MS20-P7 Glycine co-crystals at low temperature and high pressure: X-ray diffraction and spectroscopic study

Evgeniy A. Losev[1], Boris A. Zakharov[1,2], Elena V. Boldyreva[1,2]

1. Institute of Solid State Chemistry and Mechanochemistry SB RAS, Kutateladze, 18, Novosibirsk, 630128, Russia
2. REC-008, Novosibirsk State University, Pirogova, 2, Novosibirsk, 630090, Russia

email: losev.88@mail.ru

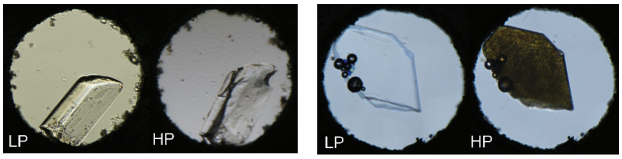
There are three “true” co-crystals of glycine with carboxylic acids (with no proton transfer from acidic component to basic one) reported up to now: those with glutaric (GG), DL-tartaric (GT) and phthalic (GP) acids. The co-crystal of glycine with glutaric acid was obtained in two research groups independently [1, 2]. The behaviour of this co-crystal at low temperature and high pressure was investigated in our laboratory previously and first order phase transition was discovered [3, 4].

The present study was focused on the effect of variations in temperature and pressure on two other co-crystals of glycine - with DL-tartaric and phthalic acids. Both co-crystals were stable on cooling down up to 100 K. The changes of unit cell parameters and in the geometry of the hydrogen bonds were followed. No phase transitions were detected, in contrast to GG co-crystal.

The effect of pressure on selected co-crystals was much more significant. The two molecular co-crystals underwent reversible phase transformations at quite low pressures. The phase transitions were accompanied by fracture (Fig. 1). Despite this, the crystal structure of the high-pressure phase of GT co-crystal could be solved by single crystal X-ray diffraction. The changes in the structure as compared with the low-pressure phase were analysed in terms of molecular conformations and hydrogen bonded motifs. However, it was impossible to solve the structure of GP co-crystal after the high-pressure phase transition, due to a complete fracture of the single crystal, although Raman spectra could be measured for the new phase. The crystal structures of high-pressure phases of glycine co-crystals were compared with each other. The features of structural rearrangement and changes in hydrogen bond network were analysed using X-ray diffraction and spectroscopic data.

The work was supported by the Russian Foundation for Basic Research (RFBR) (Grant No. 14-03-31866 mol-a).

[1]Losev, E.A., Zakharov, B.A., Drebushchak, T.N., Boldyreva, E.V. Acta Crystallogr., Sect. C: Cryst. Struct. Commun., 2011, 67 (8), pp. o297-o300. [2]Riscob, B., Shakir, M., Kalyana Sundar, J., Natarajan, S., Wahab, M.A., Bhagavannarayana, G. Spectrochim. Acta, Part A, 2011, 78 (1), pp. 543-548. [3]Zakharov, B.A., Losev, E.A., Kolesov, B.A., Drebushchak, V.A., Boldyreva, E.V. Acta Crystallogr., Sect. B: Struct. Sci., 2012 68 (3), pp. 287-296. [4]Zakharov, B.A., Losev, E.A., Boldyreva, E.V. CrystEngComm, 2013, 15 (9), pp. 1693-1697.



I II

Figure 1. The destruction of glycine co-crystals under high pressure. I – glycine-DL-tartaric acid co-crystal, II - glycine-phthalic acid co-crystal. LP – low-pressure phase, HP - high-pressure phase

Keywords: high-pressure, glycine, co-crystal, hydrogen bond