Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

Carbon Dioxide Capture in the Presence of Water Vapour in InOF-1

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1. Representation of the binuclear [$In_2(\mu_2$-OH)] building block

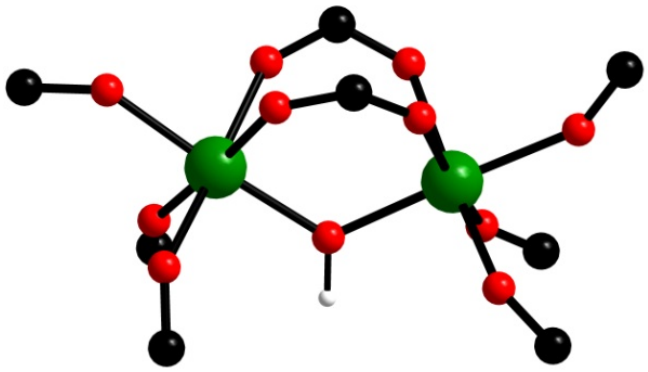

Fig. S1: Binuclear building block of two metal ions oxygen octahedra bridged by a μ_2-hydroxo group. Green, red, black and white spheres represent In(III), O, C and H atoms, respectively.

2. Materials and Measurements

All reagents and solvents were used as received from commercial suppliers without further purification. Powder X-ray diffraction (PXRD) data were collected under ambient conditions on a Bruker AXD D8 Advance diffractometer operated at 160 W (40 kV, 40 mA) for Cu $K\alpha_1$ (λ= 1.5406 Å). Thermal gravimetric analysis (TGA) was performed under N_2 at a scan rate of 2 °C/min using a TA Instruments Q500HR analyser. N_2 adsorption was carried out in a conventional volumetric technique by a Micromeritics ASAP 2020 sorptometer. The surface area was calculated using the BET method based on adsorption data in the partial pressure (p/p_0) range 0.01 to 0.04. Dynamic and isothermal experiments were performed using a humidity-controlled thermobalance (TA Instruments, model Q5000SA) at 30 ^{o}C and a relative humidity (RH) of 40%.

3. TGA plot

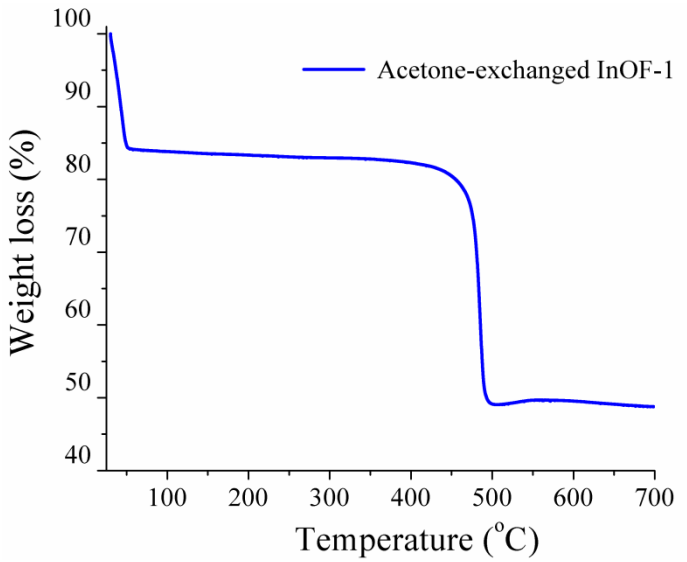

Fig. S2: TGA analysis of acetone-exchanged InOF-1 (blue line).

