Supplementary Material (ESI) for CrystEngComm

Electronic Supplementary Information（ESI）

Metal-Organic Coordination Polymers Based on a Flexible Tetrahydrofuran-2,3,4,5-tetracarboxylate Ligand: Syntheses, Crystal Structures, and Magnetic/Photoluminescent Properties

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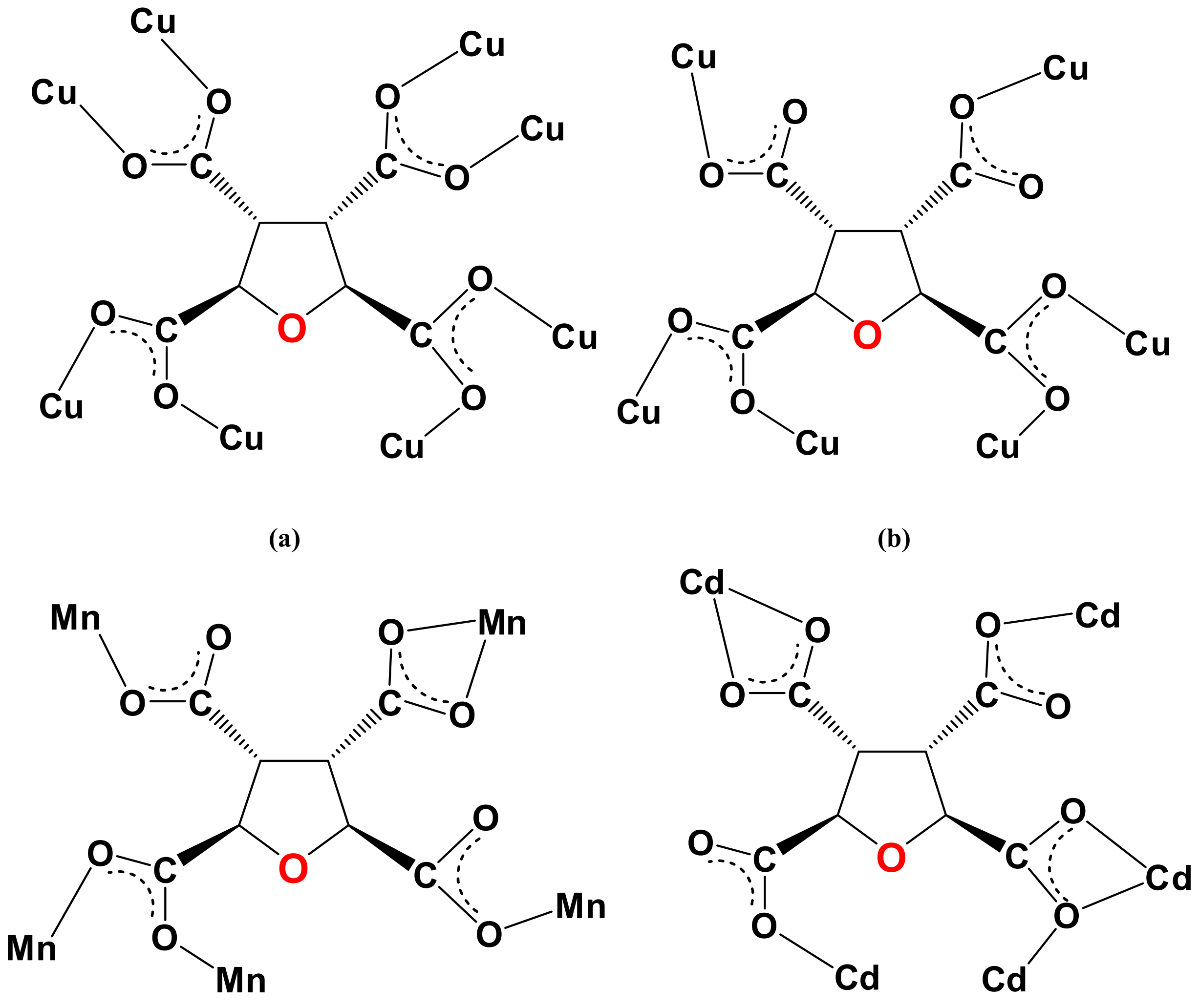
To ***CrystEngComm*** (Full Paper)



(a)

(b)

(c)

(d)

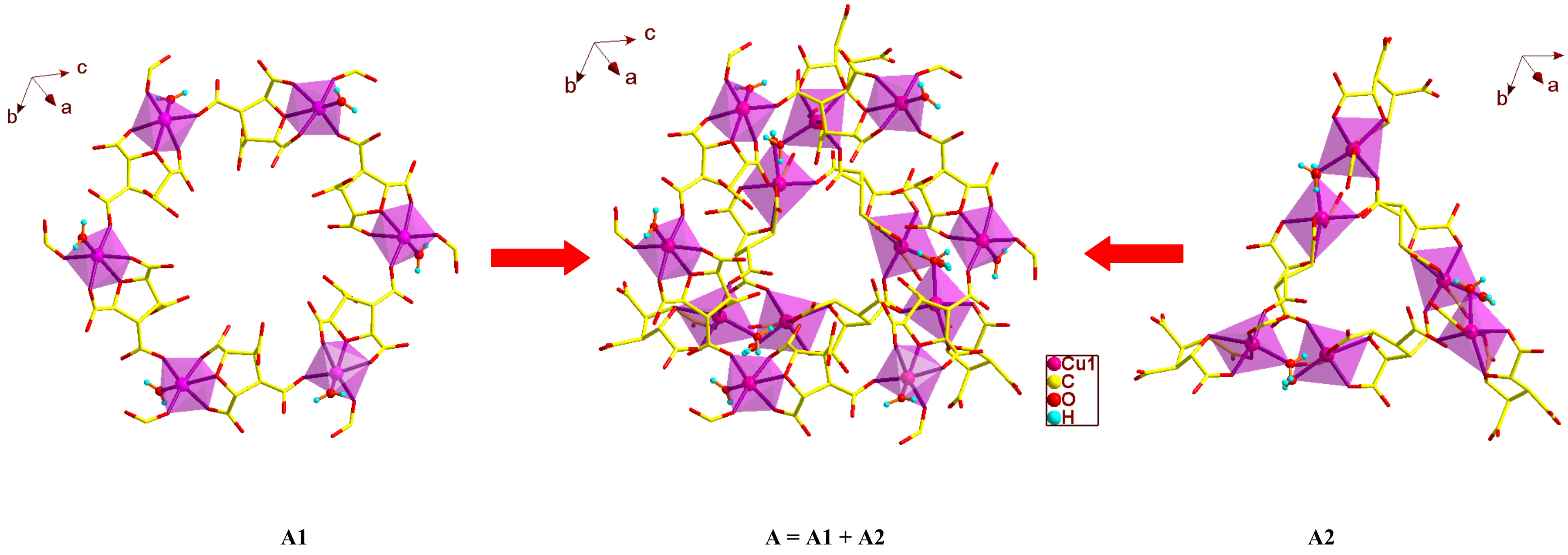
Scheme S1 Coordination modes of fully deprotonated **L** ligand in **1**–**5**:

(a) For **1**: μ_2-η^1:η^1-*syn-syn* bridging mode for the carboxylate groups at the top left and right corners as well as μ_2-η^1:η^1-*syn-anti* bridging mode for the carboxylate groups at the bottom left and right corners;

(b) For **2** and **3**: μ_1-η^1:η^0-monodentate mode for the carboxylate groups at the top left and right corners as well as μ_2-η^1:η^1-*syn-anti* bridging mode for the carboxylate groups at the bottom left and right corners;

(c) For **4**: μ_1-η^1:η^0-monodentate mode for the carboxylate groups at the top left and bottom right corners, μ_1-η^1:η^1-chelating mode for the carboxylate group at the top right corner, and μ_2-η^1:η^1-*syn-anti* bridging mode for the carboxylate group at the bottom left corner;

(d) For **5**: μ_1-η^1:η^0-monodentate mode for the carboxylate groups at the top right and bottom left corners, μ_1-η^1:η^1-chelating mode for the carboxylate group at the top left corner, and μ_2-η^1:η^2-chelating/bridging mode for the carboxylate group at the bottom right corner.

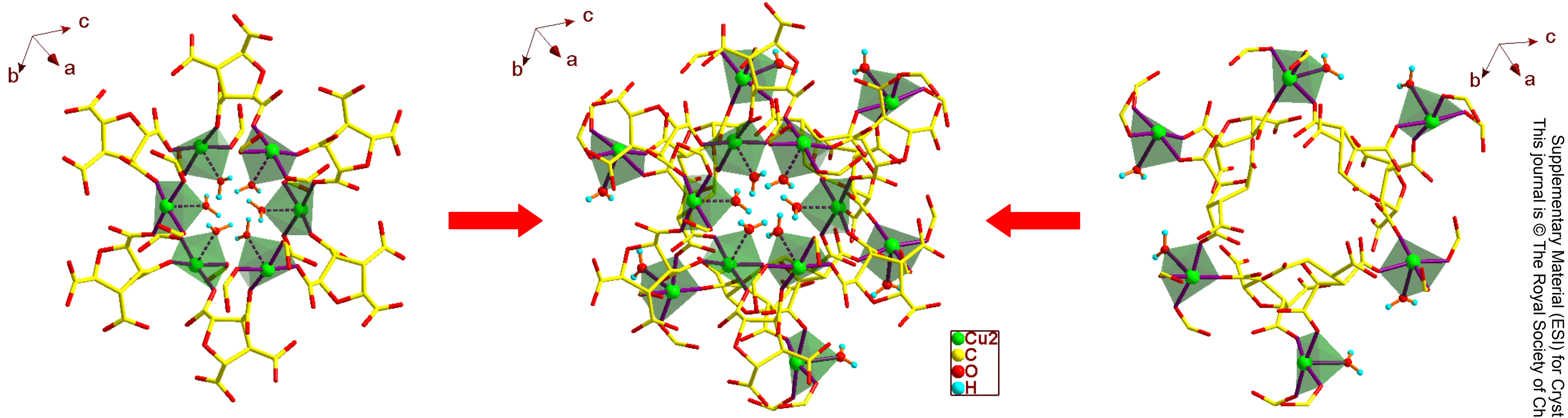


A1

A = A1 + A2

A2

Fig. S1 View of the 3-D fragment **A** in the coordination network of **1**, which contains Cu(1) centers and **L** ligands and exhibits the same crystallographic direction artificially as that in Figure 1(c). Please see the main text for more details.



B1

B = B1 + B2

B2

Fig. S2 View of the 3-D fragment **B** in the coordination network of **1**, which contains Cu(2) centers and **L** ligands and exhibits the same crystallographic direction artificially as that in Figure 1(c) (violet dashed lines represent weak Cu(2)···O(1W) interactions). Please see the main text for more details.

