Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.


# Electronic Supplementary Information

## Water Adsorption Properties of a Sc(III) Porous Coordination Polymer for $CO_2$ Capture Applications

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## 1. Representation of the binuclear [$Sc_2(\mu_2$-OH)] building block

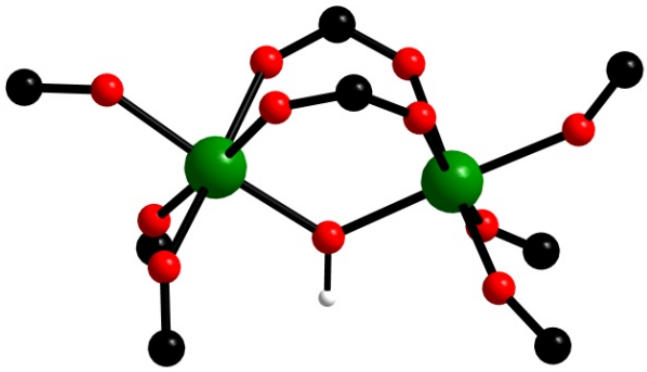

**Figure S1**: Binuclear building block of two metal ions oxygen octahedra bridged by a $\mu_2$-hydroxo group. Green, red, black and white spheres represent Sc(III), O, C and H atoms, respectively.

## 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 $K\alpha_1$ ($\lambda$= 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 $^oC$ and different relative humidities (RH).

