

## Supporting information for

# A series of reaction-controlled coordination polymers constructed from bis(imidazole) and tetrafluoroterephthalic acid ligands: syntheses, structural diversities, properties

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1. **Table S1** The selected bond distances (Å) and angles (°) for **1-7**.
2. **Table S2** Hydrogen-bonding lengths (Å) and angles (°) in **1, 4-7**.
3. **Table S3** cell parameters of **1a** and **1b**.
4. **Fig. S1** View of O-H...O intermolecular interactions in **1**.
5. **Fig. S2** View of C-H...F intermolecular interactions in **1**.
6. **Fig. S3** View of C-H...F intramolecular interactions in **2**.
7. **Fig. S4** View of C-H...F intermolecular interactions in **3**.
8. **Fig. S5** View of C-H...F intermolecular interactions in **6**.
9. **Fig. S6** PXRD patterns of **1-7**.
10. **Fig. S7** TGA curves of **1-7**.
11. **Fig. S8** PXRD patterns of **1, 1a** and **1b**.

1. **Table S1.** Selected bond distances (Å) and angles (°) for **1-7**.

<b>1</b>			
Co(1)-O(1)	1.9413(17)	Co(1)-O(1)#1	1.9413(17)
Co(1)-N(1)#1	2.001(2)	Co(1)-N(1)	2.001(2)
O(1)-Co(1)-O(1)#1	113.19(11)	O(1)-Co(1)-N(1)#1	104.20(8)
O(1)#1-Co(1)-N(1)#1	111.46(8)	O(1)-Co(1)-N(1)	111.46(8)
O(1)#1-Co(1)-N(1)	104.20(8)	N(1)#1-Co(1)-N(1)	112.57(12)
<b>2</b>			
Cd(1)-O(4)	2.202(12)	Cd(1)-N(1)	2.209(12)
Cd(1)-O(2)#1	2.281(10)	Cd(1)-O(3)	2.316(11)
Cd(1)-O(1)	2.363(11)	Cd(1)-O(2)	2.401(10)
Cd(2)-N(3)	2.200(12)	Cd(2)-O(7)	2.249(11)
Cd(2)-O(6)	2.258(10)	Cd(2)-O(5)#2	2.313(10)
Cd(2)-O(8)	2.390(11)	Cd(2)-O(5)	2.562(10)
O(2)-Cd(1)#3	2.281(10)	O(5)-Cd(2)#6	2.313(10)
O(4)-Cd(1)-N(1)	95.7(5)	O(4)-Cd(1)-O(2)#1	87.1(4)
N(1)-Cd(1)-O(2)#1	108.5(4)	O(4)-Cd(1)-O(3)	169.7(5)
N(1)-Cd(1)-O(3)	91.6(5)	O(2)#1-Cd(1)-O(3)	83.7(4)
O(4)-Cd(1)-O(1)	88.8(5)	N(1)-Cd(1)-O(1)	158.2(4)
O(2)#1-Cd(1)-O(1)	92.9(4)	O(3)-Cd(1)-O(1)	87.0(5)
O(4)-Cd(1)-O(2)	94.6(4)	N(1)-Cd(1)-O(2)	104.2(4)
O(2)#1-Cd(1)-O(2)	146.9(2)	O(3)-Cd(1)-O(2)	90.6(4)
O(1)-Cd(1)-O(2)	54.1(4)	N(3)-Cd(2)-O(7)	98.4(5)
N(3)-Cd(2)-O(6)	156.9(4)	O(7)-Cd(2)-O(6)	92.5(4)
N(3)-Cd(2)-O(5)#2	104.9(4)	O(7)-Cd(2)-O(5)#2	88.3(4)
O(6)-Cd(2)-O(5)#2	95.7(4)	N(3)-Cd(2)-O(8)	92.8(5)
O(7)-Cd(2)-O(8)	164.2(5)	O(6)-Cd(2)-O(8)	81.2(4)
O(5)#2-Cd(2)-O(8)	78.0(4)	N(3)-Cd(2)-O(5)	103.8(4)
O(7)-Cd(2)-O(5)	107.3(4)	O(6)-Cd(2)-O(5)	53.3(4)