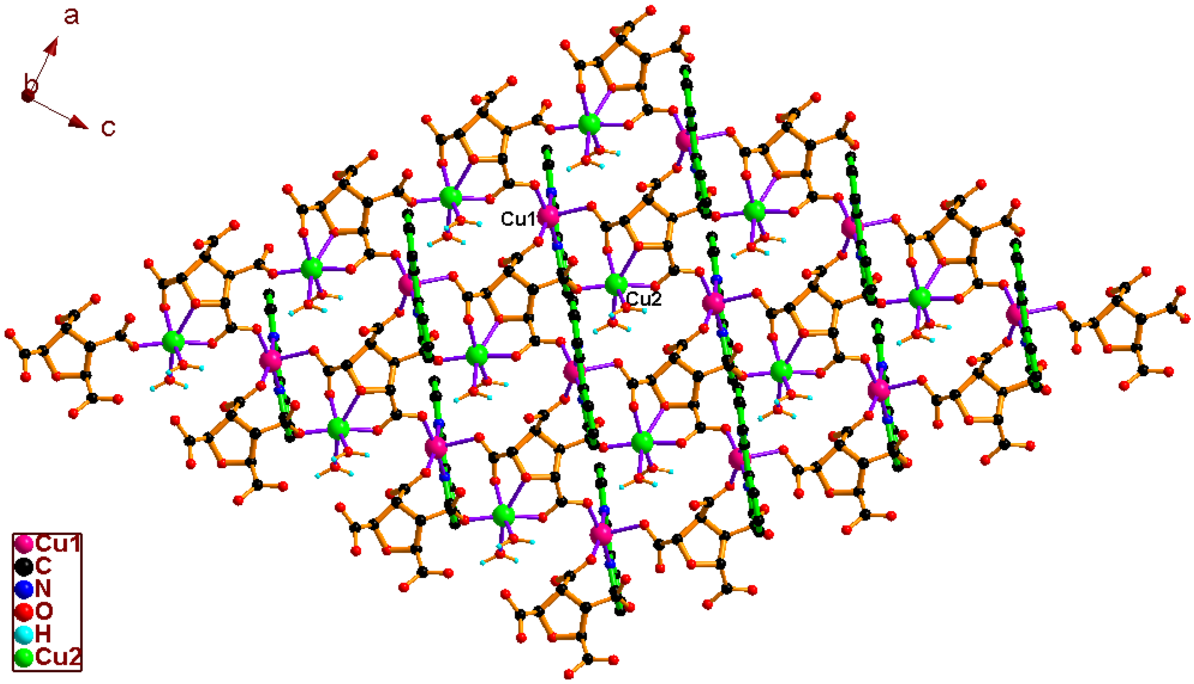


Fig. S3 View of the two-dimensional (2-D) layer in **2** running parallel to the (010) plane.

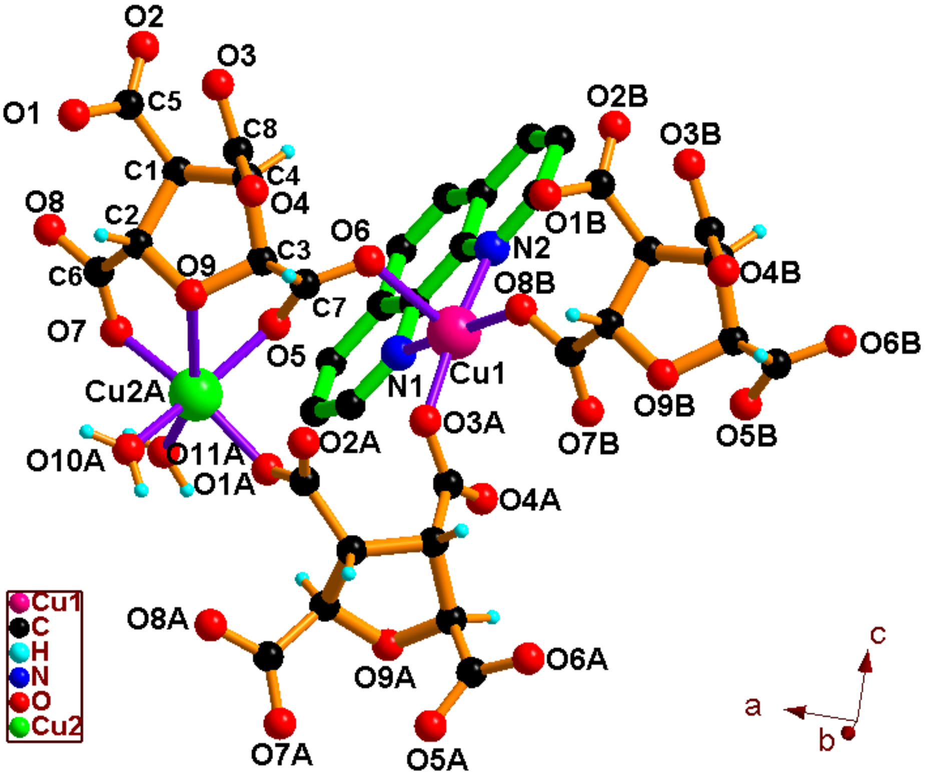


Fig. S4 View of the local coordination environments of Cu^{II} atoms in **3** [pink and green spheres correspond to Cu(1) and Cu(2) centers with different coordination geometries, respectively]. The symmetry-related atoms labeled with the suffixes A and B are generated by the symmetry operations (x, $-y + 3/2$, $z - 1/2$) and ($x + 1$, y, z). Lattice water and methanol molecules as well as all H atoms except coordinated aqua molecules and tetrahydrofuran rings of **L** ligands were omitted for clarity.

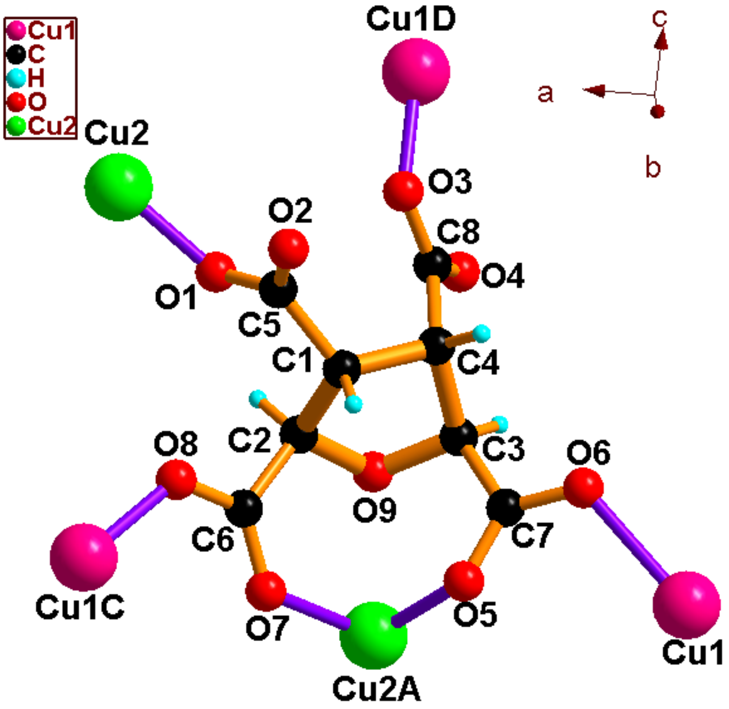


Fig. S5 View of coordination modes of **L** in **3**: μ_2-η^1:η^1-*syn-anti* bridging mode for O(5)–C(7)–O(6) and O(7)–C(6)–O(8) carboxylate groups and μ_1-η^1:η^0-monodentate mode for O(1)–C(5)–O(2) and O(3)–C(8)–O(4) carboxylate groups. The symmetry-related atoms labeled with the suffixes A, C, and D are generated by the symmetry operations (*x*, –*y* + 3/2, *z* – 1/2), (*x* – 1, *y*, *z*), and (*x*, –*y* + 3/2, *z* + 1/2).

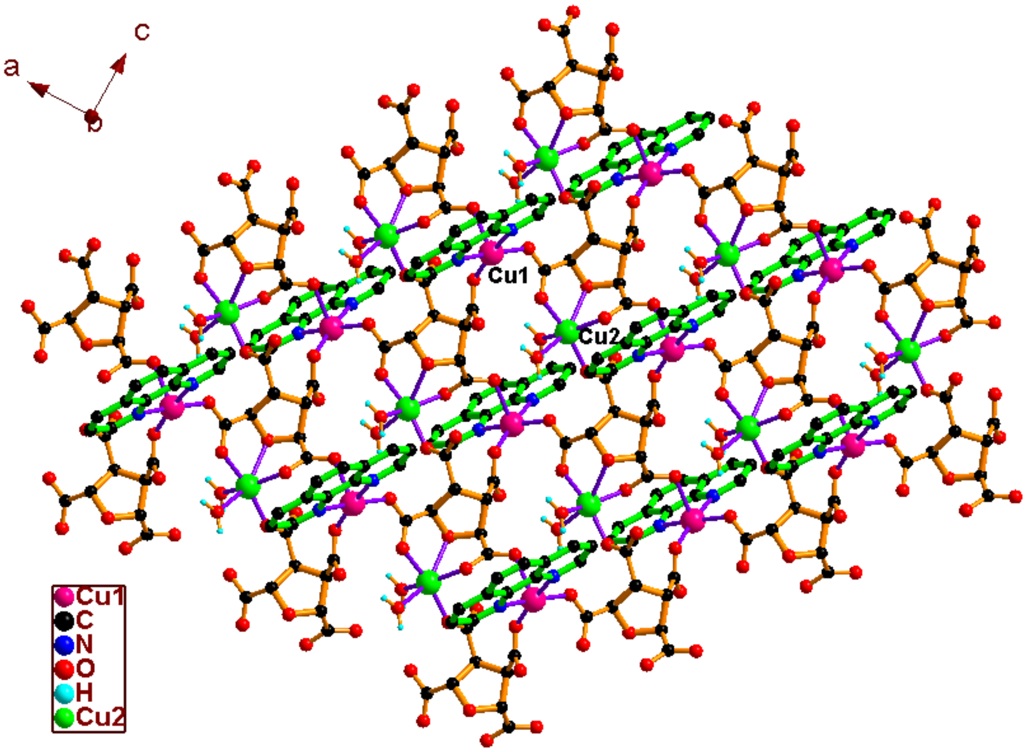


Fig. S6 View of the two-dimensional (2-D) layer in **3**, running parallel to the (010) plane. Lattice water and methanol molecules as well as all H atoms except coordinated aqua molecules were omitted for clarity.

