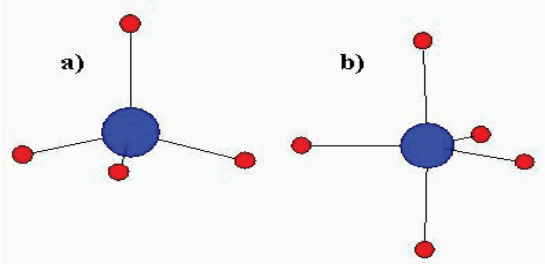

Fig.1. Coordinates polyhedra around Fe atoms: a) tetrahedron, b) trigonal bipyramid

The Rietveld analysis gives us information about changes of avarage structures (cubic ↔ monoclinic) but Pair distribution Function (PDF) methods let us describe the local configuration of deuterium atoms wich stays almost the same in order and disordere phases (fig.2). Neutron Time-of-Flight (ToF) data were collected at IPNS, Argonne, and Lujan Center, Los Alamos on series of samples with different deuterium content. Each sample was measured below and above the temperature of deuterium ordering. The local deuterium configuration in disordered phase have been modeled by DISCUS using Revers Monte Carlo technique [3].

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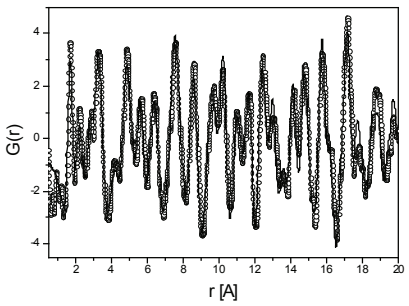

Figure 2. Observed PDF (points) of $YFe_2D_{4.2}$ in disordered state and modeled (solid line) by same local order of deuterium atoms around iron as in the ordered phase.

FA5-MS01-O4

Structural Investigations of $LnBO_3$ (Ln= Y, La, Nd, Sm, Eu, Gd, Dy, Ho, Er,Yb, Lu) by Rietveld Method. Semih Seyyidoglu[a], Katrin Hoffmann[b], Barbara Albert[b], Aysen Yılmaz[a]. [a]*Department of Chemistry, Middle East Technical University, 06531, Ankara, Turkey.* [b]*Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Petersenstr. 18, 64287, Darmstadt, Germany.*
E-mail: semihseyyidoglu@yahoo.com

Numerous efforts have been devoted to the structure determination of these compounds in literature. While $LaBO_3$ and $NdBO_3$ exhibit the aragonite type (orthorhombic Pnma) structures [1-2], the structure vaterite type rare earth borates (Y, Gd-Yb) are still under investigation since the structure of these compounds are directly related with their synthesis method. The structure of $GdBO_3$ were defined in rhombohedral space group R32 by Lin and coworkers [3]. While in Sheptyakov's work[4], Eu doped yttrium orthoborate structure is monoclinic space gropu C2/c, Chadeyron produced YBO_3 single crystals with P63/m space group [5]. Since there is no systematic structural analysis work of whole rare earth borate series, in this work we synthesized and solved their stucture by using Rietveld Method [6] with GSAS program[7]. We prepared $LnBO_3$ (Ln=Y, La, Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb, Lu) powder samples by using Ln_2O_3 and H_3BO_3 (ratio=1:2) heated at 900 °C for 10 hour and 1000 °C for 5. Then, their XRD patterns were collected on a PANalytical X'PERT PRO diffractometer equiped with PIXCEL detector. Among these rare earths, $LaBO_3$ and $NdBO_3$ were solved based on Pnma orthorhombic structure. The crystal structure of YBO_3, $DyBO_3$ and $HoBO_3$ were C2/c monoclinic and $SmBO_3$ showed P-1 triclinic structure. The structure of $TbBO_3$, $TmBO_3$ and $YbBO_3$ were solved based on P21/m.

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FA5-MS01-O5

Metal and Chemical Hydrides: Highlights and Pitfalls of Powder Diffraction. Radovan Černý. *Laboratory of Crystallography, University of Geneva, 24, quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland.*
E-mail: Radovan.Cerny@cryst.unige.ch

The methods of structural characterization of metal and chemical hydrides are reviewed (see also [1]). It is shown that powder diffraction is essential component of hydrides research where the structural characterization is currently undertaken by X-ray and neutron diffraction. In the case of chemical hydrides like borohydrides of light alkaline metals/earths X-ray diffraction alone can provide the structural parameters with sufficient accuracy. A crystallographer analyzing hydrides has to face numerous crystallographic challenges which include complex structures, superstructures, pseudo-symmetries, twinning,