Electronic Supplementary Information (ESI)

How do substituent groups in the 5-position of 1,3-benzenedicarboxylate affect the construction of supramolecular frameworks? †

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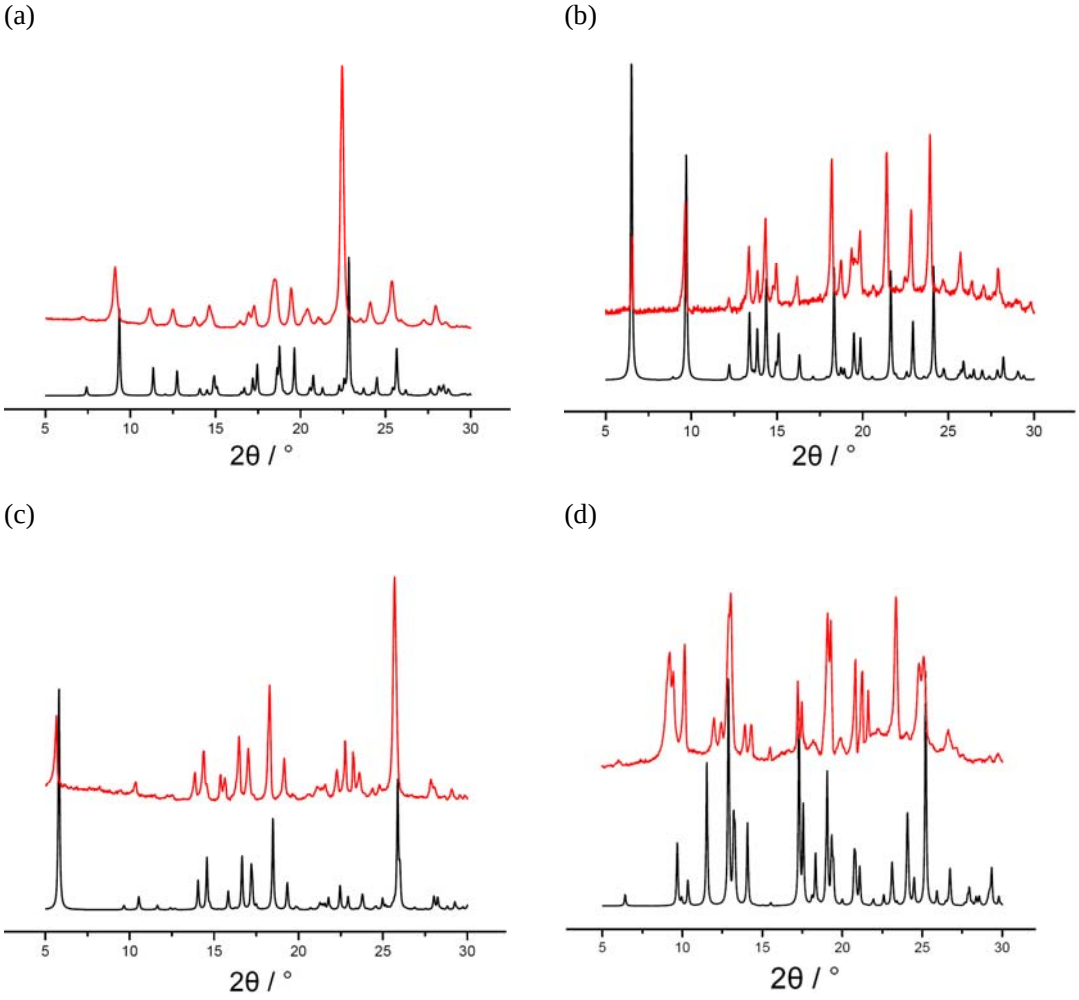
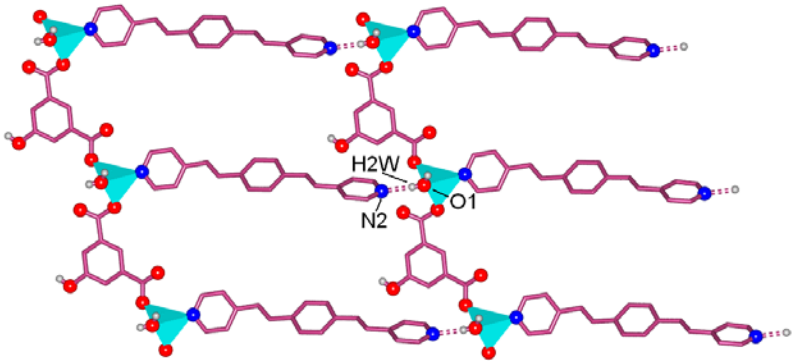
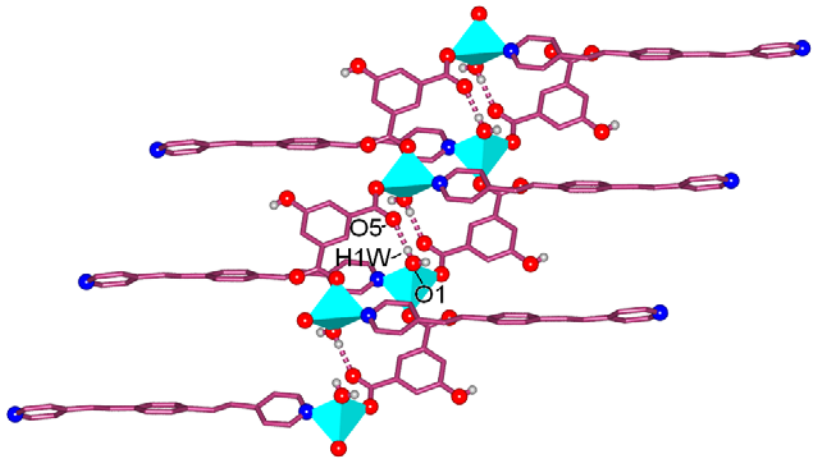


