

# Laboratory Astrophysics in the Age of ALMA and JWST

799. WE-Heraeus-Seminar

18 - 21 September 2023

at the

Max-Planck-Institut für Kernphysik,  
Heidelberg

**WILHELM UND ELSE  
HERAEUS-STIFTUNG**



# Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see <https://www.we-heraeus-stiftung.de>

## Aims and scope of the 799. WE-Heraeus-Seminar:

The physics and chemistry of molecules in interstellar space are at the forefront of astronomical research. Almost 300 different molecular species have been identified in interstellar environments to date, ranging in size from simple diatomics to complex organic molecules and even fullerenes. The pace of new detections has been accelerating in recent years, owing to the availability of modern observatories and techniques. It has been recognized that in order to make the most of the observational data that await us in the next decades, a major push toward laboratory astrophysics – including theoretical efforts to understand fundamental astrophysical processes and modelling of interstellar and exoplanetary environments – will be needed.

This WE-Heraeus-Seminar will bring together experts and young researchers in the emerging field of Molecular Astrophysics to discuss data needs as well as new experimental and theoretical developments to address urgent questions regarding the formation, destruction, and identification of molecules in space.

## Scientific Organizers:

PD Dr. Holger Kreckel

MPI für Kernphysik Heidelberg, Germany  
E-mail: [holger.kreckel@mpi-hd.mpg.de](mailto:holger.kreckel@mpi-hd.mpg.de)

Prof. Dr. Paola Caselli

MPI für extraterrestrische Physik, Garching,  
Germany  
E-mail: [caselli@mpe.mpg.de](mailto:caselli@mpe.mpg.de)

Prof. Dr. Melanie Schnell

Universität zu Kiel und DESY Hamburg, Germany  
E-Mail: [melanie.schnell@desy.de](mailto:melanie.schnell@desy.de)

# Introduction

## Administrative Organization:

Dr. Stefan Jorda  
Marion Reisinger

Wilhelm und Else Heraeus-Stiftung  
Kurt-Blaum-Platz 1  
63450 Hanau, Germany

Phone +49 6181 92325-18

Fax +49 6181 92325-15

E-mail [reisinger@we-heraeus-stiftung.de](mailto:reisinger@we-heraeus-stiftung.de)

Internet: [www.we-heraeus-stiftung.de](http://www.we-heraeus-stiftung.de)

## Venue:

MPI for Nuclear Physics  
Saupfercheckweg 1  
69117 Heidelberg  
Germany

Phone +49 6221 516-0

<https://www.mpi-hd.mpg.de/mp/de/>

## Registration:

Foyer Otto Hahn Lecture Hall, Building 12  
Monday 12:30 – 14:00

**Program**

# Program

**Monday, 18 September 2023**

12:30 - 14:00	Arrival at the MPIK and Registration (Foyer Otto Hahn Lecture Hall, Building 12)	
14:00	<b>Session 1: Overview and current developments</b>	
14:00 – 14:15	Scientific organizers	<b>Welcome Words</b>
14:15 – 15:00	Thomas Henning	<b>JWST Observations of Star and Planet Formation</b>
15:00 – 15:45	Evelyne Roueff	<b>Physics and chemistry of photon-dominated regions: current challenges</b>
15:45 – 16:30	Paul Molliere	<b>Molecules in Exoplanet Atmospheres</b>
16:30 – 17:00	<i>COFFEE BREAK</i>	
17:00	<b>Contributed Talks</b>	
17:00 – 17:20	Gayatri Batra	<b>Exploring the silicon derivatives of aromatic hydrocarbons for facilitating astronomical searches</b>
17:20 – 17:40	Hayley Bunn	<b>Millimeter/submillimeter spectroscopy and interstellar search for singly and doubly deuterated methyl mercaptan (CH<sub>2</sub>DSH/CHD<sub>2</sub>SH)</b>
17:40 – 18:00	Parker Crandall	<b>Optical Spectrum of the Urotropin Radical Cation</b>
18:00 – 18:20	Lisa Gamer	<b>MOCCA: a 4-kilo-pixel microcalorimeter detector for CSR</b>
18:20 – 18:40	Miguel Jiménez-Redondo	<b>Reactions of CN<sup>+</sup>, HCN<sup>+</sup> and HNC<sup>+</sup> with H<sub>2</sub> studied in a low-temperature ion trap</b>
18:40 – 19:00	Daniel Strasser	<b>Formation of new bonds in ionization of isolated molecules</b>
19:00	<i>BUFFET DINNER AND POSTER SESSION (MPIK Foyer)</i>	

# Program

Tuesday, 19 September 2023

09:00	<b>Session 2: Spectroscopy</b>	
09:00 – 09:45	Silvia Spezzano	Laboratory spectroscopy - From clouds to planets
09:45 – 10:30	Stephan Schlemmer	Misslons: Missing Ions in Laboratory and Space
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:45	Donatella Loru	A multispectroscopic approach to underline the role of polycyclic aromatic hydrocarbons in the interstellar medium
11:45 – 12:30	Guido Fuchs	Old stars with new matter: Watching the infrared sky at high spectral resolution
12:30 – 14:00	<i>LUNCH BREAK</i>	
14:00	<b>Labtour MPIK</b>	
16:00	<i>COFFEE BREAK</i>	
16:30	<b>Contributed Talks</b>	
16:30 – 16:50	Alexey Potapov	Trapped water on silicates in the laboratory and in astrophysical environments
16:50 – 17:10	Tamar Stein	Computational exploration of the oxygen( <sup>1</sup> D) reactivity with C <sub>2</sub> H <sub>x</sub> hydrocarbons: astrochemical reaction pathways
17:10 – 17:30	Taarna Studemund	Small Silicon Oxide Cations as Precursors for Interstellar Dust: Optical Absorption and Photodissociation Properties

# Program

**Tuesday, 19 September 2023**

17:30 – 17:50	Akemi Tamanai	<b>Experimental verification for effect of dust agglomeration on MIR spectra: What do individual dust agglomerates tell us about observed spectra?</b>
17:50 – 18:10	Richard Thomas	<b>Probing charge-transfer neutralization reactions in cool plasmas using the ion storage facility DESIREE</b>
18:10 – 18:30	Xavier Urbain	<b>Merged beams experiments with neutral atoms and stored molecular ions at the CSR</b>
18:45	<b>Bus transfer to S’Kastanie</b>	
19:30	<i>CONFERENCE DINNER</i>	

# Program

Wednesday, 20 September 2023

09:00	<b>Session 3: Gas phase experiments</b>	
09:00 – 09:45	Oldrich Novotny	<b>Recombination of molecular ions at the Cryogenic Storage Ring</b>
09:45 – 10:30	Brianna Heazlewood	<b>Studying ion–neutral reaction dynamics at low temperatures</b>
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:45	Sandra Brünken	<b>Infrared Action Spectroscopy as a Tool for Probing Gas-Phase Dynamics</b>
11:45- 12:30	Henning Zettergren	<b>Astrophysical studies at the DESIREE facility</b>
12:30- 14:00	<i>LUNCH BREAK</i>	
14:00	<b>Session 4: Fundamental processes</b>	
14:00 – 14:45	Jennifer Meyer	<b>Ion molecule reactive scattering for astrophysics?</b>
14:45 – 15:30	Roman Curik	<b>Indirect dissociative recombination of cold molecular ions</b>
15:30 – 16:15	Alexandre Faure	<b>Electron collisions with interstellar molecules and molecular ions</b>
16:15	<i>COFFEE BREAK</i>	
17:00	<b>Poster Session</b>	
19:00	<i>BUFFET DINNER AND POSTER SESSION (MPIK Foyer)</i>	



# Program

Thursday, 21 September 2023

09:00	<b>Session 5: From Complex Molecules to Dust Grains</b>	
09:00 – 09:45	Harold Linnartz	<b>Inter- and circumstellar ice research in the era of JWST - the laboratory perspective</b>
09:45 – 10:30	Veerle Sterken	<b>Cosmic dust in the solar system</b>
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:45	Otto Dopfer	<b>Photochemical Properties of Astrochemically-Relevant Silicon Clusters: Bridging the Gap Between Diatomics and Silicate Grains</b>
11:45- 12:30	Annemieke Petrignani	<b>Zooming in on photo-processing of PAHs</b>
12:30- 14:00	<i>LUNCH BREAK</i>	
14:00	<b>End of the seminar and departure</b>	

**Posters**

## Posters

- Mitsunori Araki      **Millimeter and submillimeter spectroscopy of the deuterated molecular ion  $SD^+$**
- Romain Basalgète      **Experimental diffusion of water through porous amorphous carbon dust analogues**
- Lukas Berger      **Characterization of a simple supersonic expansion source for small molecular ions**
- Jonas Bosmann      **Double resonance excitation of overtones and combination bands in jet-cooled  $N_2O$**
- Petr Dohnal      **Ion trap study of nuclear spin state-changing collisions of  $H_3^+$  with  $H_2$  at low temperatures**
- Selina Gaisser      **Modeling detection efficiency for microcalorimetry at CSR**
- Varazdat Grigorian      **The newly set-up spectroscopic molecular beam apparatus : Conceptual and technical overview**
- Florian Grussie      **Merged beams experiments between neutral atoms and molecular ions at the Cryogenic Storage Ring**
- Felix Herrmann      **The CSR-ReMi – A cryogenic in-ring reaction microscope**
- Pierre-Michel Hillenbrand      **Single-pass merged-beams experiments on molecular ion-neutral reactions for astrochemistry**
- Leonard Isberner      **First Dielectronic Recombination Measurements at the Cryogenic Storage Ring**
- Cornelia Jäger      **The evolution of molecular ice into kerogen-like carbon**
- Christopher Alexander Jakob      **MOCCA - A 4k-Pixel Microcalorimeter Detector for the Cryogenic Storage Ring CSR**

## Posters

- Abel Kalosi      **Dissociative recombination of  $\text{OH}^+$  and  $\text{ArH}^+$  at the Cryogenic Storage Ring**
- Matin Kaufmann      **The newly set-up spectroscopic molecular beam apparatus: Applications towards multiphoton resonance**
- Hunarpreet Kaur      **Investigating Prebiotic Chemistry with Cryogenic Action Spectroscopy**
- Stav Knaffo      **Toward a new type of gas phase spectroscopy for complex organic ions**
- Franciele Kruczkiewicz      **Probing Life's Building Blocks: Thermal Desorption and Infrared Spectroscopy of Amino Acids**
- Christine Lochmann      **Temperature dependent reactions of atomic hydrogen with astrochemically relevant anions**
- Alberto Macario      **How fast are the first stages of nucleation? Reaction kinetics of the formation of heterodimers**
- Damian Müll      **Radiative cooling of small isolated cluster ions in the slow exchange limit**
- Kai Pollow      **Optical Spectra of the Smallest Silicon Carbide Cations**
- Sruthi Purushu Melath      **Photodetachment spectroscopic studies of cold, trapped negative ions**
- Fabio Ribeiro      **Complex refractive index of water ice analogues measured by terahertz time-domain spectroscopy**
- Vincent Richardson      **IR-PD Spectroscopy of the Astrochemically-Relevant  $\text{HCCS}^+$  Ion**
- Gaël Rouillé      **Carbonated silicate grains: Photodissociation of carbonate groups with Lyman- $\alpha$  irradiation**

## Posters

- Viviane Charlotte Schmidt      **Resonant photo-dissociation studies of  $C^4O^-$  at the Cryogenic Storage Ring**
- Dian Schrauwen      **Infrared irradiation of mixed interstellar ice analogues**
- Sebastian Schwetje      **The newly set-up spectroscopic molecular beam apparatus: Producing transient molecules in a cold supersonic jet**
- Dasarath Swaraj      **New Setup for High-Resolution Ion-Molecule Crossed Beam Imaging**
- Richard Tuffs      **Radiative transfer modelling of the photoelectric heating of gas in the nearby spiral galaxy NGC628**
- Lise von Rötzel      **Rotational Spectroscopy of 2-Cyanobiphenyl**
- Aigars Znotins      **Electron recombination of deuterated triatomic hydrogen ions at the Cryogenic Storage Ring**

# **Abstracts of Talks**

(in alphabetical order)

# Exploring the silicon derivatives of aromatic hydrocarbons for facilitating astronomical searches

**G. Batra,<sup>1</sup> D. Loru,<sup>1</sup> and M. Schnell**

<sup>1</sup>*Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany*

Silicon is one of the most abundant elements in the Earth's crust and is also prevalent in space in the form of gaseous molecules, interstellar dust, and ice grains. To date, more than 15 silicon-containing molecules have been detected in space, accounting for ~7% of total detections [1]. Considering the presence of silicon in the interstellar medium, silicon-containing aromatic molecules are likely targets of future astronomical searches. To aid these searches and understanding the silicon chemistry in space, laboratory data are crucial. In the laboratory, exotic silicon-containing molecules can be produced and spectroscopically characterized by combining spectroscopic techniques with electrical discharge sources. The aim is to investigate the variety of products generated by the electrical discharge experiment of silicon-substituted aromatic molecules. Numerous fragments, products, and reaction intermediates are identified by gas-phase spectroscopic techniques like rotational spectroscopy and mass-selective IR-UV spectroscopy combined with quantum-chemical calculations. The spectroscopic analysis of these molecules can aid their detection in the interstellar medium using modern telescopes like ALMA and JWST.

## References

[1] B.A. McGuire, 2021 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules, *ApJS*. 259 (2022) 30.

# Infrared Action Spectroscopy as a Tool for Probing Gas-Phase Dynamics

S. Brünken<sup>1</sup>

<sup>1</sup>*FELIX Laboratory, Radboud University, Nijmegen, The Netherlands*

Complex organic molecules, including aromatics and polycyclic aromatic hydrocarbons (PAHs), are found in a large variety of astronomical environments, including low temperature and low density molecular clouds in the interstellar medium which are the birthplaces of new stars and planets. Laboratory astrophysical studies on chemical reaction pathways and rate coefficients under astronomically relevant conditions are crucial to interpret astronomical observations and as input for simulations in astrochemical networks. Of similar importance are spectroscopic studies of the often elusive, but essential, molecular reaction partners, intermediates and products that yield fundamental insights on their structure, and provide spectroscopic signatures needed for their identification in space.

Cryogenic ion traps have proven to be ideal tools for studying ion-molecule reactions under controlled conditions and enable sensitive spectroscopic studies of mass-selected, cold, and isolated molecular ions. Here, I will describe the combination of such a cryogenic 22-pole ion trap instrument with the widely tunable infrared free-electron lasers at the FELIX Laboratory [1]. Cryogenic infrared action-spectroscopy is used to structurally characterize isomeric ions formed upon (dissociative) ionization of neutral species, allowing us to unravel their fragmentation processes (top-down processes), e.g. [2,3]. Very recently, we developed a combination of ion-molecule reactivity studies and infrared spectroscopy to elucidate and disentangle formation routes of complex molecules (bottom-up processes) at astronomically relevant temperatures, and have in this way identified an efficient low-temperature PAH-growth pathway from mono- to polycyclic aromatic hydrocarbons [4].

## References

- [1] P. Jusko, S. Brünken, O. Asvany, S. Thorwirth, A. Stoffels, L. van der Meer, G. Berden, B. Redlich, J. Oomens, S. Schlemmer, *Faraday Discuss.* **217**, 172-202 (2019)
- [2] D.B. Rap, A. Simon, K. Steenbakkens, J.G.M. Schrauwen, B. Redlich, and S. Brünken, *Faraday Discuss.*, **in press**, (2023). Doi: 10.1039/D3FD00015J
- [3] S. Banhatti, D.B. Rap, A. Simon, H. Beloucher, G. Wenzel, C. Joblin, B. Redlich, S. Schlemmer, and S. Brünken, *Phys. Chem. Chem. Phys.* **24**, 27434-27535 (2022).
- [4] D.B. Rap, J.G.M. Schrauwen, A.N. Marimthu, B. Redlich, S. Brünken, *Nat. Astron.* **6**, 1059 (2022)



# Millimeter/submillimeter spectroscopy and interstellar search for singly and doubly deuterated methyl mercaptan (CH<sub>2</sub>DSH/CHD<sub>2</sub>SH)

**H. A. Bunn<sup>1</sup>, S. Spezzano<sup>1</sup>, L. H. Coudert<sup>2</sup>, C. Endres<sup>1</sup>, J.-C. Guillemin<sup>3</sup>, V. Lattanzi<sup>1</sup>, and P. Caselli<sup>1</sup>**

<sup>1</sup>*The Center for Astrochemical Studies, Max-Planck Institut für extraterrestrische Physik, Garching, Germany*

<sup>2</sup>*Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay, CNRS, Orsay, France*

<sup>3</sup>*UMR 6226, CNRS-ENSCR, Institut des Sciences Chimiques de Rennes, Rennes France*

Isotopic fractionation is an essential tool for tracing the formation and evolution of molecules throughout the process of star and planet formation (1). The detection of singly and doubly deuterated complex organic molecules (COMs), is steadily rising (e.g. 2-5), and show the deuterium fractionation to be very similar amongst these species, thereby implying a similar formation process. The deuterium fractionation of sulphur-based COMs, however, has not yet been investigated. Methyl mercaptan, CH<sub>3</sub>SH, is the sulphur analog of methanol and has been detected in the interstellar medium (ISM) with abundances that make detection of deuterated isotopologues plausible. While the microwave spectrum of CH<sub>2</sub>DSH and CHD<sub>2</sub>SH has been reported (e.g. 6), insufficient rotational information for extension up to the higher frequencies needed for astronomical detection was provided. Therefore, we have collected spectra of singly and doubly deuterated methyl mercaptan (CH<sub>2</sub>DSH/CHD<sub>2</sub>SH) in the 80-500 GHz range. The spectrum of CH<sub>2</sub>DSH and CHD<sub>2</sub>SH is complicated by the hindered torsional rotation of the CH<sub>2</sub>D/CHD<sub>2</sub> group. The torsional potential resulting from the internal motion of the deuterated methyl group has three minima corresponding to three different substates, two gauche (e<sub>0</sub> and o<sub>1</sub>) and one anti (e<sub>1</sub>). The Hamiltonian needed to account for this unsymmetrical methyl rotor requires an accurate potential, which is to be extracted from the torsional substates present in the far infrared, observed using the high resolution far infrared facilities at the Canadian Light Source and SOLEIL. So far, we have assigned ~1800 transitions for the singly deuterated isotopologue, including *a*-type R-branch and *b*-type Q-branch transitions for all three substates, along with interstate transitions between the two gauche substates. Furthermore, we have identified the strong *a*-type R-branch transitions for the doubly deuterated isotopologue. I will present an update on the analysis of this complex spectra along with our attempts at their detection in the ISM.

