

MO 17: Posters 2: Cold Molecules and Clusters

Time: Wednesday 16:15–18:15

Location: Orangerie

MO 17.1 Wed 16:15 Orangerie

A high density source of cold, slow and rotationally pure polar molecules — ●MANUEL KOLLER, THOMAS GANTNER, XING WU Ø, MARTIN ZEPPENFELD, SOTIR CHERVENKOV, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Garching 85748, Germany

Cold polar molecules provide fascinating research possibilities in physics and chemistry. However, densities of cold and slow molecules, achieved in past experiments have been insufficient for many applications. By combining cryogenic buffer gas cooling and centrifuge deceleration we put an end to this problem. Our source delivers a record high flux exceeding 10^{10}s^{-1} and densities up to 10^9cm^{-3} of internally cold polar molecules with a single state purity of up to 92% [1] at kinetic energies corresponding to less than 1K [2]. The generality of our method makes it applicable to a wide range of molecular species (ND_3 , CH_3F , CHF_3 , etc.). Beside enabling detailed collision studies our technique could serve as an ideal source for optoelectrical Sisyphus cooling and testing fundamental physics.

[1] X. Wu et al., *ChemPhysChem* 2016, 17, 3631

[2] X. Wu et al., *Science* 2017, 358, 645-648

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MO 17.2 Wed 16:15 Orangerie

A Molecular Zeeman slowing scheme — ●PAUL KAEBERT, NIKLAS REINHARDT, MAURICE PETZOLD, PHILIPP GERSEMA, MIRCO SIERCKE, and SILKE OSPELKAUS — Institut für Quantenoptik

We report on our progress in implementing a novel scheme for slowing laser-coolable, buffer-gas cooled molecules, reminiscent of Zeeman slowing. We show the results of our proof of principle experiment, realizing the scheme on the D1-line of ^{39}K , and detail our progress on performing the experiment on molecules. From our theoretical simulations and our experimental results we expect the technique to outperform current slowing methods, and hope that the resulting large flux of trappable molecules will be the enhancement needed to produce large, ultra-cold ensembles of directly cooled molecules.

MO 17.3 Wed 16:15 Orangerie

Generation of charged water clusters for hybrid trap experiments — ●JAN TRAUTMANN¹, NINA BEIER¹, HENRY LOPEZ¹, JONAS TAUCH¹, BASTIAN HOLKEMEIER¹, ROLAND WESTER², and MATTHIAS WEIDEMÜLLER^{1,3} — ¹Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — ²Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstraße 25/3, A-6020 Innsbruck, Austria — ³University of Science and Technology of China, Shanghai Branch, Shanghai 201315, China

We present a novel design of a pulsed plasma discharge ion source for the creation of a vast variety of anions, especially hydrated water clusters. The ions are produced inside a glow discharge plasma and characterised via a Wiley-McLaren mass spectrometer. We report the successful creation of different species of anions from various gas compositions. In future experiments, the water clusters ions will be stored in a hybrid atom-ion trap for studies of chemical reactions at ultralow temperatures.

MO 17.4 Wed 16:15 Orangerie

Laser induced fluorescence detection of ultracold formaldehyde — ●MARTIN IBRÜGGER, ALEXANDER PREHN, MAXIMILIAN LÖW, MARTIN ZEPPENFELD, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

Ultracold molecules offer ideal perspectives for a variety of exciting applications. Proposed experiments range from the investigation of ultracold chemistry over quantum simulation to high-precision spectroscopy. Optoelectrical Sisyphus cooling has proven to be capable to provide a sizeable number of $3 \cdot 10^5$ molecules of formaldehyde (H_2CO) at temperatures below 1 mK [1]. However, in the past the experiment has suffered from a low detection efficiency of the quadrupole mass spectrometer employed for counting the molecules, thus severely increasing measurement times.

Here, we present a scheme for continuous detection of formaldehyde based on laser induced fluorescence (LIF). Molecules are electronically excited by a UV-laser and successively fluoresce. No cycling transition

is available due to bad Franck-Condon overlap and thus light collection optics covering a large solid angle is mandatory. We present techniques to reduce stray light by many orders of magnitude in order to allow for a high signal to noise ratio. This setup should enable detection of formaldehyde with a sensitivity increased by about a factor of 30 and thus bring many of the proposed applications within reach and open up the way for fascinating new experiments.