Fig. S1 Powder XRD patterns of (a) $[Zn(OH_2)(5\text{-}HO\text{-}1,3\text{-}BDC)(1,4\text{-}bpeb)]_n$ **(1)**; (b) $[Zn(HBTC)(1,4\text{-}bpeb)]_n$ **(2)**; (c) $\{[Zn(5\text{-}NO_2\text{-}1,3\text{-}BDC)(1,4\text{-}bpeb)]\cdot 2(H_2O)_{0.5}\}_n$ **(3)**; (d) $[Zn(5\text{-}Me\text{-}1,3\text{-}BDC)(1,4\text{-}bpeb)]_n$ **(4)**. Black: simulated from single crystal analysis and experimental; Red: as synthesized.

(a)



(b)



(c)

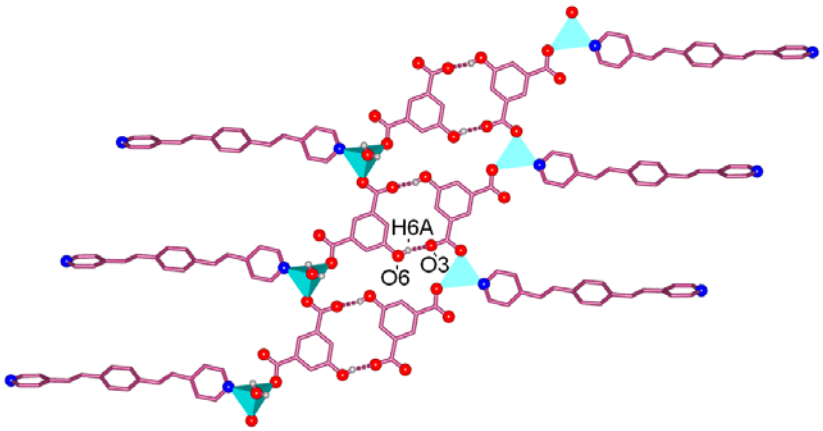


Fig. S2 (a) The O1–H2W···N2 H-bonding interaction in **1.** (b) The O1–H1W···O5 H-bonding interaction in **1.** (c) The O6–H6A···O3 H-bonding interaction in **1.**