## 3. TGA plot

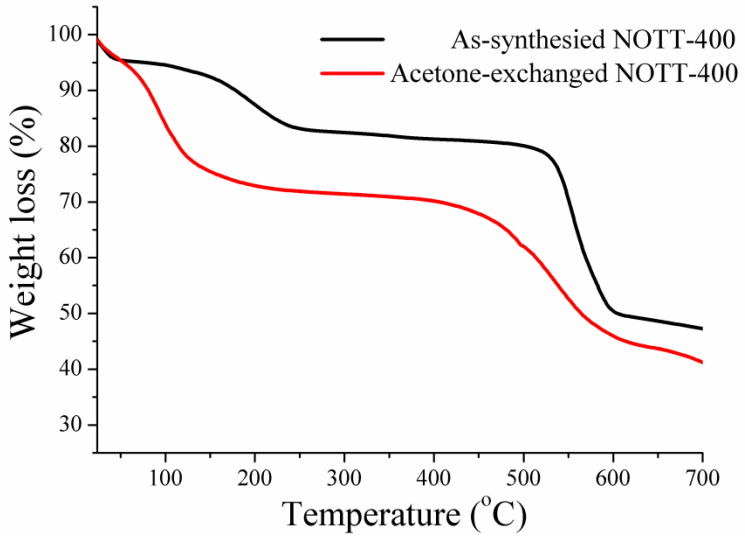


**Figure S2**: TGA analyses of as-synthesised NOTT-400 (black line) and acetone-exchanged NOTT-400 (red line).

## 4. Powder X-ray Diffraction Patterns

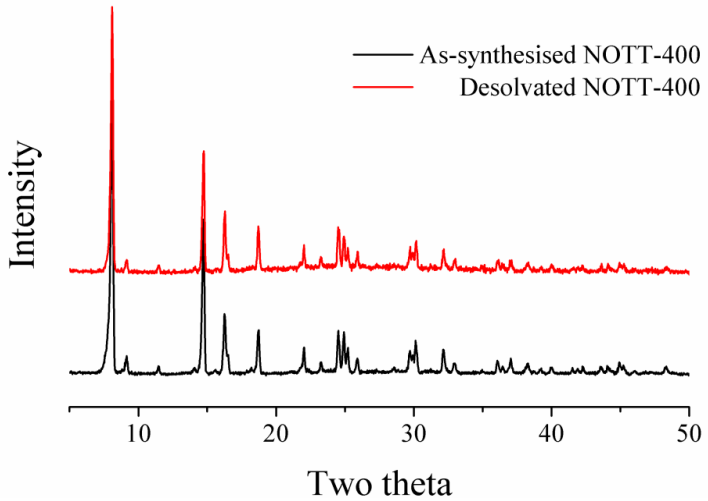


**Figure S3**: PXRD patters of as-synthesised (black) and desolvated (red) NOTT-400.

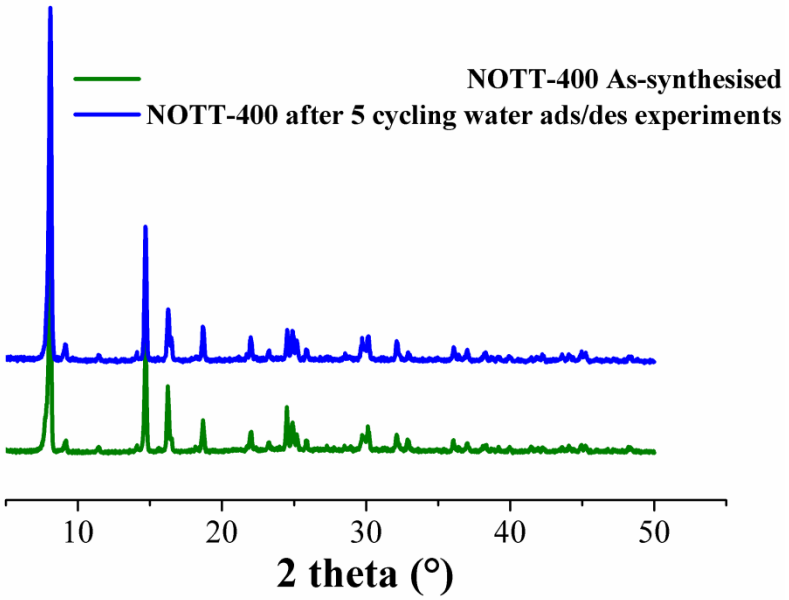


**Figure S4**: PXRD patters of as-synthesised (green) and after five cycling water adsorption/desorption experiments (blue) of NOTT-400.

## 5. Calculation of the hydroxo functional groups ($\mu_2$-OH) and the water molecules adsorbed per unit cell

| | | |
|---|---|---|
| Po | 4256.3854 | Pa |
| $m_{ref}$ | 22.9705 | mg |
| $sc2(C_{16}H_8O_8)(OH)_2$ | 450.1418 | g/mol |
| MW $H_2O$ | 18.015 | g/mol |
| Z | 4 | |
| OH/cell | 8 | |

$$\frac{Molecules}{Cell} = \frac{n_{H_2O}}{n_{cell}} = \frac{\frac{m_{H_2O}}{MW_{H_2O}}}{\frac{\overline{m}_s}{Z\,MW_m}} = \frac{m_{H_2O}}{\overline{m}_s}\frac{Z\,MW_m}{MW_{H_2O}}$$

