2018 Conference on Cold and Controlled Molecules and Ions (CCMI)

University of Georgia, Athens, GA
March 25 – March 29, 2018

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Tanya Zelevinsky, Columbia University (USA)
Agenda

Sunday, March 25th

Registration, 4:30 pm – 5:30 pm, Conference Registration Desk

Welcome Reception, 5:00 pm – 6:00 pm, Pecan Tree Galleria

Dinner, 6:00 pm – 8:00 pm, Banquet Area

Keynote Lecture, 8:00 pm – 9:30 pm, Masters Hall

8:00 pm: Introductory Remarks

8:10 pm: John Doyle, Towards Ultracold Polyatomic Molecules via Laser Cooling: N Atoms Too Many

Monday, March 26th

Session 1 (Chair: Jonathan Weinstein), 9:00 am – 12:15 am, Masters Hall

9:00 am: Tanya Zelevinsky, Photodissociation and Precision Spectroscopy with Ultracold Diatomic Molecules in an Optical Lattice

9:40 am: Stefan Truppe, Laser Cooling Molecules to Below the Doppler Limit

Coffee Break, 10:20 am – 10:45 am, Pecan Tree Galleria Break Area

10:45 am: Brianna R. Heazlewood, Cold Ion-Molecule Reactions in Coulomb Crystals

11:25 am: Aaron Calvin, Rovibronic Spectroscopy of CaH\(^+\) in a Coulomb Crystal

11:50 am – 12:15 am: Simon L. Cornish, Coherent Control of Ultracold Ground-state \(^{87}\text{Rb}^{133}\text{Cs}\) Molecules in an Optical Trap

Lunch, 12:30 pm – 1:30 pm, Banquet Area

Session 2 (Chair: Bas van de Meerakker), 2:00 pm – 5:20 pm, Masters Hall

2:00 pm: Martin Centurion, Ultrafast Electron Diffraction from Aligned Molecules
2:40 pm: Zhi Gao, *Observation of Correlated Excitations in NO-O₂ Inelastic Collisions*

**Coffee Break**, 3:05 pm – 3:35 pm, Pecan Tree Galleria Break Area

3:35 pm: Xing Wu, *A Cryofuge for Cold-collision Experiments with Slow Polar Molecules*

4:15 pm: Andreas Osterwalder, *Merged Beam Study of the Ne(³P₂) + Ar Reaction: Cold Stereodynamics*

4:40 pm – 5:20 pm: Kang-Kuen Ni, *Building Single Molecules*

**Dinner (off-site)**, 5:20 pm – 8:00 pm

**Poster Session 1**, 8:00 pm – 11:00 pm

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**Tuesday, March 27th**

**Session 3 (Chair: Anastasia Borschevsky)**, 9:00 am – 12:15 am, Masters Hall

9:00 am: Robert Berger, *Cold Molecules as Probes for Fundamental Physics: Predictions for Diatomic Molecules and Perspectives for Chiral Systems*

9:40 am: Andreas W. Hauser, *Molecular Collisions in Helium Droplets: From Spatial Hindrance to Controlled Molecular Synthesis*

**Coffee Break**, 10:20 am – 10:45 am, Pecan Tree Galleria Break Area

10:45 am: Balakrishnan Naduvalath, *Quantum Dynamics and State-to-State Chemistry of Ultracold Molecules*


11:50 am – 12:15 am: Sharly Fleischer, *The Ramifications of Coherent Radiative Decay on Periodically Orienting Molecular Ensembles*

**Lunch**, 12:30 pm – 1:30 pm, Banquet Area

**Session 4 (Chair: Michael Duncan)**, 2:00 pm – 5:20 pm, Masters Hall

2:00 pm: Dietrich Leibfried, *Preparation and Coherent Manipulation of Pure Quantum States of a Single Molecular Ion*

2:40 pm: Martin Zeppenfeld, *Electric Field Controlled Collisions between Polar Molecules and Rydberg Atoms*
**Coffee Break**, 3:05 pm – 3:35 pm, Pecan Tree Galleria Break Area

3:35 pm: **Pierre-Nicholas Roy**, *Dynamics of Confined Molecules*

4:15 pm: **David T. Anderson**, *Quantum Diffusion-Controlled Chemistry in Solid Parahydrogen*

4:40 pm – 5:20 pm: **Stephan Schlemmer**, *New Methods in Molecular Spectroscopy*

**Dinner (off-site)**, 5:20 pm – 8:00 pm

**Poster Session 1**, 8:00 pm – 11:00 pm

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**Wednesday, March 28**th

**Session 5 (Chair: Phillip Stancil)**, 9:00 am – 12:15 am, Masters Hall

9:00 am: **Wesley C. Campbell**, *Optical Deceleration and Cold Hydrocarbon Chemistry*

9:40 am: **Heather J. Lewandowski**, *Isomer Specific Ion-Molecule Reactions*

**Coffee Break**, 10:20 am – 10:45 am, Pecan Tree Galleria Break Area

10:45 am: **David Patterson**, *Quantum Control of Polyatomic Molecules*

11:25 am: **Mikhail Lemeshko**, *The Angulon Quasiparticle: From Molecules in Superfluids to Ultrafast Magnetism*

11:50 am – 12:15 am: **Shimshon Kallush**, *Directional Quantum-Controlled Chemistry: Generating Aligned Ultracold Molecules via Photoassociation*

**Lunch**, 12:30 pm – 1:30 pm, Banquet Area

**Break**, 1:30 pm – 4:00 pm

**Poster Session 2**, 4:00 pm – 6:00 pm

**Cash Bar Reception**, 6:00 pm – 7:00 pm, Pecan Tree Galleria

**Dinner**, 7:00 pm – 8:30 pm, Banquet Area
Thursday, March 29th

Session 6 (Chair: Andreas Osterwalder), 9:00 am – 12:15 am, Masters Hall

9:00 am: Daniel M. Reich, *Understanding the Dynamics of Molecular Ions after Cold Penning Ionization*

9:40 am: Katrin Dulitz, *Towards the Study of Quantum-state-selected Penning Reactions*

Coffee Break, 10:20 am – 10:45 am, Pecan Tree Galleria Break Area

10:45 am: Jun Ye, *Exploring a New Frontier of Molecular Structure and Interactions*

11:25 am: Jutta Toscano, *Cold State-selected Radicals for the Study of Low Temperature Chemistry*

11:50 am – 12:15 am: Philipp C. Schmid, *Quantum-state Controlled Ion Chemistry*

Lunch, 12:30 pm – 1:30 pm, Banquet Area

Session 7 (Chair: Sadiq Rangwala), 2:15 pm – 4:15 pm, Masters Hall

2:15 pm: Ardita Kilaj, *Observation of Different Reactivities of para- and ortho-water Towards Cold Diazenylium Ions*

2:40 pm: Masato Morita, *Quantum Spin-dynamics in Ultracold Atom-molecule and Atom-ion Collisions*

Coffee Break, 3:05 pm – 3:35 pm, Pecan Tree Galleria Break Area

3:35 pm – 4:15 pm: Stephen D. Hogan, *Resonant Energy Transfer in Collisions of Rydberg Atoms with Polar Molecules*

Dinner (off-site), 4:15 pm – 8:00 pm

Poster Session 2, 8:00 pm – 11:00 pm
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Towards Ultracold Polyatomic Molecules via Laser Cooling: N Atoms Too Many

John Doyle

Department of Physics, Harvard University, Cambridge, MA, 02138, USA

For quantum control of molecules, cooling their external and internal degrees of freedom is a near necessity. Exquisite quantum state control has already been achieved with atomic species, leading to great progress in quantum computation, simulation, searches for physics beyond the Standard Model, and novel collisions and chemical reactions. Molecules are now a current frontier in cold matter science, with diatomic molecules taking center stage at the moment. Moving to the next frontier, the creation of ultracold polyatomic molecules presents new laboratory challenges. One of our key long-term scientific goals is to achieve for a wide variety of polyatomic molecules the kind of single-state control and high phase space density now available with atoms. This talk will center on laser cooling of diatomic and polyatomic molecules. Recent results will be presented, along with some prospects for the future.
Photodissociation and Precision Spectroscopy with Ultracold Diatomic Molecules in an Optical Lattice

Tanya Zelevinsky

Department of Physics, Columbia University, New York

Atomic-clock style control of the internal and motional quantum states of diatomic molecules enables new measurements on multiple fronts. We apply this control to one- and two-photon, bound-continuum and bound-bound transitions in strontium dimers trapped in an optical lattice. The bound-continuum light-induced transitions correspond to photodissociation, or the breaking of the interatomic bond. By controlling the quantum state of the initial molecules, essential features of ultracold quantum chemistry are observed. These include tunneling through reaction barriers and matter-wave interference of coherently created reaction products. By applying small magnetic fields that correspond to Zeeman energies of a similar magnitude to the potential-barrier and kinetic energies, we can predictably control the photodissociation process. Furthermore, by tuning the kinetic energy of the fragments in the 0-5 mK range we directly observe a transition from the distinctly quantum mechanical to the quasiclassical chemistry regime. On the other hand, two-photon bound-bound transitions between vibrational states can yield a high-precision measurement of the van der Waals interatomic force, for testing molecular QED at a high level and searching for new physics. We show that by tuning the wavelength of the optical lattice, coherence time of the molecule-light interaction can be increased by several orders of magnitude, leading to hertz-level vibrational spectroscopy.
Laser Cooling Molecules to Below the Doppler Limit


Centre For Cold Matter, Blackett Laboratory, Imperial College London, London, SW7 2BW, UK

*Present address: Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany

We demonstrate and characterize a two-frequency\(^1\) magneto-optical trap (MOT) of CaF molecules and show how to cool these molecules to 50µK, well below the Doppler limit, using a three-dimensional blue-detuned optical molasses.\(^2,3\) We then coherently control their rotational, hyperfine and Zeeman states and demonstrate magnetic trapping of the molecules in a single, selectable quantum state.\(^4\)

These ultracold molecules can be loaded into optical tweezers to trap arbitrary arrays for quantum simulation, launched into a molecular fountain for testing fundamental physics, and used to study collisions and chemistry between atoms and molecules at ultracold temperatures.