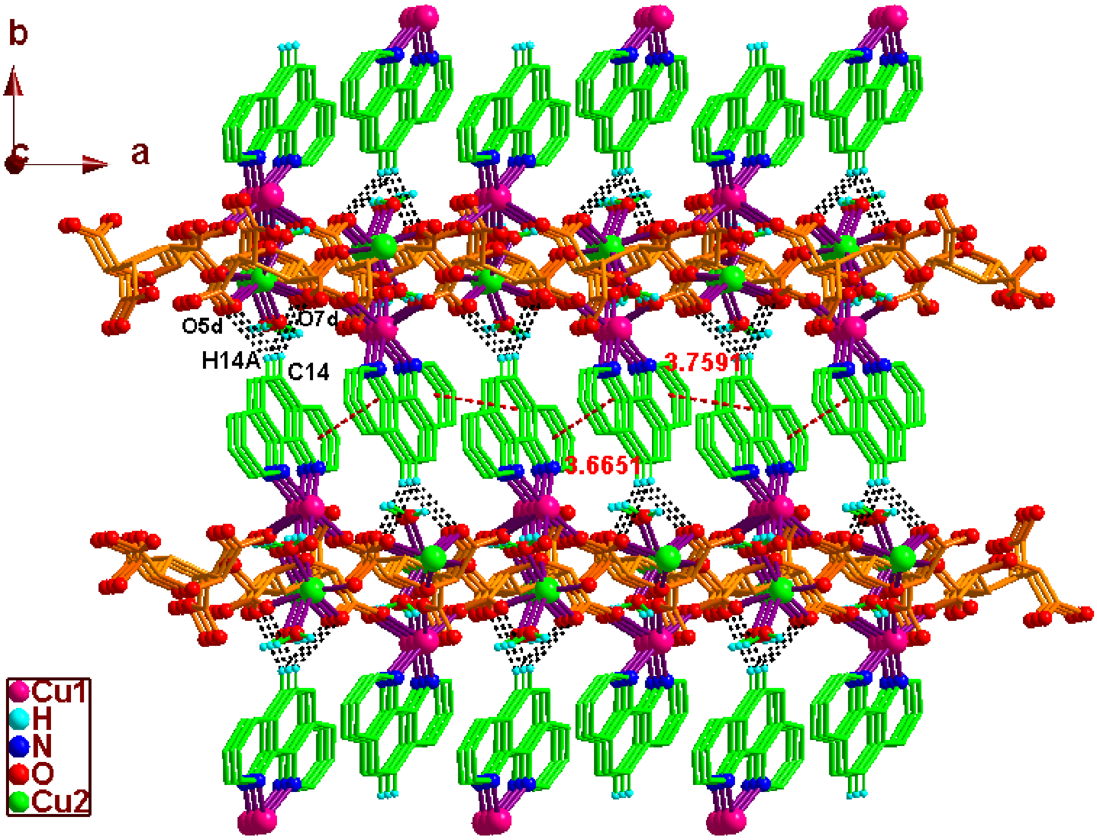


Fig. S7 View of the three-dimensional (3-D) framework in **3**, viewed along the [001] direction, formed by the co-effects of inter-layer C–H···O hydrogen-bonding interactions (black dashed lines) between phenyl rings of phen ligands and carboxylate groups of **L** ligands as well as inter-layer π···π stacking interactions (red dashed lines) between pyridyl rings of phen ligands. For clarity, lattice water and methanol molecules were omitted and only H atoms involved in the interactions and the coordinated aqua molecules were shown.

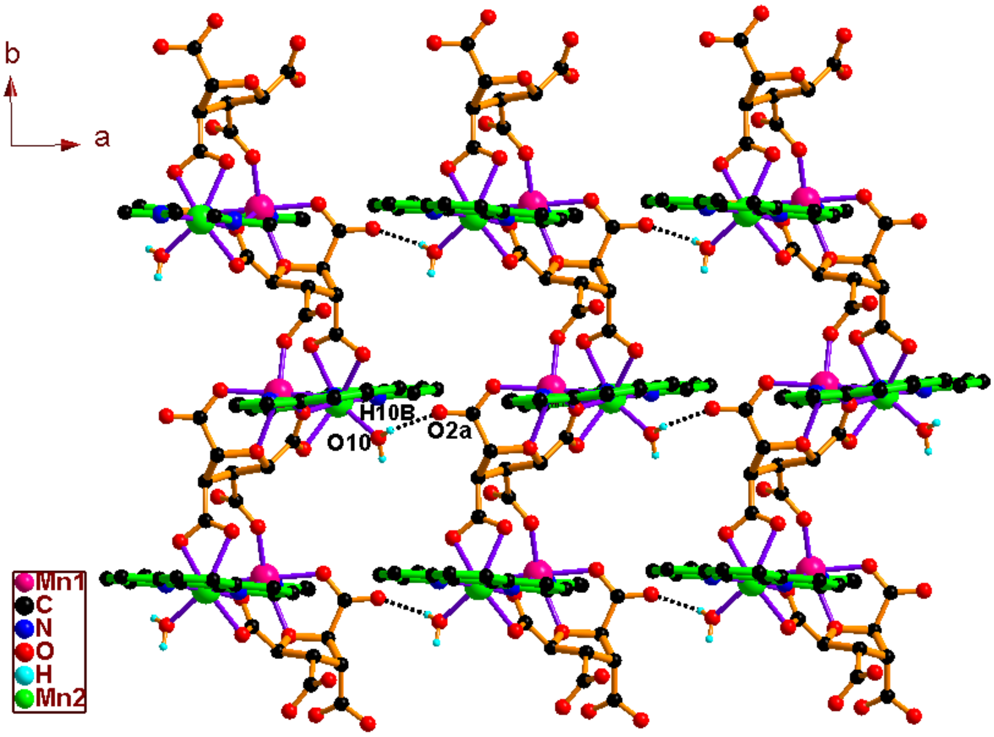


Fig. S8 View of the two-dimensional (2-D) network in **4**, parallel to the (001) plane, formed by the inter-chain O–H···O hydrogen-bonding interactions (black dashed lines),.

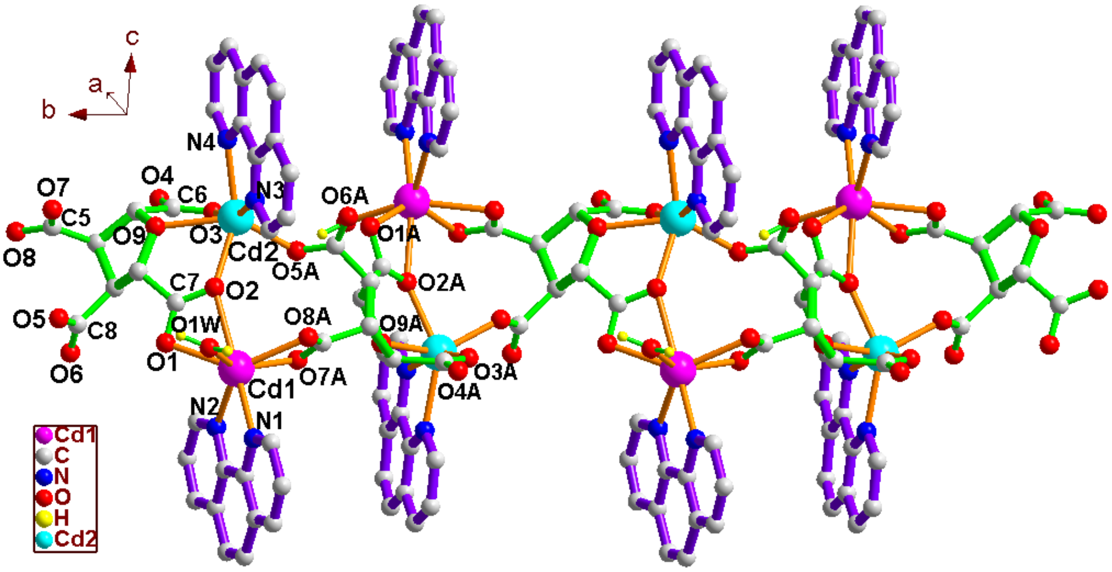


Fig. S9 View of the one-dimensional (1-D) chain in **5**, running along the [010] direction (*b*-axis), showing the local atom-numbering coordination environments of Cd^{II} atoms [magenta and cyan spheres correspond to Mn(1) and Mn(2) centers with different coordination geometries, respectively]. The symmetry-related atoms labeled with the suffix A are generated by the symmetry operation (–*x* + 1, *y* –1/2, –*z* + 3/2). For clarity, only H atoms of coordinated aqua molecules were shown.

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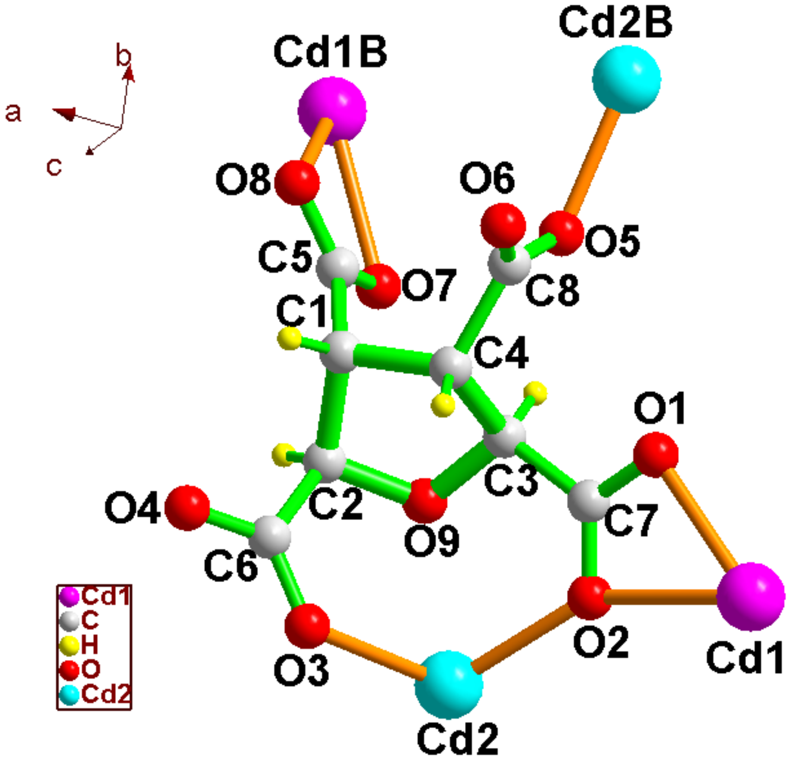


Fig. S10 View of coordination modes of **L** in **5**: μ_1-η^1:η^1-chelating mode for O(7)–C(5)–O(8) carboxylate group, μ_2-η^1:η^2-chelating/bridging mode for O(1)–C(7)–O(2) carboxylate group, and μ_1-η^1:η^0-monodentate mode for O(3)–C(6)–O(4) and O(5)–C(8)–O(6) carboxylate groups. The symmetry-related atoms labeled with the suffix B are generated by the symmetry operation (–*x* + 1, *y* +1/2, –*z* + 3/2).

