

# Laboratory Astrophysics Workshop 2021

Dust, Ice, Complex and Prebiotic Molecules in the  
ISM, Disks and Exoplanet Atmospheres

22. - 24. November 2021

in the Dornburger Castles near Jena,  
Germany

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## **Program, Day 1 (22.11.2021). Dust, ice, and molecules**

8:45 – 9:05 Registration

### **Session 1.**

09:05 – 09:15 Introduction. **Cornelia Jäger**

09:15 – 10:00 Invited talk. **Rens Waters** “Molecules, Ice and Dust: from the Interstellar Medium to Planets” ([online](#))

10:00 – 10:45 Invited talk. **Harald Mutschke** „Measurements of dust optical constants at long wavelengths and low temperatures” ([online](#))

10:45 – 11:30 Coffee break + Registration

11:30 – 12:15 Invited talk. **Belen Mate** “Physical and chemical processes on interstellar ice and dust analogues: recent results at IEM-CSIC”

12:15 – 12:35 Contributed talk. **Jiao He** “Refractive index and extinction coefficient of vapor deposited water ice in the UV-Vis range”

12:35 – 12:55 Contributed talk. **Franciele Kruczkiewicz** “Merging THz-TDS and FTIR data for direct reconstruction of CO dielectric properties”

12:55 – 13:15 Contributed talk. **Will Rocha** “Getting ready for JWST: introducing the new Leiden Ice Database and the ENIIGMA fitting tool”

13:15 – 14:30 Lunch

### **Session 2.**

14:30 – 15:15 Invited talk. **Otto Dopfer** “Photochemical Properties of Silicon Clusters: Bridging the Gap Between Diatomics and Grains”

15:15 – 16:00 Invited talk. **Paul Scheier** “Helium-tagging spectroscopy as a tool for the identification of diffuse interstellar band carriers”

16:00 – 16:45 Coffee break

16:45 – 17:05 Contributed talk. **Robert Radloff** “Astrochemically-Relevant Silicon Carbide Clusters: Photodissociation and Electronic Properties”

17:05 – 17:25 Contributed talk. **Eileen Döring** “High Resolution IR Spectroscopy on small metal bearing molecules”

17:25 – 17:45 Contributed talk. **Guido Fuchs** “Mid-Infrared Observations of Late-type Stars at High Spectral Resolution”

17:45 – 18:05 Contributed talk. **Miguel Jiménez-Redondo** “Study of low-temperature ion-neutral interactions in a 22-pole ion trap”

18:05 – 18:25 Contributed talk. **Valerio Lattanzi** “High-Resolution Gas-Phase Spectroscopy for Astrophysics at CAS@MPE” ([online](#))

19:30 Conference dinner

## **Program, Day 2 (23.11.2021). Complex organic molecules and the Origin of Life.**

### **Session 1.**

09:00 – 09:45 Invited talk. **Cornelia Meinert** “The cosmic origin of biomolecular chirality” ([online](#))

09:45 – 10:30 Invited talk. **Angela Ciaravella** “Formation of complex organic molecules in ices triggered by X-rays”

10:30 – 11:15 Coffee break + Poster session

11:15 – 12:00 Invited talk. **Guillermo Munoz Caro** “Formation of N-heterocycles and S-chains in UV-photoprocessed interstellar ice analogs”

12:00 – 12:20 Contributed talk. **Ko-Ju Chuang** “Formamide formation in H<sub>2</sub>O-rich and CO-rich interstellar ice analogs”

12:20 – 12:40 Contributed talk. **Riccardo Urso** “Energetic processing of methanol-rich ices”

12:40 – 13:00 Contributed talk. **Gayatri Batra** “Exploring silicon chemistry in the electrical discharge of methyl phenyl silane (MPS) using chirped-pulse Fourier-transform microwave spectroscopy” ([online](#))

13:00 – 14:30 Lunch

### **Session 2.**

14:00 – 14:45 Invited talk. **Wolf Geppert** “Astrobiology and the origin of life” ([online](#))

14:45 – 15:30 Invited talk. **Kathrin Altwegg** “Cometary chemistry”

15:30 – 16:15 Coffee break + Poster session

16:15 – 16:35 Contributed talk. **Diksha Garg** “Fragmentation Dynamics of Fluorene, on Femtosecond Timescales” ([online](#))

16:35 – 16:55 Contributed talk. **Tushar Suhasaria** “A novel UHV setup with MALDI-high resolution mass spectrometry for the in-situ detection of biomolecules”

16:55 – 17:15 Contributed talk. **Parker Crandall** “Optical Properties of Simple Diamondoid Cations and Their Astrochemical Relevance”

17:15 – 17:35 Contributed talk. **Taarna Studemund** “Small Si<sub>n</sub>O<sub>m</sub><sup>+</sup> Clusters - Photodissociation & Optical Absorption Properties”

17:35 – 17:55 Contributed talk. **Dima Semenov** “Sensitivity of gas-grain chemical models to surface reaction barriers: Effect from a key carbon-insertion reaction, C + H<sub>2</sub> → CH<sub>2</sub>”

### **18:00 – 19:00 Poster session**

18:00 – 18:05 **Donatella Loru** “Revealing the chemistry of polycyclic aromatic hydrocarbons by plasma sources” ([online](#))

18:05 – 18:10 **Holger Kreckel** “Astrochemistry at the Cryogenic Storage Ring” ([online](#))

18:10 – 18:15 **Annika Oetjens, Aigars Znotins** “Preparations for experiments with triatomic hydrogen ions at the Cryogenic Storage Ring” ([online](#))

18:15 – 18:20 **Philipp Schmid** “Sneaking into the astrochemistry of chlorine: Gas-phase IR action spectroscopy of CH<sub>2</sub>Cl<sup>+</sup> and CH<sub>3</sub>ClH<sup>+</sup>” ([online](#))

### In presence

**Oskar Asvany** “Rotational action spectroscopy of  $\text{CN}^+$ ,  $\text{CH}_2\text{NH}_2^+$  and  $\text{CH}_3\text{NH}_3^+$ ”

**Stefan Bergmeister** “Atomic and molecular clusters embedded in helium nanodroplets”

**Luis Bonah** “LLWP – A new Loomis-Wood Software at the Example of Propanone- $^{13}\text{C}_1$ ”

**Cesare Cecchi-Pestellini** “Chemical and physical processes caused by electrons impacting on  $\text{H}_2\text{O}$ - $\text{CO}$  mixed ices”

**Elham Ghavidel** “Electronic transitions in  $\text{Rb}_2^+$  dimers solvated in Helium”

**Victor Herrero** “Polymerization in  $\text{C}_2\text{H}_2$  plasmas used for the generation of interstellar dust analogues”

**Bettina Heyne** “Characterizing home-built chirped-pulse spectrometers for complex molecules of astrophysical interest”

**Matin Kaufmann** “Spectroscopy of molecular glow discharge products using REMPI”

**Christian Kranhold** “Semiconductor- & Metallic-Behavior of Iron(II) Sulfides: A Multi-Wavelengths Study”

**Miriam Meyer** “Action Spectroscopy of PAH Ions Using the Helium Droplet Technique”

**Fabian Peterß** “Mid Infrared CW Cavity Ring Down Spectroscopy in a Supersonic Jet”

**Gael Rouillé** “Gas-phase condensation of carbonated silicates”

**Karel Vávra** “Rotational Spectrum of Vinyl Isocyanate”

### Program, Day 3 (24.11.2021). Exoplanetary atmospheres and extraterrestrial life

#### **Session 1.**

09:00 – 09:45 Invited talk. **Christiane Helling** “Physics and Chemistry of planetary atmospheres” ([online](#))

09:45 – 10:30 Invited talk. **Paul Molliere** “Modeling and Characterization of Cloudy Exoplanet Atmospheres” ([online](#))

10:30 – 11:00 Coffee break

11:00 – 11:20 Contributed talk. **Dominic Samra** “Mineral Snowflakes on Exoplanet and Brown Dwarf Atmospheres”

11:20 – 12:05 Invited talk. **Jeroen Bouwman** “Observational constraints on dust processing in circumstellar media and exoplanetary atmospheres” ([online](#))

12:05 – 13:05 Discussion on laboratory experiments relevant to exoplanetary atmospheres.

13:05 – 13:15 Final remarks. **Cornelia Jäger**

13:15 – 14:30 Lunch

14:30 Departure to Jena

## **Abstracts. Day one**

# Molecules, Ice and Dust: from the Interstellar Medium to Planets

L.B.F.M. (Rens) Waters<sup>1,2</sup>

<sup>1</sup>*Department of Astrophysics, IMAPP, and IMM/Felix, Radboud University*

<sup>2</sup>*SRON Netherlands Institute for Space Research*

Molecular gas and solids play a crucial role in the life cycle of matter in galaxies, and show an intricate interplay. Their presence, even at low abundance, determines heating and cooling of interstellar gas; Vice-versa, their presence can be used as a probe of the local conditions. Molecular gas and solid (refractory) particles are ejected by evolved stars and supernovae. In the diffuse Interstellar Medium, molecules do not survive and the refractory dust is processed by shocks and high energy particles. In denser parts of the ISM, solid particles can grow again, and provide a surface that allows the formation of molecular hydrogen, which subsequently drives a very rich (ion) chemistry. Shielding of the interstellar radiation field and cooling by molecules results in the formation of interstellar ices, with a very rich (organic) grain surface chemistry. Upon heating near forming stars, these icy mantles release complex organic molecules to the gas phase. In planet forming disks that surround young stars, solids, inherited from the molecular cloud, are the starting point of planet formation. The planet formation process drives a partitioning between (molecular) gas and solids that sets the chemical composition of planetary atmospheres. Icy objects, formed in the outer parts of disks, contain a record of the complex chemistry in the environment they formed in, and can be dynamically injected into the warm inner regions of disks, where rocky planets form. Temperatures and densities vary by many orders of magnitude between the diffuse ISM and the densest regions of planet forming disks, or the atmospheres of exoplanets. These variations are reflected in the amazingly rich chemistry that can be observed in these diverse environments. In this review, this rich variety will be discussed from an observational point of view.

# Measurements of dust optical constants at long wavelengths and low temperatures.

**H. Mutschke, C. Kranhold, D. Häßner, J. Greif, and P. Mohr**

*Astrophysical Institute and University Observatory, Friedrich Schiller University Jena, Schillergäßchen 2-3, 07745 Jena, Germany*

Most of the dust in the interstellar medium, in planetary systems, and in protoplanetary disks is cold and emits thermal radiation at far-infrared and sub-millimeter wavelengths. The emission efficiency of dust particles at these wavelengths, however, is quite poorly known for many possible constituent materials, especially at low temperatures.