[1] A. Prehn et al., *Phys. Rev. Lett.* **116**, 063005 (2016).

MO 17.5 Wed 16:15 Orangerie

Towards Direct Laser Cooling of Barium Monofluoride — ●TOBIAS SIXT, LUCAS HOFER, ANNA GRIBBON, TOBIAS REINSCH, RALF ALBRECHT, and TIM LANGEN — 5. Physikalisches Institut und Center for Integrated Quantum Science and Technology (IQST), Universität Stuttgart, Germany

We present a new experimental setup for the laser cooling and trapping of barium monofluoride molecules. Laser cooling of molecules had long been considered impossible due to their complex vibrational and rotational level structure. However, beneficial Franck-Condon factors and selection rules allow for optical cycling in many molecular species, including barium monofluoride. The molecules will be generated through laser ablation in cryostat and precooled by collisions with a 4K helium buffer gas. This results in a cold and intense beam that provides ideal starting conditions for transversal laser cooling, laser slowing and subsequent loading of a 3D magneto-optical trap. The resulting cold molecular gas will pave the way for a large number of novel and interdisciplinary applications ranging from few- and many-body physics to cold chemistry and tests of fundamental symmetries.

MO 17.6 Wed 16:15 Orangerie

Near threshold photodetachment spectroscopy of CN^- and C_3N^- in a cryogenic multipole trap — MALCOLM SIMPSON¹, ●MARKUS NÖTZOLD¹, ALICE SCHMIDT-MAY¹, ROBERT WILD¹, VITACHESLAV KOKOULINE², and ROLAND WESTER¹ — ¹Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, A-6020, Innsbruck (Austria) — ²Department of Physics University of Central Florida Orlando, FL 32816, USA

Molecular anions often exist only in a single bound electronic state. However, neutral molecules with a permanent dipole moment greater than the critical value of 1.625 D interacting with a single electron are expected to possess additional weakly bound states close to the detachment threshold (dipole bound states)[1] and metastable resonance states in the continuum (dipole scattering states) [2]. Using a cryogenic 22-pole trap we are able to probe anionic cyanides, study their interaction with light and search for evidence of dipole bound states. Current experiments of near-threshold photodetachment of the C_3N^- ($\mu \sim 3.6$ D) anion and the CN^- ($\mu \sim 1.4$ D) anion are presented and future prospects are given.

[1] Carelli, F.; Gianturco, F. A.; Wester, R.; Satta, M., *J. Chem. Phys.* **141** (2014) 054302.

[2] Carelli, F.; Satta, M.; Grassi, T.; Gianturco, F. A., *Astrophys. J.* **774** (2013) 97.

MO 17.7 Wed 16:15 Orangerie

Towards reaction studies of CN^- with atomic hydrogen in a cryogenic multipole trap — ●ELIN CARAPOVIC, ROBERT WILD, MALCOLM SIMPSON, ALICE SCHMIDT-MAY, MARKUS NÖTZOLD, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, A-6020 Innsbruck, Austria

After the radioastronomical discovery of the first interstellar anions, interest has grown in understanding the formation and destruction pathways of negative ions in the interstellar medium. Our group has previously performed photodetachment studies on C_nH^- [1], CN^- and C_3N^- anions [2], but reactions with hydrogen may also play a significant role. Reaction rate studies of C_nH^- with molecular hydrogen show vanishing rates [3]. Here we focus on the role of atomic hydrogen in reactions with interstellar anions. Our 22-pole cryogenic ion trap is a versatile tool to simulate interstellar conditions, and we have incorporated a hydrogen atom source into our system. This allows us to study the reaction rates of CN^- with atomic hydrogen at cold temperatures.

[1] T. Best, R. Otto, S. Trippel, P. Hlavenka, A. von Zastrow, S.

Eisenbach, S. Jézouin, R. Wester, E. Vigren, M. Hamberg, *Astrophys. J.* **742**, (2011).

[2] S. S. Kumar, D. Hauser, R. Jindra, T. Best, Š. Roučka, W. D. Geppert, T. J. Millar, and R. Wester, *Astrophys. J.* **776**, (2013).

[3] E. S. Endres, O. Lakhmanskaya, D. Hauser, S. E. Huber, T. Best, S. S. Kumar, M. Probst, and R. Wester, *J. Phys. Chem. A*, **118**, (2014).

