Experimental report

14/02/2025

Proposal: 7-05-598 **Council:** 10/2023

Title: Tuning the pore-chemistry of Zr¿¿-C4 Metal-Organic Frameworks for gasadsorption: unraveling the host-guest interactions via INS

Research area: Materials

This proposal is a new proposal

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Samples: C24H16O32Zr6 Based-MOF hcp Topology
C24H16O32Zr6 Based-MOF fcu Topology

Instrument	Requested days	Allocated days	From	To
IN1 LAG	7	3	04/03/2024	06/03/2024
			14/06/2024	16/06/2024

Abstract:

The transition to a civilization without carbon emissions depends on the storage and separation of gas from the atmosphere and environment. As a result of its adaptable pore shape and customizable chemistry, Metal-Organic Frameworks (MOFs) have become potential adsorbents for gases including CO2 and CH4. With regard to customised gas adsorption, Zr¿¿-C4 MOFs with pendant functional groups show enormous promise. It was investigated the green synthesis of Zr-C4 MOFs with various pendant groups (-SH, -NH¿, Br, and COOH) that resulted in both cubic (BCM-1) and hexagonal (BCM-2) topologies. The objective of this research is to unravel the host-guest interactions of CO2, CH4, and water at high and low pressures within the most promising cubic and hexagonal Zr-C4 MOF variants. A detailed experimental plan, including Inelastic Neutron Scattering (INS) experiments and DFT calculations, has been outlined to achieve this goal. Hence, this project contributes to the development of advanced adsorbents for gas capture and separation, a critical step in achieving a sustainable and carbon-neutral future.

Tuning the pore-chemistry of Zr^{IV}-C4 Metal-Organic Frameworks for gas adsorption: unraveling the host-guest interactions via INS

In this experiment was measured 5 different Zr-microporous MOFs based on C4-linkers with different pedant functions. These MOFs are composed of $[Zr_6(OH)_4O_4]^{12+}$ units connected to twelve thiomalate linkers and the pendant functions decorating the organic linker were —SH (thiomalic), —NH_3 (aspartic), —COOH (transaconitic), —SH and —NH3 (trans-thiomalic), and —Br (bromine). It was utilized the monochromator Cu(220) to capture energy transfers of E_i = 26-500 meV (k_i = 210-4000 cm^{-1}) with an energy resolution of $\Delta E/E$ = 2%. All measurements were done at 10 K, using aluminum sample holders, which were also measured empty. Fig. 1 shows the spectra obtained for the 5 samples.

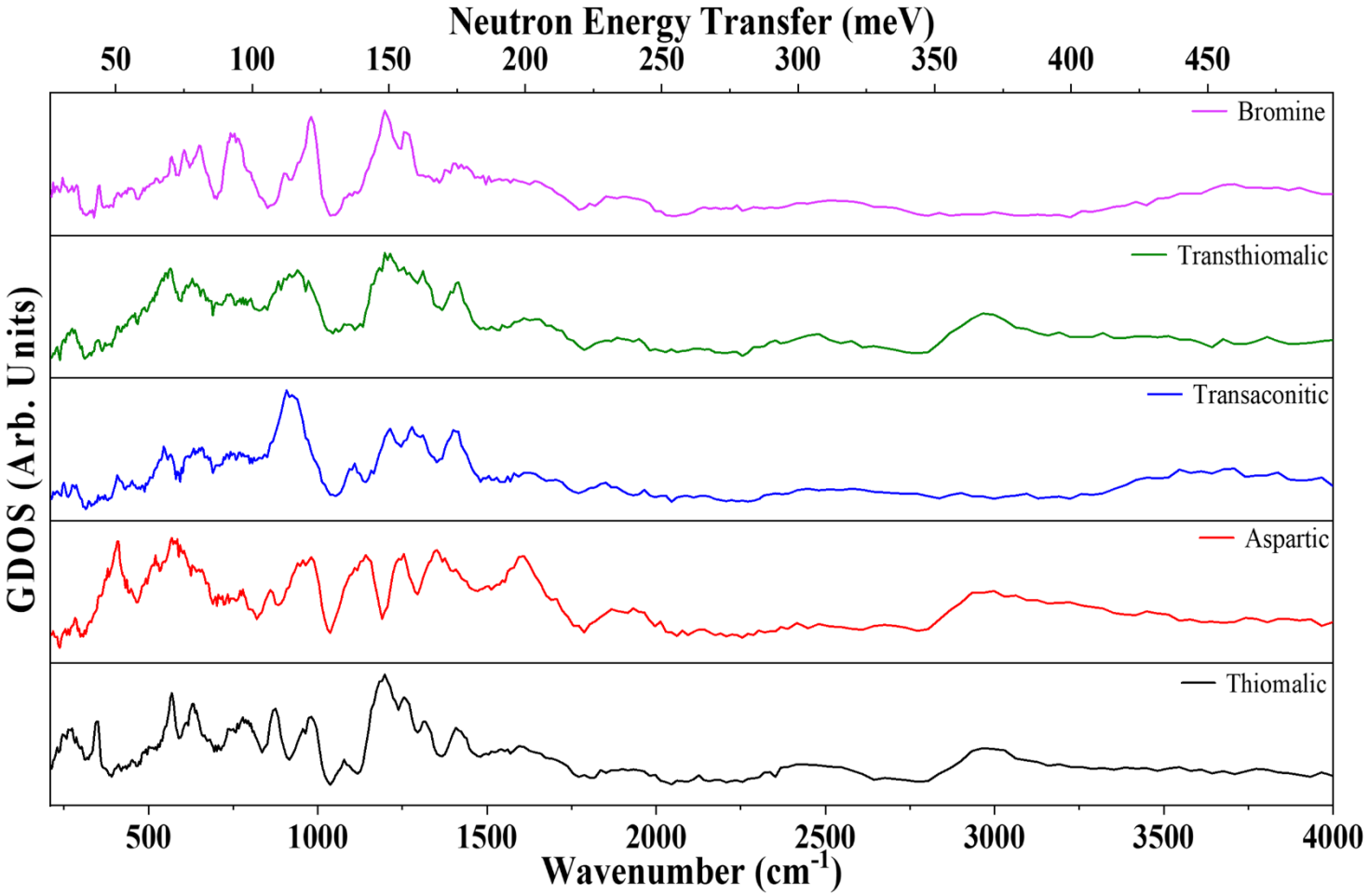

Figure 1: INS spectra for Zr-C4-MOFs with the linkers decorations —SH (thiomalic, black line), —NH3 (aspartic, red line), —COOH (transaconitic, blue line), —SH and —NH3 (transaconitic-thiomalic, green line), and —Br (bromine, magenta line).