Supplementary Material (ESI) for CrystEngComm

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Supporting Information

Structural diversity of coordination polymers assembled from adamantane dicarboxylates and conformational bis-triazole ligand †

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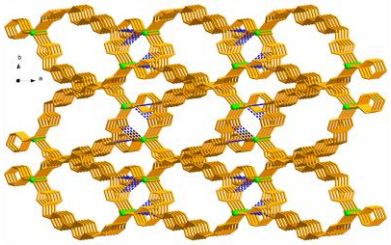


Fig. S1 View of 3D supramolecular architecture in **1**. Blue dotted lines show intermolecular C–H···O interactions.

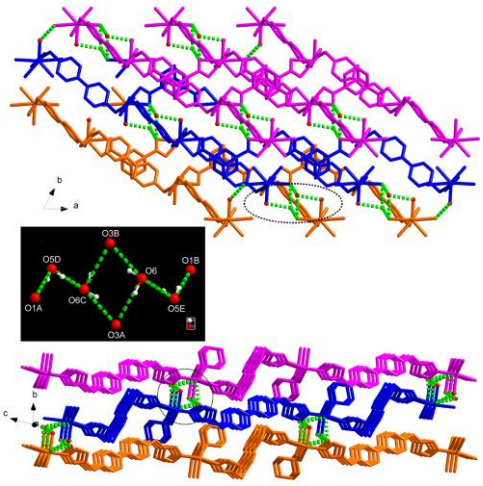


Fig. S2 Perspective view of hydrogen bonding interaction (green dotted lines) and 3D supramolecular architecture in *a*/*c* axis (Symmetry code: A = 1-x, 1-y, 1-z; B = 1+x, y, -1+z; C = 2-x, 1-y, -z; D = x, y, -1+z; E = 2-x, 1-y, 1-z.).

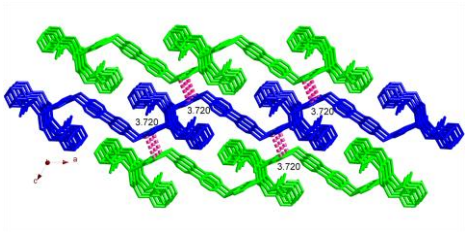


Fig. S3 A schematic view of 3D supramolecular architecture was formed by intermolecular π–π stacking interactions.

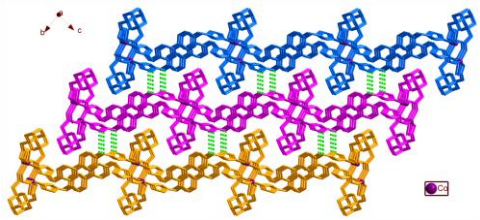


Fig. S4 A schematic view of 3D supramolecular architecture along the *a*-axis. Green dotted lines show intermolecular C–H···N interactions.

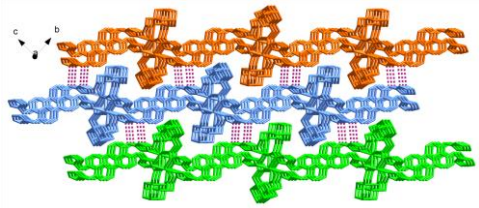
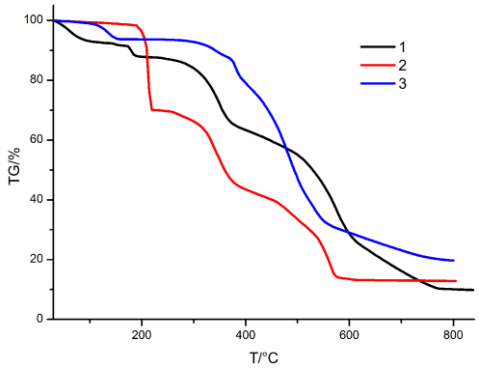
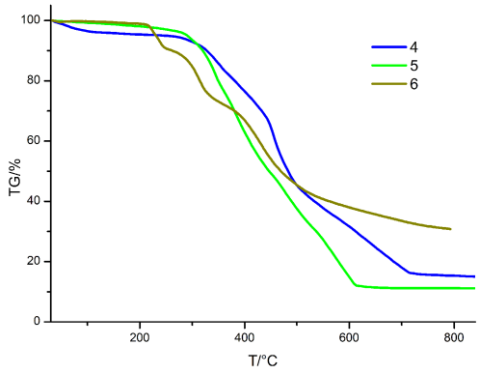