## References

1. Caselli, P. and Ceccarelli, C., *A&AR*, **20**, 1 (2012)
2. Ferrer Asensio, J. F. *et al.*, *A&A*, **670**, A177 (2023)
3. Manigand, S. *et al.*, **623**, A69 (2019)
4. Richard, C. *et al.*, *A&A*, **651**, A120 (2021)
5. Drozdovskaya, M. N. *et al.*, *A&A*, **659**, A69 (2022)
6. Su, C. F. *et al.*, *JCP*, **79**, 5828 (1983)

# Optical Spectrum of the Urotropin Radical Cation

P. Crandall<sup>1</sup>, A. Breier<sup>1</sup>, and O. Dopfer<sup>2</sup>

<sup>1</sup>*Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany*

Urotropin, or hexamethylenetetramine (HMT), has gained significant attention in astrochemistry due to its potential relevance in interstellar environments. Previous experiments have shown that urotropin can form in high abundance when ices containing methanol, carbon monoxide, ammonia, and water are exposed to ionizing radiation. [1,2] The detection of urotropin in these experiments is significant because it provides insights into the synthesis of complex organic molecules in space and raises questions about its role in prebiotic chemistry and the origins of life. However, its detection in the gas phase is not possible by radio astronomy. Instead, novel observations in the infrared (using JWST, for example) or the visible to UV are more suited for this search, but laboratory measurements are still needed for assignments. Here, we report the first optical spectrum of the urotropine radical cation ( $((\text{CH}_2)_6\text{N}_4^+)$ ) between 300 and 400 nm in the gas phase. Measurements were taken in a tandem mass spectrometer by photodissociation of mass-selected ions cooled in a cryogenic 22-pole ion trap held at 5 K. The experimental results are compared to its photoelectron spectrum and time-dependent DFT calculations for interpretation. The astrophysical implications of these results are also discussed.

## References

- [1] M.P. Bernstein *et al.*, *Astrophys J* **454**, 327 (1995)
- [2] Y. Oba *et al.*, *Astrophys J* **849**, 122 (2017)

# Indirect dissociative recombination of cold molecular ions

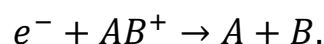
**R. Čurík<sup>1</sup>, D. Hvizdoš<sup>1,2</sup>, M. Váňa<sup>2</sup>, K. Houfek<sup>2</sup>, C.H. Greene<sup>3</sup>**

<sup>1</sup> *J. Heyrovský Institute of Physical Chemistry, Dolejškova 3, 18223 Prague, Czech Republic*

<sup>2</sup> *Institute of Theoretical Physics, Faculty of Mathematics and Physics, Charles University in Prague, V Holešovičkách 2, 18000 Prague, Czech Republic*

<sup>3</sup> *Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA*

Dissociative recombination (DR) is a process in which a free electron with a positive kinetic energy is captured by a molecular ion while breaking one or several chemical bonds,



This is a very efficient chemical process, but is rarely described in chemical textbooks. It is considered to be the most complex of gas-phase reactions leading to the production of neutral atoms and molecules [1].

Historically, we distinguish two different mechanisms for the DR process. In the direct mechanism the reaction is mediated by an electronic resonant state  $AB^*$  (shape or core-excited resonance), while in the indirect mechanism no such electronic state exists in the Frank-Condon region and the  $AB^*$  state is formed by an internal rovibrational excitation (rovibrational Feshbach resonance).

While there is a number of successful applications [2] that describe the indirect DR with the multichannel quantum defect theory (MQDT) [3], the recent experimental advances [4] put the accuracy of these models to a test. In this contribution we report on our progress in development of accurate indirect DR theory and its application to several molecular targets.

## References

- [1] A. E. Orel and M. Larsson, *Dissociative recombination of molecular ions* (Cambridge University Press, New York, 2008).
- [2] R. Čurík and C. H. Greene, *Phys. Rev. Lett.* **98**, 173201 (2007).
- [3] A. Giusti, *J. Phys. B: Atom. Molec. Phys.* **13**, 3867 (1980).
- [4] O. Novotný, P. Wilhelm, D. Paul, et al., *Science* **365**, 676 (2019)

# Photochemical Properties of Astrochemically-Relevant Silicon Clusters: Bridging the Gap Between Diatomics and Silicate Grains

**O. Dopfer**<sup>1</sup>

<sup>1</sup> *Institut für Optik und Atomare Physik, TU Berlin, Berlin, Germany*  
*E-mail: dopfer@physik.tu-berlin.de*

Interstellar dust is part of the universal recycling process of matter. A major component of interstellar dust are silicon carbides, silicon oxides, and metal-containing silicates, as inferred from IR emission and the detection of grains in meteorites. On the other hand, small silicon-containing molecules (<10 atoms) have firmly been detected in circumstellar shells by radio astronomy. Linking these two size limits from small molecules to micron-sized grains is a longstanding and still open issue. Although some hypotheses assume nucleation of seed particles, details of the growth mechanism(s), potential intermediates, and the impact of physical parameters such as radiation field, temperature, and chemical composition, remain largely unexplored. To shed further light on the nucleation process from the laboratory point of view, we investigate physical and chemical properties of small to medium-sized silicon carbide and silicon oxide clusters as a function of composition and charge state. To this end, the clusters are produced by laser vaporization techniques of various targets in molecular beams and probed by mass spectrometry, laser spectroscopy, and quantum chemistry. In a first step, geometric structures and chemical bonding of the clusters in the ground electronic state are obtained by IR spectroscopy using photodissociation and photoionization schemes, along with global optimization techniques in quantum chemical calculations [1-4]. In a second step, optical and photochemical properties are obtained by UV-VIS photodissociation spectroscopy, providing important information about electronic structure and fragmentation properties (appearance energies, competing fragmentation channels and branching ratios, particularly stable fragments) [5-7]. Results will be presented for selected  $\text{Si}_n\text{C}_m^{(+)}$  and  $\text{Si}_n\text{O}_m^{(+)}$  clusters as well as bare  $\text{Si}_2^+$ .

## References

- [1] M. Savoca et al., *J. Phys. Chem. A* **117**, 1158 (2013).
- [2] M. Savoca et al., *J. Chem. Phys.* **141**, 104313 (2014).
- [3] N.X. Truong et al., *PCCP* **16**, 22364 (2014).
- [4] N.X. Truong et al., *PCCP* **17**, 18961 (2015).
- [5] M. Förstel et al., *J. Mol. Spectrosc.* **377**, 111427 (2021).
- [6] T. Studemund et al., *J. Phys. Chem. Lett.* **13**, 7624 (2022).
- [7] T. Studemund et al., *PCCP* **25**, 17609 (2023).

# Electron collisions with interstellar molecules and molecular ions

A. Faure<sup>1</sup>

<sup>1</sup>*Institute of Planetology and Astrophysics of Grenoble, Grenoble, France*

In astrophysical molecular plasmas where the electron fraction exceeds about  $10^{-5}$ , free electrons can compete with neutral particles in driving the non-LTE excitation of molecules. Such electron fractions are found, for example, in diffuse interstellar clouds, photon-dominated regions and comets. A good knowledge of electron-impact inelastic cross sections is thus essential to extract accurate molecular column densities and to derive the gas kinetic temperature and density. Recent theoretical studies based on the UK **R**-matrix method have revisited the electron-impact rotational and vibrational excitation of many species, including key astrophysical molecules such as  $\text{HeH}^+$ ,  $\text{CH}^+$  or  $\text{H}_2\text{O}$  (see e.g. Refs. [1-3]). We will review these works and provide comparisons between state-to-state theoretical and experimental data for some benchmark species. We will also discuss the importance of the competition between inelastic collisions and dissociative recombination, both in space and in the laboratory. Finally, we will present non-LTE excitation calculations to illustrate the impact of electron collisions in actual astrophysical environments (see e.g. Refs. [4, 5]).

## References

- [1] J. Hamilton, A. Faure & J. Tennyson, *MNRAS* **455**, 3281 (2016)
- [2] R. Čurík & C. Greene, *J. Chem. Phys.* **147**, 054307 (2017)
- [3] M. Ayouz et al., *Atoms* **9**, 62 (2021)
- [4] A. Faure et al., *MNRAS* **469**, 612 (2017)
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# Old stars with new matter: Watching the infrared sky at high spectral resolution

**G.W. Fuchs<sup>1</sup>, E. Döring, and T.F. Giesen,  
and  
T.K. Greathouse<sup>2</sup>, R.S. Giles<sup>2</sup>, and J.H. Lacy<sup>3</sup>  
and  
E.J. Montiel<sup>4</sup> and M.J. Richter<sup>5</sup>**

*<sup>1</sup>University of Kassel, Institute of  
Physics, Heinrich-Plett-Str. 40, 34132 Kassel, Germany*

*<sup>2</sup>Space Science Department, Southwest Research  
Institute, San Antonio, TX, USA*

*<sup>3</sup>Department of Astronomy, The University of Texas at Austin, Austin, TX, USA*

*<sup>4</sup>USRA, NASA Ames Research Center, Moffett Field, CA, USA*

*<sup>5</sup>Department of Physics, University of California, Davis, Davis,  
USA*

Our universe is full of molecules. Most molecules have been discovered with the help of radio or MM telescopes based on their rotational spectra in the interstellar medium or in circumstellar envelopes around old stars. But molecules can also be detected unambiguously in the infrared (IR) range, and even those that do not have a permanent electric dipole moment. This is an advantage of IR astronomy. Once IR high-resolution laboratory spectra are available, they can be used to identify molecules from astrophysical observational data provided that these are also available at high spectral resolution. The molecular envelopes around aging stars provide an excellent opportunity to study molecular species and also the dynamics of their environment like the expansion of molecular shells or the infall of material into a star. For this purpose, own observations were made at the IRTF telescope on Mauna Kea, Hawaii and with the SOFIA aircraft telescope on selected astronomical objects. Example IR spectra from hypergiant stars such as VY CMa and NML Cyg, as well as observations of variable AGB stars such as Mira (o Cet), Chi Cyg, IK Tau, and R Cas will be presented. With the help of the high-resolution spectra, molecular abundances, ambient temperatures, and dynamical processes can be determined. This will be demonstrated on the molecule silicon monoxide (SiO) and others.

# **MOCCA: a 4-kilo-pixel microcalorimeter detector for CSR**

**L. Gamer<sup>1</sup>, C. Enss<sup>2</sup>, A. Fleischmann<sup>2</sup>, O. Heber<sup>3</sup>, C. A. Jakob<sup>1</sup>,  
D. Kreuzberger<sup>2</sup>, A. Lowack<sup>2</sup>, M. Rappaport<sup>3</sup>, A. Reifenberger<sup>2</sup>,  
D. Schulz<sup>2</sup>, A. Shahi<sup>3</sup>, Y. Toker<sup>4</sup>, A. Wolf<sup>1</sup>, O. Novotný<sup>1</sup>**

*<sup>1</sup>Max-Planck-Institut für Kernphysik, Heidelberg, Germany*

*<sup>2</sup>Kirchhoff-Institut für Physik, Universität Heidelberg, Germany*

*<sup>3</sup>Weizmann Institute of Science, Rehovot, Israel*

*<sup>4</sup>Bar-Ilan University, Ramat Gan, Israel*

At the cryogenic storage ring CSR at the Max-Planck Institute for Nuclear Physics in Heidelberg, various molecular ions can be stored long enough to deexcite to their vibrational and rotational ground states. Thus, reactions of molecular ions, such as dissociative recombination with electrons, can be investigated at conditions similar to those in interstellar molecular clouds. In order to mass-identify the resulting neutral reaction products as well as to determine the kinetic energy released in these reactions, a position and energy resolved detection of the fragments is necessary. For this purpose, the MOCCA detector was developed and fabricated at the Kirchhoff-Institute for Physics in Heidelberg, which encompasses 64 x 64 Metallic Magnetic Calorimeter pixels, adding up to a comparatively large square sensitive area of about 4.5 cm x 4.5 cm.

The detector will be first implemented in a CSR-independent standalone setup. There the unique cryogenic scheme and the novel detection principle will be tested at realistic conditions, collecting heavy molecular fragments from collision- or photon-induced fragmentation processes. Then the detector and the surrounding setup can be implemented in the CSR downstream of the electron cooler. In the presentation the status of the project will be reviewed.

# Studying ion–neutral reaction dynamics at low temperatures

J. A. Diprose<sup>1</sup>, R. Pandey, P. Regan<sup>1</sup>, V. Richardson<sup>1</sup>, M. Roman<sup>1</sup>, L. Y. Wu<sup>1,2</sup> and B. R. Heazlewood<sup>1</sup>

<sup>1</sup>*Department of Physics, University of Liverpool, UK*

<sup>2</sup>*Department of Chemistry, University of Oxford, UK*

In spite of their real-world importance, it is difficult to study gas-phase reactions between ions and radicals at low temperatures. Here, I will present a new method for generating beams of velocity- and state-selected radicals with tuneable properties [1-2]. We are in the process of combining our radical beam source with a cryogenic ion trap, for the study of ion–radical reactions under cold and controlled conditions (see fig. 1). Reactions will take place within Coulomb crystals, enabling us to monitor processes with exceptional sensitivity (down to the single-ion level). Recent ion–neutral reaction studies performed using this approach will be discussed [3], revealing the advantages of studying reactions within a Coulomb crystal environment.

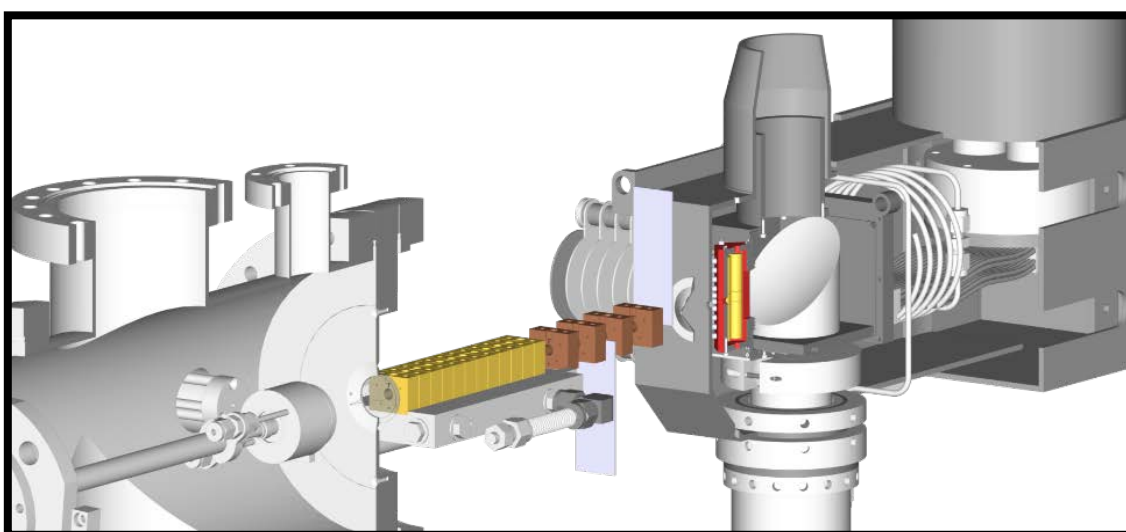


Fig. 1. Schematic illustration of the combined radical beam and cryogenic ion trap apparatus.

