New Frontiers at Heavy Ion Storage Rings: From Atomic Collisions to Many-Body Systems

738. WE-Heraeus-Seminar

20 - 24 June 2022

HYBRID
at the Physikzentrum Bad Honnef/Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

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

Aims and scope of the 738. WE-Heraeus-Seminar:

Charged particles are ubiquitous in nature and they are highly relevant in a diverse range of fields and disciplines, ranging from atomic physics all the way to biochemistry. To study the properties and reactions of atomic and molecular ions in the laboratory often presents a formidable challenge. Owing to their high reactivity they need to be separated from their surroundings and prepared in controlled quantum states for meaningful experiments.

In this context heavy ion storage rings have proven to be extremely versatile instruments for detailed studies of ionic systems in a variety of fields. Originally intended for storage of atoms and nuclei, heavy ion storage rings have also become invaluable tools in the field of electronic collisions and molecular physics. With the advent of electrostatic storage rings, which allow for mass-independent storage, even experiments with heavy clusters ions and bio-molecules have become feasible.

The goal of the seminar is to bring together experts from experiment and theory in the field for a constructive discussion of the most promising paths to maximize the impact of the available facilities and exploit synergies among the groups. Besides invited presentations on the status at the leading facilities, also the potential of new technological developments will be discussed. Students and young researchers in the field will have the opportunity to present their ideas in two series of contributed talks.

Scientific Organizers:

Prof. Dr. Klaus Blaum	Max-Planck-Institut für Kernphysik, Heidelberg, Germany E-mail: klaus.blaum@mpi-hd.mpg.de
Dr. Holger Kreckel	Max-Planck-Institut für Kernphysik, Heidelberg Germany E-mail: holger.kreckel@mpi-hd.mpg.de
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Introduction

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Registration:

Mojca Peklaj (WE Heraeus Foundation)
at the Physikzentrum, Reception Office
Monday (09:00 h – 12:00 hrs)

Program

Program *(CEST)*

Sunday, 19 June 2022

18:00	*BUFFET SUPPER for attendees arriving on Sunday*	

Monday, 20 June 2022

08:00	*BREAKFAST for attendees arriving on Sunday*	
09:00 – 12:00	ARRIVAL and REGISTRATION	
12:30 – 14:00	*LUNCH*	
14:00 – 14:15	Organizers	**Welcome**
Session 1: Magnetic Storage Rings (Chair: Andreas Wolf)		
14:15 – 15:00	Daniel Zajfman	**The Test Storage Ring @ MPIK and Molecular Ions: A Thirty-Year Perspective**
15:00 – 15:45	Gerard Tranquille	**AD-ELENA, The Low Energy Antiproton Facility at CERN**
15:45 – 16:15	*COFFEE BREAK*	
16:15 – 17:00	Michael Lestinsky	**First Experiments with CRYRING@ESR**
Contributed Talks 1 (Chair: Claude Krantz)		
17:00 – 17:20	Weronika Biela-Nowaczyk	**Dielectronic Recombination in He-like Oxygen Ions Investigated at CRYRING@ESR**
17:20 – 17:40	Leonard Isberner	**First Dielectronic Recombination Measurements at the Cryogenic Storage Ring**
17:40 – 18:00	Pierre-Michel Hillenbrand	**Experimental Studies of Nonperturbative Dynamics in Heavy-Ion-Atom Collisions**

Program *(CEST)*

18:00 – 18:20	Paul Fischer	**Time-Resolved Cluster Photo-dissociation in a Multi-Reflection Time-of-Flight Mass Spectrometer**
18:20 – 18:40	*Åsa* Larson	**Ab Initio Studies on Charge Recombination Scattering Processes**
19:00	*DINNER*	

Program *(CEST)*

Tuesday, 21 June 2022

08:00	*BREAKFAST*	
Session 2: Experiments at Electrostatic Facilities (Chair: Viviane Schmidt)		
09:00 – 09:45	Toshiyuki Azuma	**Slow Deexcitation Dynamics of Molecular Ions Stored in RICE and TMU E-Ring**
09:45 – 10:30	Lars H. Andersen	**Femtosecond Dynamics of Molecular Ions, Studied by Time-Resolved Action Spectroscopy in an Ion-Storage Ring**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Oldrich Novotny	**The Cryogenic Storage Ring CSR**
11:45 – 12:30	Henning T. Schmidt	**Mutual Neutralization Studies with Merged Beams of Stored Ions**
12:30 – 14:00	*LUNCH BREAK*	
Session 3: Collisions (Chair: Abel Kalosi)		
14:00 – 14:45	Alfred Müller	**The Role of Ion Storage Rings in Studying Electron-Ion Collisions**
14:45 – 15:30	Emily Lamour	**Ion-Ion Collisions for Atomic Cross Sections Measurements: The FISIC Project at CRYRING**
15:30 – 16:15	Ioan F. Schneider	**Electron Impact Excitation and Recombination of Molecular Cations: Theoretical Studies and Comparison with Storage Ring Experiments**
16:15 – 16:30	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
16:30 – 19:00	**Poster Session / *COFFEE***	
19:00	*DINNER*	

Program *(CEST)*

Wednesday, 22 June 2022

08:00	*BREAKFAST*	
Session 4: Understanding Astrophysical Complexity (Chair: Xavier Urbain)		
09:00 – 09:45	Christine Joblin	**Study of PAH Photophysics in an Astrophysical Context: The Role of Storage Devices**
09:45 – 10:30	Daniel W. Savin	**Astrophysically Motivated Electron-Ion Merged-Beams Studies Using the MPIK Heavy Ion Storage Rings**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Alicia Domaracka	**Ion Processing of Molecular Clusters: A Way to Form Complex Systems in Space**
11:45 – 12:30	Annemieke Petrignani	**Spectroscopy of Interstellar Complex Organic Molecules**
12:30 – 13:30	*LUNCH BREAK*	
13:30	**Excursion:** **Hike to Drachenfels vista point and Schloss Drachenburg with refreshments in the park. Details will be announced.**	
19:00	*DINNER* at the Physikzentrum	

Program *(CEST)*

Thursday, 23 June 2022

08:00	*BREAKFAST*	
Session 5: Understanding Atoms and Molecules (Chair: Åsa Larson)		
09:00 – 09:45	Sadia Bari	**Spectroscopy of Biomolecular Ions at the Advanced Light Sources**
09:45 – 10:30	Carsten Brandau	**Towards Storage Ring Studies of Highly Charged 229Th Using Nuclear Hyperfine Mixing**
10:30 – 11:00	COFFEE BREAK	
11:00 – 11:45	Eva Lindroth	**Resonances in the Time and Frequency Domain**
11:45 – 12:30	Robert E. Continetti	**Reaction Dynamics and Particle Impact Studies with Linear Electrostatic Storage Devices**
12:30 – 14:00	*LUNCH BREAK*	
Session 6: New Instruments and Techniques (Chair: Felix Nuesslein)		
14:00 – 14:45	Lisa Gamer	**MOCCA: A 4-Kilo-Pixel Microcalorimeter Detector for CSR**
14:45 – 15:30	Oded Heber	**Merged Beams with Electrostatic Ion Beam Traps (EIBT)**
15:30 – 16:15	Robert Moshammer	**Prospects of the CSR Reaction Microscope for In-Ring Electron and Ion Spectroscopy**
16:15 – 17 :00	COFFEE BREAK	

Program *(CEST)*

Contributed Talks 2 (Chair: Lutz Schweikhard)

17:00 – 17:20	Arnaud Dochain	**Measuring Differential Cross Sections with the Merged Beam Method**
17:20 – 17:40	Stephan Fritzsche	**A Community Platform for Just Atomic Calculations (JAC)**
17:40 – 18:00	Sebastian Fuchs	**High-resolution Dielectronic Recombination Spectroscopy with Slow Cooled Pb78+ Ions in the CRYRING@ESR Storage Ring**
18:00 – 18:20	Zsolt Mezei	**New Insights in the Low Energy Electron-driven Reactivity of Hydride Cations**
18:20 – 18:40	Viviane Schmidt	**Identification and Removal of Molecular Contaminations at CSR Using Isochronous Mass Spectrometry**
19:00	*HERAEUS DINNER* at the Physikzentrum (cold & warm buffet, with complimentary drinks)	

Program *(CEST)*

Friday, 24 June 2022

08:00	*BREAKFAST*	
Session 7: New Challenges from Astrophysics to Atmospheric Processes (Chair: Annemieke Petrignani)		
09:00 – 09:45	James Babb	**Radiative Association of Atomic and Ionic Carbon**
09:45 – 10:30	Roland Wester	**Controlled Interactions of Cold Trapped Negative Ions**
10:30 – 11:00	COFFEE BREAK	
11:00 – 11:45	Viatcheslav Kokoouline	**Recent Progress in Theoretical Description of Dissociative Recombination of Polyatomic Molecular Ions**
11:45 – 12:30	Richard D. Thomas	**Probing Charge-Transfer Reactions of Atmospheric Importance Using the Ion Storage Facility DESIREE**
12:30 – 12:45	Organizers	**Closing Remarks**
12:45	*LUNCH*	

End of seminar and departure

Posters

Poster Session – Tuesday, 21 June, 16:30 h (CEST)

1	Saroj Kumar Barik	**Gas-phase Formation of FeCN- in Astrophysical Environment**
2	Lukas Berger	**Dielectronic Recombination of Neon in the Polar-X-EBIT**
3	Joshua Forer	**Dissociative Recombination and Rovibrational Excitation of CF+ and CH+ in Collisions with Low-Energy Electrons**
4	Selina Gaisser	**Enhanced Detection Rate for a 3D-imaging Detector at CSR**
5	Florian Grussie	**Merged Beams Experiments Between Neutral Atoms and Molecular Ions at the Cryogenic Storage Ring**
6	Felix Herrmann	**Current Status of the Reaction Microscope for the Cryogenic Storage Ring CSR**
7	Jannis Himmelsbach	**Completion and Commissioning of an LVAP Ion Source for CSR**
8	Christopher Jakob	**MOCCA - A 4k-Pixel Microcalorimeter for the Cryogenic Storage Ring CSR**
9	Ábel Kálosi	**Dissociative Recombination of OH+ at the Cryogenic Storage Ring**
10	Claude Krantz	**The CRYRING@ESR Electron Cooler**

Poster Session – Tuesday, 21 June, 16:30 h (CEST)

11	Damian Müll	**Photodetachment of Al4- Clusters in a Cryogenic Storage Ring**
12	Felix Nuesslein	**New Lifetime Limit for the Ground State Vinylidene Anion H_2CC^-**
13	Daniel Paul	**Dissociative Recombination of Internally Cold CH+ Molecules**
14	Lutz Schweikhard	**Production and Study of Polyanionic Metal Clusters with Ion Traps**
15	Abhishek Shahi	**VMI Photoelectron Spectroscopy Probing the Rotational Cooling Dynamics of Hot Trapped OH^- Ions**
16	Deepak Sharma	**2DCyIPIC Technique to Study the AR Cooling of Ions in an Electrostatic Ion Beam Trap**
17	Xavier Urbain	**State-Selected Ion Beams for Storage Ring Studies**
18	Shuxing Wang	**Precise Determination of the 2s22p5-2s2p6 Transition Energy in Fluorine-like Nickel Utilizing a Low-lying Dielectronic Resonance**
19	Zhongwen Wu	**Hyperfine-Induced Effects on Angular Distribution of X-Ray Lines Following EIE of Heliumlike Tl79+ Ions**
20	Ilja Zebergs	**TrapREMI: A Reaction Microscope Inside an Electrostatic Ion Beam Trap**

Poster Session – Tuesday, 21 June, 16:30 h (CEST)

