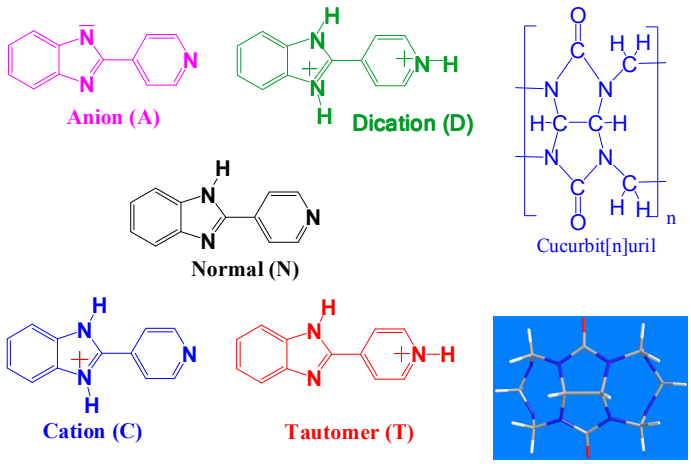
The formation of inclusion complex with cucurbit[n]uril family: A host-guest interaction with [CB]n and 2-(4'-Pyridyl)benzimidazole

Vijaykant Khorwal, Uma Nudurupati, Sohidul Islam Mondal and Anindya Datta*
Department of Chemistry, Indian Institute of Technology Bombay
vijayikant@chem.iitb.ac.in

Abstract

In the present study, we report the modulation of the ground- and excited state proton transfer processes of 2-(4'-pyridyl)benzimidazole (4PBI) in aqueous solutions by CB5, CB6, CB7 and CB8 in acidic and alkaline media and in order to examine if the protonation-deprotonation equilibria involving different forms of 4PBI are affected by inclusion in macrocyclic hosts of this class. Given a choice between a cation, anion and a neutral it is known that CB would selectively stabilize the cation, but the question we have addressed here concerns the choice between two monocations of the same molecule. 2-(4'-Pyridyl)benzimidazole (4PBI) guest comprising two binding sites, one benzimidazole group and one pyridyl group, proved could form inclusion complexes with cucurbit[n]uril (CB[n]) in aqueous solution. The binding in the cavity and at the portals of cucurbit[n]uril, absorption and fluorescent response of a guest could be dramatically changed, so by the steady state and time resolved fluorescence spectroscopy, it very easy to demonstrate that the 2-(4'-Pyridyl)benzimidazole could be interact with both cavity and portal. ^{1}H NMR spectroscopy is also proving the formation of inclusion complexes. ^{1}H NMR of both the guest and the host indicates that guests might enter in CB[n] from the benzimidazole side with in hydrophobic cavity.

Graphics



Different forms of 2-(4'-Pyridyl)benzimidazole and the glycouril unit of Cucurbit[n]uril