We produce the CaF molecules in a cryogenic buffer gas cell via pulsed laser ablation of Ca into a continuous flow of helium mixed with SF\(_6\).\(^5\) The molecules leave the cell with an average speed of 140 m/s and are slowed to about 10 m/s by a frequency-chirped counter-propagating laser beam. The molecules are then loaded into the MOT where they cool to 10 mK via Doppler cooling. By decreasing the intensity of the MOT laser beams the molecules cool further to below 1 mK. We then shift the frequencies of the MOT laser beams to positive detuning, turn-off the magnetic field and cool the molecules in a blue-detuned optical molasses to below the Doppler limit. We can then select a single quantum state via optical pumping and coherent microwave control and trap the molecules in a magnetic quadrupole trap for up to 2s.


Cold Ion-Molecule Reactions in Coulomb Crystals

Brianna R. Heazlewood, Lorenzo S. Petralia, Jutta Toscano, Timothy P. Softley

Department of Chemistry, University of Oxford, OX1 3QZ, UK

Reactive collisions are studied between Coulomb-crystallised ions held within a linear Paul ion trap and cold neutral molecules. For quantitative analysis, a mass-sensitive detection method is adopted – with the ejection of all ions onto an external detector at a selected time. This time-of-flight mass spectrometry (ToF-MS) approach removes ambiguity about the identities of dark ions: both the masses and relative numbers of all trapped species at the point of ejection can be ascertained directly from the ToF spectrum.\(^1\) Combining ToF-MS detection capabilities with real-time imaging of the Coulomb crystal enables one to examine both the kinetics and the dynamics of ion-molecule reactions. In this way, accurate reaction rate constants and branching ratios can be calculated. The combination of a range of different cold molecular sources with linear Paul ion traps is discussed, along with the potential for controlling more than just the velocity of the neutral reactant species.\(^2\)


Ultrafast Electron Diffraction from Aligned Molecules

Martin Centurion

Department of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588

Gas electron diffraction can be used to determine the structure of isolated molecules with high spatial resolution, which is important for understanding their function. With the advent of ultrafast laser and electron sources, it has become possible to capture the structure of transient states in photoexcited molecules using Ultrafast Electron Diffraction (UED). Recently, the temporal resolution of UED has reached the femtosecond scale needed to capture coherent nuclear motion during a reaction, and thus reveal the reaction path with sub-Angstrom resolution. In both static and time-resolved gas diffraction experiments, the random orientation of the molecules limits the amount of information contained in the diffraction patterns. If the molecules can be aligned, the information content of the patterns increases significantly, and in some cases it becomes possible to retrieve the full three-dimensional structure. Using impulsive laser alignment, the molecules reach maximum alignment after interacting with the laser pulse. This method has the important advantage that the molecules can be probed in a field-free environment, however, it produces a limited degree of alignment.

We will discuss three applications for diffraction from aligned molecules. In the first, we have used multiple diffraction patterns corresponding to different orientations of the alignment axis to retrieve the three-dimensional structure, even though the angular distribution in each pattern is fairly broad\textsuperscript{1,2}. In the second application, we have seen that it is possible to retrieve a diffraction pattern corresponding to a very narrow angular distribution by combining two diffraction patterns with similar angular distribution\textsuperscript{3}. In the third case, we have used the alignment due to photoexcitation (selective alignment) to distinguish the dynamics in two different excited states.

\textsuperscript{1} C. J. Hensley, J. Yang, M. Centurion "Imaging of Isolated Molecules with Ultrafast Electron Pulses" \textit{Physical Review Letters} 109, 133202 (2012).

\textsuperscript{2} J. Yang, V. Makhija, V. Kumarappan, M. Centurion "Reconstruction of three-dimensional molecular structure from diffraction of laser-aligned molecules" \textit{Structural Dynamics} 1, 044101 (2014).

A Cryofuge for Cold-collision Experiments with Slow Polar Molecules

Xing Wu*, Thomas Gantner, Manuel Koller, Martin Zeppenfeld, Sotir Chervenkov, Gerhard Rempe

Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, 85748 Garching, Germany.
*Present address: Department of Physics, Yale University, New Haven, CT 06520, USA.

Ultracold molecules represent a fascinating research frontier in physics and chemistry, but it has proven challenging to prepare dense samples at low velocities. Here, we present a solution to this goal by means of a nonconventional approach dubbed cryofuge. Cryofuge denotes successive cryogenic buffer-gas cooling\(^1\),\(^2\) and centrifuge deceleration\(^3\). In this scheme, polyatomic molecules are first cooled to very few rotational and vibrational states, and then brought to kinetic energies below 1 K × k\(_B\) in the laboratory frame, with corresponding fluxes exceeding 10\(^{10}\) s\(^{-1}\) at velocities below 20 m·s\(^{-1}\). By attaining densities higher than 10\(^9\) cm\(^{-3}\) and interaction times longer than 25 ms in samples of fluoromethane (CH\(_3\)F), as well as deuterated ammonia (ND\(_3\)), we observed cold dipolar collisions between molecules and determined their collision cross sections\(^4\). In addition, we illustrate the generality of this approach by extending it to other organic molecules, including methanol (CH\(_3\)OH), (trifluoromethyl)acetylene (CF\(_3\)CCH), and isopropanol (C\(_3\)H\(_7\)OH).


Building Single Molecules

Kang-Kuen Ni

Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

I will present our work to create single molecules. We started by tweezing and merging single cesium and sodium atoms into a single dipole trap. We studied their collisions and reactions at the ultracold regime. We built a molecule out of two atoms by photoassociation. And currently, we have tamed the individual atoms with full quantum control and are learning to create many single molecules coherently for quantum simulation, quantum information processing, and ultracold chemistry with precise initial reactant preparation.
Cold Molecules as Probes for Fundamental Physics: Predictions for Diatomic Molecules and Perspectives for Chiral Systems

Robert Berger

Fachbereich Chemie, Philipps-Universität Marburg, Germany

Combined systems of electrons and nuclei can serve as versatile probes for fundamental physics. Precision spectroscopy of atoms and molecules has for instance the potential to deliver detailed information on fundamental symmetries and fundamental interactions. For atomic systems, sophisticated experimental techniques like direct laser cooling or sympathetic cooling are well established such that spectroscopic measurements can in principle be performed under ideal conditions on individual trapped atoms. In an effort to unravel fundamental interactions, atoms are exposed to carefully tailored external fields. Fields on the atomic scale, however, are best controlled on the atomic level itself. Consequently, one favourably can let specifically designed molecules do the job! The special electronic situation in open-shell diatomic molecules, for instance, suppresses nuclear-spin independent parity-odd (P-odd) effects as compared to their nuclear-spin dependent counterparts. And chiral molecules feature a wealth of P-odd signatures in various frequency regimes, which can in principle be detected directly as energy differences rather than transition matrix elements. One of the usual disadvantages of molecules over atoms, however, is the challenge to obtain ultracold samples for precision spectroscopy. To address this problem, we have outlined classes of molecules with possible candidates for cooling with lasers\textsuperscript{1,2} and have pointed to the special situation in open-shell polyatomic molecules, which might give access to a variety of interesting properties.\textsuperscript{2}

In this talk, I will discuss the situation of open-shell diatomic molecules in general and RaF in particular. I will present predictions for P-even molecular properties, P-odd effects and possible P,T-odd signatures (with T referring to time-reversal symmetry) in this molecule\textsuperscript{1,3,4} as computed within a quasi-relativistic approach to electroweak quantum chemistry\textsuperscript{1,4,5} and outline experimental routes towards lasercooled RaF. I will also point to particular challenges and opportunities for lasercooled chiral molecules.