In this talk, I will present a number of results from laboratory spectroscopy of, e.g., silicate minerals and glasses, amorphous carbonaceous materials, water ice, and iron sulfide, which have been obtained at AIU Jena within the last decade, often in collaboration with colleagues in Jena, at Univ. Cologne, and TU Braunschweig. These results are in many cases based on transmission spectroscopy of powders and I will discuss some problems related to the extraction of the materials' optical constants from such measurements.

For all the materials, we found a quite strong temperature dependence of the optical constants, i.e. a decrease of the extinction constant at low T with respect to room temperature. The physical mechanisms behind these effects are different, e.g. based on reduction of active phonons for crystalline materials, on semiconductivity for amorphous carbon, and on relaxation absorption for amorphous silicates. In some cases, the measured extinction constants and their T dependencies have been compared to predictions from corresponding models.

## References

- [1] H. Mutschke, P. Mohr, 2019, "Far-infrared continuum absorption of forsterite and enstatite at low temperatures", *Astron. Astrophys.*, 625, A61
- [2] D. Häßner, H. Mutschke, J. Blum, T. Zeller, B. Gundlach, 2018, "Laboratory measurements of the sub-millimetre opacity of amorphous and micro-particulate H<sub>2</sub>O ices for temperatures above 80 K", *MNRAS*, 481, 5022F

# Physical and chemical processes on interstellar ice and dust analogues: recent results at IEM-CSIC

B. Maté<sup>1</sup>, I. Tanarro<sup>1</sup>, V. J. Herrero<sup>1</sup>, M. Jiménez-Redondo<sup>1,2</sup>, R. Peláez<sup>1</sup>.

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<sup>2</sup>*Present address, Max Planck Institut für Extraterrestrische Physik, Gißenbachstraße 1, 85748 Garching, Germany*

In this talk I will show some selected results of our investigation over the last years at IEM-CSIC. First, motivated by recent identification of ammonium salts on comet 69P/C-G-C surface, I will present infrared spectra of  $\text{NH}_4^+$  salts on amorphous solid water, generated by hiperquenching of water solutions on cold surfaces **(1)**. Then, I will show the studies on infrared spectroscopy and survivability of some interstellar complex organic molecules on ices in astrophysical environments. We have provided IR spectra of glycine, methyl isocyanate, 2-amino-oxazole **(2)**, and urea in ices, with the goal to help the in the possible identification of these species in the solid phase with the JWST. The destruction of these molecules by the interstellar UV field or by cosmic rays were also estimated, To this aim, a  $\text{D}_2$  UV lamp and a 5 keV electron gun were used for the derivation of the relevant destruction cross sections. Finally, the dehydrogenation of hydrogenated amorphous carbon interstellar dust analogues induced by cosmic rays was investigated by processing carbonaceous deposits generated in our plasma laboratory with 5 keV electrons **(3)**. The binding energies of some volatile species on these carbonaceous dust surfaces were also explored **(4)**.

## References

- [1] B. Maté, O. Gálvez, V. J. Herrero, et al., ApJ **703**:L178-182 (2009)
- [2] B. Maté, R. Carrasco-Herrera, V. Timón, et al., ApJ **909**:123 (2021)
- [3] B. Maté, G. Molpeceres, M. Jiménez-Redondo, et al. ApJ **831**:51, 2016.
- [4] B. Maté, M. Jiménez-Redondo, R. J. Peláez, et al. MNRAS **490**, 2936 (2019)



# Refractive index and extinction coefficient of vapor-deposited water ice in the UV-Vis range

**J. He<sup>1</sup>, S. Diamant<sup>2</sup>, S. Wang<sup>2</sup>, H. Yu<sup>2</sup>, W. Rocha<sup>2</sup>, M. Rachid<sup>2</sup>, and  
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Laboratory results of the optical properties of vapor-deposited water ice, specifically the refractive index and extinction coefficient, are available mainly for a selective set of wavelengths and a limited number of deposition temperatures. Experimental limitations are the main reason for the lack of broadband data, which is unfortunate as these quantities are needed to interpret and predict astronomical and planetary observations. We address these lacking data, using an experimental broadband method that is capable of rapidly providing reliable water ice data across the entire UV-visible range [1]. This approach combines the simultaneous use of a monochromatic HeNe laser and a broadband Xe-arc lamp to record interference fringes of water ice during deposition at astronomically relevant ice temperatures. Analyzing the period and intensity patterns combining both the monochromatic and broadband interference patterns allows the determination of the wavelength-dependent refractive index and extinction coefficient. We present accurate refractive index and extinction coefficient graphs for wavelengths between 250 and 750 nm and ices deposited between 30 and 160 K. From our data, we find a possible structural change in the ice in the 110-130 K region that has not been reported before. We also discuss that the data presented in this paper can be used to interpret astronomical observations of icy surfaces.

## References

- [1] Kofman, V., He, J., Loes ten Kate, I., et al. 2019, ApJ, 875, 131.  
doi:10.3847/1538-4357/ab0d89

# Merging THz-TDS and FTIR data for direct reconstruction of CO dielectric properties

**F. Kruczkiewicz<sup>1,2</sup>, A. A. Gavdush<sup>3</sup>, B.M. Giuliano<sup>1</sup>, A. V. Ivlev<sup>1</sup>, T. Grassi<sup>1</sup>, B. Müller<sup>1</sup>, K. Zeytsev<sup>3</sup>, P. Theulé<sup>2</sup> and P. Caselli<sup>1</sup>**

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Dust plays an important role in the radiative transfer, thermal balance and chemistry, in various galactic and extragalactic regions. The observational data increasingly available in the millimeter and sub-millimeter range can be used to advance our knowledge about the gas and dust properties in star- and planet-forming regions. To properly interpret these observations, one needs to combine models, theory, and laboratory experiments and put all the pieces of the bigger context together. For example, we can measure the physical structure of cold and dense regions such as prestellar cores and protoplanetary disks by combining dust continuum observations in the mm and sub-mm with radiative transfer models, if the optical properties of ices are known. However, directly measured optical properties of astrophysical ice analogs in the infrared and terahertz (THz) range are missing from the literature. The interpretation of dust continuum emission measurements relies on calculated opacity values, such as those tabulated in Ossenkopf & Henning (1994) [1].

In this work we merge two techniques, the THz Time-Domain Spectroscopy (THz TDS) and Fourier Transform Infrared Spectroscopy (FTIR), to determine the optical properties of CO ice in a broad range of wavelengths. Thick CO ices are expected within prestellar cores (where CO catastrophically freezes out onto dust grains) and at the CO snow line of protoplanetary disks. We developed an algorithm to reconstruct the real and imaginary parts of the refractive index of ices from the Time-Domain THz data [2] and now we extend the frequency range by using FTIR data. The complex refractive index of CO ice was determined in the wavelength range 1mm – 16  $\mu$ m (0.3 – 18 THz) and compared with available data in the literature. These data are used to calculate the opacity of dust grains covered by a CO ice mantle. They will be useful to model sources that show a drastic CO depletion, such as prestellar cores and protoplanetary disks mid-planes.

## References

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- [2] B.M. Giuliano et al., *A&A* **629**, A112 (2019)

# Getting ready for JWST: introducing the new Leiden Ice Database and the ENIGMA fitting tool

Will R. M. Rocha and Harold Linnartz

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Given the upcoming launch of the James Webb Space Telescope (JWST), with hundreds of hours dedicated to observe ices in GO, GTO and ERS programs, the development of tools to interpret those data is needed. For example, databases focused on astrochemistry (e.g., CDMS [1]) have been crucial to derive the chemical properties of astronomical regions. In this context, we introduce here the upgrades on the Leiden Ice Database (LID; <https://icedb.strw.leidenuniv.nl/>), that has played for years an important role to interpret ice observations in space. The new LID hosts IR spectra (2.5-20  $\mu\text{m}$ ) and UV/vis optical constants (0.3-0.7  $\mu\text{m}$ ) of many different ice constituents (pure and mixed) and for a range of astronomically relevant temperatures. New online tools are introduced as well. These allow the calculation of the complex refractive index of ices and also the simulation of synthetic spectra towards protostars that are useful in astrochemical models. Next, we will present the ENIGMA (dEcomposition of Infrared Ice features using Genetic Modeling Algorithms) fitting tool. It aims for the unbiased decomposition of the protostellar spectrum by combining laboratory spectra of ices. As a proof of concept we will show the analysis of two protostars Elias 29 [2] and EC92 (Rocha et al. *subm*), and the tentative detections of  $\text{CH}_3\text{CH}_2\text{OH}$  and  $\text{CH}_3\text{CN}$  in ices.

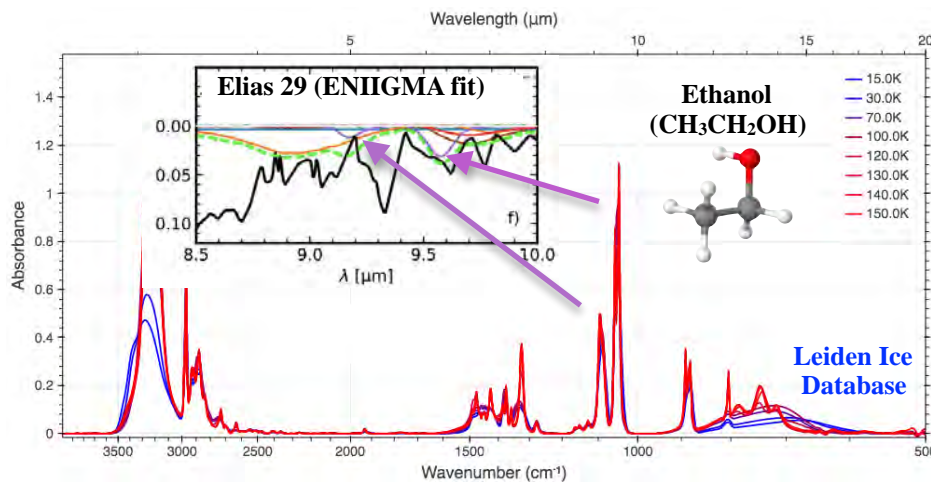


Fig. 1:  $\text{CH}_3\text{CH}_2\text{OH}$  ice spectra in the LID (Rocha et al. *in prep.*) and a global fit of the Elias 29 ISO (*Infrared Space Observatory*) spectra indicating two ethanol bands.

## References

1. Müller, H. S. P et al. *A&A*, **370**, L49 (2001)
2. Rocha et al. *A&A*, DOI: 10.1051/0004-6361/202039360 (2021)

# Photochemical Properties of Silicon Clusters: Bridging the Gap Between Diatomics and Grains

**O. Dopfer**

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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 radioastronomy. 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].

