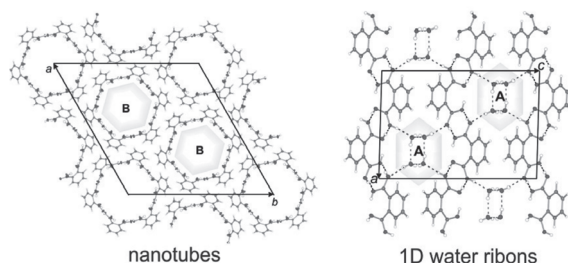
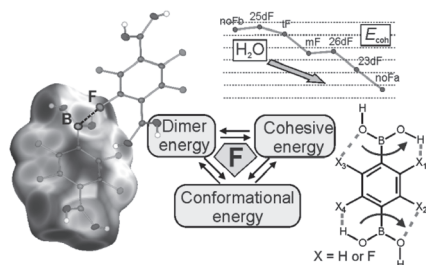


MS23-P4 Structural and energetic landscape of diboronic acids. Krzysztof Durka,^a Katarzyna N. Jarzemska,^b Radosław Kamiński,^b Sergiusz Luliński,^a Janusz Serwatowski,^a Krzysztof Woźniak,^b ^aDepartment of Chemistry, Warsaw University of Technology, ^bDepartment of Chemistry, University of Warsaw, Poland, E-mail: kdurka@gmail.com

The understanding of molecular organization in the solid state enables to control supramolecular entity formation and to produce crystal networks with desired structural features and properties. On particular interest are molecular building units, which by strong and directional intermolecular hydrogen interactions tend to form open networks (HOF) with substantial space for the inclusion of guests.^[1] Such situation occurs for 1,2-phenylenediboronic acid. We found that this compounds crystallizes in three different pseudopolymorphic forms: a) closely packed structure, b) microchannel structure with unique arrangement of water molecules, regarded as a 1D ribbons and c) nanotubular HOF structure (see below).



Apart from relatively strong hydrogen bonds, as these present in the structures of boronic and diboronic acids, also weaker interactions, e.g. involving fluorine atom, are of current interest in modern supramolecular chemistry.^[2] We present the results of X-ray crystallographic and computational studies of a series of fluorinated 1,4-phenylenediboronic acids. It seems that fluorine substituents tend to interact with the electropositive boron atom. Furthermore, intramolecular interactions significantly affect the torsion angle of the B(OH)₂ group. The constrained energy scan revealed that stronger interactions with substituents stabilize the planar conformation and hamper the rotation of the boronic group. This, in turn, has a further impact on the interactions within selected crystal motifs and supposedly rules the proton disorder within boronic fragments. The energy of appropriate dimers vary from -15 kJ·mol⁻¹ to -25 kJ·mol⁻¹.



- [1] Fournier J.-H., Maris T., Wuest J. D., Guo W., Galoppini E., (2003) *J. Am. Chem. Soc.*, 125, 1002-1006,
 [2] Chopra D., (2012) *Cryst. Growth&Des.*, 12, 541-546.

Keywords: boronic acids, organic fluorine, hydrogen-bonded organic framework

MS23-P5 High pressure crystallography 2.0: harnessing the power of the crystallographers' community. Kamil F. Dziubek, Andrzej Katrusiak Faculty of Chemistry, Adam Mickiewicz University, ul. Grunwaldzka 6, 60-780 Poznań, Poland E-mail: rumianek@amu.edu.pl

Although the interest in high pressure structural studies steadily grows, the fraction of crystals investigated at elevated pressure is still very low. Of over 600,000 structures deposited in Cambridge Structural Database [1] only about 1.5 per mil is associated with the 'pressure' descriptor. Therefore, we have decided to encourage the participants of the "Frolic Goats Workshops on High-Pressure Diffraction" (the event held in our Department annually since 2008 [2]) to work together on a common goal [3]. Since the contributors are coming from different places, equipped with various facilities (radiation sources, diffractometers, diamond anvil cells, computer software), the project assesses the reproducibility of high pressure single-crystal measurements and is a kind of round robin test evaluating the different procedures used to determine the crystal structure. Last but not least, the project promotes high pressure as an experimental tool and consolidates the high-pressure crystallographic community in the region.

As a test sample we have chosen toluene, a common compound used in chemical laboratories. Toluene is known to crystallize at ambient pressure and low temperature in two different crystal forms: the stable monoclinic *a* polymorph, space group *P2₁/c*, *Z* = 8 [4], and the metastable orthorhombic *β* modification, space group *Pbcn*, *Z* = 8 [5]. The addition of the methyl group to the benzene ring perturbs the molecular arrangement found in benzene and introduces C-H... π interactions as the cohesive forces. The high pressure investigation of toluene is particularly interesting in comparison with our former high pressure studies of benzene [6] and ethynylbenzene [7].

- [1] <http://www.ccdc.cam.ac.uk>
 [2] <http://hpc.amu.edu.pl/hpd2012>
 [3] <http://hpc.amu.edu.pl/fgsp2012>
 [4] Nayak, S. K., Sathishkumar, R. & Guru Row, T. N. (2010) *CrystEngComm* 12, 3112-3118
 [5] Andre, D., Fourme, R., Bruneaux-Pouille, J. & Bosio, L. (1982) *J. Mol. Struct.* **81**, 253-259.
 [6] Katrusiak, A., Podsiadlo, M. & Budzianowski, A. (2010) *Cryst. Growth Des.* **10**, 3461-3465.
 [7] Dziubek, K. F., Podsiadlo, M. & Katrusiak, A. (2007) *J. Am. Chem. Soc.* **129**, 12620-12621.

Keywords: high-pressure crystallography; CH...d interactions; methodology