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Thomas Henning

Max Planck Institute for Astronomy, Heidelberg

**JWST Observations of Star and Planet Formation**

The James Webb Space Telescope (JWST) is the most powerful space-based infrared observatory ever built. The first part of the talk will discuss the main structures of the telescope and its assembly after launch. The talk will then highlight the first extremely exciting science results, ranging from the high-redshift universe to the spectra of exoplanets and planet-forming disks. A special emphasis will be placed on the star and planet formation process and what we can learn from infrared spectroscopy regarding the inventory of material in the terrestrial planet-forming zone.

# Reactions of $\text{CN}^+$ , $\text{HCN}^+$ and $\text{HNC}^+$ with $\text{H}_2$ studied in a low-temperature ion trap

**M. Jiménez-Redondo<sup>1</sup>, P. Dohnal<sup>2</sup>, P. Jusko<sup>1</sup> and P. Caselli<sup>1</sup>**

<sup>1</sup>Max Planck Institute for Extraterrestrial Physics, Gießenbachstraße 1, 85748 Garching, Germany

<sup>2</sup>Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, Prague 18000, Czech Republic

$\text{HCN}$  and its higher energy isomer  $\text{HNC}$  are presumably the two simplest isomers in chemistry. Both have been detected in a variety of interstellar environments with comparable abundances. Some of the main production channels for these molecules include ionic chemistry, with mechanisms involving  $\text{HNC}^+$  and its higher energy isomer  $\text{HCN}^+$ . The lack of experimental studies for many of these processes hinders current astrochemical models involving  $\text{HCN}/\text{HNC}$  [1].

In this work, we used a 22-pole trap to determine the reaction rate coefficients for production and destruction of  $\text{HCN}^+$  and  $\text{HNC}^+$  in collisions with  $\text{H}_2$  in the range of 17 – 250 K, using chemical probing to differentiate the two ionic isomers [2]. The rate coefficients for  $\text{CN}^+$  and  $\text{HCN}^+$  reactions with  $\text{H}_2$  are stable with temperature and close to the Langevin value, while the one for  $\text{HNC}^+ + \text{H}_2$  presents a noticeable increase at lower temperatures. The product branching ratios for the  $\text{CN}^+ + \text{H}_2$  reaction also show a marked temperature dependence, favoring the production of  $\text{HNC}^+$ , the lower energy isomer, at lower temperatures.

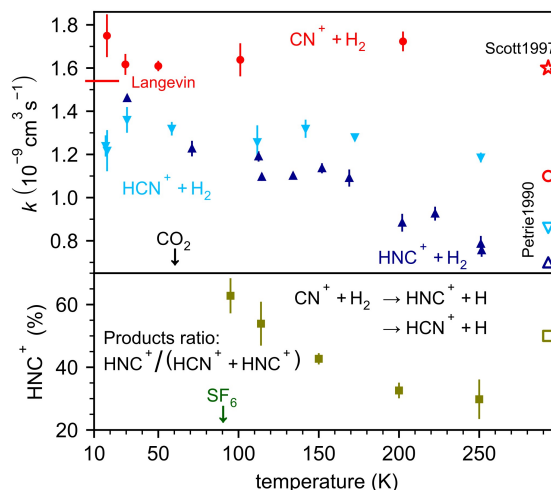


Fig. 1. Upper panel: Rate coefficients for the different reactions studied as a function of temperature. Lower panel: branching ratio for the reaction of  $\text{CN}^+$  with  $\text{H}_2$ .

## References

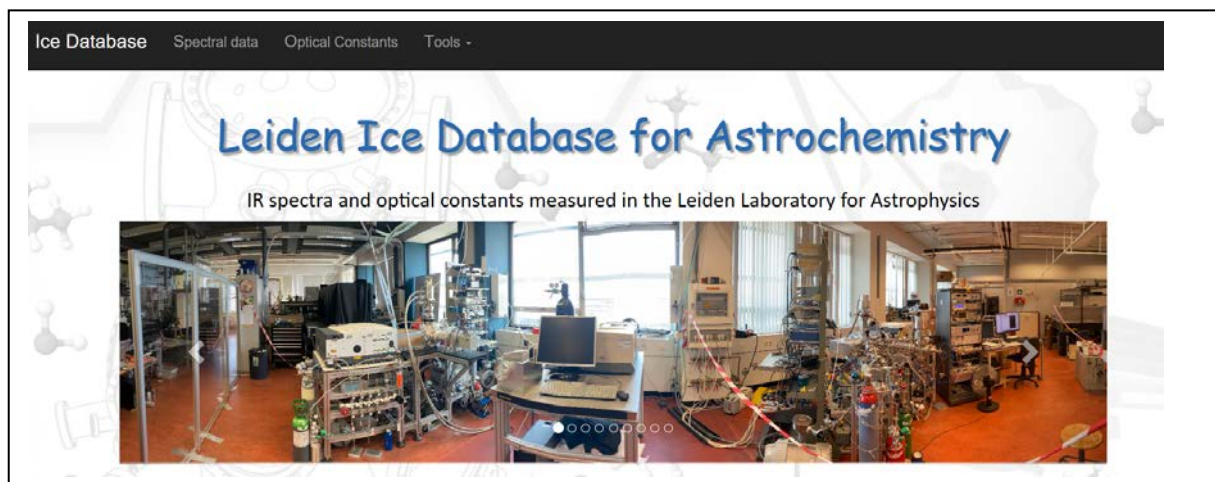
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# Inter & circumstellar ice research in the era of JWST - the laboratory perspective -

**Harold Linnartz**

*Laboratory for Astrophysics, Leiden Observatory, Leiden University  
PO Box 9513, NL2300 RA Leiden, the Netherlands*

With the launch of JWST inter & circumstellar ice research has entered a new era. In this talk the first results are presented obtained within the framework of ICE AGE [1], a JWST ERS program. It is shown how laboratory data add in assigning and interpreting the physical and chemical properties of icy grains in space, with a focus on frozen COMs (complex organic molecules). The laboratory data – spectra and optical parameters are largely online available from LIDA, the Leiden Ice Database for Astrochemistry [2, <https://icedb.strw.leidenuniv.nl/>] that is shortly introduced. This also comprises a recently introduced technique to effectively record wavelength dependent optical constants of ices [3]. In order to link the solid state with the gas phase, the results of two recent studies are presented. First an IR photodesorption study of CO and CH<sub>3</sub>OH ices using FELIX, the free electron facility in Nijmegen [4] and second an extended study of reactive desorption in Sulphur containing ices [5].



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# A multispectroscopic approach to underline the role of polycyclic aromatic hydrocarbons in the interstellar medium

**D. Loru<sup>1</sup>, A. L. Steber<sup>2</sup>, M. Schnell<sup>1</sup>**

<sup>1</sup> *Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany.*

<sup>2</sup> *Universidad de Valladolid, Valladolid, Spain.*

Polycyclic aromatic hydrocarbons are a class of molecules whose presence in the interstellar medium had been established via mid-IR emission detected through several interstellar objects and recently confirmed by the astronomical detection of the PAHs indene [1,2], cyanoindene [3], and the two isomers of cyanonaphthalene [4]. The ubiquitous nature of PAHs suggests that these molecules can be major players in interstellar chemistry. Their roles are thought to be quite diverse, from bridging the gap between gas and solid-state phases of interstellar molecular matter to forming the connection between small hydrocarbons and large fullerenes and contributing to the formation of complex organic molecules, such as nitrogen containing molecules.

Because of the impact that these roles would have in the interstellar medium, we are using cutting-edge spectroscopic techniques, such as chirped-pulse Fourier transform microwave spectroscopy [5-7] and IR-UV ion dip spectroscopy, to study the first interactions between PAHs and astrochemical relevant molecules, such as water. Furthermore, we are investigating the formation/ destruction mechanisms of PAHs and their reactivity with other astrochemical constituents under the energetic conditions generated by an electrical discharge source.

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# Ion molecule reactive scattering for astrophysics?

**J. Meyer<sup>1</sup>**

<sup>1</sup>*Fachbereich Chemie und Landesforschungszentrum OPTIMAS,  
RPTU Kaiserslautern-Landau, Kaiserslautern, Germany*

Reaction dynamics open a window into the fundamental process of elementary reactions, that is reactive collisions. Understanding chemistry at this level will help us to derive detailed structure reactivity relations with the final aim at controlling chemical reactivity using a bottom up approach. We use gas phase methods to study the intrinsic atomistic dynamics of chemical reactions, that is how atoms rearrange during the chemical reaction. Our experimental approach uses a combination of crossed beams with 3D velocity map imaging to record energy and angle differential cross sections of ion molecule reactions [1].

Here, I will present the capabilities of crossed beam imaging to look into dynamics of astrochemically relevant ion molecule reactions, involving cations as well as anions.  $C_{2n}^-$  ( $n > 1$ ) anions are among the few anions found in space. I will present a crossed beam imaging study investigating a possible formation pathway via a chain elongation mechanism in reaction with  $C_2H_2$  [2]. The second example features the isomeric ratio of  $HCO^+/HOC^+$ . Three different reaction pathways have been investigated via crossed-beam imaging showing the capabilities of the technique [3-5]. I will finish, with a short glimpse into transition ion molecule reactive scattering by showing the first results from our new crossed beam set-up in Kaiserslautern investigating the oxygen atom transfer reaction between the tantalum cation and  $CO_2$ [6].

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# Molecules in Exoplanet Atmospheres

**P. Mollière**<sup>1</sup>

*<sup>1</sup>Max-Planck-Institut für Astronomie, Heidelberg, Germany*

With the successful launch of JWST a new era in the characterization of exoplanet atmospheres has begun. The infrared wavelengths probed by JWST are sensitive to the transitions of many molecular absorbers. Consequently, JWST has started to reveal the presence of species such as H<sub>2</sub>O, CO, CO<sub>2</sub>, SO<sub>2</sub>, CH<sub>4</sub>, and NH<sub>3</sub>. The atmospheric composition determined from such detections is key towards understanding planet formation, which may leave discrete compositional imprints. However, atmospheric abundances can be affected by disequilibrium processes such as transport by winds, photo-dissociation, or condensate rainout. In my presentation I will give an overview of the compositional diversity of exoplanets that can be probed with JWST, and how the above-mentioned disequilibrium processes require careful modeling. I will also give a small sneak preview of new atmospheric isotopologue detections, which represent a new formation tracer for exoplanets, similar to the use of isotope ratios in the solar system.

# Recombination of molecular ions at the Cryogenic Storage Ring

**O. Novotný<sup>1</sup> for the CSR team**

<sup>1</sup>*Max Planck Institute for Nuclear Physics, Heidelberg, Germany*

Dissociative recombination (DR) of molecular ions plays a key role in controlling the charge density and composition of cold plasmas, such as the cold interstellar medium (ISM). Experimental data on DR rate coefficients are required in order to understand the abundance of molecules in such astrophysical media. Experimentally, the main challenge is to acquire DR data at conditions relevant for the cold ISM, i.e., at collision temperatures of 10-100 K and at correspondingly low internal excitation. While past storage ring studies did reach collisional temperatures in the desired range, they did not have well-controlled access to internal excitation temperatures of the molecules below 300 K. This limitation was removed with the advent of electrostatic cryogenic storage rings.

The Cryogenic Storage Ring (CSR) [1] at the Max Planck Institute for Nuclear Physics, Heidelberg, is a multi-purpose electrostatic facility for studies with stored atomic, molecular and cluster ion beams. The cryogenic chamber temperatures of <6 K, and the corresponding low residual gas densities, provide for beam lifetimes of hundreds to thousands of seconds. For many molecular ions this time is sufficient to relax down to their lowest ro-vibrational states by spontaneous photon emission [2,3]. Various experimental setups providing laser-, electron-, or even neutral atomic beams can be used for collision studies or as diagnostics for internal state populations. Furthermore, techniques for ion beam phase space cooling and isobaric purification [4] are available.

The cryogenic environment and the excellent vacuum mimic the conditions in the cold ISM, making CSR an outstanding experimental setup for laboratory astrochemistry and for quantum dynamics studies with individual molecular state definition. In the talk, recent CSR measurements on DR of molecular ions in their lowest rotational states will be discussed, including  $\text{TiO}^+$  [5],  $\text{OH}^+$ ,  $\text{H}_2\text{D}^+$ ,  $\text{D}_2\text{H}^+$ , and  $\text{ArH}^+$ .

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# Zooming in on photo-processing of PAHs

S.D. Wiersma<sup>1,2,3</sup>, J.M. Bakker<sup>2</sup>, G. Berden<sup>2</sup>, W.J. Buma<sup>1</sup>, A. Candian<sup>1</sup>,  
J.R. Eyler<sup>4</sup>, J. Martens<sup>2</sup>, J. Oomens<sup>2</sup>, M. Rapacioli<sup>3</sup>, A.G.G.M.  
Tielens<sup>5</sup> and A. Petrignani<sup>1</sup>

<sup>1</sup>University of Amsterdam, PO Box 94157, 1090 GD, Amsterdam, The Netherlands

<sup>2</sup>FELIX Laboratory, Radboud University, Nijmegen, The Netherlands

<sup>3</sup>Institut de Recherche en Astrophysique et Planétologie (IRAP), CNRS, Université de  
Toulouse, Toulouse, France

<sup>4</sup>Department of Chemistry, University of Florida, Gainesville, FL 32611-7200, USA

<sup>5</sup>Leiden Observatory, Leiden University, Leiden, The Netherlands

Polycyclic Aromatic Hydrocarbons (PAHs) are a key component of interstellar chemistry, representing not only a major sink and processor of cosmic carbon, but possibly also of cosmic deuterium. We present UV photodissociation and IR multiple photodissociation (IRMPD) studies of ionic PAHs revealing their photochemical behavior. The irregularly shaped dibenzo[a,l]pyrene cation loses hydrogen alone upon irradiation, despite its ‘exposed’ pendant rings [1]. Its armchair edges may be facilitating hydrogen loss while resisting hydrocarbon loss. This contrasts with phenyl, where isomerization of the carbon skeleton, i.e., facile ring opening, prevents direct H loss, leading, instead, to loss of small hydrocarbon fragments [2]. For deuterated PAHs, fragmentation is preceded by isotopomerization, causing deuterium enrichment [3]. Upon excitation, the H and D atoms scramble across the PAH perimeter with H atoms more mobile and more prone to fragmentation, shielding its isotope. Furthermore, spectral studies show several PAHs to possess some surprisingly strong and narrow bands with little to no spectral congestion in the FIR [4], providing possible fingerprints and benchmarking. The above studies shed light on crucial behavior relevant for the interpretation of JWST observations, where the capacity to characterize spatial progressions in nebula allows unravelling interstellar chemistry like never before.

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# Trapped water on silicates in the laboratory and in astrophysical environments

**A. Potapov**

*Laboratory Astrophysics Group of the Max Planck Institute for Astronomy at the  
Friedrich Schiller University Jena, Jena, Germany*

Existence of strongly bound water molecules on silicate surfaces, above the desorption temperature of water ice, has been first predicted by ab initio calculations and recently demonstrated by laboratory experiments (see [1] and references therein). Such trapped water may be present in various astrophysical environments and there is now evidence for its presence in the diffuse interstellar medium and in extraterrestrial particles [1, 2]. I present new results of a laboratory study of the phenomenon of trapping (strong bonding) of water molecules by silicates. The results show that the efficiency of trapping is strongly dependent on the properties and composition of the surface. The results point out that the presence of trapped water should be due to the hydrophilic properties of the silicate surface and that the nature of trapping is physical (physisorption rather than chemisorption). It's demonstrated that water can be trapped on silicates up to the temperatures of about 470 K, which speaks for the presence of wet silicate grains in the terrestrial planet formation zone in planet-forming disks. Studying the thermal and UV stability of trapped water, it's concluded that the detection of trapped water in the diffuse ISM speaks for its efficient continuous formation. I discuss the results as relevant to fundamental scientific questions, such as the oxygen depletion problem, the origin of water on Earth, and the formation of rocky planets.

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# Physics and chemistry of photon-dominated regions: current challenges

E. Roueff

*Observatoire de Paris, LERMA,  
5 place Janssen, 92190 Meudon, France*

The atomic to molecular transition driven by the attenuation of the vacuum ultra violet (VUV) InterStellar Radiation Field (ISRF) delineates the interface between molecular gas, where stars form and the surrounding galactic environment. The considerable overabundance of Hydrogen in the Universe compared to the other elements is decisive: molecular hydrogen ( $H_2$ ) provides the mass reservoir of interstellar clouds and is the main collisional excitation partner of the different available atoms, ions and molecules.

The answer of  $H_2$  to interstellar vacuum ultra-violet photons ( $h\nu < 13.6\text{eV}$ ) is also very specific and entails a two-photon mechanism involving VUV discrete line absorption followed by occasional continuum emission leading to dissociation, which produces a very efficient self-shielding of the UV radiation. Formation takes place essentially on grain surfaces involving adsorbed H atoms, as no efficient gas phase mechanism is available in the low density conditions of interstellar environments. These opposite mechanisms counterbalance themselves in the so-called translucent clouds and Photon-Dominated Regions (PDRs) [1].