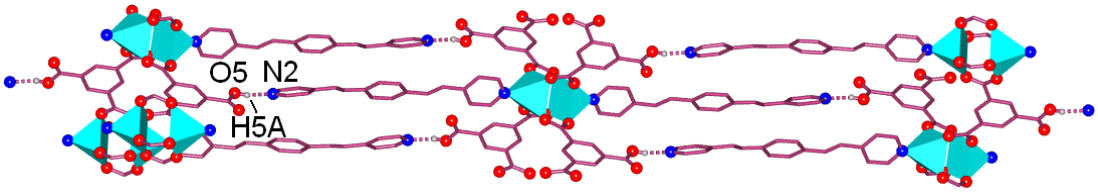


Fig. S3 The O5–H5A···N2 H-bonding interaction in **2.**

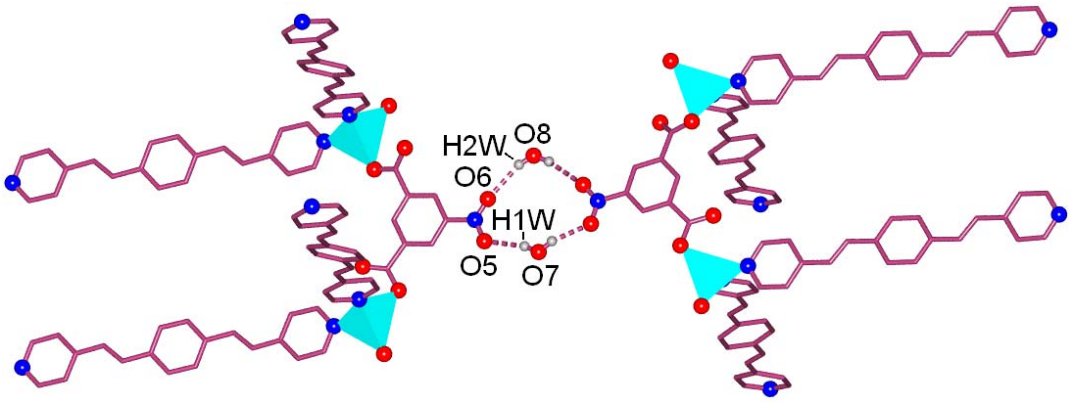


Fig. S4 The O7–H1W···O5 and O8–H2W···O6 H-bonding interactions in **3.**

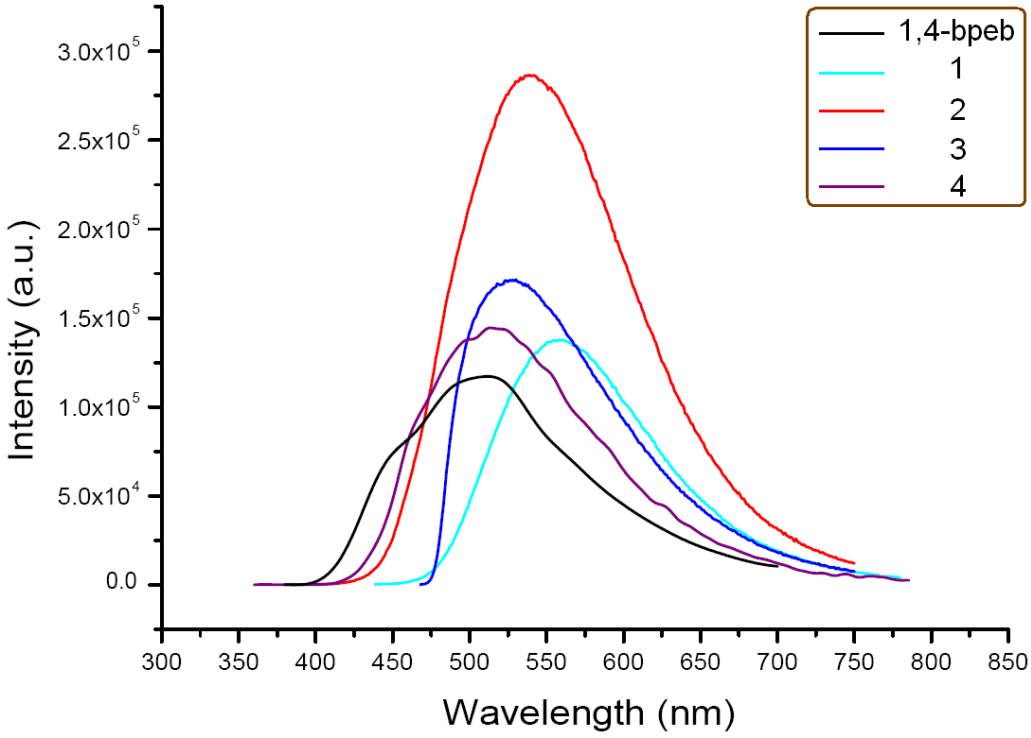


Fig. S5 Emission spectra of **1**–**4** in the solid state at ambient temperature.