O(5)#2-Cd(2)-O(5)	144.8(3)	O(8)-Cd(2)-O(5)	80.6(4)
C(2)-N(1)-Cd(1)	129.9(11)	C(3)-N(1)-Cd(1)	123.1(10)
C(16)-N(3)-Cd(2)	128.6(10)	C(17)-N(3)-Cd(2)	124.7(11)
C(7)-O(1)-Cd(1)	93.3(10)	C(7)-O(2)-Cd(1)#3	124.5(9)
C(7)-O(2)-Cd(1)	88.1(8)	Cd(1)#3-O(2)-Cd(1)	115.4(4)
C(28)#4-O(3)-Cd(1)	141.7(11)	C(28)#5-O(4)-Cd(1)	131.6(11)
C(21)-O(5)-Cd(2)#6	122.4(9)	C(21)-O(5)-Cd(2)	83.2(8)
Cd(2)#6-O(5)-Cd(2)	109.9(4)	C(21)-O(6)-Cd(2)	100.6(9)
C(14)-O(7)-Cd(2)	112.3(9)	C(14)#2-O(8)-Cd(2)	162.7(12)

### 3

Ni(1)-N(1)#1	2.018(3)	Ni(1)-N(1)	2.018(3)
Ni(1)-O(1)	2.097(3)	Ni(1)-O(1)#1	2.097(3)
Ni(1)-O(2)#1	2.204(3)	Ni(1)-O(2)	2.204(3)
N(1)#1-Ni(1)-N(1)	95.8(2)	N(1)#1-Ni(1)-O(1)	167.11(13)
N(1)-Ni(1)-O(1)	91.40(13)	N(1)#1-Ni(1)-O(1)#1	91.40(13)
N(1)-Ni(1)-O(1)#1	167.11(13)	O(1)-Ni(1)-O(1)#1	83.63(17)
N(1)#1-Ni(1)-O(2)#1	96.02(12)	N(1)-Ni(1)-O(2)#1	107.35(12)
O(1)-Ni(1)-O(2)#1	91.98(11)	O(1)#1-Ni(1)-O(2)#1	61.13(11)
N(1)#1-Ni(1)-O(2)	107.35(12)	N(1)-Ni(1)-O(2)	96.02(12)
O(1)-Ni(1)-O(2)	61.13(11)	O(1)#1-Ni(1)-O(2)	91.98(11)
O(2)#1-Ni(1)-O(2)	144.99(15)		

### 4

Co(1)-O(1)#1	2.094(4)	Co(1)-O(1)	2.094(4)
Co(1)-O(3)#1	2.094(4)	Co(1)-O(3)	2.094(4)
Co(1)-O(1W)	2.120(4)	Co(1)-O(1W)#1	2.120(4)
O(1)#1-Co(1)-O(1)	180.0(2)	O(1)#1-Co(1)-O(3)#1	93.88(18)
O(1)-Co(1)-O(3)#1	86.12(18)	O(1)#1-Co(1)-O(3)	86.12(18)
O(1)-Co(1)-O(3)	93.88(18)	O(3)#1-Co(1)-O(3)	180.000(2)
O(1)#1-Co(1)-O(1W)	92.34(15)	O(1)-Co(1)-O(1W)	87.66(15)

O(3)#1-Co(1)-O(1W)	90.42(15)	O(3)-Co(1)-O(1W)	89.58(15)
O(1)#1-Co(1)-O(1W)#1	87.66(15)	O(1)-Co(1)-O(1W)#1	92.34(15)
O(3)#1-Co(1)-O(1W)#1	89.58(15)	O(3)-Co(1)-O(1W)#1	90.42(15)
O(1W)-Co(1)-O(1W)#1	180.000(1)		