## References

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- [5] M. Förstel et al., J. Mol. Spectrosc. **377**, 111427 (2021)

# Helium-tagging spectroscopy as a tool for the identification of diffuse interstellar band carriers

M. Meyer<sup>1</sup>, A. Schiller<sup>1</sup>, P. Martini<sup>1,2</sup>, M. Gatchell<sup>1,2</sup>, F. Zappa<sup>1</sup>, S.A. Krasnokutski<sup>3</sup>, and P. Scheier<sup>1</sup>

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Messenger type spectroscopy of rare gas tagged ions is a powerful tool to investigate electronic or vibrational excitation of ions [1-5]. Helium nanodroplets containing typically at average several million He atoms are multiply charged via electron impact and doped with molecules or atoms of interest. Singly charged dopants or their clusters are extracted from the droplets either via evaporation of helium in a RF-collision cell filled with room temperature [6] He or by splashing of the droplets upon surface collisions. Depending on the conditions chosen, ions tagged with up to a few hundred He atoms are ejected. Photo dissociation of these weakly bound complexes leads to a strong increase of the bare dopant (cluster) ion which is a measure for the absorption cross section of these ions. The depletion of individually tagged ions provides information on the matrix shift from a single He atom to the bulk value of liquid He [5]. Quantum chemical simulations, such as path integral molecular dynamics calculations are performed to unravel the structure of solvation layers of He [7]. Results will be presented for C<sub>60</sub> [5] and various polycyclic aromatic hydrocarbons [8,9].

This work was supported by the Austrian Science Fund FWF (projects P31149, and I4130), the Deutsche Forschungsgemeinschaft DFG (grants No. KR 3995/4-1) and the Swedish Research Council (contract No. 2016-06625)

## References

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- [6] L. Tiefenthaler, *Rev. Sci. Instrum.* **91**, 033315 (2020)
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- [9] M. Meyer, *Astrophys. J.* **913**, 136 (2021)

# Astrochemically-Relevant Silicon Carbide Clusters: Photodissociation and Electronic Properties

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

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The occurrence of molecules in a given region of interstellar space is strongly dependent on the conditions and the abundance of elements in that particular region. In the outer layers of carbon stars like IRC+10216, carbon is more abundant than oxygen ( $C/O > 1$ ). The excess carbon can thus form a variety of other carbon-bearing molecules. We focus our research on silicon carbide (SiC) molecules. Small SiCs like SiC [1], Si<sub>2</sub>C [2], SiC<sub>2</sub> [3], SiC<sub>3</sub> [4] etc. have already been identified in the circumstellar medium around IRC+10216 by radioastronomy. Another emission feature in the IR spectrum of IRC+10216 is attributed to  $\mu\text{m}$ -sized SiC dust grains [5]. We employ photodissociation spectroscopy of mass-selected cryogenic ions in a tandem mass spectrometer coupled to a laser vaporization source, along with density functional theory (DFT) calculations, to obtain a better understanding of the potential link between small SiC molecules and large SiC dust grains as well as the photochemistry of potential intermediate species and dust precursors. In this contribution, we give an overview of the results of our experimental investigation of the photofragmentation of various cationic SiC clusters and compare them with our computational results. Furthermore, we present ground-state structures of cationic SiCs found via a global optimization algorithm and present the recently published first optical spectrum of Si<sub>4</sub>C<sub>2</sub><sup>+</sup> recorded by photodissociation spectroscopy [6].

## References

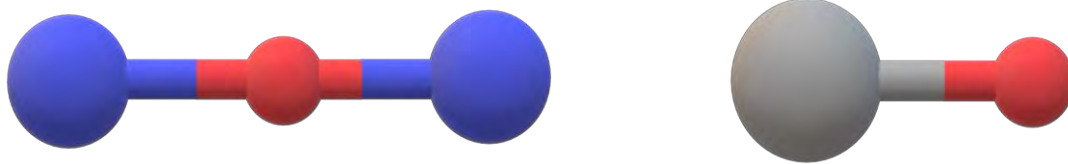
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# High resolution IR spectroscopy on small metal bearing molecules

**E. Döring<sup>1</sup>, D. Witsch<sup>1</sup>, L. Blum<sup>1</sup>, A.A. Breier<sup>1</sup>,  
T.F. Giesen<sup>1</sup>, G.W. Fuchs<sup>1</sup>**

*<sup>1</sup>Universität Kassel, Kassel, Deutschland*

The molecule and dust formation in late-type stars is still not entirely understood. Since cosmic dust forms via nucleation processes in the close vicinity of evolved stars, the investigation of small di- and triatomic molecules can help elucidating the first steps of dust formation. Especially molecules made of refractory elements are thought to act as seed molecules for dust grains, since they form molecules at an early stage when temperatures are still well above thousand Kelvin. With high-resolution IR instruments like TEXES at IRTF and EXES onboard SOFIA new insights into the chemistry of the warm regions around stars are given. In this work ro-vibrational spectra of small metal bearing molecules around 10  $\mu\text{m}$  are investigated. We recorded absorption spectra of linear dialuminum monoxide (Al-O-Al) and vanadium oxide (VO) by using a frequency modulated quantum cascade laser in combination with Herriott-type multipass optics. The molecules are produced by a laser ablation process resulting in an ablation plume which is purged with a N<sub>2</sub>O/He buffer gas mixture that subsequently undergoes an adiabatic expansion into a vacuum chamber. Due to this adiabatic expansion the molecules are rotationally cooled down to around 120 K. The here presented transition frequencies will allow for astrophysical searches of these molecules in space.

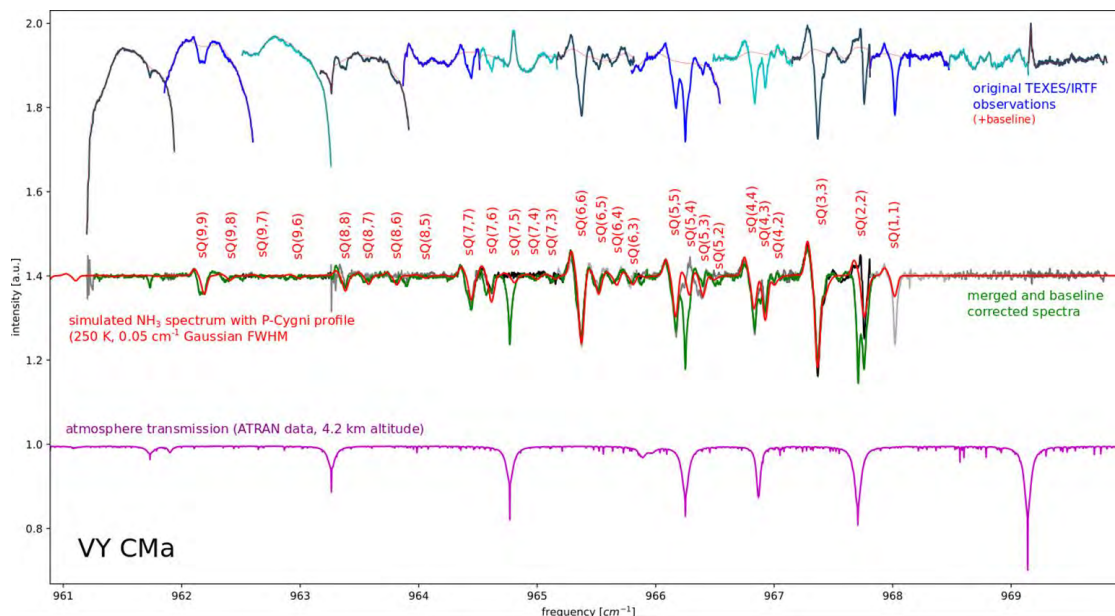


# Mid-Infrared Observations of Late-type Stars at High Spectral Resolution

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Stars on the asymptotic giant branch (AGB) and red super giants are thought to be a major source of interstellar dust. The dust formation process in the envelope surrounding these stars, especially M- and S-type stars, is still not well understood, but is most likely driven by small molecules formed from refractory material like metal, carbon, or silicon. To better understand the chemical composition of gas-phase species in these environments molecules are observed at mid-infrared wavelengths, i.e. at the typical IR fingerprint region, at high spectral resolution. In that way, possible pathways to dust formation can be found via the detection of molecular intermediates. We will present observations of late-type stars using the TEXES spectrograph on the infrared telescope IRTF. We have investigated typical molecules like SiO and NH<sub>3</sub> to learn about the abundance, dynamics and distribution of these species, but also to look for new yet undetected molecules in these environments. Driven by own laboratory investigations on TiO, VO and Al<sub>2</sub>O astrophysical searches for these molecules will be discussed.



Ammonia transitions at IR wavelengths observed towards VY Canis Majoris using TEXES/IRTF.



# Study of low-temperature ion-neutral interactions in a 22-pole ion trap

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Radio-frequency traps are very useful tools for the study of astrochemical processes. They allow the storage of charged particles for long times, during which they can interact with photons, electrons or neutral species [1]. Ion traps can be used to study the ion-neutral processes prevalent in interstellar environments, and, with cryogenic cooling, temperatures close to those found in such regions can be achieved. In this work, a 22-pole cryogenic trap is used to confine ions produced in an electron impact storage ion source with a quadrupole mass selector, and ion detection is carried out with a second quadrupole mass spectrometer and a channel electron multiplier.

The aim of this work is to investigate collisions of  $H^+$  ions with  $H_2$  at a temperature of  $\sim 15$  K in order to study the proton exchange reaction leading to the ortho-para conversion of the molecule. In this process, which is expected to be dominant compared to the inverse at low temperatures [2], the nascent ion gains a translational energy of 0.015 eV, which can be enough to allow it to leave the trap with careful selection of the voltages of the ring electrodes. The results show that ions leave the trap faster as the density of molecular hydrogen is increased. Further experiments with different neutral species show that the effect of the gas density in the trap on the ion extraction should not be disregarded.

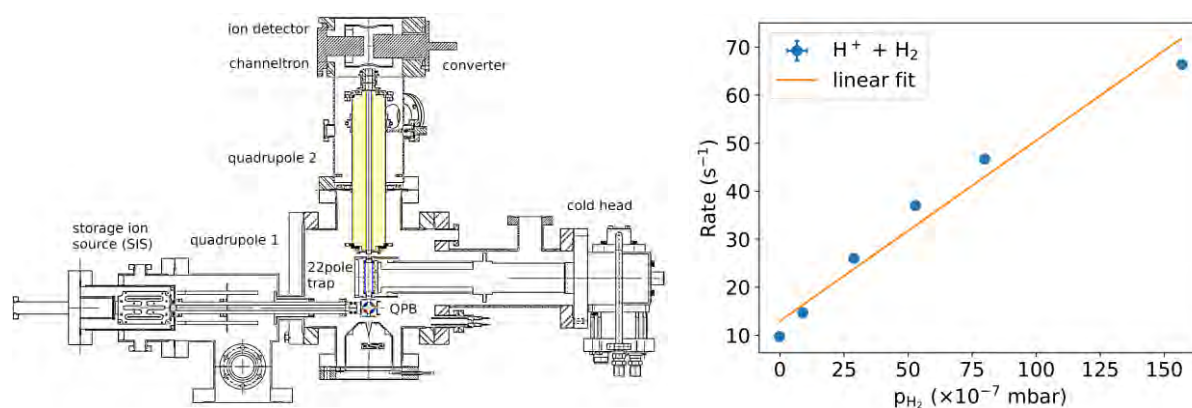


Figure 1. Left panel: diagram of the experimental setup. Right panel: measured process rate as a function of  $H_2$  pressure for  $H^+ + H_2$  collisions.