4. Powder X-ray Diffraction Patterns

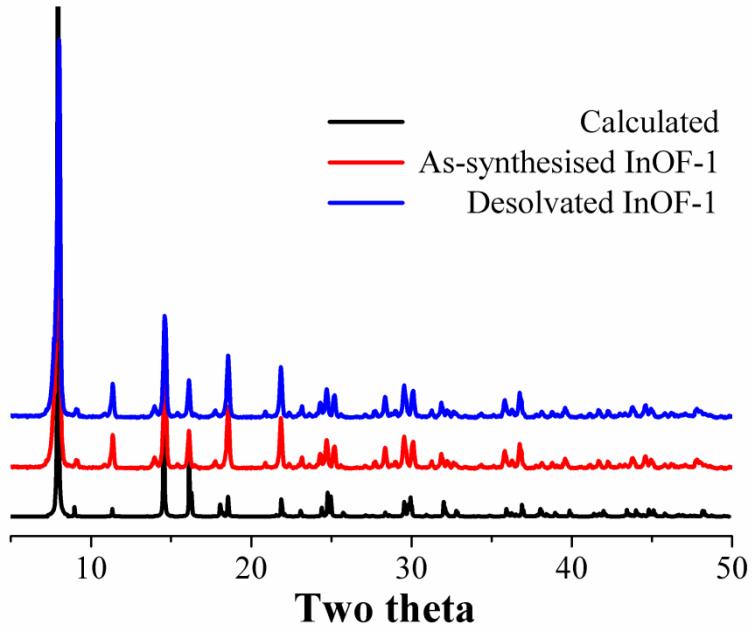

Fig. S3: PXRD patters of calculated (black), as-synthesised (red) and desolvated (blue) of InOF-1.

5. Kinetic Isotherms

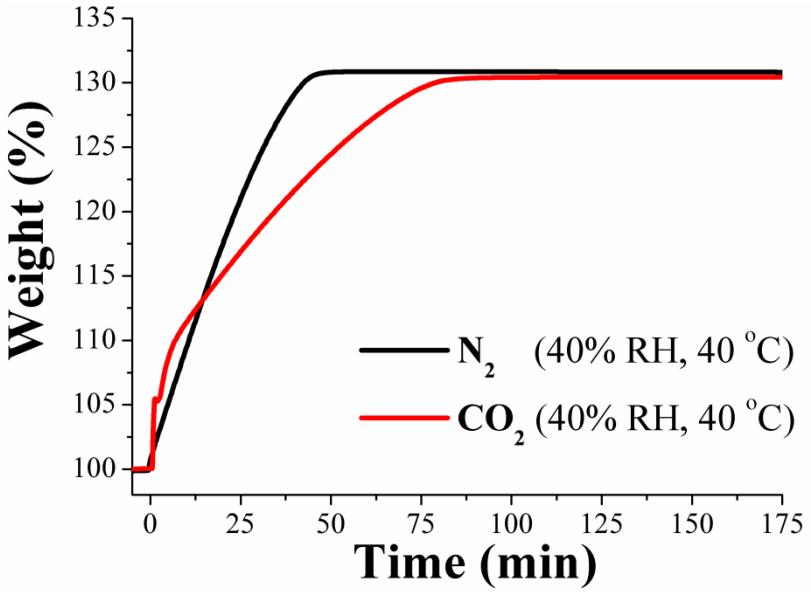

Fig. S4: Kinetic uptake experiments carried out at 40 °C and 40% RH with CO_2 (red line) and N_2 (black line) flows of 60 mL/min, respectively.