Fig. S5 A schematic view of 3D supramolecular architecture along the *a*-axis in **6**. Purple dotted lines show intermolecular C–H···N interactions.

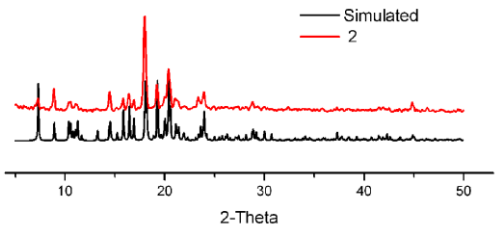


(a)

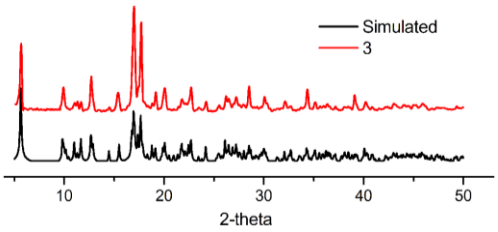


(b)

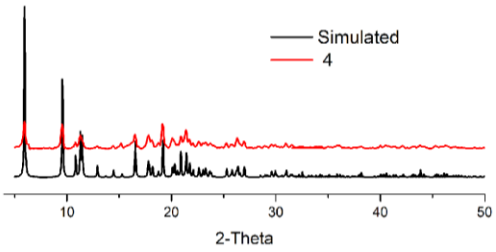
Fig. S6 The TGA curves of coordination polymers, (a) for **1**–**3**, (b) for **4**–**6.**



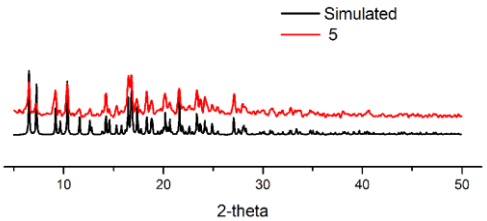
(a) Complex **2**



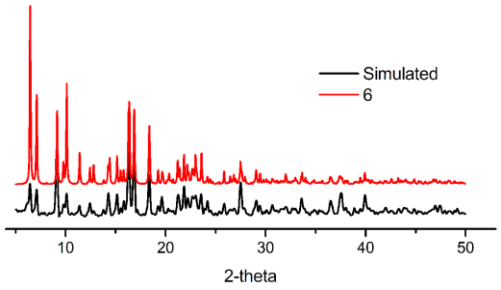
(b) Complex **3**



(c) Complex **4**



(d) Complex **5**



(e) Complex **6**

Fig. S7 XRD for complexes **2**–**6.**

Table S1 Selected bond lengths [Å] and angles [°] for complexes **1**–**6**.

