LabAstro Meeting 2024
Book of Abstracts

From Cryostats in the Basement to Stars and Galaxies

RINGBERG CASTLE
KREUTH, BAVARIA, GERMANY
25. – 28. SEPTEMBER 2024

Scientific Organizing Committee

Pavol Jusko, Paola Caselli, Sandra Brünken, Holger Kreckel, Thomas Henning

Edited by Pavol Jusko

MAX-PLANCK-GESELLSCHAFT

MPE

Ernst-Rudolf-Schloessmann-Stiftung

2024

Max-Planck-Institut für extraterrestrische Physik
Gießenbachstraße 1, 85748 Garching, Germany

NOTES:

LabAstro Meeting – Ringberg, 25. – 28. September 2024

Wednesday (25.)	Thursday (26.)	Friday (27.)
	8:00 – 9:00 Breakfast	
	T1 Large Molecules II	F1 Ices and Surfaces
Train[t] from München Hbf. to Tegernsee runs twice per hour, always around :04 and :30. Platforms 27–36.	**9:00** T1.1 J. Kamer (i)	**9:00** F1.1 T. Suhasaria
	9:35 T1.2 L. Isberner	**9:25** F1.2 F. Kruczkiewicz
	10:00 T1.3 D. Schleier	**9:50** F1.3 A. Vyjídák
	10:30 – 11:00 Coffee	
	T2 Techniques	cont.
	11:00 T2.1 L. Gamer (i)	**11:00** F1.4 J. Schrauwen
	11:35 T2.2 G. Fuchs	**11:25** F1.5 A. Tamanai
	12:00 T2.3 G. Lakatos	**11:50** F1.6 M. Nonne
	12:30 – 13:30 Lunch	
	D.: Lab and Astron. Facilities	D.: Gas vs. Solid
	13:30 D.1 S. Spezzano	**13:30** D.3 A. Potapov
	T3 Reactions	F2 Spectroscopy
14:30 Bus from Tegernsee[T]	**14:15** T3.1 Š. Roučka	**14:15** F2.1 H. Bunn
15:00 Castle opened	**14:40** T3.2 M. Jiménez-Redondo	**14:40** F2.2 M. Gerlach
check-in + coffee	**15:05** T3.3 H. Quitián-Lara	**15:05** F2.3 D. Gupta
	15:30 – 16:00 Coffee	
Opening	cont.	cont.
16:00 O.1 P. Caselli	**16:00** T3.4 A. Breier (i)	**16:00** F2.4 T. Giesen
W1 Large Molecules I	**16:35** T3.5 K. Li	**16:35** F2.5 S. Marlton
16:15 W1.1 E. Gruber (i)	**17:00** T3.6 L. Berger	**17:00** F2.6 H. Kaur
16:50 W1.2 G. Wenzel (i)(h)	D.: Quo vadis DE LabAstro	D.: Towards CDMS for IR?
17:30 Castle Tour[s]	**17:25** D.2 S. Schlemmer	**17:25** D.4 S. Brünken
Posters Placing[p]		
	18:10 – 18:30 Posters[p]	
	18:30 – 19:30 Dinner	

Notes: Contributed talks are mostly 25 min. long (including questions). Invited talks 35 min. (i) – invited talk. (h) – hybrid talk (with a remote speaker)

D.1–4 – Discussion sessions have a "free" format and are 45 min. long. The speaker will introduce the subject and gradually turn into a moderator around the topic. Anyone is encouraged to contribute to the discussion (verbally, but also a slide, etc.).

t – Duetschland-Ticket, alternatively get the M-7 zones ticket in the ticket machines (€ 17,10). Same from the airport. Attention: The trains are composed of several "parts", which end up in different places. Only enter the coaches displaying "Tegernsee"!

T – Last train with guaranteed connection to the bus is leaving Munich Hbf. at 13:04.

p – posters will be displayed on Wed. after the last talk. On Thu. and Fri., the border between the discussions and the poster session will become more "fluid".

s – on Wed. evening a "tour of the Ringberg castle" is going to be offered for anyone interested (no registration needed).

Saturday morning departure around 9:20.

LIST OF PARTICIPANTS

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46. Wild, Robert P.9, p. 21

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[1] online only

WEDNESDAY 25. SEPTEMBER

W1. LARGE MOLECULES I – FULLERENES AND PAHS

Chair: Pavol Jusko

W1.1. On the search for carriers of the diffuse interstellar bands

16:15–16:50

Elisabeth Gruber[1], Lisa Ganner[1], Miriam Kappe[1], Stefan Bergmeister[1], Paul Scheier[1]
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– invited talk –

One of the big mysteries of observational astronomy are the carriers of the diffuse interstellar bands (DIBs). Although these bands were first observed over a century ago, only five of the approximately 600 known bands have been conclusively assigned to a specific carrier, namely the C_{60}^{+} ion [1]. Other carbon-based molecular ion species, such as exohedral and endohedral fullerenes, polycyclic aromatic hydrocarbons (PAHs), and carbon chains, are considered promising candidates for explaining additional bands. To achieve unambiguous identification of these carriers, laboratory experiments under well-defined conditions are essential. However, due to technical limitations, most spectroscopic investigations are currently confined to the infrared wavelength range. Despite this, electronic spectra in the UV/visible-NIR range are crucial for unambiguous identification.

In this contribution, we will focus on novel instrumental setups that facilitate messenger-type spectroscopy of various cold ions formed within the superfluid environment of multiply-charged helium nanodroplets [2, 3]. We will discuss the advantages of the novel methods and present recent spectroscopic investigations of fullerene analogues [4, 5] as well as PAHs.

Acknowledgment This research was funded by the Austrian Science Fund (FWF) [10.55776/I6221, 10.55776/V1035, 10.55776/P34563, 10.55776/W1259]. This contribution is based upon work from COST Action NanoSpace, CA21126, supported by COST (European Cooperation in Science and Technology).

[1] E. K. Campbell et al., *Nature* **2015**, *523*, 322–323, DOI `10.1038/nature14566`.
[2] P. Martini et al., *Physical Review Letters* **2021**, *127*, 263401, DOI `10.1103/PhysRevLett.127.263401`.
[3] S. Bergmeister et al., *Review of Scientific Instruments* **2023**, *94*, DOI `10.1063/5.0144239`.
[4] M. Kappe et al., *The Journal of Chemical Physics* **2023**, *159*, DOI `10.1063/5.0176407`.
[5] M. Kappe et al., *Physical Review Research* **2024**, *6*, L012045, DOI `10.1103/PhysRevResearch.6.L012045`.

W1.2. Spectroscopically Exploring Interstellar PAHs: From Laboratory to Space

16:50–17:25

Gabi Wenzel
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– invited talk –

About 10 – 20 % of the cosmic carbon content is locked up in a molecular family called polycyclic aromatic hydrocarbons (PAHs). As part of cosmic dust, PAHs are ubiquitous species in the interstellar medium (ISM), the space between the stars, and have recently been unambiguously detected in radio astronomical observations of the dark molecular cloud TMC-1 [1]. In photodissociation regions (PDRs) of the ISM that are illuminated by nearby stars, PAHs are photoprocessed by the interaction with ultraviolet (UV) photons. Upon absorption of a UV photon, an isolated PAH can undergo a range of relaxation processes, i.e., ionization, dissociation, and radiative cooling through the emission of infrared photons [2]. The latter gives rise to the aromatic infrared bands (AIBs) observed in many astronomical objects, but also radiative cooling via recurrent fluorescence, also known as Poincaré fluorescence, represents a relevant relaxation mechanism [3]. All these processes influence the charge state and photodissociation dynamics of PAHs, ultimately determining their photostability in the ISM [4]. In return, this impacts the energy balance of the interstellar gas by photoelectric heating in PDRs. Here, PAHs potentially contribute to the formation of the most abundant molecule in space, H_2. PAHs therefore play an important role in the physics and chemistry of PDRs and the ISM in general. In this presentation, we will focus on astrochemically relevant PAHs, how to assess their characteristic properties employing spectroscopic techniques in the astrophysics laboratory [5, 6], and our search for them in space.

[1] B. A. McGuire et al., *Science* **2021**, *371*, 1265–1269, DOI `10.1126/science.abb7535`.

[2] C. Joblin et al., *J. Phys. Conf. Ser.* **2020**, *1412*, 062002, DOI `10.1088/1742-6596/1412/6/062002`.

[3] A. P. Rasmussen et al., *Astronomy & Astrophysics* **2023**, *674*, A103, DOI `10.1051/0004-6361/202346003`.

[4] G. Wenzel et al., *Astronomy & Astrophysics* **2020**, *641*, A98, DOI `10.1051/0004-6361/202038139`.