After recalling the basic physico-chemical features of interstellar  $H_2$  under PDR conditions, I will focus on current challenges raised by recent observational infra-red capabilities such as IGRINS (Immersion Grating Infrared Spectrograph) on ground observatories, NIRSpc (Near Infrared Spectrograph) and MIRI (Mid-InfraRed Instrument) on board JWST (James Webb Space Telescope) coupled to high spatially resolved ALMA submillimeter observations.

- ◇  $H_2$  heating at the edge of dense PDRs probed by high-J CO transitions [2]
- ◇ Chemical impact of UV pumped vibrationally excited  $H_2$  on the formation of hydrides [3] and the recent detection of  $CH_3^+$  by JWST [4]
- ◇ Temperature diagnostics from ortho/para ratios [5]

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# Misslons: Missing Ions in Laboratory and Space

O. Asvany, T. Salomon, P.C. Schmid, S. Thorwirth, W.G.D.P. Silva,  
M. Fatima, D. Gupta, and S. Schlemmer

*I. Physikalisches Institut, Universität zu Köln, Zùlpicher Straße 77, 50937 Köln,  
Germany*

Ions play a key role in the chemical evolution of our universe. The process of star and planet formation is tightly connected to the presence and abundance of these species. Their spectra are diagnostic tools for various astrophysical environments and their temporal evolution. However, laboratory spectra of most ions relevant to astrophysics are not available. Moreover, predicted spectra from ab-initio theory are not accurate enough to guide astrophysical searches. Therefore, laboratory spectra of molecular ions are needed. I will report on progress towards recording high-resolution spectra from the microwave to visible range using our unique and innovative methods in ion traps [1]. These methods are molecule specific through mass selection, many orders of magnitude more sensitive and less complex due to buffer gas cooling as compared to conventional spectroscopy methods.

Recent examples concern the first molecule observed in space, CH<sup>+</sup> [2] but also ions which can play an important role in the chemical development producing more complex species, e.g., C<sub>3</sub>H<sup>+</sup> [3], C<sub>3</sub>H<sub>2</sub><sup>+</sup> [4] as well as other small hydrocarbon ions [5-7]. For many reasons H<sub>3</sub><sup>+</sup>, including its deuterated siblings, is a corner stone in ion chemistry. It gives away its proton to most other species. As a result, protonation of more complex species, like methanol, could be another key towards the formation of complex organic species, molecules which are observed with today's telescopes but how they come into existence is under debate. I will discuss the newest tools to record the spectra [8] and to understand the relevant reactions in the laboratory.

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# Laboratory spectroscopy - From clouds to planets

## Silvia Spezzano<sup>1</sup>

<sup>1</sup>*Max Planck Institute for Extraterrestrial Physics, Garching bei Muenchen, Germany*

Laboratory spectroscopy is one of the pillars of Astrochemistry because it provides the necessary data to interpret astronomical observations of star and planet forming regions. By studying the abundance, distribution, and fractionation of molecules in star-forming regions we can in fact derive information on their chemistry, physics, dynamics, and evolution<sup>1</sup>.

Moreover, new and upcoming facilities like the JWST<sup>2</sup>, ELT<sup>3</sup> and ARIEL<sup>4</sup> will allow us to draw the chemical link from star-forming regions to a large sample of exoplanets by providing an unprecedented sample of spectra of exoplanetary atmospheres. The interpretation of these spectra is heavily reliant on laboratory data.

In my talk I will present some of the latest results from the CAS (Center for Astrochemical Studies) laboratories at MPE (Max Planck Institute for Extraterrestrial Physics). I will talk about our work on the rotational spectroscopy of astrophysical relevant molecules in the cm, mm and submm-wave range. I will highlight the importance of complex organic molecules in star and planet forming regions, and discuss challenges posed by their spectral analysis.

I will also discuss the impact of dominant gases on trace species in exoplanetary atmospheres and present our work on high resolution laboratory infrared spectroscopy to determine pressure broadening effects.

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# **Computational exploration of the oxygen(<sup>1</sup>D) reactivity with C<sub>2</sub>H<sub>x</sub> hydrocarbons: astrochemical reaction pathways**

T. Stein

Fritz Haber Research Center for Molecular Dynamics, The Hebrew University of  
Jerusalem, Jerusalem, Israel, 9190401

Understanding how complex organic molecules are formed in the harsh environment of the interstellar medium has long presented a significant puzzle to scientists. In molecular clouds, irradiation of ice plays a crucial role in producing complex organic molecules. In this work, we present ab-initio molecular dynamics (AIMD) simulations to model reaction taking place on ice with astronomical compositions. Specifically, we model the reactions between oxygen(<sup>1</sup>D) and C<sub>Y</sub>H<sub>X</sub> on the ground and excited electronic states. We observe which organic molecules are formed and find several possible pathways along the potential energy surface for their formation. To predict relevant photochemical reaction pathways, we perform non-adiabatic ab-initio molecular dynamics and demonstrate the important role of the dynamics on the excited states by identifying secondary products that form on those surfaces. Additionally, we model the effect of the ice environment on the resulting products.

# Cosmic dust in the solar system

**V.J. Sterken**<sup>1</sup>

<sup>1</sup>*ETH Zürich, DPHYS, Wolfgang-Paulistrasse 27, CH-8093 Zürich, Switzerland*

In situ measurements of cosmic dust in the solar system were initially performed in the context of the onset of space exploration, but quickly became a research method to seek “ground truth information” on the cosmic dust particles that otherwise were investigated by remote astronomical methods. Many different types of dust in the solar system have been investigated, from nanodust coming from the interiors of active moons, to impact ejecta from planetary surfaces, cometary dust, dusty rings and interstellar dust passing through the solar system. For enabling this, also laboratory calibrations are necessary, usually with a dust accelerator or a light gas gun, and hence, cosmic dust analogs have to be fabricated and characterized in the lab.

This talk reviews the different types of dust investigated in situ in the solar system, their characteristics, interaction with the space environment, and the methods best suited for measuring them. We discuss the state-of-the-art in situ instrumentation, science questions that can be addressed, and current challenges and limitations. We particularly focus on the largest particles (micrometer size) and smallest ones (nanodust) measured so far, and on calibration efforts in the laboratory. Finally, we give a preview on near-future space missions and mission concepts with new dust instrumentation, like *Destiny+*, *Europa Clipper*, the *Interstellar Probe* concept, and opportunities for (interstellar) dust research from the Lunar Gateway.

# Formation of new bonds in ionization of isolated molecules

**D. Strasser**<sup>2</sup>

<sup>1</sup>*Institute of chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel*

Ionization is a powerful trigger for structural rearrangement and formation of new chemical bonds. It is particularly important for the chemical evolution of isolated low temperature molecules. Recently, we explored dynamics initiated by double ionization of several organic species.[1-4] In a combined experimental and theoretical study, we reveal a rich variety of competing proton and electron transfer mechanisms leading to different Coulomb explosion product channels.

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# Small Silicon Oxide Cations as Precursors for Interstellar Dust: Optical Absorption and Photodissociation Properties

**T. Studemund<sup>1</sup>, K. Pollow<sup>1</sup>, M. Förstel<sup>1</sup> and O. Dopfer<sup>1</sup>**

<sup>1</sup>*Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany*

Interstellar dust is a crucial ingredient in astrophysical investigations of the still poorly understood mechanism of star and planet formation which is also of great interest to answer open questions related to processes in space. The origin as well as the evolutionary formation mechanism of those dust grains, which contain a large amount of  $\mu\text{m}$ -sized silicon-containing particles are still barely known. A possible starting point to form those silicate dust grains are silicon and oxygen containing molecules which are not well investigated so far. Just silicon monoxide ( $\text{SiO}$ ) is identified in the interstellar medium (ISM) and closer examined in further laboratory studies. However, no information about larger silicon-containing molecules or ions is available. [1]

The photodissociation and optical absorption properties, molecular structures, and energies of possible  $\text{Si}_n\text{O}_m^+$  ions that are suitable candidates as precursors for dust grains are obtained by experimental data and quantum chemical calculations. Our experimental setup relies on action spectroscopy via mass spectrometry and resonant laser photodissociation of size-selected  $\text{Si}_n\text{O}_m^+$  clusters. These are generated by laser vaporization in a molecular beam expansion coupled to a quadrupole/time-of-flight tandem mass spectrometer and a broadly tunable UV/VIS-OPO laser. [2]

Initial results demonstrate rival fragmentation channels, their appearance energies and branching ratios, and the abundance and stability of neutral fragments. In particular, we emphasize the  $\text{Si}_3\text{O}_2^+$  molecule and discuss the first optical spectrum of a silicon oxide molecule (neutral and ion) larger than  $\text{SiO}$ . [3]

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# Experimental verification for effect of dust agglomeration on MIR spectra: What do individual dust agglomerates tell us about observed spectra?

**A. Tamanai<sup>1</sup>, R. Tazaki<sup>2</sup>, H. Mutschke<sup>3</sup>, W. Klauser<sup>4</sup>, S. Zimmerman<sup>4</sup>,  
N. M. Murillo<sup>1</sup>, S. Ohashi<sup>5,1</sup>, T. Oyama<sup>1</sup>, Z. Zhang<sup>1</sup>, S. Zeng<sup>1</sup>,  
Y. Watanabe<sup>6</sup>, N. Sakai<sup>1</sup>**

<sup>1</sup> *RIKEN Cluster for Pioneering Research, Wako-shi, Saitama, Japan*

<sup>2</sup> *Institut de Planétologie et d'Astrophysique de Grenoble, Grenoble, France*

<sup>3</sup> *AIU Jena, Friedrich-Schiller-Universität Jena, Jena, Germany*

<sup>4</sup> *Mikrorobotik und Regelungstechnik, Universität Oldenburg, Oldenburg, Germany*

<sup>5</sup> *National Astronomical Observatory of Japan, Mitaka, Tokyo, Japan*

<sup>6</sup> *Materials Science and Engineering, Shibaura Institute of Technology, Tokyo, Japan*

Interpretation of the observed mid-infrared (MIR) spectra of dust grains is not straightforward since these spectra are strongly influenced by not only chemical/mineralogical properties, but also physical ones. Specifically, the morphology of dust grains (e.g., individual particle size, shape, agglomeration state) has a great effect on optical properties<sup>1</sup>. In order to interpret the observed spectra in detail, it is crucial to have a well-defined experimental data and theoretical models. Still, it is not easy to incorporate all physical conditions (e.g., individual grain shapes, size heterogeneity, complex agglomerate structures) into theoretical models such as light scattering simulations. Using experimental approaches, we have performed MIR spectroscopic extinction measurements for systematically arranged individual agglomerates consisting of micron-sized particles<sup>2</sup>. This time, we used an IR microscope with synchrotron radiation at the Super Photon ring-8 GeV (SPring-8), the Japanese synchrotron facility located in Hyogo. This allowed us to obtain experimentally the details of the changes in the MIR band profiles caused by the morphological effect. Our target samples are astronomically relevant silicate materials such as amorphous SiO<sub>2</sub>, crystalline forsterite (Mg<sub>2</sub>SiO<sub>4</sub>) and enstatite (MgSiO<sub>3</sub>). We focused on the wavelengths between 8 and 12 μm where the strongest stretching vibration bands take place. Here, we demonstrate (1) to what extent the agglomeration and the particle orientation affect the stretching vibration band profile; (2) the deviation between the experimental spectra and theoretical simulations, applying Mie theory, the discrete dipole approximation (DDA), and the transition matrix approach (T-matrix). By comparing the results with spectra obtained from observation, we aim to improve our understanding of the physical properties of dust grains and contribute to the clarification of the initial stage of the dust growth process.

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# Probing charge-transfer neutralization reactions in cool plasmas using the ion storage facility DESIREE

M. Poline<sup>1</sup>, A. Dochain<sup>2</sup>, J. Grumer<sup>3</sup>, S. Rosén<sup>1</sup>, MC Ji<sup>1</sup>, G. Eklund<sup>1</sup>, A. Simonsson<sup>1</sup>, P. Reinhed<sup>1</sup>, M. Blom<sup>1</sup>, N. S. Shuman<sup>4</sup>, S. G. Ard<sup>4</sup>, A. A. Viggiano<sup>4</sup>, M. Larsson<sup>1</sup>, H. Cederquist<sup>1</sup>, H. T. Schmidt<sup>1</sup>, H. Zettergren<sup>1</sup>, X. Urbain<sup>2</sup>, P. S. Barklem<sup>1</sup>, and R. D. Thomas<sup>1</sup>

*1 Department of Physics, Stockholm University, SE-114 21 Stockholm, Sweden.*

*2 Institute of condensed Matter and Nanosciences, Université catholique de Louvain, Louvain-la-Neuve, Belgium*

*3 Theoretical Astrophysics, Department of Physics and Astronomy, Uppsala University, SE-751 20, Uppsala, Sweden*

*4 Air Force Research Laboratory, 1451 Fourth Street, Albuquerque, New Mexico, 87116, United States*

*Email: rdt@fysik.su.se*

The Double ElectroStatic Ion Ring ExpEriment (DESIREE) facility located at Stockholm University, Sweden, uniquely allows for studies of interactions between cations and anions at low and well-defined internal temperatures and centre-of-mass collision energies down to about 20 K and ~50 meV, respectively [1-5].

Using this facility, we aim for a better understanding of how small and large molecules are formed and processed in astrophysical, atmospheric, and combustion plasmas, where we combine several novel experimental methods to build a fundamental understanding of the transfer of charge-, energy- and mass in collisional reactions. Control over the reaction environment means that desired information, e.g., reaction products, can be obtained over many of the conditions needed to accurately model plasmas where these processes are important.

This talk highlights how this facility, which is the only one of its kind currently in the world, can play a crucial role in studying in mutual neutralisation reactions relevant to cool plasmas.

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# Merged beams experiments with neutral atoms and stored molecular ions at the Cryogenic Storage Ring

X. Urbain<sup>1</sup>, F. Grussie<sup>2</sup>, L. Berger<sup>2</sup>, M. Grieser<sup>2</sup>,  
D. Müll<sup>2</sup>, A. Znotins<sup>2</sup>, F. Dayou<sup>3</sup>, and H. Kreckel<sup>2</sup>

<sup>1</sup>*Institute of Condensed Matter and Nanosciences,  
Université Catholique de Louvain, Louvain-la-Neuve B-1348, Belgium*

<sup>2</sup>*Max Planck Institute for Nuclear Physics,  
Saupfercheckweg 1, D-69117 Heidelberg, Germany*

<sup>3</sup>*Sorbonne Université, Observatoire de Paris, PSL University, CNRS, LERMA,  
F-92195 Meudon, France*

Reactions between neutral atoms and molecular ions play an important role for the formation of molecules in interstellar space, where they initiate an active network of ion-neutral chemistry. However, these reactions are particularly difficult to study in the laboratory, as both reactants are highly reactive and have to be prepared in defined quantum states for meaningful experiments.

We have constructed a dedicated ion-neutral collision setup at the Cryogenic Storage Ring (CSR) of the Max Planck Institute for Nuclear Physics in Heidelberg, Germany. This setup allows for energy-resolved studies of collisions between ground term neutral atoms and cold molecular ions. The neutral atoms are produced by photodetachment of a negative ion beam and merged with the stored ions in one of the straight sections of the storage ring.

We will describe the merged beams setup and the challenges of neutral beam experiments at a heavy ion storage ring and its validation with proof-of-principle experiments of collisions between  $D_2^+$  and C, for which single-pass merged beams measurements exist.

Our recent studies of reactions of cold  $HD^+$  ions with C atoms reveal an unexpected kinetic isotope effect for the  $CH^+$  and  $CD^+$  product channels, namely the complete switch-off of  $CD^+$  production at higher collision energies. The reaction dynamics is fully accounted for by quasi-classical trajectory (QCT) calculations performed on newly computed potential energy surfaces of various symmetries. Such kinetic isotope effects have been described in the literature for collisions between HD and various cations, and may be rationalized with the so-called spectator stripping model. Their observation with molecular ions was so far hindered by the rovibrational excitation of the reactants. Preliminary results for  $H_3^+$  will be presented at the conference.

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# Astrophysical studies at the DESIREE facility

H. Zettergren<sup>1</sup>

<sup>1</sup>*Department of Physics, Stockholm University, Sweden*

Cryogenic electrostatic ion beam storage ring devices offer new opportunities to address key open questions related to how isolated molecules may survive and interact in astrophysical environments [1]. Here, I will present results from such studies at the DESIREE (Double ElectroStatic Ion Ring ExpERiment) storage ring facility at Stockholm University. These include studies of radiative cooling processes where we monitor the spontaneous decays of internally hot molecular ions and use laser probing techniques [2] to determine their cooling rates on timescales ranging from milliseconds to seconds and beyond [3,4]. The results highlight the importance of recurrent fluorescence for the survival of internally hot Polycyclic Aromatic Hydrocarbons (PAHs), i.e. inverse internal conversion followed by photon emission from the thermally populated electronically excited state. Small PAHs are therefore much more resilient against fragmentation than previously assumed in astrochemical models [5], which may have important consequences for their abundances in space.