*The authors acknowledge Dieter Gerlich, who greatly helped in the construction of the ion trap at MPE and for his inspiring discussions, which still resonate among us.*

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# High-Resolution Gas-Phase Spectroscopy for Astrophysics at CAS@MPE

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The Center for Astrochemical Studies at the Max Planck Institute for Extraterrestrial Physics is build around three subgroups tightly connected to each other, with focus on observations, theory, and laboratory research.

In the present talk an overview of the experiments and techniques used to obtain high-resolution rotational and ro-vibrational spectra of molecular species of astronomical interest will be presented. Some example of recent results will be also briefly reviewed, including updates on the hardware and the spectroscopy of complex organic molecules. Finally, the future planning of our laboratories will be addressed.

## **Abstracts. Day two**

# Astrophysical origins of biomolecular homochirality

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'How did life choose its handedness?' Just like our hands mirror each other, but cannot be superimposed on each other, amino acids and sugars exist in left- and right-handed forms. Even if there appears to be no biochemical reason to favor one enantiomer over the other, life on Earth uses almost exclusively *left-handed* amino acids and *right-handed* sugars. This is called biological homochirality and it is inevitable for building functional proteins and RNA/DNA. Numerous experiments have confirmed that simple prebiotic molecules could have been synthesized both in space as well as on the early Earth. However, the preferential selection of one enantiomer over the other remains to date most likely explained by asymmetric interactions of stellar ultraviolet circularly polarized light (UV CPL) with chiral organics. The astrophysical origin of homochirality is strengthened by *i*) the detection of L-enriched amino and D-enriched sugar acids in meteoritic samples, *ii*) the detection of CPL in several star-forming regions as well as *iii*) experiments studying the interaction of UV CPL with prebiotically relevant chiral species. In this talk, I will highlight significant results on electronic circular dichroism/anisotropy spectroscopy as a key tool to decipher the response of chiral molecules to UV CPL. Moreover, I will present our major findings on recent asymmetric photo-synthesis/photolysis experiments to discuss whether stellar UV CPL could have induced a common chiral bias across molecular families?

Support by the European Research Council under the EU's HORIZON 2020 research & innovation programme [grant agreement 804144] is gratefully acknowledged.



# Soft X-ray irradiation of bilayered ice mantles: photo-desorption and diffusion

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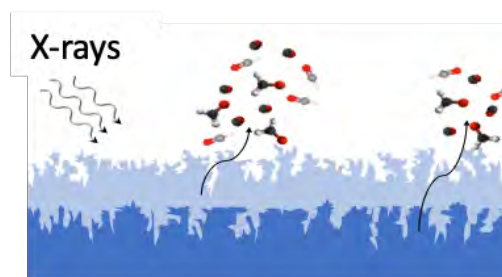
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X-rays from young solar-type stars are thousands of times higher than today's sun. Such energetic radiation can penetrate into the outer regions of a protoplanetary disk, with chemical implications, so far, relatively unexplored. Such a copious energy transfer must have played an important, perhaps crucial role in the synthesis and selection of organic prebiotic molecules in protoplanetary discs. Since all the species in the inventory of interstellar ices have different condensation temperatures, the information delivered by ice band absorption profiles can be interpreted as the ices were organized in a bi-layered structure of segregated components.

We consider a stratified ice composed of a H<sub>2</sub>O:CH<sub>4</sub>:NH<sub>3</sub> mixture, covered by a layer made of CH<sub>3</sub>OH and CO simulating a "realistic" evolved ice mantle, and we have irradiated it with synchrotron soft X-rays ranging from 250 to 1250 eV.

The photo-products found desorbing from both ice layers to the gas phase during the irradiation converge with those detected in higher abundances in the gas phase of protoplanetary disks, providing important insights on the nonthermal processes that drive the chemistry in protoplanetary discs. The irradiation induces diffusion within the ice at very low temperatures, leading to an efficient mixing of the ice molecular content. Such molecular dynamics facilitates chemical reactions from which complex organic species can be formed. Diffusion also drives the desorption of species that would otherwise remain buried near the silicate/carbon dust nucleus<sup>[1]</sup>.



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# Formation of N-heterocycles and S-chains in UV-photoprocessed interstellar ice analogs

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Certain N-heterocycles can be made by irradiation of interstellar ice analogs, among them are species of astrobiological interest related to biological cofactors and nucleobases<sup>1,2</sup>. S-chains are a possible reservoir of the missing sulfur which is likely depleted in interstellar dust. Recent work on the synthesis of the simplest N-heterocycles will be presented. Methylamine is a precursor of hexamethylenetetramine (HMT, (CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub>), an abundant photoproduct in interstellar ice analogs with mass 140 amu and a beautiful cage-structure. For this study we compare the better known irradiation products of H<sub>2</sub>O:CO/CH<sub>3</sub>OH:NH<sub>3</sub> ice to those formed by irradiation of methylamine (CH<sub>3</sub>NH<sub>2</sub>), either pure or mixed with H<sub>2</sub>O in the ice. In these experiments, it was possible to monitor the formation sequence of the simplest N-heterocycles<sup>3</sup>. Similarly, in our study of sulfur photochemistry, we followed the formation of S-chains produced from irradiation of H<sub>2</sub>S molecules in the ice. Monte Carlo simulations served to reproduce the experimental results and permitted an extrapolation to the real astrophysical scenario. It is proposed that S<sup>+</sup> in translucent clouds contributes to S depletion in denser regions by forming long S-chains on dust grains. In comets, the S<sub>2</sub> to S<sub>4</sub> molecules are probably made by UV-photoprocessing of H<sub>2</sub>S-bearing ice in molecular clouds, or from short S chains formed during the translucent cloud phase<sup>4</sup>.

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# Formamide formation in H<sub>2</sub>O-rich and CO-rich interstellar ice analogs

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Formamide (NH<sub>2</sub>CHO) is one of the most observed N-bearing complex organic molecules (COMs) toward various star-forming regions and comets [1]. This simplest amide (-HNCO-) species has been suggested to be a key ingredient forming nucleobases. Several laboratory studies have shown an efficient solid-state route (i.e., NH<sub>2</sub>+HCO) to form formamide on dust grains [2]. However, they have often questioned whether such radical-radical reactions are still valid in an interstellar H<sub>2</sub>O-rich environment, given the stronger binding/diffusing barrier expected on water surfaces. This work experimentally investigates the formamide formation following the proposed reactions in astronomically relevant H<sub>2</sub>O-rich and CO-rich ice compositions upon energetic vacuum UV-photons (VUV) impact under molecular cloud conditions. The experimental results obtained from FTIR spectroscopy and QMS-TPD spectrometry show that the photolysis of CO:NH<sub>3</sub> ice mixtures with/without H<sub>2</sub>O at 10 K results in several N-bearing products, including formamide, isocyanic acid (HNCO), and aminomethanol (NH<sub>2</sub>CH<sub>2</sub>OH). The kinetic analysis suggests that the final product composition depends on interstellar ice ratios and compositions (see Figure 1), and explicitly, formamide yield is favored in H<sub>2</sub>O-rich ice.

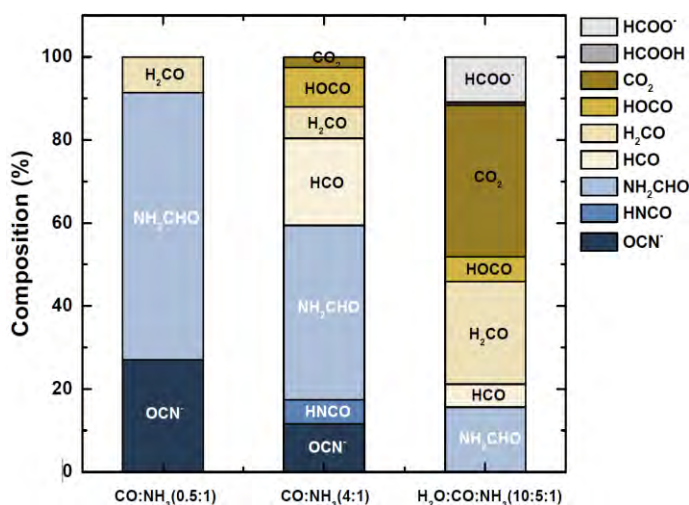


Figure 1. Product composition obtained after the VUV irradiation of CO:NH<sub>3</sub> (0.5:1), CO:NH<sub>3</sub> (4:1), and H<sub>2</sub>O:CO:NH<sub>3</sub> (10:5:1) for a fluence of 8.2E17 photons cm<sup>-2</sup> at 10 K.

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# Energetic processing of methanol-rich ices

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Frozen methanol is detected in various sources in the ISM, with abundance up to 30 % with respect to water [1]. Frozen methanol is also detected in the outer Solar System, on the surfaces of the Centaur Pholus, the Trans-Neptunian Object VE95, and on the kuiper-belt object Arrokoth [2]. Such small bodies formed by accreting the materials present in the outer Solar cloud and thus they are expected to preserve information on its physico-chemical properties. Small bodies in the outer Solar System are also characterized by the red colour of their surfaces, possibly due to the presence of complex organic materials. Such organic materials could have been inherited from the solar cloud or could have formed later on, thanks to the interaction with cosmic rays and solar particles, and favoured by thermal processing [3, 4].

I will present recent results obtained in laboratory experiments to simulate the ion bombardment and the subsequent warm-up of methanol-rich frozen surfaces in space. Ices exposed to ion bombardment are analysed by means of FT-IR, and the spectroscopic data are compared to astronomical observations to obtain information on the extent of processing experienced by frozen surfaces.

We also warm-up the irradiated ices to produce organic residues. Residues are analysed by means of very high-resolution mass spectrometry to study their chemical composition and their high molecular diversity, including the presence of astrobiologically-relevant compounds.

We find that the amount of processing experienced by a frozen surfaces determines the composition of the residue and thus of the organic materials in the ism as well as in the outer Solar system.

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# Exploring silicon chemistry in the electrical discharge of methyl phenyl silane (MPS) using chirped-pulse Fourier-transform microwave spectroscopy.