[5] G. Wenzel et al., *Journal of Molecular Spectroscopy* **2022**, *385*, 111620, DOI `10.1016/j.jms.2022.111620`.

[6] S. Banhatti et al., *Physical Chemistry Chemical Physics* **2022**, *24*, 27343, DOI `10.1039/D2CP03835H`.

THURSDAY 26. SEPTEMBER

T1. LAEGE MOLECULES II – PAHS AND SI/N-PAHS

Chair: Silvia Spezzano

T1.1. Mid-IR spectroscopy and Photoprocessing of Polycyclic Aromatic Nitrogen Heterocycles

9:00 – 9:35

Jerry Kamer,[1] Domenik Schleier,[1,2] Andy Jiao,[3] Grégory Schneider,[3] Merel Donker,[1] Jonathan Martens,[4] Giel Berden,[4]
Patrick Hemberger,[5] Andras Bodi,[5] Harold Linnartz,[1] Jordy Bouwman [6]
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– invited talk –

Infrared emission features are observed towards diverse astronomical objects in the interstellar medium (ISM) [1, 2]. Generally, the consensus is that these IR features originate from polycyclic aromatic hydrocarbons (PAHs) and are hence named aromatic infrared bands (AIBs) [3–5]. It has been proposed that nitrogen substituted PAHs (PANHs) contribute to the AIBs as well, as nitrogen inclusion in PAHs can improve the match with the AIBs, specifically around the 6.2 μm emission feature [6, 7]. So far only a few PANHs have been investigated experimentally, despite their astronomical relevance. In this talk I will present our latest experimental results on the photodissociation pathways and gas-phase mid-IR spectroscopy of several cationic PANHs and their derivatives. The dissociation mass spectra and mid-IR spectra will be compared to those of their carbon homocyclic PAH congeners. I will show that these spectra contain remarkable similarities and also some insightful differences. Also, I will show that cationic PANHs and their derivatives may contribute to the IR emission bands and that nitrogen-containing dissociation fragments of cationic PANHs are potential tracers of PANH dissociation in the ISM.

[1] A. G. G. M. Tielens, *Annu. Rev. Astron. Astrophys.* **2008**, *46*, 289–337, DOI `10.1146/annurev.astro.46.060407.145211`.

[2] Chown, R. et al., *A&A* **2024**, *685*, A75, DOI `10.1051/0004-6361/202346662`.

[3] A. Leger, J. L. Puget, *A&A* **1984**, *137*, L5–L8.

[4] L. J. Allamandola, A. G. G. M. Tielens, J. R. Barker, *Astrophys. J.* **1985**, *290*, L25–L28, DOI `10.1086/184435`.

[5] L. J. Allamandola, A. G. G. M. Tielens, J. R. Barker, *Astrophys. J.* **1989**, *71*, 733, DOI `10.1086/191396`.

[6] E. Peeters et al., *A&A* **2002**, *390*, 1089–1113, DOI `10.1051/0004-6361:20020773`.

[7] D. M. Hudgins, C. W. Bauschlicher, L. J. Allamandola, *Astrophys. J.* **2005**, *632*, 316–332, DOI `10.1086/432495`.

T1.2. Electron collisions with C_{60}^{+} ions

9:35–10:00

Leonard Isberner,[1,2] Bhalchandra Sitaram Choudhari,[2] Manfred Grieser,[2] Florian Grussie,[2] Claude Krantz,[3] Holger Kreckel,[2] Viviane Schmidt,[2] Andreas Wolf,[2] Stefan Schippers,[1] Oldřich Novotný[2]
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The Fullerenes C_{60}, C_{60}^{+}, and C_{70} are the largest molecules found in space so far [1–3]. A lot of interest was attracted by the charged C_{60}^{+} as it is the only identified carrier of diffuse interstellar bands. In astrophysical models, due to a lack of experimental data, the interplay between neutral C_{60} and charged C_{60}^{+}, their formation and destruction, so far relies on assumptions about the underlying reaction rates.

We stored C_{60}^{+} ions for up to 500 s in the Cryogenic Storage Ring CSR [4], located at the Max-Planck-Institut für Kernphysik in Heidelberg. In a merged-beams setup utilizing the CSR electron cooler, we studied electron collisions with C_{60}^{+} at collision energies between ~1 meV and 85 eV. Two single-particle detectors allowed for simultaneous detection of charged and neutral reaction products. We observed recombination, fragmentation, ionization, and fragmentation-ionization processes, for which absolute rate coefficients have been derived. Compared to electron collisions of small molecular ions, C_{60}^{+} displays strongly different reaction dynamics.

[1] J. Cami et al., *Science* **2010**, *329*, 1180–1182, DOI `10.1126/science.1192035`.

[2] E. K. Campbell et al., *Nature* **2015**, *523*, 322–323, DOI `10.1038/nature14566`.

[3] `https://cdms.astro.uni-koeln.de/classic/molecules`, Accessed: 27.05.2024.

[4] R. von Hahn et al., *Review of Scientific Instruments* **2016**, *87*, 063115, DOI `10.1063/1.4953888`.

T1.3. The role of phenylnitrene in the formation of polycyclic aromatic nitrogen heterocycles

10:00–10:25

Domenik Schleier
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Molecular growth reactions are driven by small resonance stabilized radicals (RSRs), like propargyl (C_3H_3), and ultimately produce polycyclic aromatic hydrocarbons (PAHs) and soot. The influence of reactive nitrogen species in these processes has not yet been investigated, although they have been proven to efficiently synthesize C−N bonds in organic chemistry. Here, we present the reaction between phenyl nitrene and propargyl radicals as a possible molecular growth mechanism that leads to polycyclic aromatic nitrogen heterocycles (PANHs). The two reactants are generated in a pyrolysis microreactor and the composition of the reaction products is isomer-selectively analyzed using mass-selected threshold photoelectron spectra recorded on a photoelectron photoion coincidence (PEPICO) setup. We find that the reaction leads to multiple isomeric products, among them quinoline, that all have submerged barriers with respect to the isolated reactants. As such, nitrenes are promising candidates that facilitate molecular growth reactions under nitrogen-rich conditions like in the atmosphere of Titan.

T2. TECHNIQUES AND HIGH "LOW" ENERGY

Chair: Silvia Spezzano

T2.1. MOCCA: a 4-kilo-pixel microcalorimeter detector for the cryogenic storage ring CSR

11:00 – 11:35

L. Gamer[1], C. Enss[2], A. Fleischmann[2], S. Gaisser[1], O. Heber[3], D. Hengstler[2], C. A. Jakob[1], D. Kreuzberger[2], A.Lowack [2], A. Özkara[2], M. Rappaport[3], A. Reifenberger[2], D. Schulz[2], A. Shahi[3], Y. Toker[4], A. Wolf[1], O. Novotný[1]
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[3]*Weizmann Institute of Science, Herzl St 234, Rehovot, Israel*
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– invited talk –

The cryogenic storage ring CSR at the Max Planck Institute for Nuclear Physics in Heidelberg is capable of storing various molecular ions for an extended period of time, allowing them to de-excite into their vibrational and rotational ground states. This enables investigation of molecular-ion reactions, such as dissociative recombination with electrons, at conditions similar to those in interstellar molecular clouds. For the mass-identification of the resulting neutral reaction products and the determination of the kinetic energy released in these reactions, a position and energy resolved detection of the fragments is required. For this purpose, the MOCCA detector, 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, was developed and microfabricated at the Kirchhoff-Institute for Physics in Heidelberg.

Prior to the integration of MOCCA and the surrounding setup in the CSR downstream of the electron cooler, it 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 resulting from collision- or photon-induced fragmentation processes. The current status of the project will be discussed in the presentation.

T2.2. Multi-level excitation diagram analysis of circumstellar molecules seen in the infrared

11:35 – 12:00

Guido W. Fuchs,[1] Eileen Döring,[1] Rohini S. Giles,[2] Thomas K. Greathouse,[2] John H. Lacy,[3] Ed Montiel,[4] Curtis DeWitt,[4] Matt Richter,[5] Thomas F. Giesen,[1]
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The standard spectroscopic tool "rotation diagram" assumes local thermal equilibrium conditions, which are not always fulfilled in practice. We present an extended version ('multi-level excitation diagram method') that also works in non-equilibrium ($T_{rot} \neq T_{vib}$) environremnts, assuming that the concept of temperature is still valid per vibrational level. The method can be applied to laboratory data, like high-resolution spectra produced in supersonic jets but also to data from astrophysical observations. We demonstrate this technique using high-resolution infrared data of circumstellar molecules around the hyper-giant star VY CMa, like SiO and NH_3.

