MS36-P9 Hydrogen bonding in a benzimidazole derivate - what is in a name ? A combined use of powder diffraction, solid state and molecular DFT study.

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Apart for obvious electrostatic interactions the molecules of methyl 3-((benzimidazol-4(7)-yl) amino)-2-cyano-prop-2-enoate are in the structure (solved from powder diffraction data and refined by high quality energy minimization in the solid state) also held by N-H…N and C-H…N hydrogen bonds, remarkably differing in their strengths and roles. To evaluate the strength of these hydrogen bonds in the structure molecular DFT calculations applying dispersion corrected functional B97-D3 (environment-dependent D3 scheme with haVDZ basis set) as well as wave-function based SCS-MP2 method with def2-TZVPP basis set were done. Because wave-function based methods treat intermolecular electron correlation (a quantum-mechanical origin of dispersion interaction) in a different way than DFT does, application of the methods differing in their nature provides a stringent test of consistency of the resulting values. To estimate the interaction energy of infinite chain of N-H..N hydrogen bonded molecules a standard procedure based on extrapolation to infinity was applied. First, the interaction energies in a dimer, a trimer and in a tetramer of molecules of linked by one, two and three N-H...N bonds, were calculated. However, rather than the absolute value of the interaction energy it is the size of one its ingredients, of a dispersion interaction, which is of main interest here. For a dimer this contribution represents 78% of the interaction energy and this share slightly increases for the trimer (83%) and than just marginally for the tetramer (86%). Dispersion interaction calculated for pairs of molecules bound by the weaker C-H..N hydrogen bond is at DFT level of theory also relatively large, ~55%. It can be thus concluded that although from pure formal geometrical point of view the ribbons of the molecules in the structure are connected by hydrogen bonds, it should be clearly understood that in addition to the "pure" H-bond mechanism of interaction, it is dispersion interaction, which plays important role.

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MS36-P10 Structural diversity in supramolecular compounds of *para*-sulfonatocalix[8]arene with phenanthroline

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para-Sulfonatocalix[*n*]arenes are anionic, water soluble derivatives of calix[*n*]arenes, which are supramolecular hosts and 'building blocks' in crystal engineering. An important feature of these compounds is their ability to co-crystallize with variety of molecular species. They form a series of complexes with polar and non-polar molecules and/or metal cations both in solution and solid-state. They create a variety of supramolecular architectures such as bilayers, molecular capsules, polymers stabilized by hydrogen bonds, one or two-dimensional coordination polymers, motifs like 'ferris wheel' and 'Russian doll', helical arrays, channels filled with water molecules as well as nanometer-sized spheres or tubes[1].

Calix[8]arenes themselves may adopt sixteen 'up-down' conformations[1] and numerous others in which one or more of the aryl rings projects outward from the average plane of the molecule, depending on the functionalization of the macrocycle, the solvent used for the crystallization or the shape and nature of complexed guest molecules. The most common conformation, both in solution and in the solid state, is pleated loop conformation (Fig.1), stabilized by intramolecular hydrogen bonds O–H···O.

Calixarenes, due to their diversity and conformational mobility are important receptors in molecular recognition. The goal of this paper is to show structural diversity of *para*-sulfonatocalix[8]arene in complexes with 1,10-phenanthroline in solid state.

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