PS08.01.45 Li_xB - A LITHIUMBORIDE CONTAINING LINEAR BORON CHAINS. Michael Wörle, Reinhard Nesper, Laboratorium für anorganische Chemie, ETH Zürich, Universitätsstr. 6, CH-8092 Zürich.

The structure, magnetic and spectroscopic properties of Li_xB ($0.67<x<1.22$) are reported. The composition of this compound has earlier been described as Li_5B_4 [1] or Li_7B_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]-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.

[1] F. E. Wang, M. A. Mitchell, R. A. Sutula; J. Less Common Met., **57**,(1978), 161
[2] R. Szwark, R. D. Walton, S. Dallek, B. F. Larrick; J. Electrochem. Soc. **129**, (1982),1168
[3] D. W. Ernst; J. Electrochem. Soc., **129**, (1982), 1513

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 Rutherford Appleton Laboratory, England

The specific features of structure and electron density distribution have been studied in the temperature range 10-296 K in the $Na_{0.39}Y_{0.61}F_{2.22}$ fluorite crystal.

The structure refinements of the crystal were realized to R~ 0.5 % 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 (0.29, 0.29, 0.29) and supplementary (48i) F' with coordinates (0.5, 0.13, 0.13). Cationic sites are splitted about 0.1 A in the directions 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 $Na_{0.39}Y_{0.61}F_{2.22}$ 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 ~ 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/A^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_xWO_3 BRONZE SYNTHESIZED UNDER HIGH PRESSURE. Zibrov I.P.[1], Filonenko V.P.[2].[1]Institute of Crystallography, Russian Academy of Sciences, 117333 Moscow, Leninsky pr.59, Russia. [2]Institute for High Pressure Physics, Russian Academy of Sciences, 142092 Troitsk, Moscow Region, Russia.

A new intergrowth tungsten bronze (ITB), Ca_xWO_3 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_xWO_3(ITB)+ $CaWO_4$ were revealed in the samples with x<0.15, the mixture of $CaWO_4$+ Ca_xWO_3(HTB[1]+PTB[2])- in the samples with x>0.15. The calculated unit cell parameters of the ITB phase are: a=10.152, b=7.423 and c=3.790Å.

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_xWO_3(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.

[1]. P.E.Bierstedt et. al., Solid State Commun. 4, 25, 1966.
[2]. D.Vandeven et. al., Mater. Res. Bull., 2, 809,1967.
[3]. A.Hussain and L.Kihlborg, Acta Cryst. A32, 551 (1976).
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 CRYSTALLOCHEMICAL ANALOGS STRONTIUM ANORTITE AND THEIR INTERRELATIONS. Arifov P.A. Inst. of Chemistry, Tashkent, Uzbekistan.

The results of syntesis and investigation of some strontium anortite varieties and their analogs interrelations are given. $SrAl_2Si_2O_8$ and $SrAl_2Ge_2O_8$ triclinnic forms were obtained by solid phase reactions, differently from the former, $SrAl_2Ge_2O_8$ was obtained close to the melting temperature. Anortite hexagonal and orthorombic forms and their analogs were obtained by glass or melt crystallization. $SrAl_2Si_2O_8$ a=8,21; b=12,84; d=3120 kg/m^3 tricl. $SrAl_2Ge_2O_8$ a=8,562; b=13,27; c=7,28; d=3740 kg/m^3 tricl. The synthesis temperature of $SrAl_2Si_2O_8$ corresponds to 1500° C and for $SrAl_2Ge_2O_8$ - 1450°C, the melting temperature is respectivety 1710 and 1515°C. Also, studed the interrelations of hexagonal varieted of solid solution in the system $SrAl_2Si_2O_8$ - $BaAl_2Si_2O_8$ (Table).

Compound	Dens	Prms	elem. cell,A		Ind/refr.	
	kg/m^3	a	c	V, A^3	Ng	Np
$SrAl_2Si_2O_8$	2980	5,25	7,56	180	1,573	1,571
$Sr_{0,9}Ba_{0,1}Al_2Si_2O_8$	3010	5,25	7,58	181	1,573	1,571
$Sr_{0,7}Ba_{0,3}Al_2Si_2O_8$	3080	5,25	7,64	182	1,573	-
$Sr_{0,5}Ba_{0,5}Al_2Si_2O_8$	3150	5,25	7,68	183	1,573	-
$Sr_{0,3}Ba_{0,7}Al_2Si_2O_8$	3220	5,25	7,74	184	1,573	-
$Sr_{0,1}Ba_{0,9}Al_2Si_2O_8$	3300	5,25	7,76	185	1,573	-
$BaAl_2Si_2O_8$	3320	5,25	7,82	186	1,573	-

The crystallochemical similarities in the homological series system of $SrGa_2Si_2O_8$ - $SrGa_2Ge_2O_8$ have also been studied.