T2.3. Low-energy proton implantation induced chemical changes in calcium-carbonate

12:00–12:25

Gergő Lakatos,[1,2], Sándor Biri,[2] Robert W. McCullough,[3] Péter Heczku,[2] Sándor Kovács,[2] Duncan V. Mifsud,[2] Nigel J. Mason,[2,4] Richárd Rácz,[2] Béla Sulik,[2] Zoltán Juhász,[2]
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[2]*HUN-REN Institute for Nuclear Research (ATOMKI), Debrecen, Bem tér 18/c H-4026, Hungary*
[33]*Department of Physics and Astronomy, School of Mathematics and Physics, Queen's University Belfast, Belfast, BT7 1NN, United Kingdom*
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Calcite has been observed in many astronomical environments within and beyond the Solar System. [1, 2] Previous radiolysis studies on this carbonate mineral shed light to the formation of a plethora of interesting radiolysis products (e.g. small molecular weight carboxylic acids and other organic molecules) from an astrochemical point of view.[3] Although, to our knowledge, no experiments were addressed to directly simulate the physical-chemical effects of stellar activity on this mineral.

The HUN-REN Institute for Nuclear Research in Debrecen, Hungary hosts the AQUILA Irradiation Chamber, which makes possible the irradiation of various target materials at low temperatures, by single or molecular ions of different charge states (Q) with kinetic energies ranging from Q*500 eV to Q*20 keV. In our experiments we investigated the chemical changes in $CaCO_3$ induced by 10 and 2 keV proton implantation mimicking the effect of solar wind, at 20 K. For the detection of the newly formed particles, we utilized Fourier-transformed Infrared (FTIR) Spectroscopy and quadrupole mass spectrometry (QMS) techniques.

We observed the formation and entrapment of carbon-dioxide and carbon-monoxide in the irradiated layers as main radiolysis products. The ratio of these molecules showed significant dependance on the projectile energy. Some characteristic changes in the infrared spectra of the irradiated samples suggest that proton radiation can induce recrystallization in calcite even at very low temperatures.

[1] K. Tomeoka, P. R. Buseck, *Science* **1986**, *231*, 154–1546, DOI `10.1126/science.231.4745.1544`.
[2] C. Ceccarelli et al., *A&A* **2002**, *395*, L29–L33, DOI `10.1051/0004-6361:20021490`.
[3] G. Albarrán, K. E. Collins, C. H. Collins, *J. Mol. Evol.* **1987**, *25*, 12–14, DOI `10.1007/BF02100035`.

T3. REACTIONS AND CHEMICAL PROCESSES

Chair: Christian Endres

T3.1. Ion Trap Study of Nuclear-Spin-Changing Collisions Between H_3^+ and H_2

14:15–14:40

Štěpán Roučka[1], Octavio Emmanuel Hernandez Alvarez[1], Serhiy Rednyk[1], Lilia Uvarova[1], Petr Dohnal[1], Radek Plašil[1], Juraj Glosík[1]
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The nuclear spin states of H_2 and H_3^+ have extremely long lifetimes in the cold and dilute conditions of the interstellar medium. Therefore, the observed populations of the ortho and para nuclear spin states of H_2 and H_3 are often far from equilibrium and their relaxation rate can even be used as astrophysical clock [1, 2]. A major process contributing to the relaxation of H_2 nuclear spin states in the interstellar medium are inelastic collisions with H_3^+[3, 4]:

$$ {}^{\mathrm{p}}H_3^+ + H_2(f_2) \xrightarrow{k^{\mathrm{p}\to\mathrm{o}}(f_2)} {}^{\mathrm{o}}H_3^+ + H_2, \tag{1}$$

$$ {}^{\mathrm{o}}H_3^+ + H_2(f_2) \xrightarrow{k^{\mathrm{o}\to\mathrm{p}}(f_2)} {}^{\mathrm{p}}H_3^+ + H_2, \tag{2}$$

where the relaxation rate coefficients $k^{\mathrm{p}\to\mathrm{o}}(f_2)$ and $k^{\mathrm{o}\to\mathrm{p}}(f_2)$ depend on the population of the para state of the H_2 reactant, f_2. In the present contribution, we will demonstrate the experimental determination of the rate coefficients of these state-changing collisions at the astrophysically relevant temperature of 65 K. We have used the cryogenic radiofrequency 22-pole trap with a catalytic para-H_2 generator combined with chemical probing and action spectroscopy for determination of the H_2 and H_3^+ nuclear spin states, respectively.

[1] S. Brünken et al., *Nature* **2014**, *516*, 219–221, DOI `10.1038/nature13924`.

[2] F. Grussie et al., *Astrophys. J.* **2012**, *759*, 21, DOI `10.1088/0004-637X/759/1/21`.

[3] E. Hugo, O. Asvany, S. Schlemmer, *J. Chem. Phys.* **2009**, *130*, 164302, DOI `10.1063/1.3089422`.

[4] J. Le Bourlot et al., *Mol. Phys.* **2023**, *122*, e2182612, DOI `10.1080/00268976.2023.2182612`.

T3.2. Ion-molecule chemistry of HCO^+/HOC^+ isomers studied in a low-temperature ion trap

Miguel Jiménez-Redondo,[1] Robin Dahl,[1] Petr Dohnal,[2] Paola Caselli,[1] Pavol Jusko[1] 14:40–15:05
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HCO^+ and its higher energy isomer, HOC^+, are one of the simplest pairs of molecular ion isomers. HCO^+ was detected in the interstellar medium more than 50 years ago [1, 2], with HOC^+ following a decade later [3]. The HCO^+ / HOC^+ column density ratio has been found to be significantly smaller towards photodissociation regions and diffuse clouds compared to dark clouds, suggesting a more efficient HOC^+ formation in warmer environments. In this work, we used a 22 pole ion trap [4] to determine the reaction rate coefficients and branching ratios of some of the main ion-molecule processes for the production and destruction of HOC^+ in astrophysical environments, using chemical probing to differentiate the two isomers. The reaction of $CO^+ + H_2$, previously considered an efficient way to produce HOC^+ [5], was found to yield negligible amounts of this ion [6]. In contrast, $H_3{}^+ + CO$ results in a $\sim 20\%$ branching ratio for the high energy isomer. The isomerization reactions of HOC^+ with both H_2 and CO have also been characterized, obtaining rate coefficients of 4.2×10^{-10} cm^3 s^{-1} and 1.2×10^{-9} cm^3 s^{-1} respectively, highlighting the efficiency of these destruction mechanisms.

[1] D. Buhl, L. E. Snyder, *Nature* **1970**, *228*, 267–269, DOI `10.1038/228267a0`.

[2] R. C. Woods et al., *Phys. Rev. Lett.* **1975**, *35*, 1269–1272, DOI `10.1103/PhysRevLett.35.1269`.

[3] R. C. Woods et al., *ApJ* **1983**, *270*, 583–588, DOI `10.1086/161150`.

[4] P. Jusko, M. Jiménez-Redondo, P. Caselli, *Mol. Phys.* **2024**, *122*, e2217744, DOI `10.1080/00268976.2023.2217744`.

[5] M. A. Smith et al., *ApJ* **2002**, *578*, L87, DOI `10.1086/344404`.

[6] M. Jiménez-Redondo et al., *ChemPhysChem* **2024**, *n/a*, e202400106, DOI `10.1002/cphc.202400106`.

T3.3. Ethanolamine: precursor of prebiotic molecules and potential key to understanding the formation of unsaturated molecules in the ISM

Heidy M. Quitián-Lara,,[1] Jhoan Londoño-Restrepo,[2] Santiago Gómez,[3], Nigel J. Mason[1], Heloisa M. Boechat-Roberty[4],
Felipe Fantuzzi[5] and Albeiro Restrepo[3] 15:05–15:30
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Ethanolamine (C_2H_7NO), a complex organic molecule of prebiotic significance, detected in the molecular cloud G+0.693–0.027, is an excellent candidate for investigating chemical processes in primitive interstellar regions. The experimentally determined fragmentation patterns of C_2H_7NO produce significant chemical precursors necessary for synthesising other complex species. Additionally, these experiments suggest that X-ray radiation could produce the extended networks of π bonds in highly unsaturated molecules commonly observed in the interstellar medium.

[1] J. Londoño-Restrepo, et. all, "X-Ray & UV Photoinduced Fragmentation of Prebiotic Molecules in Interstellar Clouds: Ethanolamine", in preparation.

[2] J. Londoño-Restrepo, et. all, "More π, Please: What Drives the Formation of Unsaturated Molecules in the Interstellar Medium?", in preparation.