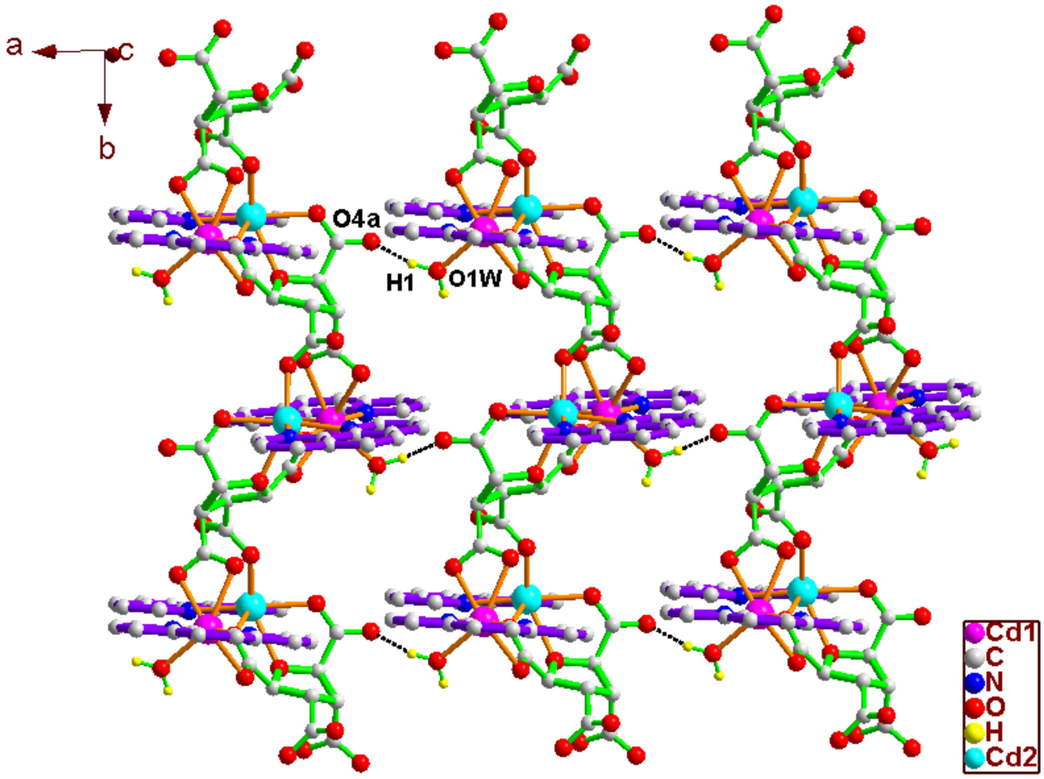


Fig. S11 View of the two-dimensional (2-D) network in **5**, running parallel to the (001) plane, formed by the inter-chain O–H···O hHydrogen-bonding interactions (black dashed lines). Lattice water molecules and all H atoms except coordinated aqua molecules were omitted for clarity.

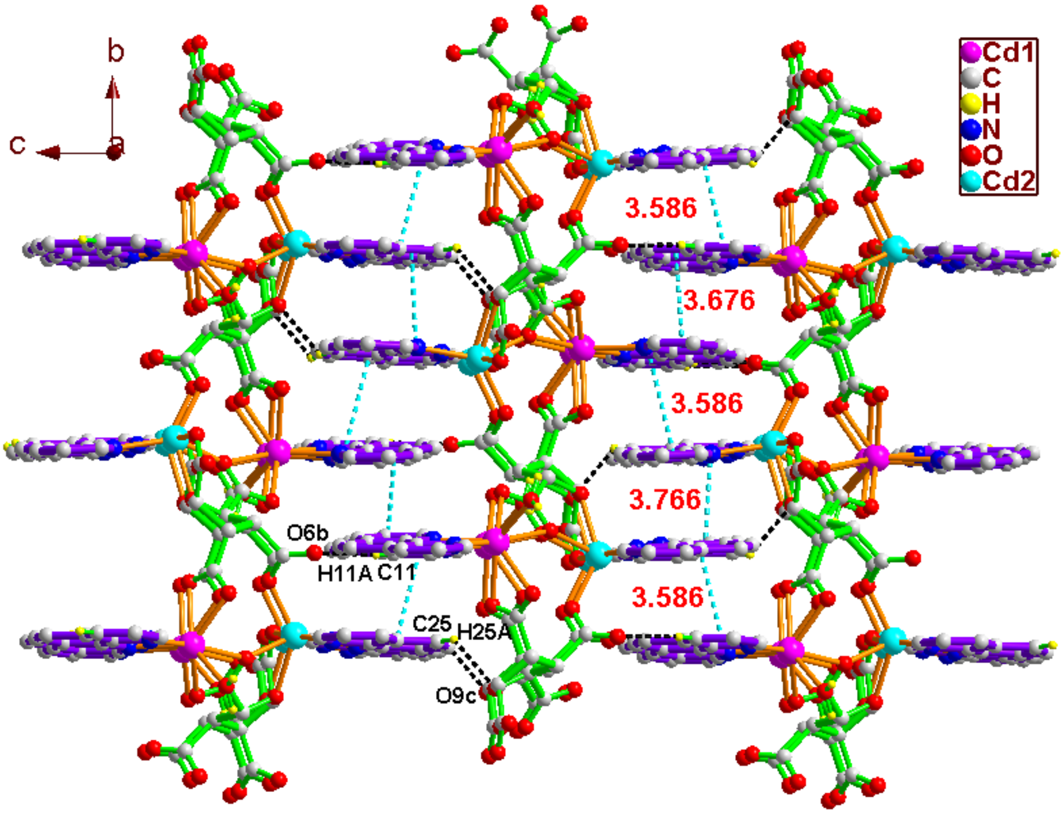
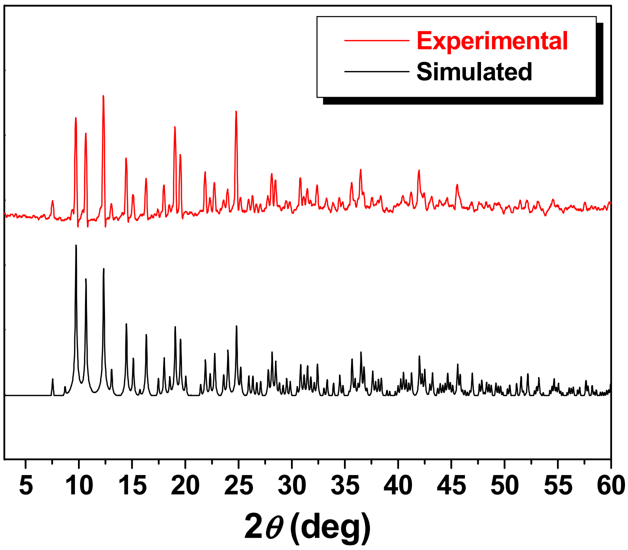
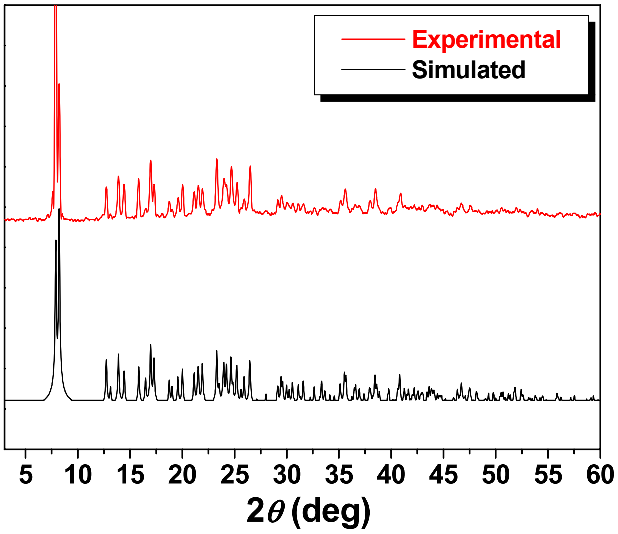


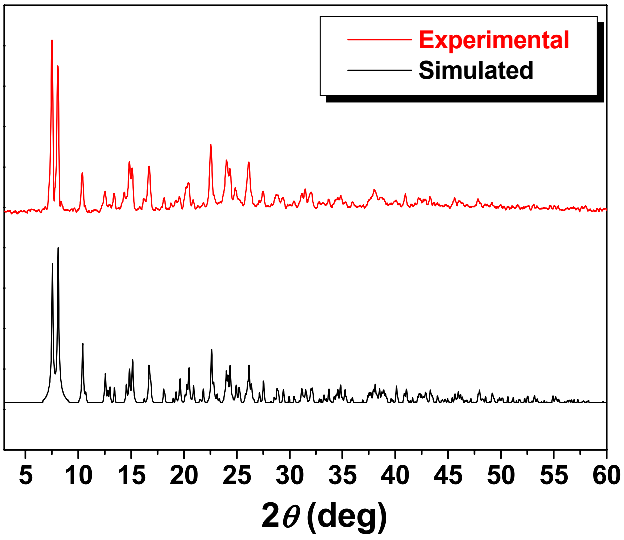
Fig. S12 View of the three-dimensional (3-D) framework in **5**, formed by the inter-chain π···π stacking (cyan dashed lines) and C–H···O hydrogen-bonding (black dashed lines) interactions. For clarity, only H atoms involved in the interactions and the coordinated aqua molecules were shown.


