Electronic Supplementary Information

Solvent-free porous framework resulted from 3D entanglement of 1D zigzag coordination polymer

Goutam Kumar Kole,[a] Amy J. Cairns,[b] Mohamed Eddaoudi*[,b,c] and Jagadese J. Vittal*[,a]

[a]*Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore-117543. E-mail: chmjjv@nus.edu.sg; Fax: +65 6779 1691; Tel: +65 6516 2975*

[b]*Department of Chemistry, University of South Florida, 4202 East Fowler Avenue (CHE205), Tampa, Florida 33620*

[c]*Chemical and Life Sciences and Engineering Division, King Abdullah University of Science and Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia. Email: mohamed.eddaoudi@kaust.edu.sa*

Experimental section:

trans-4,4'-Stilbenedicarboxylic acid (H_2SDC) was synthesized *via* dehydro-dimerization reaction as reported in literature.[1] All other chemicals were purchased from various commercial sources and were used without further purification.

Thermogravimetric analyses (TGA) were carried out on a TA Instrument SDT 2960 TGA Thermal Analyzer. The samples were heated at a constant rate of 5°C min^{-1} from room temperature and the atmosphere was maintained with continuous flow of nitrogen. Elemental analyses were performed in the Micro-analytical Laboratory, Department of Chemistry, National University of Singapore. Powder X-ray diffraction (PXRD) patterns were obtained by using a D5005 Bruker X-ray diffractometer equipped with Cu Kα radiation (λ = 1.5410 Å). The accelerating voltage and current were 40 KV and 40 mA respectively.

Low Pressure Gas Sorption Measurements: Volumetric gas sorption studies were conducted at the University of South Florida (USF) on a fully automated micropore gas analyzer Autosorb-1 MP (Quantachrome Instruments) at relative pressures up to 1 atm. The cryogenic temperatures were controlled using liquid nitrogen and liquid argon at temperatures of 77 and 87K, respectively. All gases used were of 99.999 % purity. The as-synthesized sample was loaded (dry) into a 6-mm cell and evacuated at room temperature and 10^{-5} Torr for 24 h. The sample was subsequently evacuated at 100°C for 8 h, increasing at a rate of 1.0°C/min. The estimated BET and Langmuir surface areas were determined from the Ar adsorption at 87 K. The pore volume was determined by applying the Dubinin-

Radushkevich (D-R) equation. The isosteric heat of adsorption was calculated from the hydrogen sorption data at 77 and 87 K by applying the Clausius-Clapeyron equation.

X-ray crystallography:

Intensity data for **2** was collected on a Bruker APEX diffractometer attached with a CCD detector and graphite-monochromated MoKα (λ = 0.71073 Å) radiation. Empirical absorption corrections were applied with the data using the program SADABS[2] and the crystallographic package SHELXTL[3] was used for all calculations.

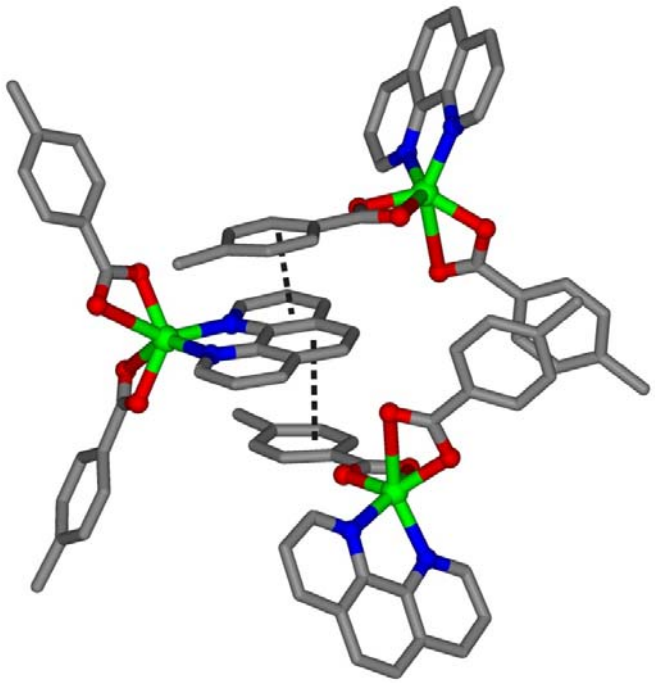

Fig. S1. Strong interchain π-π stacking interactions (distances are between 3.4 – 3.6 Å) that contribute for the robustness of framework.

