

Electronic Supplementary Information

Water Adsorption Properties of NOTT-401 and CO₂ Capture under Humid Conditions

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1. Representation of the binuclear $[\text{Sc}_2(\mu_2\text{-OH})]$ building block

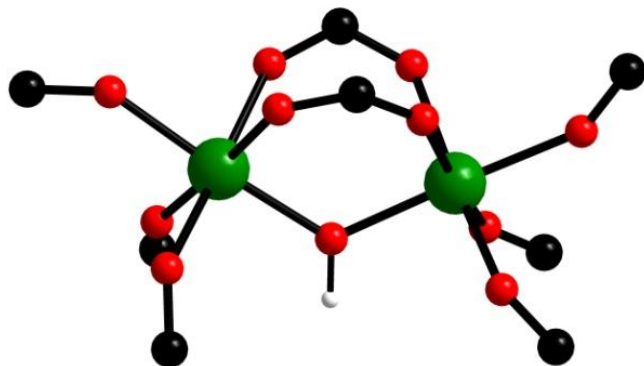
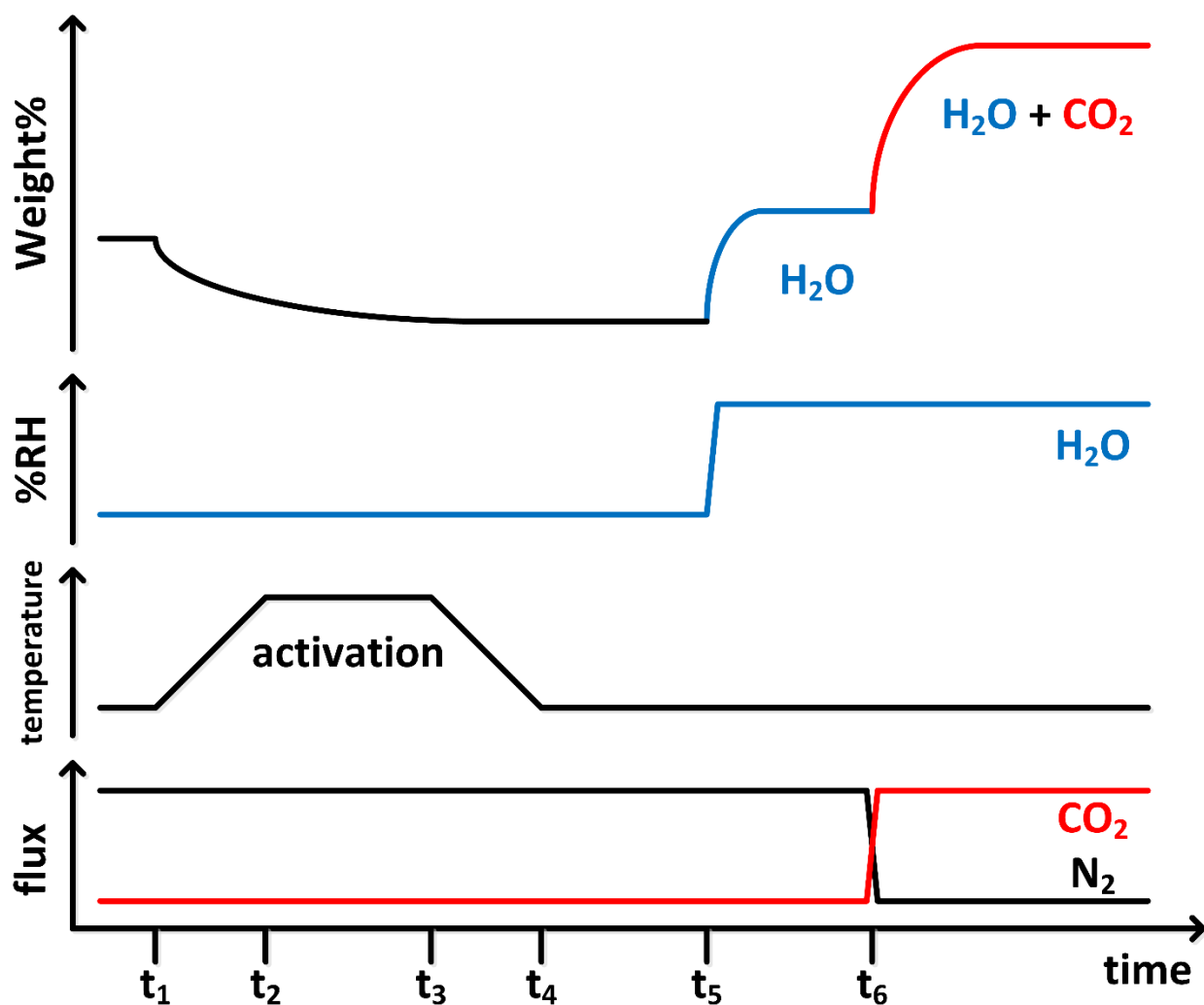


