

MO 10: Experimental Techniques

Time: Tuesday 14:30–16:15

Location: PH/SR106

MO 10.1 Tue 14:30 PH/SR106

Luminescence Characterization of Mass-Selected Electro-sprayed Ions Embedded in Rare-Gas Matrices — ●BASTIAN KERN¹, JEAN-FRANCOIS GREISCH^{1,2}, DMITRY STRELNIKOV¹, ARTUR BÖTTCHER¹, PATRICK WEIS¹, DETLEF SCHOSS^{1,2}, BERHARD SCHÄFER², MARIO RUBEN^{2,3}, and MANFRED M. KAPPES^{1,2} — ¹Physikalische Chemie Mikroskopischer Systeme, Karlsruhe Institute of Technology, Fritz-Haber Weg 2, 76131 Karlsruhe, Germany — ²Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — ³Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Engesserstr. 15, 76131 Karlsruhe, Germany

The combination of electrospray ionization (ESI), laser-induced luminescence, and matrix isolation is demonstrated for the first time using lanthanide diketone ions. The accumulation of mass-selected ions over several hours into a cryogenic rare-gas matrix yields material amounts large enough for sensitive measurements on elusive species whose properties are typically masked in standard condensed-phase measurements. With the additional advantage of measurements at 5K, spectra were obtained which display sharp emission lines. Comparison of matrix laser induced luminescence measurements with those on trapped ions in the gas phase show a remarkable agreement, i. e. the vibronic bands are close to identical. This suggests that the neon matrix used induces only negligible geometrical and electronical perturbations to the species studied.

MO 10.2 Tue 14:45 PH/SR106

Polarisation Infrared Spectroscopy on Oriented Substrates (PIROS) - A case study on Phenazine — MICHAELA BRAUN, GERNOT ENGLER, KATHARINA HUNGER, ●ALEXANDER WOHLERT, KARL KLEINERMANN, and MICHAEL SCHMITT — Universität, Düsseldorf, Germany

Vibrationally induced changes of the molecular dipole moment give rise to different band types in infrared spectroscopy. According to the projection of the molecule's normal modes onto the inertial axes of the molecule these bands can be classified as a, b or c types. In case of molecules with C_{2v}, D₂- or D_{2h}-symmetry the inertial axes and the components of the dipole moment are parallel to each other and therefore the molecules normal modes can easily be classified. In crystals or molecules oriented in films on surfaces, the absorption of polarized IR light depends on the orientation of the molecules with respect to the surface and the plane of polarization of the light. Since the dipole moment changes have a well-defined orientation with respect to the molecular frame, defined by the main inertial axes, the orientation of the molecules on a surface can be determined from the dependence of the IR intensities using polarized IR light, while rotating the sample along the axis of the He-Ne-Laser-beam. To test this method we chose the phenazine molecule since it has D_{2h} symmetry.

MO 10.3 Tue 15:00 PH/SR106

Non-destructive State Detection and Identification of Molecular Ions — ●AMY GARDNER, WILLIAM GROOM, and MATTHIAS KELLER — Ion Trap Cavity QED and Molecular physics (ITCM) group, University of Sussex, UK

The nature of ion traps allow for extremely well localised atomic and sympathetically cooled molecular species; leading to a variety of applications - most notably cold chemistry, testing fundamental theories, searching for changes in fundamental constants and, potentially, the development of methods for quantum computing. Prerequisite for these applications is the cooling of the molecule's motion and its non-invasive identification. Furthermore, the internal quantum state of the molecule needs to be prepared and, at readout, non-destructively detected.

While blackbody assisted laser cooling was recently demonstrated, the non-destructive state detection of trapped molecules is still beyond current experiments. Employing state selective laser induced dipole forces we aim to detect the internal state of molecular ions by mapping the state information onto the ions motion.

We can also identify different ionic species within a coulomb crystal by measuring the average charge-to-mass ratio of trapped ions with high precision. This is a tool that can be used to investigate chemical reactions between neutral molecules/atoms and trapped molecular

ions. The same means can also be achieved by using only laser forces.