## 5

Cd(1)-O(1)#1	2.251(3)	Cd(1)-O(1)	2.251(3)
Cd(1)-O(3)	2.278(3)	Cd(1)-O(3)#1	2.278(3)
Cd(1)-O(1W)#1	2.312(3)	Cd(1)-O(1W)	2.312(3)
O(1)#1-Cd(1)-O(1)	180.000(1)	O(1)#1-Cd(1)-O(3)	94.07(16)
O(1)-Cd(1)-O(3)	85.93(16)	O(1)#1-Cd(1)-O(3)#1	85.93(16)
O(1)-Cd(1)-O(3)#1	94.07(16)	O(3)-Cd(1)-O(3)#1	180.00(19)
O(1)#1-Cd(1)-O(1W)#1	91.07(13)	O(1)-Cd(1)-O(1W)#1	88.93(13)
O(3)-Cd(1)-O(1W)#1	87.85(13)	O(3)#1-Cd(1)-O(1W)#1	92.15(13)
O(1)#1-Cd(1)-O(1W)	88.93(13)	O(1)-Cd(1)-O(1W)	91.07(13)
O(3)-Cd(1)-O(1W)	92.15(13)	O(3)#1-Cd(1)-O(1W)	87.85(13)
O(1W)#1-Cd(1)-O(1W)	180.000(1)		

## 6

Cd(1)-N(4)	2.247(5)	Cd(1)-O(4)	2.282(4)
Cd(1)-N(2)	2.318(5)	Cd(1)-O(3)	2.319(5)
Cd(1)-O(2)	2.407(4)	Cd(1)-O(1)	2.460(5)
Cd(2)-N(6)	2.266(5)	Cd(2)-O(6)	2.274(4)
Cd(2)-N(8)	2.315(5)	Cd(2)-O(8)	2.333(5)
Cd(2)-O(9)	2.422(5)	Cd(2)-O(10)	2.423(5)
Cd(3)-N(12)	2.221(5)	Cd(3)-O(12)	2.262(5)
Cd(3)-N(10)	2.288(5)	Cd(3)-O(15)	2.323(6)
Cd(3)-O(13)	2.332(4)	Cd(3)-O(11)	2.580(5)
N(4)-Cd(1)-O(4)	105.94(18)	N(4)-Cd(1)-N(2)	88.62(18)
O(4)-Cd(1)-N(2)	161.85(19)	N(4)-Cd(1)-O(3)	105.9(2)
O(4)-Cd(1)-O(3)	84.56(19)	N(2)-Cd(1)-O(3)	81.0(2)

N(4)-Cd(1)-O(2)	150.44(18)	O(4)-Cd(1)-O(2)	77.69(17)
N(2)-Cd(1)-O(2)	95.08(18)	O(3)-Cd(1)-O(2)	103.62(19)
N(4)-Cd(1)-O(1)	96.13(18)	O(4)-Cd(1)-O(1)	87.44(17)
N(2)-Cd(1)-O(1)	101.99(18)	O(3)-Cd(1)-O(1)	157.84(19)
O(2)-Cd(1)-O(1)	54.39(17)	N(6)-Cd(2)-O(6)	104.06(18)
N(6)-Cd(2)-N(8)	89.14(19)	O(6)-Cd(2)-N(8)	163.28(19)
N(6)-Cd(2)-O(8)	107.2(2)	O(6)-Cd(2)-O(8)	84.36(19)
N(8)-Cd(2)-O(8)	81.9(2)	N(6)-Cd(2)-O(9)	153.12(18)
O(6)-Cd(2)-O(9)	77.69(16)	N(8)-Cd(2)-O(9)	95.25(18)
O(8)-Cd(2)-O(9)	99.70(19)	N(6)-Cd(2)-O(10)	98.47(17)
O(6)-Cd(2)-O(10)	87.44(16)	N(8)-Cd(2)-O(10)	100.92(19)
O(8)-Cd(2)-O(10)	154.27(19)	O(9)-Cd(2)-O(10)	54.65(16)
N(12)-Cd(3)-O(12)	146.02(19)	N(12)-Cd(3)-N(10)	87.97(19)
O(12)-Cd(3)-N(10)	105.24(19)	N(12)-Cd(3)-O(15)	118.3(2)
O(12)-Cd(3)-O(15)	94.7(2)	N(10)-Cd(3)-O(15)	82.42(19)
N(12)-Cd(3)-O(13)	89.79(18)	O(12)-Cd(3)-O(13)	87.63(18)
N(10)-Cd(3)-O(13)	159.72(19)	O(15)-Cd(3)-O(13)	80.93(17)
N(12)-Cd(3)-O(11)	93.71(18)	O(12)-Cd(3)-O(11)	52.83(17)
N(10)-Cd(3)-O(11)	105.63(19)	O(15)-Cd(3)-O(11)	147.5(2)
O(13)-Cd(3)-O(11)	94.63(18)		