Furthermore, I will present results from DESIREE experiments demonstrating that defect PAHs [6] and fullerenes will survive indefinitely in isolation. These highly reactive species are formed in collisions typical of those in interstellar shocks and can thus act as important intermediates in the formation of larger molecules from smaller ones [6]. Finally, I will highlight studies of neutralization of atomic, PAH, and fullerene cations in sub-eV collisions with atomic and molecular anions. In these studies we take full advantage of the unique DESIREE features [7] to determine the excited states being populated in such reactions as well as the relative reaction rates as a function of center-of-mass collision energy. These results are important to benchmark theory and models for reliable predictions of e.g. the ionization balance in molecular clouds [8].

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# **Abstracts of Posters**

(in alphabetical order)

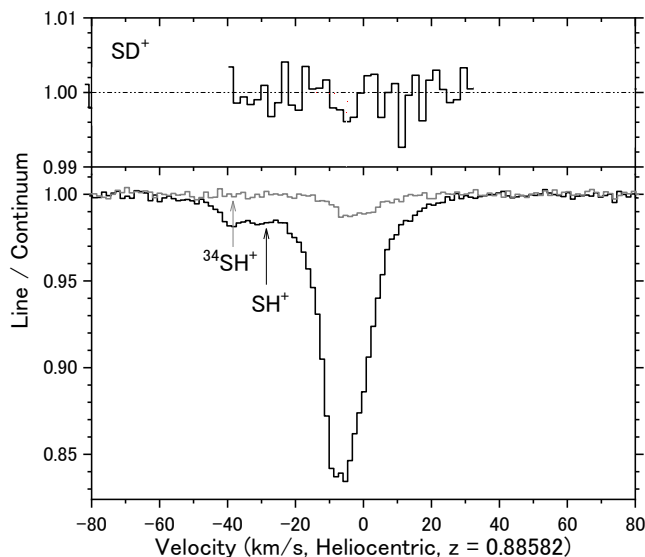
# Millimeter and submillimeter spectroscopy of the deuterated molecular ion $\text{SD}^+$

Mitsunori Araki, Valerio Lattanzi, Christian Endres, and Paola Caselli

*Max-Planck-Institut für extraterrestrische Physik, Garching, Germany*

To detect interstellar molecules in space, the laboratory production of molecules, followed by measurements of precise rest frequencies, is essential. In this work, seven rotational transitions of the deuterated molecular ion  $\text{SD}^+$  have been measured in the 271–863 GHz region in the laboratory. This ion has been produced by DC-glow discharge using a mixture of  $\text{D}_2\text{S}$  and Argon in a free space cell under a temperature range of  $-140$  to  $-160^\circ\text{C}$ . The rotational, centrifugal distortion, spin-spin interaction, spin-rotation, and hyper-fine constants have been determined; the standard deviation of the residuals in the fitting is 68 kHz. The measured frequencies can now be used for astronomical detection.

By using the ALMA archive, we have investigated the line of  $\text{SD}^+$  toward the quasar PKS 1830-211. The  $z = 0.89$  molecular absorber exits in front of this quasar.  $\text{SH}^+$  has been detected in the molecular absorber [1,2]. There is a data set covering the 297 GHz region [3], which includes the  $N, J = 2, 3-1, 2$  transition of  $\text{SD}^+$  at 561 GHz under redshift. A weak feature having an S/N of 2 is located at the same velocity with the peaks of  $\text{SH}^+$  and  $^{34}\text{SH}^+$  as shown in the following figure. The feature shows the column density of  $3 \times 10^{12} \text{ cm}^{-2}$  using a dipole moment of 1.087D [4] and assuming the excitation temperature of 5.14 K [1]. However, the column density provides an abundance ratio  $\text{SD}^+/\text{SH}^+$  of 7%, which is overlarge considering the know deuterated species of ND (0.07-0.7%) and HDO (0.1%) [5]. Therefore, the present column density should be regarded as an upper limit of  $\text{SD}^+$ . To detect this deuterated ion, the transitions that come from the lowest rotational level  $N, J = 0, 1$  are awaited to be investigated because of the low excitation temperature of this absorber.



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# Experimental diffusion of water through porous amorphous carbon dust analogues

**R. Basalgète, G. Rouillé, C. Jäger**

*Laboratory Astrophysics Group of the Max Planck Institute for Astronomy at the Friedrich Schiller University Jena, Institute of Solid State Physics, Jena, Germany*

Interstellar dust plays a crucial role in the chemistry of the interstellar medium by providing catalytic surfaces for the formation of molecules. The surface reactions involved are of primary importance since they have explained a variety of gas phase abundances in the interstellar medium. These reactions depend primarily on how the atoms and molecules diffuse on the surface and/or through the dust grains. To date, laboratory experiments have focused on the diffusion of volatiles (CO, NH<sub>3</sub>, CO<sub>2</sub>, ...) in water ice (e.g. [1]) and very little is known on the influence of the dust grains on such processes. Gas transport through porous media analogous to interstellar dust is also an important topic in cometary science [2].

Interstellar dust analogues synthesized in the laboratory [3] offer a unique opportunity to better understand the diffusion processes in dust grains. Here we propose to study such processes for water, which is a major component of interstellar and cometary ices. Thin layers of water ice were deposited on a cold substrate and covered by carbon or silicate dust grains produced by pulsed laser ablation of a solid target in a quenching gas atmosphere. The diffusion of water through the dust layers was activated by heating up the substrate. Isothermal modifications of the infrared bands of the water over time enabled us to quantify the diffusion process and to measure physical parameters of primary importance for astrochemical models, such as the diffusivity. In this context, I will present the main findings of the studies and I will discuss their astrophysical implications.

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# Characterization of a simple supersonic expansion source for small molecular ions

L. Berger<sup>1</sup>, A. Znotins<sup>1</sup>, F. Grussie<sup>1</sup>, D. Müll<sup>1</sup>, A. Dochain<sup>2</sup>,  
J. Fréreau<sup>2</sup>, X. Urbain<sup>2</sup> and H. Kreckel<sup>1</sup>

<sup>1</sup>Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg

<sup>2</sup>Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain,  
Louvain-la-Neuve, B-1348 Belgium

The Cryogenic Storage Ring (CSR) [1] at the Max-Planck-Institute for Nuclear Physics allows for the storage of molecular ions of almost arbitrary mass at extreme vacuum (residual gas densities on the order of  $1000 \text{ cm}^{-3}$ ) and at low temperature ( $T < 5\text{K}$ ). In this environment, small infrared-active molecular ions will cool to their lowest rotational states within minutes, and studies of astrophysically relevant reactions can be performed under true interstellar conditions. However, some astrophysically relevant molecular ions lack a permanent dipole moment (e.g.,  $\text{H}_2^+$ ,  $\text{H}_3^+$ ,  $\text{H}_3\text{O}^+$ ) and have to be produced in cold ion sources prior to injection, as they do not cool in experimentally accessible time scales.

Here we present the design of a simple supersonic expansion source based on a commercial pulsed valve and an electric discharge. It allows for the production of intense pulses of small molecular ions. We use high-resolution photodissociation spectroscopy of  $\text{N}_2\text{O}^+$ , employing the STARGATE setup [2] at the Université Catholique de Louvain, to characterize the internal excitation of the molecular ions and extract their rotational temperature.

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## DOUBLE RESONANCE EXCITATION OF OVERTONES AND COMBINATION BANDS IN JET-COOLED N<sub>2</sub>O

**J. BOSMANN, F. PETERS, K. VAVRA, G. W. FUCHS,  
T. F. GIESEN**, *Laborastrophysik, Universität Kassel, Heinrich-Plett-Straße  
40, 34132 Kassel, Germany*

Propylene oxide (PO) is one of the most discussed chiral molecules since its astronomical detection<sup>1</sup>. For future applications such as chiral detection of PO by infrared three-wave mixing (IR-3WM) techniques we would like to acquire its ro-vibrationally resolved spectrum. In our investigations we found the ro-vibrationally resolved spectrum of PO to be quite complex and thus the assignment of ro-vibrational transitions relying solely on an IR cavity ring-down spectrometer is not straight forward. Infrared (IR) and microwave (MW) double resonance excitation, using well known microwave transitions to assign unknown IR-transitions, is a strategy to overcome the problem of spectral complexity.

In a first step we present the proof of principle concept of combining an IR cavity ring-down spectrometer (2.7-4.0  $\mu\text{m}$ ) and a MW chirped-pulse Fourier transform (100-112 GHz) spectrometer to excite double resonance processes in jet-cooled N<sub>2</sub>O. In our setup the three components IR, MW and molecular jet are aligned perpendicular to each other and both excitation sources are linearly polarized with arbitrary orientation. We observed pure rotational transitions in the vibrational ground state (00<sup>0</sup>0), the first overtone of the symmetric stretching mode (20<sup>0</sup>0) around 3.9  $\mu\text{m}$  and the combination band of symmetric and asymmetric stretching mode (10<sup>0</sup>1) at 2.875  $\mu\text{m}$ <sup>2</sup> and their decay into lower states. Next a racemic mixture and pure enantiomers of PO are probed with the same setup. The double resonance procedure allows for precise assignment of the ro-vibrationally resolved spectrum. Results will be compared to theoretical predictions.

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# Ion trap study of nuclear spin state-changing collisions of $\text{H}_3^+$ with $\text{H}_2$ at low temperatures

Š. Roučka, S. Rednyk, O. E. Hernandez Alvarez, L. Uvarova,  
J. Palacký, P. Dohnal, R. Plašil, J. Glosík

*Department of Surface and Plasma Science, Faculty of Mathematics and Physics,  
Charles University, Prague, Czech Republic*

The most abundant molecule in the interstellar medium,  $\text{H}_2$ , exists in ortho and para nuclear spin states. The thermalization of the  $\text{H}_2$  nuclear spin states is so slow, that it can be used as a proxy for measurements of the age of interstellar objects. The major process contributing to the relaxation of  $\text{H}_2$  nuclear spin states are state-changing collisions with  $\text{H}_3^+$  molecules. The  $\text{H}_3^+$  molecule also exists in ortho and para nuclear spin states. However, the state-specific rate coefficients of nuclear spin state changing collisions have not been determined experimentally yet. We present the results of our ongoing effort to measure the rate coefficients of these astrophysically relevant processes using a time-resolved action spectroscopy experiment in a cryogenic 22-pole ion trap. This work is supported by Czech Science Foundation grant 21-28560S and Charles University Grant Agency 376721.

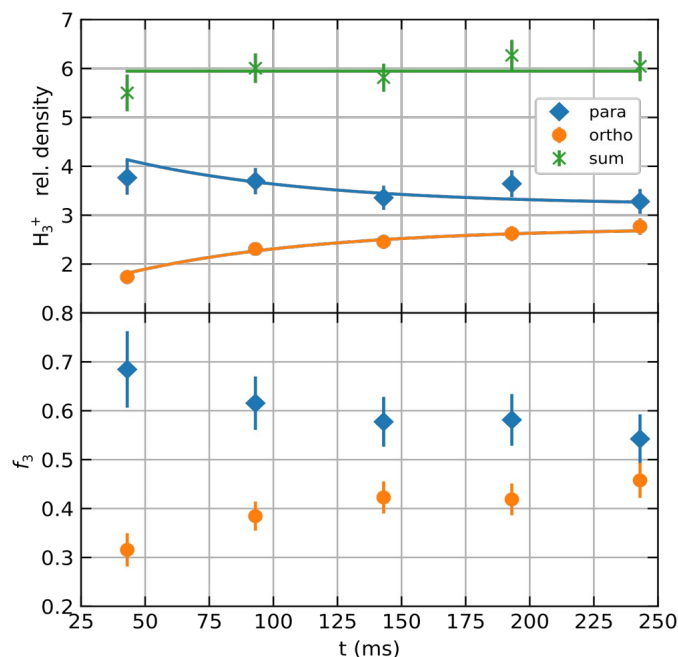


Fig. 1: Time evolution of the relative numbers of trapped  $\text{H}_3^+$  ions in the ortho and para nuclear spin states at 60 K.

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# Modeling detection efficiency for microcalorimetry at CSR

**S. K. Gaisser<sup>1</sup>, K. Blaum<sup>1</sup>, C. Enss<sup>2</sup>, A. Fleischmann<sup>2</sup>, L. Gamer<sup>1</sup>,  
C. A. Jakob<sup>1</sup>, A. Lowack<sup>2</sup>, D. Schulz<sup>2</sup>, A. Wolf<sup>1</sup>, and O. Novotný<sup>1</sup>**

<sup>1</sup> *Max-Planck-Institut for Nuclear Physics, Saupfercheckweg 1,  
69117 Heidelberg, Germany*

<sup>2</sup> *Kirchhoff-Institute for Physics, Im Neuenheimer Feld 227,  
69120 Heidelberg, Germany*

In interstellar clouds, an important chemical reaction is Dissociative Recombination (DR), the products of which lead to the formation of various complex organic molecules [1]. To understand such interstellar processes, a number of key DR reactions need to be studied experimentally under conditions similar to those in the interstellar medium. A facility capable of such measurements is the electrostatic Cryogenic Storage Ring (CSR) [2] at the Max Planck Institute for Nuclear Physics in Heidelberg. With temperatures below 10 K and a particle density of  $\sim 1000$  particles per  $\text{cm}^3$  the setup is close to the conditions given in interstellar clouds. In addition to the ambient conditions, a detector is needed to collect the DR products with high energy, time, and position resolution to obtain an accurate picture. For this purpose, the MOleCule Camera Array (MOCCA) [3], based on Metallic Magnetic Calorimeters (MMCs), was designed at the Kirchhoff Institute for Physics in Heidelberg. With  $64 \times 64$  pixels, the readout is only performed with 32 Superconducting QUantum Interference Devices (SQUIDs). To achieve an efficient and correct allocation of impinged pixel out of a total of 4096 pixels, two different readout schemes for MOCCA have been developed and tested. Due to the high requirements concerning the detection efficiency, it is of utmost importance to thoroughly examine both designs. In addition to laboratory test, the efficiency of both MOCCA versions have been examined by simulating the response of the detector readout scheme to impacts of fragments from a DR reaction. In the presented model, the DR channels studied focused on protonated methanol, which was detected not only in cold interstellar clouds but also in various other interstellar sources [4, 5].

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# **The newly set-up spectroscopic molecular beam apparatus : Conceptual and technical overview**

**V. Grigorian<sup>1</sup>, J. Jakob<sup>1</sup>, S. Schwetje<sup>1</sup>, M. A. Kaufmann<sup>1</sup>,  
A. A. Breier<sup>2</sup>, G. W. Fuchs<sup>1</sup> and T. F. Giesen<sup>1</sup>**

<sup>1</sup> *Laboratory Astrophysics, Kassel, Germany*

<sup>2</sup> *Molecular Spectroscopy/Environmental Physics, Berlin, Germany*

Molecular chirality is an established phenomenon and an extensive field of modern interdisciplinary research. In particular, the usage of light for the identification and control of chirality on a molecular level constitutes fundamental challenges and represent the main research goal of the SFB 1319 ELCH (Extreme light for sensing and driving molecular chirality). Aspects of these challenges are the distinction between enantiomers, enantiomer switching, and enantio-selective state preparation, which demand the development of precision spectroscopic tools and techniques. We aim to employ a combination of microwave and infrared radiation to achieve chirality sensing.

Here, we present our new spectrometer capable of production and cooling of chiral species adiabatically in a molecular beam and subsequent manipulation and detection via resonance-enhanced multi-photon ionization (REMPI). A conceptual and technical overview of the experimental setup and its various components is presented. For the production and cooling of chiral molecules an Even-Lavie valve is utilized. REMPI-schemes are employed with optical radiation for state selective ionization and mass selective detection of the species by ion time-of-flight spectrometry.

Manipulation and state preparation techniques are outlined, and technical specifications as well as performance data of the nozzle (pulse shape, temperature profile) and of the employed optical lasers (spectral line widths) are presented.

# Merged beams experiments between neutral atoms and molecular ions at the Cryogenic Storage Ring

F. Grussie<sup>1</sup>, L. Berger<sup>1</sup>, M. Grieser<sup>1</sup>, D. Müll<sup>1</sup>,  
A. Znotins<sup>1</sup>, X. Urbain<sup>2</sup>, and H. Kreckel<sup>1</sup>

<sup>1</sup>*Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany*

<sup>2</sup>*Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Belgium*

Reactions between neutral atoms and molecular ions play an important role for the formation of molecules in interstellar space, driving an active network of ion-neutral chemistry. However, experimental data are scarce since both reactants need to be prepared in defined quantum states for meaningful measurements. To address this important class of reactions, we have constructed a merged beams experiment [1] to study ion-neutral collisions at the Cryogenic Storage Ring (CSR) [2] of the Max Planck Institute for Nuclear Physics in Heidelberg, Germany. In a dedicated transfer beamline, ground term atomic beams are produced via laser photodetachment [3], merging the stored molecular ions in one of the straight sections of the CSR. Varying the kinetic energy of the neutral atom beam allows for energy-resolved studies of collisions between ground term neutral atoms and ro-vibrationally cold molecular ions. We will present recent studies of reactions between cold HD<sup>+</sup> ions and C atoms, revealing a pronounced intramolecular kinetic isotope effect.

