

Soutenance de thèse

Ananya Sen

Institut des Sciences Moléculaires d'Orsay (ISMO), Orsay

Chiral recognition in neutral and ionic molecular complexes

The main objective of this thesis is a spectroscopic study of molecules or complexes bearing multiple chiral centres in the gas phase, to understand the effects of stereochemistry on their structural properties. Neutral *Cinchona* alkaloids have been introduced intact in gas phase by laser-ablation. They have been studied by combining supersonic expansion with laser spectroscopy. The two pseudo-enantiomers Quinine and Quinidine show similar electronic and vibrational spectra, in line with similar structure. Their properties in solution differ more, as shown by Vibrational Circular Dichroism (VCD) experiments. This difference is further enhanced in Hydroquinine and Hydroquinidine.

Lastly chiral recognition has been studied in ionic complexes in an ion trap. A homochiral preference has been shown in the stability of the complexes formed between S-Camphor and R and S protonated Alanine. However, the calculated interaction energy as well as the IRMPD spectrum in the fingerprint region are identical. The role of higher energy conformers in chiral recognition has been discussed.

Key words: Chiral Recognition Laser ablation Vibrational Circular Dichroism (VCD)

Pseudo-enantiomers Supersonic Expansion Infrared multiple-photon dissociation (IRMPD)



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