MS34. Growth, structure and application of multi-component crystals

Chairs: Christopher Frampton, Tomislav Friščić

MS34-P1 Structure, stability and physicochemical properties of phenyleneboronic acids cocrystals with NO-compounds

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Organoboron compounds have been known for about 150 years and found a widespread use in synthetic organic chemistry,[1] in supramolecular chemistry, or medicine. In turn, N-oxides of various heterocyclic compounds are important due to their vast applications as protective groups, oxidants or ligands in coordination complexes.[2] Both classes of compounds are eager to form hydrogen bonds. It is therefore interesting to testify whether it is possible to combine them together into solid-state systems of desired properties (e.g. increased biological activity or solubility). Consequently, the purpose of this study was to co-crystallize phenylenediboronic acids with a series of aromatic N-oxides. 12 new cocrystals were obtained and structurally characterized. Their crystal networks are stabilized by an extended net of hydrogen bonds usually forming layers further interacting via pi-stacking. Most of the structures contain water molecules biding acid and N-oxide molecules together. Ortho- diphenyloboronic acid is much more resistant to form cocrystals with N-oxides than its para-analogue and creates much less predictable cocrystal structures. A truly remarkable result of the fused ortho-phenylenediboronic acid and its semi-anhydride incorporated into the cocrystal structure is reported. For all of the studied systems a comprehensive analysis of crystal packing and energetic features was conducted. The nature of intermolecular interactions was additionally investigated via the Hirshfeld surface approach. The obtained theoretical results were confronted with that of the TGA-DSC experiments.

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