These results show that a combination of MOMAs with X-ray and neutron diffraction measurement is of great use for single crystal analyses of protein crystals that do not grow to required sizes.

![X-ray diffraction images](image)

**Figure 1.** X-ray diffraction images, (a) and (b), taken at two different angles 90° apart. The edges of the images correspond to resolution of 1.79 Å. The averaged full width of half maximum (FWHM) of the diffraction spots are 2.14 and 2.77° for (a) and (b), respectively.

**Keywords:** X-ray crystallography, Neutron crystallography, Micro-crystallography, Magnetic orientation

**MS11-P2 Adsorption of hydrocarbons in the porous borohydrde framework γ-Mg(BH₄)₂**

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The first porous hydride, γ-Mg(BH₄)₂, was discovered recently [1]. It has about 1/3 of space in a form of small pores available to guest molecules, such as H₂, N₂, or CH₄,Cl₂ [1]. It is expected that the hydridic nature of the borohydrde ligands, exposed by H² into the pores, gives rise to specific guest-host interactions and thus to a selectivity of adsorption. In this work we study adsorption of methane, ethane, propane and butane into γ-Mg(BH₄)₂.

**In situ** X-ray diffraction data show that only methane and ethane are adsorbed into the pores, while propane and butane are too large to enter. Variable temperature diffraction under different gas pressures allowed us not only to localize the guests, but also to extract the isosteric heats of adsorption directly from the diffraction data [1, 2]. Neutron powder diffraction was done on doubly isotope substituted γ-Mg(¹⁵BD₄)₂, loaded with CD₄ (NIST) and C₂H₆ (HZB). Accurate localization of the guest molecules allows to determine the nature and the role of the guest-host interactions.

On saturation, 2/3 of methane and ethane molecules are adsorbed per Mg atom. The isosteric heats of adsorption, 22 (CH₄) and 32 (C₂H₆) kJ/mol of gas, allow to store 15–30 weight % of fuel gases at room temperature. This work will be complemented by volumetric studies of the adsorption enthalpies, as well as by theoretical calculations aiming to understand perfectly clear the nature of the intermolecular interactions.


**Keywords:** adsorption, in situ powder diffraction, porous hydride, thermodynamics