STRUCTURAL STUDY OF GAS ADSORPTION IN POROUS SOLIDS: γ-$Mg(BH_4)_2$ AND DERIVATIVES

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Several porous metal borohydrides are reported: γ-$Mg(BH_4)_2$[1], *c*-$Ce(BH_4)_3$[2], γ-$Mn(BH_4)_2$[4], β-$Y(BH_4)_3$, and α-$Mg(BH_4)_2$. Porous γ-$Mg(BH_4)_2$ is the first light metal hydride capable of storing hydrogen both chemically, due to the existence of the covalent B-H bonds, and physically due to its porosity (33% of empty space at high pressure). Physisorption of H_2, N_2, CH_4, C_2H_6, C_2H_4 and C_2H_6 has been studied by X-ray and neutron diffraction[1].

Now we study the adsorption of those gazes by γ-$Mg(BH_4)_2$ by volumetric methods and by TGA/DSC, aiming to compare the equilibrium curves with those obtained from *in situ* X-ray powder diffraction[3]. We also study the physisorption of a monoatomic gas, argon, by X-ray diffraction. Interestingly, while only one larger molecule occupies the pore, the smaller hydrogen and argon may take up to 2 crystallographically independent molecules. Furthermore, we study and compare the adsorption of those gazes in similar porous compounds, implying a change of the metal: γ-$Mn(BH_4)_2$; or a change of the ligand: $MgIm_2$ (Im = imidazolate).

The synthesis of solvent free γ-$Mn(BH_4)_2$ is described in the literature[4]. A metathesis $2LiBH_4 + MnCl_2$ in DMS/toluene followed by a filtration conduct to the formation of the solvate $Mn(BH_4)_2 \cdot 1/2S(CH_3)_2$, which after vacuum gives porous γ-$Mn(BH_4)_2$. Porous $MgIm_2$ has been synthesized in our laboratory, the optimal experimental conditions to obtain the porous phase are still being investigated.

The physisorption of argon in γ-$Mg(BH_4)_2$ is investigated using synchrotron powder diffraction data measured at the Swiss–Norwegian Beam Lines of the ESRF. The volumetry and TGA/DSC measurements are made at UCL.

Bibliography:

(1) Filinchuk, Y.; Richter, B.; Jensen, T. R.; Dmitriev, V.; Chernyshov, D.; Hagemann, H. *Angew. Chem. Int. Ed.* **2011**, *50* (47), 11162. and not yet published work.
(2) Ley, M. B.; Jørgensen, M.; Černý, R.; Filinchuk, Y.; Jensen, T. R. *Inorg. Chem.* **2016**, *55* (19), 9748.
(3) Filinchuk, Y. *27th Eur. Crystallogr. Meet. ECM 27 Bergen Nor.* **2012**. for the methodology.
(4) Richter, B.; Ravnsbæk, D. B.; Tumanov, N.; Filinchuk, Y.; Jensen, T. R. *Dalton Trans* **2015**, *44* (9), 3988.