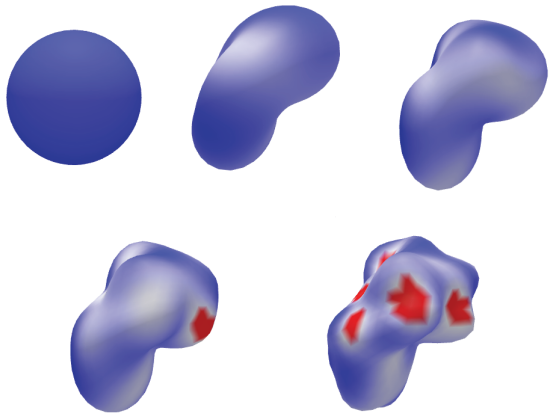

Figure 1. Reconstruction (from the resultant shape coefficients) of a sucrose molecule Hirshfeld surface along with a property on the surface (in this case d_{norm}) for angular momentum l = 1, 4, 6, 8, 9

Keywords: spherical harmonics, Hirshfeld surface, crystal packing, intermolecular interactions, cluster analysis

MS36-P16 Cyclohexylhemicucurbit[8]uril - a chiral macrocyclic host for anionic guests

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Cucurbituril chemistry has gained considerable interest over the last decades. Classical cucurbit[*n*]uril (CB[*n*]) homologues, known to encapsulate neutral or positively charged molecules, have already been employed in stimuli responsive systems and in CB[*n*] mediated catalysis.[1][2] Accounts of anion binding within CB[*n*] homologues are scarce, with the exception of hemicucurbit[*n*]urils (HC[*n*]), a sub-group of the CB[*n*] family, known to preferentially bind anions.[3][4]

Chiral cyclohexylhemicucurbit[*n*]urils (cycHC[*n*]) have been synthesized and investigated by our group.[5][6] The electron-poor cavity of cycHC[*n*] renders these macrocycles capable of anion recognition.[7] Our recent efforts to gain insight into the binding of anionic guests by cycHC[8] have resulted in a number of successfully crystallized and structurally characterized complexes. Crystal structures of 1:1 complexes with a number of singly charged tetrahedral and octahedral anions have been successfully obtained, demonstrating the remarkable ability of cycHC[8] to accommodate guests of different shapes and sizes. The flexible nature of the cycHC[8] portals allows for tight sealing of the encapsulated guests. Additionally, the binding of anionic guests to cycHC[8] has been complementarily evaluated by ESI-TOF MS and NMR spectroscopy.

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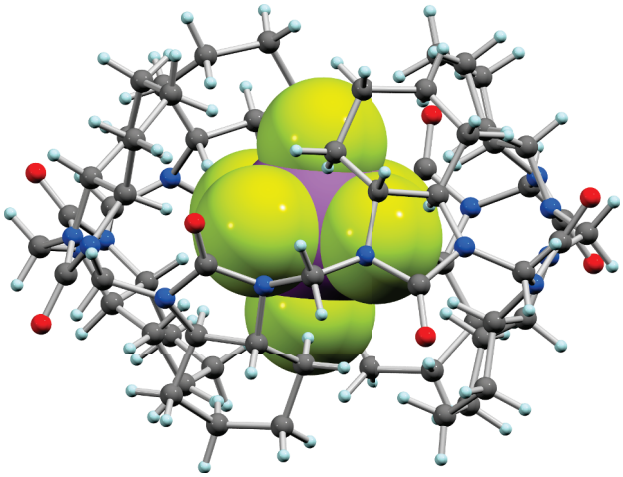

Figure 1. The structure of an inclusion complex of cycHC[8]:SbF_6^- from X-ray diffraction analysis

Keywords: hemicucurbiturils, host-guest chemistry, anion binding

MS36-P17 Shortest intermolecular contacts in crystals of organic compounds

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The intermolecular interactions are one of the most important factor governing the formation of crystal structures.[i],[ii] Therefore characterization of the shortest contacts is extremely important for understanding this process, developing methods of crystal engineering[iii] and predicting the crystal structures.[iv] The investigation of the shortest contacts population reveals bimodal distribution and a clear distinction between strong and weak interactions. Further deconvolution, show that populations are sum of Gaussian-like distributions for specific intermolecular contacts (Fig. 1).[v] Fitting to correct function gave parameters, like mean distance and standard deviation, very useful for validating crystal structures. Moreover, we have found group of crystal structures which does not have any van der Waals contacts,[vi] according to Bondi.[vii] The existence of such population is an important input in discussion of van der Waals radii values, and can be starting point for their recalculation.

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