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.

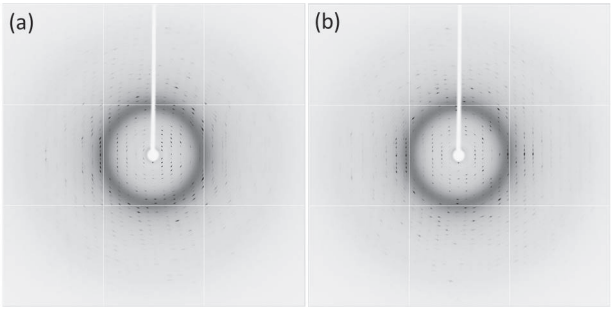

Figure 1. X-ray diffraction images, (a) and (b), taken at two different angles 90° apart. The edges of the images correspond to resolution of 1.79 Å. The averaged full width of half maximum (FWHM) of the diffraction spots are 2.14 and 2.77° for (a) and (b), respectively.

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

MS11-P2 Adsorption of hydrocarbons in the porous borohydride framework γ-$Mg(BH_4)_2$

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The first porous hydride, γ-$Mg(BH_4)_2$, was discovered recently [1]. It has about 1/3 of space in a form of small pores available to guest molecules, such as H_2, N_2 or CH_2Cl_2 [1]. It is expected that the hydridic nature of the borohydride ligands, exposed by $H^{\delta-}$ 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-$Mg(BH_4)_2$.

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 isotopically substituted γ-$Mg(^{11}BD_4)_2$, loaded with CD_4 (NIST) and C_2H_6 (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 (CH_4) and 32 (C_2H_6) 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.

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