Structure of Halogens@bambus[6]uril caviplexes

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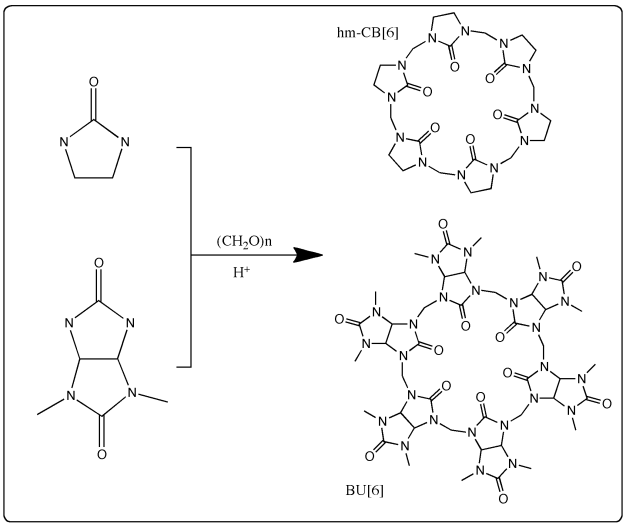
Bambus[n]urils[1] are a new class of organic cavitands, composed by dimethyl-glycoluril units, linked together by methylene bridges. These macrocycles, mainly bambus[6]uril (**BU[6]**) ressemble somehow to cucurbiturils (**CB[n]**) and hemi-cucurbiturils (**hm-CB[n]**), but their monomers are arranged in a picket fence conformation. This feature affects their shape (as a bamboo segment) and also the charge distribution inside their cavity. Differently from cucurbiturils, **BU[6]** displays enormous affinity for anions, instead of cations. Species such as Cl^-, I^-, SCN^- among others, may form very stable inclusion compounds with **BU[6]** and It is very difficult to remove chloride ions during its synthesis for example.



The structures of Hemi-cucurbit[6]uril and bambus[6]uril

Our group has developed several applications with included halogens in cucurbiturils (**$(X_2)_n$@CB[n]**), especially as selective halogenating agents for organic synthesis[2]. This time we have studied the inclusion of iodine and bromine into bambusurils and we have obtained colored inclusion compounds as one could expect. These inclusions compounds are not as stable as their analogues with cucurbiturils, and the halogens are totally released in less than a week at room N.C.T.P. For our surprise, we could form very stable inclusion compounds with Cl^-@BU[6] and iodine or bromine, that lasted for much longer periods enduring minimal weight losses. We suspect that the BU[6] cavity favors and stabilizes uneven trihalide structures like $ClBr_2^-$ and ClI_2^- inside the macrocycles. Our objective is to unravel these caviplexes structure, and how it will affect their reactivity.

1) J Svec, M Necas, and V Sindelar. Bambus[6]uril. Angew. Chem. Int. Ed. Engl., 49(13):2378–2381, 2010. doi: 10.1002/anie.201000420.
2) K R K K Reddy, T S Cavallini, G J F Demets, and L F Silva Jr. Bromine and iodine–cucurbit[6]uril complexes: preparation and applications in synthetic organic chemistry. New J. Chem., 38:2262-2262, 2014. doi: 10.1039/c4nj00284a

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