Electronic Supplementary Information (ESI)

Structural diversification and metal-directed assembly of coordination architectures based on tetrabromoterephthalic acid and a bent dipyridyl tecton 2,5-bis(4-pyridyl)-1,3,4-oxadiazole

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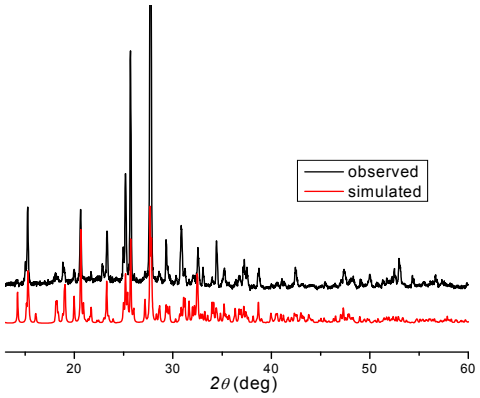
CrystEngComm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simulated
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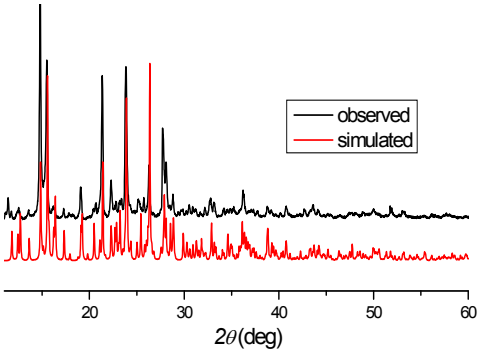
2θ(deg)

(a)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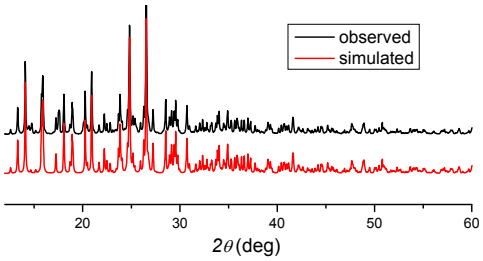
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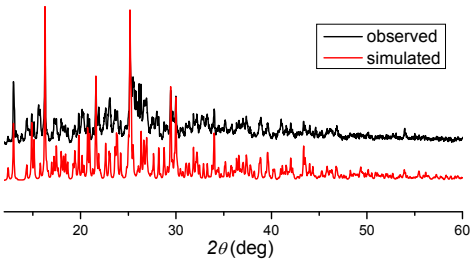
(c)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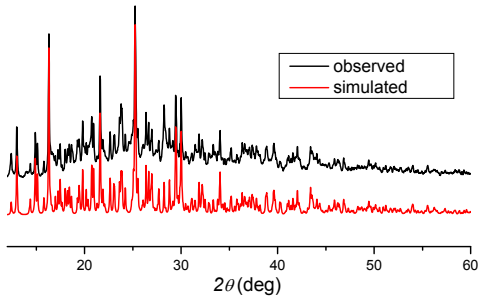
(d)



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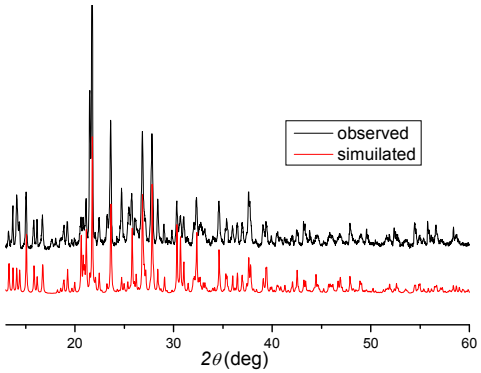

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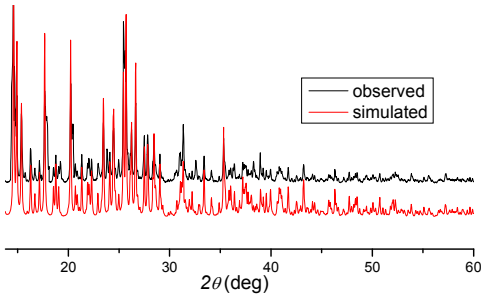

