu2–O13	172.80(16)	O22A–Cu2–N12	90.78(16)
O13–Cu2–N12	86.74(16)	O22A–Cu2–N6B	92.67(16)
O13–Cu2–N6B	90.95(16)	N12–Cu2–N6B	169.54(17)
O22A–Cu2–O28	84.97(15)	O13–Cu2–O28	89.09(15)
N12–Cu2–O28	104.32(15)	N6B–Cu2–O28	85.82(16)
O19–Cu3–O18C	179.07(14)	O19–Cu3–N19	91.95(15)
O18C–Cu3–N19	88.91(15)	O19–Cu3–N18	88.33(16)
O18C–Cu3–N18	90.82(16)	N19–Cu3–N18	177.88(17)
O19–Cu3–O26	90.13(15)	O18C–Cu3–O26	89.51(15)
N19–Cu3–O26	90.85(15)	N18–Cu3–O26	91.25(15)
O19–Cu3–O27	84.91(15)	O18C–Cu3–O27	95.43(15)
N19–Cu3–O27	90.21(14)	N18–Cu3–O27	87.73(15)
O26–Cu3–O27	174.96(13)	O9–Cu4–O6D	178.30(15)
O9–Cu4–N13	91.81(16)	O6D–Cu4–N13	89.89(16)
O9–Cu4–N24B	88.60(15)	O6D–Cu4–N24B	89.69(15)
N13–Cu4–N24B	176.90(18)	O9–Cu4–O29	85.05(15)
N13–Cu4–O29	82.06(15)	O6D–Cu4–O29	95.35(13)
N24B–Cu4–O29	101.02(15)		

2c

Cu1–O2	1.938(2)	Cu1–O6A	1.950(2)
Cu1–N6	2.026(3)	Cu1–N1B	2.035(3)
Cu1–O7	2.318(3)		
O2–Cu1–O6A	159.73(9)	O2–Cu1–N6	88.55(10)

O6A–Cu1–N6	90.07(10)	O2–Cu1–N1B	89.84(10)
O6A–Cu1–N1B	91.31(10)	N6–Cu1–N1B	178.34(9)
O2–Cu1–O7	92.47(9)	O6A–Cu1–O7	107.78(9)
N6–Cu1–O7	91.06(10)	N1B–Cu1–O7	89.39(10)

Symmetry codes for **2a**: A x, $y - 1$, z; B x, $y + 1$, $z - 1$; C $-x + 1$, $-y + 2$, $-z + 1$. **2b**: A x, $y + 1$, z; B x, $y + 1$, $z + 1$; C x, $y - 1$, $z - 1$; D x, y, $z - 1$. **2c**: A $x - 1/2$, $-y + 1/2$, $z - 1/2$; B $x - 1/2$, $-y + 1/2$, $z + 1/2$.

Table S3 Selective bond lengths (Å) and angles (°) for complexes **3a**–**3c**

3a

Cd1–O4A	2.258(2)	Cd1–O5	2.305(2)
Cd1–N1B	2.331(2)	Cd1–O1	2.363(2)
Cd1–N2	2.376(2)	Cd1–O2	2.540(2)
O4A–Cd1–O5	81.55(6)	O4A–Cd1–N1B	136.04(6)
O5–Cd1–N1B	85.70(7)	O4A–Cd1–O1	88.38(6)
O5–Cd1–O1	96.31(6)	N1B–Cd1–O1	134.94(6)
O4A–Cd1–N2	87.47(6)	O5–Cd1–N2	169.02(6)
N1B–Cd1–N2	102.42(7)	O1–Cd1–N2	83.26(6)
O4A–Cd1–O2	138.88(6)	O5–Cd1–O2	88.85(6)
N1B–Cd1–O2	82.24(6)	O1–Cd1–O2	52.90(5)
N2–Cd1–O2	99.48(6)		