T3.4. Exploring $Si_nC_m^+$ molecules: First laboratory detection of SiC^+ via EPD

16:00–16:35

Alexander A. Breier,[1] Taarna Studemund,[1] Kai Pollow,[1] and Otto Dopfer [1]
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– invited talk –

The detection of SiC, a challenging endeavor both in laboratory and space-based settings, saw a breakthrough with collaborative efforts between radio astronomy and laboratory astrophysics, culminating in its definitive identification in the circumstellar shell of the evolved carbon star IRC+10216 [1]. SiC's presence, confirmed through millimeter-wave spectral lines, emphasizes its relevance in cosmic dust formation processes, particularly in carbon-rich environments [2] where photochemistry also plays an important role. Notably, the identification of SiC will likely soon extend to cationic species, offering insights into the ionization- and the non-equilibrium processes within the environment of evolved stars [3].

Nevertheless, SiC and its ionic counterparts can be seen as the starting pieces in silicon-carbide dust formation reactions, serving as crucial precursors in the nucleation and growth of dust grains. This presentation focuses on the experimental investigation of the smallest cationic silicon-carbide molecule, SiC^+, synthesized in our laboratory by evaporating a solid SiC rod using a pulsed laser in a carbon-enriched buffer gas environment. The adiabatic expansion of the gas jet facilitates the observation of its electronic photodissociation fragments, shedding light on its electronic structure and vibrational motions. This is conducted within a tandem mass spectrometer integrating a quadrupole and a time-of-flight mass spectrometer, alongside a widely tunable UV/VIS-OPO laser [4, 5]. Subsequently, the experimental observations are compared and evaluated with computational predictions using high-level quantum chemical calculations [6].

As observational techniques advance and spectroscopic information is recorded in laboratory environments, SiC^+ may emerge as a significant component, offering valuable insights into key aspects of astrophysical processes and cosmic evolution.

[1] J. Cernicharo et al., *ApJ* **1989**, *341*, L25, DOI 10.1086/185449.

[2] M. Frenklach, C. Carmer, E. Feigelson, *Nature* **1989**, *339*, 196, DOI 10.1038/339196a0.

[3] D. Gobrecht, *Front. Astron. Space Sci.* **2021**, *8*, 662545, DOI 10.3389/fspas.2021.662545.

[4] T. Studemund et al., *J. Phys. Chem. Lett.* **2022**, *13*, 7624–7628, DOI 10.1021/acs.jpclett.2c02200.

[5] M. Förstel et al., *Rev. Sci. Instrum.* **2017**, *88*, DOI 10.1063/1.5010853.

[6] D. Zhou et al., *Spectrochim. Acta A* **2018**, *204*, 164, DOI 10.1016/j.saa.2018.06.041.

T3.5. Investigating Possible NCO^- Formation Pathways Using a 22 Pole Ion Trap

16:35–17:00

Kevin Li[1], Miguel Jiménez-Redondo[2], Paola Caselli[2], Jozef Lengyel[1], Pavol Jusko[2]
[1]*Lehrstuhl für Physikalische Chemie, TUM School of Natural Sciences, Technische Universität München, Garching, Germany*
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The Cyanate ion is thought to be the origin of the XCN band that can be found in interstellar ices as well as high-mass young stellar objects. However, attempts to observe it directly in dark clouds were not successful. This could indicate the lack of an efficient formation pathway through the gas-phase.[1] Theoretical calculations predict transition states that inhibit the reaction towards NCO^-.[2] Using the laboratory CAS ion trap setup at the Max Planck Institute for Extraterrestrial Physics[3] we investigated possible reactions with negative enthalpy towards the formation of NCO^-. Our experiments indeed confirm that most the reactions are not producing NCO^-. Generally, whenever HCN is involved, the reaction towards CN^- is strongly preferred, with reaction rate constants of about $k \approx 5 \cdot 10^{-9}$ $cm^3\,s^{-1}$. One reliable way to produce NCO^- is through the reaction of $NH_2^- + CO_2 \rightarrow NCO^- + H_2O$. Additionally the reaction of O^- with HCN has a small branching ratio of about 10% NCO^-/CN^-. In conclusion, our experiments show that NCO^- is likely not produced through anionic gas phase reaction in the interstellar medium.

[1] L. Dore et al., *The Journal of Physical Chemistry A* **2022**, *126*, 1899–1904, DOI 10.1021/acs.jpca.2c00313.

[2] E. Yurtsever, F. A. Gianturco, R. Wester, *The Journal of Physical Chemistry A* **2016**, *120*, 4693–4701, DOI 10.1021/acs.jpca.5b10472.

[3] P. Jusko, M. Jiménez-Redondo, P. Caselli, *Mol. Phys.* **2024**, *122*, e2217744, DOI 10.1080/00268976.2023.2217744.

T3.6. A simple supersonic expansion ion source for intense pulses of cold molecular ions

17:00–17:25

Lukas Berger[1], Aigars Znotins[1], Florian Grussie[1], Felix Nuesslein[1], Xavier Urbain[2], Holger Kreckel[1]
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[2]*Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve B-1348, Belgium*
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We developed a simple pulsed supersonic gas expansion ion source for operation at the Cryogenic Storage Ring (CSR) of the Max Planck Institute for Nuclear Physics in Heidelberg. The CSR is an electrostatic storage facility that is cooled to cryogenic temperatures by a closed cycle liquid helium unit (~ 5 K). Residual gas densitys of about 1000 particles per cm^3 can be reached, and black body radiation is strongly reduced compared to room temperature experiments. Small infrared-active molecular ions cool down to their lowest vibrational and rotational states within minutes, and measurements under conditions mimicking those of interstellar space are possible. However, some astrophysically relevant ions do not cool down in accessible storage times due to the lack of a permanent dipole moment (e.g. H_2^+, H_3^+) [1]. Therefore, it is necessary to prepare those ions as cold as possible prior to injection into the CSR [2]. To adress this issue, we characterized the performance of a home-built supersonic expansion ion source, using N_2O^+ ions in the STARGATE setup at the UCLouvain [3]. We measured the internal rotational temperature using resonant photodissociation, which resulted in temperatures between 40 K and 200 K. The design and performance of the source will be presented.

[1] F. Grussie et al., *Rev. Sci. Instrum.* **2022**, *93*, 053305, DOI `10.1063/5.0086391`.

[2] F. Grussie et al., “Merged beams study of the reaction of cold HD$^+$ with C atoms reveals pronounced intramolecular kinetic isotope effect”, *Phys. Rev. Lett.*, in press.

[3] R. Bejjani et al., *Rev. Sci. Instrum.* **2021**, *92*, 033307, DOI `10.1063/5.0039627`.

FRIDAY 27. SEPTEMBER

F1. ICES AND SURFACE PROCESSES

Chair: Valerio Lattanzi

F1.1. Formation of precursors to biomolecules after irradiation of ethanolamine ice at low temperature

9:00 – 9:25

Tushar Suhasaria
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Can prebiotic molecules relevant to the origin of life form under the conditions of dense interstellar clouds? This question remains open. In our experimental investigation, we studied the UV photo-processing of solid ethylamine (EA) ice at low temperatures (around 10 K). Using FTIR and mass spectrometry, we observed the formation of glycinal, a precursor to glycine, along with other simple molecules. Upon warming the ice to room temperature, high-resolution Orbitrap mass spectrometry analysis of the resulting residue revealed the presence of several amino acids and even small peptides.

F1.2. How chemical complexity flourishes in the ISM: the role of H_2 and atomic carbon

9:25 – 9:50

Franciele Kruczkiewicz,[1], Julia C. Santos,[1] Ko-Ju Chuang[1]
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The molecular makeup of the Interstellar Medium (ISM) is crucial for understanding the birth of our solar system and the potential for life elsewhere. In translucent and dense molecular clouds, chemical complexity begins to flourish on the surface of cold dust grains that act as chemical reservoirs and catalytic surfaces. These surfaces facilitate essential reactions under energy-limited conditions, forming icy mantles rich in water (H_2O), methane (CH_4), and ammonia (NH_3), and Complex Organic Molecules. Despite advancements, gaps remain in our understanding of COMs formation routes, particularly the role of molecular hydrogen (H_2) and atomic carbon. This study experimentally investigate H_2 and atomic carbon contribution to solid-state reactions and COMs formation.
In this study, we concentrate on the experimental analysis of sulfur-bearing species utilizing the SURFRESIDE^3 setup [1]. The uniqueness of this setup relies on its beamlines that can co-deposit atomic (H/D, C, O, and N) and molecular species (H_2, CH_3OH, NH_3...), optimally designed to study solid-state formation under conditions found in translucent and molecular clouds. Interstellar ice analogues are grown on a gold-plated substrate within an ultra-high vacuum (UHV) chamber (P_{base} = 10^{-10} hPa), monitored via reflection absorption infrared spectroscopy (RAIRS) and analyzed with a quadrupole mass spectrometer (QMS) during temperature-programmed desorption (TPD) measurements.
As a result, this work will contribute to the development of more comprehensive astrochemical models and algorithms, enhancing our ability to predict and explain the formation of COMs in interstellar ices and their gas-phase abundances in star-forming regions.

