Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information

Acid-base directed supramolecular isomers of isophthalate based MOFs for CO_2 adsorption and transformation

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Experiments and Instruments.

Ligand Synthesis: 20 mmol of 5-aminoisophthalic acid, 10 mmol of 1,4,5,8-naphthalenetetracarboxylate dianhydride and five drops of N,N-dimethylformamide were added to a mortar and ground together with a pestle before a purple powder was heated at 180 °C for four hours to achieve a similar yield of H_4L.[1]

MOF Synthesis: $Cu(NO_3)_2 \cdot 2.5H_2O$ (11.6 mg, 0.05 mmol) and H_4L (14.8 mg, 0.025 mmol) heated to 80 °C for up to 48 h. TFA was added from 5 to 40 μL to perform the acid controlled syntheses and pyridine (0.05 mmol) was added for the base controlled synthesis.

Measurements from 4000-400 cm^{-1} were taken on a Perkin Elmer FT-IR Spectrometer Spectrum Two (UATR Two) with 4 cm^{-1} resolution. TA Instruments TGA Q50 was used to record thermal gravimetric analysis (TGA) data from room temperature to 800 °C at a 10 °C/min rate. Gas adsorption measurements were performed using a Micromeritics ASAP 2020 surface area analyzer to collect N_2 (surface area measurement at 77 K) and CO_2 isotherms at 273 K and 298 K, using high purity gas. Powder X-ray diffraction (PXRD) data was collected at room temperature using a Bruker D8 Advance theta-2theta diffractometer with copper radiation (Cu Kα, λ = 1.5406 Å) operating at 40 kV and 40 mA and a secondary monochromator; whereby samples were measured between 3° and 25° at 0.5 second/step and step size of 0.01°.

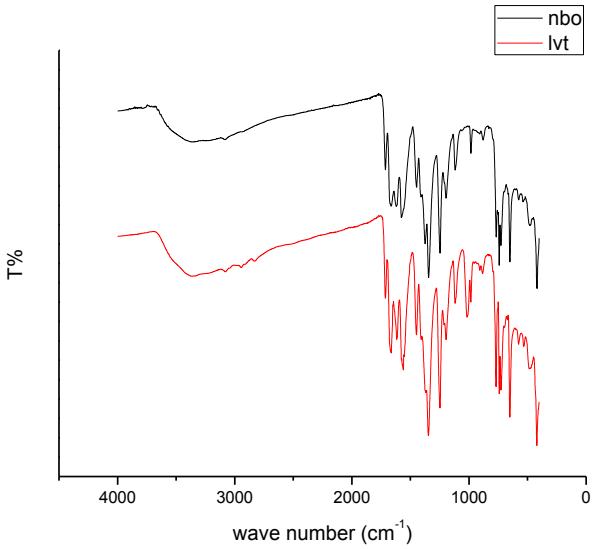

Fig. S1. Infrared spectra of $[Cu_2\mathbf{L}]_n$ **nbo** and **lvt**.

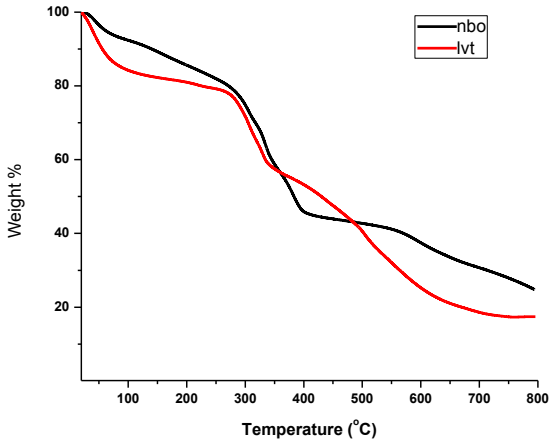

Fig. S2. TGA plots of $[Cu_2\mathbf{L}]_n$ **nbo** and **lvt**.

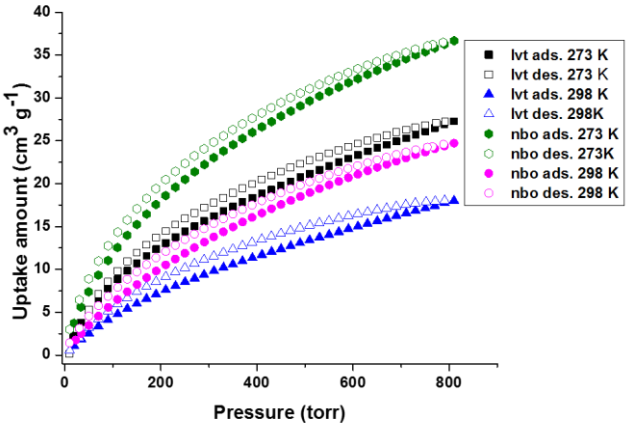

Fig. S3. CO_2 sorption isotherms for $[Cu_2\mathbf{L}]_n$ **nbo** and **lvt**.

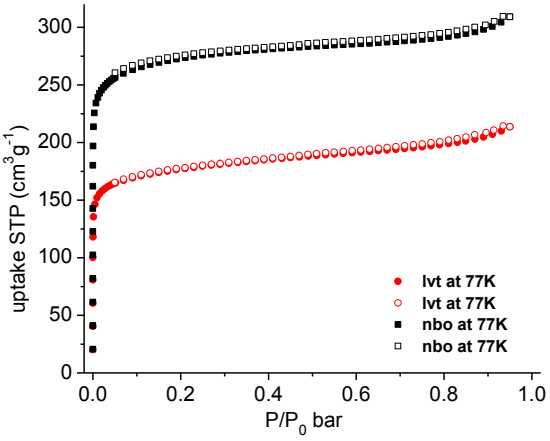

Fig. S4. N_2 sorption isotherms for for $[Cu_2\mathbf{L}]_n$ **nbo** and **lvt**.

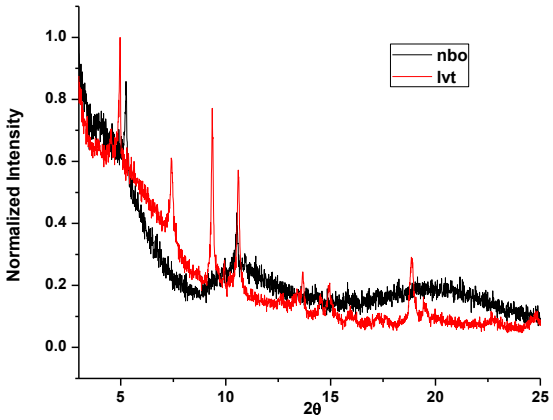

Fig. S5. PXRD patterns after catalyzing propylene oxide into propylene carbonate. High

background due to low loading (<5 mg) of MOF along with pipetted reagents.

Reference:

1. J. A. Perman, A. J. Cairns, L. Wojtas, M. Eddaoudi and M. J. Zaworotko, CrystEngComm, 2011, 13, 3130