7

Cd(1)-N(3)	2.244(8)	Cd(1)-N(1)#1	2.269(7)
Cd(1)-O(5)	2.312(7)	Cd(1)-O(4)	2.383(7)
Cd(1)-O(2)	2.468(6)	Cd(1)-O(3)	2.545(7)
Cd(1)-O(1)	2.545(6)	N(1)-Cd(1)#2	2.269(7)
N(3)-Cd(1)-N(1)#1	175.2(3)	N(3)-Cd(1)-O(5)	90.6(3)
N(1)#1-Cd(1)-O(5)	91.4(3)	N(3)-Cd(1)-O(4)	92.0(3)
N(1)#1-Cd(1)-O(4)	89.7(3)	O(5)-Cd(1)-O(4)	133.9(2)
N(3)-Cd(1)-O(2)	84.1(3)	N(1)#1-Cd(1)-O(2)	91.6(3)

O(5)-Cd(1)-O(2)	143.0(2)	O(4)-Cd(1)-O(2)	83.0(2)
N(3)-Cd(1)-O(3)	91.7(3)	N(1)#1-Cd(1)-O(3)	92.9(3)
O(5)-Cd(1)-O(3)	81.1(2)	O(4)-Cd(1)-O(3)	52.8(2)
O(2)-Cd(1)-O(3)	135.5(2)	N(3)-Cd(1)-O(1)	89.5(2)
N(1)#1-Cd(1)-O(1)	86.1(3)	O(5)-Cd(1)-O(1)	91.3(2)
O(4)-Cd(1)-O(1)	134.8(2)	O(2)-Cd(1)-O(1)	52.2(2)
O(3)-Cd(1)-O(1)	172.3(2)		

symmetrical codes: **1:** #1  $x, -y+1/2, -z+1/2$ . **2:** #1  $-x+1/2, y-1/2, -z+1/2$ ; #2  $-x+3/2, y+1/2, -z+1/2$ ; #3  $-x+1/2, y+1/2, -z+1/2$ ; #4  $-x+1, -y+1, -z$ ; #5  $x-1/2, -y+3/2, z+1/2$ ; #6  $-x+3/2, y-1/2, -z+1/2$ . **3:** #1  $-x+1/2, y, -z+1/2$ . **4:** #1  $-x+1, -y+1, -z+1$ . **5:** #1  $-x, -y, -z+1$ . **7:** #1  $x+1, y, z+1$ ; #2  $x-1, y, z-1$ .

## 2. Table S2 Hydrogen-bonding lengths (Å) and angles (°) in **1**, **4-7**.

D-H $\cdots$ A	d(D-H)	d(H $\cdots$ A)	d(D $\cdots$ A)	$\angle$ (DHA)
<b>1</b>				
O(1W)-H(1) $\cdots$ O(2)	0.824(10)	2.125(17)	2.929(3)	165(5)
<b>4</b>				
O(1W)-H(1WA) $\cdots$ O(2)#1	0.83	1.81	2.633(6)	168.3
O(1W)-H(1WB) $\cdots$ O(4)#1	0.83	1.93	2.726(6)	160.6
O(5)-H(5) $\cdots$ O(4)#1	0.822(10)	2.41(15)	2.845(9)	114(13)
<b>5</b>				
O(1W)-H(1WA) $\cdots$ O(2)	0.84	2.17	2.660(5)	117.4
O(1W)-H(1WB) $\cdots$ O(4)#1	0.83	1.99	2.742(5)	150.6
O(5)-H(5) $\cdots$ O(4)#2	0.822(10)	2.09(9)	2.836(9)	152(17)
<b>6</b>				
O(3)-H(3W) $\cdots$ O(7)#1	0.818(10)	1.93(5)	2.677(6)	152(11)
O(8)-H(8W) $\cdots$ O(5)#2	0.820(10)	2.04(9)	2.645(6)	130(10)
O(15)-H(15W) $\cdots$ O(14)	0.822(10)	1.82(3)	2.591(7)	157(8)