[1] D. Qasim et al., *Review of Scientific Instruments* **2020**, *91*, 054501, DOI `10.1063/5.0003692`.

F1.3. Investigating Deuterated Methanol Species in Interstellar Ice Analogues via Infrared Spectroscopy

Adam Vyjídák,[1], Barbara Michela Giuliano,[1] Paola Caselli[1] 9:50–10:20
[1] *Max-Planck-Institut für extraterrestrische Physik, Garching, Germany*
vadam@mpe.mpg.de

Interstellar ices serve as reservoirs of crucial organic molecules, with methanol (CH_3OH) playing a central role as a precursor to complex organics. In this work done at the Centre for Astrochemical Studies at the Max Planck Institute for Extraterrestrial Physics, we utilize IR spectroscopy to analyze interstellar ice analogs containing mixtures of non-deuterated and deuterated methanol species across a broad spectral range from 6000 cm^{-1} to 30 cm^{-1}. Using a custom Vertex v70 spectrometer coupled to a closed-cycle cryostat in a vacuum chamber, we deposit ices at 10 K to mimic interstellar conditions. Futhermore, our investigation includes spectral analysis of ices comprising of water and deuterated methanol mixtures in different ratios, offering insights into the composition and structure of interstellar ices. Moreover, considering the significance of methanol deuteration highlighted in recent observations, our experiments address the importance of understanding deuteration processes, which can provide crucial insights into the chemistry and evolution of interstellar environments.

[1] Bizzocchi, L. et al., *A&A* **2014**, *569*, A27, DOI 10.1051/0004-6361/201423858.

[2] Parise, B. et al., *A&A* **2002**, *393*, L49–L53, DOI 10.1051/0004-6361:20021131.

[3] Parise, B. et al., *A&A* **2004**, *416*, 159–163, DOI 10.1051/0004-6361:20034490.

F1.4. Infrared irradiation of two-component H_2O-rich interstellar ice analogues

Johanna G. M. Schrauwen,[1] Sergio Ioppolo,[2] Herma M. Cuppen,[3] Britta Redlich [1] 11:00–11:25
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[2] *InterCat, Department of Physics and Astronomy, Aarhus University, Denmark*
[3] *Institute of Molecules and Materials (IMM), Radboud University Nijmegen, The Netherlands*
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Interstellar ices and their energy dissipation dynamics play an important role in advancing the chemical complexity in space. Interstellar ices are a mix of numerous molecular species and it is generally assumed that the energy dynamics in the ice structure depend strongly on its contents. We tested the influence of mixing components in H_2O-rich ices on the energy dissipation of vibrational energy in the hydrogen-bonding network. By focusing on the effect of infrared irradiation particularly, we try to relate our results to the release of excess energy from an exothermic reaction on the ice surface or direct infrared irradiation in space. Irradiation on-resonance with the OH-stretching vibration of all mixtures we investigated results in quantitatively identical changes compared to pure amorphous solid water. The restructuring closely resembles local ordering reported for amorphous solid water before [1, 2]. Weaker changes are observed for 5:1 H_2O:X mixtures with CO_2 and CH_4, whereas in a 5:1 with NH_3-mixture the changes are identical to pure water. This suggests a dependence on the ability to form hydrogen-bonds of the mixing component. Our experiments show that pure water ices qualitatively approximate the behaviour of H_2O-rich mixtures well and that it might not always be necessary to work with complex systems in the case of energy dissipation in the hydrogen-bonding network.

[1] J. A. Noble et al., *The Journal of Physical Chemistry C* **2020**, *124*, 20864–20873, DOI 10.1021/acs.jpcc.0c04463.

[2] H. M. Cuppen et al., *J Phys Chem A* **2022**, *126*, 8859–8870, DOI 10.1021/acs.jpca.2c06314.

F1.5. Effect of individual agglomerates on mid-infrared extinction spectra examined at SPring-8

11:25 – 11:50

Akemi Tamanai[1], Ryo Tazaki[2], Harald Mutschke[3], Waldemar Klauser[4], Sören Zimmerman[4], Nadia M. Murillo[5,1], Satoshi Ohashi[6,1], Takahiro Oyama[1], Ziwei Zhang[1], Shaoshan Zeng[1], Yoshimasa Watanabe[7], Nami Sakai[1]
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[2]*Institut de Planétologie et d'Astrophysique de Grenoble, Université Grenoble Alpes, Grenoble France*
[3]*AIU Jena, Friedrich-Schiller-University Jena, Jena, Germany*
[4]*Division of Microrobotics and Control Engineering, University of Oldenburg, Oldenburg, Germany*
[5]*Instituto de Astronomia Ensenada, Universidad Nacional Autónoma de México, Ensenada, Mexico*
[6]*National Astronomical Observatory of Japan, Mitaka, Tokyo, Japan*
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For interpretation of the observed spectra of dust grains in detail, it is essential to take into account of not only physical properties of dust grains, but also chemical properties of them [e.g., 1]. Even among those, dust grain morphology (individual size, shape, agglomeration state) is one of the factors that strongly influences on the infrared band profiles [2], and thus this makes the interpretation of observed spectra exceedingly difficult. In particular, the extent to which differences in agglomerate structure affect infrared spectra is not yet fully understood. Hence, we focus on the agglomerate structure consisting of micron-sized fine particles and have performed laboratory-based spectroscopic extinction spectrum measurements of each agglomerate having different structure at a Japanese synchrotron facility, the Super Photon ring-8 GeV (SPring-8). Is it really correct that agglomerates and clumps will have the same band profile if they are the same overall size? Verification has been carried out by comparing light scattering simulations with our experimental results which may provide a clue to understand the dust grain growth mechanism and its surrounding environment.

[1] J. Olofsson et al., *AA* **2012**, *A90*, DOI 10.1051/0004-6361/201118735e.

[2] A. Tamanai et al., *AA* **2018**, *619*, DOI 10.1051/0004-6361/201833119.

F1.6. Rotational Spectroscopy of Deuterated Species: Bis Deuterated Glycolaldehyde and (Z)-1,2-Ethenediol

11:50 – 12:15

Michela Nonne[1], Mattia Melosso[2], Francesca Tonolo[2], Luca Bizzocchi[2], Silvia Alessandrini[2], Jean-Claude Guillemin[3], Luca Dore[2] and Cristina Puzzarini[2]
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[2]*Dipartimento di Chimica "Giacomo Ciamician", Università di Bologna, Via F. Selmi 2, 40126 Bologna, Italy*
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In some regions of the Interstellar Medium (ISM) the D/H ratio of molecules has been observed to be much higher than the elemental one ($\sim 10^{-5}$). The study of deuterated species is thus a precious tool for elucidating the formation mechanisms of Complex Organic Molecules (COMs) and whether they form in the gas phase or on the icy surface of interstellar dust grains. Glycolaldehyde is considered an important prebiotic molecule and it is a highly investigated COM which has been detected in the ISM [1] along with its enolic form (Z)-1,2-ethenediol [2]. Here we report on the acquisition and characterization of the rotational spectra of doubly-deuterated glycolaldehyde (CHD–ODCHO) and of the singly- and doubly-deuterated forms of (Z)-1,2-ethenediol (CHOD=CHOD, CHOD=CHOH and CHOH=CHOD). These species have been generated through flash vacuum pyrolysis at ca. 750°C. Our analysis covers the spectral regions between 80–115 GHz and 250–300 GHz and yielded accurate determination of the rotational and centrifugal distortion constants. These findings allowed for the calculation of an improved semi-experimental equilibrium structure of glycolaldehyde, by providing an additional set of rotational constants (those of CHD–ODCHO). Furthermore, from our results we have computed new spectral line catalogues for guiding astronomical observations.

[1] J. M. Hollis, F. J. Lovas, P. R. Jewell, *Astrophys. J.* **2000**, *540*, L107, DOI 10.1086/312881.

[2] M. Melosso et al., *Chem. Commun.* **2022**, *58*, 2750–2753, DOI 10.1039/d1cc06919e.

