

Laser Spectroscopic and Theoretical Study of Encapsulation Complexes in the Gas Phase Toward Molecular Level Understanding of the Encapsulation Mechanism of Host-Guest Complexes

Frontiers in Chemical Physics and Analysis Seminar Series

Presented by...

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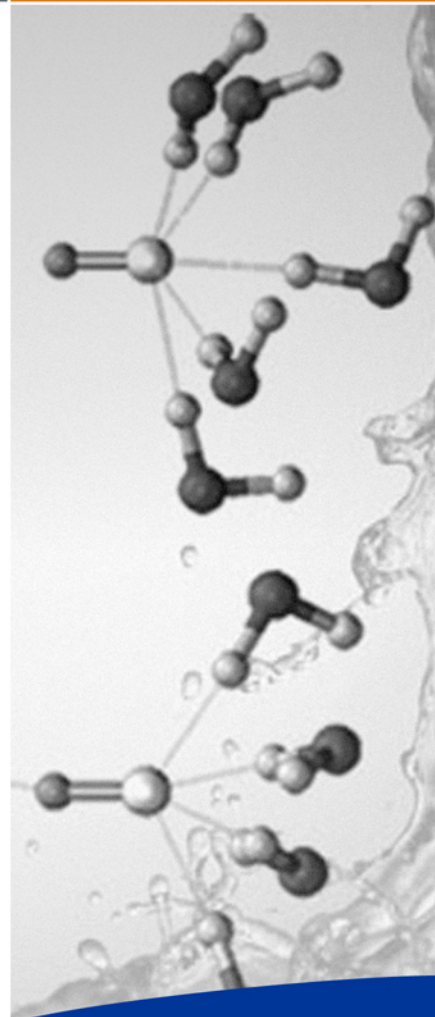
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Abstract

Laser spectroscopic and theoretical study will be presented for elucidating the structures and complexation mechanism of gas phase host-guest complexes formed in supersonic jets and electrospray ionization cold 22 ion-trap. The examined hosts include crown ethers and calix[4]arene, and for the guest species various neutral molecules and alkali metal cations are chosen. We measure the electronic spectra by laser-induced fluorescence (LIF), mass-selected resonance enhanced multiphoton ionization (REMPI) and ultraviolet-ultraviolet hole-burning (UV-UV HB) spectroscopy. The vibrational spectra are measured by infrared-ultraviolet double resonance (IR-UV DR) and fragment detected infrared photodissociation (IRPD) spectroscopy. For the ionic complexes, ultraviolet photodissociation (UVPD) and IR-UV DR spectroscopy has been applied. The obtained results are analyzed by density functional theory and first principles electronic structure calculations. We discuss how the host molecule changes its conformation or which conformer is preferred for forming stable encapsulation complex as well as the key interactions, leading to the molecular recognition.

More info?

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Auditorium

Time: 11 am