for all types of guests molecules which are ordered in the middle of the channel, whereas inflexible $[V(O)(bdc)]_n$ can adsorb only a little amount of the guest (5-10 mol. %). In the first case, the stoichiometry of inclusion compound is $Guest_{0.5}@[Al(OH)(bdc)]$ or $Guest_{0.25}@[Al(OH)(bdc)]$. In the case of $[V(O)(bdc)]_n$, only cobaltocene forms inclusion phase composition $cobaltocene_{0.5}@[V(O)(bdc)]_n$ due to the formation of charge-transfer complex [4]. Hydrogen bonds, host-guest and guest-guest interactions as well as structural effects of the substitute group inside the guest molecule have been studied in details for all inclusion compounds.

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Keywords: coordination polymers, host-guest complexes, powder structure determination

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Dimensional Encapsulation of Halogen-Bonded Supramolecular Anions. Pierangelo Metrangolo[a,b], Gabriella Cavallo[a], Manu Lahtinen[c], Tullio Pilati[d], Kari Rissanen[e], Giuseppe Resnati[a,b,d], Giancarlo Terraneo[a,b].
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Halogen bonding [1] has increasingly facilitated the assembly of diverse host-guest solids. In this contribution, we show that a well-known class of organic salts, bis(trimethylammonium) alkane diiodides, can reversibly encapsulate I_2 [2] and a series of α,ω-diiodoperfluoroalkanes (DIPFAs) through intermolecular interactions between the host's I^- anions and the guest's terminal iodine substituents [3]. In particular, bis(trimethylammonium)hexane diiodide encapsulates I_2 yielding in a predictable and controllable manner the selective formation of the rare polyiodide species $I^-\cdots I–I\cdots I^-$. Similarly, the process is highly selective for the DIPFA that forms an $I^-\cdots I(CF_2)_m I\cdots I^-$ superanion, which matches in length to the chosen dication. DIPFAs that are 2 to 12 carbons in length can thereby be isolated from mixtures by means of crystallization from solution upon addition of the dissolved size-matched ionic salt. The solid-state salts can also selectively capture I_2 and the DIPFAs from the vapour phase, yielding the same product formed from solution despite a lack of porosity of the starting lattice structure.
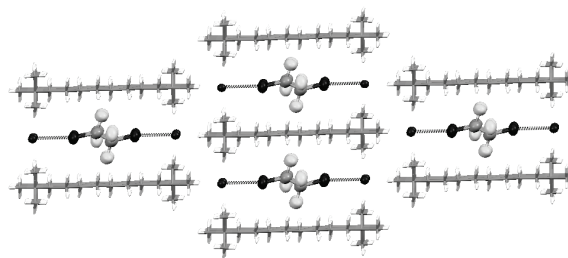
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Towards docking-based prediction of host-guest framework systems Peter A. Wood, Oliver Korb.
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The design and prediction of multi-component organic crystal structures is of interest to many areas of the chemical industry. Host-guest framework structures can, for example, be used to tune the physicochemical properties of a solid form, to achieve selective separation and even as catalysts. Current design and prediction methods have limitations though; crystal structure prediction (CSP) can be very computationally expensive for each individual multi-component system and there is also a limit to the number of experimental screens that can be carried out.

These multi-component structures do, however, essentially represent a form of host-guest binding related to that seen when a ligand interacts with a protein binding site. In this study we investigate whether established techniques for predicting protein-ligand binding can be applied to the challenge of modelling small molecule host-guest crystalline frameworks.

In order to examine the general applicability of this technique, an off-the-shelf docking package (GOLD [1]) is used with a standard scoring function (CHEMPLP [2]) that has been trained for interactions in protein-ligand binding sites. A range of experimentally-determined channel-based test structures are used to evaluate the effectiveness of the docking package. The test structures include API frameworks, well-known organic inclusion compounds and metal-organic frameworks. This work shows that the principles of docking can be successfully applied to the crystal engineering problem of predicting host-guest systems.

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