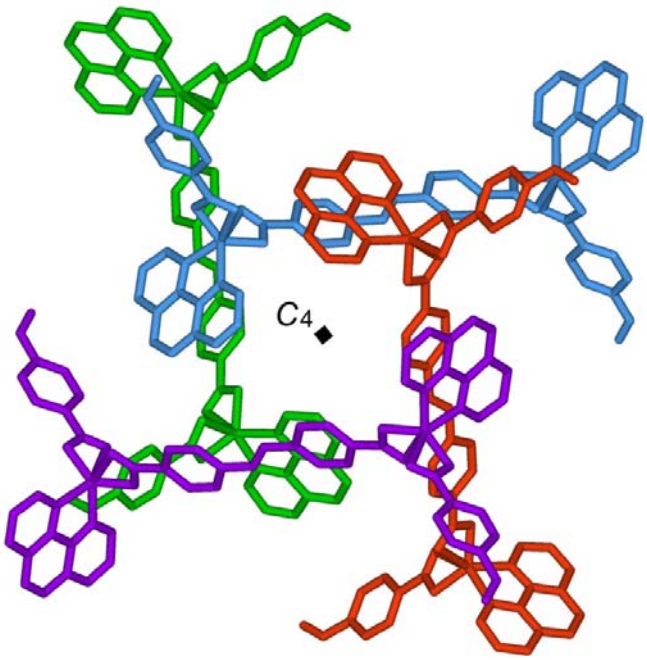

Fig. S2. 1D zigzag chains propagate in four non-coplanar directions around 4-fold axes.

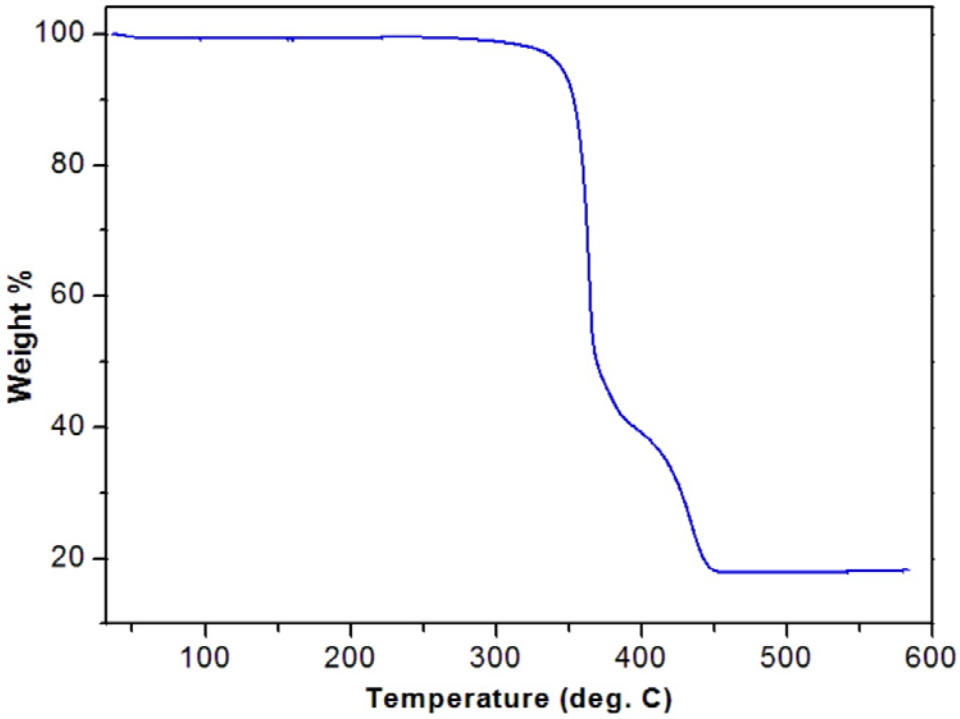

Fig. S3. Thermogravimetric analysis (TGA) of **2** shows no solvent loss.