F2. SPECTROSCOPY

Chair: Mitsunori Araki

F2.1. High resolution laboratory spectroscopy of deuterated complex organic molecules (COMs)

14:15 – 14:40

Hayley A. Bunn,[1] Silvia Spezzano,[1] Laurent Coudert,[2] Jean-Claude Guillemin [3], Christian Endres,[1] Valerio Lattanzi,[1] Paola Caselli ,[1]
[1] *Max-Planck-Institut für extraterrestrische Physik, Gießenbachstraße 1, D-85748 Garching bei München, Germany*
[2]*Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Université Paris-Sud, Université Paris-Saclay, 91405 Orsay, France*
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Isotopologue abundance ratios are pivotal for tracing the origin and evolution of the molecular material in the process of star and planetary system formation. By following the isotopic fractionation of some crucial molecules, we now have observational evidence that the chemistry does not undergo a complete reset with the formation of the protostar, and hence pre-stellar cores provide the budget of matter that will finally form stars and planets [1]. In order to correctly determine the formation of inheritance of complex organic molecules (COMs) we, therefore, must also identify the associated isotopologues and their relative abundance. Our group has previously measured the laboratory spectrum of doubly deuterated acetaldehyde allowing for its first identification and quantification in the pro-stellar region, IRAS 16293 [2]. We are continuing this study into deuterated complex organic molecules, in particular methyl mercaptan (CH_2DSH/CHD_2SH), methyl formate (CH_2DOCOD/CHD_2OCOD), and methanol (CH_2DOD/CHD_2OD), where all molecules contain an asymmetric methyl rotor resulting in complex spectral patterns. I will present our efforts to collect and analyse the rotational spectrum of these species and potential searches for these species in IRAS 16293.

[1] L. I. Cleeves et al., *Science* **2014**, *345*, 1590–1593, DOI 10.1126/science.1258055.

[2] Ferrer Asensio, J. et al., *A&A* **2023**, *670*, A177, DOI 10.1051/0004-6361/202245442.

F2.2. Progress report on the vibrational and rotational spectra of protonated isothiocyanic acid, $H_2NCS^+/HNCSH^+$

14:40 – 15:05

Marius Gerlach,[1] Bryan Changala,[2] Noël Schneider,[1] Britta Redlich,[1] Sandra Brünken[1]
[1]*HFML-FELIX Laboratory, Radboud University, Toernooiveld 7, 6525 ED Nijmegen, The Netherlands*
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Isothiocyanic acid, HNCS, was detected for the first time in 1979 in Sagitarrius B2.[1] Since then it has been detected in other star forming regions[2] and molecular clouds[3] and its isomer thiocyanic acid, NCSH, could be identified in Sagitarrius B2.[4] Most recently, thiofulminic acid (HNCS) was also discovered in TMC-1.[5]

The formation of HNCS is proposed to proceed via the ionic intermediates NCS^+, $H_2NCS^+/HNCSH^+$ and $HNCS^+$, analogous to the formation chemistry of isocyanic acid, HNCO.[3] In this contribution, we present our progress towards investigating these ions in the laboratory, beginning with the protonated intermediates $H_2NCS^+/HNCSH^+$. At the FELIX (Free Electron Lasers for Infrared Experiments) laboratory we form these ions by electron impact ionization of a HNCS sample in a radiofrequency storage ion source. Broadband infrared spectra are then recorded in the FELion 22-pole ion trap instrument coupled to FELIX[6] and analyzed by comparison to high-level quantum-chemical calculations. Additionally, we conduct measurements in a Fourier Transform Microwave spectrometer located at the Harvard-Smithsonian Center for Astrophysics, providing high-resolution rotational transition frequencies of $H_2NCS^+/HNCSH^+$.

The reference data provided by these experiments will enable the detection and investigation of these ions in the interstellar medium, which according to theoretical studies is promising.[7]

[1] M. A. Frerking, R. A. Linke, P. Thaddeus, *Astrophys. J.* **1979**, *234*, L143–L145, DOI 10.1086/183126.

[2] L. Velilla Prieto et al., *Astron. Astrophys.* **2015**, *575*, A84, DOI 10.1051/0004-6361/201424768.

[3] G. R. Adande et al., *Astrophys. J.* **2010**, *725*, 561, DOI 10.1088/0004-637X/725/1/561.

[4] D. T. Halfen et al., *Astrophys. J. Lett.* **2009**, *702*, L124–L127, DOI 10.1088/0004-637x/702/2/L124.

[5] J. Cernicharo et al., *Astron. Astrophys.* **2024**, *682*, L4, DOI 10.1051/0004-6361/202349105.

[6] P. Jusko et al., *Faraday Disc.* **2019**, *217*, 172–202, DOI `10.1039/C8FD00225H`.

[7] M. Gronowski, R. Kołos, *Astrophys. J.* **2014**, *792*, 89, DOI `10.1088/0004-637X/792/2/89`.

F2.3. High-resolution infrared spectroscopy of protonated diacetylene, $H_2C_4H^+$

15:05 –15:30

Divita Gupta,[1] Marcel Bast,[1] Samuel J. P. Marlton,[1] Sven Thorwirth [1] Oskar Asvany [1] Thomas Salomon [1] Philipp C. Schmid [1] Stephan Schlemmer [1]
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Molecular ions are long known to be key intermediates in the evolution of molecular complexity in the interstellar medium (ISM). Ion-neutral reactions involving hydrocarbon ions can play an important role in the bottom-up approach towards cyclic and polycyclic aromatic hydrocarbons. High-resolution rovibrational and pure rotational spectra are essential to obtain crucial inputs for an unambiguous identification of ions in space. So far, three unsaturated hydrocarbon cations with a linear carbon backbone, C_3H^+, C_5H^+ and $H_2C_3H^+$, have been detected in the ISM towards the cold molecular cloud TMC-1 [1–3].

Here, I will present the high-resolution rovibrational spectrum of protonated diacetylene ($H_2C_4H^+$) measured using the recently developed leak-out spectroscopy (LOS) method [4]. With the combined use of a quantum cascade laser and a cw-OPO, the fundamental acetylenic C–C stretch, the acetylenic C–H stretch, as well as the symmetric and anti-symmetric CH_2 stretches were measured in two cryogenic 22-pole ion trap setups. The rotational constants for the ground state and the four vibrational states could aid future astronomical searches for this hydrocarbon ion. Protonated diacetylene exists in two nuclear spin configurations with an *ortho*/*para* ratio of 3:1. By selectively leaking out one, nuclear-spin state selective samples could be prepared in the ion trap. The future potential of LOS to isolate nuclear spin configurations and structural isomers will also be discussed.

[1] S. Brünken et al., *The Astrophysical Journal* **2014**, *783*, L4, DOI `10.1088/2041-8205/783/1/L4`.

[2] J. Cernicharo et al., *Astronomy & Astrophysics* **2022**, *657*, L16, DOI `10.1051/0004-6361/202142992`.

[3] W. Silva et al., *Astronomy and Astrophysics* **2023**, *676*, DOI `10.1051/0004-6361/202347174`.

[4] P. C. Schmid et al., *The Journal of Physical Chemistry A* **2022**, *126*, 8111–8117, DOI `10.1021/acs.jpca.2c05767`.

F2.4. Infrared-Millimetre Wave Double Resonance Spectroscopy in Supersonic Jets

16:00 –16:35

Guido Fuchs, Eileen Döring, Fabian Peterß, Jan Jakob, **Thomas Giesen**
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With the launch of the James Web Space Telescope (JWST), an outstanding new instrument is available for astronomical observations in the infrared spectral region. The spectral resolution of the telescope enables the detection of rotationally resolved vibrational spectra of small molecules and their assignment to the molecular carriers. For medium-sized molecules, at least the band contours can be resolved with JWST, giving inside to the molecular abundance, excitation mechanism, and dynamics of the gas. Precise laboratory data is required for the astronomical detection of molecules using IR spectroscopy. There is a lack of laboratory infrared data, especially for hot, vibrationally excited states.

The talk presents our current laboratory efforts to measure and analyze ro-vibrational spectra of medium size molecules. IR-MM double resonance excitation of cold molecules in a supersonic jet is used to identify rotational-vibrational transitions in excited vibrational states. Recent results on propylene oxide and related species will be presented.