| Target, % P/Po | Change In Mass (%) - ref | p, Pa | m, mg | molec/cell | |
|---|---|---|---|---|---|
| 0 | 0 | 0 | 22.9705 | 0 | 8 |
| 5 | 0.38 | 21281.927 | 23.0577879 | 0.37980324 | 8 |
| 10 | 0.67 | 42563.854 | 23.1244024 | 0.66965308 | 8 |
| 15 | 1.01 | 63845.781 | 23.2025021 | 1.00947703 | 8 |
| 20 | 1.47 | 85127.708 | 23.3081664 | 1.46923885 | 8 |
| 25 | 2.2 | 106409.635 | 23.475851 | 2.19886086 | 8 |
| 30 | 4.32 | 127691.562 | 23.9628256 | 4.31776314 | 8 |
| 32 | 6.64 | 136204.333 | 24.4957412 | 6.63656187 | 8 |
| 34 | 10.95 | 144717.104 | 25.4857698 | 10.9443302 | 8 |
| 36 | 18.57 | 153229.874 | 27.2361219 | 18.5603846 | 8 |
| 38 | 28.67 | 161742.645 | 29.5561424 | 28.6551549 | 8 |
| 40 | 36.57 | 170255.416 | 31.3708119 | 36.5510644 | 8 |
| 42 | 37.33 | 178768.187 | 31.5453877 | 37.3106709 | 8 |
| 44 | 37.59 | 187280.958 | 31.605111 | 37.5705362 | 8 |
| 46 | 37.85 | 195793.728 | 31.6648343 | 37.8304016 | 8 |
| 48 | 38.1 | 204306.499 | 31.7222605 | 38.0802722 | 8 |
| 50 | 38.32 | 212819.27 | 31.7727956 | 38.3001583 | 8 |
| 55 | 39.01 | 234101.197 | 31.9312921 | 38.989801 | 8 |
| 60 | 39.89 | 255383.124 | 32.1334325 | 39.8693453 | 8 |
| 65 | 40.75 | 276665.051 | 32.3309788 | 40.7289 | 8 |
| 70 | 41.54 | 297946.978 | 32.5124457 | 41.518491 | 8 |
| 75 | 42.44 | 319228.905 | 32.7191802 | 42.418025 | 8 |
| 80 | 43.36 | 340510.832 | 32.9305088 | 43.3375486 | 8 |
| 90 | 44.93 | 383074.686 | 33.2911457 | 44.9067357 | 8 |