1 Isaev, T.A.; Berger, R. “Laser-cooled RaF as a promising candidate to measure molecular parity violation” Physical Review A, (2010), 82, 052521.


“Coupled-cluster study of radium monofluoride, RaF, as a candidate to search for P- and T,P-violation effects” Physical Review A, (2014), 90, 052513.


Molecular Collisions in Helium Droplets: From Spatial Hindrance to Controlled Molecular Synthesis

Andreas W. Hauser,† María Pilar de Lara-Castells,‡ Wolfgang E. Ernst†

† Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria; ‡ Instituto de Física Fundamental, CSIC, Serrano 123, 28006 Madrid, Spain

The dotation of superfluid helium droplets is particularly well suited for studies of unstable or highly reactive molecules such as radicals and molecular fragments. On one hand, the droplets act as a nearly ideal cryogenic matrix, providing a sub-Kelvin temperature bath for the dopants with a minimum of interaction, which greatly simplifies the interpretation of optical spectra. On the other hand, the spherical helium environment also acts as a spatial confinement for immersed molecules and can be used as a reaction container due to its non-vanishing, typically attractive interaction with most impurities. Recently, this property has been exploited for the synthesis of tailor-made bimetallic clusters.

All growth processes start with a molecular or atomic collision event. In this talk, I will focus on the impact of the He environment on the collision process from a theoretical point of view for situations of weak and strong interaction involving either “heliophilic” (sinkers) or “heliophobic” (swimmers) reaction partners.

Cases of both reactants being heliophobic (e.g. alkali metal atoms) can be omitted as they are conceptually identical with reaction mechanisms of gas molecules on surfaces. The He droplet does not provide any spatial hindrance. Cases of both reactants being heliophilic (e.g. coinage metal atoms) are particularly interesting as such processes are the foundation of metal cluster formation in helium droplets.1 We look at Cu, Ag and Au collision times in comparison with dotation rates and discuss the effect of He droplet size on the size distribution of metallic nanoparticles produced.2 Cases of mixed reactants, one immersed, one remaining on the surface, offer a rich playground for the investigation of reaction kinetics regarding very slow molecular motion at almost zero Kelvin (below the Landau velocity limit) and additional spatial hindrance due to separating layers of helium. We pick two scenarios: The first describing a weak interaction between heliophilic Xe and heliophobic Rb,3 the second an ionic interaction between heliophilic C60 and heliophobic Cs involving a harpoon-type electron transfer.4,5


Quantum Dynamics and State-to-State Chemistry of Ultracold Molecules

Balakrishnan Naduvalath

Department of Chemistry, University of Nevada, Las Vegas, NV 89154

In the ultracold regime quantum effects are the norm rather than the exception. Both the internal quantum states and orientation of the molecules can be controlled in this regime and chemistry triggered by selective preparation of initial quantum states. The first such experiments were performed on the K+KRb and KRb+KRb systems by research groups at JILA and universal models based on long-range behavior of the interaction potentials have been successfully applied to explain the overall reactivity. However, explicit quantum dynamics of these systems remains computationally challenging due to the high density of states of the reaction intermediates. Here, I will present results of numerically exact quantum dynamics of the K+KRb chemical reaction with quantum state resolution of the reaction products\(^1\). While the universal model describes the overall reaction rate, the product rotational states display a Poisson distribution, owing to chaotic nature of the reaction complex. We attribute such long-lived complexes to the cause of trap-loss involving ultracold molecules, even when inelastic and reactive channels are not energetically accessible. We illustrate this for Rb+K\(_2\) collisions that display many long-lived resonances in the elastic scattering cross section due to the formation of K\(_2\)Rb complexes with µs lifetimes\(^2\). I will also discuss how the geometric phase effect manifests and controls chemical reactivity in the ultracold regime.


Preparation and Coherent Manipulation of Pure Quantum States of a Single Molecular Ion*

Dietrich Leibfried, Chin-Wen Chou, Christoph Kurz, David Hume, David Leibrandt

National Institute of Standards and Technology, Boulder CO 80305, USA

An amazing level of control is routinely reached in modern experiments with atoms, but similar control over molecules has been an elusive goal. We recently proposed a method based on quantum logic spectroscopy\textsuperscript{1} to address this problem for a wide class of molecular ions\textsuperscript{2}. We have now realized the basic elements of this proposal.

In our demonstration, we trap a calcium ion together with a calcium hydride ion (CaH\textsuperscript{+}) that has a simple structure and is convenient to trap. However, the same apparatus and methods work in principle for a large class of molecular ions, including polyatomic molecules. We cool the two-ion crystal to its motional ground state and then drive the motional sidebands of Raman transitions in the molecular ion. A transition of the molecule is indicated by a single quantum of excitation in the secular motion of the pair. We can efficiently detect this single quantum with the calcium ion, which projects the molecule into the final state of the attempted sideband transition, leaving the molecule in a known, pure quantum state.

The molecule can be coherently manipulated after the projection, and its final state read out by quantum logic state detection \textsuperscript{3}. We demonstrate this by driving Rabi oscillations between rotational states. All transitions we address in the molecule are either driven by a single, far off-resonant continuous-wave laser or by a far-off-resonant frequency comb. This makes our approach applicable to control and precision measurement of a large class of molecular ions.

\textsuperscript{1} P.O. Schmidt, et al. Science 309, 749 (2005)

\textsuperscript{2} D. Leibfried, New J. Phys. 14, 023029 (2012)


*Supported by ARO, IARPA, ONR, and the NIST Quantum Information program.
Dynamics of Confined Molecules

Pierre-Nicholas Roy

Department of Chemistry, University of Waterloo, Waterloo, ON, Canada, N2L 3G1

Molecular assemblies are often described using classical concepts and simulated using Newtonian dynamics or Classical Monte Carlo methods. At low temperatures, this classical description fails to capture the nature of the dynamics of molecules, and a quantum description is required in order to explain and predict the outcome of experiments. In this context, the Feynman path integral formulation of quantum mechanics is a very powerful tool that is amenable to large-scale simulations. We will show how path integral simulations can be used to predict the properties of molecular rotors trapped in superfluid helium and hydrogen clusters. We will show that microscopic Andronikashvili experiments can be viewed as a measurement of superfluidity in a quantum mechanical frame of reference. We will also show that path integral ground state simulations can be used to predict the Raman spectra of parahydrogen clusters and solids. We will present ongoing work on the simulation of molecular rotors confined in endohedral fullerene materials such as H$_2$O@C$_{60}$ and HF@C$_{60}$. The questions we will address include symmetry breaking, spin conversion, the nature of dipole correlations and dielectric response, and entanglement measures.
New Methods in Molecular Spectroscopy

Stephan Schlemmer and Oskar Asvany

I. Physikalisches Institut, Universität zu Köln, Germany

The Cologne Center for THz Spectroscopy invites guests to use a wide variety of instruments to obtain spectra from the far-infrared to the mid-infrared region. The improvement of sensitivity, frequency coverage and spectral resolution are technical aims to record ever weaker transitions of species (complex organic molecules, radicals and ions) which shall be found in future astronomical observations.

The method of light induced reactions (LIR) in ion traps has been developed continuously over the last 20 years in our group in order to record spectra of only a few thousand mass selected, cold molecular ions. The spectral resolution of our IR measurements is high enough to predict THz spectra at sub-MHz accuracy which is sufficient to identify those ions in astronomical observations. Changing the population of the rotational states and interrogating them by LIR in double resonance experiments leads to predictions of THz transition frequencies at the $10^{-9}$ level, which challenges observations. IR spectra of cold ions in the range of 250 – 3200 cm$^{-1}$ are recorded with the ion trap instrument FELion operated at the FELIX free electron laser in Nijmegen (NL). Identifying the vibrational bands of mass selected molecular ions challenges quantum chemical predictions and is used as a basis for high resolution studies in order to ultimately find those molecules in space.

A particular interest concerns the spectroscopy of very fluxional molecules like protonated methane, CH$_5^+$. Obtaining spectra of such molecules is challenging but likewise is their interpretation. Due to the restrictions of standard Hamiltonian descriptions model independent methods are applied but also new Hamiltonians are explored.