Figure S1: Binuclear building block of two metal ions oxygen octahedra bridged by a μ_2 -hydroxo group. Green, red, black and white spheres represent Sc(III), O, C and H atoms, respectively.

2. Measurements



Scheme S1. Experimental variables diagram over the time for the CO_2 capture experiment. First the sample activation step at 180 °C under N_2 atmosphere (t_1 to t_3), then a stabilization step at 30 °C (t_4), after relative humidity setting (t_5), and capture of CO_2 under controlled humidity (t_6).

3. TGA plot

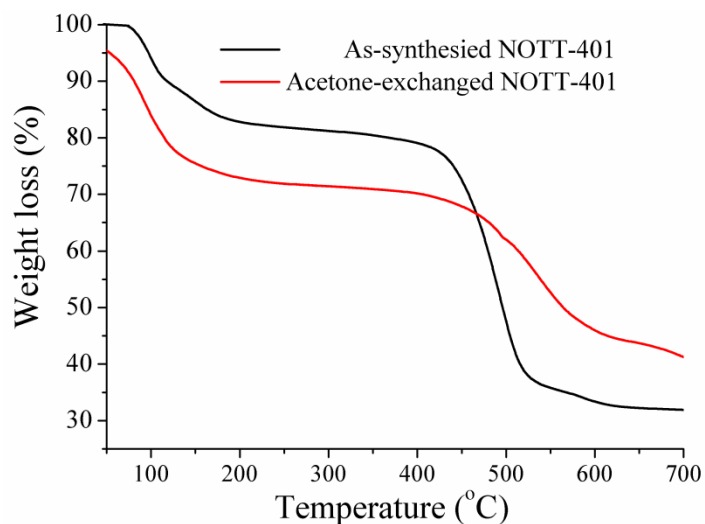


Figure S2: TGA analyses of as-synthesised NOTT-401 (black line) and acetone-exchanged NOTT-401 (red line).

4. Powder X-ray Diffraction Patterns

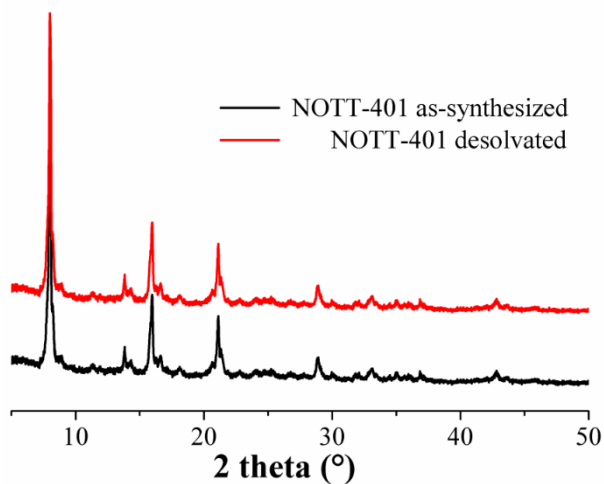


Figure S3: PXRD patterns of as-synthesised (black) and desolvated (red) NOTT-401.

