The structure, magnetic and spectroscopic properties of Li$_3$B (0.67 < x < 1.22) are reported. The composition of this compound has earlier been described as Li$_3$B$_4$ [1] or Li$_3$B$_6$ [2,3]. Hitherto published structural data are wrong.

The compound crystallizes in the space group P6$_3$/mmc. The lattice constants are with $a = 402.86$ pm and $c = 290.2$ pm (for x=1) or $a = 401.81$ pm and $c = 279.4$ pm (for x=1.22) dependent on the lithium content. The crystal structure was determined from X-ray powder diffraction data.

The structure consists of a distorted hexagonal closed packing of lithium atoms. The stacks of octahedra are centered by linear chains of boron atoms along the crystallographic c-axis.

This is the first compound known to contain isolated linear [B]$_n$-chains in the ideal case. However, crystal defects limit the average chain length to about 67 boron atoms and lead to variations of the stoichiometry. These chains are the first examples of carbinoid systems (boryne) of a really large size.


SPECIFIC FEATURES OF DEFECT STRUCTURE OF N$_{0.39}$Y$_{0.61}$F$_{2.22}$ CRYSTALS. Zhurova, E. A., Maximov, B. A., Hull S., Keen, D. A., Wilson, C. C., Sobolev B. P., Simonov, V. I. Inst. of Crystallography RAS, Moscow, Russia

The specific features of structure and electron density distribution have been studied in the temperature range 0-296 K in the N$_{0.39}$Y$_{0.61}$F$_{2.22}$ fluorite crystal.

The structure refinements of the crystal were realized to $R$-0.3 % for the X-ray experiment and to $R$ ~ 3-7 % for the neutron ones at different temperatures. It was found, that there are three different F atom sites, the main one (8c) F, relaxed (32f) FR with coordinates (0.5, 0.13, 0.13). Cationic sites are splitted about $\pm 0.1$ A in the direction of the coordinate axes. If we take into account the multiplicity of the (32f) site, the occupancy of the FR atom per one formula unit is close to Na content, and we can suppose that there are two sublattices in the N$_{0.39}$Y$_{0.61}$F$_{2.22}$ crystal. One of them contains Y and F atoms, the other one contains Na and FR, and one of the sublattices is displaced relative to the other by a distance of about 0.1 A.

The temperature dependence of the lattice parameter indicates a possible change in the crystal structure model at ~110 K. However, such a specific feature was not revealed in the course of structure refinement.

On the deformation electron density maps there are peaks ~0.1 e/Å$^3$ in height, which are slightly displaced from Na(Y)-F line. They can be due to partial covalent character of the Y-F chemical bond.

The crystallochemical similarities in the homological series system of SrGa$_2$Si$_2$O$_6$ - SrGa$_2$Ge$_2$O$_6$ have also been studied.