Experimental
Simulated
5 10 15 20 25 30 35 40 45 50 55 60
2θ (deg)

(a)


Experimental
Simulated
5 10 15 20 25 30 35 40 45 50 55 60
2θ (deg)

(b)


Experimental
Simulated
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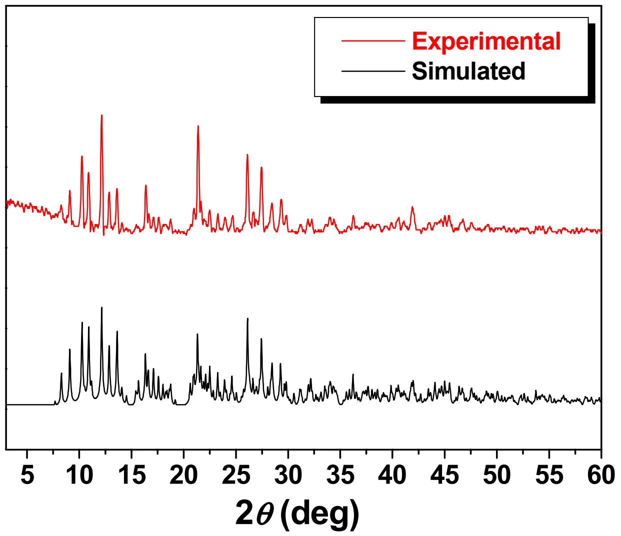
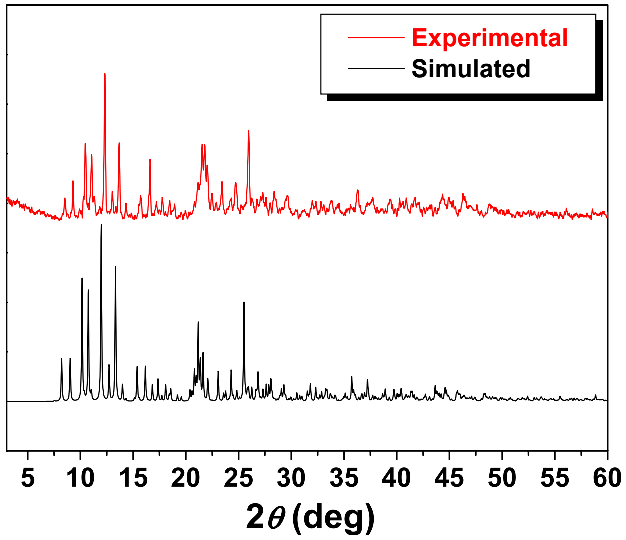
2θ (deg)

(c)



(d)



(e)

Fig. S13 XRPD patterns of (a) for **1**, (b) for **2**, (c) for **3**, (d) for **4**, and (e) for **5**.

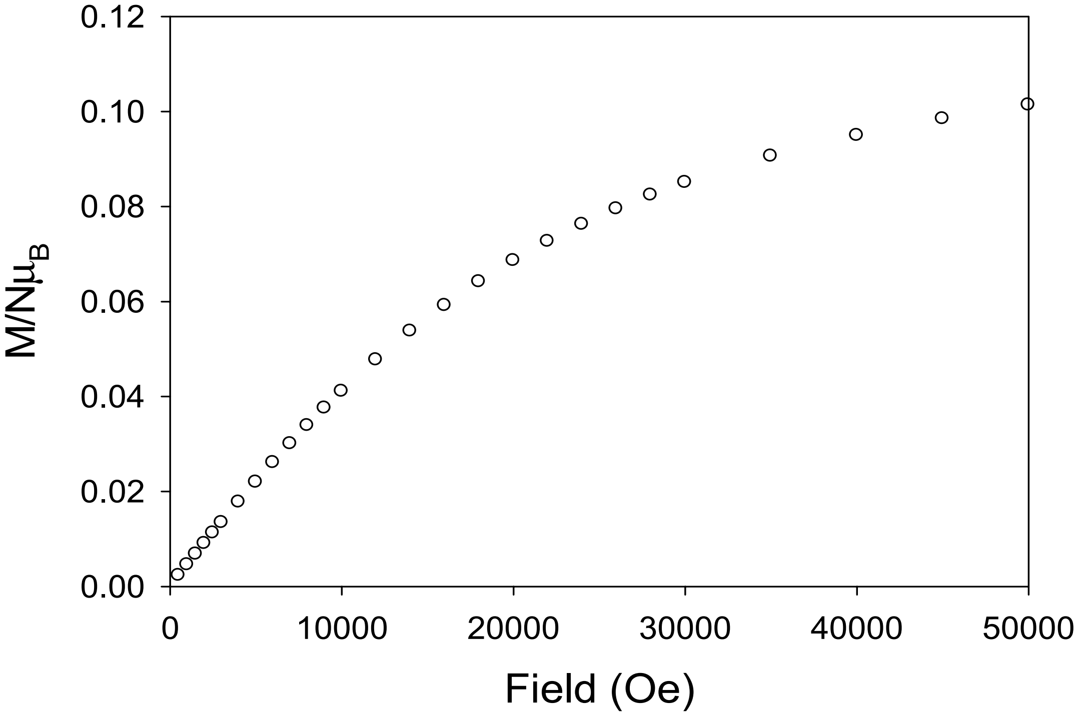


Fig. S14 Magnetization vs. field plot for **1** at 2 K.

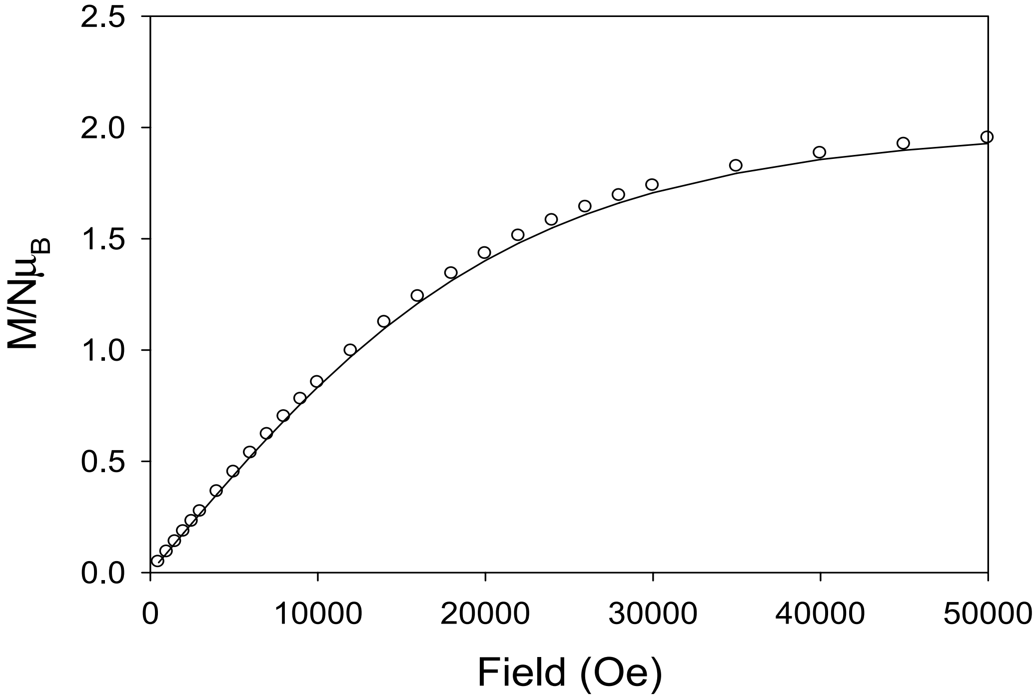


Fig. S15 Magnetization vs. field plot for **2** at 2 K. The solid line is the Brillouin function for $S = 1$ and $g = 2.0$ and is only there to aid in visualization of the curve.

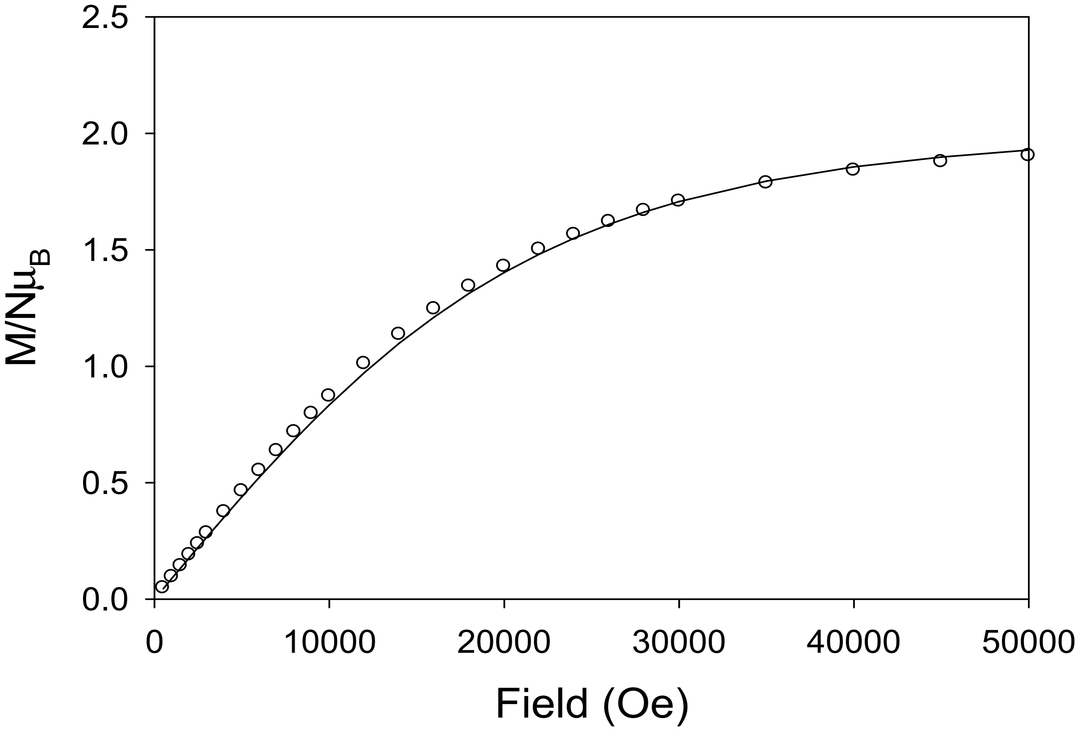


Fig. S16 Magnetization vs. field plot for **3** at 2 K. The solid line is the Brillouin function for $S = 1$ and $g = 2.0$ and only there to aid in visualization of the curve.