21 Aigars Znotins **Electron Collisions and Spectroscopy with Triatomic Hydrogen Ions at the Cryogenic Storage Ring**

Abstracts of Lectures

(in alphabetical order)

Femtosecond dynamics of molecular ions, studied by time-resolved action spectroscopy in an ion-storage ring

Lars H. Andersen

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Storage rings offer many attractive possibilities related to the long observation time of stored ions. In this presentation, we shall see how rather slow ground-state dissociation may be used in action-spectroscopy studies of biochromophores. As a more recent development, we use time-resolved action spectroscopy in combination with fast femtosecond lasers. [1] In this way, we trace the time evolution of electronically excited states and follow the transition from an excited state to the electronic ground state of ions stored in the SAPHIRA ion-storage ring. [2] The technique has been applied to biochromophores of for example chlorophylls, [3] the green fluorescent protein (GFP), [4] and protonated Schiff-base retinal, where fast 11-*cis* -> *all-trans* isomerization is important for vision. [5] Fluorescence of the GFP chromophore in the gas phase has not been detected so far. We see, however, that there is evidence that cold GFP chromophores may indeed be fluorescent in the gas phase, where excited-state energy barriers determine the rate-limiting decay by internal conversion. [4] We shall also see that, contrary to immediate expectations, locking the retinal chromophore structure may steer and accelerate the excited-state dynamic rather than slowing it down. [6]

References

[1] H. V. Kiefer, *et al.* Phys. Rev. Lett. **117** 243004 (2016)
[2] H. B. Pedersen, *et al*. Rev. Sci. Instrum. **86** 063107(1-9) (2015)
[3] E. Gruber *et al.* Phys. Chem. Chem. Phys. **24** 149-155 (2022).
[4] A. Svendsen *et al.* J. Am. Chem. Soc. **139** 8766 (2017)
[5] H. V. Kiefer *et al.* Nature Communications, **10** 1210 (2019)
[6] E. Gruber *et al.* J. Am. Chem. Soc. **144**, 1, 69-73 (2022)

Slow deexcitation dynamics of molecular ions stored in RICE and TMU E-ring

T. Azuma[1]

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We have studied isolated molecular ions in a vacuum by taking advantage of two electrostatic ion storage rings, RICE in the cryogenic condition and TMU E-ring at room temperature over the years. We have focused on the deexcitation dynamics of laser-excited carbon clusters (C_n^-) and understood them based on statistical descriptions. This strategy was successfully applied for larger molecules, i.e., pentacene anions ($C_{22}H_{14}^-$) [1].

Recently, we have started rovibrational state-selective observation of the deexcitation of small molecular ions using a wavelength-tunable pulsed laser. The first example is the vibrational cooling of triatomic molecular ions N_2O^+ in the range of several seconds. We found that the deexcitation dynamics drastically deviate from the statistical description based on a Boltzmann-type distribution [2,3]. We also observed deexcitation of the simple iso-nuclear diatomic negative molecule C_2^- in the tens of millisecond range. An iso-nuclear diatomic molecule has zero dipole moment, and the vibration transition is prohibited due to its symmetry. However, it is de-excited via spontaneous infrared radiation between electric excited and ground states. The time evolution of the population at specific vibrational states was measured up to 60 milliseconds, providing the first quantitative experimental support for long-standing theoretical predictions [4]. We also tackled Si_2^- on the micro-second time region. To our surprise, the excitation spectra show well-resolved rovibronic structures exclusively in the delayed time region [5].

References

[1] S. Iida, T. A., et al., Phys. Rev. A 104, 043114 (2021)
[2] R. Igosawa, T. A., et al., J. Chem. Phys. **153**, 184305 (2020)
[3] A. Hirota, T. A., et al., Phys. Rev. A **102**, 023119 (2020)
[4] S. Iida, T. A., et al., J. Phys. Chem. Lett. **11**, 10526-10531 (2020)
[5] S. Iida, T. A., et al., J. Phys. Chem. Lett. **11**, 5199-5203 (2020)

Radiative association of atomic and ionic carbon

J. F. Babb

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The rate coefficients for the formation of the dicarbon cation C_2^+ by the radiative association process are calculated [1]. At 100 K the rate coefficient is 2×10^{-18} cm^3/s. We will discuss potential applications and review progress on other ionic systems.

Reference

[1] J.F. Babb, R.T. Smyth, and B.M. McLaughlin, Ap. J. **876**, 38 (2019)

Spectroscopy of biomolecular ions at the advanced light sources

S. Bari[1,2]

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Biomolecules are the building blocks of life and it is important to understand how exactly their physical properties are responsible for their functionality and responses to stressors. A very suitable method is to study isolated biomolecules with cutting-edge mass spectrometry techniques at advanced light sources to unravel their intrinsic properties, i.e. in an environment-free and controlled chemical state. In particular, Near-Edge X-ray Absorption Mass Spectrometry (NEXAMS), which is an action-spectroscopy technique based on fragment-resolved absorption upon resonant photoexcitation of core atomic levels, has been of growing interest in recent years for investigating the spatial and electronic structure of biomolecules.
In this talk, I will present the latest results from NEXAMS studies on peptides [1, 2] and related molecules like porphyrins [3]. Not only spatial and electronic structures, but also damage processes, site-selective dissociation and orbital-dependent deexcitation pathways will be discussed.

References

[1] S. Dörner, L. Schwob, K. Atak, K. Schubert, R. Boll, T. Schlathölter, M. Timm, C. Bülow, V. Zamudio-Bayer, B. von Issendorff, J. T. Lau, S. Techert and S. Bari, J. Am. Soc. Mass Spectrom. **32**, 670 (2021)

[2] L. Schwob, S. Dörner, K. Atak, K. Schubert, M. Timm, C. Bülow, V. Zamudio-Bayer, B. von Issendorff, J. T. Lau, S. Techert and S. Bari, J. Phys. Chem. Lett., **11**, 1215 (2020)

[3] K. Schubert, M. Guo, K. Atak, S. Dörner, C. Bülow, B. von Issendorff, S. Klumpp, J. T. Lau, P. S. Miedema, T. Schlathölter, S. Techert, M. Timm, X. Wang, V. Zamudio-Bayer, L. Schwob, S. Bari, Chem. Sci. **12**, 3966 (2021)

Dielectronic recombination in He-like oxygen ions investigated at CRYRING@ESR

W. Biela-Nowaczyk[1*], P. Amaro[2], S. Fuchs[3,4], F. Grilo[2],
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Electron-electron interaction is a crucial aspect of atomic reactions involving electron-ion collisions. An effective way to investigate this interaction is to study the higher order recombination processes, which are only allowed by the electron-electron interaction. Among the recombination processes the dielectronic recombination (DR) especially affects the dynamics of astrophysical objects [1, 2]. Therefore, the accurate experimental recombination cross-sections are particularly important for astrophysical models.

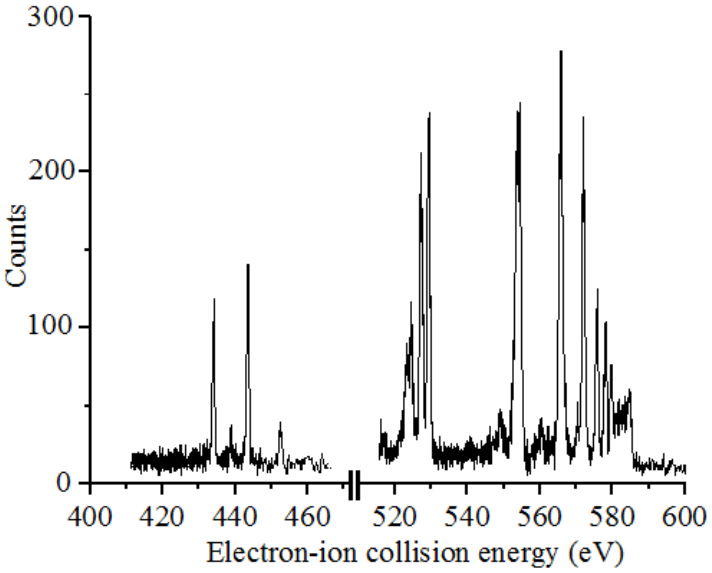

Figure 1: Preliminary results of measured DR resonances of O^{6+} ions at CRYRING@ESR electron cooler.

DR is a two-step process. The first step, called dielectronic capture (DC), is essentially the time reversal of the Auger process, producing an excited state. To complete the DR process a radiative deexcitation takes place in a second step.

To provide the experimental data for high temperature plasmas, DR has been investigated in the $\Delta n=1$ regime. The data presented in Figure 1 was collected for K-Ln (n=L, M, N, …) DR of He-like oxygen ions. Oxygen is one of the most abundant elements in the Universe and, therefore, is of particular importance for astrophysics [1, 2]. The experiment took place at the low-energy storage ring CRYRING@ESR. DR spectra were measured by applying collision spectroscopy of ions merged in a cold electron beam [3]. He-like oxygen ions were passing hundred thousand times per second through a cold electron beam. This beam was essentially a target, and as a signature for recombination, O^{5+} ions were detected. The resonant condition was achieved by changing the relative electron-ion energy. This high-precision spectroscopy method has been successfully used before [3] and is of special importance within the research program of the SPARC Collaboration [4].

References

[1] A. Burgess, Astron. J. **139**, 776 (1964)
[2] S. Schippers, J. Phys.: Conf. Ser. **388** 012010 (2012)
[3] C. Brandau, C. Kozhuharov, M. Lestinsky *et al.*, Phys. Scr. **T166**, 014022 (2015).
[4] M. Lestinsky *et al.*, Eur. Phys. J. Special Topics **225**, 797 (2016)

Towards storage ring studies of highly charged ^{229}Th using nuclear hyperfine mixing

C. Brandau[1,2]

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229-Thorium is the only known candidate for a frequency standard based on a nuclear transition. Such a "nuclear clock" can be used for ultraprecise metrology, enhanced precision in GPS and geodesy or as a means to find answers to fundamental questions in science such as: "Have the fundamental constants of nature changed since the birth of the universe?" [1].

At GSI, an alternative approach to the physics of 229-Th is under development: We propose to investigate and utilize a phenomenon that is unique to very highly charged ^{229}Th such as one-electron $^{229}Th^{89+}$. In high thorium charge states, in addition to the ordinary hyperfine structure, the very strong magnetic field of ~28 MT of the unpaired s-electron mediates a mixing of the F = 2 levels of ground state (g.s.) and isomeric state (i.s.) [2,3]. The mixing results in an additional small energy shift. But more notable, the lifetime of the i.s. decreases drastically by 5-6 orders of magnitude, from a few hours down to a few 10 ms. In two-electron $^{229}Th^{88+}$ (2e) the effective field of the paired electrons is zero. As a consequence, mixing is "switched off" and τ_γ is the same as for the bare nucleus. In essence, depending on the electronic configuration, the lifetime of the nucleus can be gradually or instantaneously manipulated on purpose. This manipulation of nuclear gamma-decay rates by orders-of-magnitude simply by altering the number or the configuration of electrons is a fascinating effect beyond the common motivations to study ^{229}Th. Furthermore, the vastly accelerated decay, e.g., in $^{229}Th^{89+}$ implies that the excitation probability with a laser and the detection of fluorescense light are each enhanced by these 5-6 orders of magnitude.

It is proposed to investigate nuclear hyperfine mixing using laser spectroscopy and dielectronic recombination at the storage rings ESR and the CRYRING of GSI/FAIR. The ^{229}Th ions will be produced in-flight between SIS18 and the ESR and cleanly separated in the ESR.

References

[1] P. Thirolf, B. Seiferle, and L. von der Wense, Ann. Phys. **531**, 1800381 (2019)

[2] F.F. Karpeshin, S. Wycech, I.M. Band and M.B. Trzhaskovskaya, M. Pfützner and J. Zylicz, Phys. Rev. C **57**, 3085 (1998).

