

Supporting Information

Monitoring Adsorption-Induced Switching by ^{129}Xe NMR Spectroscopy in a new Metal-Organic Framework



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Thermogravimetric analysis

The thermogravimetric analysis was carried out using a Netzsch STA 409 PC Luxx thermal analyser with heating in air. An as synthesised sample ($\text{Ni}_2(2,6\text{-ndc})_2(\text{dabco})(\text{DMF})_{6.5}(\text{MeOH})_3$, **1**) was dried in argon flow and heated at a constant rate 5 °C /min in air from 30 °C to 600 °C.

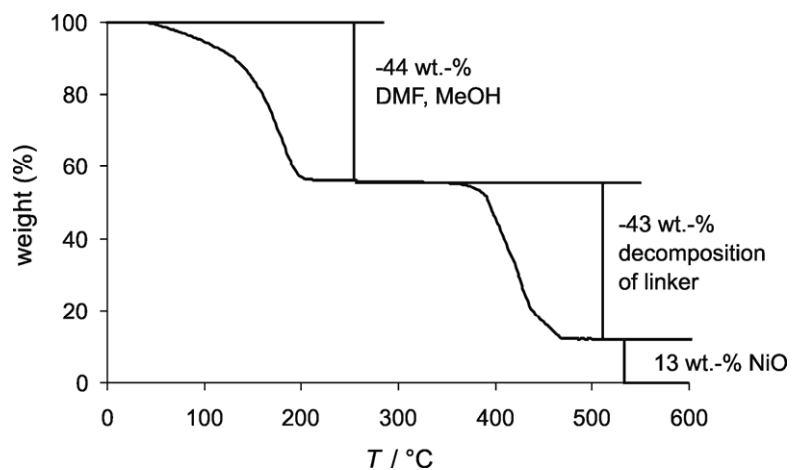


Fig. 1: TGA of phase 1 in air.

FT-IR-Spectra

The FT-IR-Spectra are measured in air with a Magna-IR 550 series II spectrometer from Nicolet. A small amount of the sample was mixed with KBr in a ratio of 1:100 in a ball mill and afterwards formed to a tablet that was measured right away.

The characteristic valence vibrations bands of the bridging carboxylate groups ν_s (COO) and ν_{as} (COO) are the same for phase **1** and the activated sample ($\text{Ni}_2(2,6\text{-ndc})_2(\text{dabco})$, **2**) (1608 cm^{-1} , 1410 cm^{-1}). The band at 1670 cm^{-1} in the spectrum of **1** indicates the CHO-vibration of the solvent molecule DMF. This signal is missing for the solvent free phase **2**.

