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Supporting Information

Construction of variable dimensional cadmium(II) coordination polymers from pyridine-2,3-dicarboxylic acid

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Contents

Table S1. Crystal data and structure refinement of compounds **1-5.**

	1	**2**	**3**	**4**	**5**
Chemical formula	$C_{20}H_{18}Cd_2N_8O_{13}$	$C_7H_3CdNO_4$	$C_{27}H_{29}Cd_2N_7O_{15}$	$C_{14}H_8Cd_2N_2O_9$	$C_6H_8CdN_2O_7$
Formula weight	803.22	277.50	916.37	573.02	332.54
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P\,2_1/n$	$P\,2_1/c$	$P\,2_1/c$	$P\,2_1/n$	$C2/c$
a /Å	13.3217(2)	10.7212(1)	15.5653(18)	8.3601(2)	21.032(2)
b /Å	11.7975(2)	7.7259(1)	15.3856(18)	8.4793(2)	7.9734(8)
c /Å	23.3963(5)	8.6780(1)	14.8364(17)	21.4434(4)	12.5404(13)
α/°	90	90	90	90	90
β/°	123.480(2)	110.0370(10)	109.7250(10)	93.9090(10)	110.1920(10)
γ/°	90	90	90	90	90
V/Å^3	3066.93(10)	675.30(1)	3344.6(7)	1516.54(6)	1973.7(4)
Z	4	4	4	4	8
T/K	298(2)	298(2)	298(2)	298(2)	298(2)
F(000)	1576	528	1824	1096	916
Dcalcd/g·cm^{-3}	1.740	2.729	1.820	2.510	2.238
μ/mm^{-1}	1.458	3.206	1.353	2.864	2.238
R_{int}	0.0231	0.0183	0.0446	0.0180	0.0199
data/restraint/parm	5513 / 0 / 388	1253 / 0 / 119	4767 / 3 / 466	2815 / 3 / 251	1790 / 0 / 154
GOF	1.076	1.082	1.025	1.059	1.077
$R_1[I=2\sigma(I)]$[a]	0.0384	0.0235	0.0399	0.0178	0.0227
$wR_2[I=2\sigma(I)]$[b]	0.0827	0.0596	0.0896	0.0429	0.0181
Largest diff. peak and hole(e·Å^{-3})	0.764 and -0.743	0.793 and -1.013	0.769 and -0.634	0.683 and -0.491	1.114 and -1.224

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table S2. Selected bond lengths (Å) and bond angles (º) for compounds **1-5**.

Compound **1**			
Cd(1)-O(7)	2.256(3)	O(7)-Cd(1)-O(2)	119.25(12)
Cd(1)-O(2)	2.274(3)	O(7)-Cd(1)-O(2)	119.25(12)
Cd(1)-N(3)	2.326(3)	O(7)-Cd(1)-N(3)	94.06(12)
Cd(1)-N(4)#1	2.330(3)	O(2)-Cd(1)-N(3)	86.48(12)
Cd(1)-O(5)	2.363(3)	O(7)-Cd(1)-N(4)#1	89.14(12)
Cd(1)-O(4)	2.391(3)	O(7)-Cd(1)-N(4)#1	89.14(12)
Cd(2)-N(1)	2.315(3)	O(2)-Cd(1)-N(4)#1	87.15(12)
Cd(2)-O(8)	2.325(3)	N(3)-Cd(1)-N(4)#1	173.63(12)
Cd(2)-N(2)#2	2.327(3)	O(7)-Cd(1)-O(5)	93.12(11)
Cd(2)-O(1)	2.422(3)	O(2)-Cd(1)-O(5)	147.60(12)
Cd(2)-O(11)	2.489(3)	N(3)-Cd(1)-O(5)	92.96(12)
Cd(2)-O(2)	2.489(3)	N(4)#1-Cd(1)-O(5)	92.37(12)
N(1)-Cd(2)-O(1)	93.41(11)	O(7)-Cd(1)-O(4)	148.21(11)
O(8)-Cd(2)-O(1)	131.94(14)	O(2)-Cd(1)-O(4)	92.53(12)
N(2)#2-Cd(2)-O(1)	86.71(11)	N(3)-Cd(1)-O(4)	88.34(13)
O(10)-Cd(2)-O(1)	138.13(10)	N(4)#1-Cd(1)-O(4)	91.84(13)
N(1)-Cd(2)-O(11)	92.56(12)	O(5)-Cd(1)-O(4)	55.08(11)
O(8)-Cd(2)-O(11)	144.37(15)	N(1)-Cd(2)-O(8)	90.79(12)
N(2)#2-Cd(2)-O(11)	90.77(11)	N(1)-Cd(2)-N(2)#2	176.65(12)
O(10)-Cd(2)-O(11)	54.89(10)	O(8)-Cd(2)-N(2)#2	86.65(12)
O(1)-Cd(2)-O(11)	83.24(10)	N(1)-Cd(2)-O(10)	89.00(12)
N(1)-Cd(2)-O(2)	81.96(12)	O(8)-Cd(2)-O(10)	89.75(14)
O(8)-Cd(2)-O(2)	80.03(14)	N(2)#2-Cd(2)-O(10)	93.15(12)
N(2)#2-Cd(2)-O(2)	95.46(11)	O(1)-Cd(2)-O(2)	53.40(10)
O(10)-Cd(2)-O(2)	166.20(11)	O(11)-Cd(2)-O(2)	135.54(11)

