[Supplementary Information]

A novel metal-organic framework with the diamondoid topology constructed from pentanuclear zinc-carboxylate clusters

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Figure S1. Thermal ellipsoid plot (50 %) showing an asymmetric unit of 1. Selected bond lengths [Å] and angles [°]: Zn(1)-O(9) 1.990(3), Zn(2)-O(1) 2.085(3), Zn(2)-O(3) 2.116(3), Zn(2)-O(9) 2.072(3), Zn(2)-O(10) 2.088(4), Zn(2)-O(11) 2.073(4), Zn(3)-O(2) 1.965(3), Zn(3)-O(4) 1.981(4), Zn(3)-O(9) 2.016(3); O(10)-Zn(2)-O(9) 89.34(16), O(10)-Zn(2)-O(11) 89.10(17), O(9)-Zn(2)-O(11) 178.04(13), O(10)-Zn(2)-O(1) 179.19(16), O(9)-Zn(2)-O(1) 90.75(12), O(11)-Zn(2)-O(1) 90.81(13), O(10)-Zn(2)-O(3) 85.88(16), O(9)-Zn(2)-O(3) 92.46(13), O(11)-Zn(2)-O(3) 86.23(14), O(1)-Zn(2)-O(3) 94.93(12), O(2)-Zn(3)-O(4) 108.66(14), O(2)-Zn(3)-O(9) 104.94(12), O(4)-Zn(3)-O(9) 101.61(13).
Figure S2. IR spectrum of the polymer 1. FT-IR (KBr): $\tilde{\nu} = 3388$ (s), 1658 (s), 1581 (s), 1531 (s), 1400 (s), 1178 (w), 1103 (m), 1007 (w), 850 (m), 768 (s), 685 (m), 578 (w), 538 (w), 469 (w) cm$^{-1}$.
Figure S3. Powder XRD patterns of the polymer 1: (a) simulated, (b) experimental and (c) exchanged with CH$_2$Cl$_2$ for 24 h and then calcinated at 60 °C for 1 h.
Figure S4. The thermogravimetric analysis (TGA) curve of 1 in air. The TGA curve for 1 shows that the weight loss of 22.11 % during the first step between 35 and 115 °C corresponds to the loss of five guest H\textsubscript{2}O, three guest EtOH and three guest DMF (calculated 22.31 %), and the weight loss of 11.93 % during the second step between 150 and 270 °C corresponds to the loss of two coordinated EtOH and two coordinated DMF (calculated 11.88 %). Decomposition of 1 began above 270 °C. The residue was ZnO (experimental: 20.14 % and calculated: 20.29 %). Elemental analysis and ICP analysis for C\textsubscript{81}H\textsubscript{107}N\textsubscript{5}O\textsubscript{33}Zn\textsubscript{5} (2005.65): C 48.53, H 5.22, N 3.44, Zn 16.25 % (calcd: C 48.51, H 5.38, N 3.49, Zn 16.30 %).
**Figure S5.** The 3D frameworks of 1 viewed along the [001] direction. (DMF and EtOH groups have been omitted for clarity.)
Figure S6. N$_2$ adsorption isotherm for 1.