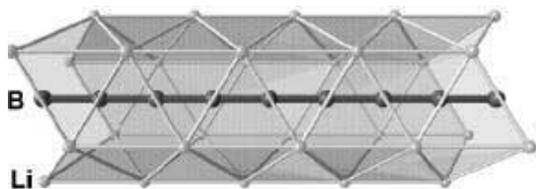


**s1.m1.p11**  $\text{LiB}_x$  – An Incommensurate Composite Structure at Low Temperatures. M. Wörle\*, R. Nesper\*, T. Chatterji<sup>†</sup>, \*Laboratory of Inorganic Chemistry, ETH Zürich, Universitätstr. 6, CH-8092 Zürich; <sup>†</sup>Institut Laue Langevin, BP156, F-38042 Grenoble Cedex 9.  
Keywords: aperiodic, incommensurate.

The lithium boride  $\text{LiB}_x$  ( $0.82 < x < 1.0$ ) the first boride known to contain linear boron chains, isoelectronic to carbyne which are embedded and stabilized in a lithium matrix<sup>1</sup>. Indeed, this compound contains a surprising solution to the famous carbyne problem. At room temperature the boron chains are disordered, giving rise to diffuse scattering in the corresponding X-ray and neutron powder diffraction patterns. At about 150 K a second order phase transition takes place which leads finally to the formation of an incommensurate composite structure. The crystal structures at 2 K of both sublattices were determined from the neutron diffraction experiment and refined in the space group  $P-1(\alpha\beta\gamma)$ .



[1] Wörle M., Nesper R. "Infinite Linear Unbranched Borynide Chains in  $\text{LiB}_x$  – Isoelectronic to Polyene and Polycumulene", *Angewandte Chemie*, in press

**s1.m1.p12** New incommensurate misfit layer oxides in the system (Bi, Ca, Co, O). S. Lambert, H. Leligny, D. Grebille, Lab. CRISMAT (UMR CNRS 6508), ISMRA, 14050 CAEN Cedex.  
Keywords: misfit, incommensurate, oxide.

Recently, a new family of oxide composite structures has been discovered in the  $[\text{Bi}-(\text{Sr,Ca})\text{-Co-O}]$  and  $[\text{Tl}-(\text{Sr,Ca})\text{-Co-O}]$  systems and characterized by E.M. and EXAFS observations<sup>1,2</sup>. It shows strong analogies with the well known family of misfit layered chalcogenides  $(\text{MX})_{1+x}(\text{TX}_2)_m$  with the alternate stacking along *c* of pseudo-hexagonal layers and rock-salt type layers, sharing the same *a* parameter but exhibiting two incommensurate periodicities along *b*.

A first structural study of the  $[\text{Bi}_{0.87}\text{SrO}_2]_2[\text{CoO}_2]_{1.82}$  phase in the 5D superspace formalism was carried out using single crystal X-ray diffraction data.<sup>4</sup>

A more systematic investigation of these families has been carried out. Single crystals and powder samples of the prototype phase  $\text{Ca}_3\text{Co}_4\text{O}_9$  and of a Bi substituted phase ( $\text{Bi}_{0.11}\text{Ca}_3\text{Co}_{3.7}\text{O}_9$ ) have been synthesized. A characterization of the symmetry of these phases will be presented using Weissenberg or precession photographs and synchrotron X-ray diffraction patterns. The symmetry of the Bi free phase is monoclinic ( $a = 4.85 \text{ \AA}$ ,  $b = 4.55 \text{ \AA}$ ,  $c = 10.74 \text{ \AA}$ ,  $\beta = 98^\circ$ ) and the sample presents a twinning phenomenon. Some extra reflections are observed in the common  $(a^*, c^*)$  plane and can be explained assuming an intrinsic modulation within the RS sublattice. The Bi substituted phase, in spite of a weak substitution rate and of very close values of the cell parameters, shows a different orthorhombic symmetry. A first description of this structure is proposed.

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[2] Boullay Ph. *Chem. Mater.* Chemical and physical aspects of the misfit layer oxides  $\text{Tl}_x[(\text{Sr}_{1-y}\text{Ca}_y)\text{O}]_{1+x}(\text{CoO}_2)$  (1998) 10 : 92-102

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[4] Leligny H., A 5D structural investigation of the misfit layer compound  $[\text{Bi}_{0.87}\text{SrO}_2]_2[\text{CoO}_2]_{1.82}$ , *Acta Cryst* (2000) B56, in press.