5. Static and isothermal adsorption experiments on NOTT-401

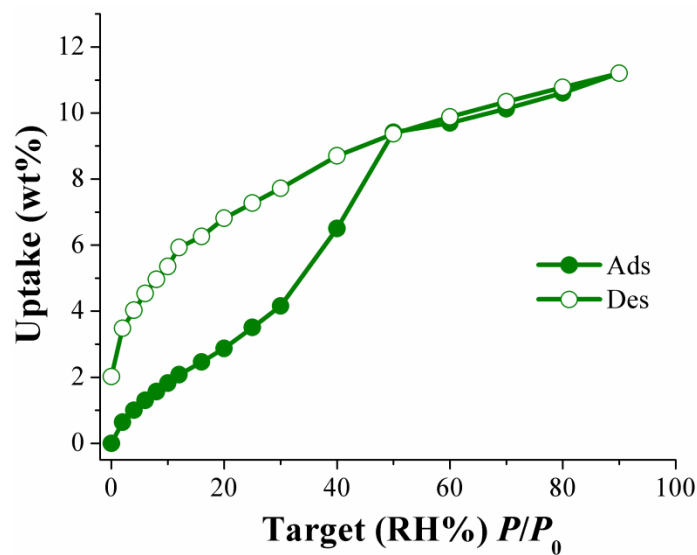


Figure S4: Static H₂O isotherm carried out at 20 °C in NOTT-401.

Enthalpy for H₂O adsorption

| | |
|---|---|
| Adsorption | kJ/mol -60.705 |
| 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 ΔH_s = enthalpy of adsorption |
| we obtain the values with | $\Delta H_s = -R [\ln (p_2/p_1) / (1/T_2) - (1/T_1)]$ |

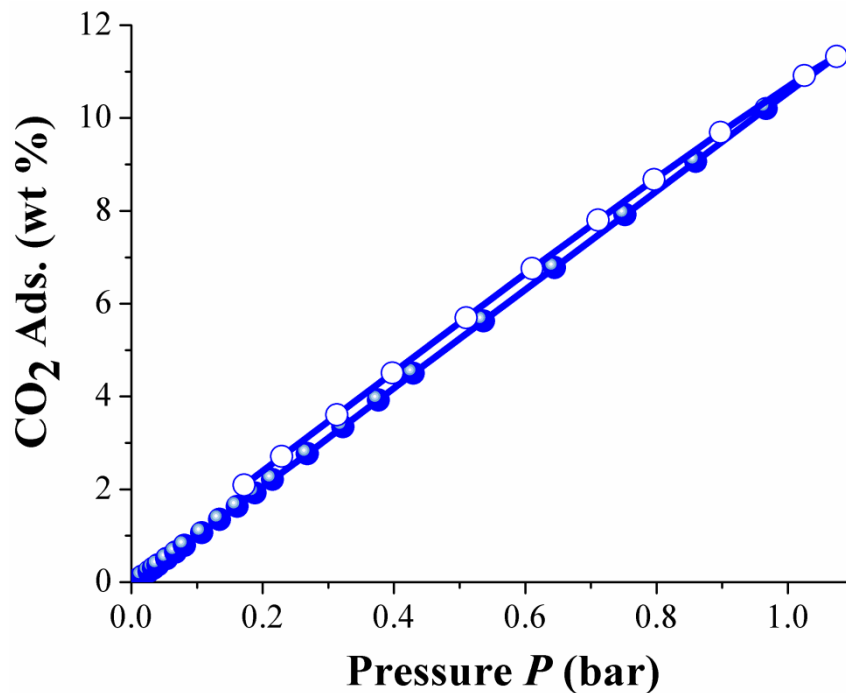


Figure S5: Static CO₂ isotherm carried out at 30 °C and 1 bar in NOTT-401.