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O(5)-H(1W)···O(1)#1      0.82(2)      1.85(2)      2.675(9)      175(12)

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symmetrical codes: **4**: #1 -x+1, -y+1, -z+1. **5**: #1 -x, -y, -z+1. #2 x+1, y, z. **6**: #1 x+1, y, z. #2 x-1, y, z. **7**: #1 -x+2, -y, -z+1.

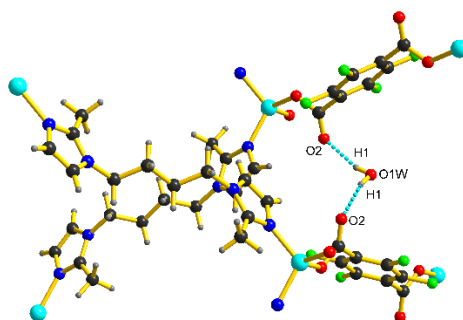
### 3. Table S3 cell parameters of **1a** and **1b**.

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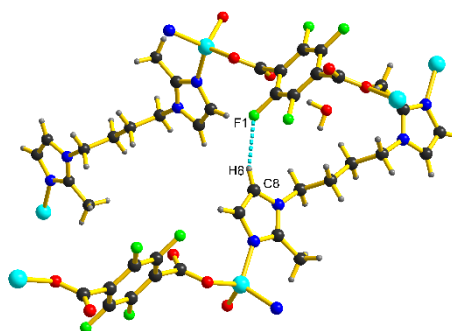
complex	<b>1a</b>	<b>1b</b>
<i>a</i> (Å)	18.135	18.05
<i>b</i> (Å)	13.852	13.75
<i>c</i> (Å)	9.347	9.41
$\alpha$ (°)	90	90
$\beta$ (°)	90	90
$\gamma$ (°)	90	90
<i>V</i> (Å <sup>3</sup> )	2348	2324

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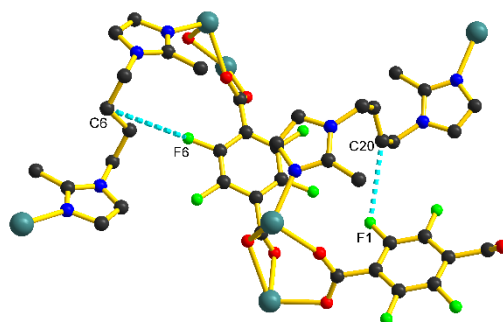
### 4. Fig. S1 View of O-H···O intermolecular interactions in **1**.



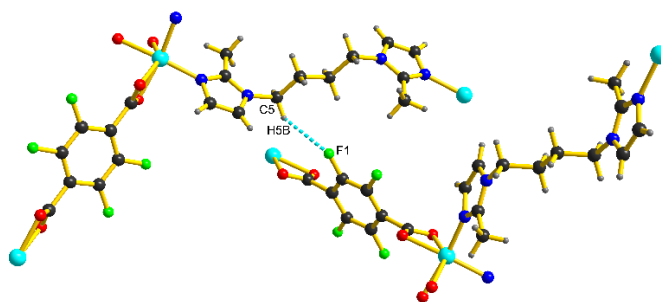
### 5. Fig. S2 View of C-H···F intermolecular interactions in **1**.



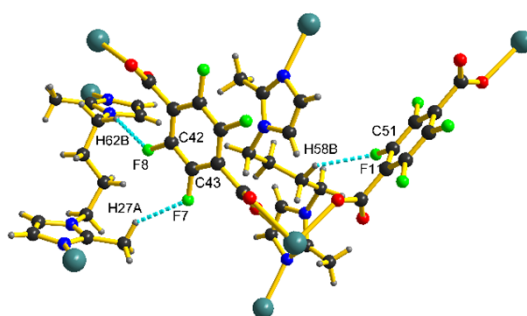
6. **Fig. S3** View of C-H...F intramolecular interactions in **2**.