[3] V.M. Shabaev, D.A. Glazov, A.M. Ryzhkov, C. Brandau, G. Plunien, W. Quint, A.M. Volchkova, and D. V. Zinenko., Phys.Rev. Lett. **128**, 043001 (2022).

Reaction Dynamics and Particle Impact Studies with Linear Electrostatic Storage Devices

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This presentation will briefly review applications of linear electrostatic storage devices to studies of the photoinduced reaction dynamics of light molecular anions as well as impact studies of submicron particles, providing two diverse use cases for these versatile tools. Studies of light molecular anions will focus on the use of the process of dissociative photodetachment to reveal details of the reaction dynamics of hydroxyl radical reactions, including the photodetachment of $HOCO^-$ to probe the HOCO radical intermediate in the $OH + CO \rightarrow H + CO_2$ reaction, and studies of the exit channel of the $OH + CH_3OH \rightarrow H_2O + CH_3O$ reaction by photodetachment of $CH_3O^-(H_2O)$. In the former case, detailed information about the HOCO intermediate and tunneling to form $H + CO_2$ was learned,[1,2] and in the latter case, the exit channel $CH_3O\text{-}H_2O$ complex was identified, as well as the existence of long-lived vibrational Feshbach resonances in the neutral complex.[3] The second part of the presentation will focus on applications of the Aerosol Impact Spectrometer, a device that combines charge detection mass spectrometry in a linear electrostatic ion beam trap with a particle-specific linear acceleration scheme to allow studies of the coefficient of restitution, fragmentation and chemical speciation of polystyrene latex spheres,[4] submicron tin/tin oxide particles,[5] and ice grains doped with organic compounds. This work has been supported in part by the US DOE under grant DE-FG03-98ER14879 and ASML US, San Diego, CA, Tin Management Research Program under project number 2271-1007-F.

References

[1] C.J. Johnson, B.B. Shen, B.L.J. Poad and R.E. Continetti, Rev. Sci. Instrum. 82 105105 (2011).
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Measuring differential cross sections with the merged beam method

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The differential cross section is important for collision processes such as e^-/ion and atom/atom collision as it gives an insight of dominant and interfering pathways reflected in partial wave emissions.
Measuring low collision energy differential cross sections in merged beam geometry leads to higher complexities than other methods as the angular and energetic collision distribution is neither uniform nor Maxwellian, meaning that extracting differential cross section requires extensive beam simulations.
Additionally, as the mutual neutralization (MN) is driven by the Coulomb potential during half of the collision, the differential cross section cannot easily be described by a sum of Legendre polynomials. In order to overcome this problem, we propose a simple analytic model for the MN which derives from the hypothesis above.
Using the UCLouvain merged beam setup, we measured the angular distribution of the $Na^+(^1S) + O^-(^2P°) \rightarrow Na(3p\ ^2P°) + O(^3P)$ mutual neutralization (MN) as a function of the c.m. collision energy (from 5 to 500 meV). At the lowest collision energy, we see that the angular distribution is rather uniform. This comes from the combination of the broad angular collision distribution convoluted with the broad differential cross section; when the collision energy increases (below 100 meV), the angular collision distribution sharpens faster than the differential cross section. We also observe that the deflection decreases rapidly around 100 meV, leading to nearly no deflection above 1 eV (meaning that the eikonal approximation becomes inscreasingly valid).

References

[1] A. Dochain, N. de Ruette, R.D. Thomas and X. Urbain, *in preparation.*

Ion processing of molecular clusters: a way to form complex systems in space

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In space, the molecular matter is energetically processed by ionizing radiation and two scenarios are proposed to explain the emergence of new molecular species. On the one-hand, the *bottom-up* approach proposes the growth of larger molecules from smaller subunits. On the other hand, the *top-down* scenario considers the emission of molecular species from a large piece of matter. In order to study the processes leading to the formation of complex organic molecules, we have considered an intermediate approach, ion interaction with molecular clusters.

During my talk, I will present an overview of experimental studies performed at GANIL in Caen leading to molecular complexification within molecular clusters induced by low-energy ion collisions: (i) intra-cluster molecular growth processes in clusters of polycyclic aromatic hydrocarbons or fullerenes [e.g. 1-3]. This growth is driven by the prompt fragmentation of molecules in loosely bound clusters when the impacting projectile ion deposits a large amount of energy and momentum to individual atoms through nuclear scattering *(knock-out processes*) leading to the formation of reactive species. These molecular fragments may form covalent bonds with neighboring molecules in the cluster on sub-picosecond time scales, well before the excited cluster dissociates. (ii) formation of peptide bonds in collisions of a single He^{2+} ion with amino acid β-alanine clusters [4]. We attribute the formation of polypeptides to specific energy transfers resulting from the collision with He^{2+} ions, which are in contrast to photon collisions not localized but rather distributed along the ion trajectory in the cluster. Excitation and ionization processes in the collision, are followed by proton transfer that leads to weakly bound protonated molecular clusters. They are stabilized through the formation of peptide bonds, releasing water molecules, via low energy barriers.

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Time-resolved cluster photodissociation in a multi-reflection time-of-flight mass spectrometer

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Multi-reflection time-of-flight (MR-ToF) mass spectrometers—devices in which ions are stored between two opposing electrostatic mirrors—are used for precision mass measurements and high-resolution isobar separation of exotic nuclei. In molecular physics research they are used as electrostatic ion beam traps (EIBTs) to probe molecular reactions in a fashion similar to electrostatic storage rings.

In-trap photoexcitation in an MR-ToF mass spectrometer is applied at the University of Greifswald to both select atomic clusters and study their dissociation with high mass resolving powers [1,2]. Due to the electrostatic nature of the device, the ions' flight paths are governed by their kinetic energy. This feature is used to track delayed dissociation events by observing fragment signals with distinct revolution periods after photoexcitation [3]. Continuous decay over multiple revolutions leads to a series of fragment bunches, the relative abundances of which reflect the time-resolved decay rate. Measurements performed on indium-cluster anions indicate a power-law behavior. This is understood in the context of a hot cluster ensemble with a broad distribution of internal energies and, thus, decay constants.

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A community platform for just atomic computations

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Electronic structure calculations of atoms and ions have a long tradition in physics with applications in basic research and spectroscopy. With the Jena Atomic Calculator (JAC), I here present a new implementation of a (relativistic) electronic structure code for the computation of atomic amplitudes, properties as well as a large number of excitation and decay processes for open-shell atoms and ions across the periodic table. JAC [1] is based on Julia, a new programming language for scientific computing, and provides an easy-to-use but powerful platform to extent atomic theory towards new applications.

A primary guiding philosophy in designing JAC was to develop a general and easy-to-use toolbox for the atomic physics community, including an interface that is equally accessible for working spectroscopists, theoreticians and code developers. In addition, I also wish to provide a modern code design, a reasonable detailed documentation of the code and features for integrated testing [2].

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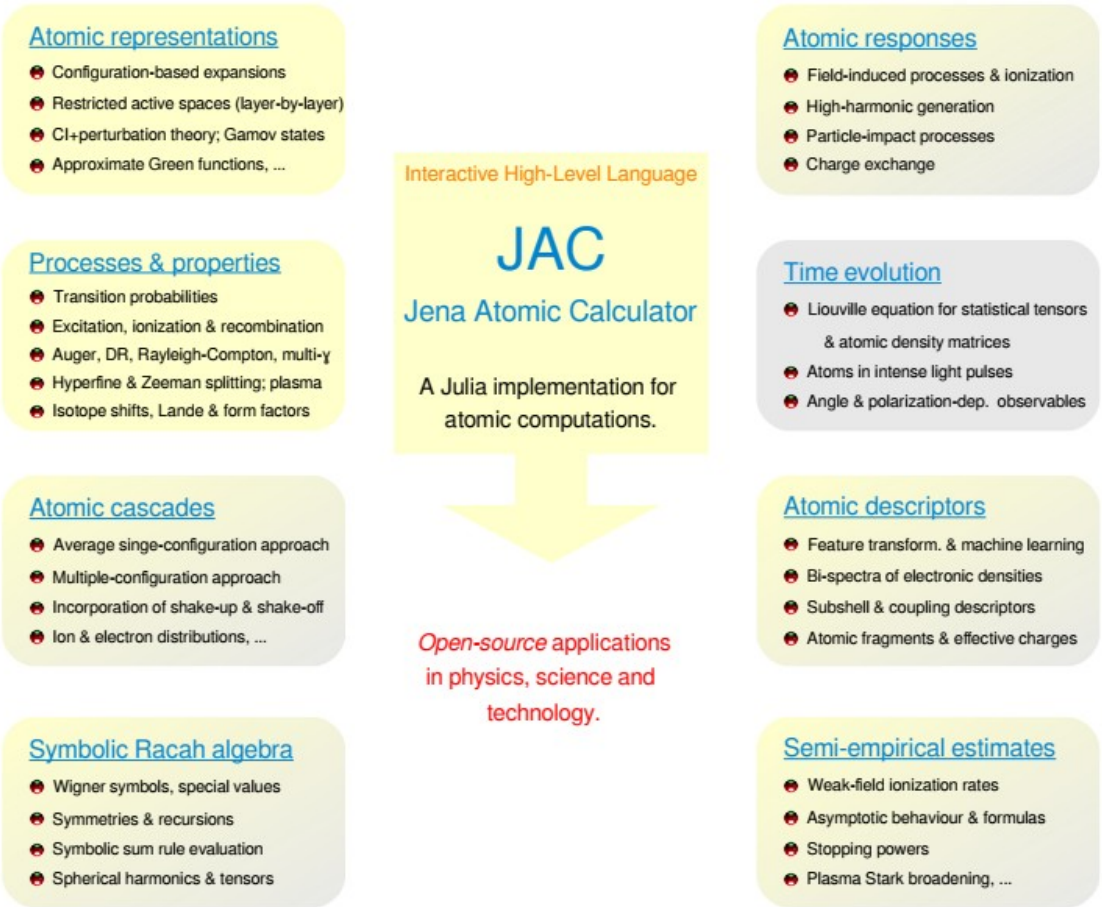

High-resolution dielectronic recombination spectroscopy with slow cooled Pb^{78+} ions in the CRYRING@ESR storage ring

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Dielectronic recombination (DR) spectroscopy is a very successful technique to study the properties of highly charged ions [1–3]. Its high precision and versatility make it an important spectroscopic tool in the physics program of the SPARC collaboration, e.g. outlined in Ref. [4]. The heavy-ion storage ring CRYRING@ESR of the international FAIR facility in Darmstadt is a very attractive machine for performing DR spectroscopy because of its electron cooler that provides an ultra-cold electron beam promising highest experimental resolving power. Here, we report on results from the first DR experiment with highly charged ions at this new facility.

The measured DR spectra of Be-like Pb^{78+} ions in the electron-ion collision energy range of 0–40 eV cover the *2s2p* ($^3P_1$) 19l and 20l resonances. The preliminary results show good agreement of relative peak positions and peak strengths with theoretical calculations using the methodology described in Ref. [5].

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

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

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

Merged Beams with Electrostatic Ion Beam Traps (EIBT)

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The merged beams method is a very useful technique to study low energy interaction between two particles. Single path apparatus where two beams interact with each other once or where the products are studied within this interaction time range are well established. However, the internal excitation states of the interacting particles are often unknown, or the lifetime of the product needs to be measured. In such cases, it would be advantageous to follow the interaction as a function of time or store the reaction product over a period of time that is of the same order of magnitude as the lifetime of the excited or metastable states. Therefore storage devices are needed, and have been developed in the last few years to incorporate merged beams for low energy molecular reactions.

In this presentation, two such experiments using an EIBT will be described.