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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. The first interstellar silicon was detected in 1971 in the form of SiO, towards Sgr B2 [1]. Since then, more than 15 silicon containing molecules have been detected in various regions of the interstellar medium (ISM), and constitute approximately 7% of the total number of molecules detected in space, to date [2].

Electrical discharge sources coupled with chirped pulse Fourier transform microwave spectroscopy have proved to be a great tool to produce in situ molecular ions, radicals, long chains and ring structures of molecules of astronomical interest. In this work, we investigate the electrical discharge chemistry of methyl phenyl silane (C<sub>7</sub>H<sub>10</sub>Si), with the aim of studying the incorporation of silicon in the framework of complex organic molecules (COMs). The new species formed in the electrical discharge of MPS are probed using the Hamburg COMPACT spectrometer in the 2-12 GHz frequency regime [3]. The newly formed species can be assigned with rotational parameters required for interstellar searches with various radio telescopes like the Radio Telescope Effelsberg and Jansky Very Large Array (JVLA).

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# The role of ion reactions in the build-up of complex organic molecules

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Among the multitude of molecules detected in space and in the atmospheres of planets, including our own, ions have been known to play an important role<sup>1,2</sup>. During the processes of star formation and evolution ion reactions of have been invoked as intermediate steps in the build-up of complex organic molecules (COMs)<sup>3</sup>, which can function as missing link in the formation of prebiotic molecules. Such biomolecule precursors can be delivered to planetary surfaces by accretion as well as comet and asteroid impacts and act as starting points for the formation of the building blocks of life. In addition, a multitude of ions including protonated nitriles and other nitrogen-containing compounds have been observed by the Cassini Plasma Spectrometer (CAPS) and the Ion and Neutral Mass Spectrometer (INMS) in the atmosphere of the Kronian satellite Titan.<sup>4</sup> It is therefore necessary to investigate possible formation and destruction pathways of these complex species in the interstellar medium and planetary atmospheres. With increasing complexity, also isomerism of ions gains importance and the different behaviour of isomers of ions upon chemical reactions has to be studied. During the last years, ion traps and guided beam devices have been successfully employed to investigate ion-neutral processes. We investigated the chemical reactions of isomers of nitrogen-containing ions using guided beam machines and their vibrational spectra using infrared photodissociation spectroscopy in a cold ion trap. The role of these species in the build-up of COMs in the interstellar medium and planetary ionospheres is discussed.

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# From supervolatiles to refractories: the composition of 67P/Churyumov-Gerasimenko

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Five years after the end of the mission, data analysis for the ROSINA mass spectrometer on Rosetta is still ongoing. By now, more than 77 parent molecules have been identified in the cometary coma [1], ranging from the highly volatile N<sub>2</sub>, Ar, CO and CH<sub>4</sub> to semi-volatiles like NH<sub>4</sub>Cl [2]. Data taken during dusty periods around perihelion reveal a wealth of organic hydrocarbons, pure and heteroatomic species like e.g. naphthalene and benzoic acid. The average elemental abundance of these organics (normalized to C) C<sub>1</sub>H<sub>1.56</sub>O<sub>0.134</sub>N<sub>0.046</sub>S<sub>0.017</sub> compares very well with the results from the Rosetta dust mass spectrometer COSIMA [3] except for the higher H/C ratio, which implies a connection between these two reservoirs. If they are connected by a bottom up or top down mechanism is not clear. The abundance is also very similar to what has been found in the Saturn rings [4].

Another surprising detection are refractory elements in the coma of 67P, namely Na, Si, S, Ca, K and Fe [5]. While these elements are clearly detected with our gas mass spectrometer, albeit some only during very specific times (e.g. Fe), no parent molecules, which could explain these elements, have been found. While sputtering from the nucleus by solar wind was suspected early in the mission, the fact that these elements are found during perihelion passage, where solar wind is heavily attenuated at the position of the comet and S/C, makes this explanation questionable. The question remains if such refractory elements can stick to nanograins and be released when these grains heat up in the coma.

Direct impacts of grains into the ROSINA mass spectrometer yield further information on the nature of these cometary grains. This is work in progress and will be discussed.

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# Fragmentation Dynamics of Fluorene, on Femtosecond Timescales

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Polycyclic aromatic hydrocarbons (PAHs) are an important class of astrochemical relevant molecules, constituting more than 20% of the total galactic carbon. Recently, substituted PAHs were identified in interstellar molecular clouds and their formation mechanisms are yet to be unraveled [1]. In order to understand the chemical processes occurring in the interstellar medium (ISM), studying the fragmentation dynamics of these molecules is crucial.

Our experiments investigated the fragmentation dynamics for the PAH, fluorene ( $C_{13}H_{10}$ ). Electronic relaxation for this molecule happens on femtosecond (fs) time scales. To investigate it, we employed pump-probe spectroscopy with 30.3 nm XUV photons from a free electron laser (FEL) and 400 nm UV photons by doubling the output of a table-top Ti:Sa laser. The experiments were performed at the Free-Electron Laser in Hamburg using the CAMP endstation [2].

Using FEL - 400 nm as pump-probe lasers, the formation of fluorene dication and its subsequent dissociation via the reaction  $C_{13}H_{10}^{2+} \rightarrow C_3H_x^+ + C_{10}H_y^+$  could be observed. The momentum profiles as a function of pump-probe delay values are presented in the figure below. The two monocation fragments clearly have the same momentum in the region marked between the white lines, demonstrating their simultaneous formation. Besides, discussing the fragmentation dynamics of fluorene, I will also present the comparison between probing the molecules with two different wavelength 400 nm and 810 nm while using FEL (XUV photons, 30.3 nm) as pump for both conditions. More detailed insights will be presented in the poster.

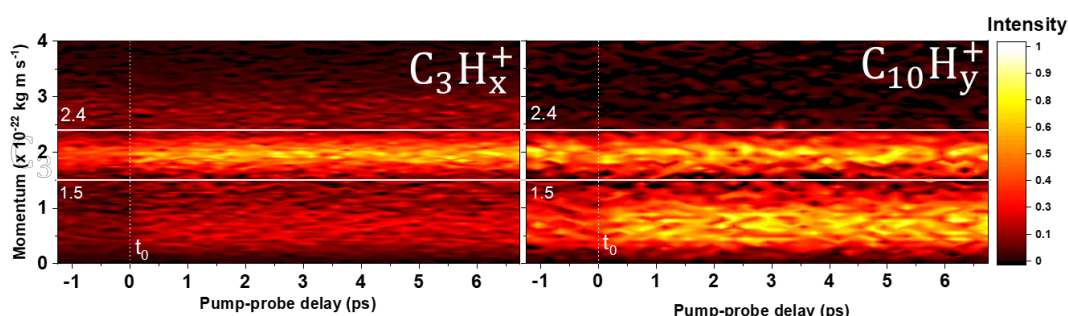


Figure: Pump-probe delay dependent momentum distribution of fluorene fragments,  $C_3H_x^+$  and  $C_{10}H_y^+$ . The subscripts x and y are the number of hydrogens involved and the  $t_0$  is the time when pump-probe laser hits the molecule at the same time.

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## **A novel UHV setup with MALDI- high resolution mass spectrometry for the in-situ detection of biomolecules**

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Over the last two decades, laboratory astrochemistry has played an immense role in elucidating how some of the complex organic molecules (COMs) are formed from simple molecular ice in the coldest depths of dense molecular cloud. Much of the chemistry in the solid state is driven by the exposure to external star radiation. Organic molecules continue to evolve as interstellar material transit from molecular clouds to planetary systems. A deeper understanding of the physical and chemical processes involved in the formation and evolution of prebiotic COMs may provide valuable insights into the origins of life. To this end, we have designed a novel ultra-high vacuum setup with a cryostat to mimic the cold extraterrestrial environments wherein single and multicomponent ices will be processed by energetic electrons or UV photons in a controlled fashion. We will use quadrupole mass spectrometer and Infrared spectroscopy to monitor changes in the ice matrix. In addition, we will also employ a tunable ns-IR laser to first desorb and then a ns-UV laser to ionize biomolecules produced in the ice mixture. The ions will then be guided to a very high resolution Orbitrap mass spectrometer for in situ detection. This set up will allow us to characterize in real time the solid state evolution of astrophysically relevant ice mixtures upon energetic processing. At the end of the processing experiments, the organic residue on the sample, after warming up to room temperature, will also be analysed in solution by the same orbitrap mass spectrometer ex situ. The work of the Origins of Life laboratory will provide crucial data to the astrochemical and astrophysical community.

# Optical Properties of Simple Diamondoid Cations and Their Astrochemical Relevance

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Diamondoids are a class of highly stable, aliphatic cycloalkanes arranged into cage-like structures by  $sp^3$  hybridization of the carbon atoms. Members of the astrochemical community have demonstrated similarities between the IR spectra of diamondoids and unidentified infrared emission bands seen in the spectra of young stars with circumstellar disks [1,2]. Due to their low ionization energy and absorption in the visible range, it is also suggested that the radical cations of these molecules might be responsible for features in the long-known but largely unassigned diffuse interstellar bands [3]. However, the optical spectra of these cations have not been measured experimentally in the laboratory, which is required for astronomical identification. To this end, we present here the first optical spectra of the two simplest diamondoid radical cations, namely the adamantane ( $C_{10}H_{16}^+$ ) and diamantane ( $C_{14}H_{20}^+$ ) radical cations [4]. These spectra were recorded in the gas phase by means of photodissociation spectroscopy using a cryogenic 22-pole ion trap (operated at 5 K) coupled to a tandem mass spectrometer and an electron ionization source. Both spectra reveal broad features that are attributed to significant lifetime broadening and Franck-Condon congestion. Geometric changes due to Jahn-Teller distortion, photodestruction processes, and the astrophysical implications of these ions will also be discussed.

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# Small $\text{Si}_n\text{O}_m^+$ Clusters - Photodissociation & Optical Absorption Properties

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Interstellar dust contains a large amount of  $\mu\text{m}$ -sized silicate particles. The origin as well as the evolutionary formation mechanisms of this dust, which eventually forms stars and solar systems like our own, is still poorly understood. A possible starting point to form large silicate particles are silicon and oxygen containing molecules. However, only silicon monoxide (SiO) has been identified in the interstellar medium (ISM) so far [1] and no information is available for larger molecules and the ions.

Here we present both, experimental data and quantum chemical calculations, that help to understand the photodissociation and optical absorption behavior as well as structures and energies of possible silicon and oxygen containing molecules that are potential precursors dust particles. The experimental approach relies on mass spectrometry and resonant photodissociation of cryogenic and size-selected  $\text{Si}_n\text{O}_m^+$  clusters 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. Initial data provide information about (competing) fragmentation channels, their appearance energies and branching ratios, as well as the abundance and stability of neutral fragments. Additionally, we present the first optical absorption spectrum of  $\text{Si}_3\text{O}_2^+$ , which we could measure via photodissociation [2]. Also, these spectral results are compared to quantum chemical calculations and discussed in an astrophysical context.

