From First Molecules to Life (SYML)

jointly organized by
the Mass Spectrometry Division (MS) and
the Molecular Physics Division (MO)

Robin Golser	Gereon Niedner-Schatteburg	Lutz Schweikhard
Fakultät für Physik	Fachbereich Chemie	Institut für Physik
Universität Wien	Technische Universität Kaiserslautern	Universität Greifswald
Währinger Str. 17	Erwin-Schrödinger-Straße	Domstr. 10a
1090 Wien	67663 Kaiserslautern	17487 Greifswald
Österreich	gns@chemie.uni-kl.de	Lutz.schweikhard@physik.uni-greifswald.de
robin.golser@univie.ac.at		

The Symposium “From first Molecules to Life” illustrates processes in space which concatenate on the way from primordial atomic and ionic matter to condensed matter and exosolar planetary atmospheres - prerequisites for subsequent evolution of life. The first session focusses explictly on astrophysical topics while the second session takes a remote stand and comprises of novel laboratory studies on molecular and ionic matter in isolation.

Overview of Invited Talks and Sessions

(Lecture room e415)

Invited Talks

SYML 1.1	Wed	11:00–11:30	e415	**Laboratory studies of interstellar molecules: from the first molecules to complex organics in space** — •Holger Kreckel
SYML 1.2	Wed	11:30–12:00	e415	**Detecting astrophysically relevant ions in laboratory and space** — •Stephan Schlemmer
SYML 1.3	Wed	12:00–12:30	e415	**Interstellar ice - a hot topic** — •Harold Linnartz
SYML 1.4	Wed	12:30–13:00	e415	**Exoplanets: The Thorny Path to Habitable Conditions** — •Manuel Güdel
SYML 2.1	Wed	14:30–15:00	e415	**Physics with keV Ion Beams in the Cryogenic Storage Ring CSR** — •Andreas Wolf
SYML 2.3	Wed	15:15–15:45	e415	**A generalized theory for rovibrational motion in cold, extremely floppy molecules** — •Hanno Schmiedt, Per Jensen, Stephan Schlemmer
SYML 2.6	Wed	16:15–16:45	e415	**Lead-cluster investigations at ClusterTrap** — Stephan König, Paul Fischer, Gerrit Marx, •Lutz Schweikhard, Markus Wolfram, Albert Vass

Sessions

SYML 1.1–1.4	Wed	11:00–13:00	e415	**From First Molecules to Life**
SYML 2.1–2.6	Wed	14:30–16:45	e415	**Molecules and Ions in Isolation**

SYML 1: From First Molecules to Life

Time: Wednesday 11:00–13:00 Location: e415

Invited Talk SYML 1.1 Wed 11:00 e415
Laboratory studies of interstellar molecules: from the first molecules to complex organics in space — •Holger Kreckel — Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Modern telescopes have detected more than 180 different molecules, bearing witness to a surprisingly rich interstellar chemistry network that operates efficiently at extremely low densities and temperatures. The key to the molecular complexity in the gas phase are reactions between molecular ions and neutral atoms and molecules, as this class of reaction is often exothermic and barrier-less and therefore proceeds even in low-temperature environments. However, many of the key interstellar species are highly reactive under terrestrial conditions and thus difficult to study in the laboratory.

I will report on laboratory studies that simulate the formation of molecular hydrogen in the early universe and describe the merged beams technique that allows for the determination of energy-resolved rate coefficients for interstellar applications. Furthermore, I will introduce the planned neutral-ion collision setup at the Cryogenic Storage Ring (CSR) of the Max Planck Institute for Nuclear Physics (Heidelberg). This new experimental development aims at the study of ion-neutral collisions relevant for the formation of key species like water and complex organic molecules, under true interstellar conditions.

Invited Talk SYML 1.2 Wed 11:30 e415
Detecting astrophysically relevant ions in laboratory and space — •Stephan Schlemmer — 1. Physikalisches Institut, Universität zu Köln

Ions play a pivotal role in the astrophysics of the interstellar medium as they are readily formed by cosmic ray ionisation. They are also key species to understand the physics and chemistry of many other environments. Todays radio telescopes like the Atacama Large Millimeter Array (ALMA) and the airborne observatory SOFIA are sensitive enough to detect those species in space. In fact, many molecules and in particular some ions are first detected in space. However, laboratory spectra are missing as they are difficult to record due to their transient, i.e. highly reactive, nature. In recent years various methods of action spectroscopy have been developed in our group to overcome these limitations. In all cases changes in the rate of chemical reactions are imposed by excitation of the parent, mass selected ion. Recording the product formation in ion traps as a function of the excitation frequency results in the respective molecular spectra. Examples include mid-resolution vibrational, as well as high-resolution ro-vibrational and pure rotational spectra. In this presentation the methods are introduced and recent examples related to astrophysical searches in the radio frequency range will be discussed.