In the first case, we used an EIBT to measure the lifetime of the ionic product of the merging (with a small angle) of two neutral beams in the reaction $Ne^{*}+Ar \rightarrow NeAr^{+} + e$. The $NeAr^{+}$ was stored in an EIBT, and its lifetime was measured. The lifetime was found to be relatively long due to the phase protection of the Fano-Feshbach resonance.[1]

The second device is a Hybrid EIBT (HEIBT). In this device, two EIBT are nested coaxially, one inside the other. The outer EIBT is for the heavier ion beam, while the inside one is trapping the lighter one. The energies of both beams are tuned such that the relative velocity in the field-free central region of the inner trap is small[2]. With such a configuration, the HEIBT is capable of trapping simultaneously any charge combination (positive and negative) of molecular ion beams. Some preliminary test results will be presented.

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Experimental Studies of Nonperturbative Dynamics in Heavy-Ion-Atom Collisions

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Experimental data for atomic collisions of highly charged ions are essential for benchmarking the theoretical description of dynamical processes in atomic physics. Of particular challenge is the accurate description of those processes that exceed the applicability of relativistic first-order perturbation theories. Recently, we have investigated two characteristic cases of such collision systems at the Experimental Storage Ring ESR of the GSI heavy-ion accelerator facility in Darmstadt, Germany:

(1) For fast collisions of U^{89+} projectiles with N_2 and Xe targets at 76 MeV/u, we studied the electron-loss-to-continuum cusp both experimentally and theoretically. We compared the continuum electron spectra of the two collision systems, which originate from the ionization of the projectile, and we were able to identify a clear signature for the nonperturbative character of the collision systems [1].

(2) For slow collisions of Xe^{54+} and Xe^{53+} with a Xe target at 30 and 15 MeV/u, we performed an x-ray spectroscopy experiment focusing on the target Kα radiation. Experimental data for such slow symmetric collision systems are important for testing relativistic two-center calculations and provide an intermediate step towards understanding heavy-ion collisions in super-critical fields. We used the target Kα satellite and hypersatellite lines to derive cross-section ratios for double-to-single target *K*-shell vacancy production and compared our experimental results to theory applying a fully relativistic time-dependent two-center approach [2].

At GSI, new prospects of investigating slow Xe^{54+}-Xe collisions under improved conditions will now be facilitates by the low-energy heavy-ion storage-ring CRYRING@ESR. Corresponding experiments are currently being devised.

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First Dielectronic Recombination Measurements at the Cryogenic Storage Ring

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Over the past three decades, electron-ion recombination has been extensively studied in heavy-ion storage rings by applying the merged-beams technique [1]. A persisting challenge of these experiments is the background induced by electron capture from residual gas. Because of the relatively high vacuum pressure of conventional room temperature magnetic storage rings, experiments so far have been restricted to ions with a high charge-to-mass ratio, which could be stored at sufficiently high velocities to suppress electron capture from the residual gas. As the charge balance in plasmas is determined by competing ionization and recombination processes, experimental recombination data – also on low-charged heavy ions – are essential for understanding and modeling of plasmas in astrophysical environments as well as terrestrial applications [2]. The electrostatic Cryogenic Storage Ring CSR [3] combines mass-independent storage with the excellent vacuum conditions of cryogenic surroundings. It is equipped with an electron cooler and a suitable single particle detector. Thus, CSR provides a unique environment that is promising for the study of electron-ion recombination with low-charged heavy ions. Here, we report on the first recombination measurements with atomic ions at CSR. Investigating the dielectronic recombination of doubly charged neon and triply charged xenon, we have observed resonant recombination features in agreement with quantum-theoretical predictions. Our results clearly demonstrate the feasibility of atomic recombination studies with heavy low-charged ions at CSR.

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Study of PAH photophysics in an astrophysical context: the role of storage devices

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The interaction of polycyclic aromatic hydrocarbons (PAHs) with VUV photons has a significant impact on the physical and chemical conditions of star and planet forming regions. The ionization of PAHs leads to the heating of the gas by thermalization of the emitted electrons. Photodissociation mainly governs the chemical evolution of these astroPAHs and their contribution to the production of H_2 and small hydrocarbons. Radiative cooling affects the dissociation efficiency and leads to emission in the well-known aromatic infrared emission bands (AIBs), which are the only direct diagnostic we have to date for the presence of astroPAHs. These AIBs will be the focus of upcoming observations by the James Webb Space Telescope [1].

In the laboratory, the molecular processes associated with the interaction of PAHs with VUV photons must be quantified in order to feed astronomical models [2]. In recent years, a major advance has been the quantification of the fast (ms time scale) cooling process called recurrent fluorescence, which occurs in addition to the slower (~s) infrared cooling [3]. Due to the extreme isolation conditions encountered in astrophysical environments, the study of radiative cooling in the laboratory requires the use of cryogenic ion traps [4,5] or, even better, cryogenic electrostatic storage devices [6]. Devices such as DESIREE from Stockholm University should therefore be used in addition to facilities operating at room temperature (e.g. the Mini-Ring) [7]. To mimic astrophysical conditions, access to tunable VUV radiation is also required. Recent experiments have been performed using the linear ion trap of the DESIRS VUV synchrotron beamline [8,9]. The coupling of a cryogenic ring with synchrotron radiation will be the objective of the new SynPAHcool project [10].

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Recent progress in theoretical description of dissociative recombination of polyatomic molecular ions

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In the presentation, I will give a short overview of recent progress in theoretical description of dissociative recombination of electrons with molecular ions at energies below a few eV. The theory, based on first principles only, is now able to give reliable cross sections of the process for ions having up to approximately ten atoms. A reliable theoretical description of this and other processes, taking place in electron-molecule collisions, is crucial for various applications, where molecular plasma is involved.

Ion-ion collisions for atomic cross sections measurements: the FISIC project at CRYRING

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Electronic processes in ion-ion collisions play an important role in astrophysical and fusion plasmas as well as in ion-matter interaction. In the so-called intermediate velocity regime where the ion stopping power is maximum, there is a lack of both experimental and theoretical data on the electronic cross sections. The FISIC set-up is a mobile experiment designed to perform collisions between slow (keV/u) ion beams coming from the FISIC platform and fast (MeV/u) ion beams from CRYRING. The FISIC platform is equipped upstream the collision zone with an ECR ion source, a low energy beam line and an omega-shaped purification system [1], and downstream the collision chamber with a home-made ion spectrometer. This set-up is inspired by the investigation of ion-ion collisions carried in the low velocity regime by the Giessen group [2]. With FISIC at CRYRING, besides the possibility to reach the pure three-body problem (bare ion on hydrogenic target) as a benchmark, the role of additional electrons bounded to the target and/or to the projectile -one by one- should allow quantifying several effects such as electron–electron interactions or the multi-electron processes for instance and this for a large variety of collision systems. The scientific goals [3] of the FISIC program and a status of the experimental set-up will be presented.

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Ab initio studies on charge recombination scattering processes

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To perform theoretical studies on processes such as dissociative recombination, mutual neutralization and associative ionization, structure calculations are combined with electron scattering calculations. There is a need to accurately and consistently describe bound valence electronic states, highly excited Rydberg states, electronic resonant states and interactions to the ionization continuum. To compute final state distributions the nuclear dynamics on the coupled states has to be followed during the scattering process from reactants to products. We here describe the procedure of the theoretical calculations and compare results with measurements in the case of the H_2 reaction complex.

First experiments with CRYRING@ESR

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As part of the Swedish in-kind contribution to the international FAIR project, the low-energy heavy-ion storage ring CRYRING was transported from Stockholm to GSI in Darmstadt in 2013 and integrated into the accelerator complex downstream of ESR. In the following years, the ring was modernised, new features added and recommissioned. Now, all major functions of the facility are in service and routine operation for experiment proposals approved by the General Program Advisory Committee is established since 2021. Either, ions in low charge states can be injected from a local ion source through a 300 keV/u RFQ linac, or in high charge states from ESR with access to all ion species which the GSI accelerator complex is capable of producing. The low-energy stored cooled beams at this machine are allowing an unprecedented access to precision spectroscopy and for studying the dynamics of slow collisions and we prepared a rich research program[1] covering e.g. atomic physics in highly charged ions, nuclear reactions and materials research.
This talk shall give an overview over the present setup of our facility, discuss the data from our first experiments and look ahead at the coming years.

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Resonances in the time and frequency domain

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When photons or particles impinge on atomic systems, the probability for charge changing processes is often very sensitive to the detailed structure of these systems. During the collisional process a resonance may form which can serve as an intermediate step between the initial and final state, hereby altering the probability for a process dramatically. A famous example is the so-called *giant resonances* seen in photoionization from the 4d-shell in several elements, and another is the enormous recombination rates[1, 2] discovered for specific ions when accurate recombination experiments became possible with the ion storage rings in the nineteen nineties.

Traditional studies of photoionization measure the cross section and are thus primarily sensitive to the amplitude for the process. Information on the phase of the ionized wave packet is nevertheless accessible in some specific cases: The angular anisotropy of the photoelectrons depends on the relative phases of different partial waves and asymmetric line profiles on that of different ionization paths. Attosecond techniques have more recently provided alternative ways to obtain phase information. With these the phase of the wave packet emerging from one particular orbital can be measured relative other orbitals in the same, or another, element, or the phase in one particular angle can be related to that in an another angle. For resonances this is particularly interesting since the very rapid phase variations over them can be compared to a region where the phase is essentially flat. The spectral derivative of the phase is connected to how much the photoelectron is delayed on its journey [3] and gives thus access to time. What new can we learn about resonance dynamics when it can be studied with high resolution in both the time and energy domain? I will give examples from the 4d-ionization in xenon [4] where the fast decaying giant resonance interfere with long lived resonances that mediate a spin-flip.

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New insights in the low energy electron-driven reactivity of hydride cations

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Electron-impact dissociative recombination, ro-vibrational (de)excitation and dissociative excitation of hydride cations

$$AB^+ + e^- \rightarrow AB^{*,**} \rightarrow \begin{cases} A + B \\ AB'^+ + e^- \\ A + B^+ + e^- \end{cases} , \quad (1)$$

are in the heart of molecular reactivity in the cold ionized media [1], being major charged particles destruction reactions and producing often atomic species in metastable states, inaccessible through optical excitations. They involve super-excited molecular states undergoing predissociation and autoionization, having thus strong resonant character. Consequently, they are subject to beyond-Born-Oppenheimer theoretical approximations, and often require rather quasi-diabatic than adiabatic representations of the molecular states. In addition, they involve particularly sophisticated methods for modelling the collisional dynamics, able to manage the superposition of many continua and infinite series of Rydberg states.

We use the Multichannel Quantum Defect Theory [2], capable to account the strong mixing between ionization and dissociative channels, open - direct mechanism - and closed - indirect mechanism, via capture into prominent Rydberg resonances [3, 4] correlating to the ground and excited ionic states, and the rotational effects. These features will be illustrated for several cations of high astrophysical and cold plasma physical relevance such as SH^+ [5] and CH^+ [4, 6, 7], comparisons with other existing theoretical and experimental results being performed.

Advancement in the theoretical treatment - as the effect of the energy-dependence of the quantum defect on vibronic interactions for the benchmark cation H_2^+, the isotopic effects for diatomic and polyatomic systems like H_2^+ [8] and N_2H^+, etc. - will be presented.