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# Sensitivity of gas-grain chemical models to surface reaction barriers:

Effect from a key carbon-insertion reaction,  $C + H_2 \rightarrow CH_2$

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We study the sensitivity of gas-grain chemical models to the energy barrier of the key surface reaction  $C + H_2 \rightarrow CH_2$ . We used the gas-grain code ALCHEMIC to model the time-dependent chemical evolution over a 2D grid of densities ( $n_H$  in  $[10^3, 10^{12}]$   $\text{cm}^{-3}$ ) and temperatures ( $T$  in  $[10, 300]$  K), assuming UV-dark ( $A_V = 20$  mag) and UV-irradiated ( $A_V = 3$  mag) conditions that are typical of the dense interstellar medium. We considered two values for the energy barrier of the surface reaction,  $E_a = 2500$  K (as originally implemented in the networks) and  $E_a = 0$  K (as measured in the laboratory and computed by quantum chemistry simulations). We find that if the  $C + H_2 \rightarrow CH_2$  surface reaction is barrierless, a more rapid conversion of the surface carbon atoms into methane ice occurs. Overproduction of the  $CH_n$  hydrocarbon ices affects the surface formation of more complex hydrocarbons, cyanides and nitriles, and CS-bearing species at low temperatures  $\lesssim 10$ -15 K. The surface hydrogenation of CO and hence the synthesis of complex organic molecules become affected as well. As a result, important species whose abundances may change by more than a factor of two at  $t = 1$  Myr include atomic carbon, small mono-carbonic ( $C_1$ ) and di-carbonic ( $C_2$ ) hydrocarbons,  $CO_2$ , CN, HCN, HNC, HNCO, CS,  $H_2CO$ ,  $H_2CS$ ,  $CH_2CO$ , and  $CH_3OH$  (in the gas and/or ice phase). The abundances of other key species such as CO,  $H_2O$ ,  $N_2$  as well as O,  $HCO^+$ ,  $N_2H^+$ ,  $NH_3$ , NO, and most of the S-bearing molecules remain barely unaffected by this change.

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# Revealing the chemistry of polycyclic aromatic hydrocarbons by plasma sources

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Polycyclic aromatic hydrocarbons (PAHs) are considered to dominate the unidentified infrared bands (UIRs) - infrared emissions, which are characteristic of the vibrational modes of aromatic species and which have been detected in many circumstellar and interstellar objects. PAHs are thought to incorporate a large fraction of the galactic carbon budget (10 to 25%) and play an extensive and ubiquitous role in interstellar chemistry. Despite their importance, the formation and destruction of PAHs, as well as their reactivity with other interstellar molecules under the harsh conditions of the ISM remain relatively unexplored.

To look at these processes in the laboratory, we have coupled an electrical discharge nozzle with chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy in the 2-12 GHz frequency range. Under plasma conditions, PAHs are expected to undergo fragmentation processes and/or a recombination chemistry. The formed species are then unambiguously identified via their unique microwave signatures.

Using this technique, we investigate PAHs of different size, shape, and degree of aromaticity to understand how these different properties can influence the plasma chemistry.

Herein, we present our results obtained from electrical discharge experiments on the PAHs naphthalene (C<sub>10</sub>H<sub>8</sub>) and phenanthrene (C<sub>14</sub>H<sub>10</sub>), both pure and in mixture with acetonitrile (CH<sub>3</sub>CN), a simple nitrogen-containing interstellar molecule. Most of the molecules that we have observed, such as the two isomers of cyanonaphthalene, have been already detected in the TMC-1. This suggests that the species generated in our experiments could be used as a basis for chemical investigation in TMC-1 and other interstellar clouds.

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# Astrochemistry at the Cryogenic Storage Ring

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The Cryogenic Storage Ring (CSR) [1] at the Max Planck Institute for Nuclear Physics in Heidelberg is the largest electrostatic storage ring project in the world. The CSR combines electrostatic ion optics with extreme vacuum and cryogenic temperatures. The storage ring has a circumference of 35 m, and all deflectors are housed in experimental vacuum chambers that can be cooled down to 5K. It has been shown that within a few minutes of storage inside the CSR infrared-active molecular ions (e.g., CH<sup>+</sup>, HeH<sup>+</sup> and OH<sup>-</sup>) cool to their lowest rotational quantum states by spontaneous emission of radiation.



Equipped with an ion-neutral collision setup and a low-energy electron cooler, the CSR offers unique possibilities for astrochemical experiments under true interstellar conditions. We will present an overview of the capabilities of the CSR, along with experimental results on collision experiments between cold molecular ions and free electrons [2], photons [3,4], and neutral atoms [5], yielding quantum state-selective rate coefficients for astrophysically important processes.

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# Preparations for experiments with triatomic hydrogen ions at the Cryogenic Storage Ring

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The triatomic hydrogen ion  $H_3^+$  is one of the most important molecules in astrochemistry. As an active proton donor, it initiates important reaction chains in cold interstellar clouds, which contribute to processes like deuterium fractionation and the onset of organic chemistry in space. In particular, the electron recombination of  $H_3^+$  has received a lot of attention, owing to the influence of its rate coefficient on the ionization balance of interstellar chemistry networks.

We will present current efforts to understand the cooling behavior of  $H_3^+$  and  $H_2D^+$  inside the Cryogenic Storage Ring (CSR), and the preparation of laser diagnostic schemes and dedicated ion sources for future studies.

# Sneaking into the astrochemistry of chlorine: Gas-phase IR action spectroscopy of $\text{CH}_2\text{Cl}^+$ and $\text{CH}_3\text{ClH}^+$

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Halogen-bearing molecules are known to be present in the interstellar medium. In this environment one of the key molecules is  $\text{CH}_3\text{Cl}$  which is predicted to form via gas-phase reactions of chloromethyl cation,  $\text{CH}_2\text{Cl}^+$ , and protonated methyl chloride,  $\text{CH}_3\text{ClH}^+$ . However, so far, no experimental vibrational or rotational gas-phase spectra of these two molecular ions are known, which are prerequisite for astronomical detection.

Here, we present first experimental gas-phase IR spectra of both,  $\text{CH}_2\text{Cl}^+$  and  $\text{CH}_3\text{ClH}^+$ , obtained using the FELion 22-pole ion trap experiment connected to the Free Electron Laser for Infrared eXperiments (FELIX) at Radboud University, Nijmegen.

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# Rotational action spectroscopy of $\text{CN}^+$ , $\text{CH}_2\text{NH}_2^+$ and $\text{CH}_3\text{NH}_3^+$

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The pure rotational spectra of the elusive  $\text{CN}^+$  [1],  $\text{CH}_2\text{NH}_2^+$  [2] and  $\text{CH}_3\text{NH}_3^+$  [3] cations have been observed in their singlet electronic ground states using a cryogenic ion trap apparatus and applying action spectroscopy schemes. Due to the cryogenic cooling to a nominal temperature of 4 K only the lowest few rotational transitions have been observed. In each case, the hyperfine structure is dominated by the quadrupolar nucleus  $^{14}\text{N}$  ( $I=1$ ), but could only be resolved for the  $\text{CN}^+$  cation. The lower figure shows overview scans of the lowest three rotational transitions of  $\text{C}^{14}\text{N}^+$  displaying the mentioned hyperfine splitting. The new measurements and the derived predictions of pure rotational transitions will enable the first radio-astronomical search for these species.

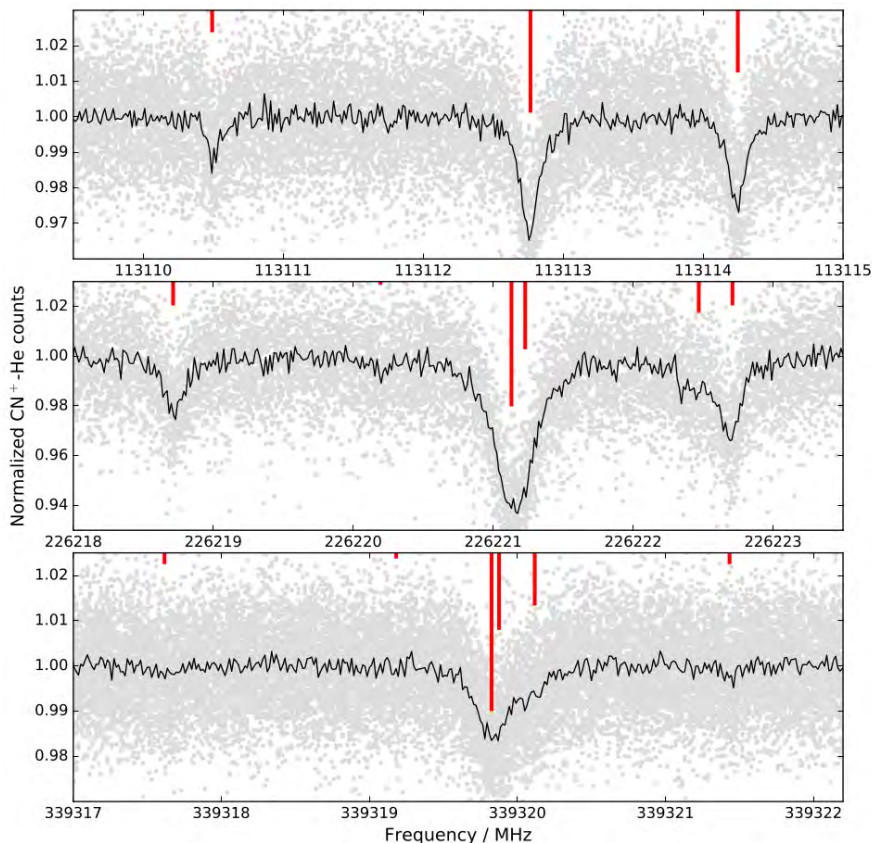


Figure 1: Overview scans of the lowest three rotational lines of  $\text{C}^{14}\text{N}^+$ , exhibiting hyperfine splittings.

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# Atomic and molecular clusters embedded in helium nanodroplets

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In this contribution, a new experimental setup will be discussed which enables mass spectrometry and laser spectroscopy of molecular ions of astrophysical and biological interest in a well-defined and ultracold environment. The setup, visible in figure 1, consists of an electrospray ionization source (ESI) and a helium nanodroplet (HND) source in combination with a time-of-flight mass-spectrometer. Fragile molecules which are produced with an ESI are captured by traversing HNDs. The latter are transparent from the deep UV to the far IR and serve as gentle matrices to provide a cryogenic environment, reducing the number of populated quantum states and freezing out structural fluctuations of the embedded molecules. A preliminary version of the setup was used to study the stabilization of  $\text{SF}_6^+$  [1] as well as neon cluster ions [2] in HNDs and will be discussed in this contribution.

