

Poster Presentations

[MS24-P03] **Serine co-crystals under extreme P-T conditions.** Sergey G. Arkhipov^{1,2}, Boris A. Zakharov^{1,2} and Elena V. Boldyreva^{1,2}

1. REC-008, Novosibirsk State University, Novosibirsk, 630090, Russian Federation;

2. Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, 630128, Russian Federation.

E-mail: arksergey@gmail.com

This work is devoted to the preparation and study of crystals of molecular complexes of amino acids. Cocrystals and salts of amino acids are very promising models to study the regularities in the formation of salts and cocrystals. The presence of amino-, carboxylic- groups, and also various side chains makes it possible to produce a rich variety of crystal structures with homomolecular and heteromolecular contacts. Multicomponent serine crystals can be considered as biomimetics when analyzing relation between crystal structures, hydrogen bonding, and sidechain mobility. Besides, some of them are promising as molecular materials with piezoelectric, ferroelectric, nonlinear optical properties, or as biologically active compounds. The systems are also of fundamental interest for crystal engineering. Their structures can help to understand the role of the presence of several potential hydrogen-bond donors and acceptors, as well as of the shapes and flexibility of molecules in forming a certain molecular packing in multicomponent crystals. Experiments with systematic temperature and pressure changes can provide valuable information about the behavior of the hydrogen bonds in the structures under study. These researches allow us to understand the relationship "structure-property" and in particular to compare the behavior of the hydrogen bonds in mixed crystals as compared with crystals of the individual components.

In the present contribution we describe crystallization of two new multi-component crystals (L-serinium semi-maleate (I), and DL-

serinium semi-maleate (II), $C_3H_8NO_3^+C_4H_3O_4^-$), and the results of solving their structures [1]. They provide the first example of the chiral and racemic anhydrous serine salts with the same organic anion. A comparison of their crystal structures with each other, and also with the structures of pure components (L-serine polymorphs, DL-serine, maleic acid, and other amino acids maleates) is important for understanding the formation of crystal structures, their response to variations of temperature and pressure, and structure-properties relations. Both in (I) and in (II), there are chains $C_2^2(12)$ and $C_2^2(12)'$. In (I) chains $C_2^2(12)'$ look like springs and account for interesting

response of this structure with respect to P, T variations, which was followed by X-ray diffraction and Raman spectroscopy. Some data were compared with the existing data obtained for the individual components constituting the mixed crystal as well as with to some of the results obtained for other structures of serine.

This work was supported by a grant from Ministry of Education and Science of Russia (14.B37.12.1093), by RFBR (grant 12-03-31541 mol_a), by Department of Chemistry and Materials Sciences of the Russian Academy of Science (projects No. 5.6.4. and No. 22.44) and by a grant of President of Russia for Russian leading Scientific Schools (project NSh-221.2012.3).

[1] Arkhipov, S., Zakharov, B., Boldyreva E. (2013) *Acta Cryst.* **C69**, 517-521.

Keywords: mixed crystals, amino acids, high pressure, low temperature.