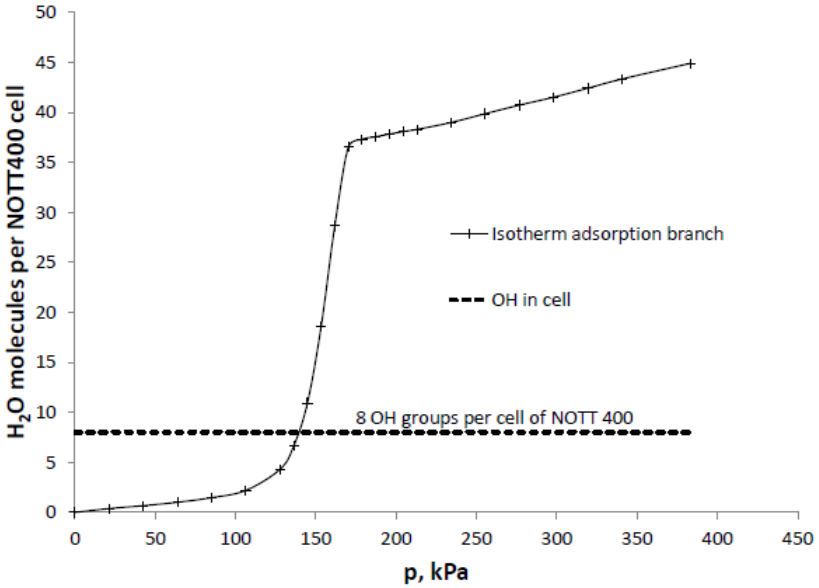


**Figure S5**: Water molecules per NOTT-400 cell *vs* water pressure.

## 6. Kinetic Isotherms

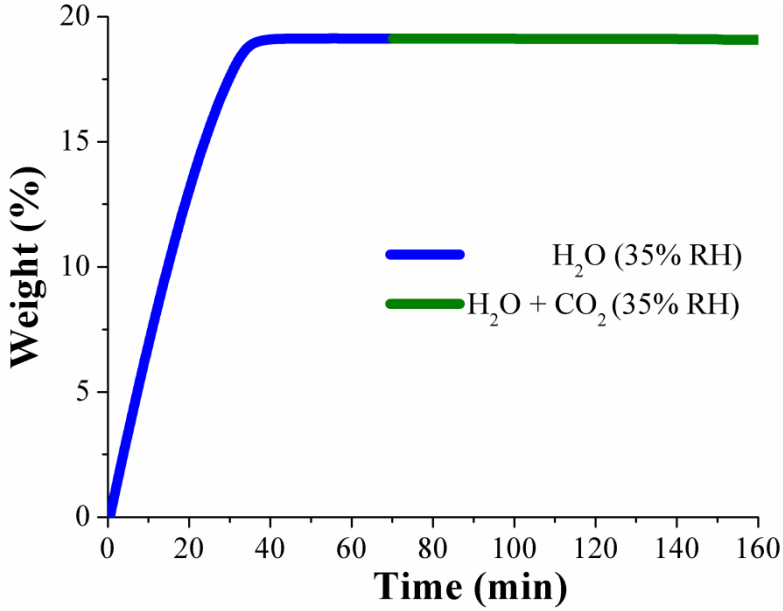


**Figure S6**: Kinetic uptake experiments carried out at 30 $^{o}$C and 35% RH with $H_2O$ (blue line) and $H_2O$+$CO_2$ (green line).

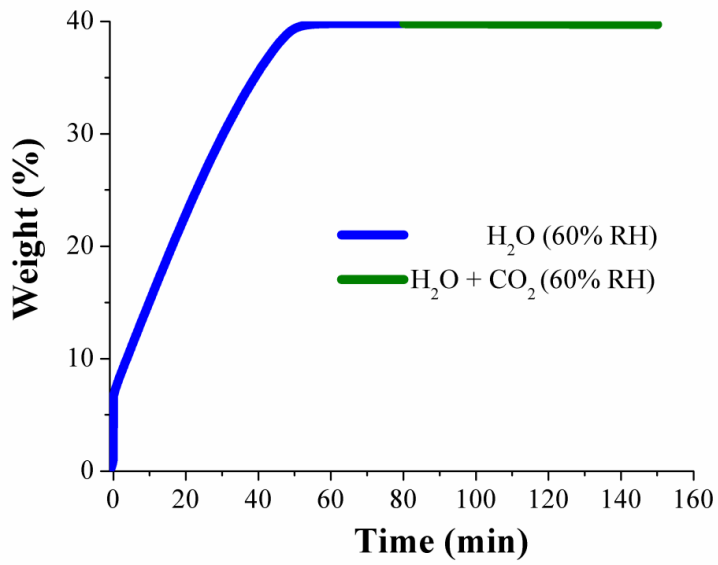


**Figure S7**: Kinetic uptake experiments carried out at 30 °C and 60% RH with $H_2O$ (blue line) and $H_2O$+$CO_2$ (green line).

