

s14.m39.p5 **Neutron Diffraction Study of Rare Earth Substituted Powdered  $YAl_3(BO_3)_4$  Crystals.** E. Sváb<sup>1</sup>, Gy. Mészáros<sup>1</sup>, Z. Somogyvári<sup>1</sup>, E. Beregi<sup>1</sup>, F. Bourier<sup>2</sup>, <sup>1</sup>Research Institute for Solid State Physics and Optics, H-1525 Budapest, POB 49, Hungary, <sup>2</sup>Laboratoire Léon Brillouin, CEA/Saclay, 91191 Gif-sur-Yvette, France. E-mail: svab@szfki.hu

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Yttrium aluminium borate  $YAl_3(BO_3)_4$  (YAB) single crystals have excellent non-linear optical properties, and doped YAB crystals have important applications in laser engineering [1]. YAB crystals have suitable sites for some rare-earth elements at the  $Y^{3+}$  site ( $Er^{3+}$ ,  $Nd^{3+}$ ,  $Yb^{3+}$ ,  $La^{3+}$ ) or other doping ions at  $Al^{3+}$  site ( $Cr^{3+}$ ,  $Ga^{3+}$ ). The knowledge of the crystallographic parameters is important when characterising the optical properties of YAB crystals. In a previous study we have reported our results on  $Ga$ -doped YAB structure [2].

The aim of this work was to investigate the crystallographic effect of the substitution of  $Er$  and  $Yb$  into  $YAl_3(BO_3)_4$ . Single crystals were grown by top-seeded high temperature solution (flux) method, and the composition was verified by atomic absorption spectroscopy [3]. The single crystals were powdered into fine grains to obtain good powder spectrum for data analysis. Three samples were investigated, namely  $YAl_3(BO_3)_4$ ,  $Y_{0.88}Er_{0.12}Al_3(BO_3)_4$  and  $Y_{0.5}Yb_{0.5}Al_3(BO_3)_4$ , by neutron diffraction at BNC/Budapest and at LLB/Saclay using the medium resolution PSD ( $\lambda=1.07\text{\AA}$ ) [4] and the high resolution 3T2 ( $\lambda=1.2251\text{\AA}$ ) [5] diffractometers, respectively.

The crystal structure of  $YAl_3(BO_3)_4$  is rhombohedral with space group  $R\bar{3}2$ . The  $Y$  atoms,  $Al$  atoms and  $B$  atoms occupy trigonal prisms, octahedra, and triangles of oxygen, respectively. Our investigations have shown that the substitution of  $Y$  atoms by  $Er$  and  $Yb$  leaves the space group invariant. The lattice parameters, atomic position parameters and interatomic distances were determined by Rietveld refinement of the neutron diffraction pattern. It was concluded that both the  $Er$  and  $Yb$  ions occupy the trigonal prismatic  $Y$ -position.

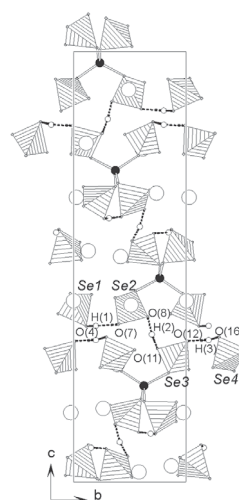
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- [1] G. Dominiak-Dzik, W. Ryba-Romanowski, M. Grinberg, E. Beregi, L. Kovacs, *J. Phys.: Condens. Matter* **14**, 5229 (2002)
- [2] Gy. Mészáros, E. Sváb, E. Beregi, A. Watterich, M. Tóth, *Physica*, **B276-278**, 310-311 (2000)
- [3] E. Beregi, E. Hartmann, L. Malicskó, J. Madarász, *Cryst. Res. Technol.* **34**, 641 (1999)
- [4] <http://www.bnc.hu/>
- [5] <http://www-llb.cea.fr/>

s14.m39.p6 **X-ray and Neutron Single Crystal Diffraction Study of  $Rb_4LiH_3(XO_4)_4$  ( $X = S, Se$ ).** S. I. Troyanov<sup>a</sup>, Ch. D. Ling<sup>b</sup>, E. Kemnitz<sup>c</sup>, <sup>a</sup>Chemistry Department, Moscow State University, <sup>b</sup>Institute Laue-Langevin, Grenoble, France, <sup>c</sup>Chemistry Institute, Humboldt University Berlin, Germany. E-mail: sergej.troyanov@rz.hu-berlin.de

**Keywords:** Hydrogen bond; Neutron diffraction; Laue method

The compounds of the general composition  $M_4LiH_3(XO_4)_4$  ( $M = K, NH_4, Rb; X = S, Se$ ) are known to exhibit ferroelastic properties at low temperatures [1]. At elevated temperatures, they undergo phase transitions to superprotonic phases [2]. X-ray single crystal investigation was performed for  $Rb_4LiH_3(SeO_4)_4$  (**1**) at 180 K. Neutron single crystal study was carried out for  $Rb_4LiH_3(SO_4)_4$  by Laue method at 298 K (**2a**) and 480 K (**2b**). Isotypic **1** and **2** crystallize in tetragonal unit cell (space group  $P4_1$ ) [3]. Hydrogen bonding systems in both compounds consist of four  $XO_4$  tetrahedra connected by three



hydrogen bonds (Fig.). The central essentially symmetrical and disordered H-bond (2.49 Å) is shorter than the both terminal (asymmetrical) H-bonds (2.52-2.54 Å). In the high temperature phase **2b**, which is known to possess a high protonic conductivity, larger thermal displacement parameters and an increased proton disorder of the central hydrogen bond are the only dissimilarities from the room temperature phase **2a** [4].

#### References

- [1] Mróz B., Kim S.M., Powell B.M., Kiefler H., Donaberger R.L. *Phys. Rev. B* 1997, **55**, 11174.
- [2] Pietraszko A., Polomska M., Pawłowski A. *Izv. AN SSSR, Phys. Ser.* 1991, **55**, 529.
- [3] Zúniga F.J., Etxebarria J., Madariaga G., Brezczewski T. *Acta Cryst. C* 1990, **46**, 1199.
- [4] Troyanov S.I., Snigireva E.M., Ling Ch.D. *Kristallografiya* 2004, **49** (in press)