

investigation of the B_2O_3 -CuO- Li_2O ternary system". [3] N. A. Kuratieva, D. Mikhailova, H. Ehrenberg, "A new polymorph of $Cu_3B_2O_6$ ", *Acta Cryst. C* 65 (2009) 185-186. [4] Behm, H. (1982). *Acta Crystallogr. B* 38, 2781, "Pentadecacopper (II) Bisborate Hexaorthoborate Dioxide".

Keywords: Jahn-Teller distortion of Cu(II), layered structure, anisotropic thermal expansion

FA2-MS16-P42

Crystallographic Orientation Relationship between Bastnaesite, Fluocerite and Cerianite in a Single Crystal from the Pikes Peak Pegmatites. Mathis M. Müller, Hans-Joachim Kleebe. *GeoScience, Technical University Darmstadt, Germany.*

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A fluocerite (Ce,La)F₃ single crystal intergrown with bastnaesite (Ce,La)[CO₃]F from the Pikes Peak area in Colorado, USA was prepared for the investigation of the crystallographic orientation relationship between the two mineral phases via transmission electron microscopy. The epitaxial overgrowth of bastnaesite on fluocerite was confirmed by evaluating the electron diffraction patterns of the relevant mineral phases. During the examination, a third mineral phase, which was unexpected in this phase assemblage, was detected and identified as cerianite CeO₂ by EDS in conjunction with electron diffraction. Its orientation relationship to the main mineral phases can be described as a syntactical growth. The La-concentration of the bastnaesite changed with the distance from the cerianite interface, as confirmed by EDS. The reduction of La-content near the interface together with the respective crystallographic relationship yielded a model explaining the formation of the encountered mineral assemblage of bastnaesite, fluocerite and cerianite. The orientation matrix and the direction-plane relation for the three mineral phases was established.

Keywords: bastnaesite, orientation relationship, orientation matrix

FA2-MS16-P43

Ordering in intercalated Co atoms and electron density distributions of layered compounds Co_xTiS₂

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A structural study of layered compounds Co_xTiS₂ (x=0.26,0.43, and 0.57) by X-ray diffraction analysis was performed to investigate both the ordered atomic arrangement and disordering behavior of intercalated Co atoms, and the nature of the chemical bond from the electron density distribution (EDD) obtained by the maximum entropy method. The 2ax2ax2c superstructure of the Co atoms is observed for x=0.26 and 0.57, and disappears at 510 and 550K, respectively. On the other hand, $\sqrt{3}ax\sqrt{3}ax2c$ superstructure of the Co atoms is observed for x=0.43, and disappears at 610 K. It is understood that the type of the transition is second-order-like. The overlapping of the EDD between Co and S atoms & Ti and S atoms are clearly seen, which are corresponding to the covalent bonding in the van der Waals gap layer and in the TiS₂ one. It is expected that nature of covalent bonding

between Co and S atoms causes decreasing of the interlayer distance.

Keywords: layered compounds, ordering of the Co atoms, EDD

FA2-MS16-P44

Structural trends in the (emim)_m[A_n(Mo₈O₂₆)] (emim = 1-ethyl-3-methylimidazolium; m=2,3; n=1,2; A=K, Rb, Cs) group of compound. Anna Pakhomova, Sergey Krivovichev. *Saint-Petersburg State University, Russian Federation.*

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Polyoxometalates (POMs) have many properties that make them attractive for applications in medicine, biology, magnetism, materials science and catalysis. POMs are a kind of competent structure-tunable building block because they exhibit a wide variety of structural motifs of different sizes and topologies. As far as we know, all known octamolybdates has been synthesized by hydro- and solvothermal methods. To the best of our knowledge, ionothermal methods were not used, although they recently have shown high promise in the preparation of novel metal-organic frameworks.¹ We have used ionic liquid (emim)Br (emim=1-ethyl-3-methylimidazolium) as both solvent and template for the purpose of construction of novel organic-inorganic polymolybdates of alkali metals. The three novel octamolybdates (emim)₃K(Mo₈O₂₆) (1), (emim)₃Rb(Mo₈O₂₆) (2) and (emim)₂Cs₂(Mo₈O₂₆) (3) (emim = 1-ethyl-3-methylimidazolium) have been obtained in the ionothermal reactions. The structures of these compounds are described on the basis of octamolybdate anions [β -Mo₈O₂₆]⁴⁻. In compounds 1 and 2, [β -Mo₈O₂₆]⁴⁻ units are linked by metal cations to form chain structures, while Cs cations in the compound 3 link to polyoxoanions to form layer structure.

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[1] Ranham E.R.; Morris R.E. *Acc. Chem. Res.* 2007, 40, 1005.

Keywords: ionothermal synthesis, alkali polyoxomolybdates, X-Ray crystal structure determination

FA2-MS16-P45

Comparison of HP data for X-ray diffraction in Beand diamond-backed DACs. Benedetta Periotto^a,

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High-pressure cells reduce significantly the accessible reciprocal space in single-crystal studies and, moreover, the parts of cells traversed by radiation produce as a rule strong background features. In order to increase the quality of measured data and accuracy of calculated structural parameters it is of primary importance to reduce these deleterious effects. In Diamond Anvil Cells (DAC) diamond anvils must be supported by a strong and X-ray transparent