[Supporting information]

Seven entangled coordination polymers assembled from triphenylamine-based bisimidazole and polycarboxylates: interpenetration, self-penetration and mixed entanglement

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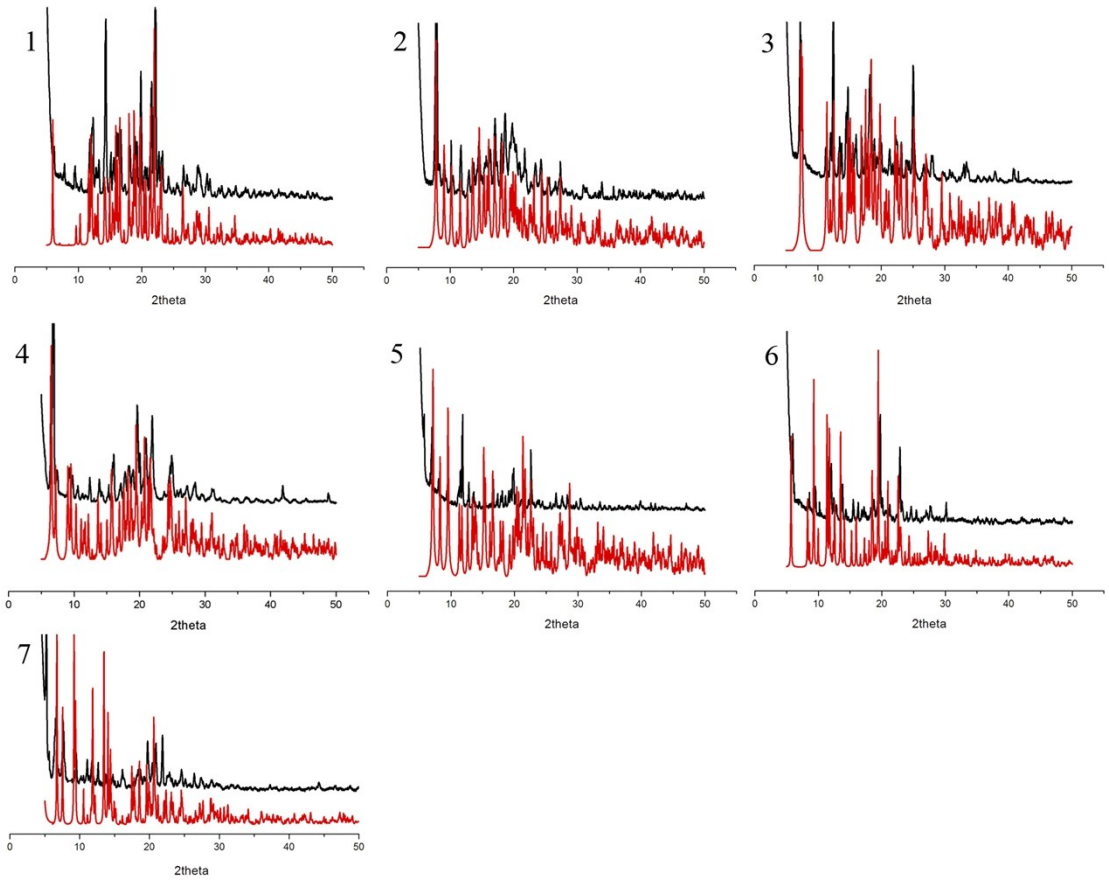

Fig. S1. The simulated (red) and experimental (black) XRPD patterns for 1-**7**.

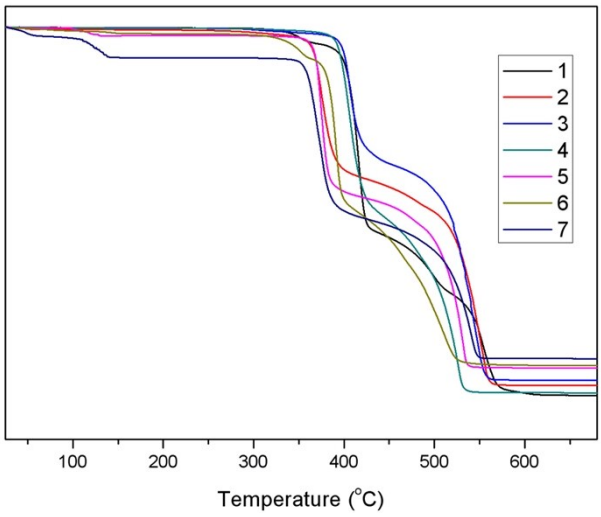

Fig. S2. TGA curves of **1-7**.