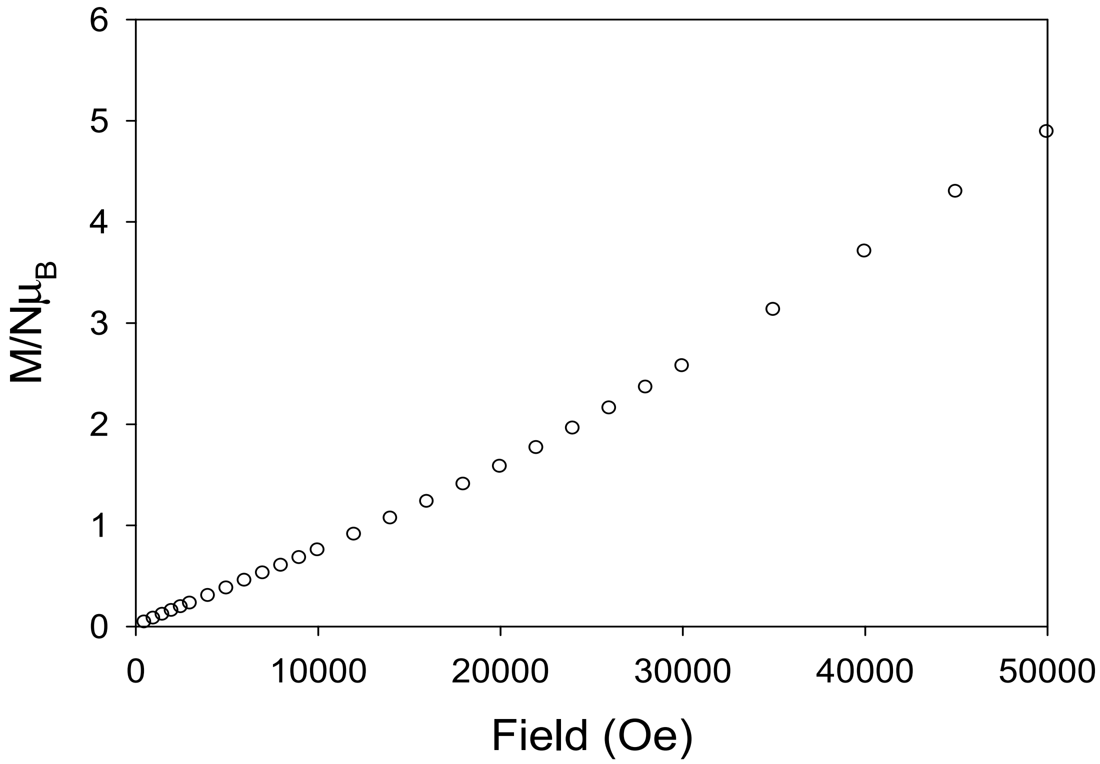
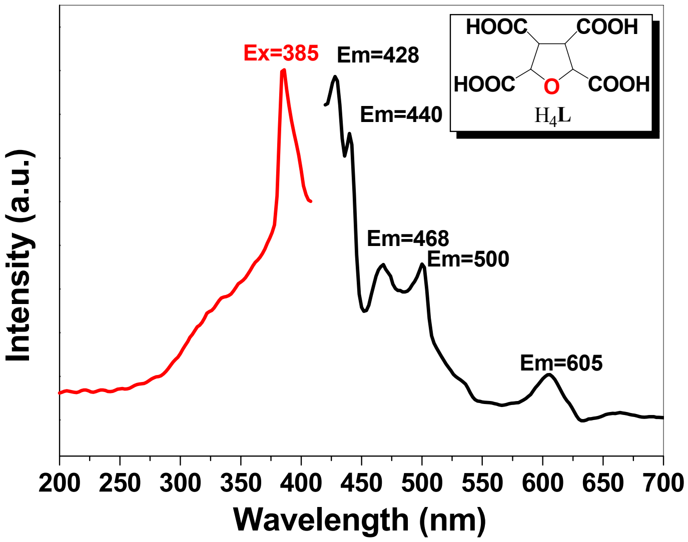
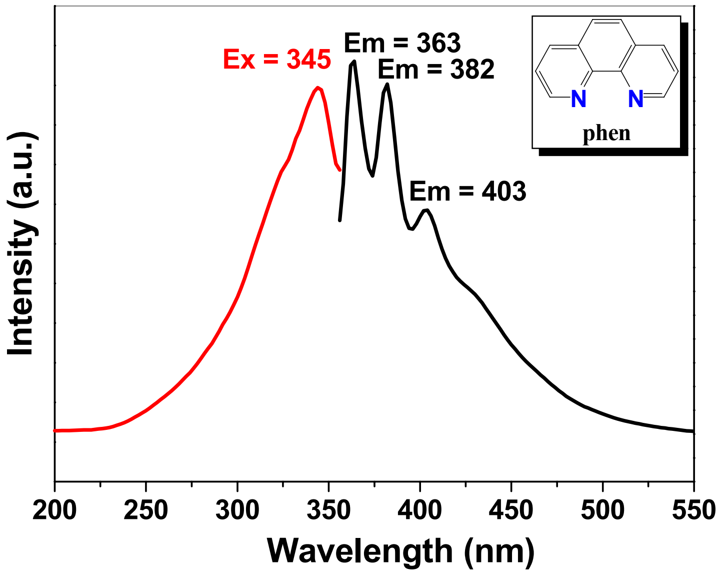


Fig. S17 Magnetization vs. field plot for **4** at 2 K.

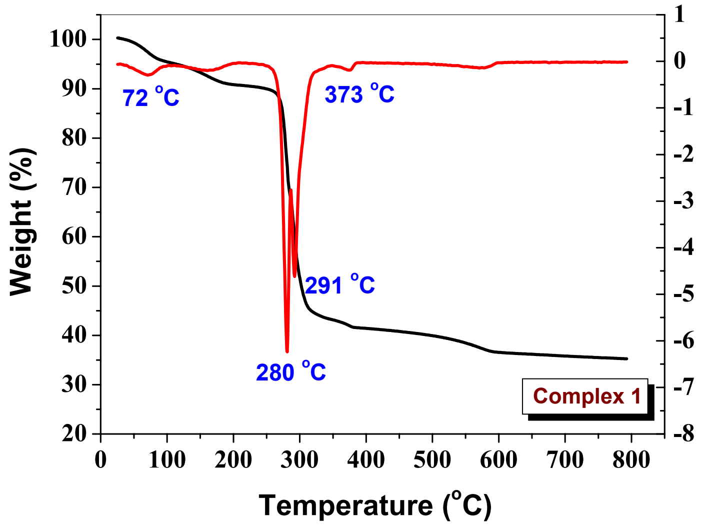


(a)

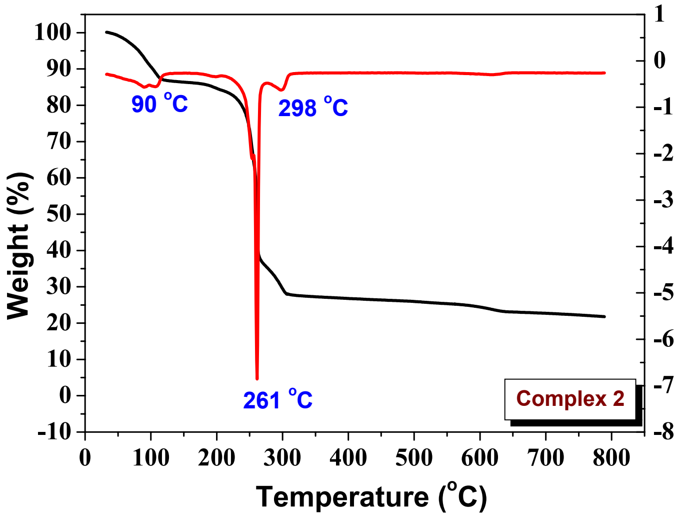


(b)

Fig. S18 Excitation and emission spectra of the free ligands in the solid state at room temperature: (a) for $H_4\mathbf{L}$ and (b) for phen.


Weight (%)
100
90
80
70
60
50
40
30
20
1
0
-1
-2
-3
-4
-5
-6
-7
-8
0
100
200
300
400
500
600
700
800
Temperature (°C)
72 °C
373 °C
291 °C
280 °C
Complex 1

(a)


Weight (%)
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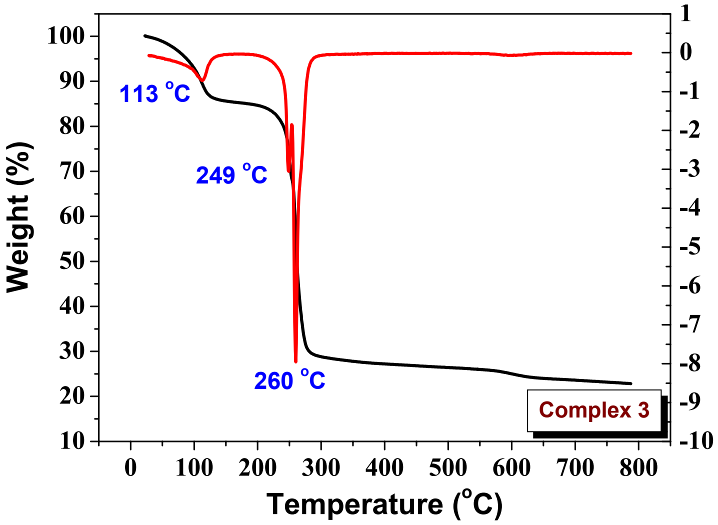
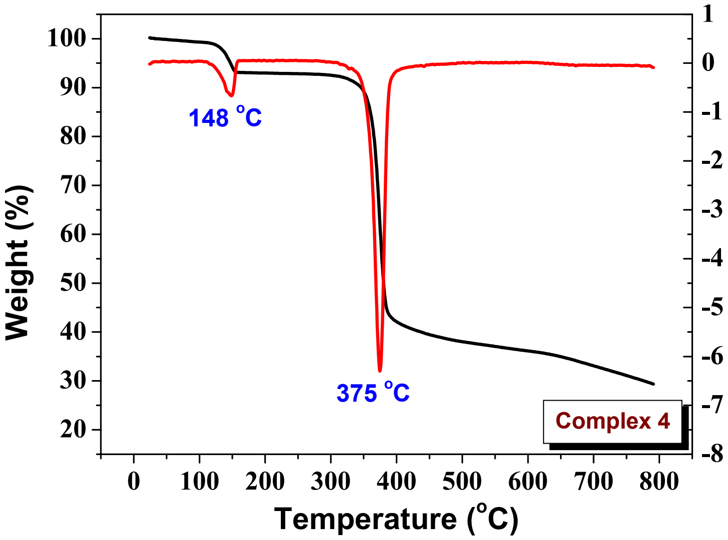
90
80
70
60
50
40
30
20
10
0
-10
1
0
-1
-2
-3
-4
-5
-6
-7
-8
0
100
200
300
400
500
600
700
800
Temperature (°C)
90 °C
298 °C
261 °C
Complex 2

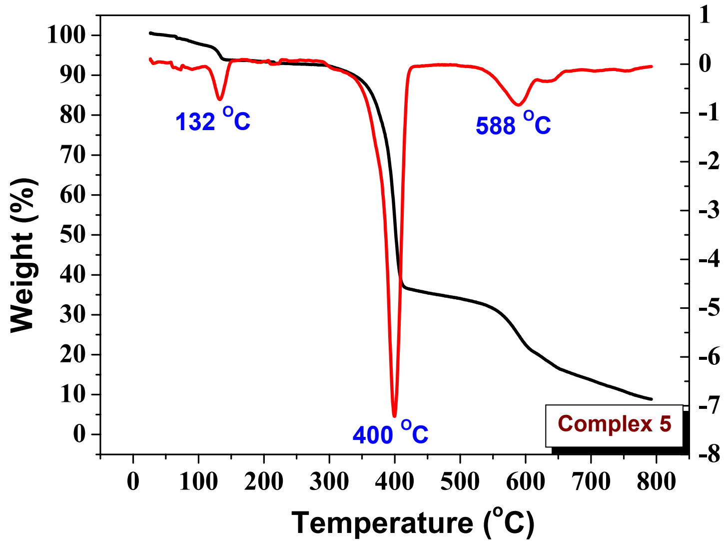
(b)


Weight (%)
100
90
80
70
60
50
40
30
20
10
1
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
0
100
200
300
400
500
600
700
800
Temperature (°C)
113 °C
249 °C
260 °C
Complex 3

(c)



(d)



(e)

Fig. S19 Thermogravimetric (TG) analysis plots of (a) for **1**, (b) for **2**, (c) for **3**, (d) for **4**, and (e) for **5**.