6. Calculation of the hydroxo functional groups (μ_2 -OH) and the water molecules adsorbed per unit cell

Adsorbent selectivity for component (1) was estimated by¹:

$$\alpha_{12} = \frac{K_1}{K_2}$$

Where K_i is the Henry's constant. The selectivity error was estimated by:

$$\delta\alpha_{12} = \frac{\delta K_1}{K_2} - \frac{K_1 \delta K_2}{K_2^2}$$

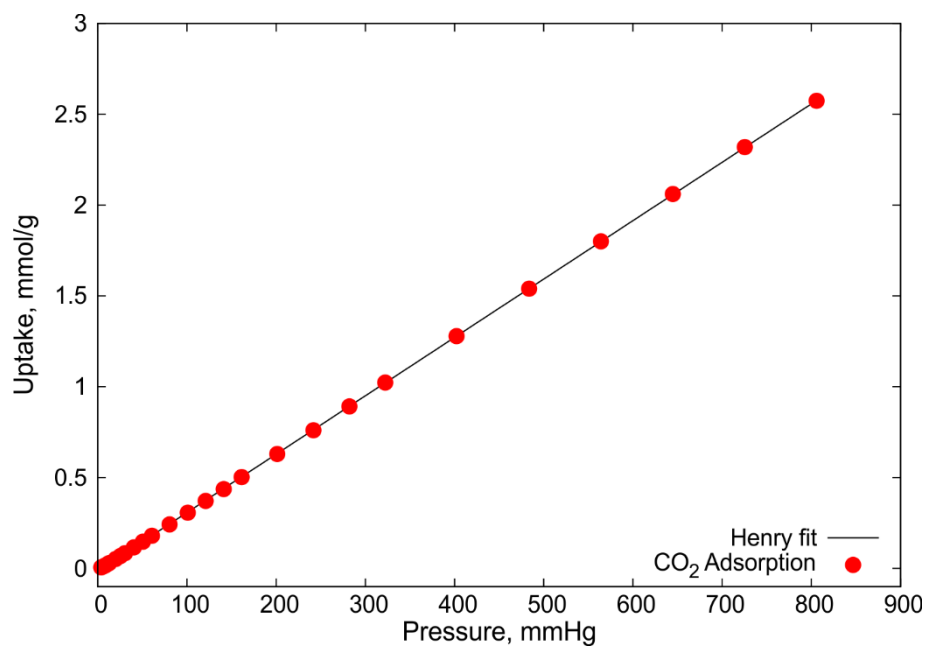


Figure S6: Experimental CO₂ isotherm at 30°C in NOTT401 and Henry's law fitted to it.