F2.5. Infrared Electronic Transition of HCN^+ Measured Using LEAK-OUT Spectroscopy

16:35 –17:00

Samuel J. P. Marlton,[1] Philipp C. Schmid,[1] Weslley G. D. P. Silva,[1] Oskar Asvany [1] Stephan Schlemmer [1]
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The spectroscopy of HCN^+ is of astronomical and fundamental interest. The HCN^+ cation has two low lying electronic states—a $\tilde{X}^2\Pi$ ground state and an excited $\tilde{A}^2\Sigma^+$ state—which are mixed by spin-orbit and vibronic coupling.[1] Although these states have been observed previously,[2] gas-phase transitions between cationic electronic states of HCN^+ have never been reported. This is predominantly because the aggressive reactivity of HCN^+ obstructs spectroscopic investigation in supersonic expansions and discharges. Furthermore, the low energy of the transition (approx 3250 cm^{-1}) complicates action spectroscopic techniques like infrared multiple photon dissociation or messenger tagging. To overcome these obstacles and measure the $\tilde{X}^2\Pi$ to $\tilde{A}^2\Sigma^+$ transition of HCN^+, we employ the novel leak-out spectroscopy technique (LOS).[3] The spectrum exhibits rotational, fine, and hyperfine structure that precisely describe the nature of these electronic states. This is the first reported electronic spectrum using the LOS method. Future measurements might demonstrate whether LOS is well suited to measuring electronic spectra of ions that resist photodissociation after being excited electronically. This could be helpful for unraveling the mystery of the unidentified absorption bands that have been detected by astronomers in the visible and near infrared—referred to as diffuse interstellar bands—which are presumed to arise from photostable molecules.[4]

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F2.6. Broadband Infrared Spectroscopy of $[C_2H_5O_2]^+$ ions: Protonated methyl formate, acetic acid and glycolaldehyde

17:00–17:25

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The astronomically observed abundances of the isomeric trio methyl formate, acetic acid offer crucial insights into the formation pathways of complex organic molecules (iCOMs). Their formation is often proposed via their protonated analogues, but limited spectroscopic data on the latter hampers their astronomical detection and the understanding of specific formation pathways. Here we present the first broadband vibrational analysis of the corresponding $[C_2H_5O_2]^+$ isomers protonated methyl formate, acetic acid, and glycolaldehyde. The ions were formed via electron impact ionization of their respective vapors (dimer for glycolaldehyde) in a storage ion source. Vibrational spectra of the mass-selected ions were recorded in the 650-1800 cm^{-1} range by Ne-tagging IRPD spectroscopy in the FELion cryogenic 22-pole ion trap instrument coupled to the infrared free-electron lasers at the FELIX Laboratory [1]. Experimental spectra are compared to vibrational frequencies calculated at the B2PLYPD3/aug-cc-pVTZ level of theory. Protonated forms of both methyl formate conformers (syn and anti) were identified, with protonation on the carbonyl oxygen in trans and cis orientations, respectively. The lowest energy conformer (E,Z) of carbonyl-protonated acetic acid was mainly observed, and a potential isomerization to protonated glycolaldehyde will be discussed. Using glycolaldehyde dimer as precursor, the lowest energy isomers of both protonated glycolaldehyde and acetic acid were observed.

[1] P. Jusko et al., *Faraday Discuss.* **2019**, *217*, 172–202, DOI 10.1039/C8FD00225H.

Discussion Sessions

D.1. Priorities of Lab Astro for the next decade(s) in connection to current and upcoming astronomical facilities

Thu. 13:30–14:15

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Selected current and future facilities:

- ALMA; NOEMA; GBT
- Yebes; 30m telescope
- JWST
- SKA
- ELT
- ngVLA

D.2. Common activities among the German LabAstro community

Thu. 17:25–18:10

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Discussion will be focused on common activities among and the future of the German LabAstro community:

- annual meeting, common proposals for funding,
- exchange of equipment (e. g.: Cologne Center for THz Spectroscopy, FELion, light sources (lasers). . .)
- strengthening of our community (exchange between laboratories); careers,
- addition of further working groups/ replacing retirements,
- engagement in / relation to european/ international activities (e. g. ECLA).

D.3. Astrochemistry: Gas Phase vs Solid State

Fri. 13:30–14:15

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One of the fundamental questions regarding astrophysical and (exo)planet atmosphere environments and small Solar System bodies (comets, asteroids and their meteoritic remains) is the nature and abundance of detected molecular species. Chemical processes leading to the formation of molecules in space can be divided into two groups, gas phase and dust grain surface reactions. Surface reaction pathways lead to a greater complexity of molecular species. Experimental and computational studies have even shown that the building blocks of biological macromolecules, such as amino acids and nucleobases, can be produced in surface reactions under astrophysically relevant conditions. These studies in combination with the detection of the aforementioned species in comets and meteorites link astrochemistry to the big scientific question - the origin of life on Earth - and motivate the search for extraterrestrial life and other habitable planets. Does this mean that exploring pathways to prebiotic molecules we should forget about gas-phase astrochemical networks? What is the level of molecular complexity that can be reached in gas-phase and solid-state experiments? Should we think about experiments combining gas-phase and solid-state chemistries as it's done in some astrochemical models? These are the questions I would like to discuss.

D.4. Towards a “cdms” for infrared spectroscopy?

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Fri. 17:25 – 18:10

The radioastronomical community profits from a decades long investment in spectroscopic databases for rotational spectroscopy, like the Cologne Database for Molecular Spectroscopy, the JPL catalogue, and recently VAMDC. This is complemented by databases adding collisional excitation data like the Leiden Atomic and Molecular Database (LAMDA). With the exciting molecular infrared spectra delivered by JWST, the question arises if a similar endeavour needs to be undertaken for (ro-)vibrational data. We should hear the opinion from our community on where data is lacking, how it can be organized, if we need databases in addition to HITRAN and EXOMOL, or how we can contribute. One example would be a compilation of experimental data on PAHs (where to date mainly calculated spectral templates are used), or on other complex hydrocarbons now detected, e.g., within the MINDS survey towards protoplanetary disks, and which species are relevant in exoplanetary atmospheres.

POSTERS

P.1. Laboratory detection of 2,5- and 2,4-cyclohexadien-1-thione

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Many aromatic compounds including bicyclic polycyclic aromatic hydrocarbons have been detected since benzonitrile was found in the dark cloud TMC-1[1]. Due to the richness of sulfide compounds in space, the presence of sulfur-containing aromatic compounds is expected. Using a combination of a chirped pulse Fourier transform microwave spectrometer and a pulsed-discharge supersonic-jet system, discharge products of thiophenol in a buffer gas of neon were unbiasedly studied in the frequency range of 8-26 GHz. The molecules are observed at rotational temperatures of about 3-5 K under these conditions. Lines of 19 and 13 rotational transitions could be assigned to the two sulfide aromatic hydrocarbons 2,5-cyclohexadiene-1-thione and 2,4-cyclohexadiene-1-thione (C_6H_6S), respectively. This first laboratory detection made it possible to determine the molecular constants of these molecules and thus precise rest frequencies in the centimeter-wave range, enabling the molecules to be searched for in space.

[1] B. A. McGuire et al., *Science* **2018**, *359*, 202–205, DOI `10.1126/science.aao4890`.

P.2. Excitation diagram analysis of high-resolution infrared TiO spectra towards the variable star χ Cyg

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Cosmic dust is formed by nucleation processes in the vicinity of evolved stars. Small molecules of refractory materials formed during these nucleation processes play an important role in dust formation and are also involved in the opacity process of variable late-type stars, as has been shown for the molecule TiO [1]. Recently we presented the high resolution infrared spectrum of TiO and its isotopologues, measured in the laboratory around 10 µm [2]. Using the TEXES instrument on IRTF in its high resolution mode [R =100,000] together with the laboratory data allow unambiguous identification of molecules and enable line shape analysis of the observed molecular spectra. Over a time period of three years various stellar phases of χ Cyg around $970\,\mathrm{cm}^{-1}$ were observed with the TEXES instrument. TiO was detected in the mid-IR region, for the first time. Using a home made data analysis software, it was possible to perform an excitation diagram analysis to determine the non-equilibrium temperature and column density of TiO in the envelope of χ Cyg.

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[2] D. Witsch et al., *J. Mol. Spectrosc.* **2021**, *377*, 111439, DOI `10.1016/j.jms.2021.111439`.

P.3. Formation of doubly- and triply-charged C_{60} dimers

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We report on the astonishing formation and stabilization of doubly- and triply-charged C_{60} dimers within superfluid helium nanodroplets (HNDs) [1]. Previously, it has been shown that cluster sizes of $n \geqslant 5$ and $n \geqslant 10$ are required for the stabilization of doubly and triply-charged cationic $(C_{60})_n$ clusters, respectively [2]. Our novel method uses efficient cooling in the superfluid helium environment and a stepwise ionization process to stabilize these clusters against Coulomb explosion [1].