3b

Cd1–N1	2.298(4)	Cd1–N7	2.316(4)
Cd1–O2	2.334(3)	Cd1–O13	2.346(3)
Cd1–O12A	2.440(3)	Cd1–O14	2.453(4)
Cd1–O11A	2.507(3)	Cd2–O16	2.294(3)
Cd2–O7	2.306(3)	Cd2–O15	2.325(4)
Cd2–O6	2.344(3)	Cd2–N12B	2.383(4)
Cd2–O8	2.500(3)	Cd2–O5	2.526(3)
N1–Cd1–N7	177.87(13)	N1–Cd1–O2	91.24(12)
N7–Cd1–O2	90.59(12)	N1–Cd1–O13	85.67(13)
N7–Cd1–O13	95.67(13)	O2–Cd1–O13	81.53(11)
N1–Cd1–O12A	92.74(12)	N7–Cd1–O12A	85.86(12)

O2–Cd1–O12A	161.18(11)	O13–Cd1–O12A	80.44(12)
N1–Cd1–O14	93.48(13)	N7–Cd1–O14	86.03(13)
O2–Cd1–O14	72.64(12)	O13–Cd1–O14	154.14(13)
O12A–Cd1–O14	125.38(12)	N1–Cd1–O11A	82.13(12)
N7–Cd1–O11A	95.74(12)	O2–Cd1–O11A	145.85(10)
O13–Cd1–O11A	130.80(11)	O12A–Cd1–O11A	52.97(10)
O14–Cd1–O11A	74.37(11)	O16–Cd2–O7	94.34(13)
O16–Cd2–O15	174.54(14)	O7–Cd2–O15	85.92(13)
O16–Cd2–O6	81.04(12)	O7–Cd2–O6	152.53(12)
O15–Cd2–O6	96.21(13)	O16–Cd2–N12B	82.72(13)
O7–Cd2–N12B	81.30(13)	O15–Cd2–N12B	102.70(15)
O6–Cd2–N12B	124.40(13)	O16–Cd2–O8	83.15(13)
O7–Cd2–O8	54.08(12)	O15–Cd2–O8	92.63(14)
O6–Cd2–O8	98.45(12)	N12B–Cd2–O8	131.65(12)
O16–Cd2–O5	101.67(13)	O7–Cd2–O5	152.98(12)
O15–Cd2–O5	80.18(13)	O6–Cd2–O5	53.04(11)
N12B–Cd2–O5	79.34(12)	O8–Cd2–O5	148.92(12)

3c

Cd1–N6A	2.295(3)	Cd1–N1	2.297(3)
Cd1–O8	2.329(3)	Cd1–O7	2.421(3)
Cd1–O1	2.468(3)	Cd1–O3A	2.492(2)
Cd1–O2	2.498(3)		

N6A–Cd1–N1	170.95(11)	N6A–Cd1–O8	94.39(12)
N1–Cd1–O8	89.25(12)	N6A–Cd1–O7	83.59(10)
N1–Cd1–O7	89.67(10)	O8–Cd1–O7	155.58(10)
N6A–Cd1–O1	92.37(12)	N1–Cd1–O1	96.46(11)
O8–Cd1–O1	79.17(11)	O7–Cd1–O1	125.17(9)
N6A–Cd1–O3A	86.17(10)	N1–Cd1–O3A	86.66(10)

O8–Cd1–O3A	76.30(10)	O7–Cd1–O3A	79.29(8)
O1–Cd1–O3A	155.23(10)	N6A–Cd1–O2	91.67(10)
N1–Cd1–O2	92.18(10)	O8–Cd1–O2	131.01(11)
O7–Cd1–O2	73.41(9)	O1–Cd1–O2	52.00(10)
O3A–Cd1–O2	152.68(9)		

Symmetry codes for **3a**: A x, $y - 1$, z; B $-x + 1$, $-y + 2$, $-z + 2$. **3b**: A x, y, $z + 1$; B $x + 1$, y, z. **3c**: A $-x + 1/2$, $y + 1/2$, $-z + 1/2$.