Table S1 Selected Bond Distances (Å) and Angles (deg) for Complexes **1-5**^{a}

1

Cu(1)–O(7)	1.932(4)	Cu(1)–O(1)$^{\#1}$	1.960(4)
Cu(1)–O(4)$^{\#2}$	1.984(4)	Cu(1)–O(5)$^{\#2}$	2.004(4)
Cu(1)–O(2W)	2.224(4)	Cu(1)–O(9)$^{\#2}$	2.353(3)
Cu(2)–O(2)	1.904(4)	Cu(2)–O(3)$^{\#3}$	1.935(4)
Cu(2)–O(8)$^{\#4}$	1.990(4)	Cu(2)–O(6)$^{\#2}$	2.035(4)
Cu(1)$^{\#4}$–O(1)	1.960(4)	Cu(2)$^{\#5}$–O(3)	1.935(4)
Cu(1)$^{\#6}$–O(4)	1.984(4)	Cu(1)$^{\#6}$–O(5)	2.004(4)
Cu(2)$^{\#6}$–O(6)	2.035(4)	Cu(2)$^{\#1}$–O(8)	1.990(4)
Cu(1)$^{\#6}$–O(9)	2.353(3)		

O(7)–Cu(1)–O(1)$^{\#1}$	100.20(17)	O(7)–Cu(1)–O(4)$^{\#2}$	167.31(15)
O(1)$^{\#1}$–Cu(1)–O(4)$^{\#2}$	84.30(15)	O(7)–Cu(1)–O(5)$^{\#2}$	86.66(17)
O(1)$^{\#1}$–Cu(1)–O(5)$^{\#2}$	171.99(16)	O(4)$^{\#2}$–Cu(1)–O(5)$^{\#2}$	88.14(16)
O(7)–Cu(1)–O(2W)	99.15(17)	O(1)$^{\#1}$–Cu(1)–O(2W)	94.39(16)
O(4)$^{\#2}$–Cu(1)–O(2W)	92.28(16)	O(5)$^{\#2}$–Cu(1)–O(2W)	88.53(16)
O(7)–Cu(1)–O(9)$^{\#2}$	92.10(14)	O(1)$^{\#1}$–Cu(1)–O(9)$^{\#2}$	99.42(13)
O(4)$^{\#2}$–Cu(1)–O(9)$^{\#2}$	75.40(13)	O(5)$^{\#2}$–Cu(1)–O(9)$^{\#2}$	76.05(13)
O(2W)–Cu(1)–O(9)$^{\#2}$	160.36(16)	O(2)–Cu(2)–O(3)$^{\#3}$	166.20(16)
O(2)–Cu(2)–O(8)$^{\#4}$	96.83(17)	O(3)$^{\#3}$–Cu(2)–O(8)$^{\#4}$	87.53(16)
O(2)–Cu(2)–O(6)$^{\#2}$	86.13(18)	O(3)$^{\#3}$–Cu(2)–O(6)$^{\#2}$	88.42(17)
O(8)$^{\#4}$–Cu(2)–O(6)$^{\#2}$	174.03(15)		

2

Cu(1)–O(3)$^{\#1}$	1.952(3)	Cu(1)–O(8)	1.978(3)
Cu(1)–N(1)	1.993(4)	Cu(1)–N(2)	2.008(4)
Cu(1)–O(2)$^{\#2}$	2.286(3)	Cu(2)–O(5)$^{\#3}$	1.903(3)
Cu(2)–O(7)	1.968(3)	Cu(2)–O(1)	2.016(3)
Cu(2)–O(10)	2.038(3)	Cu(2)–O(11)	2.280(4)
Cu(2)–O(9)	2.381(3)	Cu(1)$^{\#4}$–O(2)	2.286(3)
Cu(1)$^{\#5}$–O(3)	1.952(3)	Cu(2)$^{\#6}$–O(5)	1.903(3)

O(3)$^{\#1}$–Cu(1)–O(8)	88.20(12)	O(3)$^{\#1}$–Cu(1)–N(1)	96.83(14)
O(8)–Cu(1)–N(1)	169.49(14)	O(3)$^{\#1}$–Cu(1)–N(2)	168.52(14)
O(8)–Cu(1)–N(2)	92.00(14)	N(1)–Cu(1)–N(2)	81.24(16)
O(3)$^{\#1}$–Cu(1)–O(2)$^{\#2}$	93.10(11)	O(8)–Cu(1)–O(2)$^{\#2}$	85.64(11)
N(1)–Cu(1)–O(2)$^{\#2}$	103.23(13)	N(2)–Cu(1)–O(2)$^{\#2}$	98.36(14)
O(5)$^{\#3}$–Cu(2)–O(7)	166.51(13)	O(5)$^{\#3}$–Cu(2)–O(1)	89.57(12)
O(7)–Cu(2)–O(1)	92.18(13)	O(5)$^{\#3}$–Cu(2)–O(10)	90.85(14)
O(7)–Cu(2)–O(10)	92.36(15)	O(1)–Cu(2)–O(10)	158.62(13)
O(5)$^{\#3}$–Cu(2)–O(11)	86.43(13)	O(7)–Cu(2)–O(11)	80.29(12)
O(1)–Cu(2)–O(11)	107.55(12)	O(10)–Cu(2)–O(11)	93.81(14)
O(5)$^{\#3}$–Cu(2)–O(9)	116.53(11)	O(7)–Cu(2)–O(9)	76.74(11)

O(1)–Cu(2)–O(9)	73.85(10)	O(10)–Cu(2)–O(9)	86.90(12)
O(11)–Cu(2)–O(9)	157.03(11)		

3

Cu(1)–O(3)$^{\#1}$	1.930(3)	Cu(1)–O(8)$^{\#2}$	1.973(3)
Cu(1)–N(1)	2.002(4)	Cu(1)–N(2)	2.011(4)
Cu(1)–O(6)	2.306(4)	Cu(2)–O(1)	1.901(3)
Cu(2)–O(7)$^{\#3}$	1.965(3)	Cu(2)–O(10)	1.996(4)
Cu(2)–O(5)$^{\#3}$	1.996(4)	Cu(2)–O(11)	2.357(4)
Cu(2)–O(9)$^{\#3}$	2.417(3)	Cu(1)$^{\#3}$–O(3)	1.930(3)
Cu(2)$^{\#1}$–O(5)	1.996(3)	Cu(2)$^{\#1}$–O(7)	1.965(3)
Cu(1)$^{\#4}$–O(8)	1.973(3)	Cu(2)$^{\#1}$–O(9)	2.417(3)
O(3)$^{\#1}$–Cu(1)–O(8)$^{\#2}$	89.00(15)	O(3)$^{\#1}$–Cu(1)–N(1)	96.77(17)
O(8)$^{\#2}$–Cu(1)–N(1)	171.30(17)	O(3)$^{\#1}$–Cu(1)–N(2)	173.12(17)
O(8)$^{\#2}$–Cu(1)–N(2)	91.58(17)	N(1)–Cu(1)–N(2)	81.91(19)
O(3)$^{\#1}$–Cu(1)–O(6)	93.81(14)	O(8)$^{\#2}$–Cu(1)–O(6)	86.49(14)
N(1)–Cu(1)–O(6)	99.56(16)	N(2)–Cu(1)–O(6)	93.07(16)
O(1)–Cu(2)–O(7)$^{\#3}$	162.77(16)	O(1)–Cu(2)–O(10)	91.24(17)
O(7)$^{\#3}$–Cu(2)–O(10)	92.52(18)	O(1)–Cu(2)–O(5)$^{\#3}$	89.00(15)
O(7)$^{\#3}$–Cu(2)–O(5)$^{\#3}$	93.71(15)	O(10)–Cu(2)–O(5)$^{\#3}$	158.02(16)
O(1)–Cu(2)–O(11)	84.62(16)	O(7)$^{\#3}$–Cu(2)–O(11)	78.21(15)
O(10)–Cu(2)–O(11)	98.02(17)	O(5)$^{\#3}$–Cu(2)–O(11)	103.88(15)
O(1)–Cu(2)–O(9)$^{\#3}$	121.32(14)	O(7)$^{\#3}$–Cu(2)–O(9)$^{\#3}$	75.64(13)
O(10)–Cu(2)–O(9)$^{\#3}$	87.78(15)	O(5)$^{\#3}$–Cu(2)–O(9)$^{\#3}$	73.44(13)
O(11)–Cu(2)–O(9)$^{\#3}$	153.43(13)		

4

Mn(1)–O(4)	2.047(3)	Mn(1)–O(6)$^{\#1}$	2.150(3)
Mn(1)–O(1)$^{\#1}$	2.186(3)	Mn(1)–N(4)	2.250(3)
Mn(1)–N(3)	2.298(3)	Mn(1)–O(9)$^{\#1}$	2.345(2)
Mn(2)–O(10)	2.196(3)	Mn(2)–O(5)$^{\#1}$	2.197(3)
Mn(2)–N(1)	2.268(3)	Mn(2)–O(8)	2.291(3)
Mn(2)–N(2)	2.292(3)	Mn(2)–O(7)	2.332(3)
Mn(1)$^{\#2}$–O(1)	2.186(3)	Mn(2)$^{\#2}$–O(5)	2.197(3)
Mn(1)$^{\#2}$–O(6)	2.150(3)	Mn(1)$^{\#2}$–O(9)	2.345(2)
O(4)–Mn(1)–O(6)$^{\#1}$	88.46(11)	O(4)–Mn(1)–O(1)$^{\#1}$	90.04(11)
O(6)$^{\#1}$–Mn(1)–O(1)$^{\#1}$	107.62(11)	O(4)–Mn(1)–N(4)	95.83(11)
O(6)$^{\#1}$–Mn(1)–N(4)	88.07(12)	O(1)$^{\#1}$–Mn(1)–N(4)	163.43(12)
O(4)–Mn(1)–N(3)	118.10(11)	O(6)$^{\#1}$–Mn(1)–N(3)	148.22(11)
O(1)$^{\#1}$–Mn(1)–N(3)	90.54(12)	N(4)–Mn(1)–N(3)	73.02(12)
O(4)–Mn(1)–O(9)$^{\#1}$	146.15(10)	O(6)$^{\#1}$–Mn(1)–O(9)$^{\#1}$	71.97(9)
O(1)$^{\#1}$–Mn(1)–O(9)$^{\#1}$	70.95(9)	N(4)–Mn(1)–O(9)$^{\#1}$	110.37(10)
N(3)–Mn(1)–O(9)$^{\#1}$	90.60(10)	O(10)–Mn(2)–O(5)$^{\#1}$	80.82(11)

