

Poster Presentation

MS35.P15

Molecular Swiss Cheese: new complexes and conformations of p-sulphonato[8]arene

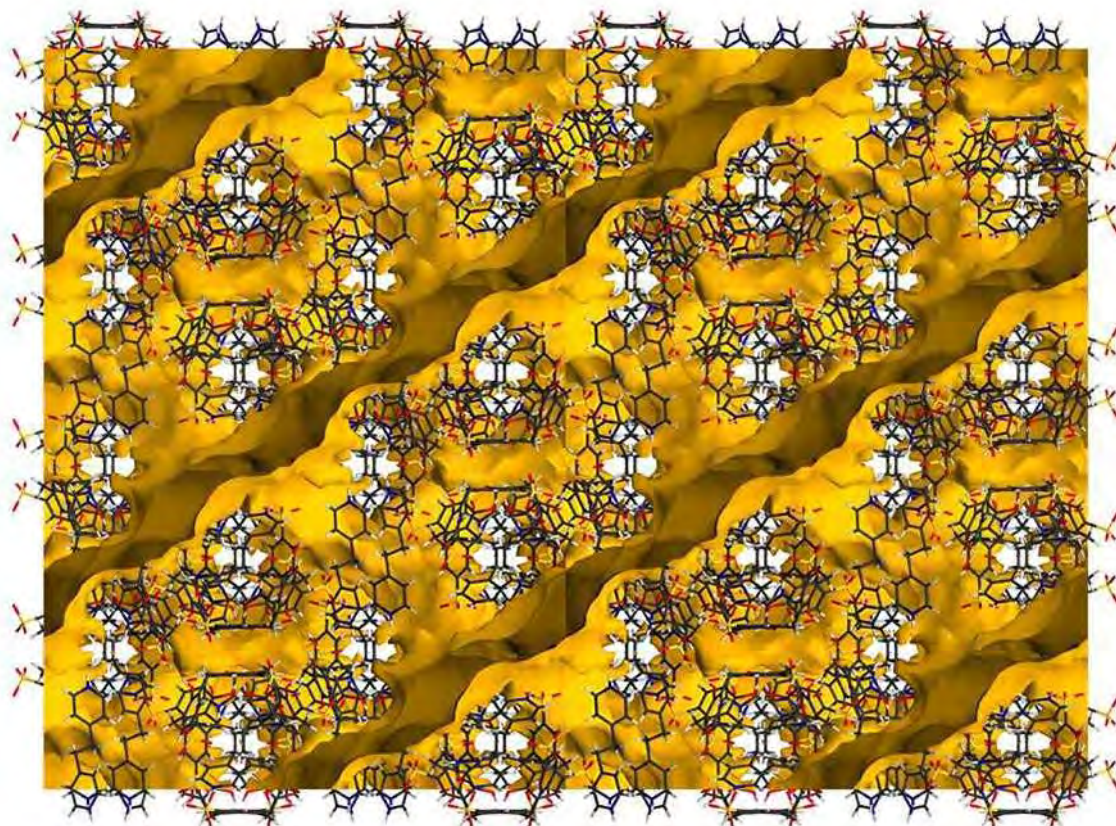
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The crystal structures of the salts of para-sulphonatocalix[8]arene with two flexible guest molecules 1,2-bis(4-pyridyl)-ethane (BPE) and 1,3-bis(4-pyridyl)-propane (BPP) are presented. para-Sulphonatocalix[8]arene molecule adopts new types of conformations: "double facing cone" in BPP complex and "up-flat-down" in BPE complex. Although the difference between BPE and BPP is only a presence or absence of a single carbon atom in the central bridge, the structures of their complexes with para-sulphonatocalix[8]arene are remarkably different. While the salt with BPE shows true porosity and can be compared to that of an extremely complex zeolite or to a solid state molecular Swiss Cheese, the second structure with BPP shows no porosity and is of the type of organic clay firstly observed for the sodium salt of para-sulphonato-calix[4]arene [1], and can be compared to a Gruyere Cheese. The structure of the para-sulphonatocalix[8]arene with BPE salt (Figure 1) shows a complex network of interconnecting channels of variable size, one of which contains a BPE cation effectively blocking this channel, the others contain water and solvents and are thus accessible. A total of six different channels are observed in this structure. Gas take-up has been demonstrated, to show the porous nature of the solid. The effect of a single carbon atom between the cations on the complexity of the Supramolecular Organic Framework (SOF), is remarkable. Work is currently underway to study other complexes of para-sulphonatocalix[8]arene with rigid and flexible organic cations and to open up the way to novel SOFs. Figure 1. Solvent accessible surface in para-sulphonatocalix[8]arene and 1,2-bis(4-pyridyl)-ethane complex: view along [001] axis.

[1] A. W. Coleman, S. G. Bott, S. D. Morley, et al., *Ang. Chem. Int. Ed.*, 1988, 27, 1361-1362.



Keywords: calixarene, host-guest complexes, molecular self-assembly