Table S4 Possible hydrogen-bonding metrics in the structures of **1a–1c**

Compound	D–H···A	D···A (Å)	H···A (Å)	D–H···A (°)
1a	O5–H5B···O3	2.709(2)	1.89	163
	O6–H6B···O2	2.697(2)	1.87	163
	O6–H6A···O3[a]	2.782(2)	1.94	173
	N5–H5'···O8[b]	2.919(2)	2.05	161
	O5–H5A···O7[c]	2.746(2)	1.93	162
	O7–H7A···N2[d]	2.755(2)	1.93	162
	O7–H7B···O8[e]	3.041(2)	2.40	132
	O8–H8A···N3[f]	2.874(2)	2.08	156
	O8–H8B···O2	2.849(2)	2.02	166
1b	N5–H5A···O3	3.005(3)	2.44	121
	N5–H5A···O5[g]	3.348(3)	2.55	148
	N5–H5B···O9[h]	3.037(3)	2.21	152
	O7–H7A···N2[i]	2.834(3)	2.00	166
	O7–H7B···O2	2.742(2)	1.93	158
	O8–H8A···O2[h]	2.776(2)	1.96	159
	O8–H8B···O3	2.637(2)	1.80	166
	O9–H9A···O7	2.986(3)	2.33	134
	O9–H9B···N3[j]	3.093(3)	2.31	153
1c	O3–H3···O1[k]	2.731(2)	1.97	154
	N5–H5A···O9	3.071(3)	2.31	141
	N5–H5B···O1[k]	3.040(3)	2.20	153
	O6–H6···N6[l]	2.578(3)	1.80	158
	O7–H7A···N3[m]	2.804(2)	1.96	176
	O7–H7B···O1[k]	2.764(2)	1.92	174
	O8–H8A···N2[n]	2.805(2)	1.98	164
	O8–H8B···O2[k]	2.641(2)	1.80	169
	O9–H9A···O5[l]	2.922(3)	2.56	107
	O9–H9B···O1[o]	3.136(3)	2.51	131

[a] $-x + 3/2, y - 1/2, -z + 1/2$. [b] $x + 1, y, z$. [c] $x + 1/2, -y + 1/2, z + 1/2$. [d] $x - 1, y, z$. [e] $-x + 1/2, y - 1/2, -z + 1/2$. [f] $-x + 3/2, y + 1/2, -z + 1/2$. [g] $-x, -y + 1, -z$. [h] $x, y + 1, z$. [i] $-x, -y + 1, -z + 1$. [j] $x + 1, y - 1, z$. [k] $x, y - 1, z$. [l] $-x + 1, -y + 1, -z$. [m] $x + 1, y + 1, z$. [n] $-x + 2, -y, -z + 1$. [o] $x - 1, y - 1, z$.

Table S5 Possible hydrogen-bonding metrics in the structures of **2a–2c**

Compound	D–H···A	D···A (Å)	H···A (Å)	D–H···A (°)
2a	O5–H5A···N2[a]	2.907(3)	2.04	164
	O5–H5B···O2	2.872(3)	2.00	176
	O6–H6A···O5[b]	2.843(3)	1.97	172
	O6–H6B···O5[c]	2.893(3)	1.99	167
2b	O25–H25A···O5[d]	2.827(6)	2.02	140
	N5–H5B···O4[d]	3.162(8)	2.46	136
	N11–H11B···O24[e]	3.036(8)	2.42	126
	N17–H17B···O11[e]	3.135(7)	2.43	137
	N5–H5A···O32	3.047(8)	2.19	162
	N11–H11A···O36[f]	2.983(7)	2.13	159
	N17–H17A···O31	3.116(7)	2.32	149
	N23–H23B···O33[g]	2.977(7)	2.11	163
	O25–H25B···O31	2.795(5)	1.87	160
	O26–H26"···O32	2.784(7)	1.84	168
	O28–H28B···O33[h]	2.908(6)	2.22	127
	O30–H30B···O8	2.699(6)	1.97	144
	O34–H34B···N12[i]	3.359(7)	2.61	147
	O35–H35A···O10	2.756(7)	1.92	168
	O35–H35B···N3[j]	2.947(7)	2.12	163
	O36–H36A···O34[k]	2.706(7)	1.85	179
	O36–H36B···N11[f]	2.983(7)	2.20	153
	O27–H27B···O17[l]	2.726(6)	2.00	131
	O28–H28A···N21[m]	2.789(6)	1.86	161
	O29–H29A···O5[j]	2.661(5)	1.86	155
	O29–H29B···N9	2.798(6)	1.97	165
2c	O3–H3···O4[n]	2.634(4)	1.82	169
	O7–H7A···O1	2.775(4)	1.94	166
	O7–H7B···O5[o]	2.766(4)	1.98	154
	O8–H8A···O1[p]	2.689(4)	1.95	145
	O8–H8B···O5[q]	3.015(5)	2.20	161
	N5–H5A···O8[o]	2.973(5)	2.16	152