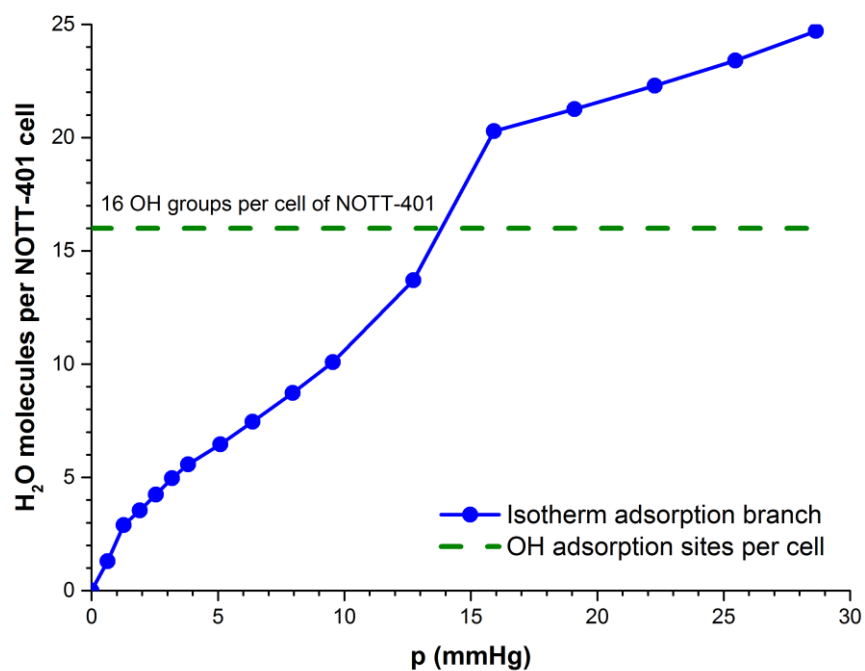


Figure S7: Representation of the water adsorption isotherm per number of H₂O molecules in a cell of NOTT-401.