## 7. Static and isothermal adsorption experiments on NOTT-400

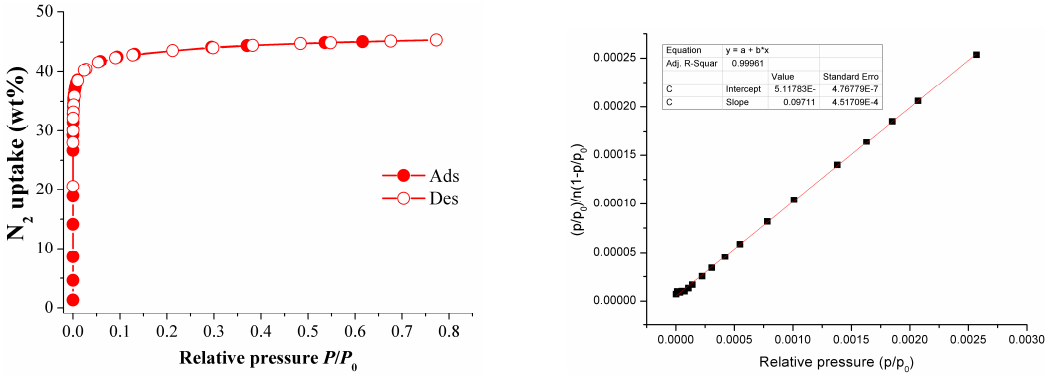


**Fig. S8**: left) Static $N_2$ isotherm carried out at 30 °C in NOTT-400; right) BET plot.

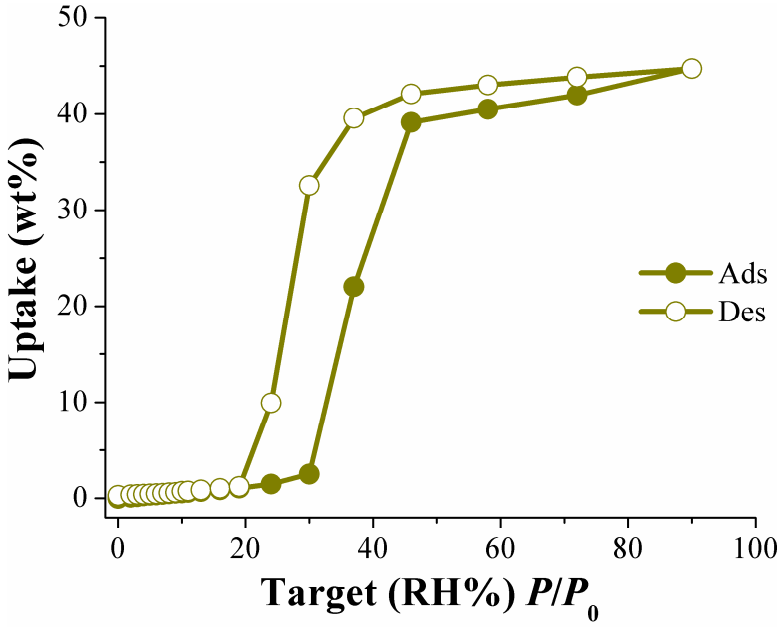


**Fig. S9**: Static $H_2O$ isotherm carried out at 20 °C in NOTT-400.

## Enthalpy for $H_2O$ adsorption

| | | |
|---|---|---|
| | kJ/mol | |
| Adsorption | **-46.815** | |
| Isosteric enthalpy of adsorption is calculated via a Clausius-Clapeyron-type equation | $(\partial \ln p/\partial T)_\theta = -\Delta H_s/RT^2$ | |
| | θ= vapour surface coverage<br>ΔHs = enthalpy of adsorption | |
| we obtain the values with | ΔHs =-R [ln (p2/p1) / (1/T2)-(1/T1)] | |

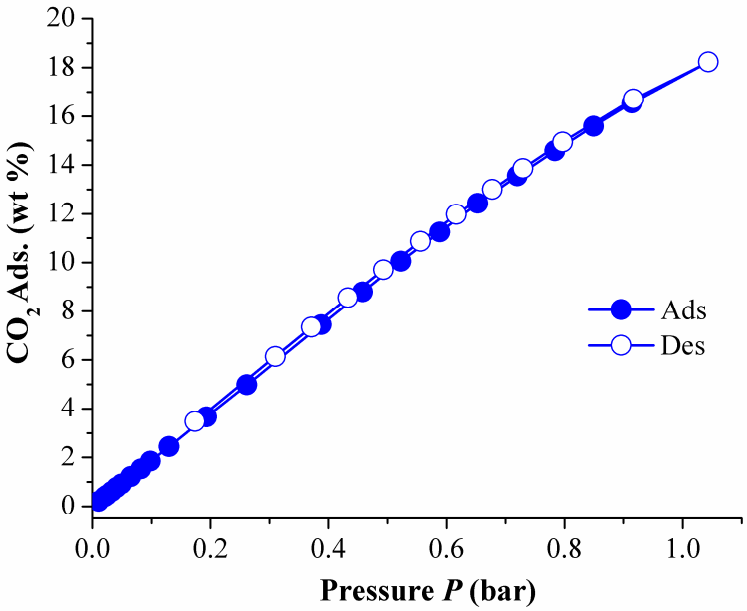


**Fig. S10**: Static $CO_2$ isotherm carried out at 30 $^{o}$C in NOTT-400.