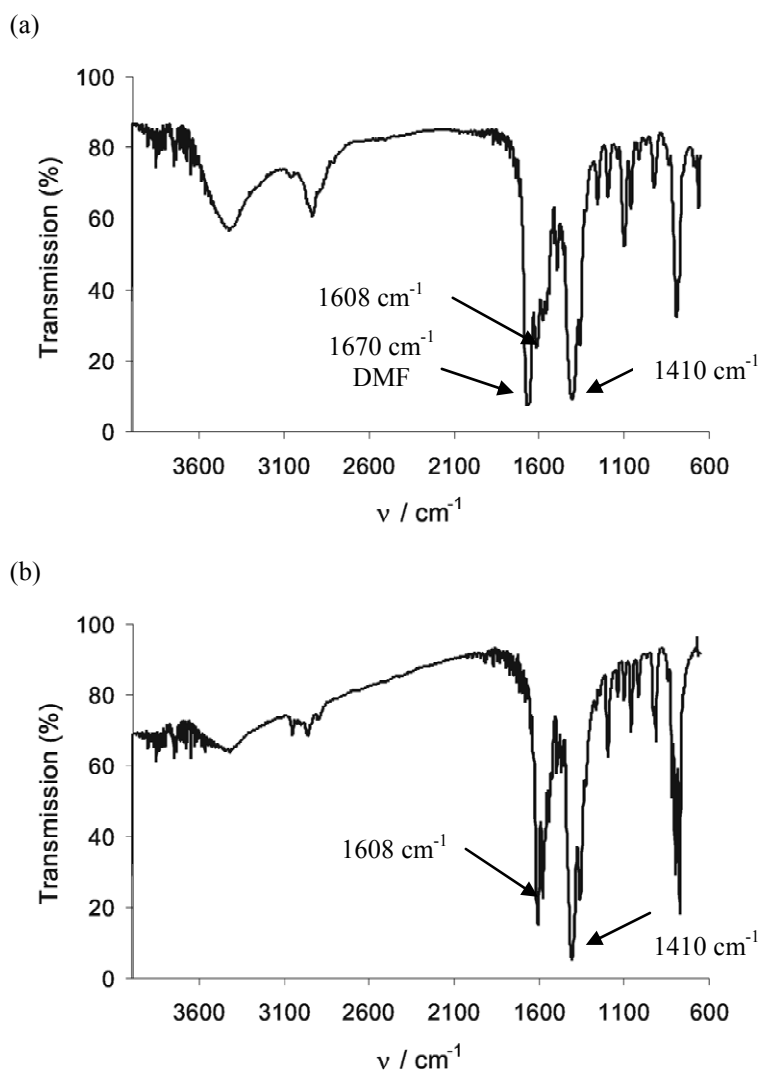


Fig. 2: IR-spectra of **1** (a) and **2** (b).

The colour change during adsorption of N₂

For the experiment with nitrogen an activated sample **2** (yellow) was filled in a typical Quantachrome adsorption measurement cell, evacuated and cooled down to 273K. At the given temperature the sample cell was filled with nitrogen up to 1 bar. In the following the sample cell was cooled down to 77K which leads to a relative pressure whereas the opening of the structure is almost completed. At this point the sample appears green again.

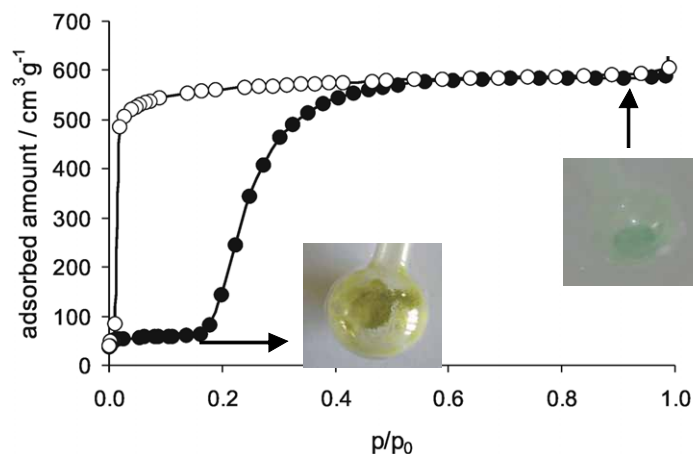


Fig. 3: N₂ adsorption/desorption (●/○) isotherm of Ni₂(2,6-ndc)₂(dabco) measured at 77K and the colour change occurring during the adsorption.

Hydrogen adsorption at 77K

Low pressure hydrogen adsorption measurement up to 1 bar at 77K was carried out using a Quantachrome Autosorb1C apparatus. The high pressure adsorption measurement up to 110 bar at 77K was performed using approximately 0.55 g sample on a volumetric BELSORP-HP apparatus.

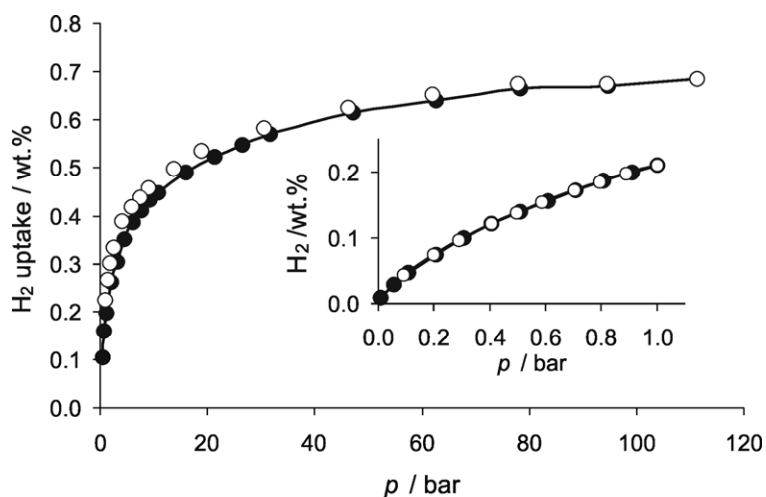


Fig. 4: High pressure H₂ excess adsorption/desorption (●/○) isotherm at 77K; insertion: low pressure H₂ adsorption/desorption isotherm of Ni₂(2,6-ndc)₂(dabco) at 77K.