In our setup, HNDs are created within the supersonic expansion of helium and subsequent electron impact ionization leads to the formation of multiply-charged HNDs [3]. The multiply-charged droplets are then doped with the C_{60} molecules which are evaporated in an oven. The C_{60} molecules are attracted by the charges in the droplet and ionized via charge transfer. Further pick-up of C_{60} molecules leads to the formation of singly charged $(C_{60})_n{}^+$ clusters embedded in HNDs. Electron bombardment from a second electron impact source creates again He^+ and metastable Helium atoms in the HND. While He^+ ions are repelled by the charged $(C_{60})_n{}^+$ clusters, metastable Helium can Penning ionize $(C_{60})_n{}^+$. The resulting multiply-charged $(C_{60})_n$ clusters are extracted from the HNDs through collisions with room-temperature helium gas and detected with a time-of-flight mass spectrometer [1]. Since neutral C_{60} and $C_{60}{}^+$ have already been detected in space [4, 5] and a stepwise ionization can also occur in space, multiply-charged fullerene complexes might be of astrophysical relevance.

Acknowledgment This research was funded by the Austrian Science Fund (FWF) [10.55776/W1259, 10.55776/V1035, 10.55776/P34563]. This contribution is based upon work from COST Action NanoSpace, CA21126, supported by COST (European Cooperation in Science and Technology).

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[5] J. Cami et al., *Science* **2010**, *329*, 1180–1182, DOI `10.1126/science.1192035`.

P.4. Synthesis of CO_2 and CO in ice-coated organic residues

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Carbonaceous matter and ices are present in dense molecular clouds [1], star forming regions and on the surface of outer solar system objects (such as icy moons [2, 3]). It is widely accepted that in these environments dust and ice are continuously processed by energetic ions such as galactic cosmic rays, stellar winds or magnetospheric ions. Ion irradiation induces physico-chemical alterations on surface materials, such as the formation of new species (like CO_2 and CO) at the interface between ice and refractory organics. This work expands previous similar experiments [4–8] on interface chemistry mechanisms by employing an isotopically labeled organic sample with a relatively flat surface geometry.

Experiments here presented have been performed in the Laboratory for Experimental Astrophysics (LASp) at INAF - Catania Astrophysical Observatory (Italy). Our study aims to characterize the evolution of the chemical species (especially of CO_2 and CO) induced by ion irradiation of ice deposited on refractory C-rich material. The initial sample (methane layers on silicon substrates), in a stainless ultra-high vacuum chamber ($\sim 10^{-9}$ mbar), at a temperature of 18 K, has been irradiated by 200 keV H^+ ions to obtain a refractory organic residue. After the formation of the organic residue, ices (H_2O, O_2) were deposited on the organic residue and irradiated by 200 keV H^+. Infrared transmission spectra were taken before irradiation and at different steps of irradiation.

As a result of the irradiation several IR bands arise. We observe the formation of CO_2 and CO at the interface between the ice and the residue. For each experiment, the CO_2 and CO effective cross section has been estimated, as well as their column density equilibrium values

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[2] F. Tosi et al., *Journal of Geophysical Research: Planets* **2023**, *128*, e2023JE007836, DOI `10.1029/2023JE007836`.

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P.5. MOCCA - A 4k-Pixel Molecule Camera for CSR

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More than 300 different molecules have been identified in interstellar clouds, despite their low pressures and temperatures of only a few kelvins. The mechanisms that lead to the formation of these molecules are not yet fully understood. However, an important reaction is the dissociative recombination, in which a molecular ion recombines with an electron and then dissociates into neutral fragments. For further investigation, the Cryogenic Storage Ring CSR was built at the Max Planck Institute for Nuclear Physics in Heidelberg. In CSR, extreme conditions similar to those in interstellar clouds can be reproduced in laboratory and reactions such as the dissociative recombination can be investigated. To reconstruct the complete reaction kinematics, a position-sensitive coincident detection of all neutral reaction products is required. For this purpose, the MOCCA detector was developed at the Kirchhoff Institute for Physics in Heidelberg. MOCCA is based on metallic magnetic calorimeters and is operated at temperatures of only a few millikelvins. It has a sensitive area of about 45 mm × 45 mm consisting of 4094 pixels which can be read out with only 32 two-stage SQUID channels. We present characterization measurements as well as the integration of MOCCA and its ^{3}He/^{4}He dilution refrigerator into a CSR-independent standalone setup, that will be used to study photon- and collision-induced ion fragmentation processes before MOCCA will be integrated into CSR.

P.6. Ion traps for public outreach

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MPE organises an open day for general public on 3. October 2024. For this occasion, engineers from mechanical and electrical workshops of MPE were involved in creating something entertaining, but at the same time useful for understanding the basics of "particle" trapping in non-stationary fields. In particular dust-trap and a rotating saddle trap are going to be displayd. Hands on experience is expected and welcome.

P.7. Laboratory Rotational Spectroscopy of Doubly Deuterated Methyl Formate (CH_2DOCDO)

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The study of isotopologues of Complex Organic Molecules (COMs) in the Interstellar Medium (ISM) provides essential insights into the chemical processes that occurred in the early solar system and their potential role in prebiotic chemistry. Here, laboratory work bridges the gap between theoretical predictions and astronomical observations. Our work focuses on building an accurate spectroscopic catalog, necessary for the interstellar detection of doubly deuterated methyl formate (CH_2DOCDO) by measuring its millimeter/submillimeter spectrum in the laboratory. Observing these transitions in space provides valuable insights into the ISM's molecular composition, dynamics, and environmental conditions. For that, we rely heavily on laboratory spectra, especially due to the complex spectral patterns caused by the molecules' asymmetric methyl rotor. Previous laboratory research has been focused on characterizing the spectral properties of CH_3OCDO [1], which has single deuteration on the aldehyde group (CHO). Prior laboratory measurements have also been taken for the singly (CH_2DOCHO) [2], and doubly deuterated methyl formate (CHD_2OCHO) [3], with deuteration occurring on the methyl group (CH_3). All three isotopologues have been identified in the ISM. CH_2DOCHO was detected in the Orion KL nebula [4], whereas CH_3OCDO and CHD_2OCHO were found towards IRAS16293-2422 [5] [6]. This provides a foundation for our current work on CH_2DOCDO. By measuring deuteration on both the methyl and aldehyde groups, our study aims to gain deeper insights into how deuteration at different sites within the molecule influences its spectral properties and the deuterium fractionation mechanisms during star formation. We will present the spectral analysis of these complex spectra.

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P.8. Hot Exozodiacal Dust: Infrared Thermal Emission Spectroscopy in the Laboratory

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We have launched a project whose aim is to contribute to the identification of the materials that make up hot exozodiacal dust disks (exozodis). Exozodis are frequent and appear to consist of submicronic grains possibly as hot as 2000 K because of their location very close to the star. The composition and therefore the origin of these grains are currently undetermined. Given that the presence of hot exozodiacal grains is revealed by their thermal emission at near- and mid-infrared wavelengths, we aim to obtain the optical constants of relevant materials at high temperatures in the infrared wavelength range. These data will allow us to compute thermal emission spectra for different grain geometries and sizes, which we will compare to astronomical observation data in order to identify or constrain the composition of hot exozodis. We will derive the optical constants of the materials from the analysis of Fourier-transform infrared (FTIR) thermal emission spectra complemented with FTIR reflection spectra. Heating the materials in steps from room temperature to 1800 K for emission spectroscopy, to 1000 K for reflection spectroscopy, will allow us to characterize the temperature dependence of the optical constants. In order to perform FTIR thermal emission measurements, an objective of the project is to bring this technique into our laboratory. We will present the project in detail and report on first measurements.

P.9. Destruction Mechanisms for Astrochemically Relevant Anions

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Eight negatively charged molecules have been thus far been detected in the interstellar medium, and more are expected to exist. The confirmed anions are nitrogen- or hydrogen-terminated carbon chains, of the form C_nN^- (n=1,3,5,7) or C_nH^- (n=4,6,8,10). Another class of substances of interest are charged polycyclic aromatic hydrocarbon (PAH) molecules, which could be the main carrier for negative charge in interstellar clouds [1] and may contribute to the aromatic infrared emission bands [2]. The destruction mechanisms for these anions require experimental determination for accurate rate models. Two important destruction mechanisms for anions are direct photodetachment and associative detachment with neutral atoms or molecules [3, 4].
We present photodetachment spectroscopy of deprotonated naphthalene ($C_{10}H_7^-$) using 2D tomography on the loss rate of the ions in our cryogenic 16-pole wire trap, extracting the absolute photodetachment cross section [5]. We also present the associative detachment reaction rates with atomic hydrogen of deprotonated naphthalene, as well as CN^- and C_3N^-, the latter showing significant deviations from the previously measured rates at 300 K [6]. Progress on near-threshold photodetachment cross-section measurements on naphthalene will also be reported.

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[5] S. Purushu-Melath et al., in preparation.

[6] C. Lochmann et al., in preparation.

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