MS21- Intermolecular interactions from structural, energetic and charge density perspective(s)

Chairs: Prof. Enrique Espinosa, Prof. Ulli Englert

MS21-P01

Crystal structure and reconstruction of charge density of 9-aminoacridine hemihydrate

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Nowadays, the most routine X-ray structure determination in crystallography is based on so-called Independent Atom Model (IAM) of electron density, which assumes both sphericity and neutrality of the atoms. Unfortunately, the quantitative topological analysis of an electron density based on IAM is inaccessible (Dittrich *et al.*, 2009). The multipolar approach, as proposed by Hansen and Coppens (Coppens, 1997) , is the method of choice in modelling of the experimental electron density distribution. High-resolution diffraction data of outstanding quality are mandatory in order to perform full structure refinement with multipolar model – a condition impossible to meet for very small crystals or macromolecules. However, the theoretical databanks of aspherical scattering factors developed in recent years, for example, UBDB databank (Jarzembska & Dominiak, 2012) based on experimental geometries, can be used in order to reconstruct the charge density with the Transferable Aspherical Atom Model (TAAM) approach.

Acridines belong to the polycyclic heteroaromatic chemical compounds and their derivatives have found a wide range of applications in clinical area as an antimicrobial, antiviral or antitumor agents as well as in chemical analysis, for example as a matrix for matrix-assisted laser desorption/ionization (MALDI). The 9-aminoacridine can be considered as a model compound from this family of chemicals. In its neutral form it crystallizes as a hemihydrate the $I\,4_1/a\ 2/c\ 2/d$ space group with several atoms in special positions. The very interesting crystal structure of title compound was described in the 1983 year by Chaudhuri and until now has not been more thoroughly investigated. Here, the reconstruction of charge density distribution with the UBDB data bank and TAAM refinement will be performed in order to obtain more accurate geometry of the compound, the quantitative topological analysis of an electron density as well as the basis for the energetic calculation (crystal lattice and dimer energies) by using *Crystal*, *CrystalExplorer* or *Pixel* approaches. This research is the part of the wider project carried out in cooperation with dr Mihails Arhangelskis.

Acknowledgments:

Polish National Science Centre MAESTRO grant decision number DEC2012/04/A/ST5/00609, DSM grant No. 501-D112-86-DSM-115 100 are acknowledged.

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Keywords: 9-aminoacridine hemihydrate, charge density, TAAM refinement

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MS21-P02

Preparation of non-covalent organic frameworks using dodecasubstituted porphyrins

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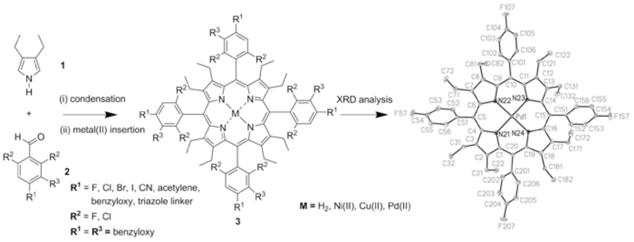
Nowadays the use of porphyrins to create highly porous, sponge-like frameworks is a well-studied field, established by the seminal work of Byrn *et al*. coining the phrase "porphyrin sponge" in 1991.[1] This initial study used a porphyrin host, trapping a variety of guests within the crystal lattice. Since then, many contributions have focused on the manipulation of planar porphyrins containing a variety of functional groups (namely carboxylic acids or halogens) to obtain directly linked porphyrin frameworks.[2] However, as of yet, there are no specific examples of the use of highly distorted porphyrins [3] being used to obtain such highly porous materials. In this work, we have synthesized a series of 5,10,15,20-tetraaryl-2,3,7,8,12,13,17,18-octaethylporphyrins with alternating halogen, alkyl, and aryl substitution patterns to probe the effects of non-planarity on the formation of non-covalent organic frameworks.

The target porphyrins were synthesized according to a modified Lindsey condensation reaction followed by metal(II) insertion. To investigate substituent interactions, modified aldehydes were used. For halogen effects, a family of derivatives with F, Cl, Br or I in either the *ortho*- or *para*-position of the meso-aryl residues were selected. Hydrogen bonding interactions were examined by incorporating a nitrile group. Steric effects were examined through the incorporation of a benzyloxy group at either the *meta*- or *para*-positions. Finally, investigations were conducted into the use of arm-extended porphyrins using a triazole linker group to further extend their functionality. Solid-state structures were determined *via* small molecule X-ray crystallography to elucidate the major distortion modes and to characterize any non-covalent interactions. These were then compared to their planar derivatives to determine effects the substitution patterns may have on the formation of non-covalent organic frameworks.



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Keywords: Porphyrin, Halogens, Macrocycles