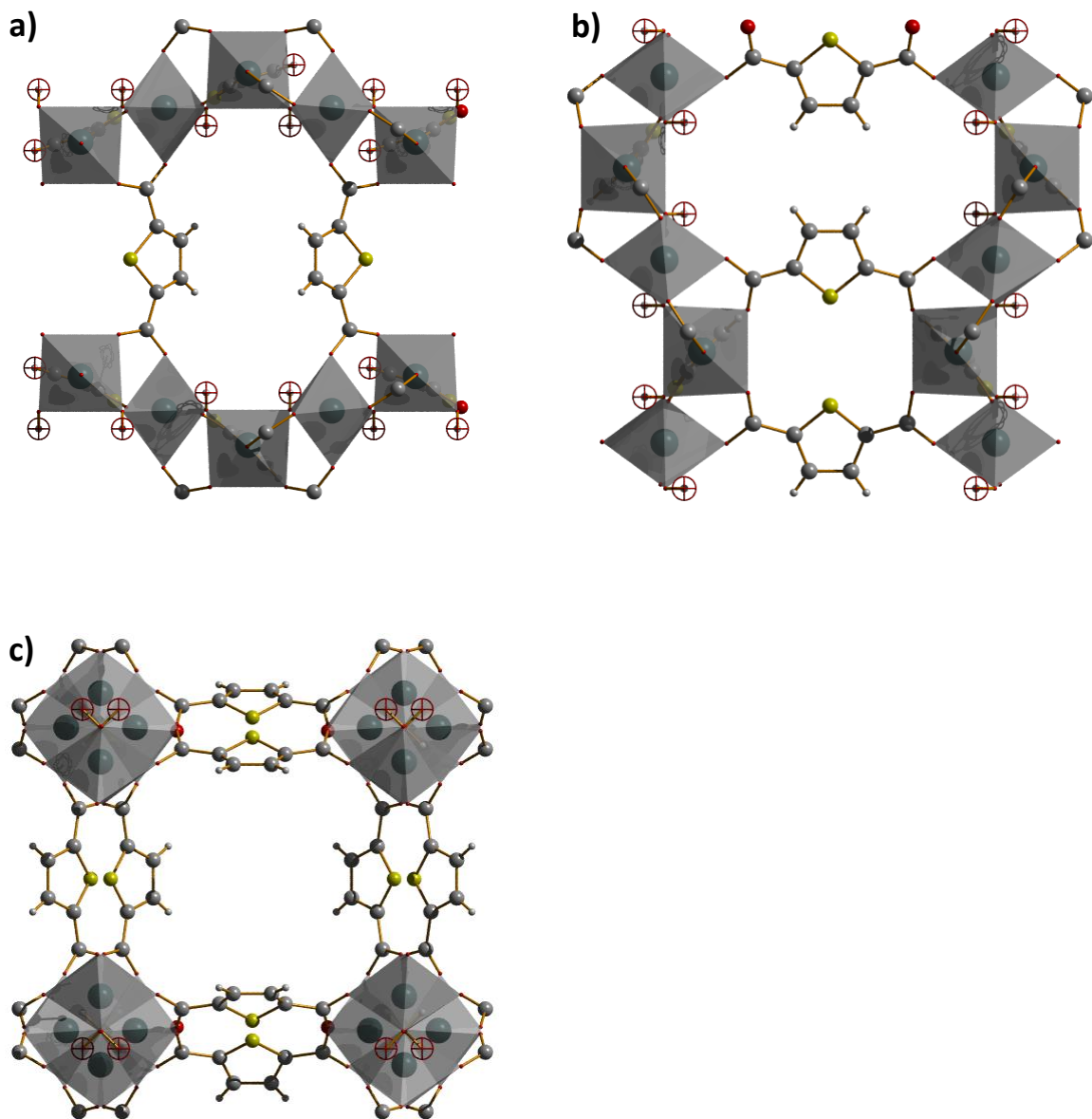


Figure S8: One pore of NOTT-401 (showing the thiophene-2,5-dicarboxylate building units) view along the: **a)** *a*-axis, **b)** *b*-axis and **c)** *c*-axis. The hydrogen atoms of OH groups are represented by principal ellipses and with bigger radius.