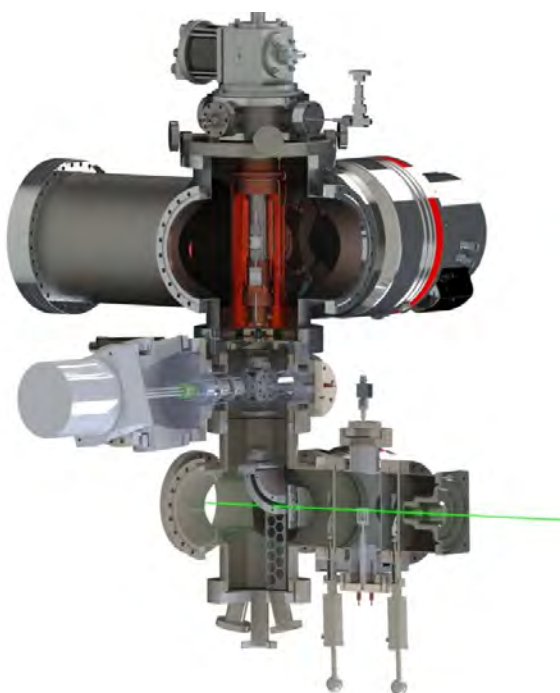


Figure 1: Rendering of the experimental setup. The colored parts are used for the first measurements, the grey parts are now in construction.

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# LLWP – A new Loomis-Wood Software at the Example of Propanone-<sup>13</sup>C<sub>1</sub>

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Spectra of complex molecules are dense and complicated, especially if isotopologues, low-lying vibrationally excited states, hyperfine structure or other interactions are present. Analysis of these spectra can be difficult due to line confusion. One approach to accommodate this challenge are Loomis-Wood plots (LWPs), which are a visual aid for displaying series of transitions in a spectrum in order to ease assignments. Programs utilizing LWPs exist already in the literature, e.g. AABS [1], Pgopher [2] and LWW [3]. Here, we present a newly developed software which focuses on being intuitive and user friendly while simultaneously allowing for fast and confident assignments of molecular spectra. The software is called LLWP and is written in Python. The core functionality and selected features are presented on the example of first results of the analysis of isotopically enriched propanone-<sup>13</sup>C<sub>1</sub> (<sup>13</sup>CH<sub>3</sub>COCH<sub>3</sub>), which was synthesized as its signal at natural abundance only allowed for a very limited analysis [4, 5]. The software and its full documentation are available at [ltotheois.github.io/LLWP](https://ltotheois.github.io/LLWP).

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# Chemical and physical processes caused by electrons impacting on H<sub>2</sub>O-CO mixed ices

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The exogenic bombardment of surface icy moons around gas giants by energetic electrons and ions may modify the ice composition and physical structure. The relevant number of Jupiter-sized exoplanets discovered so far, and the ubiquity of water in space make these environments an exciting case for studies about the emergence of life. It is thus important to quantitatively understand the effects of different weathering agents.

In the present study we exploit middle-range electrons (200 – 1000 eV) to study the radiation induced chemistry in ices of mixed composition, H<sub>2</sub>O + CO. We derive production and destruction cross-sections, and for the case of CO also the desorption cross-section. We list the products observed after irradiation with energetic electrons to understand the mechanisms and kinetics associated with the relevant reactions. A comparison is made with the results of experiments performed using different processing sources, namely X-rays, UV, and protons. Finally, we discuss the difference in the *desorption relevant depths* between the present case and that of a pure CO ice.



# Electronic transitions in $\text{Rb}_2^+$ dimers solvated in Helium

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We reported depletion spectra of the heteronuclear ( $^{85}\text{Rb}^{87}\text{Rb}^+$ ) dimer cation complexed with up to ten He atoms. The ions were formed by doping helium nanodroplets in a pickup cell filled with low-density Rb vapor and subsequent electron ionization. The weak binding between He and  $\text{Rb}_2^+$  ensures that the target ions are in their vibrational ground states. Two absorption bands were observed between 920 and 250 nm, due to transitions into the  $1^2\Sigma_u^+$  and  $1^2\Pi_u$  states. The transitions are blue- and redshifted, respectively, when the number of He atoms is increased. Spectroscopic constants and the spin-orbit (SO) splitting are deduced for the bound  $1^2\Pi_u$  state. All experimental findings are supported by ab initio calculations, using the coupled clusters singles doubles (CCSD) method for modeling the ground electronic state, and the equation of motion CCSD (EOMCCSD) and multireference configuration interaction (MRCI) for electronically excited states.

# Polymerization in C<sub>2</sub>H<sub>2</sub> plasmas used for the generation of interstellar dust analogues

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It has been conjectured that acetylene polymerization in the envelopes of evolved stars could play a significant role in the generation of interstellar (IS) carbonaceous dust, and there is great interest in establishing a relationship between gas-phase polymerization reactions of acetylene and the characteristics of the particles formed. In particular, gas discharges of acetylene are used for the production of hydrogenated amorphous carbon (a-C:H) particles, whose IR spectra are in good agreement with astronomical observations of IS dust [1]. Chemical models of C<sub>2</sub>H<sub>2</sub> plasmas [2] include radicalic, cationic and anionic routes where C<sub>2</sub>H, C<sub>2</sub>H<sub>2</sub><sup>+</sup> and C<sub>2</sub>H<sup>-</sup> are the key reactive species and show that the first steps of polymerization lead to linear polyynes, in accordance with observations, but the particles finally formed contain mostly aliphatic and aromatic functional groups.

In this work, we extend our previous study on the steady-state kinetics of plasmas of acetylene with noble gases [3] and provide time-resolved mass spectrometry measurements of the evolution of neutrals and, for the first time, also for ions at the start of polymerization in C<sub>2</sub>H<sub>2</sub>/Ar plasmas, before the onset of particle formation. A simple model of the chemistry is also advanced that accounts globally for the observations. The results confirm the usually assumed sequential polymerization through addition of C<sub>2</sub> units, but reveal also the puzzling early appearance of species with a high number of C atoms and the predominance of vinylidene (C<sub>2</sub>H<sub>2</sub><sup>-</sup>) over ethynide (C<sub>2</sub>H<sup>-</sup>) in the anionic polymerization route, contrary to the assumptions of most previous models. Properties of a-C:H particles, produced in the same reactor, are discussed in the light of the gas-phase results.

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# Characterizing home-built chirped-pulse spectrometers for complex molecules of astrophysical interest

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We present our two chirped-pulse Fourier transform spectrometers operating in different frequency ranges. The instruments are designed to achieve high stability and sensitivity, which makes it possible to measure isotopic species of molecules in natural abundance.

One spectrometer operates between 12 and 26.5 GHz, which is interesting for rotational spectra of complex molecules that are relevant for astrophysics, due to the matching frequency range of the Green Bank Telescope. In addition, many of the organic molecules present or possibly present in space have their maximum transition intensity in this region at cold temperatures. In a recent modification, 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 [1]. 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 demonstrate the performance of our spectrometer, we will present the spectra of  $^{13}\text{C}$  isotopologs of n-propyl cyanide observed in natural abundance. We have also detected the rotational spectra of 4'-methylacetophenone, for which we used a nozzle attachment with a heated reservoir [2]. The performance of our instrument and example spectra will be discussed.

The other chirped pulse spectrometer is operational in the millimeter-wave range between 75 and 110 GHz, which is coincident with the Atacama Large Millimeter/Submillimeter Array (ALMA) Band 3. Besides the possibility to detect isotopologs in natural abundance, a high voltage DC discharge in combination with a supersonic jet is incorporated to observe fragments of molecules. For this application, the first tests were performed with methyl cyanide ( $\text{CH}_3\text{CN}$ ). We observed HCN as well as HNC discharge products.

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# Spectroscopy of molecular glow discharge products using REMPI

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Diffuse interstellar bands (DIBs) are a century old spectroscopic mystery, which can be observed in the UV and visible spectral range along many astronomic sightlines [1]. The source of these rather diverse spectral features, ranging from narrow and distinct to very shallow and broad, are largely unknown. Due to the rich variety of carbon chemistry in the interstellar medium, polycyclic aromatic hydrocarbons (PAHs) contribute most likely to over 500 unidentified diffuse signals. A first breakthrough was achieved in 2015 with the assignment of  $C_{60}^+$  as one of the carriers of some DIBs [2]. Nevertheless, the majority of DIBs remains still unassigned.

In this work a glow discharge plasma is used in order to produce different molecular species in a molecular beam by introducing simple carbonaceous precursor molecules within a carrier gas, as demonstrated by T.Motylewski and H.Linnartz 1999 [3]. Resonance enhanced multi-photon ionization schemes (REMPI) combined with a time of flight mass spectrometer provide high measurement sensitivity and are predestined for spectroscopy of samples with unknown composition. We present spectra of molecular species created by a glow discharge nozzle and observe their vibrionic transitions in the UV spectral range.

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# Semiconductor- & Metallic-Behavior of Iron(II) Sulfides: A Multi-Wavelengths Study

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Iron(II) sulfides are one of the predicted sulfur reservoirs in cosmic dust. They were first found in the solar system e.g. in comet 1P/Halleys dust<sup>[1]</sup> and subsequently in protoplanetary disks around Herbig stars<sup>[2]</sup>. Spectroscopic laboratory investigations so far cover either the UV-VIS to NIR, or the FIR spectral range. Astronomical models consist of interpolated optical constants between measured regimes<sup>[3]</sup>.

In this study, reflectivity data of the spectral range from UV to FIR serve for the determination of optical constants. Low temperature measurements in the infrared are presented for the influence on free charge carriers. Samples with different iron to sulfur ratios from meteoritic troilite as stoichiometric end member to characterized terrestrial pyrrhotites were embedded in epoxy and high gloss polished.

Binary spectroscopic behavior was discovered between stoichiometric(-like) and iron depleted iron(II) sulfides. Measured specific resistances confirmed metallic-behavior for non-stoichiometric and semiconductor-behavior for the stoichiometric-like sample. For the latter, free charge carrier characteristics only appear at sub-mm wavelengths in comparison to all pyrrhotites where they are dominant from MIR to FIR. Temperature dependent reflectivity changes for the pyrrhotites were found in this wavelength regime. New, first from theory predicted<sup>[4]</sup>, phonon bands were detected for troilite in the FIR with increasing strength from 300 K to 10 K. As a result, the optical constants depend on the iron to sulfur ratio and the infrared reflectivity decreases with higher iron amount.