Optical Deceleration and Cold Hydrocarbon Chemistry

Wesley C. Campbell, Eric R. Hudson, Xueping Long, Scarlett Shijia Yu, Tiangang Yang, Gary Chen

Department of Physics & Astronomy, University of California Los Angeles, Los Angeles, CA 90095

Picosecond optical pulses from mode-locked lasers can be tailored to create robust excitation of electronic transitions in atoms and molecules. If an excitation pulse and a simulated emission pulse are counter-propagating in space, this will effect a momentum kick of $2 \hbar k$ that can be repeated at a rate that is much faster than the excited state lifetime. We present our results benchmarking this force with cold rubidium atoms and discuss the outlook for moving to a molecular beam. We also discuss cold chemical reactions between a cryogenic buffer gas beam and trapped carbon and beryllium ions. Reaction products can be controlled and analyzed by varying the quantum states and relative speeds of the reactants, thereby allowing pure internal state chemistry with hydrocarbons.
Isomer Specific Ion-Molecule Reactions

Heather J. Lewandowski, Philip Schmid, James Greenberg, and Mikhail Miller

JILA / Department of Physics, University of Colorado, Boulder, CO 80309

Ion-molecule reactions play an important role in the chemistry that drives dynamics in the interstellar medium and during combustion of hydrocarbons. We use tools borrowed from the cold atom community to measure ion-molecule reactions in a well-controlled environment. In our experiments, molecular ions are stored in a linear quadrupole ion trap and sympathetically cooled with co-trapped, laser-cooled Ca+. Coupled to the trap is a time-of-flight mass spectrometer, which enables the determination of all trapped reaction products. Thus, a reaction can be followed by the increase of reaction products and not just the loss of reactants.

Here, we focus on reactions between small molecules that are important in basic organic chemistry. We present results from the reactions between isomers of C$_3$H$_4$, propyne CH$_3$CCH and allene CH$_2$CCH$_2$, with the acetylene cation, C$_2$H$_2^+$. Measurements show a strong dependence on the structural configuration of the reactant. Additionally, we identify multiple reaction pathways and measure the reaction rates and branching ratios for this fundamental organic reaction.
Quantum Control of Polyatomic Molecules

David Patterson

Department of Physics, University of California, Santa Barbara, CA 93106

The last half decade has seen enormous progress in our ability to prepare, cool, and read out the state of both neutral diatomic molecules and trapped molecular ions. The vast majority of this work has concentrated on diatomic species, and to date, a polyatomic molecule has never been prepared in a single internal and motional quantum state.

The ability to prepare and readout polyatomic molecules in single quantum states would enable diverse experimental avenues not available with diatomics, including new applications in precision measurement and edm searches, sensitive chemical and chiral analysis at the single molecule level, and precise studies of never-observed Hz-level molecular tunneling dynamics.

I will present the tools we are developing to control polyatomic molecular ions at this level, and will argue - somewhat counterintuitively - that polyatomic molecules, with highly complex rotational Hamiltonians, may well be easier to control than diatomic species such as CaH+ and MgH+. Our method can be applied to most reasonably small (< 10 atoms) nonspherical polyatomic ion, and requires modest resources compared to challenging state of the art QLS techniques.1

Understanding the Dynamics of Molecular Ions after Cold Penning Ionization

Daniel M. Reich1, Alexander Blech1, Wojciech Skomorowski1, Yuval Shagam2, Prema Paliwal2, Markus Meuwly3, Gerrit C. Groenenboom4, Ad van der Avoird4, Edvardas Narevicius2, Christiane P. Koch1

1Theoretical Physics, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany
2Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel
3Department of Chemistry, University of Basel, Basel, Switzerland
4Theoretical Chemistry, IMM, Radboud University, Nijmegen, The Netherlands

Cold Penning ionization reactions in merged beams have opened the way to studying quantum effects in cold collisions. In addition, they also provide a launching pad for controlled dynamics on the ionic surface which can be probed experimentally using velocity map imaging. This is what we exploit here for two examples.

First, we study predissociation of molecular ions due to spin-orbit interaction which gives rise to features at high kinetic energies in the images. Predissociation is observed for some ionic species but is apparently absent for others. This raises the question of what determines the predissociation lifetimes of cationic noble gas diatoms. We find that the predissociation lifetimes of NeAr+ show a remarkable peak for certain rovibrational levels, unlike the lifetimes of, for example, HeAr+ and HeKr+. We show that the prolonged lifetime is due to destructive interference in the coupling of the metastable state to the continuum - a mechanism that we term “phase protection”.

Second, we study cold collisions between helium atoms and H2+ initiated by Penning ionization, where velocity map imaging shows a remarkable difference in the energetically resolved scattering cross sections between para- and ortho-hydrogen molecules. We study these half-collisions which are governed by a rather anisotropic three-body potential that induces large rovibrational couplings. Thus, the anisotropy leads to a significant initial-state-dependent asymmetry in the rotational distribution of the final scattering wave packet.

Towards the Study of Quantum-state-selected Penning Reactions

Jonas Grzesiak¹, Simon Hofsäss¹, Vivien Behrendt¹, Frank Stienkemeier¹, Marcel Mudrich², Katrin Dulitz¹

¹Institute of Physics, University of Freiburg, Hermann-Herder-Str.3, 79104 Freiburg i.Br., Germany
²Department of Physics and Astronomy, Ny Munkegade 120, 8000 Aarhus C, Denmark

Our goal is to study quantum-state-controlled Penning collisions between lithium atoms and metastable helium atoms at low collision energies, e.g., to study the influence of electron-spin polarization on the reaction rate and to observe quantum resonance effects. For this, we use an experimental apparatus which consists of a discharge source for the production of metastable helium atomic beams and a magneto-optical trap (MOT) for ultracold lithium atoms. Using a novel multipulse detection scheme, we are able to mass-selectively probe the ionic reaction products at improved energy resolution. In this contribution, I will give an overview of the current state of these experiments. I will also present our progress towards achieving quantum-state selectivity of the reaction partners, which includes optical quenching of the metastable He(2¹S₀) state and magnetic-hexapole focusing of the metastable He(2³S₁, M_L = 1) state into the MOT target.
Exploring a New Frontier of Molecular Structure and Interactions

Jun Ye

JILA, NIST and Department of Physics, University of Colorado

Broad advances in the capabilities of cooling molecules and molecular spectroscopy have enabled new scientific discoveries in molecular structure and interaction dynamics. We will present examples for some of the latest work.
Resonant Energy Transfer in Collisions of Rydberg Atoms with Polar Molecules

Stephen D. Hogan

Department of Physics and Astronomy, University College London, London WC1E 6BT, UK

Atoms and molecules in Rydberg states with high principal quantum number $n$ can possess large electric dipole transition moments. For $\Delta n = \pm 1$ transitions these dipole moments exceed 1000 D for $n > 30$. Such large transition dipole moments make atoms and molecules in these states ideal model systems with which to study resonant energy transfer in collisions with other species.

In this talk I will describe experiments in which the resonant transfer of energy from the inversion sublevels in the ground electronic state of ammonia, to triplet Rydberg states in helium with $n = 36 – 41$, has been studied\textsuperscript{1,2}. For this range of values of $n$ the energy transfer process can be tuned through resonance using electric fields of less than 10 V/cm. This electric-field dependence has been studied using Rydberg-state-selective detection schemes based upon state-selective electric field ionization, and microwave spectroscopy. The experimental data are in good agreement with a simple theoretical model of the energy transfer process. Microwave spectroscopy of atoms that have undergone energy transfer has allowed the environment in which the atom-molecule interactions take place to be characterized.

This first demonstration of electric-field-controlled resonant energy transfer in atom-molecule collisions, combined with the methods of Rydberg-Stark deceleration, opens new opportunities for studies of gas-phase reaction dynamics at low temperature\textsuperscript{3,4} in which long-range dipole interactions may be exploited to regulate access to short-range chemical processes. They also represent a step toward the implementation of proposals to exploit resonant dipole interactions between Rydberg atoms and polar molecules for non-destructive detection\textsuperscript{5}, characterization of rotational state populations\textsuperscript{6}, coherent control\textsuperscript{7}, and cooling\textsuperscript{8,9}.


3 Allmendinger P.; Deiglmayr, J.; Schullian, O.; Höveler, K.; Agner, J. A.; Schmutz, H.; Merkt, F., “New method to study ion-molecule reactions at low temperatures and application to the H\textsubscript{3}\textsuperscript{+} + H\textsubscript{2} \rightarrow H\textsubscript{3}\textsuperscript{+} + H reaction” \textit{Phys. Chem. Chem. Phys.} (2016) 17, 3596.


Contributed Abstracts: Hot-Topic Talks

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Rovibronic Spectroscopy of CaH$^+$ in a Coulomb Crystal

Aaron Calvin$^1$, Smitha Janardan$^1$, John Condoluci$^1$, René Rugango$^1$, Eric Pretzsch$^2$, Gang Shu$^1$, and Kenneth Brown$^3$

1. School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332
2. School of Physics, Georgia Institute of Technology, Atlanta, GA 30332
3. Department of Electrical and Computer Engineering, Duke University, Durham, NC 22701

We report the measurement of an electronic transition of CaH$^+$ with rotational resolution. This molecular ion was co-trapped with Doppler-cooled Ca$^+$ to perform vibronic spectroscopy of the $1^1\Sigma$, v = 0 $\rightarrow$ $2^1\Sigma$, v' = 0, 1, 2, 3 transitions using two-photon photodissociation with a frequency-doubled, mode-locked Ti:Sapph laser$^1$. Spectroscopy on the deuterated isotopologue, CaD$^+$ confirmed a revised assignment of the CaH$^+$ vibronic levels and an approximately 700 cm$^{-1}$ disagreement with MS-CASPT2 theoretical calculations$^2$. Updated high-level coupled-cluster calculations that include core-valence correlations reduce the disagreement between theory and experiment to 300 cm$^{-1}$. The broad bandwidth of the pulsed Ti:sapph provided an advantage for the initial search for transitions, but did not allow spectral resolution of rotational transitions. Pulse shaping was applied to spectrally narrow the linewidth of the pulsed laser to obtain rotational constants for the $2^1\Sigma$, v' = 0, 1, 2, 3 states$^3$. These measurements will allow testing methods of rotational cooling by optical pumping, cryogenic cooling, or by collisions with laser cooled atoms.