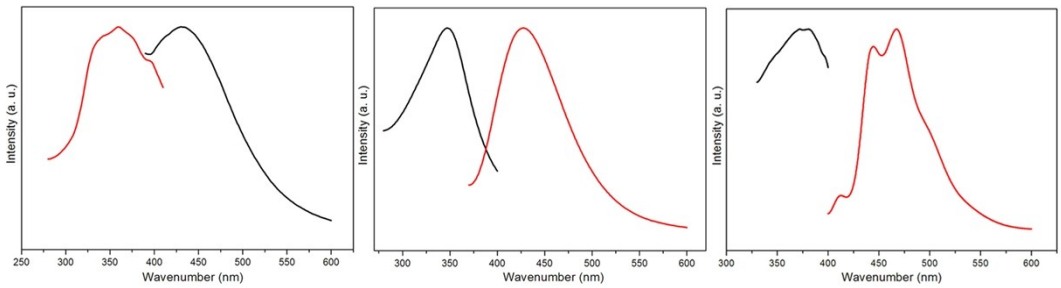

Fig. S3. Excitation (black) and emission (red) spectra of H_2sdc (left), H_2bpdc (middle) and H_2sda (right).

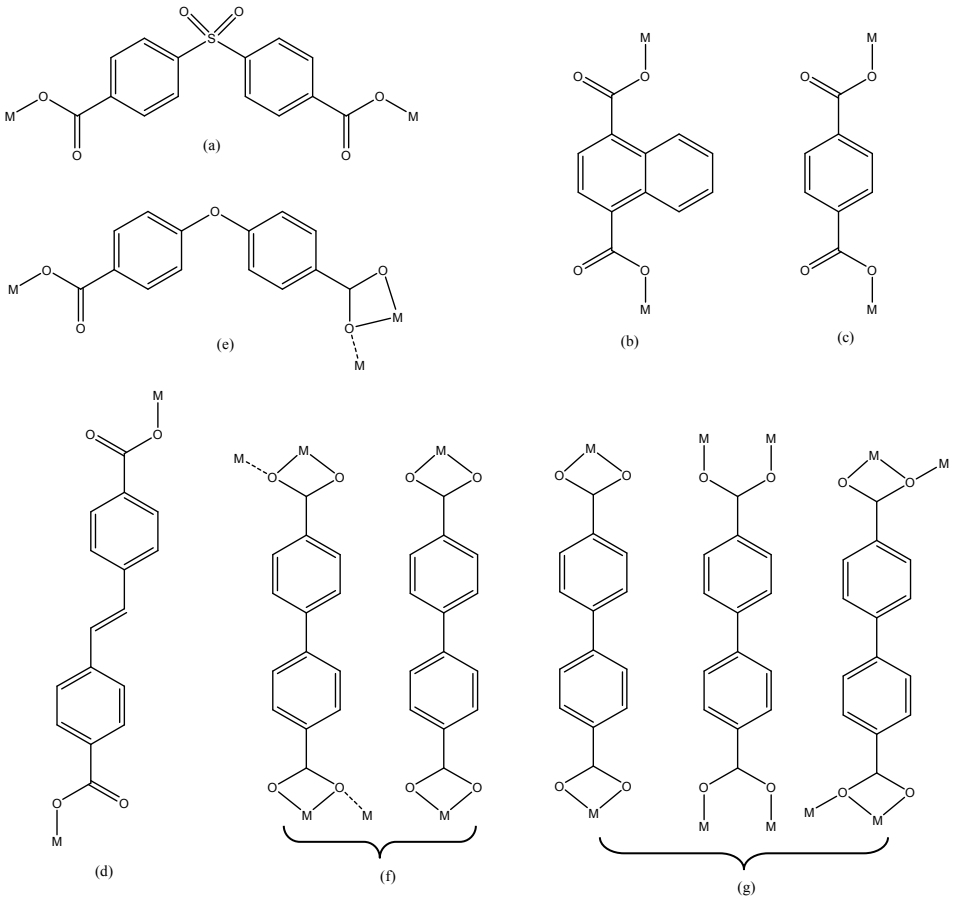

Fig. S4. The coordination modes of the dicarboxylates in compounds **1-7**. (a for **1**, b for **2**, c for **3**, d for **4**, e for **5**, f for **6** and g for **7**.

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

Zn(1) - N(1)	1.982(3)
Zn(1) - O(2)	1.927(3)
Zn(1)-N(5)#4	2.032(3)
Zn(1)-O(3)#3	1.947(3)
O(2)-Zn(1)-O(3)#3	103.26(14)
O(2)-Zn(1)-N(1)	122.88(12)
O(3)#3-Zn(1)-N(1)	116.16(13)
O(2)-Zn(1)-N(5)#4	99.16(13)
O(3)#3-Zn(1)-N(5)#4	106.41(13)
N(1)-Zn(1)-N(5)#4	106.73(13)

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

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Zn(1) - N(1)	1.998(4)
Zn(1)-N(5)#4	2.010(4)
Zn(1) - O(1)	1.924(4)
Zn(1)-O(4)#3	1.947(4)
O(1)-Zn(1)-O(4)#3	102.92(18)
O(1)-Zn(1)-N(1)	111.5(2)
O(4)#3-Zn(1)-N(1)	116.22(18)
O(1)-Zn(1)-N(5)#4	116.28(19)
O(4)#3-Zn(1)-N(5)#4	96.94(19)
N(1)-Zn(1)-N(5)#4	112.12(17)