[a] $-x+1, -y+1, -z+2$. [b] $x, y, z-1$. [c] $-x+2, -y+1, -z+1$. [d] $-x, -y+1, -z$. [e] $-x+1, -y+1, -z+1$. [f] $-x+1, -y+2, -z+1$. [g] $-x+1, -y, -z+1$. [h] $x, y+1, z$. [i] $x, y-1, z$. [j] $x, y, z+1$. [k] $x+1, y+1, z$. [l] $x, y-1, z-1$. [m] $x, y+1, z+1$. [n] $-x, -y+1, -z+1$. [o] $x+1/2, -y+1/2, z-1/2$. [p] $x-1, y, z$. [q] $x-1/2, -y+1/2, z-1/2$.

Table S6 Possible hydrogen-bonding metrics in the structures of **3a–3c**

Compound	D–H···A	D···A (Å)	H···A (Å)	D–H···A (°)
3a	O5–H5A'···O2[a]	2.775(2)	1.95	162
	O5–H5B'···O7[b]	2.747(3)	1.95	155
	N5–H5A···O1[c]	2.893(3)	2.01	172
	N5–H5B···O6[d]	3.138(5)	2.24	174
	O7–H7A···O3[e]	3.189(3)	2.44	147
	O7–H7A···N3[d]	3.137(3)	2.51	132
	O7–H7B···O3[f]	2.802(3)	1.97	167
3b	N5–H5A···O18	3.044(8)	2.17	163
	N5–H5B···O9[g]	3.110(6)	2.32	147
	N11–H11A···O17[h]	3.044(5)	2.18	164
	O14–H14A···O15[i]	3.286(6)	2.37	160
	O14–H14B···O17[h]	2.887(5)	2.20	128
	O15–H15B···N8[j]	3.219(5)	2.53	128
	O16–H16B···O1[k]	2.738(5)	1.91	164
	O17–H17A···N9[i]	2.863(6)	2.07	154
	O17–H17B···O5[c]	2.826(5)	1.98	175
	O13–H13A···O1	2.711(5)	1.89	162
	O13–H13B···N2[h]	3.005(6)	2.24	149
	O16–H16A···N6[l]	2.780(6)	1.98	157
3c	O7–H7B···O4[m]	2.572(4)	1.74	166
	O6–H6A···O5[n]	2.649(3)	1.69	173
	N5–H5A···O9[o]	2.886(5)	2.05	157
	N5–H5B···O10[p]	3.04(1)	2.14	174
	N5–H5B···O10'[p]	3.06(1)	2.21	158
	O7–H7A···O9[l]	2.731(4)	1.89	176
	O8–H8A···O10	2.650(9)	2.16	117
	O8–H8A···O10'	3.08(1)	2.38	140

[a] $-x, -y + 2, -z + 2$. [b] $-x, -y + 1, -z + 1$. [c] $x + 1, y, z$. [d] $-x + 1, -y + 1, -z + 1$. [e] $-x + 1, -y + 2, -z + 1$. [f] $x, y - 1, z - 1$. [g] $-x + 1, -y + 2, -z$. [h] $x - 1, y, z$. [i] $-x, -y + 2, -z$. [j] $-x - 1, -y + 2, -z$. [k] $-x, -y + 1, -z$. [l] $x, y, z - 1$. [m] $-x + 1/2, y + 1/2, -z + 1/2$. [n] $-x + 1, -y, -z + 2$. [o] $x, -y, z - 1/2$. [p] $-x + 1/2, y - 1/2, -z + 1/2$.