$^2$Condoluci, J.; Janardan, S.; Calvin, A. T.; Rugango, R.; Shu, G.; Sherrill, C. D.; and Brown, K. R. “Reassigning the CaH$^+$ $1^1\Sigma \rightarrow 2^1\Sigma$ vibronic transition with CaD$^+$” Journal of Chemical Physics, (2017), 147, 214309.

Coherent Control of Ultracold Ground-state $^{87}\text{Rb}^{133}\text{Cs}$ Molecules in an Optical Trap

Simon L. Cornish$^1$, Phil Gregory$^1$, Jacob Blackmore$^1$, Elizabeth Bridge$^1$, Ruth Le Sueur$^2$, Jeremy Hutson$^2$, Jesus Aldegunde$^3$

$^1$Joint Quantum Centre (JQC) Durham-Newcastle, Department of Physics, Durham University, South Road, Durham DH1 3LE, UK
$^2$Joint Quantum Centre (JQC) Durham-Newcastle, Department of Chemistry, Durham University, South Road, Durham DH1 3LE, UK
$^3$Departamento de Quimica Fisica, Universidad de Salamanca, 37008 Salamanca, Spain

The formation of ultracold heteronuclear molecules opens up many exciting areas of research spanning precision measurement, quantum computation, quantum simulation, ultracold chemistry and fundamental studies of quantum matter. Long-lived, trapped samples of molecules with full quantum control of the molecular internal state are crucial to many of these applications. Here we demonstrate coherent microwave control of the rotational and hyperfine state of ultracold, chemically stable $^{87}\text{Rb}^{133}\text{Cs}$ molecules. We create up to 4000 molecules in the rovibrational and hyperfine ground state at a temperature of ≈1.2 μK and a density of ≈10$^{11}$ cm$^{-3}$ using magnetoassociation on a Feshbach resonance$^1$ followed by optical transfer using stimulated Raman adiabatic passage.$^2,^3$ We then use precision microwave spectroscopy of the rotational transition to probe the rich hyperfine structure of the molecule and exploit coherent Rabi oscillations to transfer the total population of molecules between hyperfine levels.$^4$ We subsequently investigate the AC Stark effect due to the trapping light in low-lying rotational levels and reveal a rich energy structure with many avoided crossings between hyperfine states.$^5$ Understanding this structure allows us to trap the molecules in a range of internal states. We study the collisional lifetimes of the molecules in such traps for various rotational and hyperfine states, shedding light on the ‘sticky collision’ issue.$^6$ Finally, we describe our future plans for imaging and addressing of single molecules in ordered arrays as a basis for quantum simulation.


Observation of Correlated Excitations in NO-O₂ Inelastic Collisions

Zhi Gao, Tijs Karman, Sjoerd N Vogels, Matthieu Besemer, Gerrit Groenenboom, Ad van der Avoird, Sebastiaan Y T van de Meerakker

Radboud University, The Netherlands

Whereas collisions between atoms and molecules are largely understood, collisions between two molecules have proven much harder to study. In both experiment and theory, our ability to determine quantum state-resolved bimolecular cross sections lags behind their atom-molecule counterparts by decades. The combination of the Stark deceleration and velocity map imaging techniques allow for studies of atom-molecule collisions at very high resolution\(^1,\)\(^2\). Recently we extended this technique to molecule-molecule collisions.

Here, we report on the measurement of state-to-state differential cross sections between state-selected and velocity-controlled nitric oxide (NO) radicals and oxygen (O₂) molecules. Using velocity map imaging of the scattered NO radicals, the full product-pair correlations of rotational excitation that occurs in both collision partners from individual encounters are revealed. The correlated cross sections show surprisingly good agreement with quantum scattering calculations using \textit{ab initio} NO-O₂ potential energy surfaces. The observations show that the well-known energy-gap law that governs atom-molecule collisions does not generally apply to bimolecular excitation processes and reveal a propensity rule for the vector correlation of product angular momenta.

\(^1\) S. N. Vogels \textit{et al}., Imaging Resonances in low-energy NO-He inelastic collisions. \textit{Science} \textbf{350}, 787

\(^2\) A. von Zastrow \textit{et al}., State-resolved diffraction oscillations imaged for inelastic collisions of NO radicals with He, Ne and Ar. \textit{Nat Chem} \textbf{6}, 216
Merged Beam Study of the Ne(3P2) + Ar Reaction: Cold Stereodynamics

Sean D.S. Gordon, Junwen Zou, Silvia Tanteri, Nik Gkogkoglou, and Andreas Osterwalder

Institute for Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

I will present our recent results on merged-beam investigations of the Ne(3P2)+Ar reaction in a range of collision energies between 0.1 K – 1000 K. This reaction can proceed along two different pathways, leading either to Penning ionization and producing Ne(1S) and an Ar^+ ion, or to associative ionization, producing a NeAr^+ ion. The branching between these channels depends on the orientation of the neon J-vector relative to the interatomic axis. We have studied this steric effect by polarizing Ne(3P2) in a magnetic guide and orienting it in a static magnetic field in the interaction zone, where the neon beam was crossed or merged with a supersonic expansion of argon. By separately counting the product ions and recording the branching ratio as a function of magnetic field direction and collision energy we were able to extract energy dependent cross sections for states that differ only in W, the projection of J on the interatomic axis.

Widely Tunable Cavity Enhanced Ultrafast Spectroscopy

Yuning Chen, Myles C. Silfies, Thomas K. Allison

Department of Chemistry and Physics, Stony Brook University, Stony Brook, NY 11794

Ultrafast optical spectroscopy methods, such as transient absorption spectroscopy and 2D spectroscopy, are widely used across many disciplines. However, these techniques are typically restricted to optically thick samples, such as solids and liquid solutions. Using a frequency comb laser and optical cavities, we have developed a technique Cavity Enhanced Ultrafast Spectroscopy and demonstrated a detection limit of ΔOD as small as 2×10⁻¹⁰ (1×10⁻⁹/√Hz).[1] This enables the study of the dynamics of cold molecules and clusters in a molecular beam. In this talk, we will present results using a new widely tunable cavity-enhanced ultrafast spectrometer covering the ultraviolet and visible spectral ranges to investigate excited-state proton transfer dynamics in jet-cooled molecules. We will also discuss progress towards cavity-enhanced 2DIR spectroscopy [2] using mid-infrared frequency combs.


The Ramifications of Coherent Radiative Decay on Periodically Orienting Molecular Ensembles

Ran Damari, Dina Rosenberg, Sharly Fleischer

Department of Chemical Physics, Tel-Aviv University, Tel Aviv 6997801, Israel
Tel-Aviv University center for Light-Matter-Interaction, Tel Aviv, 6997801 Israel
e-mail address : sharlyf@post.tau.ac.il

Laser-induced molecular alignment and molecular orientation methodologies have been developed and vastly explored in order to provide on-demand access to anisotropic angular distribution of molecules in the gas phase. We have conducted time-resolved measurement of field-free alignment (induced by an ultrashort near-IR pulse) and field-free orientation (induced by an intense single-cycle terahertz field) in several gasses and in a range of gas pressures. Analyzing the decay rates of the alignment and the orientation and comparing between them, we found that transientsly oriented molecules decay at a faster rate than transientsly aligned samples (for a specific molecular sample and gas pressure). We termed this phenomenon 'coherent radiative decay' which can be, in fact, trivially explained by the most basic physical principle - conservation of energy: the radiation emitted by the macroscopic dipole oscillations upon molecular orientation dissipates energy from the molecular rotors. In aligned samples, the inversion symmetry of the medium is retained at all times thus lacking any macroscopic dipole oscillations and emission of radiation. Thus, under field-free conditions, optically-aligned molecules decay mostly due to collisions among the ensemble constituents, while in oriented molecules, an additional radiation mechanism adds to the overall observed decay rate.

I will present three complementary experimental evidences for the unveiled phenomenon from different perspectives - (1) The EM field perspective: absorbed vs. emitted THz field, (2) the molecular perspective - by direct monitoring of the rotational populations, and (3) the ramifications to the decay rate of the dynamics.