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Prospects of the CSR Reaction Microscope for in-ring electron and ion spectroscopy

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Reaction microscopes are combined electron and ion spectrometers that cover the full solid angle and allow kinematically complete studies of molecular fragmentation. The first cryogenic reaction microscope worldwide, the so-called CSR-ReMi, has is presently under construction and ready for installation into the cryogenic storage ring CSR at the MPIK in Heidelberg. After its integration, which is expected to be finalized in fall 2022, the in-ring CSR-ReMi is expected to significantly enhance the range of scientific applications of the CSR infrastructure. For example, dynamical processes occurring when atoms, molecules or clusters break up in collisions with slow and cold ions stored in the CSR can be investigated with high resolution. Furthermore, electrons resulting from interactions with ultrashort laser pulses, in photoemission or detachment reactions, will be detected with high efficiency and in coincidence with created neutral fragments in the CSR. The potential applications will range from structure determinations of molecular ions by means of photoelectron spectroscopy to femtosecond time-resolved experiments on state-prepared molecules using established pump-probe techniques. The technical challenges as well as future prospects will be discussed in the talk.

The Role of Ion Storage Rings in Studying Electron-Ion Collisions

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Ion storage rings hold the promise to preserve expensive ionic species, to prepare bright beams of such particles and to facilitate their efficient use in experiments. In particular, the use of ion-storage ring techniques has been extremely successful in studies of electron-ion collision phenomena. The existing potential for the further development of this research field has by far not yet been exhausted. New storage-ring facilities are opening a bright future for studies that address or involve electron-ion interactions.

The Cryogenic Storage Ring CSR

O. Novotný[1] for the CSR team

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Interactions of gas phase molecules and clusters with photons, electrons, and other heavy particles can trigger various types of electronic dynamics and nuclear rearrangements. Processes like vibrational and rotational relaxation, delayed electron emission, and fragmentation can span over timescales far beyond microseconds. To access these timescales in the laboratory, storage techniques for molecular ions have been developed. Long-time storage in cryogenic environments with low-radiation fields allows for the preparation of molecules in defined quantum states, before the interaction dynamics is initiated. Recently, very versatile implementations of such advanced experimental techniques became available with the advent of cryogenic electrostatic storage rings.

The Cryogenic Storage Ring (CSR) [1] at the Max Planck Institute for Nuclear Physics, Heidelberg, is a multi-purpose electrostatic facility for studies with stored atomic, molecular and cluster ion beams. The cryogenic chamber temperatures of <6K, and the corresponding low residual gas densities, provide for beam lifetimes of hundreds to thousands of seconds. For many molecular ions this time is long enough to relax down to their lowest ro-vibrational states by spontaneous emission of radiation [2,3]. Various experimental setups providing laser-, electron-, or even neutral atomic beams can be used for collision studies, or as diagnostics for internal state populations. Furthermore, techniques for ion beam phase space cooling and isobaric purification are available. The cryogenic environment and the excellent vacuum mimic the conditions in the cold interstellar medium, making CSR an outstanding experimental set-up for laboratory astrochemistry and for quantum dynamics studies with individual molecular state definition.

In this talk key experimental techniques and milestones of CSR experiments since its first operation in 2015 will be reviewed, with special emphasis on recent electron collision studies [4,5]. Furthermore, future challenges and plans for upgrades will be summarized.

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Spectroscopy of interstellar complex organic molecules

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The evolution of large organic molecules such as Polycyclic Aromatic Hydrocarbons (PAHs) in the interstellar medium is greatly governed by photochemistry. We study the spectral signatures and photolysis of these species using Resonant Enhanced MultiPhoton Ionisation (REMPI), Infrared Multiple Photon Dissociation (IRMPD), and IR-UV double resonance spectroscopy. We use these advanced techniques together with theoretical investigations to identify electronic and vibrational signatures and processes at play of (cold) neutral and ionic species. Studies revealed vibrational [1,2] and electronic [3] coupling effects to be much stronger in PAHs than expected, photolysis processes leading to isomerisation [3,4], and unexpected (F)IR [5] and electronic [6] signatures. These studies illuminate the necessity of experiment and the need to advance theoretical approaches typically used in astrochemistry.

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Astrophysically Motivated Electron-Ion Merged-Beams Studies using the MPIK Heavy Ion Storage Rings

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In astrophysical environments dominated by either atoms or molecules, electron collisions play an important role in determining the physical properties of the objects. Cosmic atomic plasmas can be divided into two broad classes: electron ionized and photoionized. Electron-ionized plasmas are formed in objects such as the sun and other stars, supernova remnants, galaxies, and the intercluster medium in clusters of galaxies. Photoionized plasmas are formed in objects such as planetary nebulae, H II regions, X-ray binaries, and active galactic nuclei. Molecular environments exist at many stages along the pathway from star formation to planetary systems. These include diffuse clouds, dense molecular clouds, pre-stellar cores, protoplanetary disks, and planetary atmospheres.

The heavy ion storage rings at the Max Planck Institute for Nuclear Physics (MPIK), both the recently decommissioned Test Storage Ring (TSR) and the recently commissioned Cryogenic Storage Ring (CSR), have played and continue to play a leading role in studying a range of electron-driven processes that are important for the above astrophysics environments. For cosmic atomic plasmas, these studies include high temperature dielectronic recombination and electron-impact ionization measurements for electron-ionized atomic plasmas and low temperature dielectronic recombination for photoionized plasmas. For molecular environments, these studies include dissociative recombination of molecular cations and inelastic rotational (de)excitation collisions. In this talk, I will review some of the many successes with TSR and CSR and discuss some potential future studies.

Mutual Neutralization studies with merged beams of stored ions

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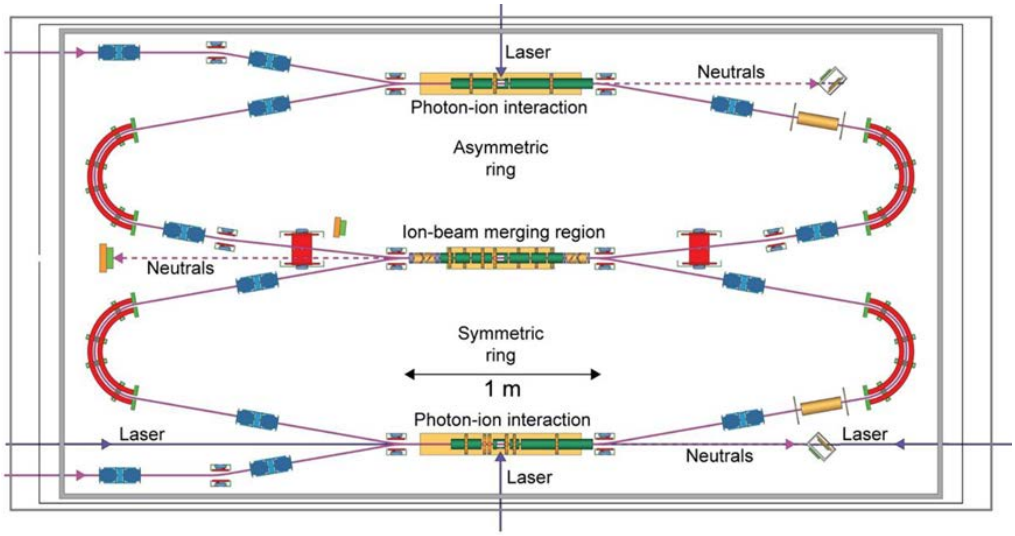
The Double Electrostatic Ion-Ring Experiment, DESIREE [1,2], at Stockholm University uniquely offers the opportunity to study interactions between positive and negatively charged ions stored for extended periods of time before interacting. In this presentation recent work on mutual neutralization of atomic ions of significance for quantitative interpretations of stellar spectra is being discussed [3-6].



Layout of the DESIREE storage rings indicating the ion-beam orbits and the electrostatic elements steering and focusing the ion beams.

Negative hydrogen ions are abundant in stellar atmospheres [7] and their mutual neutralization reactions with positive ions of other elements need to be understood in detail to deduce the abundance of the latter [8,9]. The storage rings, the experimental method and the mutual neutralization process and the results for astrophysics will be discussed.

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Identification and removal of molecular contaminations at CSR using isochronous mass spectrometry

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Electrostatic storage rings have been primarily used for collision studies of charged atoms or molecules with photons, atoms, and electrons until now. Due to the electrostatic nature and therefore mass-independent storage of the devices, multiple ion species can be stored simultaneously. The number of contaminations typically increases with the mass of the stored species. The identification and removal of these predominantly isobaric contaminations from the beam is not obvious. So far, electrostatic storage rings mostly rely on identification and purification methods prior to injection for contaminant-free measurements. Here, we report the first successful isochronous operation of an electrostatic storage ring [1] achieved at the Cryogenic Storage Ring (CSR) facility at the Max-Planck-Institut für Kernphysik in Heidelberg [2]. The isochronous operation enables a sensitive, mass-based identification of the stored beam components, information vital for all experiments conducted at CSR. Uncooled beams with typical momentum spreads of 10−3 and emittance of a few mm·mrad were investigated at non-relativistic beam energies of a few hundred keV. Mass resolutions of $\Delta m / m < 10^{-5}$ could be reached and isobaric contaminations below relative beam fractions of 10^{-4} could be identified. The proof-of-principle measurements presented here open up a new field of application in the form of ion mass measurements for these devices applicable for a large mass range. Furthermore, beam purification methods to remove the identified contaminations inside the ring have been developed.

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Electron impact excitation and recombination of molecular cations: theoretical studies and comparison with storage ring experiments

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The state-to-state study of the dissociative recombination and ro-vibrational/dissociative excitation of molecular cations on well resolved N^+,v^+ states:

$$AB^+(N^+,v^+) + e^- \rightarrow A + B,\ AB\ (N^{+'},v^{+'}) + e^- ,\ A + B^+ + e^-$$

is the object of intense experimental efforts mainly in the heavy-ion storage rings [1] and of joint theoretical work based on the Multichannel Quantum Defect Theory (MQDT) and the R-matrix method [2-4]. We will review our recent advances in modelling the major features of these processes – ro-vibrational resonant effects at low energy [5,6], capture into core-excited Rydberg states at intermediate energy[7,8], infinite series of dissociative channels and vibrational continua at high energy [9]. Our major results on diatomic – H_2, BeH, CH, CO, N_2, BF, SH, ArH - and polyatomic – BF_2, N_2H, etc. - systems (including some of their isotopologues) will be compared with the storage ring measurements.

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Probing charge-transfer reactions of atmospheric importance using the ion storage facility DESIREE

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The Double ElectroStatic Ion Ring ExpEriment (DESIREE) facility located at Stockholm University, Sweden, uniquely allows for studies of interactions between cations and anions at low and well-defined internal temperatures and centre-of-mass collision energies down to about 20 K and ~50 meV, respectively [1-3].

Using this facility, we aim for a better understanding of how small and large molecules are formed and processed in astrophysical, atmospheric, and combustion plasmas, where we combine several novel experimental methods to build a fundamental understanding of the transfer of charge-, energy- and mass in collisional reactions. Control over the reaction environment [1-5] means that desired information, e.g., reaction products, can be obtained over many of the conditions needed to accurately model plasmas where these processes are important.

This talk highlights how this facility, which is the only one of its kind currently in the world, can play a crucial role in studying in mutual neutralisation reactions relevant to cool atmospheric plasmas, and I look at reactions involving atomic and molecular oxygen and nitrogen ions [4,5].

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AD-ELENA, The Low Energy Antiproton Facility at CERN

G. Tranquille on behalf of the AD-ELENA team

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The low energy antiproton facility (Fig. 1) at CERN is a unique installation that is able to deliver high brightness antiproton beams to up to four experiments simultaneously at an energy of only 100 keV. Deceleration to this very low energy has been made possible due to the recent addition of the Extra Low ENergy Antiproton ring (ELENA) [1] to the existing Antiproton Decelerator ring, which has been operational since 2001. With this lower energy, the trapping efficiency of the experiments is improved by up to two orders of magnitude.