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z+1/2 #2 x,-y+1/2,z-1/2

Compound **2**			
Cd(1)-O(3)#1	2.220(3)	O(3)#1-Cd(1)-O(2)#2	112.32(10)
Cd(1)-O(2)#2	2.265(3)	O(3)#1-Cd(1)-O(4)#3	81.12(10)
Cd(1)-O(4)#3	2.266(3)	O(2)#2-Cd(1)-O(4)#3	92.08(10)
Cd(1)-O(1)#4	2.325(3)	O(3)#1-Cd(1)-O(1)#4	101.96(10)
Cd(1)-N(1)	2.336(3)	O(2)#2-Cd(1)-O(1)#4	81.64(10)

Cd(1)-O(2)	2.486(3)	O(4)#3-Cd(1)-O(1)#4	173.66(10)
O(2)#2-Cd(1)-N(1)	136.73(10)	O(3)#1-Cd(1)-N(1)	110.38(11)
O(4)#3-Cd(1)-N(1)	101.04(10)	O(1)#4-Cd(1)-N(1)	83.17(10)
O(3)#1-Cd(1)-O(2)	170.84(10)	O(2)#2-Cd(1)-O(2)	69.96(10)
O(4)#3-Cd(1)-O(2)	89.99(9)	O(1)#4-Cd(1)-O(2)	87.11(10)
N(1)-Cd(1)-O(2)	69.02(9)		

Symmetry transformations used to generate equivalent atoms: #1 x,y+1,z; #2 -x+1,-y+2,-z; #3 x,-y+3/2,z-1/2; #4 -x+1,y+1/2,-z+1/2.

Compound **3**

Cd(1)-O(4)#1	2.268(4)	O(4)#1-Cd(1)-N(2)	92.66(17)
Cd(1)-N(2)	2.311(5)	O(4)#1-Cd(1)-N(4)	88.72(17)
Cd(1)-N(4)	2.319(5)	N(2)-Cd(1)-N(4)	173.55(18)
Cd(1)-O(12)	2.320(5)	O(4)#1-Cd(1)-O(12)	155.54(18)
Cd(1)-O(1)	2.357(4)	N(2)-Cd(1)-O(12)	85.52(17)
Cd(1)-O(11)	2.397(5)	N(4)-Cd(1)-O(12)	95.81(17)
Cd(2)-N(3)#2	2.290(5)	O(4)#1-Cd(1)-O(1)	112.11(15)
Cd(2)-N(5)#3	2.329(5)	N(2)-Cd(1)-O(1)	86.38(16)
Cd(2)-O(3)#1	2.337(5)	N(4)-Cd(1)-O(1)	87.26(16)
Cd(2)-O(1)	2.360(4)	O(12)-Cd(1)-O(1)	92.15(16)
Cd(2)-N(1)	2.420(5)	O(4)#1-Cd(1)-O(11)	80.07(17)
Cd(2)-O(6)	2.491(5)	N(2)-Cd(1)-O(11)	92.04(18)
Cd(2)-O(5)	2.559(5)	N(4)-Cd(1)-O(11)	94.41(18)
O(3)#1-Cd(2)-N(1)	151.67(17)	O(12)-Cd(1)-O(11)	75.63(18)
O(1)-Cd(2)-N(1)	69.11(14)	O(1)-Cd(1)-O(11)	167.77(15)
N(3)#2-Cd(2)-O(6)	85.91(17)	N(3)#2-Cd(2)-N(5)#3	166.72(17)
N(5)#3-Cd(2)-O(6)	82.51(17)	N(3)#2-Cd(2)-O(3)#1	90.06(17)
O(3)#1-Cd(2)-O(6)	127.41(16)	N(5)#3-Cd(2)-O(3)#1	91.82(18)
O(1)-Cd(2)-O(6)	149.28(14)	N(3)#2-Cd(2)-O(1)	101.53(15)
N(1)-Cd(2)-O(6)	80.92(16)	N(5)#3-Cd(2)-O(1)	91.75(15)
N(3)#2-Cd(2)-O(5)	89.68(16)	O(3)#1-Cd(2)-O(1)	82.73(15)
N(5)#3-Cd(2)-O(5)	77.92(17)	N(3)#2-Cd(2)-N(1)	92.47(16)
O(3)#1-Cd(2)-O(5)	77.41(17)	N(5)#3-Cd(2)-N(1)	92.11(17)
O(1)-Cd(2)-O(5)	157.20(15)	N(1)-Cd(2)-O(5)	130.79(16)
O(6)-Cd(2)-O(5)	50.20(15)		

Symmetry transformations used to generate equivalent atoms: #1 -x, y+1/2, -z+1/2, #2 x, -y-1/2, z-1/2.

