SYHR 1: High resolution spectroscopy - modern trends and new techniques I

Zeit: Donnerstag 10:30–12:30 Raum: VMP 8 R05

Hauptvortrag SYHR 1.1 Do 10:30 VMP 8 R05

High-Resolution Rotational Spectroscopy: New Waves — •Jens-Uwe Grabow — Gottfried-Wilhelm-Leibniz-Universität, Institut für Physikalische Chemie & Elektrochemie, Lehrgebiet A, Callinstrasse 3A, 30167 Hannover

Small particles, larger molecules and clusters are of increasing technological importance with numerous fundamental questions on their structure and dynamical behavior waiting to be answered. Targeted by high resolution spectroscopy they impose a number of challenges, theoretically and experimentally.

From the theoretical point of view, e.g., internal large amplitude motions result in complicated energy level schemes. For larger species exhibiting multiple internal motions at low barriers, the resulting spectra will be rather difficult to predict. From an experimental point of view, dense spectra at the presence of wide splitting patterns are difficult to assign. With narrow-banded techniques, even though very sensitive, identification of the spectral features becomes a paramount task.

Quantitative information on the structure, charge distribution, characterization of the chemical bond, details on internal dynamics, etc. - at the highest precision available to date - are encoded in pure rotational spectra obtained by microwave spectroscopy. Right now - about a quarter century after the introduction of supersonic-jet resonator Fourier-transform microwave spectroscopy - new exciting technical developments aiming to overcome still existing limitations are expected to pave the way for a promising future of rotational spectroscopy.

Hauptvortrag SYHR 1.2 Do 11:10 VMP 8 R05

Some like it cold – aggregation and dissociation of HCl and water in helium nanodroplets — Gerhard Schwaab[1], •Ozgur Birer[2], Anna Gutberleth[1], and Martina Havenith[1] — [1]Physical Chemistry II, Ruhr University Bochum, D-44780 Bochum, Germany — [2]Chemistry Department, Koc University, Rumelifeneri Yolu, Sariyer 34450 Istanbul, Turkey

Helium nanodroplets provide a gentle, ultracold matrix for studies of agglomeration processes. Due to the superfluidity of He at 0.37 K a combination with high-resolution infrared spectroscopy provides an ideal tool to separate local and global minimum structures of aggregates.

We used Helium nanodroplets in combination with a cw OPO and a mass spectrometer as detector unit to study the aggregation and solvation of HCl in water. Besides signals of pure HCl, undissociated HCl-H_2O, and rotationally resolved HCl dimer, broadened peaks around 2670 cm^{-1} were found. Optically selective mass spectroscopy (OSMS) allowed unambiguous assignment of the according parent species as solvent separated ion pair $H_3O^+(H_2O)_3Cl^-$. A replacement of HCl by DCl produced a slight spectral shift and a further splitting. This is in excellent agreement with theoretical calculations.

The observation of, what we believe is the "smallest droplet of an acid", opens the way for spectroscopic investigation of microsolvation processes at ultracold temperatures such as zwitterion formation of amino acids.

Hauptvortrag SYHR 1.3 Do 11:50 VMP 8 R05

High resolution electronic spectroscopy of anisole dimer — •Giangaetano Pietraperzia[1], Massimiliano Pasquini[1], Nicola Schiccheri[2], Giovanni Piani[2], and Maurizio Becucci[1] — [1]LENS and Dipartimento di Chimica, Polo Scientifico e Tecnologico Università di Firenze, Via Nello Carrara 1, I-50019 Sesto Fiorentino (FI), Italy — [2]LENS Polo Scientifico e Tecnologico Università di Firenze, Via Nello Carrara 1, I-50019 Sesto Fiorentino (FI), Italy

We report the results of an experimental study of the anisole dimer, formed in a molecular beam apparatus. The dimer was studied by the resonance enhanced multiphoton ionization (REMPI) and by high resolution laser induced fluorescence (HR-LIF)techniques. From a complete assignment of the rotational structure of the band it was possible to obtain important structural information. From a comparison with the results of high level quantum calculations it was possible to infer the equilibrium structure of the complex experimentally studied. The study presented here reports on the first results of a characterization of a complex stabilized mainly by the stacking interaction, investigated at complete rotational resolution.