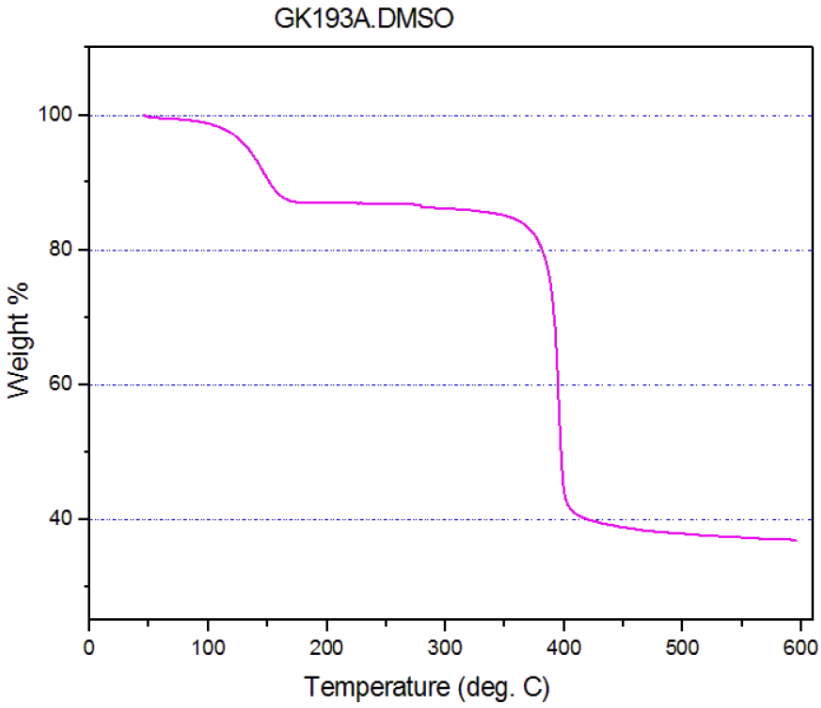

Fig. S4. TGA of **2**.DMSO. The composition $ZnC_{28}H_{18}N_2O_4.(C_2H_6SO)$ requires the weight loss 13.2%, found weight loss12.8%.