Compound **4**

Cd(1)-O(5)	2.2453(18)	O(5)-Cd(1)-O(1)	166.82(7)
Cd(1)-O(1)	2.257(2)	O(5)-Cd(1)-O(8)#1	90.11(7)
Cd(1)-O(8)#1	2.2964(19)	O(1)-Cd(1)-O(8)#1	90.68(8)
Cd(1)-N(1)	2.305(2)	O(5)-Cd(1)-N(1)	118.50(7)
Cd(1)-O(2)#2	2.3090(19)	O(1)-Cd(1)-N(1)	73.22(7)
Cd(1)-O(4)#2	2.3711(19)	O(8)#1-Cd(1)-N(1)	111.85(7)
Cd(2)-O(3)#2	2.2246(18)	O(5)-Cd(1)-O(2)#2	82.97(7)
Cd(2)-O(7)#3	2.2562(17)	O(1)-Cd(1)-O(2)#2	91.02(8)
Cd(2)-N(2)	2.276(2)	O(8)#1-Cd(1)-O(2)#2	155.86(7)
Cd(2)-O(9)	2.283(2)	N(1)-Cd(1)-O(2)#2	91.66(7)
Cd(2)-O(5)	2.3518(18)	O(5)-Cd(1)-O(4)#2	81.72(7)
Cd(2)-O(6)	2.491(5)	O(1)-Cd(1)-O(4)#2	85.72(7)
O(8)#1-Cd(1)-O(4)#2	75.86(6)	O(3)#2-Cd(2)-O(7)#3	88.75(7)
N(1)-Cd(1)-O(4)#2	157.36(7)	O(3)#2-Cd(2)-N(2)	133.43(8)
O(2)#2-Cd(1)-O(4)#2	80.26(7)	O(7)#3-Cd(2)-N(2)	119.35(7)
O(3)#2-Cd(2)-O(5)	90.72(7)	O(3)#2-Cd(2)-O(9)	136.13(8)
O(7)#3-Cd(2)-O(5)	164.94(7)	O(7)#3-Cd(2)-O(9)	92.44(7)
N(2)-Cd(2)-O(5)	71.05(7)	N(2)-Cd(2)-O(9)	82.64(7)
O(9)-Cd(2)-O(5)	77.59(7)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z; #2 -x+1/2,y+1/2,-z+1/2; #3 x+1,y,z.

Compound **5**

Cd(1)-N(1)#1	2.2710(18)	O(6)-Cd(1)-O(7)	170.21(7)
Cd(1)-O(6)	2.336(2)	O(1)-Cd(1)-O(7)	91.93(6)
Cd(1)-O(1)	2.3454(16)	O(2)-Cd(1)-O(7)	100.34(7)
Cd(1)-O(2)	2.3763(18)	N(1)#1-Cd(1)-O(4)	135.72(7)
Cd(1)-O(7)	2.3891(18)	O(6)-Cd(1)-O(4)	87.71(7)
Cd(1)-O(4)	2.416(2)	O(1)-Cd(1)-O(4)	79.58(6)
Cd(1)-O(3)	2.5461(19)	O(2)-Cd(1)-O(4)	134.67(6)
N(1)-Cd(1)#2	2.2710(18)	O(7)-Cd(1)-O(4)	84.31(7)
N(1)#1-Cd(1)-O(6)	94.10(7)	N(1)#1-Cd(1)-O(3)	85.17(7)
N(1)#1-Cd(1)-O(1)	144.31(6)	O(6)-Cd(1)-O(3)	83.53(7)
O(6)-Cd(1)-O(1)	92.19(7)	O(1)-Cd(1)-O(3)	130.48(6)
N(1)#1-Cd(1)-O(2)	89.62(6)	O(2)-Cd(1)-O(3)	170.80(7)

O(6)-Cd(1)-O(2)	89.30(7)	O(7)-Cd(1)-O(3)	87.05(7)
O(1)-Cd(1)-O(2)	55.34(6)	O(4)-Cd(1)-O(3)	51.02(6)
N(1)#1-Cd(1)-O(7)	87.71(7		

Symmetry transformations used to generate equivalent atoms: #1 x,y-1,z #2 x,y+1,z.

Table S3. Hydrogen bond parameters of compounds **1**-**3** and **5**.

D-H···A	d (D-H) (Å)	d (H···A) (Å)	d (D···A) (Å)	∠ DHA (°)
		1		
O(13)-H(13B)...O(5)#1	0.85	1.98	2.829(5)	176.5
O(13)-H(13A)...O(11)#2	0.85	1.98	2.826(4)	176.9
		2		
O(7)-H(7)...O(4)#3	0.93	2.539(3)	3.199(4)	128.3
O(6)-H(6)...O(4)#4	0.93	2.559(3)	3.456(4)	162.3
		3		
O(11)-H(11B)...O(8)	0.88	2.00	2.698(11)	135.9
O(12)-H(12B)...O(10)	0.93	2.26	2.750(9)	112.3
O(12)-H(12B)...O(8)	0.93	2.58	3.388(11)	145.4
O(13)-H(13B)...O(8)	0.85	2.64	3.398(17)	149.0
O(15)-H(15A)...O(7)#5	0.85	2.65	3.50(3)	172.4
		5		
O(6)-H(6B)...O(4)#7	0.86	2.24	2.894(3)	133.4
O(6)-H(6B)...O(5)#7	0.86	2.53	3.367(3)	167.0
O(6)-H(6A)...O(7)#4	0.81(4)	2.11(4)	2.904(3)	170(4)
O(7)-H(7B)...O(3)#5	0.92	1.96	2.830(3)	157.7
O(7)-H(7B)...N(2)#5	0.92	2.68	3.537(3)	156.3
O(7)-H(7A)...O(1)#6	0.72(3)	2.05(3)	2.766(2)	176(4)

Symmetry transformations used to generate equivalent atoms: #1 3 x+1,y,z; #2 x+1,y,z; #3 x,1+y,z; #4 –x,0.5+y,0.5-z; #5 -x,y+1/2,-z+1/2; #4 x,-y,z-1/2; #5 -x+1/2,y+1/2,-z+3/2; #6 -x+1/2,y-1/2,-z+3/2; #7 -x+1/2,-y+1/2,-z+1.

Figure S1. 2-D supramolecular layer through the hydrogen bonds O-H···O between the water molecules and nitrate oxygen atoms in *ac* plane in **1**.

