MS10.07.04 HIGH OPTICAL NONLINEARITIES IN ALUMINUM BORATE CRYSTALS. Douglas A. Keszler, Ki-Seog Chang, Department of Chemistry, Oregon State University, Corvallis, OR 97331- 4003

We have structurally characterized new aluminum borate crystals having optical second-order susceptibilities predicted to be near 2 pm/V. These nonlinearites are among the higher values for borate crystals, comparable to that of BaB_2O_4 (BBO, d_{22} = 1.8 pm/V) and exceeding those of LiB_3O_5 (LBO, d_{32} = 1.17 pm/V), and $CsLiB_6O_{10}$ (CLBO, d_{36} = 1 pm/V). Structures, crystal chemistry, optical properties, and prospects for large-scale crystal growth will be discussed.

MS10.07.05 ELECTRO-OPTIC CRYSTALS. L. Bohaty, Institut für Kristallographie, Universität zu Köln, Zülpicher Str. 49b, D-50674 Köln, Germany

A very stimulating question for crystallography and one of the most important goals of material science is to find strategies for searching for crystals with desired properties. A direct conversion of physical models into practicable criteria for "tailoring" new crystals usually fails because of the structural complexity of most crystals. Here, the application of crystallographic aspects can be very helpful. As part of our systematic investigation of nonlinear optical and electro-optic properties we have determined the complete linear electro-optic tensors (all components and signs) of more than 60 inorganic and "semiorganic" crystals in the last few years. This broad basis of experimental data enables us to analyse the linear electro-optic effect especially from the crystal-chemical point of view. In particular, we have focused our attention on the elasto-optic-piezoelectric contribution $P_{ijmn}\, d_{kmn}$ of the "unclamped" electro-optic effect ${}^{r}\sigma_{ijk} = {}^{r}\varepsilon_{ijk} + P_{ijmn}\, d_{kmn}$ and its importance for the total value of ${}^{r}\sigma_{ijk}$ ($[P_{ijmn}]$ = elasto-optic tensor, $[d_{kmn}]$ = piezoelectric tensor, $[{}^{r}\varepsilon_{ijk}]$ = "clamped" electro-optic tensor (at constant strain ε), $[{}^{r}\sigma_{ijk}]$ = "unclamped" electrooptic tensor (at constant stress σ)). One method of analysis which has proved very successful is the use of longitudinal and transverse effects, their representation as surfaces and the extraction of the extreme values. In addition, statistical analysis of more than 20.000 inorganic crystal structures with respect to the geometry and symmetry of the constituents (ions, molecules, complex groups, etc.) and to the resulting symmetry of the crystal structure make plain the important role of polar constituents and asymmetric groups for noncentrosymmetric crystals and, consequently, for new electro-optic materials. Valuable information which can be used in a systematic search for new inorganic and "semiorganic" electro-optic materials was obtained.

PS10.07.06 NEUTRON DIFFRACTION OF $KTiOPO_4$ AND ISOMORPHS. Jenni Almgren, Goran Svensson, Jorgen Albertsson, Dept of Inorganic Chemistry, Chalmers University of Technology, S-412 96 Goteborg, Sweden.

This neutron diffraction study on potassium titanyl phosphate ($KTiOPO_4$, KTP) and its analogues $RbTiOAsO_4$ (RTA) and $CsTiOAsO_4$ (CTA) was made at the Studsvik Neutron Research Laboratory (Uppsala, Sweden). Data from powder samples have been collected in the range $0< 2\theta <129°$, with a step size of 0.08° at a temperature of 295 K. Neutron diffraction has been used to retrieve a better understanding of structure and property relationships such as accurate metal to oxygen distances. Refinement of the data sets by the Rietveld method is in progress.

Crystallographic studies of the KTP isomorphic family are part of a project at our department engaged in producing the materials and then investigating physical and chemical properties. The obstacles for technological use of RTA and CTA are the difficult and expensive growth techniques needed to produce these crystals. We have built two four-zone furnaces to accomodate top seeded solution growth of single crystals of CTA and RTA from self fluxes. Our objective is to obtain single crystals of optical quality and improved size by optimizing growth parameters.

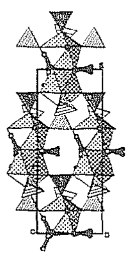
KTP has non-linear optical (NLO) properties and is commercially used as waveguides in integrated optical devices. The active site in the crystal structure, for second harmonic generation, is the slightly deformed octahedron of oxygen atoms around titanium. Arsenate isomorphs of KTP such as RTA and CTA have different NLO-properties compared to KTP and the arsenate analogues give frequency conversion in a broader wavelength region. The development of blue light generating solid state laser is needed to further increase information storage and transmission. The isomorphs RTA and CTA can be used in LIDAR technology, optical parametric oscillation devices and tunable lasers.

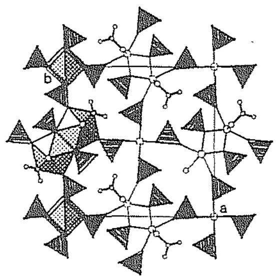
PS10.07.07 CAN SMALL ORGANIC MOLECULES INTRODUCE NONLINEARITY INTO AN INORGANIC MATRIX?— By Olyana Angelova, CL of Mineralogy and Crystallography, BAS, Rakovski 92, 1000 Sofia, Bulgaria

New addition compounds with potential nonlinear optical properties in the ternary systems $M(ReO_4)_2$-L-H_2O, where M =Ca, Sr, Ba, Pb, Cd; L = urea (U), thiourea (Tu) or similar polarizable organic molecules have been prepared and structurally characterized. Among the variety of centrosymmetric adducts of the general type $xM(ReO_4)_2.yL.zH_2O$ investigated so far the only noncentrosymmetric species are those with partial content of L, e. g. $2M(ReO_4)_2.3U.2H_2O$ (I), M = Sr, Pb, and $3Pb(ReO_4)_2.2Tu.2H_2O$ (II).

I crystallizes as a layered structure of the type $[M_2T_4f_3]f'_2$ 2, T $=ReO_4$, f = Urea, f' = H_2O (space group Fdd2) and contains specific triple M-O-M bridges imposing stable departure from centrosymmetricity.

The framework structure of **II** (P 42_1m) consists of two types of chains running along the c-axis: $[MT_4]$ and $[M_2T_2f_2]f'_2$, f = Tu, f' = H_2O. The Tu molecules are built within the pseudo-centrosymmetric $[M_2T_2f_2]f'_2$ chains but are H-bonded to the non-centrosymmetric $[MT_4]$ ones.





In both compounds the amount of organic molecules is unsufficient for achievement of centrosymmetric arrangement of the structural units but enough to perturbate the antiferroelectric ionic structure. The immanent polarizability of the organic molecule can be the key factor to obtain a large permanent crystal polarization if it is favoured by its orientation within the inorganic matrix.