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

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Zn(1) - N(1)	2.006(2)
Zn(1) - O(2)	1.941(2)
Zn(1) - O(3)	1.9667(19)
Zn(1)-N(5)#3	1.997(2)
O(2)-Zn(1)-O(3)	102.23(7)
O(2)-Zn(1)-N(5)#3	110.00(9)
O(3)-Zn(1)-N(5)#3	114.47(9)
O(2)-Zn(1)-N(1)	114.34(9)
O(3)-Zn(1)-N(1)	103.64(9)
N(5)#3-Zn(1)-N(1)	111.77(9)

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

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Zn(1) - N(1)	2.044(4)
Zn(1)-N(5)#4	2.046(3)
Zn(1) - O(1)	1.941(3)
Zn(1) - O(3)	2.278(4)
Zn(1) - O(4)	2.096(4)
O(1)-Zn(1)-N(1)	112.43(14)
O(1)-Zn(1)-N(5)#4	110.70(13)
N(1)-Zn(1)-N(5)#4	102.36(14)
O(1)-Zn(1)-O(4)	120.52(17)
N(1)-Zn(1)-O(4)	117.59(16)
N(5)#4-Zn(1)-O(4)	88.23(14)
O(1)-Zn(1)-O(3)	89.98(14)
N(1)-Zn(1)-O(3)	93.58(15)
N(5)#4-Zn(1)-O(3)	145.96(14)
O(4)-Zn(1)-O(3)	57.75(14)

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

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Cd(1) - N(1)	2.339(3)
Cd(1) - N(5)#3	2.265(2)
Cd(1) - O(1)	2.1695(19)
Cd(1)-O(4)#4	2.300(2)
Cd(1)-O(5)#4	2.556(2)
O(1)-Cd(1)-N(5)#3	128.55(8)
O(1)-Cd(1)-O(4)#4	139.37(8)
N(5)#3-Cd(1)-O(4)#4	84.82(8)
O(1)-Cd(1)-N(1)	96.76(9)
N(5)#3-Cd(1)-N(1)	96.42(9)
O(4)#4-Cd(1)-N(1)	102.08(9)
O(1)-Cd(1)-O(5)#4	96.49(8)
N(5)#3-Cd(1)-O(5)#4	134.90(8)
O(4)#4-Cd(1)-O(5)#4	53.80(7)
N(1)-Cd(1)-O(5)#4	78.15(8)

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

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Cd(1) - N(1)	2.235(3)
Cd(1) - N(5)#4	2.374(4)
Cd(1) - O(1)	2.367(3)
Cd(1) - O(2)	2.364(7)
Cd(1) - O(2')	2.397(7)
Cd(1) - O(3)	2.227(3)
O(3)-Cd(1)-N(1)	139.29(15)

O(3)-Cd(1)-O(2)	83.1(2)
N(1)-Cd(1)-O(2)	135.5(2)
O(3)-Cd(1)-O(1)	108.25(13)
N(1)-Cd(1)-O(1)	93.08(12)
O(2)-Cd(1)-O(1)	51.83(19)
O(3)-Cd(1)-N(5)#4	104.95(13)
N(1)-Cd(1)-N(5)#4	89.73(12)
O(2)-Cd(1)-N(5)#4	90.3(2)
O(1)-Cd(1)-N(5)#4	124.08(12)
O(3)-Cd(1)-O(2')	102.0(2)
N(1)-Cd(1)-O(2')	118.6(2)
O(2)-Cd(1)-O(2')	21.65(19)
O(1)-Cd(1)-O(2')	54.75(17)
N(5)#4-Cd(1)-O(2')	75.33(19)

Symmetry transformations used to generate equivalent atoms: #4 x,y,z-1.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Cd(1)-N(5)#4	2.2647
Cd(1) - O(1)	2.4484
Cd(1) - O(2)	2.3116
Cd(1) - O(3)	2.2025
Cd(1) - O(5)	2.3345
Cd(1) - O(6)	2.2905
Cd(1) - O(6')	2.3448
Cd(2) - N(1)	2.2271
Cd(2) - O(1)	2.3885

Cd(2) - O(4)	2.3717
O(3)-Cd(1)-N(5)#4	88.6
O(3)-Cd(1)-O(6)	120.4
N(5)#4-Cd(1)-O(6)	99.4
O(3)-Cd(1)-O(2)	142.5
N(5)#4-Cd(1)-O(2)	81.0
O(6)-Cd(1)-O(2)	96.9
O(3)-Cd(1)-O(5)	94.0
N(5)#4-Cd(1)-O(5)	151.4
O(6)-Cd(1)-O(5)	55.1
O(2)-Cd(1)-O(5)	112.2
O(3)-Cd(1)-O(6')	112.2
N(5)#4-Cd(1)-O(6')	97.3
O(2)-Cd(1)-O(6')	104.9
O(5)-Cd(1)-O(6')	55.5
O(3)-Cd(1)-O(1)	100.4
N(5)#4-Cd(1)-O(1)	116.5
O(6)-Cd(1)-O(1)	126.1
O(2)-Cd(1)-O(1)	54.7
O(5)-Cd(1)-O(1)	91.1
O(6')-Cd(1)-O(1)	133.4

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