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# The CSR-ReMi – A cryogenic in-ring reaction microscope

**F. Herrmann<sup>1</sup>, D. V. Chicharro<sup>1</sup>, R. von Hahn<sup>1</sup>, M. Grieser<sup>1</sup>, F. Grussie<sup>1</sup>, H. Kreckel<sup>1</sup>, O. Novotný<sup>1</sup>, A. Wolf<sup>1</sup>, K. Blaum<sup>1</sup>, R. Moshhammer<sup>1</sup>, C. D. Schröter<sup>1</sup> and T. Pfeifer<sup>1</sup>**

*<sup>1</sup>Max Planck Institute for Nuclear Physics, Saupfercheckweg 1, 69117 Heidelberg, Germany*

The CSR-ReMi is a dedicated in-ring reaction microscope to perform experiments on slow and cold molecular ions and clusters in the cryogenic storage ring CSR [1]. A reaction microscope [2] is a combined electron and ion spectrometer for energy and angular resolved particle detection created in individual collision processes. It offers multi-hit capability and provides high detection efficiency, acceptance and resolution. With coincident detection of all collision fragments, kinematically complete data sets on the reaction dynamics can be collected. This allows stringent tests of theoretical concepts for the description of molecular fragmentation and relaxation dynamics. The implementation of this first cryogenic reaction microscope worldwide will considerably extend the range of scientific applications at the CSR. In the CSR-ReMi, experiments like electron transfer, photo detachment and molecular break-up reactions are possible.

The implementation of the CSR-ReMi into the CSR started in May 2022 and its integration was recently finished. Sub-sequent final checks before commissioning and first benchmark measurements at room temperature will follow. Thereafter, first fundamental experiments on the collision dynamics of neutral targets with stored cold molecular ions are planned. In addition to the incoupling for the supersonic gas jet, which supplies the neutral target beam, the CSR-ReMi is equipped with a laser incoupling line. This contribution will present the design, main components and working principle of the complete machine.

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# Single-pass merged-beams experiments on molecular ion-neutral reactions for astrochemistry

Pierre-Michel Hillenbrand<sup>1</sup>, Caixia Bu<sup>2</sup>, Leonard W. Isberner<sup>1</sup>,  
Dmitry Ivanov<sup>2</sup>, Xavier Urbain<sup>3</sup>, and Daniel W. Savin<sup>2</sup>

<sup>1</sup>*Physikalisches Institut, Justus-Liebig-Universität, Giessen, Germany*

<sup>2</sup>*Columbia Astrophysics Laboratory, Columbia University, New York, U.S.A.*

<sup>3</sup>*Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Louvain-la-Neuve, Belgium*

Gas-phase formation of complex molecular ions in the interstellar medium at typical temperatures of 10-100 K proceeds predominantly through barrierless ion-neutral reactions. Our single-pass merged-beams apparatus at Columbia University enables us to measure energy-dependent absolute cross sections of molecular formation processes for reactions of singly-charged molecules with neutral atoms or molecules and derive temperature-dependent thermal rate coefficients for individual product channels. Focusing on key reactions implemented in astrochemical models as well as on systems of fundamental interest, we have recently studied the reactions

- (1)  $D + H_3^+ \rightarrow H_2D^+ + H$  [1],
- (2)  $D + H_2D^+ \rightarrow D_2H^+ + H$  and  $D + D_2H^+ \rightarrow D_3^+ + H$  [2],
- (3)  $C + H_2^+ \rightarrow CH^+ + H$  and  $C + D_2^+ \rightarrow CD^+ + D$  [3],
- (4)  $O + H_3^+ \rightarrow OH^+ + H_2$  and  $O + H_3^+ \rightarrow H_2O^+ + H$  [4],
- (5)  $N_2 + H_3^+ \rightarrow N_2H^+ + H$ .

Our study of reactions (1) and (2) was initially motivated by questions of  $H_3^+$  deuteration pathways in star-forming regions, but has, in addition, turned out to be a key reaction to test ab-initio quantum-mechanical calculations of molecular reaction dynamics [5]. Our study of reactions (3) was motivated by the opportunity to benchmark our results against a previously published merged-beams measurement. For reactions (4), we investigated the branching ratios of the two product channels, which are important for accurately modeling the gas-phase formation of water in diffuse and dense molecular clouds. Reaction (5) with different isotopologues of  $H_3^+$  is important for forming  $N_2D^+$  and  $N_2H^+$  in prestellar cores and protoplanetary discs, and the  $N_2D^+/N_2H^+$ -ratio is used as a chemical clock to study the evolution of these objects.

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# First Dielectronic Recombination Measurements at the Cryogenic Storage Ring

**L. Isberner<sup>1,2</sup>, M. Grieser<sup>2</sup>, R. von Hahn<sup>2</sup>, Z. Harman<sup>2</sup>, Á. Kálosi<sup>3,2</sup>, C. H. Keitel<sup>2</sup>, C. Krantz<sup>4</sup>, D. Paul<sup>3,2</sup>, D. W. Savin<sup>3</sup>, S. Singh<sup>2</sup>, A. Wolf<sup>2</sup>, S. Schippers<sup>1</sup> and O. Novotný<sup>2</sup>**

<sup>1</sup>*I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Gießen, Germany*

<sup>2</sup>*Max-Planck-Institut für Kernphysik, Heidelberg, Germany*

<sup>3</sup>*Columbia Astrophysics Laboratory, Columbia University, New York, NY, USA*

<sup>4</sup>*GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany*

Accurate modeling of astrophysical plasmas, and especially of the charge state balance, requires reliable data on the involved processes of recombination and ionization [1]. For atomic ions, recombination with free electrons has been experimentally investigated in magnetic storage rings since the 1990s using the merged-beams technique [2]. A persisting challenge in these experiments is the background signal induced by electron capture from residual gas. Due to the relatively high residual gas pressure in these room-temperature storage rings and the limited magnetic rigidity of the storage ring magnets, experiments were restricted to ions with a low mass-to-charge ratio ( $m/q$ ), which could be stored at sufficiently high energies where the rate coefficient for residual-gas-related electron capture is low [2]. But with the identification of singly charged strontium in a kilonova event, arising from the merger of two neutron stars [3], the need for recombination data also on low-charged heavy ions (high  $m/q$ ) has become apparent. As theoretical calculations for such multi-electron systems are theoretically and computationally challenging, laboratory measurements are crucial.

The electrostatic Cryogenic Storage Ring CSR [4] combines the mass-independent storage of electrostatic storage rings with the excellent vacuum conditions of a cryogenic beam environment. CSR is equipped with an electron cooler and an efficient, movable single-particle detector. Thus, CSR provides unique possibilities for the investigation of electron-ion recombination of low-charged heavy ions. Here, we report on the first recombination measurements with atomic ions at CSR. Investigating the dielectronic recombination of doubly charged neon and triply charged xenon, we have observed resonant recombination features in agreement with preliminary theoretical calculations. Our results clearly demonstrate the feasibility of atomic recombination studies with heavy low-charged ion species at CSR.

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# The evolution of molecular ice into kerogen-like carbon

**C. Jäger and A. Potapov**

*Max Planck Institute for Astronomy, Heidelberg, and Institute of Solid State Physics,  
FSU Jena, Germany  
E-mail: cornelia.jaeger@uni-jena.de*

Comets are pristine building blocks of our and extrasolar planetary systems. The nucleus of 67P/Churyumov–Gerasimenko appears to be fairly uniformly coated with dark, dehydrated, refractory and organic-rich material [1]. Comets and other solar system bodies consist of silicates, organic material, and ice. A recent study [2] has shown that comets have very different ice fractions. The silicate/organics/ice vary widely, but the organic mass fractions are very similar for different objects. The organic material can be described as kerogen-like material. Experimental studies show that grains covered with organic material can be formed by photon-induced conversion of molecular ices into kerogen-like material in molecular clouds or protoplanetary disks. IR spectroscopy, mass spectrometry, and electron microscopy have been used to characterize the organic layers and to gain more insight into the chemical pathways. The organic material formed is very complex. There are different ideas as to how these kerogen-like organics are formed. Fischer-Tropsch synthesis [3] or UV-induced photolysis and processing of ices [4]. Comparison of IR spectra of kerogen produced from different ices with meteoritic material and spectra of interplanetary dust particles shows remarkable coincidences [5].

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# **MOCCA - A 4k-Pixel Microcalorimeter Detector for the Cryogenic Storage Ring CSR**

**C. A. Jakob<sup>1</sup>, L. Gamer<sup>1</sup>, K. Blaum<sup>1</sup>, C. Enss<sup>2</sup>, A. Fleischmann<sup>2</sup>,  
S. K. Gaisser<sup>1</sup>, O. Heber<sup>3</sup>, D. Kreuzberger<sup>2</sup>, A. Lowack<sup>2</sup>,  
M. Rappaport<sup>3</sup>, A. Reifenberger<sup>2</sup>, D. Schulz<sup>2</sup>, A. Shahi<sup>3</sup>, Y. Toker<sup>4</sup>,  
A. Wolf<sup>1</sup> and O. Novotný<sup>1</sup>**

*<sup>1</sup>Max Planck Institute for Nuclear Physics, Heidelberg, Germany*

*<sup>2</sup>Kirchhoff Institute for Physics, Heidelberg, Germany*

*<sup>3</sup>Weizmann Institute of Science, Rehovot, Israel*

*<sup>4</sup>Bar-Ilan University, Ramat Gan, Israel*

The low temperatures and low gas densities in cold interstellar clouds allow the present molecules to relax into their vibrational and rotational ground states. At the Max Planck Institute for Nuclear Physics in Heidelberg, these conditions can be reproduced in the Cryogenic Storage Ring CSR, where heavy molecular ions can cool down while stored for thousands of seconds and electron-ion recombination can be investigated. To reconstruct the full kinematics of these processes, position- and energy-sensitive coincident detection of multiple neutral reaction products is required. For this purpose, MOCCA, a 4k-pixel molecule camera based on metallic magnetic calorimeters with a detection area of 45 mm×45 mm, was developed at the Kirchhoff Institute for Physics in Heidelberg. We present the detector readout scheme, characterization measurements, and the implementation of MOCCA into the CSR-independent MOCCA standalone setup, that will be used to study photon- and collision-induced ion fragmentation processes before MOCCA will be integrated into CSR.

# Dissociative recombination of OH<sup>+</sup> and ArH<sup>+</sup> at the Cryogenic Storage Ring

**Á. Kálosi<sup>1,2</sup>, L. Gamer<sup>2</sup>, M. Grieser<sup>2</sup>, R. von Hahn<sup>2</sup>,  
L. W. Isberner<sup>3,2</sup>, J. I. Jäger<sup>2</sup>, H. Kreckel<sup>2</sup>, D. Paul<sup>1,2</sup>, D. W. Savin<sup>1</sup>,  
V. C. Schmidt<sup>2</sup>, A. Wolf<sup>2</sup>, and O. Novotný<sup>2</sup>**

<sup>1</sup>*Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027, USA*

<sup>2</sup>*Max-Planck-Institute für Kernphysik, 69117 Heidelberg, Germany*

<sup>3</sup>*I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany*

The cosmic-ray ionization rate (CRIR) of atomic H is an important driver of the chemical and physical evolution of diffuse interstellar clouds. The ions from ionization by cosmic rays initiate subsequent ion-molecule reactions that lead to the gas-phase formation of complex molecules [1]. OH<sup>+</sup> and ArH<sup>+</sup> form early in these chains of reactions, but can be destroyed via dissociative recombination (DR) with free electrons. The combination of chemical models and astronomical observations of OH<sup>+</sup> and ArH<sup>+</sup> enables one to quantitatively infer the CRIR in diffuse interstellar clouds [2,3]. Such models require all relevant chemical rate coefficients that account for the internal excitation of the reactants. We have stored fast OH<sup>+</sup> and ArH<sup>+</sup> ion beams in the cryogenic environment of the Cryogenic Storage Ring (CSR), where these infra-red active diatomic hydrides relaxed to their lowest rotational states within minutes of storage [4,5], similar to the conditions of diffuse clouds. Here, we present CSR merged-beams DR experiments for OH<sup>+</sup> and ArH<sup>+</sup> interacting with free electrons produced in a low-energy electron cooler, probing collisions at translational temperatures as low as ~ 10 K.

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# The newly set-up spectroscopic molecular beam apparatus: Applications towards multiphoton resonance

J. Jakob, V. Grigorian, S. Schwetje, M. A. Kaufmann, A. A. Breier, G. W. Fuchs and T. F. Giesen

*Laborastrophysik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany*

Reconciling high spectral resolution and high sensitivity simultaneously is a daunting task. Employing the double resonance technique using a combination of microwave (MW) and infrared (IR) radiation, we have previously shown that we can transfer the precision of the MW radiation into vibrationally excited states and therefore improve the spectral resolution by up to three orders of magnitude. [1]

Now, we present a new molecular beam apparatus that allows high-resolution infrared and optical spectroscopy of cold neutral molecules, detected via resonant multiphoton ionization time-of-flight (REMPI-ToF) mass spectroscopy. A pulsed nozzle produces cold molecules in an adiabatically expanding supersonic jet. Two skimmers reduce the molecular flow to a molecular beam. We use a high-power (up to 1.5 W) continuous-wave optical parametric oscillator (cwOPO) from Qioptiq for a narrowband excitation ahead of the REMPI-ToF detection. The narrow linewidth of the cwOPO (10 - 20 kHz) in the mid-infrared (2.7 - 4  $\mu\text{m}$ ) and its frequency-stability ( $\pm 3$  MHz) ensures for ro-vibrational resolution. The subsequent detection with REMPI provides excellent detection sensitivity even for extremely small samples in addition to mass selectivity.

In a future perspective, multiphoton excitation via IR light and MW radiation in the form of three-wave mixing (3WM) schemes [2] or by photo-electron circular dichroism (PECD) [3], will allow to distinguish the enantiomers of chiral molecules in a cold molecular beam.

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# Investigating Prebiotic Chemistry with Cryogenic Action Spectroscopy

H. Kaur,<sup>1</sup> W. Wang,<sup>2</sup> J. Pérez-Ríos,<sup>3</sup> B. Redlich,<sup>1</sup> and S. Brünken<sup>1</sup>

<sup>1</sup> *Institute for Molecules and Materials, FELIX Laboratory, Radboud University, Toernooiveld 7, 6525 ED Nijmegen, The Netherlands*

<sup>2</sup> *Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany,*

<sup>3</sup> *Department of Physics and Astronomy, Stony Brook University, New York, NY, USA*

Complex organic molecules (iCOMs), such as formaldehyde, glycolaldehyde, and methyl formate, have been detected in space via astronomical observations<sup>[1]</sup>. To understand the formation of these potential prebiotic species in space it is essential to experimentally and theoretically investigate their synthesis. This work focuses on results on the synthesis of the simplest “sugar”, glycolaldehyde, using a cryogenic 22-pole ion trap stationed at FELIX<sup>[2]</sup>. We investigate the gas-phase formation of (protonated) glycolaldehyde from neutral formaldehyde and its cationic forms,  $[\text{H}_2\text{CO}]^+$  and  $[\text{H}_3\text{CO}]^+$ . Gas-phase vibrational spectra of reactant and product ions were recorded using cryogenic IR action spectroscopy and identified using quantum chemical calculations. Additionally, we employ a Markov state model, based on molecular dynamics simulations<sup>[3]</sup> to identify efficient routes for the formation of glycolaldehyde and other iCOMs under low-temperature astrophysical conditions.