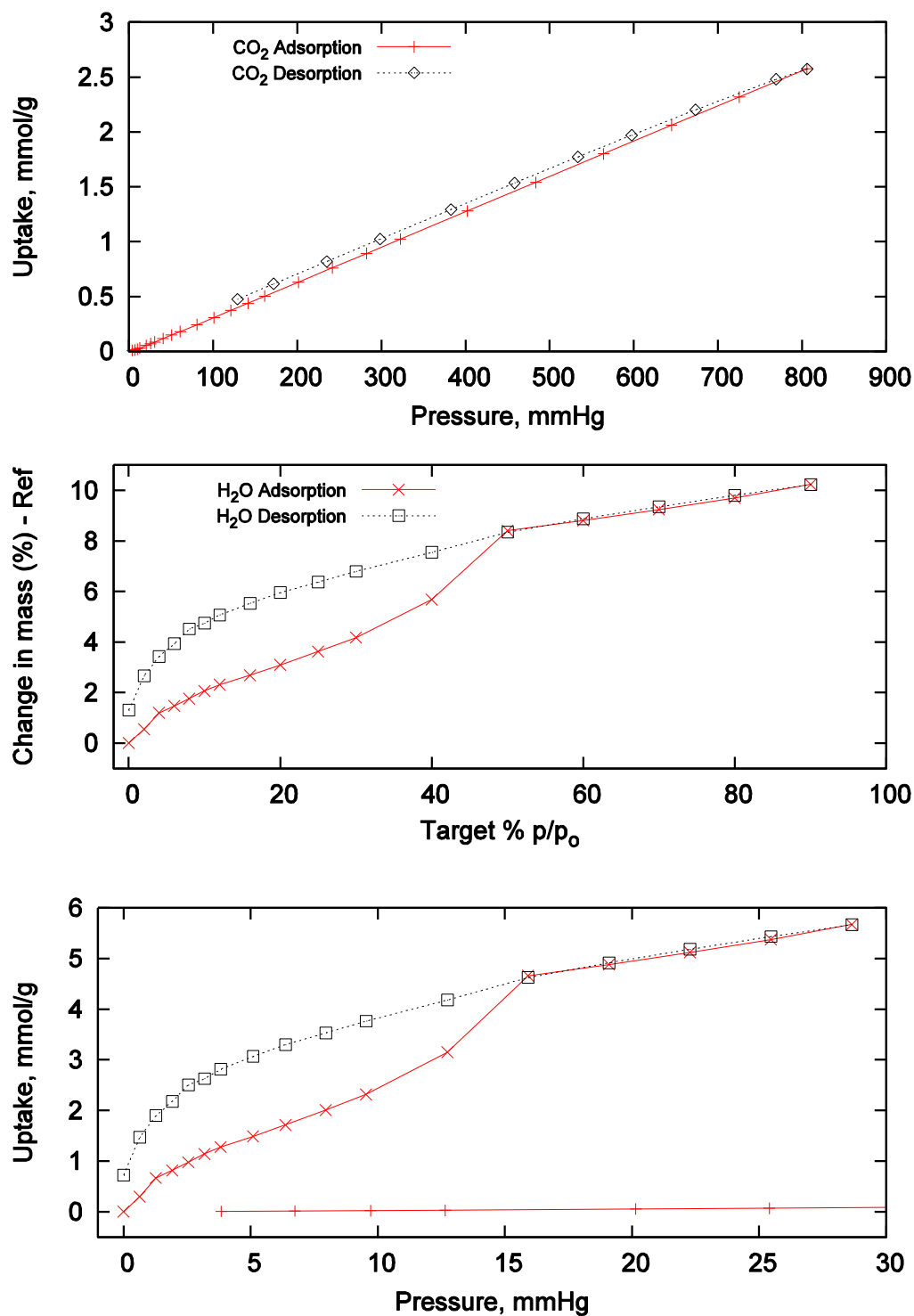


Figure S9: Carbon dioxide adsorption isotherm of NOTT-401 at 30 °C (Top); adsorption isotherm of water vapour in NOTT-401 at 30 °C (centre) and representation of both isotherms in the same coordinates and in the common pressures range (bottom).

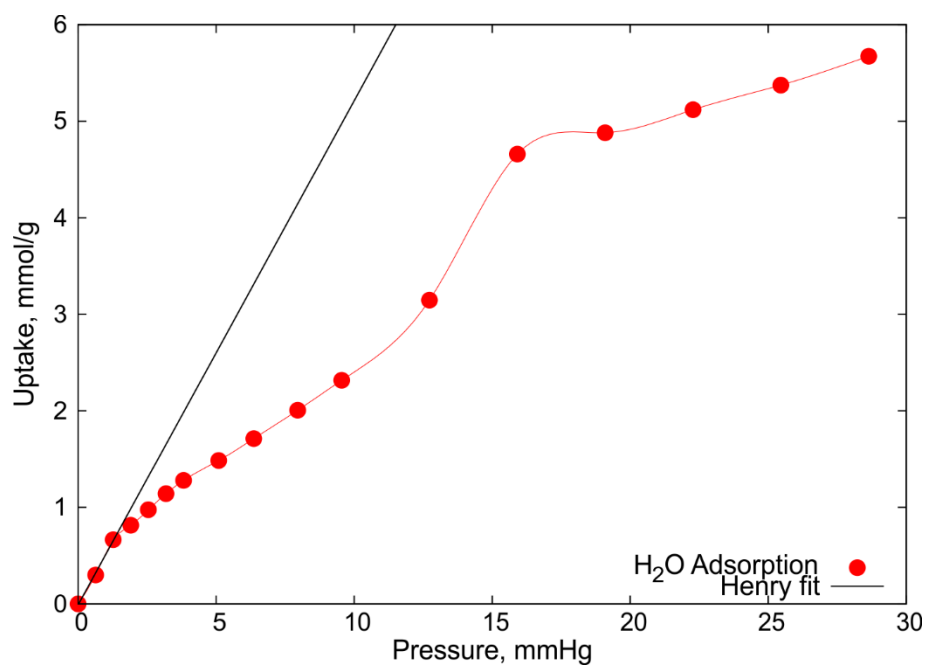


Figure S10: Experimental H₂O adsorption isotherm at 30°C of NOTT401 and Henry's law fitted to it.

References

1. Yang, R. T. Adsorbents: Fundamentals and Applications; John Wiley & Sons: Hoboken, 2003; pp 280-296.