Poster Presentation

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Low temperature and high pressure study of three molecular glycine co-crystals

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Only three glycine co-crystals with carboxylic acids were reported till now: those with glutaric[1a], DL-tartaric[1b] and phthalic acids[1c]. Co-crystallisation of glycine with some other carboxylic acids (oxalic, malonic, maleic) gives molecular salts. The reason why the three selected carboxylic acids form not salts, but co-crystals with glycine remains unclear. No obvious correlations with any physiochemical properties of acidic co-formers such as solubility, acidity, dissolution rate, geometry of molecule, etc. could be suggested. Intermolecular interactions in these crystals are of great interest and can be probed, in particular, by varying temperature and pressure in a wide range. The effect of pressure and temperature on a co-crystal of glycine with glutaric acid was investigated in our research group under low temperatures[2] and high pressure[3] and a first order phase transition giving the same new polymorph was observed (at 220 K and 1.75 GPa, respectively). No variable-temperature or variable-pressure studies of co-crystals of glycine with DL-tartaric and phthalic acids were reported. The aim of the present study was to compare the behavior of three glycinium co-crystals at low temperature and high pressure. The changes in the unit cell volumes and parameters, as well as in the geometry of the hydrogen bonds were analysed. The orientation of principal axes of strain ellipsoid with respect to the main structural motifs and relative linear strain values along these axes were calculated. The conformations and the local environment of glycine molecules, as well as the hydrogen-bonded motifs were compared for three co-crystals. The work was supported by the Russian Foundation for Basic Research (RFBR) (Grants № 14-03-31866 mol_a, 13-03-92704 IND_a), Russian Ministry of Science and Education and Russian Academy of Sciences.

[1] *E. Losev, B. Zakharov, T. Drebushchak et al., Acta Cryst., 2011, C67, o297–o300.,* ***[2]*** *B. Zakharov, E. Losev, B. Kolesov et al., Acta Cryst., 2012, B68, 287-296.,* ***[3]*** *B. Zakharov, E. Losev, E. Boldyreva, CrystEngComm, 2013, 15, 1693-1697.*

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