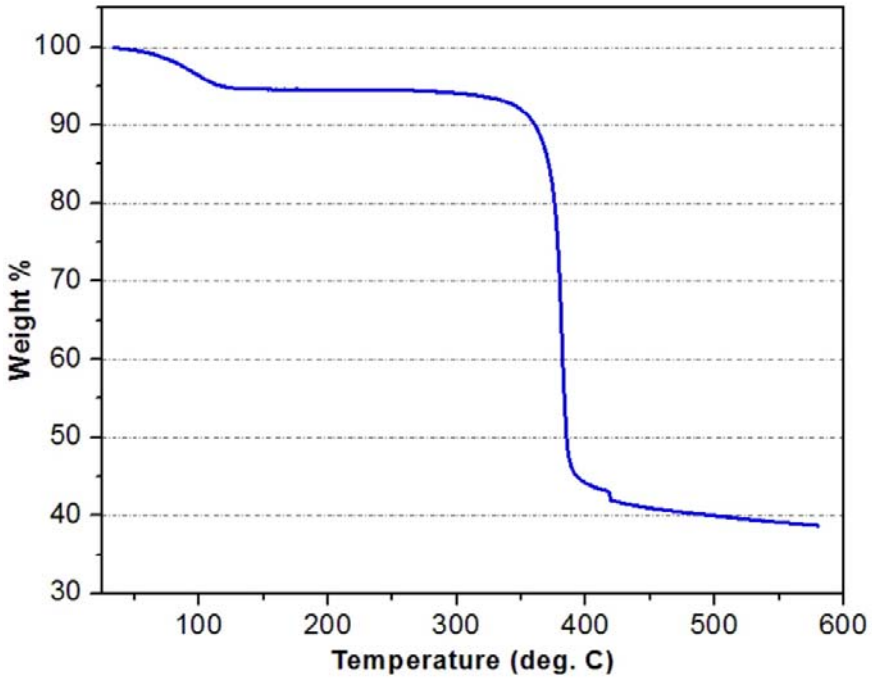

Fig. S5. TGA of **2**.DMF. The composition $ZnC_{28}H_{18}N_2O_4.\ 0.5(C_3H_7NO)$ requires the weight loss 6.6 %, found 5.4 %.

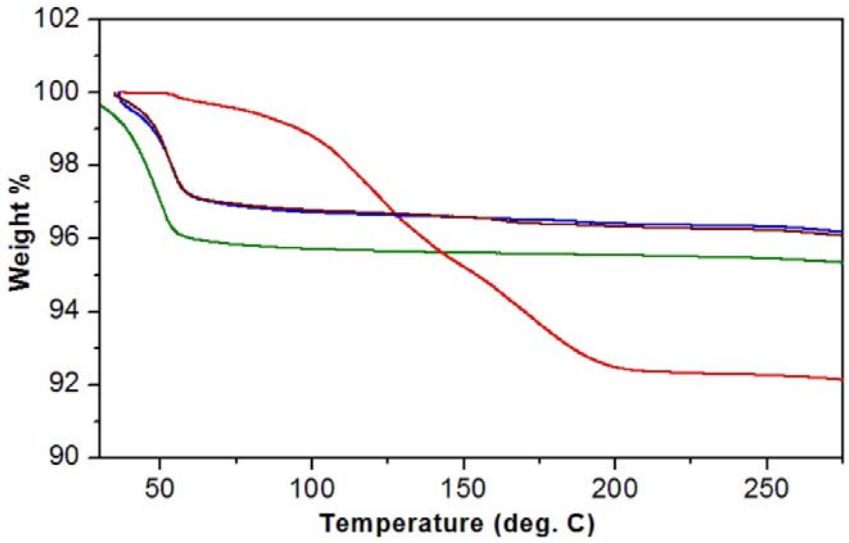

Fig. S6. TG analyses: **2**·cyclohexane - wine, **2**·benzene -blue, **2**·toluene - green, **2**·xylene - red. The respective observed weight losses of 3.0%, 2.8%, 4.1% and 7.4% can be formulated to 1.8 equivalents of each cyclohexane and benzene, 2.3 equivalent of toluene and 3.5 equivalent of xylene respectively.

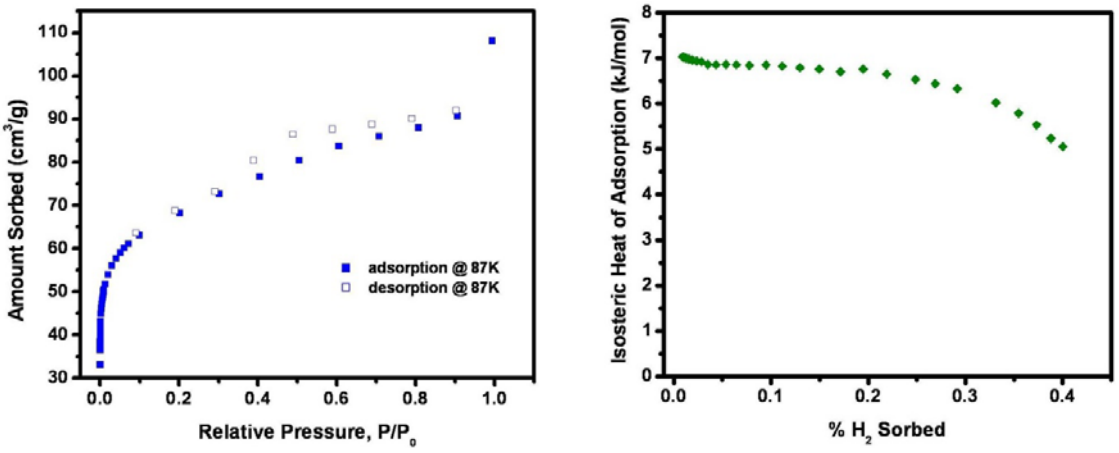

Fig. S7. (left) Argon sorption isotherm for **2** at 87 K and (right) Isosteric heat of adsorption for **2**.