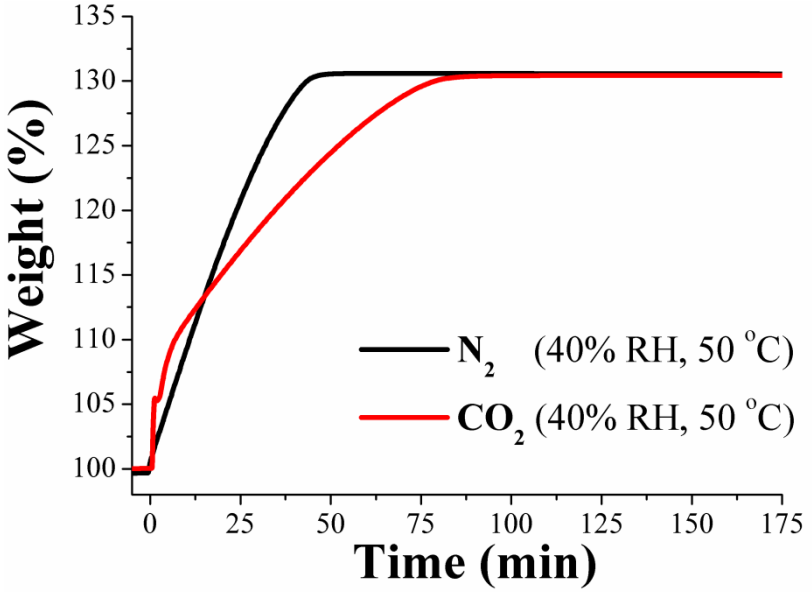

Fig. S5: Kinetic uptake experiments carried out at 50 °C and 40% RH with CO_2 (red line) and N_2 (black line) flows of 60 mL/min, respectively.

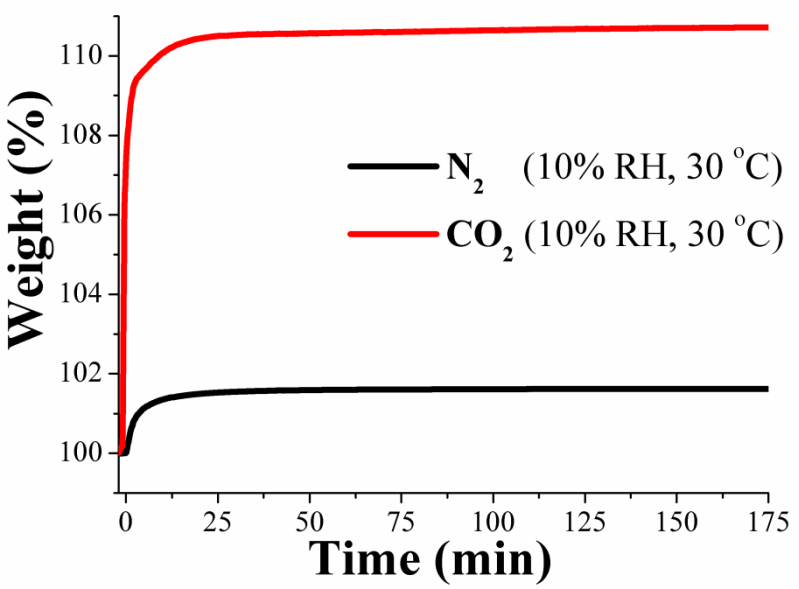

Fig. S6: Kinetic uptake experiments carried out at 30 °C and 10% RH with CO_2 (red line) and N_2 (black line) flows of 60 mL/min, respectively.

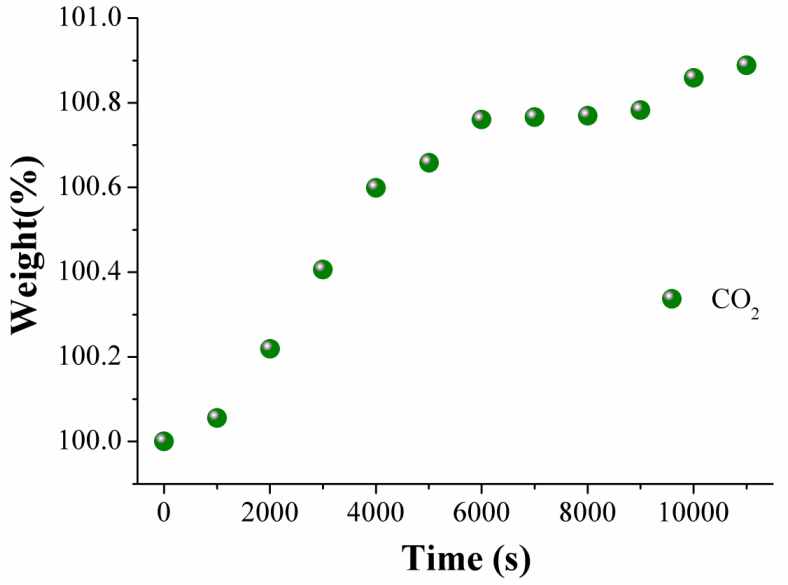

Fig. S7: Kinetic uptake experiments carried out at 30 °C and 20% RH with a CO_2 flow of 60 mL/min in PCM-14.