7. **Fig. S4** View of C-H...F intermolecular interactions in **3**.

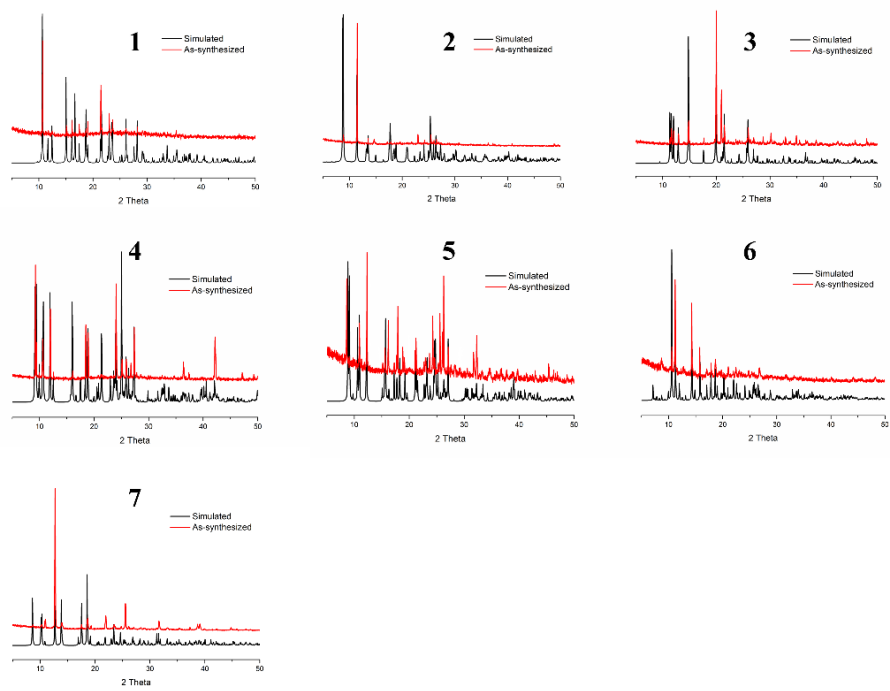


8. **Fig. S5** View of C-H...F intermolecular interactions in **6**.

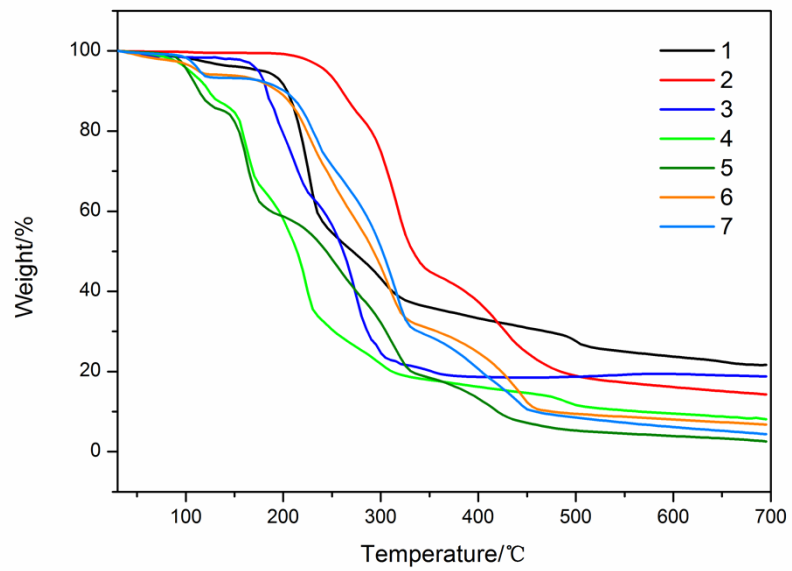


9. **Fig. S6** PXRD patterns for **1-7**.





10. Fig. S7 TGA curves of 1-7.



11. **Fig. S8** PXRD patterns of **1**, **1a** and **1b**.