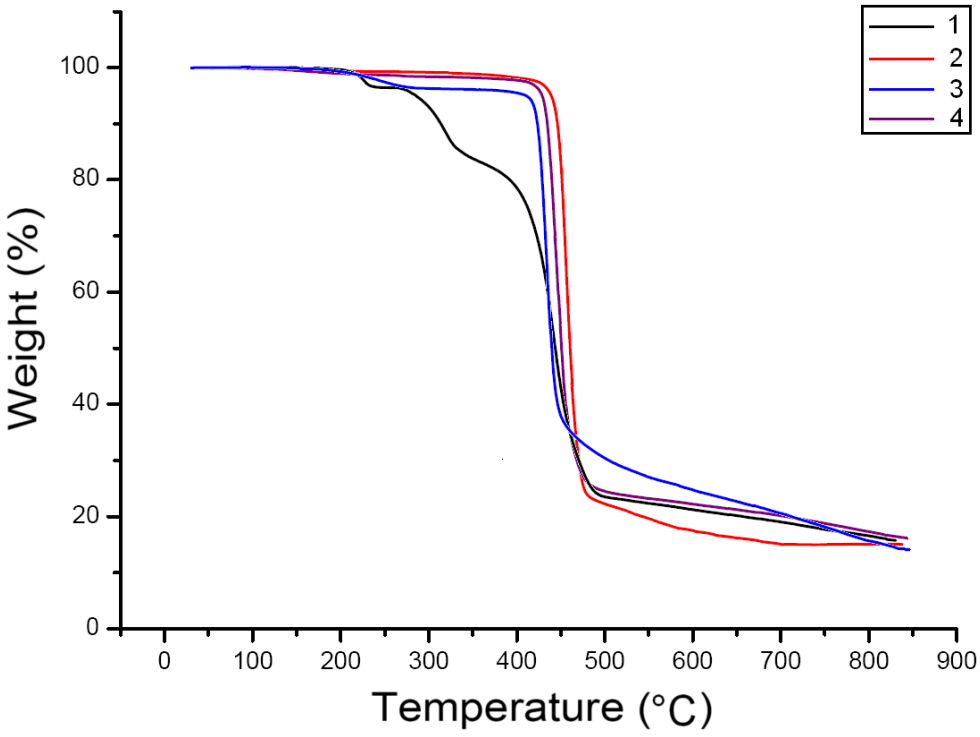


Fig. S6 The TGA curves for **1** (black), **2** (red), **3** (blue) and **4** (purple).

The thermal properties of **1**-**4** were described as follows. The thermogravimetric analyses revealed that **1**-**4** were stable up to 202 °C (**1**), 415°C (**2**), 193°C (**3**), and 400 °C (**4**) (Fig. S5†). For **1** and **3**, the first weight loss of 3.56% from 202 to 258 °C (**1**) or 3.51% from 193 to 265 °C (**3**) corresponds roughly to the loss of one coordinated water molecule per formula unit in **1** (calculated 3.29%) or two one-half of the uncoordinated water molecules per formula unit in **3** (calculated 3.12%). The second weight loss of 81.30% from 258 to 820 °C (**1**) or 82.62% from 265 to 830 °C (**3**) approximately amounts to the loss of all 1,4-bpeb and 5-HO-1,3-BDC or 5-NO_2-1,3-BDC ligands (calculated 81.85% for **1** and 82.77% for **3**). For **2** and **4**, only one weight loss of 85.38% from 415 to 820 °C (**2**) or 84.69% from 400 to 820 °C (**4**) amounts roughly to the loss of 1,4-bpeb and H_3BTC or 5-Me-1,3-BDC ligands (calculated 85.41% for **2** and 84.58% for **4**). In all cases, the decomposition residue species, according to X-ray fluorescence analysis, was asuumed to be ZnO (15.14% *vs* calculated 14.86% (**1**), 14.62% *vs* calculated 14.59% (**2**), 13.87% *vs* calculated 14.11% (**3**), and 15.31% *vs* calculated 15.42% (**4**)).