6. Cycle Stability

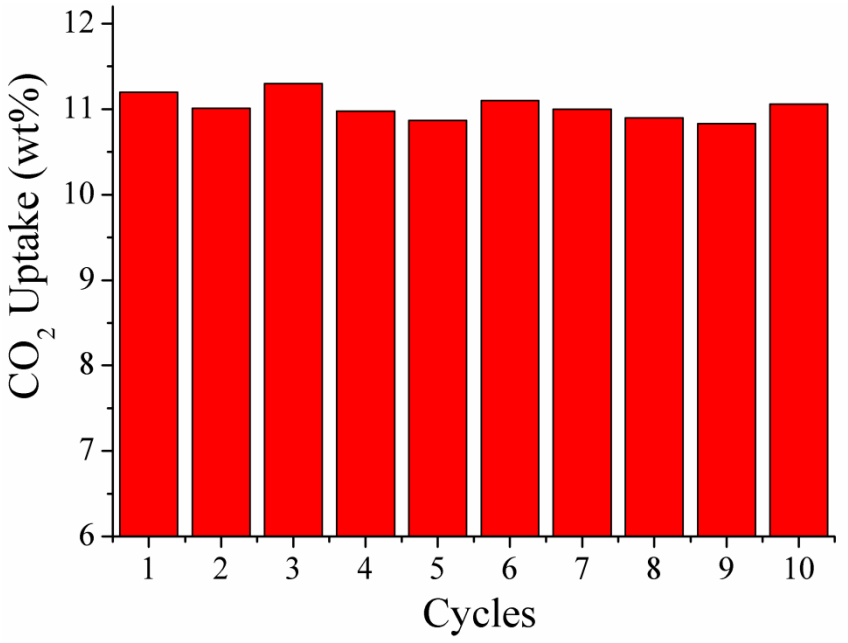

Fig. S8: Cycle Stability of the material InOF-1.

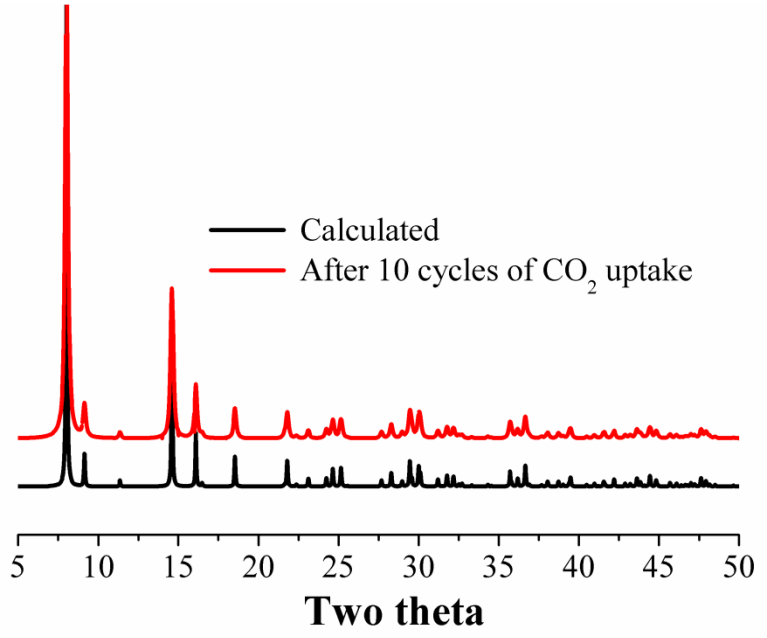

Fig. S9: Calculated PXRD pattern of InOF-1 and PXRD pattern of InOF-1 after the 10 cycles of CO_2 capture.