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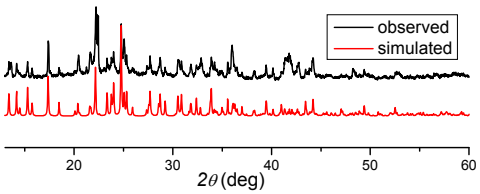

(h)

Fig. S1 Powder X-ray diffraction (PXRD) patterns for complexes **1**–**8** (**a**–**h**).

Table S1 Selective bond lengths (Å) and angles (°) for complexes **1**–**8**

		1	
Co1–N5	2.096(4)	Co1–O1	2.134(3)
Co1–N1	2.181(4)		
N5–Co1–O1	89.09(13)	N5–Co1–N1	89.41(16)
O1–Co1–N1	88.47(13)		
		2	
Ni1–O2	2.050(2)	Ni1–O4	2.066(2)
Ni1–N1	2.104(3)		
O2–Ni1–O4	88.05(10)	O2–Ni1–N1	91.64(10)
O4–Ni1–N1	88.17(11)		
		3	
Zn1–O4	2.1027(17)	Zn1–O2	2.1157(16)
Zn1–N1	2.167(2)		
O4–Zn1–O2	91.30(7)	O4–Zn1–N1	92.32(7)
O2–Zn1–N1	92.62(7)		
		4	
Ag1–O7	2.290(4)	Ag1–O5	2.312(4)
Ag1–N5	2.337(6)	Ag1–N1	2.340(6)
Ag1–O3	2.391(5)	Ag1–O4	2.468(5)
Ag1–O6	2.736(5)		
O7–Ag1–O5	134.29(17)	O7–Ag1–N5	85.0(2)
O5–Ag1–N5	90.80(19)	O7–Ag1–N1	82.02(19)

O5–Ag1–N1	92.81(18)	N5–Ag1–N1	164.87(19)
O7–Ag1–O3	140.58(17)	O5–Ag1–O3	84.98(16)
N5–Ag1–O3	92.45(19)	N1–Ag1–O3	102.50(19)
O7–Ag1–O4	86.83(17)	O5–Ag1–O4	138.60(16)
N5–Ag1–O4	88.16(19)	N1–Ag1–O4	98.72(18)
O3–Ag1–O4	53.76(16)	O5–Ag1–O6	51.20(16)
O3–Ag1–O6	135.95(14)	O4–Ag1–O6	170.19(15)
N1–Ag1–O6	78.54(17)	N5–Ag1–O6	92.41(17)
O7–Ag1–O6	83.46(17)		

5

Cd1–O7	2.286(3)	Cd1–O5	2.314(3)
Cd1–N1	2.335(3)	Cd1–N5	2.339(3)
Cd1–O3	2.390(3)	Cd1–O4	2.467(3)
Cd1–O6	2.737(3)		

O7–Cd1–O5	134.03(11)	O7–Cd1–N1	81.95(12)
O5–Cd1–N1	92.76(11)	O7–Cd1–N5	84.63(13)
O5–Cd1–N5	91.06(12)	N1–Cd1–N5	164.54(13)
O7–Cd1–O3	140.81(11)	O5–Cd1–O3	85.01(11)
N1–Cd1–O3	102.62(12)	N5–Cd1–O3	92.62(12)
O7–Cd1–O4	87.09(11)	O5–Cd1–O4	138.62(11)
N1–Cd1–O4	98.69(11)	N5–Cd1–O4	88.22(11)
O3–Cd1–O4	53.72(11)	O5–Cd1–O6	51.14(11)
O3–Cd1–O6	135.96(10)	O4–Cd1–O6	170.21(10)
N1–Cd1–O6	78.48(12)	N5–Cd1–O6	92.39(10)
O7–Cd1–O6	83.23(11)		