MO 17.8 Wed 16:15 Orangerie

Sensitive Search for an EDM on the Electron using BaF Molecules — ●THOMAS MEIJKNECHT¹, PARUL AGGARWAL¹, HENDRICK L. BETHLEM², ANASTASIA BORSHEVSKY¹, KEVIN ESAJAS¹, PI HAASE¹, STEVEN HOEKSTRA¹, KLAUS JUNGMANN¹, MAARTEN MOOIJ², ROB TIMMERMANS¹, WIM UBACHS², LORENZ WILLMANN¹, and ARTEM ZAPARA¹ — ¹Van Swinderen Institute, University of Groningen, NL, and Nikhef, NL — ²LaserLab, Department of Physics and Astronomy, Vrije Universiteit Amsterdam, NL

The observation of an electron electric dipole moment (eEDM) larger than the value allowed by the Standard Model (SM) of particle physics would be direct evidence of new physics. An upper limit of the eEDM constrains extensions to the SM. The barium monofluoride molecule (BaF) is an excellent system for electron EDM searches. Its structure gives rise to a large effective electric field \vec{E}_{eff} experienced by the valence electron, if the molecules are polarized by an external electric field. The particular structure of BaF enables their slowing down in a Stark decelerator [1] to velocities of several 10 m/s. With the addition of laser cooling a bright and slow molecular beam can be created.

The components of the experiment, from the cryogenic source of BaF to the magnetically shielded interaction zone will be discussed and the experimental strategy will be explained. The goal of the project is a statistical limit of $5 \cdot 10^{-30} e cm$. At the projected precision the results of this experiment complement results in high energy physics experiments, e.g. at LHC.

[1] J.E. van den Berg, et al., *J. Mol. Spec.* **300**, 22 (2014)

MO 17.9 Wed 16:15 Orangerie

Cryo IR Spectroscopy of N₂ and H₂ on Ru₈⁺ — SEBASTIAN DILLINGER¹, MATTHIAS P. KLEIN¹, ●ANNIKA STEINER¹, DAVID C. McDONALD II², MICHAEL A. DUNCAN², MANFRED M. KAPPES³, and GEREON NIEDNER-SCHATTEBURG¹ — ¹Fachbereich Chemie und Forschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — ²Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA — ³Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

We present the cryo IR spectra of $[Ru_8(H_2)_l]^+$ $l=1-8$, $[Ru_8(N_2)_m]^+$ $m=1-8$, and the coadsorbed $[Ru_8(H_2)_1(N_2)_4]^+$ and $[Ru_8(N_2)_4(H_2)_1]^+$ species in isolation. The $[Ru_8(H_2)_l]^+$ species with $l > 1$ reveal bands in the region of 1800 cm^{-1} to 1880 cm^{-1} , which are a strong evidence for the formation of a hydride species. The $[Ru_8(N_2)_m]^+$ species reveal features redshifted to the free N₂ vibration (2300 cm^{-1}) in the region of 2190 to 2300 cm^{-1} , which are attributed to the vibration of head on adsorbed N₂. The H₂-N₂-coadsorbates $[Ru_8(H_2)_1(N_2)_4]^+$ and $[Ru_8(N_2)_4(H_2)_1]^+$ species reveal spectral differences in the hydride region of the IR spectra. We interpret these differences to different positioning of the hydrides on the Ru cluster. This positioning is influenced by the sequence of adsorption (first H₂ and then N₂ or first N₂ and then H₂) and the possibility of migration of the hydrides on the Ru₈⁺ cluster.

MO 17.10 Wed 16:15 Orangerie

Collinear TOF electron impact for detecting high masses in cluster beam — ●AUDREY SCOGNAMIGLIO, ALEXANDER RUF, KATRIN DULITZ, BERND VON ISSENDORFF, and FRANK STIENKEMEIER — Physikalisches Institut, Universität Freiburg, Germany

The isolation of atoms, molecules and molecular complexes in rare cluster beams, and particularly in helium nanodroplets, offers a versatile method for the study of energetic and dynamical properties of these systems, because it provides low-temperature conditions with minimal perturbation by the environment. For the detection and mass selection of the needed high mass range, as well as to give insights into the mass and charge distribution, it is advantageous to use a combination of electron impact ionization, photo-ionization and time-of-flight (TOF) spectrometry in a collinear arrangement to the cluster beam. We combined an electron gun with a TOF spectrometer in order to provide a versatile ionization method and a good mass resolution. In this presentation, the characterization of the setup and first results using doped

helium nanodroplets and rare gas clusters will be discussed.