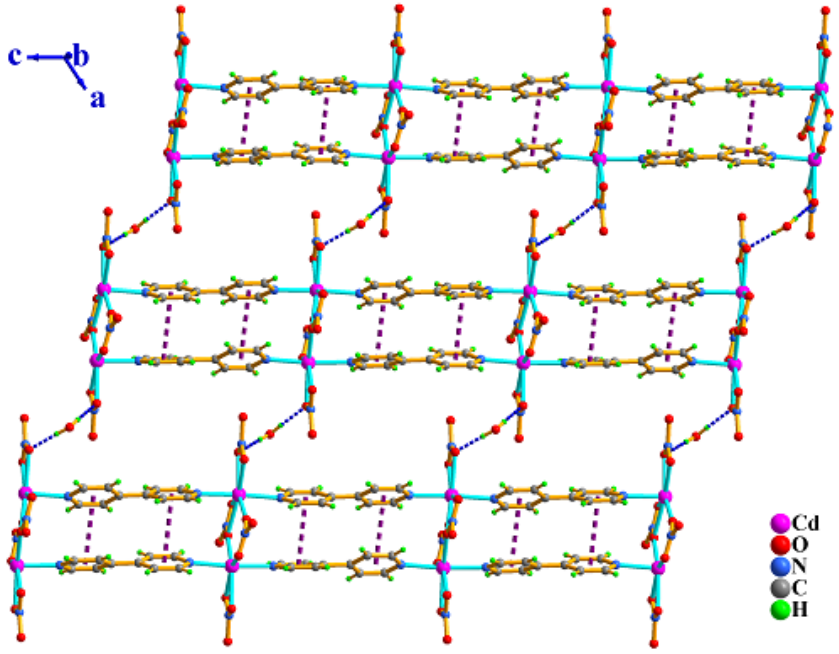


Figure S2. 3-D supramolecular network of **1** assembled through inter-chain hydrogen bonding O(C)-H···O interactions (blue dash lines) in *ab* plane.

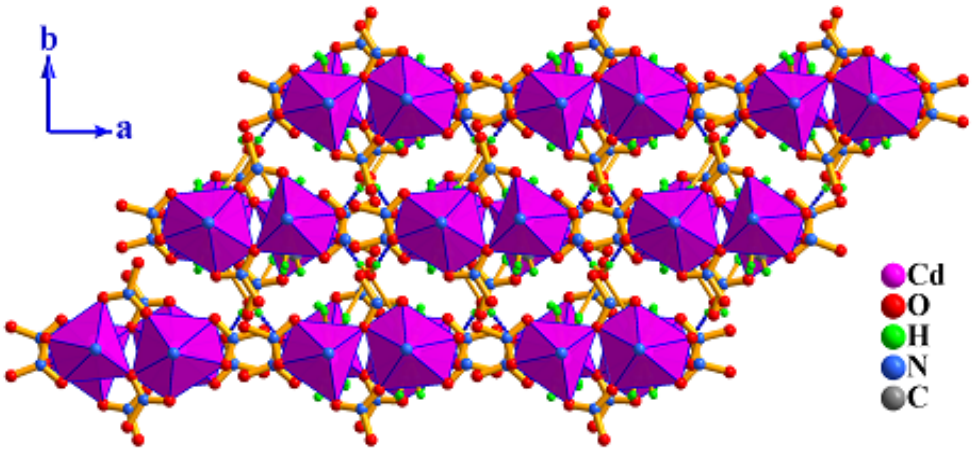


Figure S3 3-D supramolecular network via the inter-/intralayer hydrageon bonds C-H···O along *b* axis in **2**.

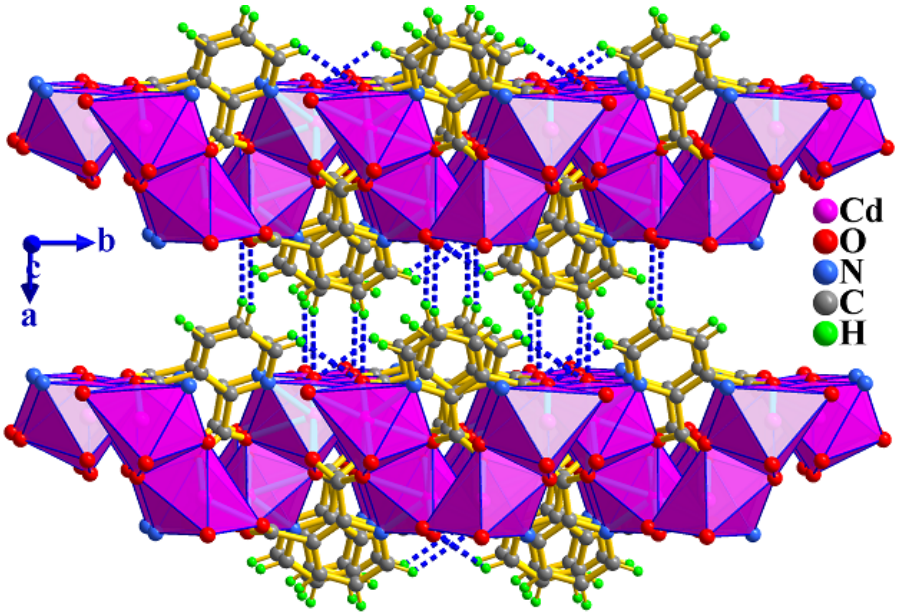


Figure S4. The coordination environment of two Cd^{2+} ions in **4**. Symmetrical codes: a) 0.5-x,0.5+y, 0.5-z; b) -x,-y, -z; c) -x,1-y,-z; d) 1+x, y, z.

