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Halogen bond driven encapsulation of tetrahalomethanes within a supramolecular host

Anssi Peuronen[1], Elina Kalenius[1], Manu Lahtinen[1]
[1]*Department Of Chemistry, University Of Jyvaskyla, Jyvaskyla, Finland*
E-mail: anssi.peuronen@jyu.fi

Amidst of organic macromolecules and their non-covalently bound aggregates, coordination cages, self-assembled from organic ligands and metal ions, are an important class of supramolecular hosts (or molecular containers).[1,2] Typically, coordination cages provide a hydrophobic binding pocket within the cage whereas selectivity towards specific types of guest molecules can be enhanced by incorporating hydrogen bonding, π-bonding or ionic sites into the ligand backbone. We have recently shown that cationic tripodal ligands promote binding of anionic guests via ionic interactions within coordination cages.[3] In this contribution we demonstrate that this ligand-guest interaction-based encapsulation can be exploited in binding of secondary guest molecules by halogen bonding interactions. In particular, this presentation will focus on the structural features of a novel tetrahedral cage with the composition of [(Cu3I4)4(L)4]8+ that is prepared via self-assembly between copper(I) iodide and a tricationic ligand (L). Analysis of this cage by means of single crystal X-ray diffraction, NMR and MS-ESI shows a structure of four endohedral iodide anions bound within the cationic pockets of the ligands thus providing an anionic interior which is selective towards encapsulation of different halomethanes via Y3C–X···I– (X = halogen, Y = halogen/hydrogen) halogen bonding (XB) interactions. These endohedral XB interactions are further analyzed by spectroscopic and computational (DFT) methods. To conclude, the broader aim in this presentation is to show that XB interaction is a viable tool in contemporary supramolecular chemistry involving coordination-driven molecular containers.

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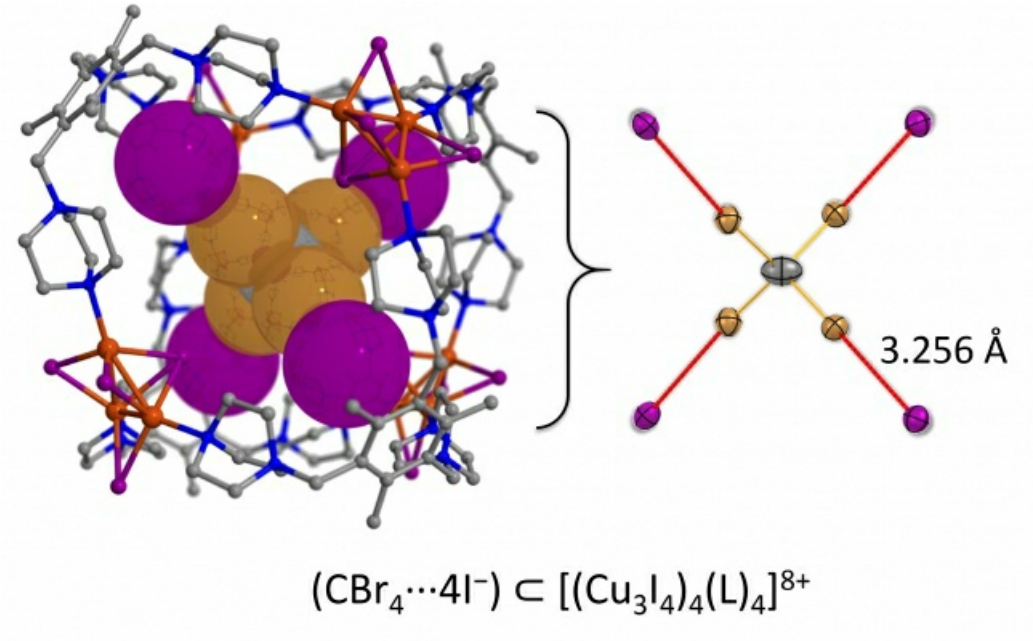

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