MO 17.11 Wed 16:15 Orangerie

Setup for production and characterization of molecular clusters from liquids — ●JOHANNES VIEHMANN, PHILIP WENZEL, ANDREAS HANS, REBECCA SCHAF, ARNO EHRESMANN, and ANDRÉ KNIE — Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology (CINSA-T), Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

In order to investigate real life processes within aqueous environments it is necessary to reconstruct natural systems of interest under laboratory conditions. Supersonic expansion is commonly used for the production of molecular clusters. Here we show how mass spectrometry enables us to adequately determine cluster sizes and characterize the parameter room of a cluster source. A setup for production and characterization of molecular clusters from liquids using a two chamber cluster source with integrated heating system is described.

MO 17.12 Wed 16:15 Orangerie

Production and analysis of micro-solvated organic molecules — ●REBECCA SCHAF, JOHANNES VIEHMANN, PHILIP WENZEL, ANDREAS HANS, ARNO EHRESMANN, and ANDRÉ KNIE — Institut für Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

The preparation of water clusters doped with organic molecules is a suited method for the experimental exploration of the behaviour of such molecules in natural (aqueous) environments. Here, we present a versatile cluster source for the production of water clusters doped with organic liquids and low-melting solids. Among others, the source enables investigations on mixing ratio effects, isotope effects, and temperature dependencies. We describe the principle of this two-chamber cluster source and present first experimental data.

MO 17.13 Wed 16:15 Orangerie

Mass Selected Water Clusters and Solvated Ions for X-Ray Spectroscopy - First Results — ●JULIUS SCHWARZ, IVAN BAEV, FRIDTJOF KIELGAST, and MICHAEL MARTINS — Institute for Experimental Physics, University Hamburg, Germany

A characterization of the geometric and electronic structure of ionized water clusters and solvated ions is crucial for a detailed understanding of Ionic Solvation and its effects on the reactivity of the solute. Such a characterization can be obtained by studying ionized water clusters and solvated ions in the gas phase using X-Ray spectroscopy. The challenge of supplying an ionized cluster beam can be solved by injecting water molecules into the flowing afterglow regime of Argon plasma to enable formation of the ionized water clusters. The same technique can be used to supply a variety of solvated ions.

Here, we present first results on commissioning a Flowing Afterglow Ion Source to supply mass-selected water clusters and solvated ions to the Photon Ion Spectrometer at PETRA III (PIPE) in Hamburg for characterization by X-Ray spectroscopy. We will report on source design, the flowing afterglow technique, mass spectra of the ion beam, as well as ion current after mass selection.

MO 17.14 Wed 16:15 Orangerie

Molecular Frame Angular Emission Distributions of Resonant ICD Electrons in Ne₂ and HeNe — ●ABIR MHAMDI¹, FLORIAN TRINTER², TILL JAHNKE², KIRILL GOKHBERG³, REINHARD DÖRNER², and PHILIPP V. DEMEKHIN¹ — ¹Institut für Physik und CINSA-T, Universität Kassel, 34132 Kassel, Germany — ²Institut für Kernphysik, Universität Frankfurt, 60438 Frankfurt am Main, Germany — ³Theoretische Chemie, Universität Heidelberg, Im Neuenheimer Feld, 69120 Heidelberg, Germany

Molecular Frame Angular Distributions (MFADs) of slow electrons released by Interatomic Coulombic Decay in van der Waals dimers are studied by the Single Center (SC) method [1] including the underlying nuclear dynamics. Specifically, we considered the spectator resonant ICD after $2s - np$ inner valence excitation of Ne dimers, which is the dominant decay pathway for $n \geq 5$ [2]. In addition, we investigated the photoionization of HeNe across the He(1s3p) excitation which is a good candidate for the antenna-receiver mechanism [3]. Theoretical predictions for HeNe are in good agreement with the results of the coincidence experiments carried out by COLTRIMS technique [4]. It is demonstrated that MFAD of the resonant ICD electrons provides a direct access to the symmetry of the intermediate electronic states.