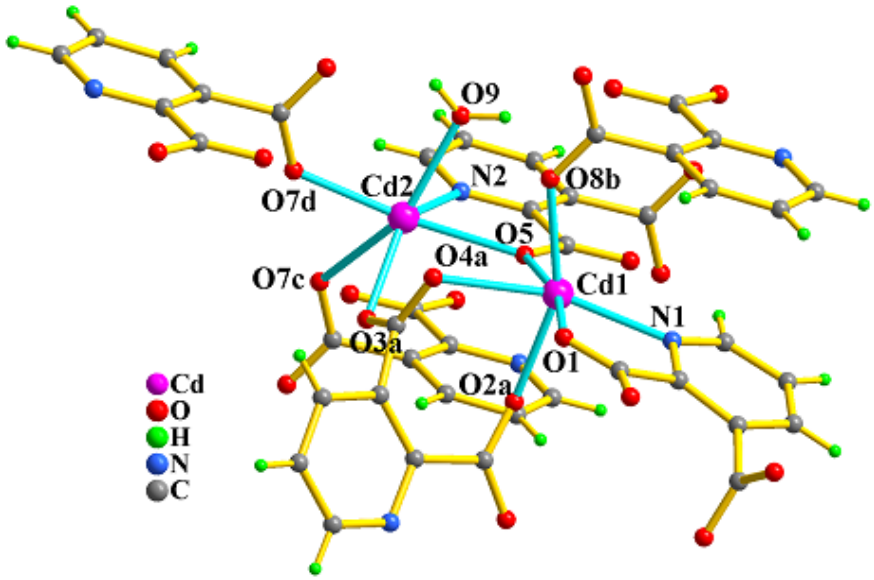


Figure S5 3-D framework structure viewed along *a* axis in **4**.

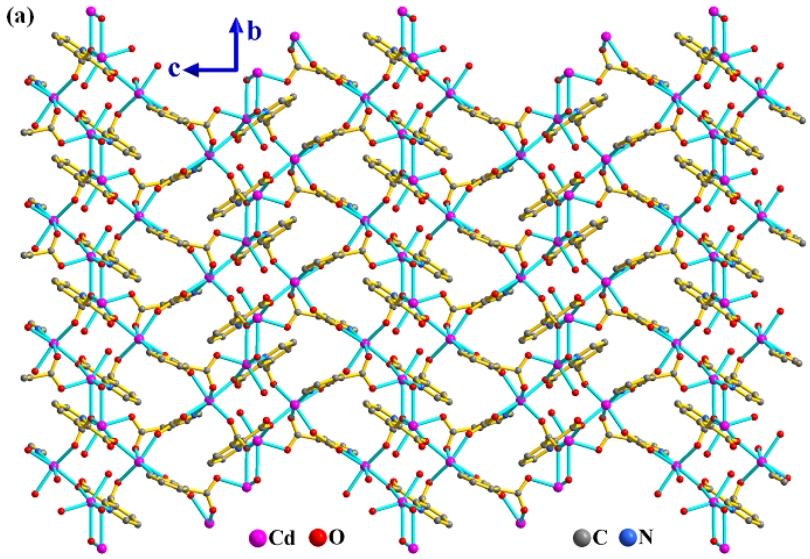
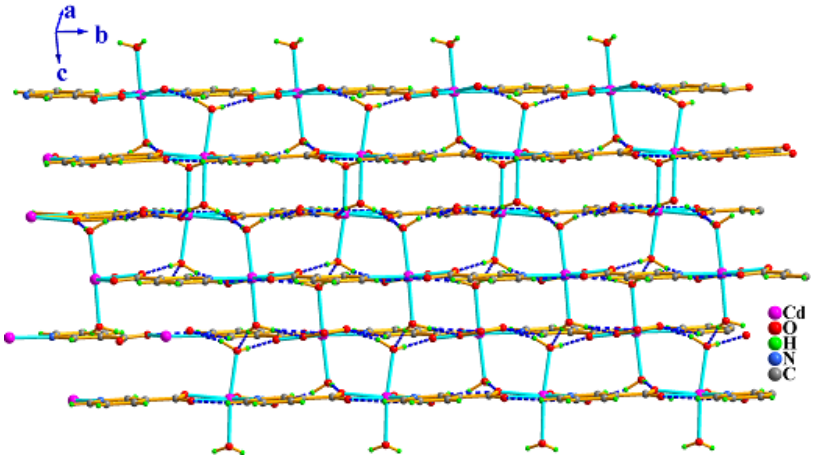


Figure S6. 2-D supramolecular layer via the hydrogen bonds O(C)-H···O between the oxygen atoms of the coordination water or nitrate or 2,3-Pydc^{2-} groups and hydrogen atoms of the coordination water and pyridyl rings in *bc* plane in **5.**

(**a**)



(**b**)

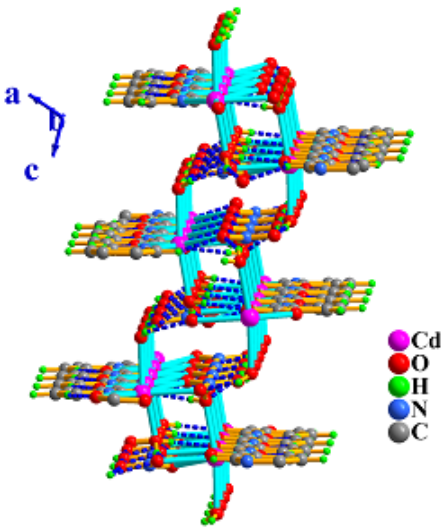


Figure S7. 3-D supramolecular framework assembled by interchain hydrogen bonding O-H···O (blue dash lines) and π···π stacking (violet dash lines) interactions in ac plane in **5**.

