Studies on Microsolvation in the Gas Phase by HR-LIF and REMPI-TOF Spectroscopy

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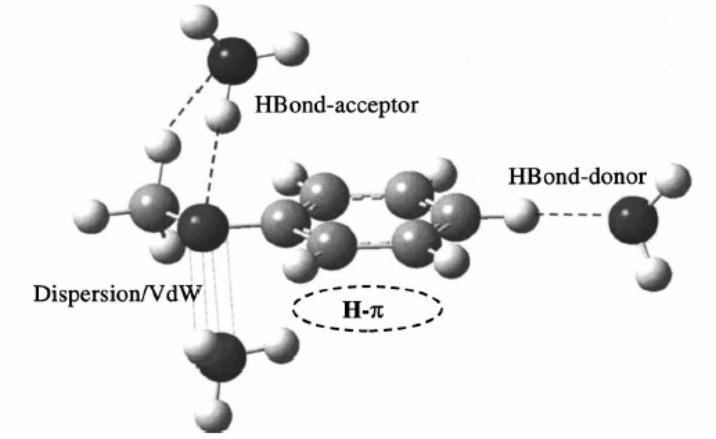
Molecular clusters are quite useful as model systems to learn about the microscopic mechanisms responsible for intermolecular interactions. Clusters of different composition make possible a detailed study of the different binding mechanism related to the existence of van der Waals, hydrogen bond and electrostatic interactions. Knowledge of these processes is of fundamental interest in order to understand the transition from isolated molecules to bulk materials and to validate models for the solvation process.

We are reporting on the spectroscopic study on different 1:1 clusters formed, in supersonic expansions, by anisole with different simple solvents and other aromatic molecules [1-4]. This allows us to probe the nature of the intermolecular bonding when many interaction mechanisms are possibly operative. These clusters have been studied by Resonance Enhanced Multi-Photon Ionization (REMPI) – Time of Flight (TOF) mass spectrometry and by high resolution (rotationally resolved) laser induced fluorescence (HR-LIF) spectroscopy. The spectroscopic parameters we derived (vibrational frequencies, rotational constants in both the ground and the excited state, frequency shift of the $S_1 \leftarrow S_0$ electronic transition with cluster formation) have been modeled with advanced *ab initio* and DFT methods (in collaboration with V. Barone and coworkers, Univ. Napoli, Italy).



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