Scientific Journey with Prof. Cornelia Bohne

From Department of Chemistry, University of Victoria, Victoria, BC, Canada

***9 de Agosto de 2016 no* IQ-05 do Instituto de Química UNICAMP**

Time	Activity	Owner
14:00 – 15:00	**Palestra**: Mechanistic Insights from Supramolecular Dynamic Studies on the Binding of Guests with Cucurbit[n]urils	
15:00 – 15:15	Coffee break	
15:15 – 15:45	Apresentação formal do Jornal ***ACS Omega*** Aberto a discussão/debate/dúvidas/questões	
15:45 – 16:00	Coffee Break	
16:00 – 17:00	Workshop sobre escrita científica e processo de revisão	

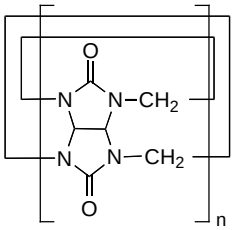
Organizado pelo ACS Brazil Chapter: www.acsbrazilchapter.org.

Mechanistic Insights from Supramolecular Dynamic Studies on the Binding of Guests with Cucurbit[n]urils

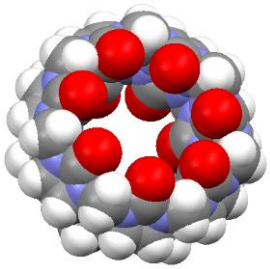
Cornelia Bohne

Department of Chemistry, University of Victoria, PO Box 3065, Victoria, BC, Canada – cornelia.bohne@gmail.com

Cucurbit[n]urils (CB[n]) are excellent macrocyclic hosts for guests that have a positive charge and a hydrophobic moiety. The positive charge is stabilized by the carbonyl groups lining the portals. Indeed the binding of CB[n]s to metal cations, such as Na^+ cations, is used to solubilize these hosts at higher concentrations. CB[n]s have been used to develop a variety of applications where the dynamics of the system, in particular the guest's association and dissociation rate constants, are essential for the intended function to be expressed.



CB[n] n = 5, 6, 7, 8



CB[7]

Our kinetic studies uncovered that different mechanisms operate in the formation of the guest complexes with CB[n]s. Guests can slip into the CB[7] cavity, or larger guests form exclusion complexes where the guest's positive charge interacts with the portal without immediate inclusion of the hydrophobic moiety of the guest into the CB[7] cavity. Different roles were observed for the Na^+ cations. The cation can cap both portals of the CB[n] removing the ability of the host to bind the guest and slowing the reaction, while in other cases Na^+ can interact with the guest@CB[n] complex expelling the guest and therefore enhancing the rate of the relaxation kinetics.

Kinetic studies are also instrumental in developing CB[n] systems as functional supramolecular systems and three proof of principle examples will be presented: (i) development of an assay to determine the association and dissociation kinetics for spectroscopically silent guests using competitive kinetics, (ii) determination of the guest ground-state protonation/deprotonation rate constants for the guest@CB[7] complex as an elementary reaction in catalysis and (iii) use of CB[6] as an additive in hydrogels to alter the distribution of small molecules between the gel's network and the constrained aqueous phase.