Poster Presentation

MS17.P05

The effects of pressure on structural strain in crystals with acetamide groups

L. McGregor^{1,2}, B. Zakharov^{2,3}, C. Boa^{1,2}, S. Goryainov⁴, E. Boldyreva^{2,3}, C. Pulham¹

¹University of Edinburgh, School of Chemistry, Edinburgh, UK, ²Novosibirsk State University, Novosibirsk, Russia, ³Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia, ⁴Institute of Geology and Mineralogy SB RAS, Novosibirsk, Russia

Polymorphism is an ever growing area of interest in chemistry. Many active pharmaceutical ingredients (APIs) have the potential to have polymorphic forms, which can subsequently be used to the advantage of the pharmaceutical industry. There are a variety of conditions in which polymorphism can be examined; one way which has sparked interest in recent years is the influence of pressure and its effect on the behaviour of intermolecular bonds. The polymorphs of paracetamol were the first solid drugs for which the properties were compared at different pressures [1-2]. Another interesting research direction involves the comparison of the structural response to pressure of a series of chemically different compounds with similar molecular fragments, but possessing different molecular packing and intermolecular interactions. This is important for crystal engineering and for understanding structure-properties relationships. In the present study, we compare the response to pressure of a series of paracetamol, two polymorphs of acetotoluidine, polymorphs and a hydrate of metacetamol, methacetin, and phenacetin. Both single-crystal Raman spectroscopy and X-ray diffraction were used. The effects of various pressure media have also undergone examination. The study was supported by the Year Abroad Programme of the University of Edinburgh (LM, CB), Russian Ministry of Science and Education and Russian Academy of Sciences (BAZ, SVG, EVB).

[1] E.V. Boldyreva, T.P. Shakhtshneider, M.A. Vasilchenko, et al., Acta Cryst. B, 2000, 56, 299-309., [2] E.V. Boldyreva, T.P. Shakhtshneider, H. Ahsbahs, et al., J. Therm. Analys. Calorim., 2001, 68, 437-452.

Keywords: phase transitions, high pressure, lattice strain