The underlying physics of the phenomenon is shared by various adjacent light-matter phenomena, where resonant fields induce polarization oscillations that give rise to radiative emission. While the ramifications to molecular rotations have been explored by us, the extent to which the phenomenon is expected to unveil in other light-matter platforms is yet to be determined.


Electric Field Controlled Collisions between Polar Molecules and Rydberg Atoms

Ferdinand Jarisch, Martin Zeppenfeld

MPI for Quantum Optics, Garching, Germany

A quantum hybrid system combining cold polar molecules with Rydberg atoms offers wide-ranging opportunities for quantum science with polar molecules. Thus, Rydberg atoms might be used to control motional\(^1\) and internal\(^2\) molecular degrees of freedom, enable nondestructive detection of molecules\(^3\), and have been suggested for quantum information processing with molecules\(^4\).

As a first step, we have experimentally investigated Förster resonant energy transfer in collisions between ammonia molecules and rubidium Rydberg atoms. Combining mm-wave state transfer with state-sensitive field ionization allows us to perform fully state-resolved measurements of the Rydberg-atom populations, enabling a detailed investigation of the energy-transfer process. A particularly fascinating aspect of the molecule-Rydberg-atom interactions is the ability to tune the interaction cross section using DC electric fields.


\(^3\) Zeppenfeld, M. “Nondestructive detection of polar molecules via Rydberg atoms” *Europhysics Letters*, (2017), 118, 13002.

Quantum Diffusion-Controlled Chemistry in Solid Parahydrogen

David T. Anderson, Morgan E. Balabanoff, Aaron I. Strom

Department of Chemistry, University of Wyoming, Laramie, WY 82071

The recombination of hydrogen atoms in solid molecular hydrogen at low temperature ($T < 4.2$ K) is controlled by quantum diffusion of the two atoms towards each other. Theories of quantum diffusion predict the timescale for diffusional jumps from one lattice site to the next depend sensitively on the energy mismatch between the hydrogen atoms in these neighboring sites (faster for small mismatch energies). This means the interatomic interaction between the two hydrogen atoms moving towards each other can slow down their tunneling motion as compared to the single-atom quantum diffusion rate at large interatomic distances. This low temperature reaction environment therefore allows reactions of hydrogen atoms with various chemical species to be studied within the quantum diffusion-controlled regime. Nitric oxide (NO) doped parahydrogen solids are formed via rapid vapor deposition and the $\text{H}^+\text{NO} \rightarrow \text{HNO/NOH}$ chemical reaction is initiated with 193 nm partial photolysis of the NO dopant. We measure the ensuing reaction kinetics as a function of temperature, parahydrogen nuclear spin enrichment, and photolysis conditions using standard FTIR spectroscopy. Surprisingly, previous studies$^1$ have shown that both HNO and NOH products are formed even though the reaction to form HNO is barrierless and the reaction to form NOH has a calculated barrier$^2$ of 12.37 kcal mol$^{-1}$. This result shows how quantum diffusion can control the reaction dynamics in non-intuitive ways and thus opens the door to study quantum diffusion-controlled chemistry. From the reverse perspective, the measured branching ratio between products provides important clues on the details of quantum diffusion of a hydrogen atom towards and an NO impurity in solid molecular hydrogen. We perform these experimental studies in collaboration with the Hinde group at the University of Tennessee who are experts in the many-body quantum mechanics of chemical species trapped in parahydrogen quantum matrices.


The Angulon Quasiparticle: From Molecules in Superfluids to Ultrafast Magnetism

Mikhail Lemeshko

*Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria*

Recently we have predicted a new quasiparticle - the angulon - which is formed when a quantum impurity (such as a molecule, an atom, or an electron) exchanges its orbital angular momentum with a many-particle environment (such as superfluid helium, lattice phonons or an electron gas) [1,2].

Soon thereafter we obtained strong evidence that angulons do exist and are formed in experiments on molecules trapped inside superfluid helium nanodroplets [3]. The angulon theory thereby provided a simple explanation for experimental data accumulated during the last two decades. Moreover, casting the many-particle problem in terms of angulons amounts to a drastic simplification and allows to tackle previously intractable problems related to quantum dynamics [4].

In this presentation we will introduce the angulon concept and discuss novel physical phenomena [1,5,6] arising from the angular momentum exchange in quantum many-particle systems. We will describe the applications of angulons to modern experiments on molecules in superfluids and on non-equilibrium magnetism.


Directional Quantum-Controlled Chemistry: Generating Aligned Ultracold Molecules via Photoassociation

S. Kallush\textsuperscript{1,2}, J.E. Carini\textsuperscript{3}, P.L. Gould\textsuperscript{3} and R. Kosloff\textsuperscript{2}

\textsuperscript{1}Department of Physics and Optical Engineering, ORT-Braude College, P.O. Box 78, 21982 Karmiel, Israel
\textsuperscript{2}The Fritz Haber Research Center, The Hebrew University of Jerusalem, Jerusalem 91904, Israel
\textsuperscript{3}Department of Physics, University of Connecticut, Storrs, Connecticut 06269, USA

Photoassociation of ultracold atoms with pulsed laser light is shown to lead to alignment of the product molecules along the excitation laser polarization axis. We theoretically investigate pulsed two-photon photoassociation of $^{87}\text{Rb}$ atoms into a specific weakly-bound level of the $a\,^3\Sigma^+_{u}$ metastable electronic state and find both stationary and time-dependent field-free alignment. Although a transform-limited pulse yields significant alignment, a frequency-chirped pulse dramatically enhances the ultracold molecular formation rate at the cost of a slight decrease in the alignment. Employing multiple pulses synchronized with the vibrational and rotational periods leads to coherent enhancement of both population and alignment of the target state. Inclusion of the rotational degree of freedom in the model gives rise to processes with multiple quantum paths, which lead to quantum effects such as interference and coherence revivals.
Cold State-selected Radicals for the Study of Low Temperature Chemistry

Jutta Toscano¹, Christopher J. Rennick², Atreju Tauschinsky¹, Katrin Dulitz³, Brianna R. Heazlewood¹ and Timothy P. Softley⁴

¹Department of Chemistry, University of Oxford, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford, OX1 3QZ, United Kingdom
²National Physical Laboratory, Teddington, Middlesex, TW11 0LW, United Kingdom
³Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, Freiburg, Germany⁴University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom

In order to obtain a source of cold state-selected radicals, we combine a Zeeman decelerator, which slows down a subset of the radicals in a supersonic beam using pulsed magnetic fields, with a newly designed magnetic guide. The latter serves to purify the output of the decelerator, yielding a pure beam of cold, state- and velocity-selected radicals which is ideal for collision studies.

We show that by optimising the deceleration switching sequences using evolutionary algorithms a 40% increase in the number of decelerated particles is obtained. Lower final velocities than it is possible to reach using standard switching sequences can also be achieved⁵. Three-dimensional particle trajectory simulations uncover a new deceleration mechanism for the optimised sequences which relies on adding particles to the phase-stable bunch as the deceleration proceeds. This novel mode of operation of a decelerator goes beyond the standard periodic phase stability approach typically adopted.

We present a novel design for a magnetic guide that can be used after a Zeeman decelerator, or after any supersonic or effusive beam, to select only radical species with a specific desired velocity within a narrow velocity distribution. In so doing, the magnetic guide skims off all other radicals, precursor and seed gases in the beam⁶. The resulting cold, state- and velocity-selected radical beam will enable us to study ion-radical collisions with enhanced control over the properties of the radical reactants.


Quantum-state Controlled Ion Chemistry

Philipp C. Schmid, James Greenberg, Mikhail I. Miller, Heather J. Lewandowski

JILA and the Department of Physics, University of Colorado, Boulder, Colorado 80309-0440, USA

Ion-molecular reactions frequently play an important role in gaseous media such as the interstellar medium, the upper atmosphere, or combustion processes. Many of these reactions are predicted to be barrier-less, thus they can occur even at low temperatures. Measurements under controlled conditions – for example by controlling translational motion, internal degrees of freedom, or even the structural isomerism - will allow for understanding of such reactions in detail.

While these molecular reactions are important, measurements of the rates and dynamics under laboratory conditions are challenging. To sensitively probe ion-molecule reactions, our experimental system\(^1\) overcomes some of these technical difficulties. Molecular ions are stored in a linear quadrupole ion trap, sympathetically cooled with co-trapped, laser-cooled Ca\(^+\). A coupled TOF-MS enables the read-out of all trapped reaction products, down to the single ion level. Thus, a reaction can be followed by the increase of reaction products and not just the loss of reactants.

In recent measurements, we utilized quantum-state control over the reactants to tune the reaction rates. This is achieved by changing the internal-state population of Ca\(^+\) by varying the detunings of the cooling lasers. Therefore, by deterministically varying the p-state and d-state populations of Ca\(^+\), the kinetics of the reactions with neutral partners such as NO or O\(_2\) are modified. We will present data on these reaction rates and branching ratios of these quantum-state controlled reactions.