References: [1] Ph. V. Demekhin, et al., *Journal of Chemical Physics*

134, 024113 (2011). [2] S. Kopelke, et al., *J. Chem. Phys.* **130**, 144103 (2009). [3] F. Trinter, et al., *Phys. Rev. Lett.* **111**, 093401 (2013). [4] R. Dörner, et al., *Physics Reports* **330**, 95 (2000).

MO 17.15 Wed 16:15 Orangerie

Investigation of the geometric and electronic structure of nitrogen clusters — ●HUDA OTTO, DANA BLOSS, ANDREAS HANS, XAVER HOLZAPFEL, CATMARNA KÜSTNER-WETEKAM, MAIK MOROWSKI, CHRISTIAN OZGA, PHILIPP SCHMIDT, ARNO EHRESMANN, and ANDRÉ KNIE — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Lately, evidence for an Intermolecular Coulombic Decay (ICD) in nitrogen van-der-Waals-dimers has been found and ICD has been suggested to widely occur in biologic tissues. While the electronic states of gaseous nitrogen have been subject of scientific investigations for decades, the geometric and electronic structure of clusters are not yet completely understood. N_2 -clusters have recently been in discussion because of a showcase, which might be a candidate for future medical applications of ICD [1, 2]. In order to investigate the ICD in N_2 -clusters in detail, it is necessary to know their electronic structure. Photon-induced fluorescence spectroscopy delivers information about the electronic states of a species. To contribute to the above-mentioned discussion fluorescence spectroscopy is introduced as a technique for investigating the geometric and electronic structure of nitrogen clusters and first data are presented.

[1] Trinter et al., *Nature* **505** 664 (2014)

[2] Gokhberg et al., *Nature* **505** 661 (2014)

MO 17.16 Wed 16:15 Orangerie

Theory of photoassociation processes of alkali metal clusters — ●JAN SCHNABEL^{1,2} and ANDREAS KÖHN^{1,2} — ¹Institut für Theoretische Chemie, Universität Stuttgart — ²Center for Integrated Quantum Science and Technology

Understanding molecular binding mechanisms on a fundamental level and creating molecules in exactly defined quantum states are major goals in the growing area of ultracold chemistry. An important method to produce ultracold molecules is photoassociation which has been demonstrated for Rb dimers in [1,2]. At the same time an experimental realization of higher associated clusters succeeded so far only with alkali metal atoms formed on helium droplets [3]. An encouraging approach for preparing isolated Rb_3 combines photoassociation with cavity QED allowing for non-destructive detection of ultracold molecules.

We use *ab-initio* calculations to investigate possible states, transitions and spin-orbit couplings to propose a realistic photoassociation scheme for realizing spin-polarized Rb_3 clusters. To this end we construct potential energy surfaces of excited states applying a general interpolation method within the framework of RKHS (reproducing kernel Hilbert space) theory. Moreover we analyze long-range interactions between Rb_2 and Rb as well as the vibrational levels of some trimer states.

[1] J. Hecker Denschlag, *Phys. Rev. A* **82**, 052514 (2010)

[2] J. Hecker Denschlag, *Phys. Rev. A* **95**, 062507 (2017)

[3] W.E. Ernst, *J. Chem. Phys.* **45**, 114501 (2008)

MO 17.17 Wed 16:15 Orangerie

3D high resolution diffractive imaging of individual silver clusters — ●J. JORDAN¹, B. LANGBEHN¹, A. ULMER¹, J. ZIMMERMANN^{5,1}, S. DOLD², B. v. ISSENDORFF², I. BARKE³, H. HARTMANN³, F. MARTINEZ³, K. OLDENBURG³, K. MEIWES-BROER³, T. FENNEL³, C. BOMME⁴, J. CORREA⁴, S. DÜSTERER⁴, B. ERK⁴, B. MANSCHWETUS⁴, R. TREUSCH⁴, T. MÖLLER¹, and D. RUPP^{1,5} — ¹TU Berlin — ²U. Freiburg — ³U. Rostock — ⁴FLASH@DESY — ⁵MBI Berlin

Short-wavelength free-electron lasers (FELs) have opened a window into the nano cosmos. Their high intensity and short pulse duration allow capturing of high resolution "snapshots" of single nanometer-sized

objects in free flight. Single silver clusters, created by a magnetron sputter source in a broad size distribution, were imaged in a diffraction before destruction approach using extreme ultraviolet (XUV) and soft x-ray pulses from the FEL in Hamburg (FLASH). In a previous work, a large variety of structural motifs were identified by using wide angle diffraction [Barke *et al.*, *Nat. Comm.* **6** (2015)]. There, the scattering signal at large angles, which contains 3D information on particle shape and orientation, was recorded in the XUV regime. However, the use of long wavelengths decreases spatial resolution. In this work, scattering images obtained at 5 nm and 13.6 nm were compared to test whether 3D information can be reliably extracted at short wavelengths while maintaining high resolution. This is key to time resolved imaging studies on light-induced electronic excitation and ultrafast melting of metal clusters, which will be further explored in an upcoming experiment.