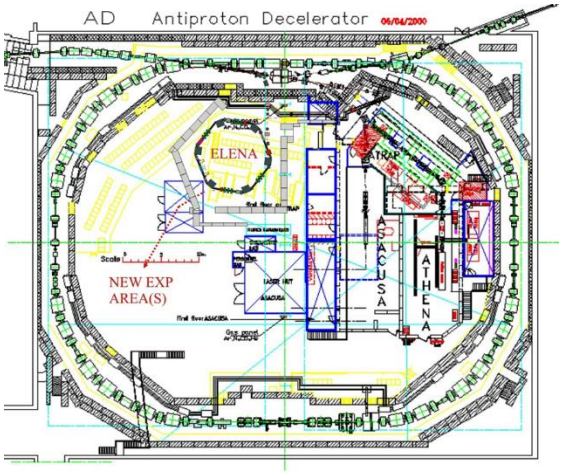

Figure 1. Layout of the Low Energy Antiproton Facility (AD and ELENA rings)

To counteract the adiabatic emittance growth and blow-up due to residual gas scattering, stochastic and electron cooling are applied at a number of steps during the deceleration process in both machines. The extracted beams are transported to the experiments through electrostatic beamlines [2] equipped with semi-destructive secondary emission grids to monitor the beam positions and profiles [3].

A dedicated H- source is also installed to setup the ELENA ring and the transfer lines. This was particularly useful during the commissioning phase in 2020 when the CERN accelerator complex was in a long shutdown period and the antiproton production beam was not available.

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Controlled interactions of cold trapped negative ions

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Negative molecular ions have drawn a lot of attention in recent years, owing to the detection of several molecular anions in cold interstellar molecular clouds. Negative ions have also attracted attention as potential candidates for sympathetic cooling of antiprotons. Radiofrequency ion traps are well suited tools to study the spectroscopy as well as cold collision processes of negative ions with high resolution and high sensitivity.

Using photodetachment spectroscopy we have probed rotational quantum states of cold trapped anions. We have used this to study rotational state-changing collisions of the negative ions OH^- and NH_2^- with neutral helium atoms at low temperature and to perform rotational terahertz spectroscopy and infrared overtone spectroscopy. Recently, we have studied photodetachment of the interstellar anions CN^- and C_3N^- near threshold and used these data to improve the accuracies of the respective electronic affinities. For CN^- the data are well described by the Wigner threshold law, if the permanent electric dipole moment of the neutral product is included in the analysis [1]. For C_3N^- the large permanent dipole moment of C_3N leads to a qualitatively different cross section behavior near threshold. Furthermore, the rotational contour of a dipole bound state was resolved slightly below the detachment threshold in agreement with calculations [2]. This state could serve as a doorway state to negative ion formation in interstellar clouds.

Recently, we have developed a two-photon scheme to probe the rotational and vibrational states of the homonuclear anion C_2^-, a candidate proposed for negative ion laser cooling. Results on accurate electronic spectroscopy and vibrational relaxation collisions of this ion will be presented [3].

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The Test Storage Ring @ MPIK and Molecular Ions

A Thirty-Year Perspective

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Many storage rings were designed and built in the 1980s, but the so-called heavy-ion storage rings (HISR) became fully operational in the early 1990s. These machines became rapidly successful and demonstrated their advantages in various fields such as nuclear, atomic, and molecular physics, beam physics, and precision measurement in relativity. Several specific techniques were developed around these machines, such as laser, electron, and stochastic cooling.

Among the many processes studied at the Test Storage Ring (TSR) at the Max-Planck Institute for Nuclear Physics in Heidelberg are the dielectronic recombination for atomic ions and the dissociative recombination of molecular ions. The experimental results yielded a better understanding of atomic or molecular structure and dynamics in both cases. Especially for molecular ions, the use of HISR allows for the control of the initial excitation (electronic, vibrational, and partly rotational) stored in the system.

Indeed, the need to ionize neutral molecular precursors to create beams of molecular ions has been, for decades, a significant impediment to the understanding of experimental results. Different ionization processes create different internal state (electronic, vibrational, and rotational) distributions, making the comparison with theory ambiguous, often yielding reaction rates differing by order of magnitude when using different experimental methods.

In this lecture, I will describe the various steps that were taken at the Max-Planck Institute for Nuclear Physics under the leadership of Prof. Andreas Wolf to overcome the fundamental difficulties described above and how heavy-ion storage rings became a tool of choice for the study of reactions of small and cold molecular ions.

Abstracts of Posters

(in alphabetical order)

Gas-phase formation of $FeCN^-$ in astrophysical environment

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The vast space between stars is called interstellar medium (ISM). Clouds of ISM consist of neutral atoms/molecules, ions and dust particles. More than 200 molecules have been detected in the ISM. Several authors discussed the role of negative ions in the formation of smaller molecules in the interstellar clouds. Despite the importance of negative ions in molecular astrophysics, only six negative ions have been detected to date. Because of the low-density interstellar medium, radiative electron attachment (REA) is a prominent pathway for anion formation. A low lying resonance state can be a door way for the formation of negative ions through REA. A molecule with more than 1.6D dipole moment can accommodate low-lying dipole stabilised state. This dipole stabilised state can couple to negative ion ground state through Intramolecular vibrational redistribution (IVR). If IVR can compete with autodetachment, the formation of stable anion can enhance. The IVR is dominant in bigger molecules since they have large degrees of freedom. Therefore it is of paramount importance to search for such resonance states for which the neutral is already detected in the ISM. FeCN has been detected in the carbon-rich star IRC+10216. In this work, we have probed the low-lying resonance of $FeCN^-$ using the photoelectron velocity map imaging technique and established that the resonance could be a dominant pathway for the formation of $FeCN^-$ in the ISM. The non-Franck-Condon nature of resonance transition, resonance photoelectron angular distribution, and the resonance state's vibrational spacing indicate that the resonance state is a dipole-stabilised state. An active intramolecular vibrational redistribution (IVR) was observed in the triatomic $FeCN^-$. The results reveal the formation of the stable anion through the active IVR. The details of the work were discussed in our recent publication[1].

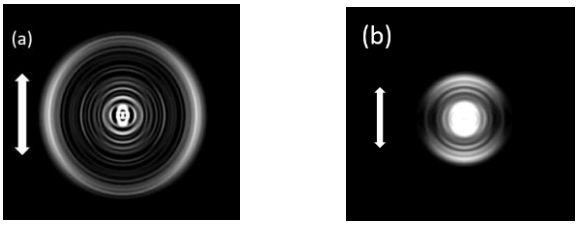

Figure 1. Abel inverted VMI image obtained at 355 nm (a) and 580 nm (b) photon wavelengths. The VMI image at 580 nm is a resonant transition.

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Dielectronic recombination of Neon in the Polar-X-EBIT

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While highly charged ions are rarely encountered in our surroundings, they are common in our universe. Highly charged ions are very interesting for astrophysics. For example, the spectral lines of highly charged ions are so specific that, with other parameters like temperature, individual elements can be identified even for distant objects. An electron beam ion trap (EBIT) can be used to produce these highly charged ions on Earth by electron impact ionization. The highly charged ions can then be stored and investigated in the EBIT or further directed to other experiments. EBITs can be used as an ion source for highly charged ion beams in storage rings such as the Cryogenic Storage Ring (CSR). Thus, interactions between highly charged ions and, e.g., molecules could be investigated. We will present the functionality of the compact Polar-X-EBIT[1,2,3,4] and dielectronic recombination[4,5] of neon.

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Dissociative recombination and rovibrational excitation of CF^+ and CH^+ in collisions with low-energy electrons

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Theoretical approaches to studying the dissociative recombination (DR) of molecular ions with competing direct and indirect mechanisms have proven to be somewhat difficult. These ions often exhibit low-energy electronic resonances, which occur, e.g., in open-shell molecular cations. We present our work to develop a theoretical approach that models this process by combining three different methods:

(i) fixed-nuclei electron-molecule scattering calculations with the UK R-matrix method

(ii) rovibrational frame transformation using dissociative wave functions calculated with a complex absorbing potential

(iii) molecular quantum-defect theory

We have applied this approach to the DR of CH+ and, more recently, CF+: two ions with very similar electronic structures. Prior experimental and theoretical results indicate that the Rydberg states belonging to excited electronic states and d-type partial waves play an important role in the DR mechanism for CH+. This work improves on our recent DR study of CH+, in which the results were not rotationally resolved, and is extended to CF+.

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Enhanced detection rate for a 3D-imaging detector at CSR

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The electrostatic Cryogenic Storage Ring (CSR) [1] at the Max Planck Institute for Nuclear Physics in Heidelberg is a unique device to study collision and laser interactions with fast atomic, molecular, and cluster ion beams. One of the most important processes is the Dissociative Recombination (DR), a reaction which occurs for example in interstellar clouds. To measure the products of such a reaction, the Neutral Imaging in Cold Environment (NICE) detector was installed at the CSR.

Previously, this 3D-imaging detector could detect and measure count rates up to 2×10^3 s^{-1} without stronger distortions or serious risk of damage. For future experiments, however, higher detection rates are required, including the imaging capability. Hence, a new method to operate the detector was implemented and tested. Hereby, the MCP bias voltage was switched between a nominal value (on) and a lowered value (off) with a frequency generator with 5 – 500 Hz and a varying duty cycle. Based on these tests, later experiments reached count rates up to 10^5 s^{-1}.

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

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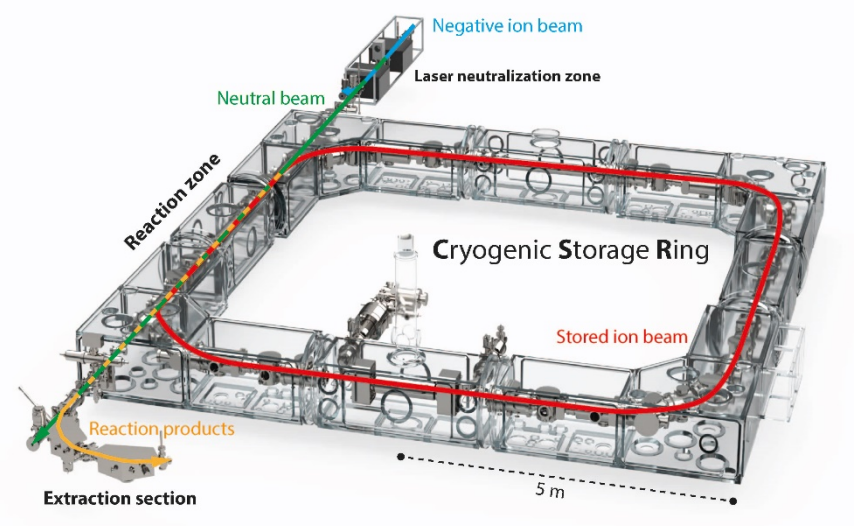
Collisions between molecular and atomic ions and neutral atoms are among the most frequent processes in the universe. To address this important class of reactions, we have developed a merged beams experiment [1] to study ion-neutral collisions at the Cryogenic Storage Ring (CSR) of the Max Planck Institute for Nuclear Physics in Heidelberg, Germany.



In a dedicated neutral beamline, ground term atomic beams are produced via laser photodetachment [2] of fast negative ions at kinetic energies ranging from 10 to 300keV. These neutral atoms are merged with stored molecular ions in one of the straight sections of the CSR. The relative collision energy of the reactants can be adjusted using a variable drift tube in which the photodetachment takes place. Several dedicated detectors and kinetic energy filters are installed in order to detect the resulting reaction products. Experiments involving infrared-active molecular ions, which decay radiatively during their storage inside CSR, will allow for collision studies with molecular ions in their lowest rotational states.