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# Action Spectroscopy of PAH Ions Using the Helium Droplet Technique

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In our experimental setup helium nanodroplets (HNDs) can get positively or negatively charged via electron ionization and are subsequently doped with polycyclic aromatic hydrocarbons (PAHs); co-doping with molecular hydrogen or other molecules is also possible. After charge transfer from the HND to the dopant, the ions are made accessible for mass spectrometry by collision of the doped droplets with a stainless steel surface. PAH ions remain decorated with up to several tens of helium atoms, or H<sub>2</sub> molecules in the case of hydrogen co-doping. These weakly bound atoms or molecules boil off after laser excitation, which results in a change in the recorded ion yield at resonant frequencies (see Figure 1).

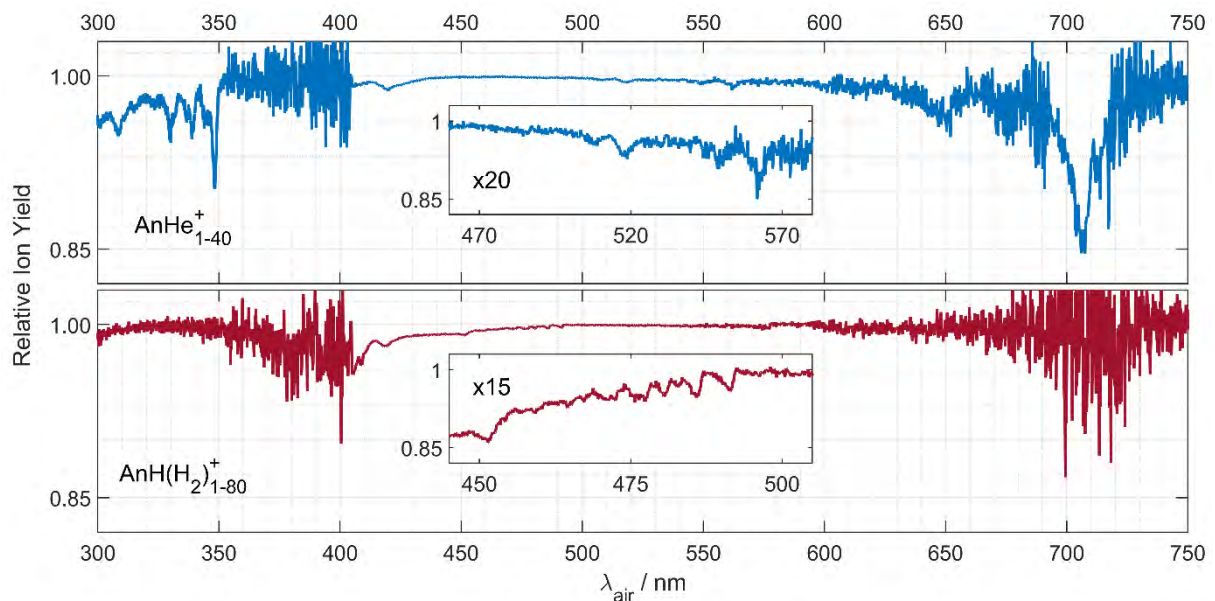


Figure 1: Absorption spectra of He<sub>n</sub> (a) and (H<sub>2</sub>)<sub>m</sub> (b) tagged An<sup>+</sup> and AnH<sup>+</sup>. The decrease of 40 (top), respectively 80 (bottom) mass channels was combined.

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# Mid Infrared CW Cavity Ring Down Spectroscopy in a Supersonic Jet

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The cavity ring down (CRD) technique is an absorption based highly sensitive spectroscopic analyzing method based on the multiple reflection of light between a pair of highly reflective mirrors (>99.99%).

Here, we report about our progress in building up a mid-infrared CRD experiment where we use a tunable cw-OPO laser system operating between 2.6 $\mu\text{m}$  - 4.0  $\mu\text{m}$  to probe a supersonic jet of gas containing molecules produced in a discharge or laser ablation source. While the cavity ring down technique itself is well known at optical wavelengths, the application to mid infrared wavelengths for spectroscopy proved to be difficult but is now constantly improving due to the availability of suitable tunable laser sources and sufficiently reflective mirrors. The mid infrared region around 3 $\mu\text{m}$ , where our CRD mirrors have their best reflectivity, is interesting from a molecular spectroscopy point of view, because -O-H, -N-H and  $\equiv\text{C-H}$  stretching vibrations can be investigated in this wavelength region.

First spectroscopic results and a brief technical characterization of our CRD setup will be presented on the poster.

# Gas-phase condensation of carbonated silicates

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Although the contribution of carbonates to the infrared spectra of cosmic dust has been episodically considered, reported, and argued against for four decades, it remains undetermined. One difficulty is to evaluate such a contribution in a wavelength range crowded with the spectral features of various silicates, hydrocarbons, and ices, all diversely composed, structured, associated, and processed. It is compounded by the lack of reference spectra for a corresponding diversity of carbonates. The other difficulty is to identify a formation mechanism for those carbonates observed in planetary nebulae [1, 2], protostars [3, 4], and young stars [5, 6]. Taking into account the low temperatures that prevail in the regions where the carbonates were found, local aqueous alteration of cosmic silicates is excluded, which is why processes that do not require liquid water were proposed [1]. Soon, the formation of carbonates was observed in experiments on the gas-phase condensation of silicates in an H<sub>2</sub>O-CO<sub>2</sub>-rich atmosphere, suggesting that they could be formed in stellar winds or in outflows of protostars [7]. In the framework of a DFG-funded project, we have started a series of experiments on the formation of carbonates without liquid water. Gas-phase condensation, gas-solid chemistry, and ice mantle-refractory core interface chemistry will be investigated. The first experiments demonstrate the gas-phase condensation of carbonated silicates in absence of water molecules. The infrared spectra of the condensates are measured for future comparison with cosmic dust observations.

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# Rotational Spectrum of Vinyl Isocyanate

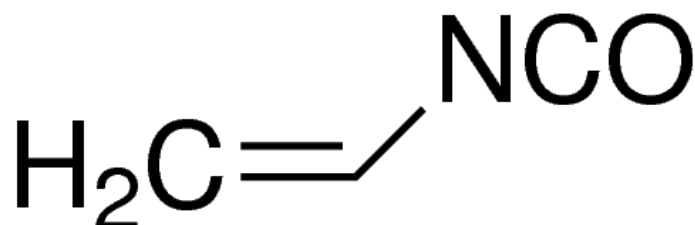
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Vinyl isocyanate (C<sub>2</sub>H<sub>3</sub>NCO) is another molecule in the group of astrophysically relevant isocyanates after well-known interstellar HNCO<sup>1</sup>, CH<sub>3</sub>NCO<sup>2,3</sup>, and very recently also C<sub>2</sub>H<sub>5</sub>NCO<sup>4</sup>. Only low-frequency data are available for vinyl isocyanate<sup>5</sup>. This makes predictions at higher frequencies rather uncertain impeding its search in space by millimetre wave astronomy.

In the present study we measured the rotational spectrum of vinyl isocyanate in the frequency ranges of 128–218 GHz and 282–330 GHz using the Prague millimetre wave spectrometer<sup>6</sup>. The sample was prepared by Curtius rearrangement of acryloyl azide<sup>5</sup>. Hundreds of new rotational transitions for both the *trans* and *cis* conformers were measured and assigned. A global fit of all the new and previously assigned transitions<sup>5</sup> was performed by Pickett's SPFIT program<sup>7</sup>. The refined rotational and centrifugal distortion constants are presented and discussed. Results of this work will allow to search for vinyl isocyanate in the interstellar medium.



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## **Abstracts. Day three**

# **Physics and Chemistry of planetary atmospheres**

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# Modeling and Characterization of Cloudy Exoplanet Atmospheres

**P. Mollière**<sup>1</sup>

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In this talk I will give an overview on how clouds affect atmospheric models of exoplanets, both in their thermal and chemical structure, focusing mostly, but not exclusively, on 1-d atmospheric prescriptions. Moreover, the effect of clouds on spectra of exoplanets will be discussed for close-in transiting planets, and for wide-separation, directly imaged planets. Lastly, I will discuss how future observatories may break cloud-related degeneracies that plague today's interpretation of exoplanet observations.

# Mineral Snowflakes on Exoplanet and Brown Dwarf Atmospheres

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Clouds remain a key challenge for exoplanet observations, altering the local atmospheric composition through condensation as well as obscuring deeper atmospheric layers. Next-generation instruments (e.g. JWST) will make spectral features of cloud particle composition observable. However, these features will be altered by the size, shape and homogeneity of cloud particles, therefore a detailed understanding of cloud formation will be required.

Cloud particle-particle collisions can significantly alter the cloud particle porosity, size and number density distributions within an atmosphere. Coagulation offers a method of building highly porous cloud particles - mineral snowflakes. Fragmentation processes existing cloud particles into a much denser cloud, composed of smaller cloud particles. We use a hybrid moment-two bin, kinetic, cloud formation model to investigate the effects of collisions induced by gravitational settling, Brownian motion and turbulence. We find that for a range of 1D pressure-temperature Drift-Phoenix profiles for exoplanet and brown dwarf atmospheres, collisions produce one of three qualitative outcomes: fragmentation dominating less dense atmospheres ( $\log_{10}(g [\text{cms}^{-2}])=3.0$ ), coagulation for cool compact atmospheres ( $T \leq 1800\text{K}$ ,  $\log(g)=5.0$ ), and growth dominating hot compact atmospheres ( $T > 1800\text{K}$ ,  $\log(g)=5.0$ ).

We investigate the optical depth of clouds, including particle-particle collisions, using Mie theory. We use effective medium theory, which can also incorporate porosity of the cloud particle, for mixed mineral cloud particle refractive indices, for which laboratory support would be beneficial. Non-spherical cloud particles are represented with a statistical distribution of hollow spheres. Irregularly shaped cloud particles enhance cloud optical depth at silicate feature wavelengths, observable with JWST MIRI. Fragmenting atmospheres enhance cloud optical depth at optical wavelengths (HST WFC3), due to an increase in cloud particle number density and decrease in surface average size. These results challenge assumptions about cloud particle material composition or size derived from observations, and show that more complex models are necessary.

# **Observational Constraints on Dust Processing in Circumstellar Media and Exoplanetary Atmospheres**

**J. Bouwman**

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In this short review, I will give an overview of the observed dust species and processing in protoplanetary disks and planetary (low mass) objects. These objects have been studied extensively from both the ground as well as space observatories like ISO, Spitzer and Herschel, identifying many dust species and showing strong processing of the circumstellar material compared to the ISM and molecular clouds. I will discuss the currently known dust species and processes and discuss the link between the composition of exoplanets and protoplanetary disks. Further, I will make the link to laboratory measurements on dust processing, required to correctly interpret these observations and identify a number of areas which required further experiments. Finally, I will briefly discuss how future JWST observations are expected to substantially enhance our knowledge of the dust processing in circumstellar media and exoplanetary atmospheres.

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