Observation of Different Reactivities of 
\textit{para-} and \textit{ortho-}water Towards Cold Diazenylium Ions

Ardita Kilaj\textsuperscript{1}, Hong Gao\textsuperscript{1}, Daniel Rösch\textsuperscript{1}, Uxia Rivero\textsuperscript{1}, Jochen Küpper\textsuperscript{2,3,4} and Stefan Willitsch\textsuperscript{1}

\textsuperscript{1}Department of Chemistry, University of Basel, 4056 Basel, Switzerland
\textsuperscript{2}Center for Free-Electron Laser Science, DESY, 22607 Hamburg, Germany;
\textsuperscript{3}Department of Physics and The Hamburg Center for Ultrafast Imaging, University of Hamburg, 22761 Hamburg, Germany; \textsuperscript{4}Department of Chemistry, University of Hamburg, 20146 Hamburg

Water, H\textsubscript{2}O, is one of the fundamental molecules in chemistry, biology and astrophysics. It exists as two distinct nuclear-spin isomers, \textit{para-} and \textit{ortho-}water, which do not interconvert in isolated molecules. The experimental challenges in preparing pure samples of the two isomers have thus far precluded a characterization of their individual chemical behaviour.

Recent progress in manipulating polar molecules using electrostatic fields has made it possible to select and spatially separate different conformers and rotational states of molecules in supersonic molecular beams\textsuperscript{1, 2}. By combining this technology with a stationary reaction target of Coulomb-crystallized ions in a linear quadrupole ion trap\textsuperscript{3} we have recently studied conformer-selected molecule-ion reaction dynamics and observed that reaction-rate constants can strongly depend on molecular conformation\textsuperscript{4, 5}.

Here, we extend this method to the separation of different nuclear-spin isomers for studies of ion-molecule reactions with control over the rotational and nuclear-spin state of the neutral reaction partner. We have studied the proton-transfer reaction of the spatially separated ground states of \textit{para-} and \textit{ortho-}water with cold ionic diazenylium (N\textsubscript{2}H\textsuperscript{+}), an important molecule in astrochemistry. We found a 23(9)% higher reactivity for the \textit{para} nuclear-spin isomer which we attribute to the smaller degree of rotational averaging of the ion-dipole long-range interaction compared to the \textit{ortho}-species. This finding is in quantitative agreement with a modelling of the reaction kinetics using rotationally adiabatic capture theory\textsuperscript{6}. The present results highlight the subtle interplay between nuclear-spin and rotational symmetry and its ramifications on chemical reactivity.


Quantum Spin-dynamics in Ultracold Atom-molecule and Atom-ion Collisions

Masato Morita\textsuperscript{a}, Maciej B. Kosicki\textsuperscript{b}, Piotr S. Żuchowski\textsuperscript{b}, Tomas Sikorsky\textsuperscript{c}, Ziv Meir\textsuperscript{a}, Ruti Ben-shlomi\textsuperscript{c}, Nitzan Akerman\textsuperscript{c}, Edvardas Narevicius\textsuperscript{c}, Roee Ozeri\textsuperscript{c}, Timur V. Tscherbul\textsuperscript{a}

\textsuperscript{a}Department of Physics, University of Nevada, Reno, 89557
\textsuperscript{b}Institute of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Toruń 87-100, Poland
\textsuperscript{c}Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 7610001, Israel

Recent advances in laser cooling and trapping of polar molecules and in the preparation of hybrid ion-atom systems have stimulated much interest in ultracold atom-molecule and atom-ion collisions in the presence of external electromagnetic fields. Quantum spin dynamics in such collisions are of particular interest, as collision-induced spin-flip transitions cause trap loss and heating, making it challenging to sympathetically cool molecular gases and single ions down to the ultracold regime (\(< 1 \mu K\)).

We explore the quantum spin dynamics of trapped SrF molecules and Sr\textsuperscript{+} ions produced in recent experiments\textsuperscript{[1,2]} colliding with ultracold Rb atoms using accurate \textit{ab initio} potential energy surfaces and rigorous quantum scattering calculations. We find that electronic spin relaxation in ultracold Rb-SrF collisions occurs more slowly than elastic scattering over a wide range of magnetic fields, suggesting favorable prospects of sympathetic cooling of laser-cooled SrF molecules with spin-polarized Rb atoms in a magnetic trap\textsuperscript{[3]}. The calculated magnetic field dependence of the inelastic cross sections displays a rich resonance structure including a low-field $p$-wave resonance, which suggests that external magnetic fields can be used to enhance the efficiency of sympathetic cooling.

We also investigate the dynamics of collision-induced spin exchange and spin relaxation of a single trapped Sr\textsuperscript{+} ion immersed in an ultracold gas of Rb atoms probed in recent experiments\textsuperscript{[2,4]}. We find that the calculated spin exchange rates are very sensitive to tiny variations of the Rb-Sr\textsuperscript{+} interaction potential even in the multiple-partial-wave regime due to an unexpected correlation between the singlet and triplet scattering phase shifts. The correlation of the scattering phase shifts induces a significant isotope dependence of the spin-exchange rate, which can potentially be observed experimentally.


\textsuperscript{[4]} Sikorsky T.; Morita M.; Meir Z.; Buchachenko A.; Ben-Shlomi R.; Akerman N.; Narevicius E.; Tscherbul T.; Ozeri R., to be submitted.
Contributed Abstracts: Poster Session 1
Rotational Echo Spectroscopy: Rephasing the Centrifugal Distortion of Rotating Gas Molecules

Dina Rosenberg$^{1,2}$, Ran Damari$^{1,2}$, Shimshon Kallush$^{3,4}$, Sharly Fleischer$^{1,2}$

$^1$Department of Chemical Physics, Tel-Aviv University, Tel Aviv 69978, Israel
$^2$Tel-Aviv University center for Light-Matter-Interaction, Tel Aviv, 6997801 Israel
$^3$Deptartment of Physics and Optical Engineering, ORT Braude College, 21982 Karmiel, Israel
$^4$The Fritz Haber Research Center and The Institute of Chemistry, The Hebrew University, Jerusalem 91904, Israel

email address: sharlyf@post.tau.ac.il

Echo spectroscopy is a central technique in magnetic resonance$^1$, electronic$^2$ and vibrational$^3$ spectroscopy, enabling researchers to decipher dynamical dephasing from decoherence phenomena. Only recently has echo spectroscopy emerged into the field of rotational dynamics, in a series of theoretical and experimental works$^4–^6$. Here we experimentally demonstrate the rephasing property of alignment echoes by utilizing the strong centrifugal distortion (CDN) of Iodomethane (CH$_3$I) as a rotational dephasing mechanism and monitor the field-free evolution of the echo signal as it rephases and dephases as a function of time. We use an ultrashort 100fs near-IR pulse (first pulse, P$_1$ at $t=0$) to induce coherent rotational dynamics in a gas of CH$_3$I molecules and let it evolve under field-free conditions. At $t = \Delta\tau$ we apply the second pulse (P$_2$) that inverts the phases of the coherences induced earlier by P$_1$ and observe an alignment echo response at $t = 2\Delta\tau$. Due to the rotational CDN of the gas, the periodic alignment signals of manifest strong distortion of the signal shape observed as 'smearing of the signal' and increased number of oscillations extending toward the positive time direction$^7$. The alignment echo signals experience the same CDN effects but in the reversed direction - i.e. the echo signals observed at $\Delta\tau < t < 2\Delta\tau$ are rephasing and their CDN effects are gradually reduced until a CDN-free echo signal is regained at $t = 2\Delta\tau$, following which the echoes continue to gradually dephase at $t > 2\Delta\tau$ but in the reversed direction.

While the multi-level rotational echoes share the underlying physics of two-level systems, several differences are identified in our simulations and experimental results (for example, while the amplitude of the echo signal in two-level systems is independent of $\Delta\tau$, it depends strongly on $\Delta\tau$ in the case of multi-level rotational systems due to interferences among multiple transition pathways). These similarities and dissimilarities and their potential utilization will be discussed.


State-to-state rotational energy transfer of CO in collision with H$_2$ and Ar at very low temperatures

Hamza LABIAD,1 Laura A. MERTENS,1,2 Martin FOURNIER,1 David CARTY,3 Otoniel DENIS-ALPIZAR,4 Thierry STOECKLIN,4 Alexandre FAURE,5 Sébastien D. LE PICARD,1 Ian R. SIMS1

1Institut de Physique de Rennes, UMR CNRS-URl 6251, Université de Rennes 1, 263 Avenue du Général Leclerc, 35042, Rennes Cedex, France
2Arthur Amos Noyes Laboratory of Chemical Physics, MC 127-72, California Institute of Technology, Pasadena, CA 91125, USA
3Joint Quantum Centre Durham-Newcastle, Durham University, South Road, Durham, DH13LE, United Kingdom
4Institut des Sciences Moléculaires, Université de Bordeaux, CNRS UMR 5255, 33405 Talence Cedex, France
5UJF-Grenoble 1/CNRS, Institut de Planétologie et d’Astrophysique de Grenoble (IPAG) UMR 5274, Grenoble F-38041, France

The study of rotational energy transfer (RET) is vital to understand and describe a wide variety of astrophysical media via radiative transfer calculations [1]. RET at the state-to-state level provides information which is very important for the understanding of many gas-phase processes, especially at very low temperatures where molecular collisions are governed by resonance phenomena and long-range forces [2][3].