O(10)–Mn(2)–N(1)	86.76(12)	O(5)$^{\#1}$–Mn(2)–N(1)	128.03(11)
O(10)–Mn(2)–O(8)	88.77(10)	O(5)$^{\#1}$–Mn(2)–O(8)	137.48(10)
N(1)–Mn(2)–O(8)	91.95(11)	O(10)–Mn(2)–N(2)	134.56(11)
O(5)$^{\#1}$–Mn(2)–N(2)	81.13(11)	N(1)–Mn(2)–N(2)	72.63(12)
O(8)–Mn(2)–N(2)	130.79(11)	O(10)–Mn(2)–O(7)	143.80(11)
O(5)$^{\#1}$–Mn(2)–O(7)	116.43(11)	N(1)–Mn(2)–O(7)	103.04(11)
O(8)–Mn(2)–O(7)	56.56(10)	N(2)–Mn(2)–O(7)	81.22(11)

5

Cd(1)–O(1)	2.314(9)	Cd(1)–O(1W)	2.330(10)
Cd(1)–N(1)	2.357(11)	Cd(1)–O(8)$^{\#1}$	2.373(10)
Cd(1)–N(2)	2.376(11)	Cd(1)–O(7)$^{\#1}$	2.464(10)
Cd(1)–O(2)	2.557(8)	Cd(2)–O(5)$^{\#1}$	2.175(9)
Cd(2)–O(2)	2.305(9)	Cd(2)–N(3)	2.327(11)
Cd(2)–O(3)	2.328(9)	Cd(2)–N(4)	2.362(11)
Cd(2)–O(9)	2.422(8)	Cd(2)$^{\#2}$–O(5)	2.175(9)
Cd(1)$^{\#2}$–O(7)	2.464(10)	Cd(1)$^{\#2}$–O(8)	2.373(10)

O(1)–Cd(1)–O(1W)	80.5(4)	O(1)–Cd(1)–N(1)	126.8(3)
O(1W)–Cd(1)–N(1)	86.2(4)	O(1)–Cd(1)–O(8)$^{\#1}$	137.6(3)
O(1W)–Cd(1)–O(8)$^{\#1}$	92.0(4)	N(1)–Cd(1)–O(8)$^{\#1}$	93.8(3)
O(1)–Cd(1)–N(2)	81.4(3)	O(1W)–Cd(1)–N(2)	132.5(4)
N(1)–Cd(1)–N(2)	70.7(4)	O(8)$^{\#1}$–Cd(1)–N(2)	129.3(3)
O(1)–Cd(1)–O(7)$^{\#1}$	117.4(4)	O(1W)–Cd(1)–O(7)$^{\#1}$	145.6(4)
N(1)–Cd(1)–O(7)$^{\#1}$	102.2(4)	O(8)$^{\#1}$–Cd(1)–O(7)$^{\#1}$	54.6(3)
N(2)–Cd(1)–O(7)$^{\#1}$	81.2(4)	O(1)–Cd(1)–O(2)	53.3(3)
O(1W)–Cd(1)–O(2)	82.0(4)	N(1)–Cd(1)–O(2)	167.9(4)
O(8)$^{\#1}$–Cd(1)–O(2)	84.3(3)	N(2)–Cd(1)–O(2)	119.5(3)
O(7)$^{\#1}$–Cd(1)–O(2)	86.5(3)	O(5)$^{\#1}$–Cd(2)–O(2)	85.2(3)
O(5)$^{\#1}$–Cd(2)–N(3)	101.8(4)	O(2)–Cd(2)–N(3)	88.0(4)
O(5)$^{\#1}$–Cd(2)–O(3)	88.0(3)	O(2)–Cd(2)–O(3)	106.5(3)
N(3)–Cd(2)–O(3)	163.2(4)	O(5)$^{\#1}$–Cd(2)–N(4)	126.1(4)
O(2)–Cd(2)–N(4)	144.8(4)	N(3)–Cd(2)–N(4)	71.4(4)
O(3)–Cd(2)–N(4)	91.9(4)	O(5)$^{\#1}$–Cd(2)–O(9)	137.5(3)
O(2)–Cd(2)–O(9)	69.7(3)	N(3)–Cd(2)–O(9)	110.6(3)
O(3)–Cd(2)–O(9)	68.3(3)	N(4)–Cd(2)–O(9)	90.8(3)

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[a] Symmetry codes for complexes **1**–**5**: **1**, #1,–*x* + 1/2, *y* – 1/2, *z*; #2, *x* – 1/2, *y*, –*z* + 1/2; #3, –*x* + 1/2, *y* + 1/2, *z*; #4, *x*, –*y* + 1/2, *z* + 1/2; #5, –*x* + 1/2, *y* – 1/2, *z*; #6, *x*, –*y*+1/2, *z* + 1/2; **2**, #1, *x* – 1/2, –*y* + 3/2, *z* + 1/2; #2, *x*, y, *z* + 1; #3, *x* – 1/2, –*y* + 3/2, *z* – 1/2; #4, *x*, *y*, *z* – 1; #5, *x* + 1/2, –*y* + 3/2, *z* – 1/2; #6, *x* + 1/2, –*y* + 3/2, *z* + 1/2; **3**, #1, *x*, –*y* + 3/2, *z* – 1/2; #2, *x* + 1, *y*, *z*; #3, *x*, –*y* + 3/2, *z* + 1/2; #4, *x* – 1, *y*, *z*; **4**, #1, –*x* + 3/2, *y* – 1/2, –*z* + 1/2; #2, –*x* + 3/2, *y* + 1/2, –*z* + 1/2; **5**, #1, –*x* + 1, *y* – 1/2, –*z* + 3/2; #2, –*x* + 1, *y* + 1/2, –*z* + 3/2.

Table S2 Hydrogen–Bonding Geometry (Å, °) for Complexes **2–5**[a]

D–H···A	***d*(D–H)**	***d*(H···A)**	***d*(D···A)**	**D–H···A**
		2		
O(1W)–H(1WA)···O(8)	0.85	2.25	3.076(5)	165
O(1W)–H(1WA)···O(3a)	0.85	2.47	3.030(5)	124
O(1W)–H(1WB)···O(6a)	0.85	1.96	2.808(9)	173
O(10)–H(10B)···O(2a)	0.85	2.10	2.798(5)	139
O(10)–H(10C)···O(2W)	0.85	1.86	2.694(8)	165
O(11)–H(11B)···O(1Wb)	0.85	1.96	2.804(5)	172
O(11)–H(11C)···O(4a)	0.85	2.10	2.934(5)	168
O(3W)–H(3WA)···O(4c)	0.85	2.17	3.023(9)	177
O(3W)–H(3WB)···O(6)	0.85	2.25	3.030(1)	153
C(12)–H(12A)···O(1d)	0.93	2.49	3.259(7)	140
C(16)–H(16A)···O(4e)	0.93	2.43	3.308(7)	156
		3		
O(1W)–H(1)···O(8a)	0.85	2.27	3.084(8)	160
O(1W)–H(2)···O(2b)	0.85	1.93	2.772(5)	169
O(2W)–H(3)···O(10a)	0.85	2.43	2.712(1)	100
O(2W)–H(4)···O(1Wa)	0.85	2.19	2.888(2)	140
O(10)–H(10B)···O(6b)	0.85	2.31	2.720(5)	110
O(10)–H(10C)···O(2Wc)	0.85	2.05	2.712(1)	134
O(11)–H(11A)···O(1Wc)	0.85	2.25	2.862(3)	129
O(11)–H(11B)···O(4b)	0.85	2.19	2.908(8)	142
C(14)–H(14A)···O(5d)	0.93	2.55	3.215(1)	128
C(14)–H(14A)···O(7d)	0.93	2.58	3.429(1)	152
		4		
O(10)–H(10B)···O(2a)	0.85	1.98	2.683(4)	140
C(26)–H(26A)···O(9b)	0.93	2.53	3.211(4)	130
C(11)–H(11A)···O(3c)	0.93	2.48	3.375(4)	162
O(1W)–H(1WA)···O(8a)	0.85	2.02	2.867(2)	173
O(1W)–H(1WB)···O(1d)	0.86	2.32	3.177(3)	177

O(2W)–H(2WA)···O(7)	0.86	2.22	3.050(9)	163
O(2W)–H(2WB)···O(1e)	0.85	2.25	2.978(2)	144
		5		
O(1W)–H(1)···O(4a)	0.85	1.85	2.695(4)	171
C(11)–H(11A)···O(6b)	0.93	2.52	3.415(9)	162
C(25)–H(25A)···O(9c)	0.93	2.54	3.221(4)	130
O(2W)–H(4)···O(8d)	0.85	2.52	2.872(3)	106
O(3W)–H(5)···O(7e)	0.85	2.44	3.141(2)	140
O(3W)–H(6)···O(2)	0.85	2.54	3.199(4)	135
O(3W)–H(6)···O(3)	0.85	2.54	3.067(8)	121

[a]Symmetry codes: for **2**: a, $x - 1/2, -y + 3/2, z + 1/2$; b, $x - 1/2, -y + 3/2, z - 1/2$; c, $x + 1/2, -y + 3/2, z + 1/2$; d, $x, -y + 1, z + 1/2$; e, $x - 1/2, y - 1/2, z + 1$; for **3**: a, $x, -y + 3/2, z + 1/2$; b, $x - 1, y, z$; c, $x, -y + 3/2, z - 1/2$; d, $-x + 2, -y + 1, -z$; for **4**: a, $-x + 1/2, y -1/2, -z + 1/2$; b, $x - 1/2, - y + 1/2, z - 1/2$; c, $x - 1/2, - y + 1/2, z + 1/2$; d, $x, y - 1, z$; e, $-x + 3/2, y -1/2, -z + 1/2$; for **5**, a, $x + 1, y, z$; b, $- x + 2, - y + 1, - z + 2$; c, $- x + 1, - y + 1, - z + 1$; d, $- x, y - 1/2, - z + 3/2$; e, $-x + 1, y - 1/2, - z + 3/2$.