MO 10.4 Tue 15:15 PH/SR106

Characterization of an electron gun for diffraction experiments on controlled gas-phase molecules — ●NELE L. M. MÜLLER¹, SEBASTIAN TRIPPEL¹, TERENCE G. MULLINS¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, DESY, Hamburg — ²The Hamburg Center for Ultrafast Imaging, Hamburg — ³Department of Physics, University of Hamburg

The aim of the presented work is to investigate the structure and dynamics of molecules in the gas-phase by electron diffraction experiments. Controlling the molecules' state and spatial orientation increases the amount of information contained in electron diffraction patterns. The contribution presents our newly set-up electron gun that will be combined with an existing controlled-molecules apparatus. In the controlled-molecules setup gas-phase molecules are state-selected by means of electric deflection and then laser-aligned to serve as a well-defined sample [1]. The developed DC electron gun can produce up to 10 million electrons per pulse and uses an electro-static lens for focusing. The focusing electrodes are arranged in a configuration similar to a velocity map imaging spectrometer. Initially, they can be used to measure the spatial and velocity distribution of the electron pulse at the cathode. In combination with electron trajectory simulations this allows for further characterization of the electron beam, as for example the determination of pulse duration and coherence length. Electron diffraction data from solid state and gaseous samples will be presented.

[1]Trippel et al., *Mol. Phys.* **111**, 1738-1743 (2013)

MO 10.5 Tue 15:30 PH/SR106

Microsolvation and coordination changes in a dinuclear iron-palladium complex in isolation — ●MAXIMILIAN GAFFGA, JOHANNES LANG, ISABEL MUNSTEIN, WERNER R. THIEL, and GEREON NIEDNER-SCHATTEBURG — Fachbereich Chemie und Forschungszentrum OPTIMAS Technische Universität Kaiserslautern, Germany

We have applied a combination of mass spectrometric and spectroscopic techniques to determine the composition and structure of isolated cationic dinuclear transition metal complexes in the gas phase. The ions are stored in a Paul trap after creation by electrospray ionization (ESI) for collision induced dissociation (CID) and Infrared Multi Photon Dissociation (IRMPD) investigations. Solvent residues after the ESI process serve as a model system for microsolvation. Fragmentation reactions of these complexes are investigated in detail by CID experiments. These studies lead to surprising information about the fragmentation behavior of the complexes. The combination of DFT calculations and CID results allow for a better understanding of these fragmentation pathways. These investigations exhibit reliable structure proposals of prominent product ions. Assignment of vibrational bands and identification of the complex coordination pattern arise from comparison of IRMPD spectra in the range of 1200-4000 cm⁻¹ to calculated spectra (B3LYP/cc-pvDZ,ECP).

MO 10.6 Tue 15:45 PH/SR106

Structural Studies of Molecular Clusters by Broadband Rotational Spectroscopy — ●CRISTOBAL PEREZ and MELANIE SCHNELL — Max-Planck Institute for the Structure and Dynamics of Cold and Controlled Molecules, Hamburg, Germany

Recent advances in high-speed digital electronics have been used to achieve unprecedented speed and sensitivity in broadband rotational spectroscopy. Such high-speed digitizers allow deep time-domain signal averaging. This new level of sensitivity allows the study of weakly bonded molecular clusters of which several examples will be shown to highlight the performance of this spectrometer.

MO 10.7 Tue 16:00 PH/SR106

Gasphase Spectroscopy of small Carbon-Bearing Molecules — ●DANIEL WITSCH, STEVEN INGUNZA, VOLKER LUTTER, GUIDO FUCHS, and THOMAS GIESEN — University of Kassel - Institute of Physics, Germany, Heinrich-Platt-Str 40, 34132 Kassel

Asymptotic giant branch (AGB) stars show a huge variety of carbon-bearing molecules. Thus, laboratory based investigations of these clusters are important to enable astrophysical detections of further species.

We present an experimental setup to study gasphase IR-spectra of these molecules at low temperatures.

For this purpose a laser ablation source is used to produce a carbon containing plasma. Helium carries the ablated material through a reaction channel, where the desired molecules are formed. Subsequent adiabatic expansion cools the molecules to a few 10 K of rotational

temperature.

This technique combined with quantum cascade lasers allows for high resolution IR-spectroscopy of carbon-bearing molecules. Especially the finger-print region from 2 to 12 microns is of great interest since many rovibrational transitions can be detected here.