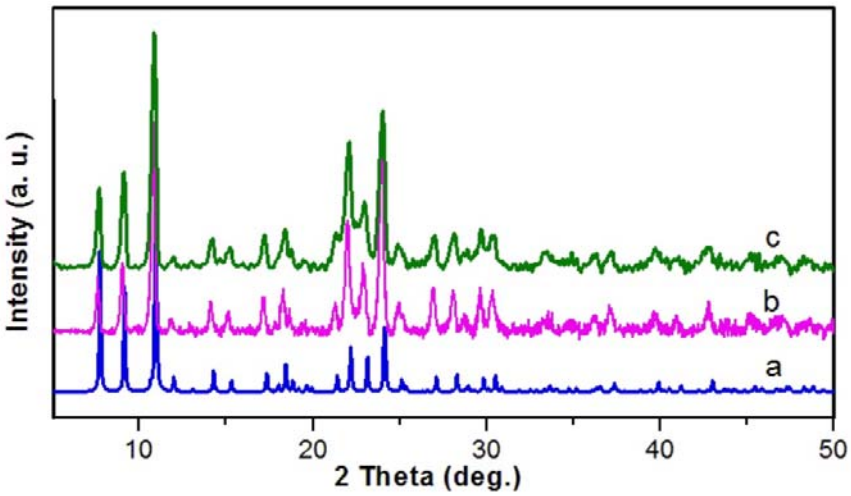

Fig. S8. PXRD patterns: (a) simulated pattern for **2**; (b) pattern observed for as-synthesized sample **2** (single crystal obtained from diffusion method); (c) pattern observed for **3** (powder sample obtained by mixing and stirring the reactants)

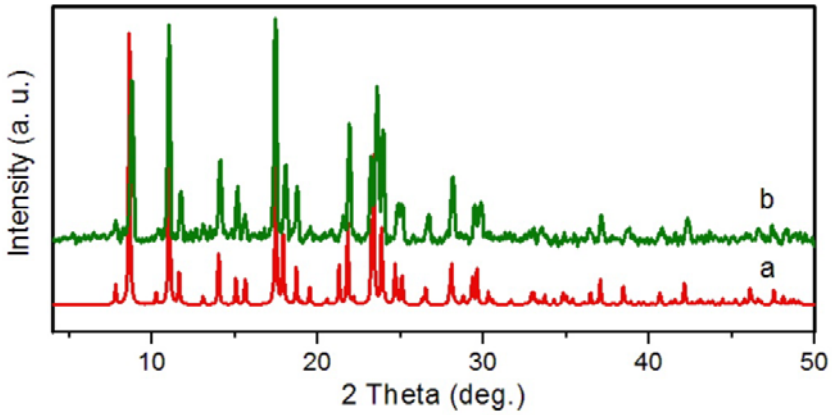

Fig. S9. PXRD patterns: (a) simulated pattern for **1**.DMSO and (b) pattern observed for the powder sample obtained by mixing and stirring the reactants in DMSO at room temperature

References:

1. W. G. Toland, J. Wilkes and F. J. Brutschy, *J. Am. Chem. Soc*., 1953, **75**, 2263; W. G. Toland, J. Wilkes and F. J. Brutschy, *J. Am. Chem. Soc*., 1954, **76**, 307.
2. G. M. Sheldrick, *SADABS, Program for Empirical Absorption Correction for Area Detector Data*; University of Göttingen: Göttingen, Germany, 2000.
3. SHELXTL References Manual, Version 5.1; Bruker AXS, Analytical X-ray Systems, Inc.: Madison, WI, **1997**.