Invited Talk SYML 1.3 Wed 12:00 e415
Interstellar ice - a hot topic — •Harold Linnartz — Leiden Observatory, University Leiden

The talk reviews laboratory based studies of interstellar ice analogues. The physical and chemical processes at play upon UV irradiation and atom bombardment are discussed. It is shown how water and complex organics - building blocks of life - form in the solid state and how photodesorption rates help to understand the formation of planets.

Invited Talk SYML 1.4 Wed 12:30 e415
Exoplanets: The Thorny Path to Habitable Conditions — •Manuel Güdel — Dept. Astrophysics, University of Vienna

Habitable conditions on planetary surfaces evolve as a consequence of complex interactions between the host star, the planet itself, and a variety of solid bodies in interplanetary space. The long journey toward habitability begins in the protoplanetary disk, the birthplace of planets; here, important molecules such as water and organics form, but also protoplanetary bodies grow and eventually accrete gas envelopes from the disk. At later stages, outgassing and colliding smaller bodies begin to form a secondary atmosphere with important molecular ingredients such as nitrogen, carbon dioxide and water. Meanwhile, the evolving stellar conditions, in particular stellar high-energy radiation and ionized winds, influence the evolution of the atmosphere, potentially leading to its severe erosion. In this presentation, I will describe the intricate interplay between these factors and discuss conditions that need to be met before a planet can become habitable.

SYML 2: Molecules and Ions in Isolation

Time: Wednesday 14:30–16:45 Location: e415

Invited Talk SYML 2.1 Wed 14:30 e415
Physics with keV Ion Beams in the Cryogenic Storage Ring CSR — •Andreas Wolf — Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany

As a cryogenic electrostatic storage ring, the CSR offers long-time storage for ion beams with energies in the multi-keV regime. The first operation [1] showed that the 35 m diam. electrostatic lattice of the ring could be successfully realized and operated at 6 K and at a residual gas density of < 100 cm^{-3}. Beam storage times reached about 10 min or more for 60 keV ion beams in the studied range of mass numbers 16–218. With this, a new tool emerges for studying internal properties and fragmentation reactions of many types of complex gas-phase ions, both anions and cations. Moreover, the ring is designed for electron cooling, presently being implemented. We discuss the experimental perspectives of this facility and of long-time stored, phase-space cooled keV ion beams more generally.

[1] S. Vogel *et al.*, this Spring Meeting, MS Division.

SYML 2.2 Wed 15:00 e415
First Cold Operation of the Cryogenic Storage Ring (CSR) — •Stephen Vogel[1], Arno Becker[1], Klaus Blaum[1], Christian Breitenfeldt[1,2], Sebastian George[1], Jürgen Göck[1], Manfred Grieser[1], Florian Grussie[1], Philipp Herwig[1], Jonas Karthein[1], Claude Krantz[1], Holger Kreckel[1], Sunil Kumar[1], Jorrit Lion[1], Svenja Lohmann[1], Christian Meyer[1], Preeti M. Mishra[1], Oldřich Novotný[1], Aodh P. O'Connor[1], Roland Repnow[1], Kaija Spruck[1,3], Stefan Schippers[3], Dirk Schwalm[1,4], Lutz Schweikhard[2], Robert von Hahn[1], and Andreas Wolf[1] — [1]Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — [2]Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, 17487 Greifswald, Germany — [3]Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [4]Weizmann Institute of Science, Rehovot 76100, Israel

CSR is an electrostatic storage ring for ions of <300 keV per unit charge kinetic energy. The ion beam optics and vacuum chambers of the 35-m circumference ring can be cryogenically cooled. The ring was cooled down with 4-K liquid He in 28 cryopumping units, starting from near 10^{-10} mbar vacuum at 300 K. Ion beams of 60–90 keV were stored for species including Ar^+, OH^-, CH^+, C_2^-, Co_2^-, Ag_2^- and Co_3^-. With the cold ring, extensive non-destructive beam diagnostics were performed including Schottky-noise and beam-position detection. Beam lifetimes up to 2500 s were measured by laser photodetachment. Inelastic collisions of the stored ions with rest gas molecules were nearly undetectable, indicating < 100 cm^{-3} rest-gas density (corresponding to $< 10^{-14}$ mbar pressure at 300 K). Rotational cooling of OH^- ions to $> 95\%$ in $J = 0$ was shown by near-threshold photodetachment.