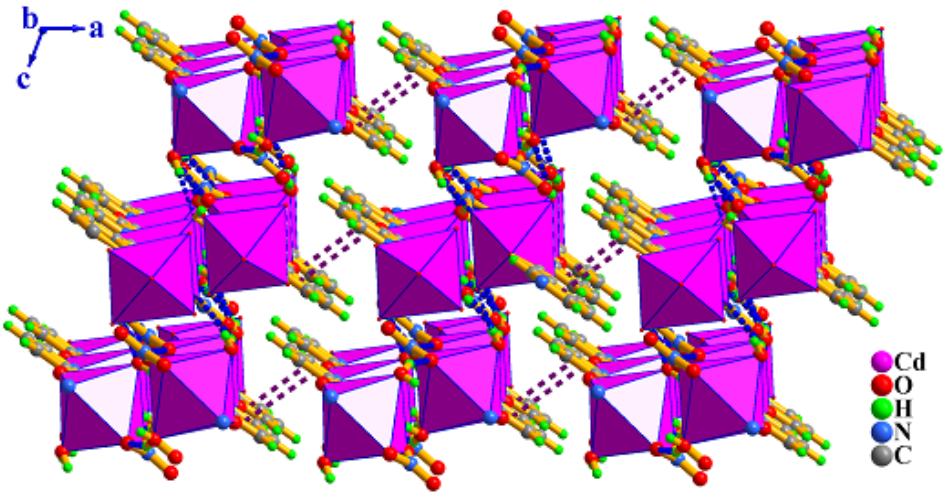
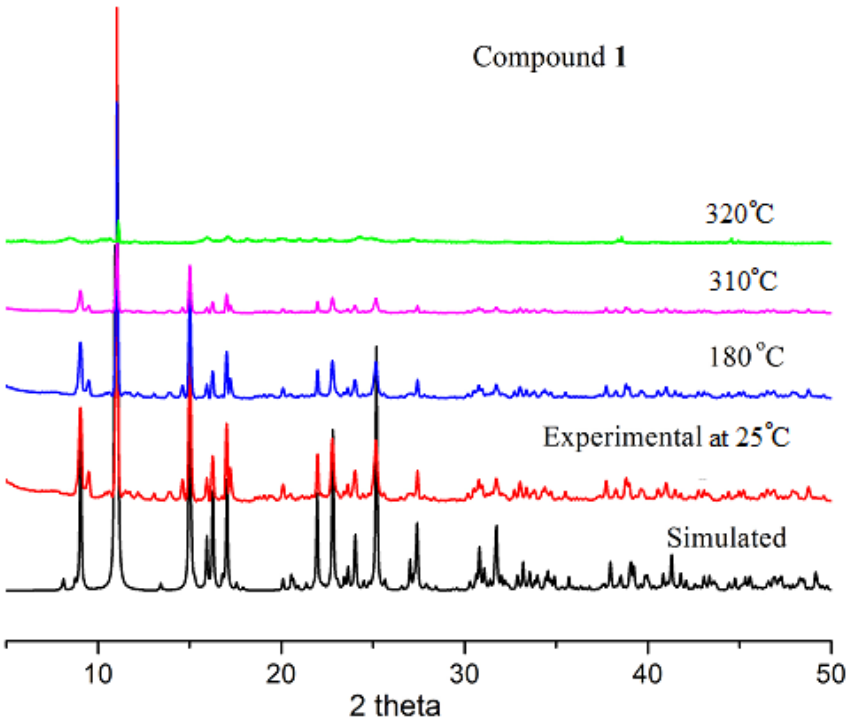
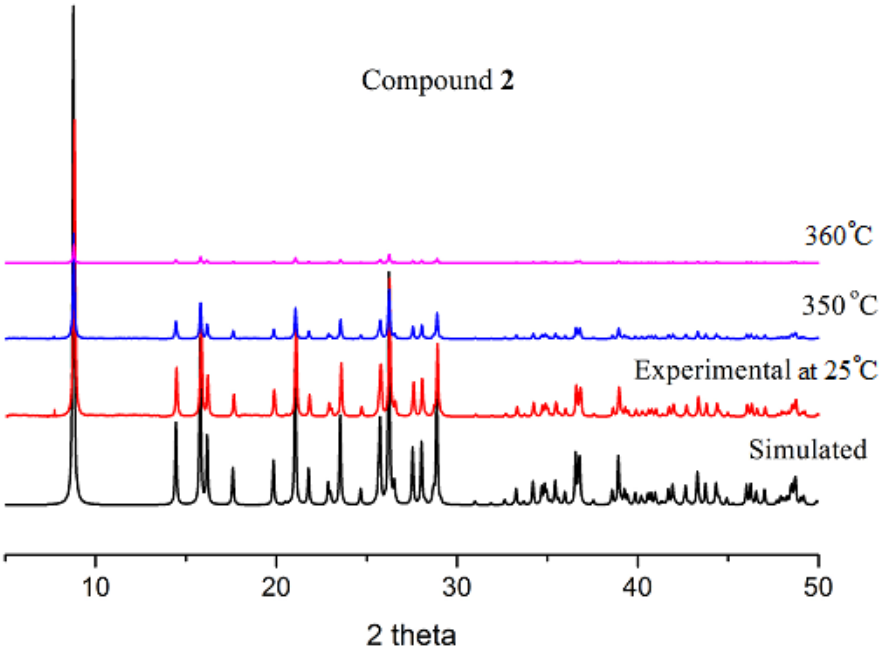
