

MS31-P3 New hybrid materials via a combination of imidazolates and complex hydrides: first compounds and further perspectives

Fabrice J. Morelle¹, Voraksmy Ban¹, Anna Miglio¹, Roman Skoryunov², Alexander Skripov², Geoffroy Hautier¹, Yaroslav Filinchuk¹

1. Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium

2. Institute of Metal Physics, Ural Branch of the Russian Academy of Sciences, Ekaterinburg 620137, Russia

email: fabrice.morelle@uclouvain.be

Since the discovery of zeolites by Axel Frederik Cronstedt in 1756, microporous materials have received an always increasing attention. In this field, the great challenges for chemists were, and still are, to tune the pore size and the pore's surface chemical nature in order to obtain materials with targeted properties while keeping the stability window as large as possible to allow practical applications. Over the past 15 years, Metal-Organic Frameworks (MOFs) received most of the attention in this field thanks to the ease of synthesizing linkers with various sizes, chemical properties, or number of coordination sites.

The recently discovered porous polymorphs of magnesium and manganese borohydride show that the tetrahydroborate anion can also have a structure directing effect as many organic ligands by preferentially making linear metal-BH₄-metal units[1], [2]. The formation of compounds containing both an organic ligand, in this case imidazolate and BH₄ group could lead to the formation of new porous hydrides having the easily tunable properties of imidazolate frameworks.

Li₂ImBH₄ (Im = imidazolate) and Li₂bImBH₄ (bIm = benzimidazolate) were successfully synthesized by liquid assisted grinding and liquid synthesis. Both structures were solved using synchrotron radiation powder diffraction and neutron powder diffraction in the case of LiImBH₄. The main features of these structures are the formation of parallel positively charged [Li₂(b)Im]_∞ fibers extending perpendicular to the (benz)imidazolate plane. The charge balancing BH₄ units are located in between these fibers and coordinate to four Li atoms in a square planar environment. Anisotropic temperature factors refined from neutron diffraction data suggests high rotational disorder of the BH₄ unit perpendicular to the square plane. This disorder was investigated and confirmed by solid state NMR and theoretical studies.

This work clearly proves that it is possible to combine hydridic and classical ligands in the same structure and that the resulting materials have original and unique properties compared to the pure borohydride or imidazolate compound.

[1] Y. Filinchuk, B. Richter, T. R. Jensen, V. Dmitriev, D. Chernyshov, and H. Hagemann, *Angew. Chem. Int. Ed.*, vol. 50, no. 47, pp. 11162–11166, Nov. 2011.

[2] B. Richter, D. B. Ravnsbæk, N. Tumanov, Y. Filinchuk, and T. R. Jensen, *Dalton Trans*, vol. 44, no. 9, pp. 3988–3996, 2015.

Keywords: metal-organic frameworks, zeolitic imidazolate frameworks, borohydride, hydrogen storage, hybrid compounds

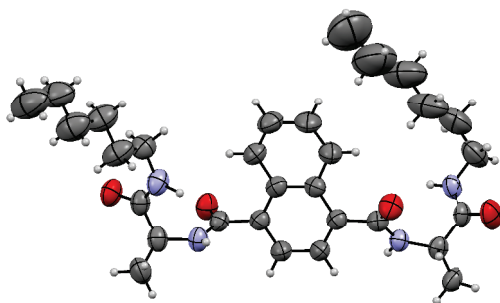


Figure 1. Molecular structure of the alanine bioconjugate.

Keywords: naphthalene, amino acid, bioconjugates, hydrogen bond