FA2-MS02-P01

The Crystal Chemistry of Huntite-like $RM_3(BO_3)_4$ Polytypes. Elena Yu. Borovikova[a], Victoria S. Kurazhkovskaya[a], Elisaveta V. Koporulina[a], Nikolay I. Leonyuk[a], Elena L. Belokoneva[a]. [a]*Department of Crystallography and Crystal Chemistry, Moscow State University. Russia.*
E-mail:amurr@mail.ru

The rare earth borates with the common formulae $RM_3(BO_3)_4$, where R – Nd, Ga, Y, and M – Al, Ga, Cr, Fe, isostructural to natural mineral huntite are studied by IR spectroscopy method. The interest to the new rare earth borates causes by the combination of their functional characteristics - nonlinear optical, laser, active-nonlinear, etc. – in a combination to high thermal, chemical both mechanical stability and unique heat conductivity [1]. The given phases crystallize in space group R32 or C2/c. Compounds with rhombohedral structure are formed at the lowest temperatures up to ~880 – 900^0, phases with symmetry C2/c crystallize at higher temteratures ~1040 - 1050^0. The comparison of structures [2] has shown that they have polytypic nature and are described in the best way in order-disorder terms [3]. Only rhombohedral phases with huntite structure (R32) possess the important physical properties. These phases cannot be divided by the powder X-ray diffractometry methods. On the basis of the prepared factor-group analysis the we have assigned the bands, characteristic for compounds with the different space groups. IR spectra of the both rhomboedral and monoclinic phases often contain bands with low intensity, characteristic for another polytype. This fact is the evidence that inclusions of one polytype in another are characteristic for studied borates. Rhombohedral polytype with different octahedral cations and different rare-earth elements can be both homogeneous, and containing inclusions of the opposite ordered layers. In borates with the small cation Al, irrespective of type of a rare-earth element, always there are fragments of monoclinic phases. Almost homogeneous rhombohedral phases can be obtained with larger octahedral cations Ga, Cr and more particularly Fe. Among the rare-earth elements the larger Nd assists the inclusion of monoclinic ordered layers to rhombohedral polytype. Nd – Al and Nd – Cr borates are characterized by monoclinic structures, but at the same time they may contain some fragments with an arrangement of layers, characteristic for rhombohedral phases. Thus, revealed earlier polytypic character of structures of investigated borates, representing uniform family, and described by the law of theory OD - an order-disorder - finds convincing acknowledgement at research IR of spectra of crystals.

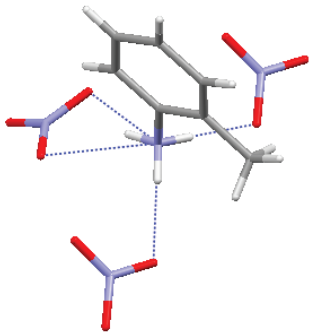
[1] Popova E.A, Leonyuk N.I., Popova M.N. et al., *Phys. Review B.* **2007**, 76, 1 [2] Belokoneva E.L., Timchenko T.I. *Crystallography* 1983, 28, 6, 1118 (in Russian). [3] Dornberger – Shiff K., *Deutsche A.*, Akad. Wiss. Berlin **1964**, 3, 1.

Keywords: infrared spectroscopy; polytypism; rare-earth compounds

FA2-MS02-P02

Structural Study of Amino Acid Salts Consisting of Mineral Anions. Rim Benali-Cherif[a], Amani Direm[a], Nourredine Benali-Cherif[a]. [a]*Institut des Sciences et Technologie. Centre Universitaire de Khenchela 40000, Algeria.*
E-mail: rym_46@hotmail.com

Amino acids are interesting materials for NLO applications. Their importance is due to the fact that all the amino acids have chiral symmetry and several compounds crystallize in noncentro-symmetric space groups [1]. Thus, salts of amino acids with different organic/inorganic acids have been explored.
Several new complexes incorporating natural amino acids and mineral anions have been recently crystallized [2] and their structural, optical [3], thermal properties and structural phase transitions [4] have been investigated.
In this present work, which is part of project of searching for potential new hybrid compounds obtained by the addition of amino acids with mineral acids, we will discuss crystalline structures of new salts based on mineral anions and natural amino acids reported in the CSD Database.
All materials of this type are characterized by the presence of strong N–H…O hydrogen bonds (Figure below) connecting anionic and cationic entities together which participate in the stability and the cohesion of crystal structures.



N–H…O interactions in 2-Methylanilinium nitrate [5].

[1] Bhat M.N., Dharmaprakash S.M., *J. Cryst. Growth*, **2002**, 236, 376–380. [2] Rodrigues V. H., Cardoso C., Paixão J. A., Costa M.M.R.R., *Acta Cryst*, **2007**, C63, o243-o245. [3] Bouchouit K., Sofiani Z., Derkowska B., Abed S., Benali-cherif N., Bakasse M., Sahraoui B., *Opt. Commun.*, **2007**, 278, 180-186. Perpétue G. J., Janczak J., *Acta Cryst*, **2004**, C60, 768. [4] Baran J., Drozd M., Głowiak T., S'ledz' M., Ratajczak H., *J. Mol. Struct*. 372, 131. Mylrajan, M. Srinivasan T.K.K., *J. Raman Spectrosc*., **1985**, 16, 412. [5] Benali-Cherif N., Boussekine H., Boutobba Z., Kateb A., *Acta Cryst*, **2007**, E63, o3287.

Keywords: natural amino acids; hydrogen bonds; hybrid compounds; X-ray diffraction

FA2-MS02-P03

New Structural Features in $RbCr^{III}(C_2O_4)_2(H_2O)_2$ (II). Malika Hamadène[a], Hamza Kherfi[a], Achoura Guehria-Laïdoudi[a], Slimane Dahaoui[b], Claude Lecomte[b]. [a]*Laboratoire de Cristallographie-Themodynamique ,USTHB, Alger, Algérie.* [b]CRM^2 ,