6

Cu1–O5A	1.977(2)	Cu1–O2	1.983(2)
Cu1–N4B	2.009(3)	Cu1–N1	2.010(3)

Cu1–O6	2.190(3)		
O5A–Cu1–O2	179.18(10)	O5A–Cu1–N4B	92.87(10)
O2–Cu1–N4B	87.25(10)	O5A–Cu1–N1	90.45(10)
O2–Cu1–N1	89.14(10)	N4B–Cu1–N1	157.90(11)
O5A–Cu1–O6	86.98(10)	O2–Cu1–O6	93.81(9)
N4B–Cu1–O6	96.73(11)	N1–Cu1–O6	105.26(11)

7

Zn1–O6	1.992(5)	Zn1–O2	2.037(4)
Zn1–N4B	2.044(5)	Zn1–N1	2.046(5)
Zn1–O4A	2.167(4)		
O6–Zn1–O2	86.53(19)	O6–Zn1–N4B	116.2(2)
O2–Zn1–N4B	98.9(2)	O6–Zn1–N1	114.7(3)
O2–Zn1–N1	97.17(19)	N4B–Zn1–N1	127.2(2)
O6–Zn1–O4A	87.52(18)	O2–Zn1–O4A	173.77(18)
N4B–Zn1–O4A	85.41(19)	N1–Zn1–O4A	83.64(19)

8

Pb1–O1	2.304(5)	Pb1–N1	2.53(3)
Pb1–N4A	2.65(2)		
O1–Pb1–N1	88.6(5)	O1–Pb1–N4A	80.3(4)
N1–Pb1–N4A	161.3(6)	O1–Pb1–O1B	77.0(3)
N1–Pb1–O1B	82.9(4)	N4A–Pb1–O1B	80.0(5)

Symmetry code: A = *x*, *y*, *z* + 1; B = –*x* + 3/2, *y* + 1/2, –*z* + 1/2 for **6**; A = *x* – 1, *y*, *z*; B = *x*, *y* – 1, *z* + 1 for **7**; A = *x* + 1, –*y* + 2, *z* – 1/2; B = –*x* + 2, *y*, –*z* + 3/2 for **8**.

Table S2 Important hydrogen-bonding geometries (Å, °)

D–H···A	$d_{D\cdots A}$	$d_{H\cdots A}$	$\angle_{D-H\cdots A}$	Symmetry code
1				
O4–H4···N4	2.643(5)	1.85	161	$-x+2, y+3/2, -z+3/2$
2				
O4–H4A···O3	2.692(3)	1.86	165	$-x, -y+1, -z$
O4–H4B···O5	2.702(4)	1.86	170	$x, y, z-1$
O5–H5A···N3	2.789(5)	2.01	158	$x-1, y, z$
3				
O4–H4A···O5	2.741(4)	1.89	174	$x-1, y, z$
O4–H4B···O3	2.646(3)	1.84	158	
O5–H5A···N2	2.954(4)	2.11	173	$-x+1, -y+1, -z+1$
4				
O7–H7A···N7	2.763(9)	1.92	173	$-x+2, -y+1, -z+1$
O7–H7B···O6	2.672(7)	1.86	160	$-x+1, -y+2, -z+1$
5				
O7–H7A···N7	2.755(6)	1.90	172	$-x+2, -y+1, -z+1$
O7–H7B···O6	2.665(4)	1.86	160	$-x+1, -y+2, -z+1$
6				
O6–H6A···O3	2.674(3)	1.98	138	
O6–H6B···O7	2.704(5)	1.90	157	
O7–H7···O4	2.693(5)	1.88	171	$x-1, y, z+1$

7

O6–H6A···O7	2.571(12)	2.15	111	$-x + 1, -y + 1, -z + 1$
O6–H6B···O5	2.585(7)	1.92	134	$x - 1, y, z$
O6–H6B···O1	3.217(8)	2.59	132	$-x + 1, -y + 1, -z$