SPECTROSCOPIC AND THEORETICAL STUDY ON THE STRUCTURES AND DYNAMICS OF FUNCTIONAL MOLECULES - TOWARDS AN UNDERSTANDING OF THE MOLECULAR RECOGNITION FOR ENCAPSULATION COMPLEXES

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Functional molecules, such as crown ethers and calixarenes, can act as hosts for encapsulating guest species through non-covalent interactions. Applications of crown ethers and calixarenes as molecular receptors, metal cation extraction agents, fluoro-ionophores and phase transfer catalytic media have been previously reported in a number of studies in the literature. One of the important aspects of these host/guest molecular assemblies is their selectivity in the encapsulation of guest species. Two important factors that control this selectivity are: (1) the size and the flexibility of the host cavity and (2) the properties of solvent molecules.

Molecular complexes formed in supersonic jets provide ideal systems for the selective study of the conformational preference and micro-solvated effects under solvent-controlled conditions. This talk will review our spectroscopic and theoretical studies of the structures of dibenzo-18-crown-6-ether (DB18C6), benzo-18-crown-6-ether (B18C6), calix[4]arene (C4A) and their complexes with guest molecules. We apply laser-induced fluorescence (LIF), resonance enhanced two-photon ionization (R2PI) and UV-UV hole-burning (HB) spectroscopy for obtaining electronic spectra and IR-UV doubleresonance and IR photodissociation (IRPD) spectroscopy for the IR spectra. The electronic and IR spectra are compared with the corresponding results obtained by DFT calculations and high-level first principles electronic structure calculations [MP2 and CCSD(T)]. Based on these joint studies we can elucidate the nature of interactions that control the encapsulation of a guest molecular species as well as how the host can adjust its conformation to accommodate a specific guest, leading to the molecular recognition.