MS43.O02

Varying experimental conditions to study interactions in the solid state

E. Boldyreva[1]

[1]*Novosibirsk State University, Chair of Solid State Chemistry, Novosibirsk, Russia; Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia*

Supramolecular interactions in the solid state attract much attention. Different experimental and computational approaches are used, to predict and to design crystal structures, to predict the properties based on molecular and crystal structures, to range different types of intermolecular interactions. Analysis of the crystal structures at fixed (e.g. ambient) temperature and pressure conditions is most common for experiments, whereas most DFT calculations are limited to 0 K, to minimize computational costs. At the same time, evolution of a crystal structure as a function of experimental conditions can contribute significantly to understanding the structure-forming role and relative energies of different types of intermolecular interactions in the same crystal structure and of similar interactions in a series of different but structurally or chemically related compounds. In the present invited contribution I attempt to illustrate this using several selected examples from my own practice and from the papers published by other research groups. I consider, in particular, the results of variable-temperature and variable-pressure studies of continuous lattice strain and phase transitions in small-molecule organic compounds, the results of variable-temperature and variable-pressure crystallization, the results of comparing the dissolution profiles of mono- and multi-component small-molecule organic crystals. I shall also discuss how variable-temperature and variable-pressure experimental diffraction data can assist in optimizing the calculations aimed at comparing the relative stability of polymorphs and predicting polymorph transitions. The study was supported by Russian Ministry of Science and Education and Russian Academy of Sciences.

Keywords: low temperature, high pressure, dissolution and crystallization