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Current Status of the Reaction Microscope for the Cryogenic Storage Ring CSR

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This poster gives an overview of the current status of the cryogenic reaction microscope (ReMi) [1], which is currently being constructed for the cryogenic storage ring (CSR) [2] at the Max Planck Institute for Nuclear Physics in Heidelberg. The CSR can be cooled down to temperatures around 2K, where molecular ions can be prepared at or close to their rotational-vibrational ground state. With the integration of the ReMi into the CSR dynamic processes occurring when atoms or molecules break up following collisions with the slow and cold ions in the CSR can be studied with high resolution.

The reaction microscope is a combined electron and ion spectrometer. Homogeneous electrostatic and magnetic fields guide the electrons and recoil-ions emerging from the collision process onto the time and position sensitive multi-channel plate (MCP) detectors. This allows for the determination of their momentum vectors within a 4 π solid angle. The coincident detection of electrons and ions provides kinematically complete data on the reaction dynamics.

The setup of one of the MCP detectors with delay-line read out and the design adaptation for operation at cryogenic temperatures will be shown. Also, the general setup of the spectrometer will be discussed. The spectrometer will be mounted perpendicular to the ion beam direction. Compensation coils are needed to correct the ion beam position after traversing the homogeneous magnetic field. Therefore, the characterization of the magnetic field inside the spectrometer is of particular interest, since the magnetic fields generated by the compensation coils overlap the homogeneous field in the spectrometer.

Integration of the ReMi into the CSR will start end of May 2022 and first in-ring test measurements at 300K are envisaged for the end of 2022. First cryogenic measurements are planned in early 2023.

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Completion and commissioning of an LVAP ion source for CSR

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Cooling processes and especially the processes of delayed electron emission and delayed atom emission have been subject to research for the past decades. For the anionic Al_4^- clusters, a lot was learned about their cooling processes from room-temperature experiments [1]. Much less is known about their cooling behavior at ambient temperatures far below room temperature. Suitable experimental conditions for further studies can be provided by the Cryogenic Storage Ring (CSR), a cryogenic electrostatic ion storage ring at the Max-Planck-Institut für Kernphysik in Heidelberg. By cooling its experimental vacuum chambers down to about 6 K, the CSR is capable of storing ion beams over timescales on the order of an hour in an environment with very low residual gas density (~100 cm^{-3}) and strongly suppressed blackbody radiation [2]. To produce cold cluster ions for the CSR, a new versatile Laser VAPorization (LVAP) ion source was designed. With this ion source, the cluster ions can be produced in already low rovibrational states. In this project, the LVAP ion source was taken into operation as a first step towards production of cold Al_4^- clusters and monitoring their cooling processes. The ion source and its auxiliary equipment were assembled and set up at a magnetic mass spectrometer dedicated to testing ion sources. All necessary tests and alignment steps were successfully performed. A roadmap of measurement steps required for commissioning the LVAP ion source was developed. The first step of the commissioning process was concluded and the production of rather stable and short (about 25 µs) ion pulses was achieved.

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MOCCA - A 4k-pixel microcalorimeter for the Cryogenic Storage Ring CSR

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In the Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics in Heidelberg, heavy molecular ions can be stored for several thousand seconds at cryogenic temperatures of only a few Kelvin, where they can relax into their vibrational and rotational ground states. This allows conditions such as those in cold interstellar plasmas to be recreated in the laboratory and electron-ion interactions such as the dissociative recombination to be studied. To reconstruct the full kinematics of these processes, position- and energy-sensitive coincident detection of multiple neutral reaction products is required. For this purpose, the MOCCA detector, a 4k-pixel molecule camera based on metallic magnetic calorimeters, was developed at the Kirchhoff Institute for Physics in Heidelberg. We present the plans for the integration of MOCCA into CSR and the CSR-independent MOCCA standalone setup that will be used to study photon- and collision-induced ion fragmentation processes, as well as a new readout scheme that reduces the spatial complexity of MOCCA and allows for better energy resolution and easier data analysis.

Dissociative recombination of OH^+ at the Cryogenic Storage Ring

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

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The CRYRING@ESR Electron Cooler

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The heavy-ion storage ring CRYRING [1] has been recommissioned at GSI, Darmstadt. Downstream of the Experimental Storage Ring (ESR), CRYRING complements the latter as a dedicated low-energy machine and provides the first operational platform for precision experiments on stored ions at FAIR [2]. A key element of CRYRING@ESR is its electron cooler, featuring one of the coldest electron beams available for the purpose [3]. This enables efficient phase-space cooling and provides very high energy resolution when used as internal electron target. We present first results from operation of the cooler at GSI/FAIR, especially with regard to handling of low-energy ion beams, which requires very precise control of the cooler and ring parameters. We also present a number of technical enhancements that have been made upon reinstallation of the cooler at FAIR or are planned for the near future.

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Photodetachment of Al_4^- clusters in a cryogenic storage ring

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We have used the Cryogenic Storage Ring (CSR) [1] at the Max Planck Institute for Nuclear Physics to study the spontaneous cooling of stored Al_4^- ions at very long time scales. Unlike the radiative cooling of macroscopic systems, the behavior of small isolated molecular clusters can no longer be described by the Stefan-Boltzmann law, since their internal energy distribution is not represented by a canonical temperature. Therefore, we try to find an alternative description, using Al_4^- as a model system.

Here, we present measurements that allow us to monitor the cluster cooling rates for up to 30 min and we compare those results to previous measurements at a room temperature [2]. We find that the cooling time scale is limited by the redistribution of vibrational energy inside the molecule, and that the cooling rates have a power law dependence on the internal energy, which can be described by a slow exchange model.

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New Lifetime Limit for the Ground State Vinylidene Anion H_2CC^-

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The molecular isomers acetylene ($HCCH$) and vinylidene (H_2CC) form one of the simplest systems for studying isomeric reactions involving hydrogen.

In anionic form, the state with lowest total energy has the vinylidene structure, H_2CC^-, with an electron affinity of about 0.5 eV. It lies 1.5 eV above the lowest neutral level of the acetylene structure, opening up the possibility that isomerization linked with electron emission could limit the lifetime of H_2CC^-.

Indeed, an experiment at a room-temperature storage ring reported a finite intrinsic lifetime of about 110 s [1], by extrapolating from collision-limited (about 10 s) to collision-free beam lifetimes of H_2CC^-, using a stable reference ion.

To access longer ion beam lifetimes, and thereby enable a better estimate of the ground state H_2CC^- lifetime, we employed the Heidelberg electrostatic Cryogenic Storage Ring (CSR) [2]. The CSR provides a cryogenic environment with strongly suppressed blackbody radiation and extremely low residual gas density, allowing to store and observe fast ion beams over time scales on the order of an hour.

We used photodetachment to monitor the decays of simultaneously stored H_2CC^- and CN^- ion beams. Here, CN^- served as a stable reference ion with nearly identical mass-to-charge ratio. Comparing the two decays at storage times of up to 3000 s allowed us to discriminate against most of the storage-ring induced loss processes. Furthermore, by using the novel isochronous mass spectrometry method [3], we were able to prove that no ion beam contaminations could significantly affect the observed lifetimes.

We present preliminary results which suggest that the intrinsic lifetime of the ground-state of H_2CC^- is several thousand seconds, i.e., at least an order of magnitude longer than assumed previously.

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Dissociative recombination of internally cold CH+ molecules

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Heavy ion storage rings provide an ideal environment for internal state preparation of atomic and molecular ions and subsequent collision experiments over a large range of collision energies using the merged-beams technique. We have studied the dissociative recombination (DR) of CH^+ in the electrostatic Cryogenic Storage Ring (CSR; [1]). In the cryogenic environment of CSR (T < 20 K), CH^+ ions radiatively decayed toward their lowest rovibrational states [2,3] and the internally relaxed ions were used for DR experiments. Merging an electron beam in the CSR electron cooler with the ion beam, low energy (meV) collisions could be probed. Measurements for different internal state populations enabled us to extract the rate coefficient for the (v=0, J=0) ground state.

DR reactions for CH^+(v=0, J=0) at meV collision energies are an important part of the chemistry in diffuse interstellar clouds, out of which stars and planets can form [4]. The DR rate coefficient is needed to model this chemistry and interpret astronomical observations. Theoretical calculations are not yet reliably able to produce the required DR data due to the large number of intermediate states involved in the dynamics. Thus, laboratory studies of DR are needed to understand the CH^+ chemistry. With our experimental results at diffuse cloud conditions, we have significantly increased the reliability of the CH^+ diffuse cloud chemistry.

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Production and Study of Polyanionic Metal Clusters with Ion Traps

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Metal-cluster sources produce mainly neutral or singly (positively or negatively) charged particles. For the study of polyanionic systems, methods have been developed to attach further electrons to anionic clusters in Penning [1,2] or Paul traps [2,3].

Due to their mutual repulsion only limited numbers of excess electrons can be hold by nanoparticles. Thus, attachment of additional electrons is observed only above element and precursor charge-state dependent appearance sizes.

Polyanionic clusters are special due to their Coulomb barrier which can lead to metastable systems where electrons have negative binding energies, i.e. they have been attached to clusters with negative electron affinities. This has been probed by laser detachment in photoelectron spectroscopy [3,4].

Alternatively, photoexcitation can lead to fragmentation, i.e. break-off of neutral pieces, or to fission into two charged products [5]. Recently, time-resolved measurements of the fragmentation of monoanionic tin clusters [6] have been extended to the investigation of delayed fission of dianions [7].

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VMI Photoelectron Spectroscopy Probing the Rotational Cooling Dynamics of Hot Trapped OH^- Ions

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The VMI photoelectron spectroscopy inside an electrostatic ion beam trap (EIBT) [1,2] is used to probe the time-dependent dynamics of rotational states relaxation (cooling) of "hot" OH^- ion, produced in a cesium sputter ion source. The photodetachment of OH^- ion results in the population of two neutral states ($\Pi_{3/2}$ and $\Pi_{1/2}$) [3-5]. The VMI photoelectron spectra of the P-branch transitions are recorded as a function of storage times in EIBT. Rotational line intestines are the direct indicative of temperature. The peak radius of the P-transition decreases with increasing the storage time, indicating the rotational population shift from high to low rotational levels i.e. cooling. The rotational temperature is estimated from rotational line intensities from 4000 to 1000K range during the 0.1-2.8 sec trapping time. We are investigating, whether a rate law model that includes the spontaneous emission, stimulated emission and absorption through blackbody radiation of many (>25) coupled rotational levels can reproduce the experimental cooling rate?

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2DCylPIC technique to study the AR cooling of ions in an electrostatic ion beam trap

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The cooling of ions is a prerequisite in several research areas. Auto-resonance (AR) cooling, where a slice from initial phase-space of ions is accelerated out, has been studied experimentally in an Electrostatic Ion Beam Trap [1]. The velocity distribution of ions within a bunch was reduced from ~1000 m/s to ~ 6 m/s. A theoretical work [2], demonstrated the AR cooling of electrons inside a static potential well. However, the interaction between the charged particles was not specifically included. Recently [3], a new technique based on two-dimensional particle in cell simulation (2DCylPIC) has been developed. Two different modes: dispersive and self-bunching, of an EIBT have been studied and the role of ion-ion interaction was demonstrated. This allows a detailed and controlled study of ions dynamics in the electrostatic ion beam trap.

Using 2DCylPIC, we study the AR process for phase-space cooling of ions in the EIBT. The preliminary results show the cooling of the ions, and they are in good agreement with the experimental observations. The ion-ion interaction strongly affects AR dragging of ions. During AR, the hot ions are continuously evaporated from the bunch, hence reducing the bunch temperature. With 2DCylPIC simulation, we demonstrate the increase in the phase-space density of ions.

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State-selected ion beams for storage ring studies

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While most storage ring studies concentrate on cold ionic species held in cryogenic environments, the time evolution of rotationally, vibrationally and electronically excited species has become a powerful tool to access state-to-state cross sections and state-specific properties. Instead of relying on the nascent excited state population, we propose to actively populate long-lived states of atomic and molecular species by different means.