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# Toward a new type of gas phase spectroscopy for complex organic ions

**S. Knaffo<sup>1</sup>\*, M.L. Rappaport<sup>1</sup>, H. Kreckel<sup>2</sup>, K. Blaum<sup>2</sup>, A.Wolf<sup>2</sup>, Th. Henning<sup>3</sup>, Y.Toker<sup>4</sup>, S.Sunil Kumar<sup>5</sup>, O. Heber<sup>1</sup>, D. Zajfman<sup>1</sup>**

<sup>1</sup>*Department of Particle Physics, Weizmann Institute of Science, Rehovot 76100, Israel*

<sup>2</sup>*Max-Planck-Institut für Kernphysik, Saupferchweg 1, 69117 Heidelberg, Germany*

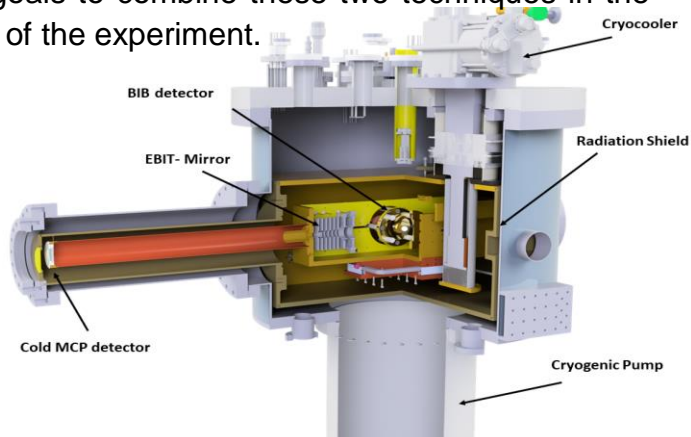
<sup>3</sup>*Max-Planck-Institut für Astronomie, Königstuhl 17, 69117 Heidelberg, Germany*

<sup>4</sup>*Department of Physics and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, 529002 Ramat-Gan, Israel*

<sup>5</sup>*Department of Physics and Center for Atomic, Molecular, and Optical Sciences and Technologies, IISER Tirupati, Tirupati 517507, Andhra Pradesh, India*

More than 300 molecules have been detected in interstellar space to date, and modern telescopes continue to add entries to the catalog of identified species at a steady pace [1]. In recent years the detection frequency of complex organic molecules (COMs) with clear pre-biotic relevance has picked up in pace, with important implications for open questions such as the possible delivery of organic material to Earth and the origin of life. However, there is currently no established technique to obtain gas phase spectra of large molecular ions. We propose to develop a novel spectroscopy technique that is based on laser excitation of electronic transitions in complex molecules, followed by internal re-distribution of the energy among vibrational states and finally the emission of mid-infrared photons [2]. We intend to detect these photons using a sensitive mid-infrared detector.

To this end, we will combine an existing cryogenic electrostatic ion trap with a mid-infrared detector module based on blocked-impurity-band (BIB) arsenic-doped silicon diodes. The ion trap and the detector have been developed and tested separately. Here, we present the challenges and goals to combine these two techniques in the laboratory and the current design stage of the experiment.



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# Probing Life's Building Blocks: Thermal Desorption and Infrared Spectroscopy of Amino Acids

F. Kruczkiewicz<sup>1</sup>, A. Schneiker<sup>2</sup>, J. Santos<sup>1</sup>, H. Linnartz<sup>1</sup>,  
and K. Chuang<sup>1</sup>

<sup>1</sup> *Laboratory for Astrophysics, Leiden Observatory, Leiden University, PO Box 9513, 2300RA Leiden, The Netherlands*

<sup>2</sup> *MTA-ELTE Lendület Laboratory Astrochemistry Research Group, Institute of Chemistry, ELTE Eötvös Loránd University, H-1518 Budapest, Hungary*

Alpha-amino acids (NH<sub>2</sub>-CHR-COOH, where -R denotes various side chains) are critical constituents in biochemistry, playing a crucial role in life as we know it. They are detected in various Solar System's bodies such as meteorites, comets<sup>1</sup>, and asteroids<sup>2</sup>. Efforts have been made experimentally to demonstrate efficient synthesis pathways for amino acids and their precursors under non-energetic conditions that replicate dark clouds<sup>3</sup> or upon irradiation<sup>4</sup>. These experiments aim to reproduce the conditions within the interstellar medium prior to our solar system's formation or in the protosolar nebula post-formation. To enhance the evaluation of these low-temperature experiments and provide supportive data for *in-situ* space missions, understanding the desorption process of these prebiotic molecules and their temperature-responsive infrared spectra is essential.

In this study, we concentrated on the experimental analysis of the desorption kinetics of three amino acids: glycine (-H), alanine (-CH<sub>3</sub>) and serine (-CH<sub>2</sub>OH). Using the SURFRESIDE<sup>3</sup> set-up and an evaporator, we prepared low-temperature (10 K) solid layers by depositing the sublimated vapor of these amino acids onto an inert gold substrate under ultrahigh vacuum conditions (10<sup>-9</sup> hPa). We employed the temperature-programmed desorption technique to characterize their desorption kinetics and used infrared spectroscopy to trace the transitions of these molecules from their neutral to zwitterionic forms. Additionally, we discuss the experimental findings and the common trends observed.

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# Temperature dependent reactions of atomic hydrogen with astrochemically relevant anions

**C. Lochmann<sup>1</sup>, S. Prusuhu-Melath<sup>1</sup>, R. Wild<sup>1</sup> and R. Wester<sup>1</sup>**

*<sup>1</sup>Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, Austria*

About 300 molecules have been identified in the interstellar medium (ISM) so far. This number is expected to rapidly increase with the introduction of the new JWST telescope and the ALMA observatory. Many of the identified molecules are carbon-containing neutral species. However, already ten negatively charged carbon-chain molecules have been found in the depths of the molecular cloud TMC-1 or in the envelope of the carbon star CW Leonis [1,2].

The driving force of chemistry in the gas phase in these regions are interactions of charged molecules with neutrals, since their long-range interaction enables much larger reaction rates. In order to understand the influence of these interactions on the chemical balance of the ISM it is necessary to support the chemical models with laboratory data. By far the most abundant neutral reaction partners in the ISM are atomic and molecular hydrogen. Previously our group showed, however, that the reaction rates of H<sub>2</sub> with carbon chain anions are too small to contribute to the ISM chemistry [3]. The same cannot be said about its atomic counterpart H [4,5].

We perform reaction experiments with atomic hydrogen in a cryogenic 16-pole radiofrequency ion trap. The hydrogen atoms are cooled to the trap temperature before entering the trap by going through a Teflon coated copper block, which is attached to the trap housing. Here, we present the temperature dependent reaction rates in the range of 300 K to 7 K of CN<sup>-</sup>, C<sub>3</sub>N<sup>-</sup> and the polyaromatic hydrocarbon naphthalene in its deprotonated state (C<sub>10</sub>H<sub>7</sub><sup>-</sup>) with atomic hydrogen.

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# How fast are the first stages of nucleation? Reaction kinetics of the formation of heterodimers

**A. Macario,<sup>1</sup> M. Drissi,<sup>1</sup> O. Abdelkader Khedaoui,<sup>1</sup> T. Guillaume,<sup>1</sup>  
B.M. Hays<sup>1</sup> and I.R. Sims<sup>1</sup>**

<sup>1</sup>*Institut de Physique de Rennes (IPR) – UMR 6251 CNRS, Université de Rennes, F-35000 Rennes, France*

Nucleation, which is the first step from vapour to condensed phase, plays an important role in a wide range of environments such as atmospheric clouds, planetary atmospheres, comets or circumstellar shells. However, its onset is still poorly understood. Under the appropriate conditions, such as low temperature and/or high degrees of supersaturation, the rate-limiting process of nucleation is the formation of the first dimer by means of these intermolecular interactions.

The kinetics of formation of homodimers have been investigated in a few previous studies, using the CRESU (reaction kinetics in uniform supersonic flow) technique mainly coupled with mass spectrometric detection. Here we have employed a completely new detection scheme, chirped-pulse Fourier transform mm-wave spectroscopy, to study for the first time the kinetics of formation of heterodimers. This innovative technique combines the ability to generate continuous cold uniform supersonic flows with the high selectivity and general applicability of rotational spectroscopy, allowing us to follow both reactant and product concentrations simultaneously. Furthermore, the high sensitivity achieved has allowed us to employ pseudo-first-order conditions to obtain absolute rate constants. We will report the first measurements of rate constants for the formation of a set of heterodimers, including formic acid, CO<sub>2</sub> and water among others, at temperatures between 35 and 80 K.

# Radiative cooling of small isolated cluster ions in the slow exchange limit

**D. Müll<sup>1</sup>, K. Blaum<sup>1</sup>, P. Fischer<sup>2</sup>, L. Gamer<sup>1</sup>, S. George<sup>1,2</sup>, M. Grieser<sup>1</sup>, F. Grussie<sup>1</sup>, O. Heber<sup>3</sup>, M. Iron<sup>3</sup>, À. Kálosi<sup>1,4</sup>, S. Knaffo<sup>3,5</sup>, O. Novotný<sup>1</sup>, F. Nuesslein<sup>1</sup>, V. C. Schmidt<sup>1</sup>, L. Schweikhard<sup>2</sup>, R. Singh<sup>3</sup>, A. Wolf<sup>1</sup>, D. Zajfman<sup>3</sup>, A. Znotins<sup>1</sup>, H. Kreckel<sup>1</sup>, Y. Toker<sup>5</sup>**

<sup>1</sup>Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69124 Heidelberg, Germany

<sup>2</sup>Institut für Physik, Universität Greifswald, 17487 Greifswald, Germany

<sup>3</sup>Department of Particle Physics, Weizmann Institute of Science, Rehovot 76100, Israel

<sup>4</sup>Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027, USA

<sup>5</sup>Department of Physics and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, 529002 Ramat-Gan, Israel

E-mail: muell@mpi-hd.mpg.de

We have used the Cryogenic Storage Ring (CSR) [1] at the Max Planck Institute for Nuclear Physics to study the spontaneous cooling of stored  $Al_4^-$  ions at ambient temperatures of  $T < 10K$ . A comprehensive understanding of the radiative cooling process of molecules is needed since it is the dominant cooling process in the interstellar medium. We present measurements employing laser-induced delayed electron detachment to monitor the internal energy of the isolated clusters for more than 30 minutes, extending the observation times compared to previous studies [2] considerably. We find that the cooling rate at long storage times cannot be explained by standard radiative cascade models, instead the limiting process at low temperatures is the internal vibrational redistribution (IVR). We devise a slow exchange model that takes the energy-dependence of the IVR rate into account. The calculated rates in the slow exchange model in combination with recurrent fluorescence -- for energies above the first electronic excited state -- provide an excellent match for the measured energy-dependence of the cooling rate.

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# Optical Spectra of the Smallest Silicon Carbide Cations

**Kai Pollow<sup>1</sup>, Taarna Studemund<sup>1</sup>, Pierluigi Moretti<sup>1</sup>,  
Alexander Breier<sup>1</sup>, Otto Dopfer<sup>1</sup>**

*<sup>1</sup> Institut für Optik und Atomare Physik, TU Berlin, Germany*

Silicon carbide (SiC) compounds play a pivotal role in both astrophysics and semiconductor development. Silicon carbide grains have been detected in the vicinity of carbon-rich stars, where their properties greatly impact our understanding of dust evolution [1]. Moreover, in the field of materials science, SiC is widely recognized for its potential as a semiconductor material. In this contribution, we investigate the optical spectra of the smallest mixed silicon carbide cations,  $\text{Si}_n\text{C}_m^+$  ( $n+m=2-4$ ), to gain valuable insights into their geometric and electronic structure.

Using advanced spectroscopic techniques (electronic photodissociation of mass-selected ions in a quadrupole/time-of-flight tandem mass spectrometer coupled to a cryogenic laser vaporization source [2]), we experimentally determine the optical spectra of these fundamental  $\text{Si}_n\text{C}_m^+$  cations [3,4]. Additionally, we compare our experimental findings with quantum chemical calculations.

By elucidating the optical spectra and electronic structure of these SiC cations, we provide crucial insights into their relevance in astrophysics, aiding in the understanding of dust evolution in the vicinity of C-rich stars. Furthermore, our findings contribute to the development of novel semiconductor materials, exploiting the bottom-up approach for enhanced material design and engineering.

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# Photodetachment spectroscopic studies of cold, trapped negative ions

S. Purushu Melath<sup>1</sup>, C. Lochmann<sup>1</sup>, M. Nötzold<sup>1</sup>, R. Wild<sup>1</sup> and  
R. Wester<sup>1</sup>

<sup>1</sup>*Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck  
Technikerstraße 25/3, 6020 Innsbruck, Austria*

Photodetachment spectroscopy is a powerful spectroscopic technique for determining the internal state distribution of a molecular anion. Previously, our group studied the threshold photodetachment spectroscopy of  $\text{CN}^-$  at both 16 K and 295 K in a 22-pole ion trap and measured the electron affinity of CN with great precision (EA: 3.864(2) eV) [1]. Here we present the threshold photodetachment spectroscopy study of  $\text{C}_2^-$ , speculated to exist in interstellar medium in a radiofrequency 16-pole ion trap at 8 Kelvin. We investigated the behaviour of the cross section near the threshold for the ground state transition,  $\text{C}_2 \text{X } ^1\Sigma_g^+ \leftarrow \text{C}_2^- \text{X } ^2\Sigma_g^+$ . We measured the electron affinity of  $\text{C}_2$  which is consistent with the previously measured values [3][4]. We also present the status of the threshold photodetachment spectroscopy of the naphthyl anion ( $\text{C}_{10}\text{H}_7^-$ ), a polyaromatic hydrocarbon anion (PAH), which may also play a role in interstellar chemistry [5].

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# Complex refractive index of water ice analogues measured by terahertz time-domain spectroscopy

F. de A. Ribeiro<sup>1,2</sup>, B. M. Giuliano<sup>1</sup>, A. A. Gavdush<sup>3</sup>, A. V. Ivlev<sup>1</sup>, K. Zeytsev<sup>3</sup>, G. Komandin<sup>3</sup> and P. Caselli<sup>1</sup>

<sup>1</sup> *Max Planck Institute for Extraterrestrial Physics, Garching, Germany*

<sup>2</sup> *Federal Institute of Rio de Janeiro, Nilópolis, Brazil*

<sup>3</sup> *Prokhorov General Physics Institute of the Russian Academy of Sciences, Moscow, Russia*

The structure and evolution of interstellar clouds and protoplanetary disks is based mainly on observations of the dust continuum emission in the millimeter and sub-millimeter wavelengths combined with radiative transfer models that require knowledge of the optical properties of the dust. This generally includes information on grain size distribution and its chemical composition, but for dense and cold molecular clouds, one also needs to consider that the presence of ice mantles, in which water is the major component, may change dust opacities. Therefore, the measurement of optical constants of astrophysical ice analogues in the infrared and terahertz range can be used to model the dust continuum emission and radiative transfer in dense and cold molecular clouds and aid in the interpretation of astronomical observations. However, due to the lack of directly measured optical properties of ice analogues at these wavelengths, the interpretation of dust continuum emission measurements generally relies on calculated opacity values. In this work, as a continuation of the work being done so far in the CASICE laboratory at the Max Planck Institute for Extraterrestrial Physics, preliminary dielectric measurements of water ice at the far infrared and terahertz frequencies will be presented. In recent investigations, the use of terahertz time domain spectroscopy (THz-TDS), Fourier transform infrared spectroscopy (FTIR) techniques, and its analysis by an algorithm developed to reconstruct the optical constants of ices allowed the direct measurement of complex refractive indices and the modelling of the opacities of CO and CO<sub>2</sub> ice mantles, respectively [1, 2]. In a similar procedure, we employ FTIR and THz-TDS to determine the complex refractive index of water ice grown at different temperatures. The effect of thermal processing and annealing on the optical constants will also be addressed. These data can be useful to model sources where water-rich ice mantles are expected to be present, such as prestellar cores in their early stages and protoplanetary disks mid-planes between the water and CO snow-lines.

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# IR-PD Spectroscopy of the Astrochemically-Relevant HCCS<sup>+</sup> Ion

J. A. Diprose<sup>1</sup>, K. Steenbakkers<sup>2</sup>, M. Michielan<sup>3</sup>, S. Brünken<sup>2</sup>, D. Ascenzi<sup>3</sup>, C. Romanzin<sup>4</sup> and V. Richardson<sup>1</sup>

<sup>1</sup>*Department of Physics, University of Liverpool, Liverpool, UK*

<sup>2</sup>*Institute for Molecules and Materials, FELIX Laboratory, Radboud University, Nijmegen, The Netherlands*

<sup>3</sup>*Department of Physics, University of Trento, Trento, Italy*

<sup>4</sup>*Université Paris-Saclay, CNRS, Institut de Chimie Physique, Orsay, France*

The recent detection of HCCS<sup>+</sup> towards the cold dark cloud TMC-1 [1] marked the first observation of a protonated radical in such an environment. Furthermore, the greater column density of the ion with respect to neutral HCCS has led to the conclusion that the major formation route in this environment is in fact the protonation of CCS [1].

This is notable as CCS has been detected in a range of different environments including Sgr B2 [2], IRC+10216 [3], the protoplanetary disk surrounding GG Tau [4], at least 14 cirrus and Clemens Barvainis cores [5], and the Horsehead nebula, a Photon-Dominated Region (PDR) [6]. Therefore, given the wide range of potential proton sources present in such environments, there is a high likelihood that HCCS<sup>+</sup> is also present in these environments. Following the launch of the JWST, an experimental IR spectrum of HCCS<sup>+</sup> could allow for further detections in either PDRs or the diffuse interstellar medium.