MO 17.18 Wed 16:15 Orangerie

Ionization dynamics of methane clusters — ●A. HEILRATH¹, M. SAUPPE¹, K. KOLATZKI^{1,2}, B. LANGBEHN¹, B. SENFFLEBEN¹, A. ULMER¹, J. ZIMMERMANN^{1,2}, L. FLÜCKIGER³, T. GORKHOVER^{1,4}, C. BOSTEDT^{5,6}, Y. KUMAGAI⁵, C. BOMME⁷, S. DÜSTERER⁷, B. ERK⁷, M. KUHLMANN⁷, C. PASSOW⁷, D. ROLLES^{7,8}, D. ROMPOTIS⁷, S. TOLEIKIS⁷, R. TREUSCH⁷, T. FEIGL⁹, T. MÖLLER¹, and D. RUPP^{1,2} — ¹TU Berlin — ²MBI Berlin — ³La Trobe University, Melbourne, Australia — ⁴SLAC Menlo Park, USA — ⁵Argonne National Lab, USA — ⁶Northwestern University, USA — ⁷FLASH@DESY — ⁸Kansas State University, USA — ⁹optiX fab, Jena

Coherent diffraction experiments using intense femtosecond short-wavelength pulses from free-electron lasers (FEL) allow to determine the structure and dynamics of individual nanoparticles. The ultrafast ionization and fragmentation dynamics of large methane clusters were studied using intense XUV double pulses from the split-and-delay unit DESC at the FLASH FEL (DESY Hamburg). With each double pulse both the cluster's initial state, and 35-650 picoseconds later the ionized state, are imaged separately on a two-detector setup. Ionic fragments are measured in coincidence with a time-of-flight spectrometer. Methane clusters, as heterogeneous model systems for biomolecules, reveal rich dynamics of higher adducts [Iwan *et al.* (2012) *PRA* **86**, 033201], unobserved in molecular methane or homogeneous clusters. The dependence of the ion spectra on cluster size and time delay will be discussed.

MO 17.19 Wed 16:15 Orangerie

THz/IR spectroscopy of glycine-water in helium nanodroplets — ●NITISH PAL¹, DEVENDRA MANI¹, RAFFAEL SCHWAN¹, GERHARD SCHWAAB¹, BRITTA REDLICH², LEX VAN DER MEER², and MARTINA HAVENITH¹ — ¹Physikalische Chemie II, Ruhr-Universität Bochum, Germany — ²Institute for Molecules and Materials (IMM), Radboud University Nijmegen, Nijmegen, Netherlands

It is well known that glycine exists in the neutral form in gaseous state and in the zwitterionic form in aqueous solution. Numerous experimental [1] and theoretical [2] studies have been carried out to understand this transformation. One of the most important goals has been to determine the minimum number of water molecules needed for such transformation.

We have already reported infrared spectra of glycine and 1:1 glycine-water complexes [3], now we are exploring the intermolecular proton transfer mechanism by stepwise adding water molecules to glycine molecule in helium droplets. The superfluid medium of helium nanodroplets allows a barrier-free diffusion of the dopant molecules and enables the formation of molecular clusters at 0.37 K temperature. The experiments are carried out using helium nanodroplet spectroscopy technique in combination with Free Electron Laser (FEL) at FELIX laboratory in Nijmegen. Herein we present the results of glycine-water infrared absorption spectra.

[1] Espinoza, C *et al.*, *J. Phys. Chem. A.*, **114**, 5919, (2010).

[2] Tudela, R *et al.*, *J. Phys. Chem. Lett.*, **7**, 5137, (2016).

[3] Kaufmann, M *et al.*, *Phys. Chem. Chem. Phys.*, **18**, 28082, (2016).