Complex 1					
Zn(1)–O(4)#1	1.952(4)	Zn(1)–O(1)	1.968(4)	Zn(1)–N(4)#2	2.018(5)
Zn(1)–N(1)	2.029(5)				
O(4)#1–Zn(1)–O(1)		96.78(17)	O(4)#1–Zn(1)–N(4)#2		109.91(18)
O(1)–Zn(1)–N(4)#2		117.95(17)	O(4)#1–Zn(1)–N(1)		111.24(19)
O(1)–Zn(1)–N(1)		110.56(17)	N(4)#2–Zn(1)–N(1)		109.8(2)
Complex 2					
Co(1)–O(4)#1	1.951(3)	Co(1)–N(4)	2.032(3)	Co(1)–O(1)	2.042(2)
Co(1)–N(1)	2.071(3)	Co(1)–O(2)	2.259(2)		
O(4)#1–Co(1)–N(4)		101.67(12)	O(1)–Co(1)–N(1)		110.02(12)
O(4)#1–Co(1)–O(1)		98.48(10)	O(4)#1–Co(1)–O(2)		158.79(11)
N(4)–Co(1)–O(1)		122.02(11)	N(4)–Co(1)–O(2)		91.11(11)
O(4)#1–Co(1)–N(1)		100.85(13)	O(1)–Co(1)–O(2)		60.31(9)
N(4)–Co(1)–N(1)		118.40(12)	N(1)–Co(1)–O(2)		87.50(11)
Complex 3					
Cd(1)–N(1)	2.284(4)	Cd(1)–O(4)#1	2.328(4)	Cd(1)–O(3)#1	2.576(4)
Cd(1)–O(2)	2.285(4)	Cd(1)–N(4)	2.353(5)	Cd(1)–O(1)	2.620(4)
Cd(1)–O(5)	2.298(4)				
N(1)–Cd(1)–O(2)		99.88(16)	O(2)–Cd(1)–O(3)#1		135.04(14)
N(1)–Cd(1)–O(5)		90.22(16)	O(5)–Cd(1)–O(3)#1		90.17(15)

O(2)–Cd(1)–O(5)	133.54(15)	O(4)#1–Cd(1)–O(3)#1	52.06(14)
N(1)–Cd(1)–O(4)#1	100.09(17)	N(4)–Cd(1)–O(3)#1	90.22(16)
O(2)–Cd(1)–O(4)#1	83.02(14)	N(1)–Cd(1)–O(1)	94.43(14)
O(5)–Cd(1)–O(4)#1	139.85(15)	O(2)–Cd(1)–O(1)	52.27(13)
N(1)–Cd(1)–N(4)	169.16(17)	O(5)–Cd(1)–O(1)	81.98(14)
O(2)–Cd(1)–N(4)	89.02(17)	O(4)#1–Cd(1)–O(1)	134.81(13)
O(5)–Cd(1)–N(4)	79.12(17)	N(4)–Cd(1)–O(1)	86.11(15)
O(4)#1–Cd(1)–N(4)	87.04(18)	O(3)#1–Cd(1)–O(1)	171.84(13)
N(1)–Cd(1)–O(3)#1	87.82(15)		

Complex 4

Zn(1)–O(1)	1.925(3)	Zn(1)–O(4)#1	1.966(3)	Zn(1)–O(3)#2	1.999(3)
Zn(1)–N(1)	2.059(4)				
O(1)–Zn(1)–O(4)#1	138.92(14)	O(1)–Zn(1)–N(1)	101.30(15)		
O(1)–Zn(1)–O(3)#2	113.04(13)	O(4)#1–Zn(1)–N(1)	106.41(14)		
O(4)#1–Zn(1)–O(3)#2	93.52(12)	O(3)#2–Zn(1)–N(1)	96.37(14)		

Complex 5

Co(1)–O(1)	2.0197(19)	Co(1)–N(4)#2	2.131(2)	Co(1)–O(4)#3	2.1605(19)
Co(1)–O(2)#1	2.0485(18)	Co(1)–N(1)	2.156(2)	Co(1)–O(3)#3	2.2405(19)
O(1)–Co(1)–O(2)#1	119.86(8)	O(2)#1–Co(1)–O(4)#3	88.35(7)		
O(1)–Co(1)–N(4)#2	91.53(8)	N(4)#2–Co(1)–O(4)#3	93.34(8)		
O(2)#1–Co(1)–N(4)#2	92.75(8)	N(1)–Co(1)–O(4)#3	89.81(8)		
O(1)–Co(1)–N(1)	86.44(8)	O(1)–Co(1)–O(3)#3	92.07(8)		
O(2)#1–Co(1)–N(1)	85.81(8)	O(2)#1–Co(1)–O(3)#3	146.75(8)		
N(4)#2–Co(1)–N(1)	176.50(8)	N(4)#2–Co(1)–O(3)#3	95.62(8)		
O(1)–Co(1)–O(4)#3	151.10(8)	N(1)–Co(1)–O(3)#3	87.30(8)		
O(4)#3–Co(1)–O(3)#3	59.12(7)				