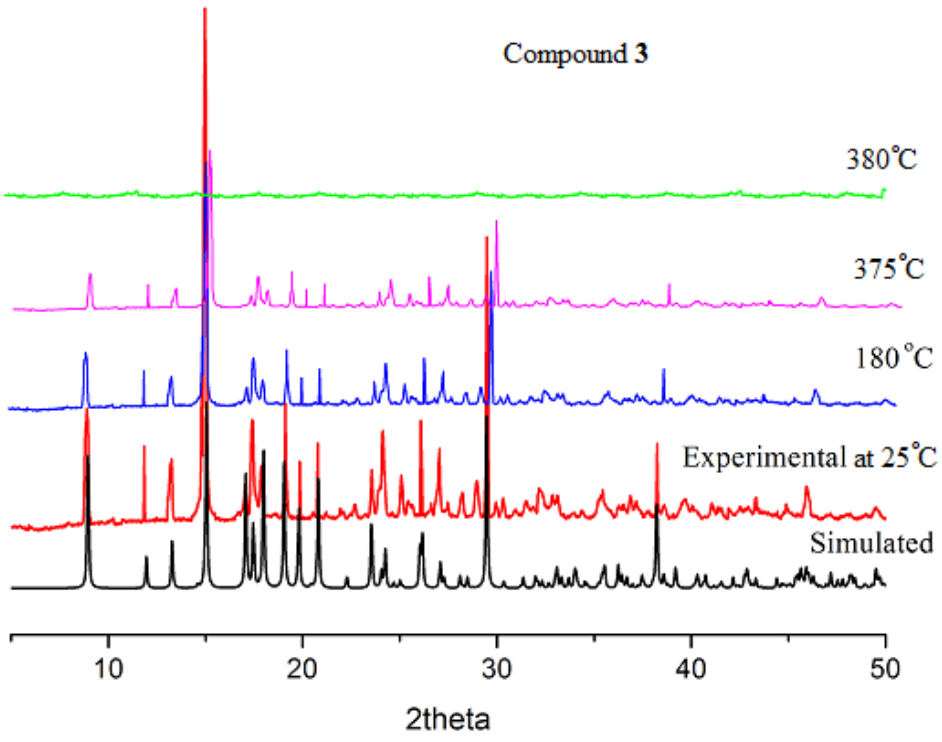
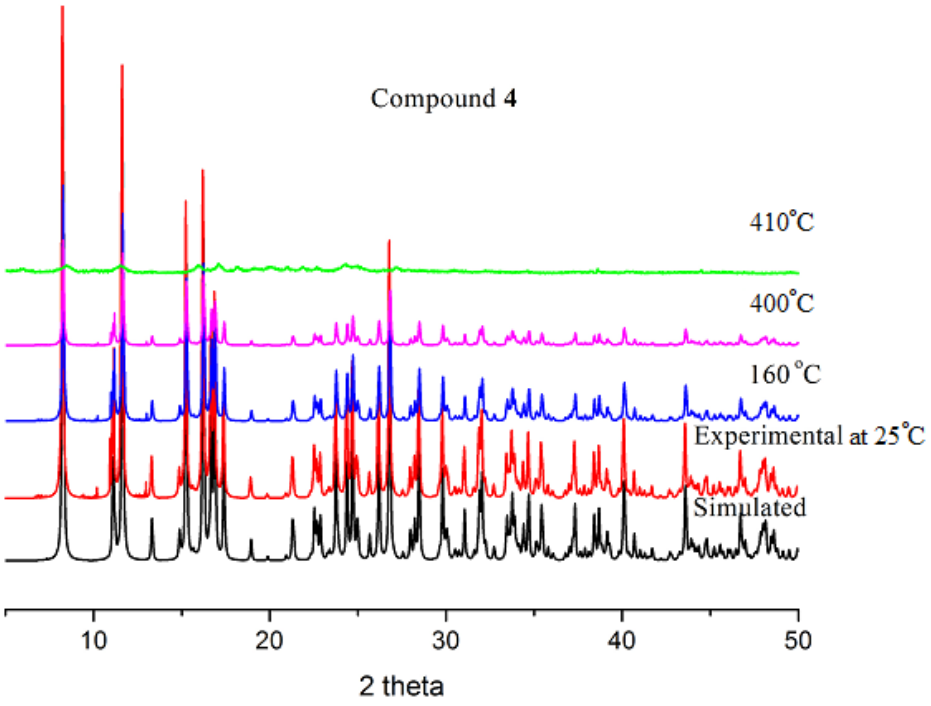


