PS08.01.45 Li$_2$B - A LITHIUMBORIDE CONTAINING LINEAR BORON CHAINS. Michael Wörle, Reinhard Nesper, Laboratorium für anorganische Chemie, ETH Zürich, Universitätstr. 6, CH-8092 Zürich.

The structure, magnetic and spectroscopic properties of Li$_2$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$_7$B$_9$ [2,3]. Hitherto published structural data are wrong.

The compound crystallizes in the space group P6$_3$/mmc. The lattice constants are with $a = 401.81$ pm and $c = 279.4$ 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.

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 reasonable size.


PS08.01.46 SPECIFIC FEATURES OF DEFECT STRUCTURE OF Na$_0.39$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 Na$_0.39$Y$_0.61$F$_{2.22}$ fluorite crystal.

The structure refinements of the crystal were realized to determine electron density maps there are peaks for the X-ray experiment and 3-7 % for the neutron experiment. Cationic sites are splitted about 0.5 coordinates in the Na0.39Y0.61F$_2$2.22 fluorite 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 ~ 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.

PS08.01.47 Ca$_3$WO$_7$ BRONZE SYNTHESIZED UNDER HIGH PRESSURE. Zibrov I.P., Filonenko V.P.: Institute of Crystallography, Russian Academy of Sciences, 117333 Moscow, Leninovy pr.39, Russia.

A new intergrov tungsten bronze (ITB), Ca$_3$WO$_7$ x=0.04-0.06 has been prepared by solid state reaction (CaO+WO$_3$+W) at P=50-80 kbar and T>1300 C. The compounds were studied by X-ray powder diffraction and high resolution transmission electron microscopy. The samples with starting composition x=0.05-0.5 were investigated. Ca$_3$WO$_7$(ITB)+ CaWO$_4$ were revealed in the samples with x<0.15, the mixture of CaWO$_4$+ Ca$_3$WO$_7$(HTB)[1]+PTB[2]-in the samples with x>0.15. The calculated cell parameters of the ITB phase are: a=10.152, b=7.423 and c=3.790 Å.

According to the nomenclature of the ITB families of related phases introduced in [3], the structure of this compound is denoted (2)-ITB and belongs to the (n)-ITB family of related phases. The number n corresponds to the number of WO$_6$-octahedra across the WO$_3$-type slabs in the structure. The theoretical upper limit of x is 0.20. However, in the Ca$_3$WO$_7$(ITB) phase the sixsided tunnels seems to be filled to about 25%. The (2)-ITB structure can be considered to consist of hexagonal tungsten bronze (HTB) slabs, one single hexagonal tunnel row wide, which are mutually linked by corner-sharing.


This research was made possible in part by Grant N 95-03-08146a from Russian Foundation of Fundamental Investigations.

PR08.01.48 SYNTHESIS OF SOME CRYSTALLOGEICAL ANALOGS STRONTIUM ANORITIAND THEIR INTERRELATIONS. Arifov P.A. Inst. of Chemistry, Tashkent, Uzbekistan.

The results of synthesis and investigation of some strontium anorite varieties and their analogs interrelations are given. SrAl$_2$Si$_2$O$_8$ and SrAl$_2$Ge$_2$O$_8$ triclinic forms were obtained by solid phase reactions, differently from the former, SrAl$_2$Ge$_2$O$_8$ was obtained close to the melting temperature. Anorite hexagonal and orthorombic forms and their analogs were obtained by glass or solid state reaction.

The synthesis temperature of SrAl$_2$Si$_2$O$_8$- SrAl$_2$Ge$_2$O$_8$ have also been studied. In the homological series system SrAl$_2$Si$_2$O$_8$- SrAl$_2$Ge$_2$O$_8$ (Table).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Dens</th>
<th>Pms/Prms</th>
<th>elem. cell</th>
<th>Ind/refr.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>kg/m$^3$</td>
<td>a</td>
<td>c</td>
<td>V,$A^3$</td>
</tr>
<tr>
<td>SrAl$_2$Si$_2$O$_8$</td>
<td>2980</td>
<td>5.25</td>
<td>7.56</td>
<td>180</td>
</tr>
<tr>
<td>Sr$_2$Ba$_4$Al$_4$Si$_2$O$_8$</td>
<td>3010</td>
<td>5.25</td>
<td>7.58</td>
<td>181</td>
</tr>
<tr>
<td>Sr$_2$Ba$_4$Al$_2$Si$_2$O$_8$</td>
<td>3080</td>
<td>5.25</td>
<td>7.64</td>
<td>182</td>
</tr>
<tr>
<td>Sr$_2$Ba$_4$Al$_2$Si$_2$O$_8$</td>
<td>3150</td>
<td>5.25</td>
<td>7.86</td>
<td>183</td>
</tr>
<tr>
<td>Sr$_2$Ba$_4$Al$_2$Si$_2$O$_8$</td>
<td>3220</td>
<td>5.25</td>
<td>7.74</td>
<td>184</td>
</tr>
<tr>
<td>Sr$_2$Ba$_4$Al$_2$Si$_2$O$_8$</td>
<td>3300</td>
<td>5.25</td>
<td>7.76</td>
<td>185</td>
</tr>
<tr>
<td>Ba$_2$Al$_4$Si$_2$O$_8$</td>
<td>3320</td>
<td>5.25</td>
<td>7.92</td>
<td>186</td>
</tr>
</tbody>
</table>

The crystallogechemical similarities in the homologous series system of SrGa$_2$Si$_2$O$_8$ - SrGa$_2$Ge$_2$O$_8$ have also been studied.