Complex 6

Cd(1)–O(3)	2.240(4)	Cd(1)–N(7)	2.369(5)	Cd(1)–N(1)	2.327(5)
Cd(1)–O(8)#1	2.286(5)	Cd(1)–O(5)	2.411(5)	Cd(1)–O(6)	2.355(4)

Cd(2)–O(8)	2.342(4)	Cd(2)–O(2)	2.311(4)	Cd(2)–N(4)#4	2.344(4)
Cd(2)–N(10)#3	2.318(4)	Cd(2)–O(4)#2	2.317(5)	Cd(2)–O(1)	2.470(4)
Cd(2)–O(7)	2.584(4)				
O(3)–Cd(1)–O(8)#1		113.27(16)	O(3)–Cd(1)–N(7)		87.07(17)
O(3)–Cd(1)–N(1)		96.81(17)	O(8)#1–Cd(1)–N(7)		85.75(17)
O(8)#1–Cd(1)–N(1)		87.24(17)	N(1)–Cd(1)–N(7)		172.9(2)
O(3)–Cd(1)–O(6)		143.97(19)	O(6)–Cd(1)–N(7)		84.26(17)
O(8)#1–Cd(1)–O(6)		100.88(16)	O(3)–Cd(1)–O(5)		90.68(17)
N(1)–Cd(1)–O(6)		95.90(17)	O(8)#1–Cd(1)–O(5)		155.65(15)
N(1)–Cd(1)–O(5)		94.48(17)	O(4)#2–Cd(2)–O(8)		81.94(17)
O(6)–Cd(1)–O(5)		54.77(15)	N(10)#3–Cd(2)–O(8)		84.71(16)
N(7)–Cd(1)–O(5)		91.42(17)	O(2)–Cd(2)–N(4)#4		87.81(17)
O(2)–Cd(2)–O(4)#2		144.26(17)	O(4)#2–Cd(2)–N(4)#4		86.35(17)
O(2)–Cd(2)–N(10)#3		95.85(17)	N(10)#3–Cd(2)–N(4)#4		176.16(19)
O(4)#2–Cd(2)–N(10)#3		89.99(17)	O(8)–Cd(2)–N(4)#4		93.62(16)
O(2)–Cd(2)–O(8)		133.65(15)	O(2)–Cd(2)–O(1)		54.19(14)
O(4)#2–Cd(2)–O(1)		90.20(17)	O(4)#2–Cd(2)–O(7)		132.22(17)
N(10)#3–Cd(2)–O(1)		95.44(16)	N(10)#3–Cd(2)–O(7)		96.46(17)
O(8)–Cd(2)–O(1)		172.14(15)	O(8)–Cd(2)–O(7)		51.90(15)
N(4)#4–Cd(2)–O(1)		85.75(16)	N(4)#4–Cd(2)–O(7)		85.17(17)
O(2)–Cd(2)–O(7)		82.20(15)	O(1)–Cd(2)–O(7)		135.70(15)

Symmetry codes: For 1: #**1** x, y, z+1; #2 -x+2, -y, -z+1. For **2**: #1 x+1/2, -y+1/2, z+1/2. For **3**: #1 x+1, y, z. For **4**: #1 -x+1/2, y-1/2, -z+1/2; #2 x, y-1, z. For **5**: #1 -x+1, -y, -z+2; #2 x+1, y-1, z+1; #3 x+1, y, z. For **6**: #1 x+1, y, z; #2 x-1, y, z; #3 -x+2, -y, -z+1; #4 -x, -y+2, -z.