Invited Talk SYML 2.3 Wed 15:15 e415
A generalized theory for rovibrational motion in cold, extremely floppy molecules — •Hanno Schmiedt[1], Per Jensen[2], and Stephan Schlemmer[1] — [1]I. Physikalisches Institut, Universität zu Köln — [2]Physikalische und Theoretische Chemie, Bergische Universität Wuppertal

We present a fundamentally new theory of the non-separable [1] rotational and vibrational motion in the class of extremely floppy molecules, with a special focus on its most prominent member, protonated methane (CH_5^+). Based on the molecular symmetry, we find the rotation group in *five* dimensions, O(5), to be the underlying dy-

namical group. For protonated methane, it is now possible to predict for the very first time (i) energy levels in a zero-order approximation, (ii) dipole selection rules, and (iii) branching rules for the still valid three-dimensional angular momentum quantum number. Additionally, a classification of the eigenstates of the O(5) theory in the finite molecular symmetry group can be established.
Most astonishing, two new quantum numbers are identified to be the basis of the new theory. In this talk, we will show its very first application to experimental data, published only recently [2], and show how they fit surprisingly well within the zero-order approximation.

[1] Schmiedt, H., Schlemmer, S., Jensen, P., J. Chem. Phys. 143 (15),154302 (2015)
[2] Asvany, O., Yamada, K.M.T., Brünken, S., Popatov, A., Schlemmer S., Science 347, 1346-1349 (2015)

SYML 2.4 Wed 15:45 e415

Control of small water clusters — •Helen Bieker[1,2], Daniel Horke[1,2], Daniel Gusa[1], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, DESY — [2]The Hamburg Center for Ultrafast Imaging, University of Hamburg — [3]Department of Physics, University of Hamburg

To unravel the microscopic details of intermolecular interactions in water, we prepare controlled samples of size- and isomer-selected water clusters. The spatial separation of neutral molecules can be achieved using inhomogeneous electric fields, allowing us to create pure samples of individual structural isomers or of size-selected clusters and to disperse molecules in a beam according to their quantum states [1].

Here, we aim to develop an understanding of the structures of water clusters containing a few monomer units. We present our first results on the production of size-selected samples using supersonic expansions and subsequent dispersion of the various clusters in strong electric fields, extending previous studies [2]. Future experiments aim at utilizing x-ray and electron diffractive imaging to study the structures and the ultrafast dissociation/fragmentation dynamics of these polymolecular systems.

[1] Y.P. Chang, D. A. Horke, S. Trippel and J. Küpper, *Int. Rev. Phys Chem.* **34**, 557-590 (2015)
[2] R. Moro, R. Rabinovitch, C. Xia, and V.V. Kresin, *Phys. Rev. Lett.* **97**, 123401 (2006)

SYML 2.5 Wed 16:00 e415

Chiral rotational spectroscopy — •Robert Cameron[1,2], Jörg Götte[1,2], and Stephen Barnett[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Deutschland — [2]School of Physics and Astronomy, University of Glasgow, Glasgow, UK

We present a new technique for the rotational spectroscopy of chiral molecules which enables the determination of individual components $G'_{XX}, G'_{YY}, G'_{ZZ}, A_{X,YZ}, A_{Y,ZX}$ and $A_{Z,XY}$ of the optical activity polarisability. Knowledge of these components fully characterises the enantiomeric constitution of a molecule. Our method gives an incisive signal for molecules with multiple chiral centres and even if the various stereoisomers of the chiral molecule are in a racemic mixture.

The necessary requirements on which our technique is based can also be found in space, which is why our method can also be exploited in the search for the molecular chirality in the interstellar medium, which, if found, could explain the existence of the biological homochirality of life as we know it.

Invited Talk SYML 2.6 Wed 16:15 e415

Lead-cluster investigations at ClusterTrap — Stephan König, Paul Fischer, Gerrit Marx, •Lutz Schweikhard, Markus Wolfram, and Albert Vass — Institut für Physik, Universität Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald

During the last couple of years the Penning-trap setup ClusterTrap has been further extended and used for studies of the production and properties of poly-anionic metal clusters, focusing mainly on the elements gold and aluminum. Recent experiments reached out to further elements including lead. As before, the lead clusters were exposed to an "electron bath": Mono-anionic lead clusters were produced in a laser vaporization source and were transferred and captured in the trap; by shooting primary electrons axially through the trap, argon buffer-gas atoms are ionized. The argon cations immediately leave the trap while the secondary electrons stay stored and can attach to the clusters - provided they overcome the repulsing Coulomb barrier. The measurements as a function of cluster size yield the appearance sizes for doubly and triply charged anionic clusters. In addition, and unlike the other clusters, the lead clusters show distinct dissociation patterns, with very prominent peaks at the (monoanionic) dodecamer and in particular the decamer. These clusters are also dominant in photodissociation spectra of larger mono-anions and apparently also of the dianions. The experiments are still ongoing and will be extended with respect to further charge states, including cationic species.