Figure S8. powder X-ray diffraction (PXRD) patterns of **1-5**.




Compound 2
360°C
350 °C
Experimental at 25°C
Simulated
10
20
30
40
50
2 theta


Compound 3
380°C
375°C
180 °C
Experimental at 25°C
Simulated
10
20
30
40
50
2theta


Compound 4
410°C
400°C
160 °C
Experimental at 25°C
Simulated
10
20
30
40
50
2 theta

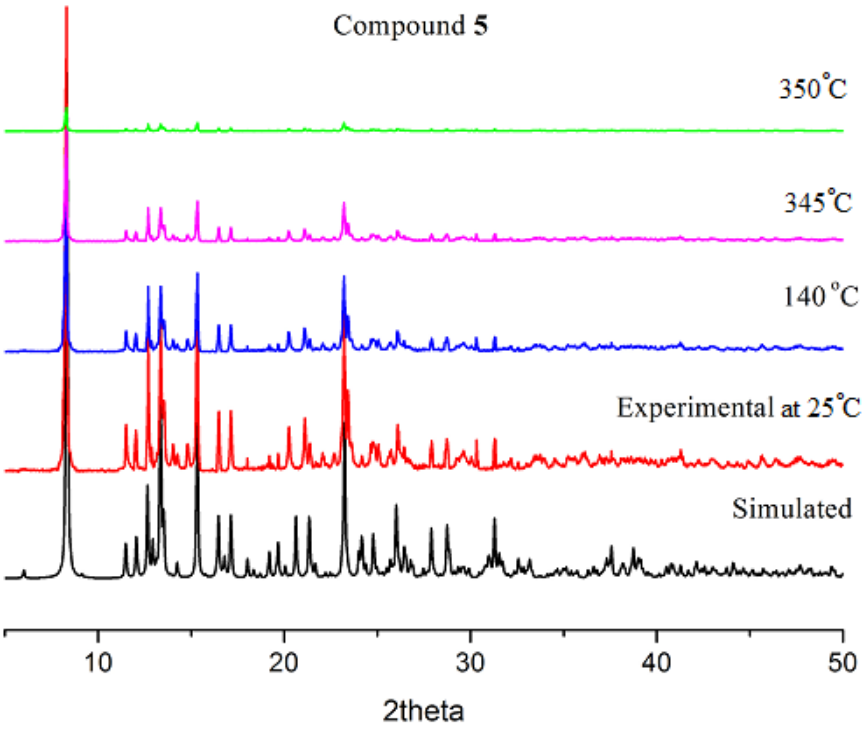

Compound 5
350°C
345°C
140 °C
Experimental at 25°C
Simulated
10
20
30
40
50
2theta

Figure S9. TGA curves of complexes **1-5**.

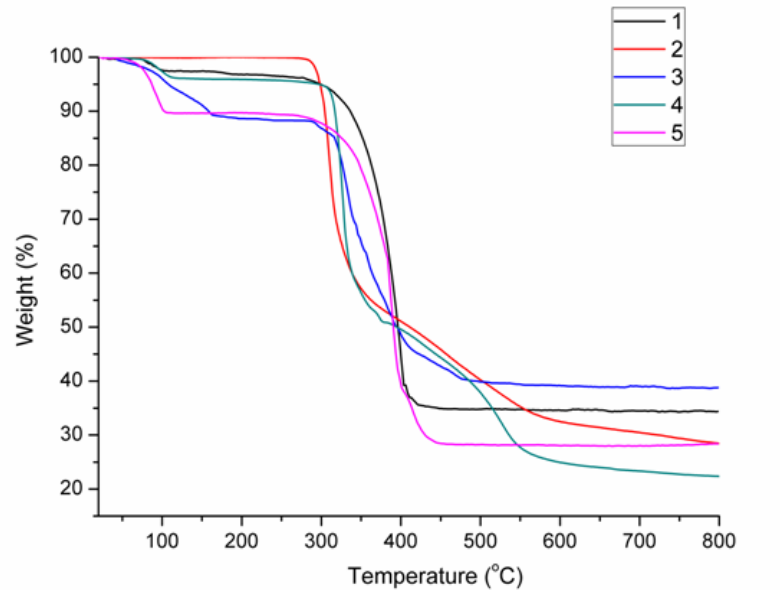


Figure S10. Solid-state emission spectrum of three complexes **2-4** and ligand 2,3-Pyridine-dicarboxylic acid excitation at the same wavelength at room temperature.

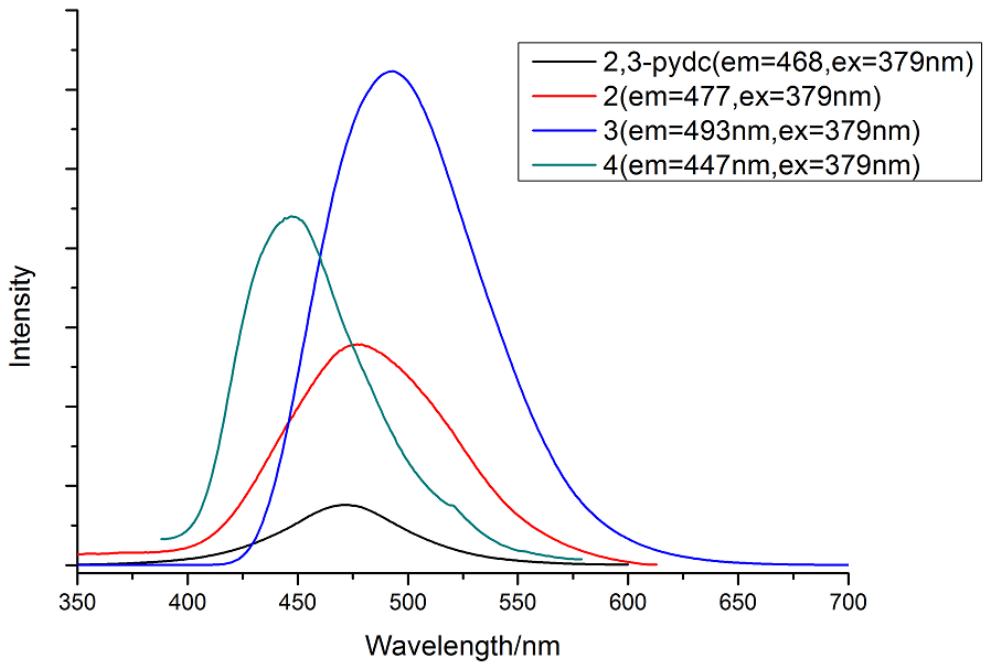


Figure S11. The selective sorption of compound **3** between H_2 and N_2 at 1 bar and 77 K.