To this end, we present preliminary IR-PD spectra of both the HCCS<sup>+</sup> ion (formed by dissociative ionization of 2,5 dibromothiophene) and [C<sub>2</sub>H<sub>2</sub>S]<sup>+</sup> (formed by dissociative ionization of thiophene). The spectra have been measured via the irradiation of H<sub>2</sub>-tagged complexes in a cryogenic 22-pole trap within the FELion instrument at the FELIX light source. While no isomers of [C<sub>2</sub>H<sub>2</sub>S]<sup>+</sup> have yet been observed in astrophysical environments, these ions could be formed by protonation of HCCS—both in dark clouds such as TMC-1 and in other environments where HCCS is present—motivating the need to record [C<sub>2</sub>H<sub>2</sub>S]<sup>+</sup> IR spectra.

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# Carbonated silicate grains: Photodissociation of carbonate groups with Lyman- $\alpha$ irradiation

**G. Rouillé<sup>1</sup>, C. Jäger<sup>1</sup>, and Th. Henning<sup>2</sup>**

<sup>1</sup> *Laboratory Astrophysics Group of the Max Planck Institute for Astronomy at the Friedrich Schiller University Jena, Institute of Solid State Physics, Jena, Germany*

<sup>2</sup> *Max Planck Institute for Astronomy, Heidelberg, Germany*

Carbonates represent the second most abundant minerals on Earth. They are also present on other planets and on asteroids, and in the fragments of these bodies, namely, meteorites and interplanetary dust particles. These carbonates are the product of aqueous alteration of silicates.

The detection of carbonate bands in the spectra of planetary nebulae [1, 2] and protostars [3, 4] suggests that the compounds can form in stellar winds and outflows. As aqueous alteration cannot occur in such environments, another mechanism must produce these carbonates [5].

We have produced amorphous, carbonated silicate nanograins by gas-phase condensation following the pulsed laser ablation of metal targets in CO<sub>2</sub> gas. Thus, we have shown that carbonated silicates –silicate grains in which carbonate groups are embedded– can form without water, either liquid or gaseous. We have also found that irradiation of the grains with Lyman- $\alpha$  photons dissociates the carbonate groups that are at, or close to, the surface of the grains, resulting in the formation of CO<sub>2</sub> molecules. The estimated photodissociation cross section is  $6.2 \times 10^{-16} \text{ cm}^2$ , a relatively high value.

We will present the laboratory study and its astrophysical implications.

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# Resonant photo-dissociation studies of $C_4O^-$ at the Cryogenic Storage Ring

**V. C. Schmidt<sup>1</sup>, M. Ončák<sup>2</sup>, S. George<sup>1</sup>, K. Blaum<sup>1</sup>, J. Göck<sup>1</sup>,  
M. Grieser<sup>1</sup>, P. Fischer<sup>3</sup>, R. von Hahn<sup>1</sup>, Á. Kálosi<sup>4,1</sup>, H. Kreckel<sup>1</sup>,  
P. M. Mishra<sup>1</sup>, D. Müll<sup>1</sup>, O. Novotný<sup>1</sup>, F. Nuesslein<sup>1</sup>, L. Schweikhard<sup>3</sup>,  
and A. Wolf<sup>1</sup>**

<sup>1</sup>Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany

<sup>2</sup>Universität Innsbruck, 6020 Innsbruck, Austria

<sup>3</sup>Universität Greifswald, 17487 Greifswald, Germany

<sup>4</sup>Columbia University, New York, 10027 New York, USA

The study of cooling dynamics and ground-state properties of molecular ions is one of many research goals at the Cryogenic Storage Ring (CSR) at the Max-Planck-Institut für Kernphysik in Heidelberg [1]. The CSR is a fully electrostatic storage ring, which can be cooled down to a few kelvin and reaches residual gas densities down to  $1000\text{ cm}^{-3}$ . Thus, the ring provides a unique research environment enabling the study of gas-phase ion species in a very low radiation field and almost free of collisional background.

Here we present investigations of the carbon-based molecule  $C_4O^-$ , which is predicted to be observable in interstellar clouds [2]. Its detection requires a detailed knowledge of the anion's vibronic structure. Past studies of this molecule have left open questions about its geometry as well as its electron affinity. A previous measurement of photon absorption properties of  $C_4O$  in a neon matrix revealed multiple absorption resonances attributed to vibronic transitions [3]. For our measurement internally hot  $C_4O^-$  ions were produced in a sputter source and injected into the CSR. They were probed with different photon energies at various storage times to monitor their internal excitations. Neutral and charged fragments were measured in coincidence by two detectors.

The results include resonant fragmentation in the photon energy region of about  $21\,300\text{ cm}^{-1}$  to  $29\,000\text{ cm}^{-1}$ . The resonance curves exhibit changes in shape and height attributed to cooling dynamics of the anions inside the CSR. One feature is attributed to the radiative cooling of a vibrational hot band. Furthermore, the possible onset of the electron detachment channel is visible around  $29\,000\text{ cm}^{-1}$ . We will present our experimental results together with a theoretical investigation of the observed features. In particular, the molecule's geometry and vibronic structure were calculated, revealing that both initial and final electronic state of the observed transitions suffer from a Renner-Teller interaction.

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# Infrared irradiation of mixed interstellar ice analogues

**Schrauwen, J.G.M.,<sup>1</sup> Traspas-Muiña, A.,<sup>2</sup> Ioppolo, S.,<sup>3</sup> Cuppen, H.M.,<sup>4</sup> Redlich, B.<sup>1</sup>**

<sup>1</sup>*FELIX laboratory, IMM, Radboud University, Nijmegen, The Netherlands*

<sup>2</sup>*EECS, Queen Mary University of London, United Kingdom*

<sup>3</sup>*InterCat, Department of Physics and Astronomy, Aarhus University, Denmark*

<sup>4</sup>*Institute of Molecules and Materials (IMM), Radboud University, Nijmegen, The Netherlands*

Previously, astronomical observations have unambiguously identified 6 small molecules in the solid state in space - H<sub>2</sub>O, CO, CO<sub>2</sub>, CH<sub>3</sub>OH, NH<sub>3</sub> and CH<sub>4</sub> [1,2]. These ices play an important role in the physical and chemical processes in the interstellar medium (ISM). The recent launch of the James Webb Space Telescope promises high resolution data sensitive to the morphology, mixing environment and thermal history of interstellar ices and possibly the detection of additional solid-state molecular species in the ISM. In order to interpret this data, a thorough understanding of the dependence of the ice structure on its physical and chemical environment is required. Here, we focus on the effect of infrared irradiation on the interstellar ices, specifically.

Ices in the ISM are generally exposed to infrared irradiation, as well as UV and cosmic ray background. In addition, exothermic reactions in and on these ice layers can release vibrational energy in the bonding network of the ice. Understanding how this energy can dissipate in an interstellar ice is key in investigating changes in the ice structure as a result of this energetic processing, as well as grain-surface reactions. The Laboratory Ice Surface Astrophysics (LISA) end station at the free electron laser (FEL) facility FELIX in the Netherlands has been designed to study these fundamental processes [3,4]. Our recent studies focused on the resonant irradiation of mixed ices of H<sub>2</sub>O and CO<sub>2</sub>. From our set of observations, it appears that H<sub>2</sub>O and CO<sub>2</sub> restructure together, i.e. when irradiating CO<sub>2</sub> changes are observed in H<sub>2</sub>O and vice versa, which implies an energy exchange mechanism between the species. In addition, irradiation of CO<sub>2</sub>-rich ices on-resonance with the CO<sub>2</sub>-stretch results in the appearance of additional bulk H<sub>2</sub>O features in the infrared spectra, which could possibly result from a desorption induced clustering of H<sub>2</sub>O molecules.

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# THE NEWLY SET-UP SPECTROSCOPIC MOLECULAR BEAM APPARATUS: PRODUCING TRANSIENT MOLECULES IN A COLD SUPERSONIC JET

**S. SCHWETJE, J. JAKOB, V. GRIGORIAN, M. A. KAUFMANN, A. A.  
BREIER, G. W. FUCHS and T. F. GIESEN**

*Laborastrophysik, Universität Kassel, Heinrich-Plett-Straße 40, 34132  
Kassel, Germany  
E-mail: sebastian.schwetje@outlook.com*

Diffuse interstellar bands, or DIBs, are features in absorption spectra of astronomical objects. Probable carriers of those bands are various, yet unassigned molecules found in the visible and near-infrared spectra of interstellar gas and dust clouds. Complex organic molecules may contribute to the DIBs as shown in recent work by Campbell et al. when they assigned some of the near-infrared DIBs to the molecular ion  $C_{60}^+$ . [1] To assign more DIBs, laboratory experiments are required. Therefore, it is necessary to employ a powerful source which is capable of producing astrochemically relevant molecules coupled with high resolution spectroscopy. The Even-Lavie high-pressure pulsed valve provides a supersonic jet with cooling properties below 1 K, backing pressures up to 100 bars, repetition rates up to 600 Hz and gas pulse widths of 20 microseconds. [2] Together with a mountable AC discharge source it is capable of producing both stable and transient molecules in a jet to approach the production of astrochemically relevant species. Here we present preliminary data from a molecular beam setup coupled with a discharge source and REMPI spectroscopy as the detection technique.

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# New Setup for High-Resolution Ion-Molecule Crossed Beam Imaging

**Dasarath Swaraj<sup>1</sup>, Tim Michaelsen<sup>1</sup>, Fabio Zappa<sup>1</sup>, Robert Wild<sup>1</sup> and Roland Wester<sup>1</sup>**

*<sup>1</sup>Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, 6020 Innsbruck, Austria*

Crossed-beam reactive scattering experiments offer a detailed understanding of the dynamics involved in elementary reactions occurring in the gas phase. By employing velocity map imaging (VMI), it is possible to acquire angle and energy differential cross-sections, as demonstrated in previous studies [1], [2]. In this study, we present a comprehensive design plan and relevant simulations for an experimental setup intended to investigate ion-molecule reactions with enhanced precision to achieve state-to-state resolution for ion-molecule reactions.

Initially, we are concentrating on the experimental studies on the ion-molecule reaction  $\text{H}_2^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{H}$ . Additionally, Monte Carlo simulations were conducted to determine the expected resolution of the product energy for the reaction [3]. To generate  $\text{H}_2^+$  ions, we employ laser-induced ionization of  $\text{H}_2$  using the 3rd or 4th harmonic of a pulsed Nd:YAG laser, ensuring that the ions primarily occupy the vibrational ground state[4]. The ion beam is then overlapped with a beam of neutral molecules, and the resulting collision products are collected and analyzed using the VMI spectrometer. Furthermore, we plan to implement coincidence detection to simultaneously observe both the ionic and neutral products subsequent to the reaction.

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# Radiative transfer modelling of the photoelectric heating of gas in the nearby spiral galaxy NGC628

Richard Tuffs<sup>1</sup>, Mark Rushton<sup>1,2,3</sup>, and Yu Fung Wong<sup>1</sup>

<sup>1</sup>*MPI fuer Kernphysik, Heidelberg, Germany*

<sup>2</sup>*Astronomical Institute of the Romanian Academy, Bucharest, Romania*

<sup>3</sup>*Jeremiah Horrocks Institute, University of Central Lancashire, Preston, UK*

We introduce a new model for the heating of interstellar gas by photoelectrons ejected from polycyclic aromatic hydrocarbons (PAHs) and dust particles following the absorption of UV/optical photons in the interstellar radiation field (ISRF). Our model takes into account not only the intensity of the ISRF but, for the first time, its colour. In particular, this allows us to consider the increased efficiency of the photoelectric (PE) heating by the absorption by negatively charged PAHs by redder photons, in regions where the ISRF has been reddened through obscuration by dust, and/or is intrinsically red due to a local predominance of more evolved stars.

We apply the model to calculate the PE heating of gas in the nearby spiral galaxy NGC628, for which we have a solution for the global variation of intensity and colour of the diffuse ISRF obtained by a self-consistent radiative transfer modelling of the direct- and dust-reradiated starlight throughout the galaxy. As a first application, we critically compare and contrast our predictions for the CO pure rotational lines from passive (non-starforming) clouds, calculated using a simple chemical reaction network, under the hypothesis that PE heating is the dominant heating mechanism for gas, with observations of the same lines, utilising data from ALMA and JWST. We also identify the main areas in which better laboratory data are needed to improve models of PE heating, both for the calculation of the ionisation balance in PAH and dust, as well as for predicting the yield and energies of photoelectrons under interstellar conditions.

# Rotational Spectroscopy of 2-Cyanobiphenyl

Lise von Rötzel, Bettina Heyne, Mariyam Fatima, Sven Thorwirth,

Stephan Schlemmer

I. Physikalisches Institut, Universität zu Köln, Cologne, Germany

The class of polycyclic aromatic hydrocarbons (PAHs) presents an important motif in building the chemical environment of the interstellar medium. Around 10 to 25% of all interstellar carbon is thought to be locked up as PAHs. Recently benzonitrile [1] as well as 1- and 2- cyanonaphthalene ( $C_{10}H_7CN$ ), have been identified in radio observations of TMC-1 [2] based on their laboratory rotational spectra. The detection of these molecules raises possibilities for the presence/formation of other cyano-aromatic molecules in the interstellar medium.

In this work, we present chirped-pulse Fourier transform microwave (CP-FTMW) spectra of 2-cyanobiphenyl (CBP) [ $C_{12}H_9CN$ ], that is a cyano-aromatic molecule. They are measured in the frequency range from 11.5 to 27 GHz. The Cologne CP-FTMW instrument has been designed to achieve high stability and sensitivity. In a recent modification to the instrument, we are using state-of-the-art RF modulation and detection technology to directly generate and receive signals in this frequency range, thus abandoning the up- and down-mixing processes of our previous chirped-pulse microwave spectrometer setup [3]. As a result, the tedious side-band separation is no longer needed. Moreover, the number of elements influencing the intensities is reduced to a minimum. To achieve faster measurements and an improved signal-to-noise ratio multiple chirped pulses per gas pulse are implemented in the experimental setup. The setup and the results of the 2-CBP measurements will be presented.

## References

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# Electron recombination of deuterated triatomic hydrogen ions at the Cryogenic Storage Ring

A. Znotins<sup>1</sup>, A. Faure<sup>2</sup>, J. Forer<sup>3</sup>, C. H. Greene<sup>4</sup>, F. Grussie<sup>1</sup>, L. W. Isberner<sup>5,1</sup>, Á. Kálosi<sup>6,1</sup>, V. Kokoouline<sup>3</sup>, M. Pezzella<sup>7</sup>, D. Müll<sup>1</sup>, O. Novotný<sup>1</sup>, D. Paul<sup>6,1</sup>, D. W. Savin<sup>6</sup>, S. Schippers<sup>5</sup>, J. Tennyson<sup>7</sup>, X. Urbain<sup>8</sup>, A. Wolf<sup>1</sup>, H. Kreckel<sup>1</sup>

<sup>1</sup> Max-Planck-Institut für Kernphysik, Heidelberg, Germany

<sup>2</sup> University Grenoble Alpes, CNRS, IPAG, Grenoble, France

<sup>3</sup> Department of Physics, University of Central Florida, Orlando, USA

<sup>4</sup> Department of Physics and Astronomy, Purdue University, West Lafayette, USA

<sup>5</sup> I. Physikalisches Institut, Justus-Liebig-Universität, Gießen, Germany

<sup>6</sup> Columbia Astrophysics Laboratory, Columbia University, New York, USA

<sup>7</sup> Department of Physics and Astronomy, University College, London, UK

<sup>8</sup> Institute of Condensed Matter and Nanosciences, Louvain-la-Neuve, Belgium

The triatomic hydrogen ion  $\text{H}_3^+$  is one of the most important molecules for the gas phase chemistry of interstellar clouds. As an active proton donor, it is a primary driver of ion-neutral chemistry in interstellar environments. Moreover, as the simplest polyatomic molecule,  $\text{H}_3^+$  is an important benchmark system for theoretical molecular calculations.

Considerable focus has been given to the dissociative electron recombination (DR) of triatomic hydrogen ions, as the rate coefficient for this reaction is crucial in determining the ionization balance of interstellar clouds. Although earlier studies have established that the DR rate coefficients of  $\text{H}_3^+$  and its isotopologues are influenced by rotational excitation, state-selective measurements have not been feasible thus far.

Here we present ongoing efforts aimed at understanding electron collisions and recombination of deuterated variants of triatomic hydrogen – namely  $\text{H}_2\text{D}^+$  and  $\text{D}_2\text{H}^+$  – inside the Cryogenic Storage Ring (CSR) [1]. Radiative cooling models, based on comprehensive line-lists [2], predict that the rovibrational populations of  $\text{H}_2\text{D}^+$  and  $\text{D}_2\text{H}^+$  become confined to a handful of identifiable states after storage times of several hundreds of seconds. Our models also include inelastic electron collisions and selective depletion by electron recombination.

We will present recent DR experiments performed with cold  $\text{H}_2\text{D}^+$  and  $\text{D}_2\text{H}^+$  ions, combined with new theoretical calculations for all relevant processes.

## References

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