MS36-O2 Systematic investigations on molecular crystals of boronic acids

Izabela D. Madura[1], Karolina Czerwińska[1], Janusz Zachara[1]

1. Warsaw University of Technology, Faculty of Chemistry

email: izamadura@gmail.com

Boronic acids of general formulae *R* -$B(OH)_2$ (*R* either aromatic or aliphatic) are the compounds of widespread applications starting from organic synthesis (including Suzuki-Miyaura cross-coupling reactions[1]) through medicinal chemistry[2] to molecular recognition processes[3] and crystal engineering[4]. The role in the latter will be discussed on the basis of systematic investigations on boronic acids crystals. Up-to-date there are around 300 boronic acids structurally characterized, thus comprising a valuable set for statistical survey.

The data will be analyzed using a bond-valence vector approach[5] to ascribe the observed subtle molecular changes. Further, a hierarchical structure of these crystals will be presented with a discussion of a role of basic and large supramolecular synthons.[6,7] It is important to note that in the case of boronic acids the basic synthons are mainly formed by O–H…O hydrogen bonds, which in combination with other interactions can form large synthons of variable dimensionality. In the case of fluoro-substituted phenylboronic acids the structure of the basic synthon was shown to interplay with the form of large synthons.[8] In turn, the latter are said to act as intermediates between small synthons and crystal growth units, thus their investigation may comprise a preliminary studies on crystallization processes.[9]

The general rules will be illustrated with our own results of newly designed co-crystals and obtained polymorphic forms. The results of temperature dependant studies on the large synthons' structure will be also presented.

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Keywords: crystal engineering, co-crystals, molecular crystals, hierarchical structure, large supramolecular synthons, hydrogen bonding, boronic acids, weak interactions

MS36-O3 In situ visualisation & evaluation of intermolecular interactions in 3D

Peter A. Wood[1], Ghazala Sadiq[1], Colin R. Groom[1], Suzanna C. Ward[1]

1. Cambridge Crystallographic Data Centre

email: wood@ccdc.cam.ac.uk

The crystallographic community has now shared over 750,000 small molecule structures and these structures contain many millions of intermolecular interaction observations within them. By using this structural information to best effect we can both predict likely intermolecular interaction behaviour prior to crystallisation and also evaluate observed interactions in a new crystal compared to the structures that have been determined before.

Using the CSD interaction knowledge base IsoStar as the underlying data, Full Interaction Mapping in Mercury provides rapid visualisation of interaction preferences within a small molecule crystal structure. This approach provides a visual and intuitive way to understand and investigate intermolecular interactions in a crystal including hydrogen bonds, halogen bonds, stacking interactions and van der Waals contacts.

This presentation, timed to coincide with the 50th anniversary of the Cambridge Structural Database, will demonstrate the breadth of applicability of Full Interaction Mapping and the depth of insight that can be gained, using recently published structures as examples.

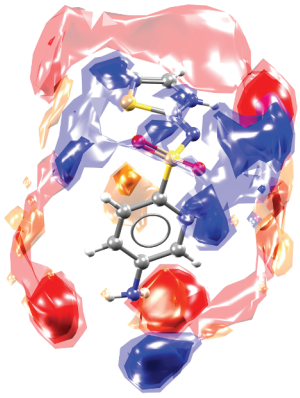

Figure 1. Full Interactions Maps displayed around the molecular conformation of sulfathiazole

Keywords: crystal engineering, intermolecular interaction, hydrogen bond, halogen bond