Regarding atomic cations, a close examination of the kinetic energy release spectra measured for mutual neutralization both in single pass and at the DESIREE storage ring has revealed the presence of metastable N^+ and O^+ cations in unknown proportion, at the percent level [1]. Strategies for boosting that electronically excited population must be explored to better constrain the theoretical predictions.

Concerning molecular species, previous experiments at the TSR with a laser ion source utilized the rovibrational selectivity of resonance enhanced ionization of H_2 for the measurement of state- specific dissociative recombination. Similar performance was demonstrated for O_2^+ [2]. Changing the ionization source for an argon ion beam allowed for the selective production of O_2^+ in its first metastable state.

Finally, a recent study of the ^4S and ^2D state of the C^- anion was conducted to obtain photodetachment cross sections and anisotropy parameters overs a wide wavelength range [3,4]. The ^2D population was enhanced by double electron capture by C^+ on cesium vapor, and measured by velocity map imaging of saturated photodetachment. This technique will be applied to the five bound states of Si^- that were recently investigated at the CSR [5].

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Precise determination of $2s^2p^5 \rightarrow 2s2p^6$ transition energy in fluorine-like nickel utilizing a low-lying dielectronic resonance

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Electron-ion recombination spectrum of fluorine-like nickel ion (Ni^{19+}) has been measured at the heavy-ion storage ring HIRFL-CSRm [1]. The measured DR resonances are identified by comparing the experimental data with relativistic calculations utilizing the flexible atomic code (FAC). The experimental determination of the collision energy for the first resonance via the $(2s2p^6[^2S_{1/2}]6s)_{J=1}$ intermediate state at 86 meV reaches an uncertainty as low as ±4 meV. By employing the multi-configurational Dirac-Hartree-Fock (MCDHF) approach and stabilization method (SM), the binding energies of the 6*s* electron in the $(2s2p^6[^2S_{1/2}]6s)_{J=1}$ state are calculated, and yielding the following values of $149.056(4)_{exp}(20)_{MCDHF}$ eV and $149.032(4)_{exp}(6)_{SM}$ eV, respectively, for the $2s^2p^5\ ^2P_{3/2} \rightarrow 2s2p^6\ ^2S_{1/2}$ transition energy in fluorine-like nickel ion [2]. The *ab initio* theoretical calculations with two different starting potentials reveal that second-order QED contributes by about -0.03 eV to the total transition energy, and can, thus, be assessed by the present precision DR spectroscopic measurement.

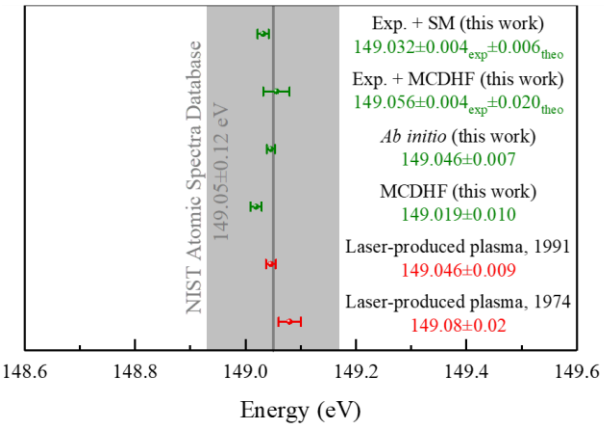

Figure 1: A comparison of present experimental and theoretical transition energies with previous plasma observations and the NIST recommended data.

Table I: Individual contributions to the transition $2s^2p^5\ ^2P_{3/2} \rightarrow 2s2p^6\ ^2S_{1/2}$ energy in fluorine-like nickel ion (in eV).

Contribution	Core-Hartree	Kohn-Sham
Dirac	123.911	128.743
Correlation (1)	27.190	22.723
Correlation (2)	−1.536	−1.972
Correlation (3)	0.032(2)	0.102(2)
QED (1)	−0.506	−0.510
QED (2)	−0.033(6)	−0.028(6)
Recoil	−0.012(3)	−0.012(3)
Total	149.046(7)	149.046(7)

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[2] S. X. Wang, Z. K. Huang, W. Q. Wen *et al.*, arXiv:2205.01334 and references therein

Hyperfine-induced effects on angular distribution of x-ray lines following EIE of heliumlike Tl^{79+} ions

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For isotopic atoms or ions with nonzero nuclear spin, the hyperfine interaction results in splittings of their fine-structure levels and, thus, affects their radiative properties. In the past decades, hyperfine structure and transition properties of various atoms and ions have been explored extensively, while the hyperfine-induced effects on angular and polarization properties of characteristic lines were rarely explored. In this work[1], we study the electron-impact excitation of heliumlike zero-spin and spin-1/2 Tl^{79+} ions and the subsequent M2 ($1s2p\,^3P_2 \rightarrow 1s^2\,^1S_0$) and $K\alpha_1$ ($1s2p\,^{1,3}P_{1,2} \rightarrow 1s^2\,^1S_0$) radiative decay using the multiconfigurational Dirac-Fock method and the relativistic distorted-wave theory. It has been found that the hyperfine interaction remarkably weakens the anisotropy of the M2 line for all the impact electron energies considered. In contrast, the hyperfine interaction makes the $K\alpha_1$ line more anisotropic for low impact energies, whereas for higher energies the $K\alpha_1$ angular distribution is hardly affected, as shown in Figure1. Moreover, the angular distribution of the M2 line was found to be more or less sensitive to the magnetic dipole moment of the spin-1/2 Tl^{79+} ions, whereas the $K\alpha_1$ angular distribution behaves insensitively.

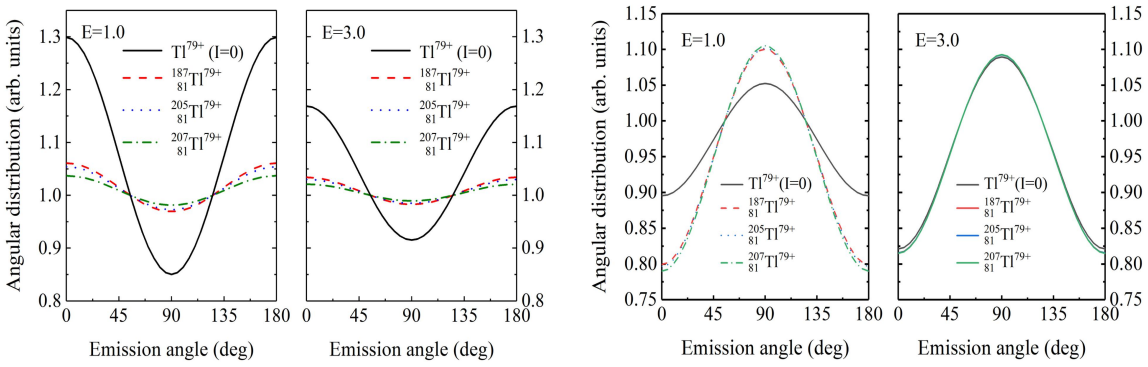

Figure 1. Angular distribution of the M2 (left panel) and $K\alpha_1$ (right) lines as functions of heliumlike zero-spin Tl^{79+} and spin-1/2 $^ATl^{79+}$ (A=187, 205, and 207) ions. Results are shown for two impact electron energies: 1.0 and 3.0 times the excitation threshold of the $1s2p\,^3P_1$ level.

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TrapREMI: a reaction microscope inside an electrostatic ion beam trap

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A novel setup has been developed in our group to investigate the reaction dynamics of molecular ions with a variety of projectiles in kinematically complete crossed-beam experiments. The setup combines an electrostatic ion beam trap (EIBT) with a reaction microscope (REMI). The EIBT stores ions in an oscillatory motion at several keV and allows further target preparation e.g. cooling, relaxation, pulsing, mass and/or charge selection. Reactions are induced by crossing the ion beam with a projectile beam in the field-free region of the EIBT, where the REMI is located. The REMI, oriented along the target beam axis, allows for detection of all fragments in coincidence, including neutral particles. By reconstructing all particles' initial momenta we obtain kinematically complete information of the observed event. During setup tests a laser pulse was used as the projectile to induce photodissociation in molecular ions. Positive and neutral fragments from these dissociation events were detected in coincidence. Currently a gas jet is being assembled to provide an atomic/molecular beam as a projectile. Near-term goals include performing collision experiments with a neutral atom/molecule beam and testing the electron detection.

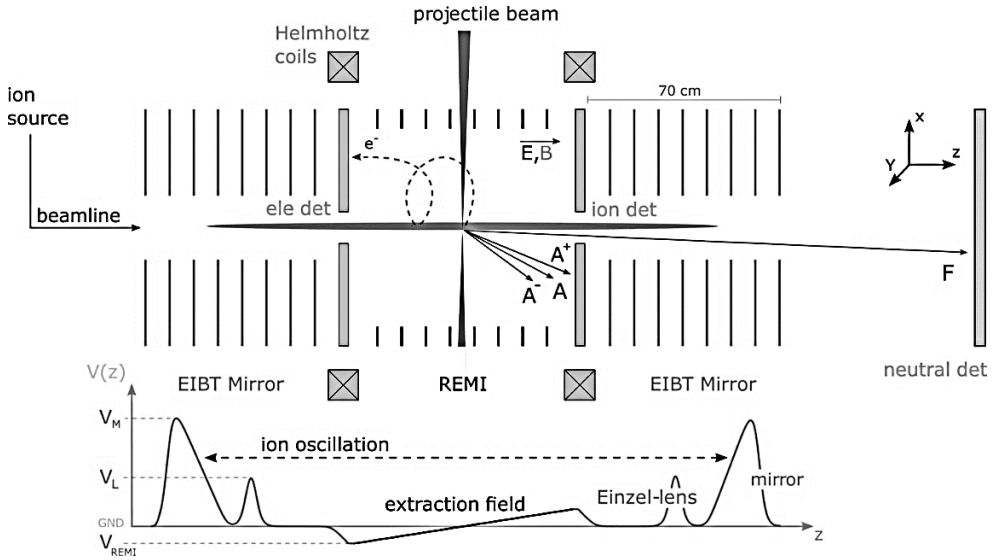

Fig. 1: *TrapREMI experimental scheme in cross-sectional view. The setup is cylindrically symmetric. The electrodes generate a typical electrostatic potential for ion storage V(z) and a homogenous electric field in REMI as depicted in lower plot. Helmholtz coils generate a magnetic field in the REMI. Heavy reaction products of different charge (A, A^+, A^-) and electrons (e^-) can be detected by the corresponding REMI detectors. Neutral fragments emitted at low angles to the trap axis (F) can be detected by an additional detector behind the EIBT. The scheme is not to scale and the number of electrodes is reduced for illustrative purposes.*

Electron collisions and spectroscopy with triatomic hydrogen ions at the Cryogenic Storage Ring.

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The dissociative recombination of triatomic hydrogen ions with electrons has received considerable attention, owing to the fact that its rate coefficient is of paramount importance for the ionization balance of interstellar clouds. While previous studies have shown that the dissociative recombination rate coefficients of H_3^+ and it isotopologues depend on rotational excitation, state-selective measurements have not been possible thus far.

In this work we present current efforts to understand the cooling behavior of H_2D^+ and D_2H^+ within the Cryogenic Storage Ring (CSR). Radiative cooling models of H_2D^+ and D_2H^+ suggest that the population becomes confined to a few distinct identifiable states after few hundreds of seconds of storage. We will show preliminary data on recent DR experiments with cold H_2D^+ and D_2H^+ ions performed at the CSR, as well as preparations for a new approach toward spectroscopy of high-lying states of H_3^+.

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