Using an Infrared Vacuum Ultraviolet Double Resonance (IRVUVDR) technique, implemented with the CRESU technique (a French acronym for reaction kinetics in uniform supersonic flow), we present experimental state-to-state rate coefficients and thermally averaged cross sections for RET of CO ($v=2$, $j=0, 1, 4, 6$) in collision with the most abundant partner in the interstellar medium, H$_2$, from 293 K down to 5.5 K, and in collision with Ar from 293 K to 30 K.

The experimental results for CO – H$_2$ are compared with inelastic scattering calculations using the new high quality diatomic-diatomic six-dimensional potential energy surface PES of Faure et al [4]. The CO – Ar experimental results are compared with inelastic scattering calculations employing the new three-dimensional PES for the CO – Ar complex of Sumiyoshi and Endo [3][5].

Theoretical investigation of the sympathetic cooling feasibility for the C₂⁻ diatomic anion

M. Kas*, J. Loreau, J. Liévin and N. Vaeck

Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, Brussels, Belgium. *milakas@ulb.ac.be

Sympathetic cooling of molecular ions using ultracold atoms is one of the possible way to reach the ultracold regime for molecular species. The co-trapping experiment of OH and Rb is currently under investigation by the HAITrap team of the university of Heidelberg. Their experimental setup consist of a radio frequency ion trap with a magneto optical trap (MOT) that allows the OH cloud to be immersed in a ultracold Rb cloud. In such environment, elastic and inelastic (including reactive) collisions can occur. In our previous work [1], we showed that the associative detachment channel Rb(2P)+OH⁻ → RbOH+e⁻ is energetically accessible and lead to a loss of OH⁻ ions. Our results agrees with the first obtained experimental value [2]. In addition, we have also investigate the excited state channel Rb(2P)+OH for which loss is to be expected [1,3]. Comparison between theoretical and experimental rate constant are under investigation for the Rb+OH⁻ system.

In order to avoid loss, one possibility is to use another alkali or alkali-earth atom has buffer gas [5], a closed-shell anions with larger EA than OH⁻ [6] or hydrated OH⁻ cluster [7]. Here we propose the use of the C₂⁻ molecular anion as the trapped specie. The internal structure of C₂⁻ is well characterized and has been the subject of many experimental and theoretical studies, for example, in the context of astrochemistry [8] and laser cooling [9]. In the present study, we have used ab initio method to study the structure of the Rb-C₂⁻ and Li-C₂⁻ molecular species. The potential energy surfaces of both singlet and triplet states have been obtained at the MRCI level of theory. We have used our PES to perform close coupling calculations of elastic and inelastic cross-sections (rotational quenching) and compare our result to several other systems. In addition we also show that the neutral PES corresponding to the ground state of RbC₂ and LiC₂ are above their respective anion’s PES, suggesting that the AD cross section should be very small. Finally, we discuss the possibility of using excited state of C₂⁻ to perform Doppler broadening thermometry in order to measure the translational temperature of the ions.

[3] M. Kas, J. Loreau, J. Liévin and N. Vaeck, to be published, see other poster
[7] see other poster
Theoretical study of excited state dynamics in a hybrid trap: Rb(2P)+OH−

M. Kas*, J. Loreau, J. Liévin and N. Vaeck

Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, Brussels, Belgium. milakas@ulb.ac.be

Sympathetic cooling of molecular ions using ultracold atoms is one of the possible way to reach the ultracold regime for molecular species. The co-trapping experiment of OH− and Rb is currently under investigation by the HAITrap team of the university of Heidelberg. Their experimental setup consist of a radio frequency ion trap with a magneto optical trap (MOT) that allows the OH− cloud to be immersed in a ultracold Rb cloud. In such environment, elastic and inelastic (including reactive) collisions can occur. In our previous work [1], we showed that the associative detachment channel Rb(2S)+OH− → RbOH+e− is energetically accessible and lead to a loss of OH− ions. Our results agrees with the first obtained experimental value [2]. In addition, we have also investigate the excited state channel Rb(2P)+OH− for which loss is to be expected [1,3]. Comparison between theoretical and experimental rate constant are under investigation for the Rb+OH− system.

Experimental evidences of interesting collision processes via excited channels in hybrid traps have been pointed out by several groups [5,6]. In the present study we extend our previous work [1] and investigate the potential energy surfaces (PES) of the low lying states of the RbOH− molecular anions. Several reaction are energetically accessible:

\begin{align*}
\text{Rb}(^{2}\text{P}) + \text{OH}^{-} & \rightarrow \text{RbOH} + e^{-} \quad (1) \text{ (Associative electronic detachment)} \\
\text{Rb}(^{2}\text{P}) + \text{OH}^{-} & \rightarrow \text{Rb}(^{2}\text{S}) + \text{OH}^{-} + E_k \quad (2) \text{ (electronic to kinetic energy transfer)} \\
\text{Rb}(^{2}\text{P}) + \text{OH}^{-} & \rightarrow \text{Rb}^{-} + \text{OH} \quad (3) \text{ (charge transfer)} \\
\text{Rb}(^{2}\text{P}) + \text{OH}^{-} & \rightarrow \text{Rb}(^{2}\text{P}) + \text{OH}^{-} \quad (4) \text{ (non reactive channel)}
\end{align*}

We used conventional ab initio approaches (MCSF/MRCI) to compute the relativistic PES of both the neutral and anionic low lying states. The PES exhibit numerous crossings and avoided crossings between anionic states. Some interesting features of the PES are discussed and comparison with other alkali and alkali earth hydroxide anion are made. Furthermore, we carefully investigate the autodetachment region i.e the region where \( E_{\text{neutral}} < E_{\text{anion}} \), which leads to reaction (1). Using a capture model that takes into account appropriate long range interaction, and Landau-Zener transition probabilities, we discuss the branching ratio between the different exit channels.

State selection, magnetic trapping and coherent control of laser-cooled molecules


Centre for Cold Matter, Blackett Laboratory, Imperial College London, Prince Consort Road, London, SW7 2AZ UK

In the last few years, magneto-optical traps (MOTs) for simple diatomic molecules have been realised for the first time\textsuperscript{1,2,3}. Further cooling in an optical molasses has proven an effective method to produce samples of molecules in the ultracold regime\textsuperscript{2}. Most applications, including simulation of strongly interacting quantum many-body hamiltonians, precision tests of fundamental physics and utilisation in quantum information processing, require coherent control over the internal state of the molecular sample. We present optical pumping of ultracold CaF molecules into a single internal state, transfer to a conservative trap and coherent microwave control over their rotational, hyperfine and Zeeman sub levels\textsuperscript{4}.

Ramsey spectroscopy for CaF molecules confined in a magnetic quadrupole trap and prepared in a coherent superposition of $|N=0, F=1, M_F=1\rangle$ and $|N=1, F=2, M_F=2\rangle$ states. Two 27 μs microwave π/2 pulses are separated by a free evolution time of 493 μs. Plots show the percentage recaptured into the MOT, proportional to the number in $N=1$, as a function of microwave frequency, $f$, relative to the transition frequency measured in free space, $f_0$. The vertical dashed line in the central lower plot indicates the position of the central fringe; the transition frequency in the magnetic trap is shifted by -404(1) Hz from $f_0$.

A DC magneto-optical trap of CaF molecules

Noah Fitch, Hannah Williams, Luke Caldwell, Stefan Truppe, Ed Hinds, Ben Sauer, and Mike Tarbutt

Centre for Cold Matter, Blackett Laboratory, Imperial College London, Prince Consort Road, London, SW7 2AZ UK

The last few years have seen the first successful attempts at making magneto-optical traps (MOTs) of molecules\textsuperscript{1,2,3}. Such systems are omnipresent in experiments and technologies based on cold atoms, where they provide a launching point for a myriad of applications, and it is expected that molecular MOTs will play a similar role in experiments based on cold and ultracold molecules. This endeavor is hampered by the fact that molecular MOTs are much more challenging to produce, due mostly to the additional degrees of freedom and the presence of quantum states that are “dark” to the cooling/trapping light. One solution to this problem is the so-called rf MOT\textsuperscript{4}, where dark states are destabilized by synchronously switching the trapping magnetic field and laser polarization. A second approach, which we use for CaF, is a dual frequency MOT, where no switching is needed. I will present the properties of this MOT, showing how the scattering rate, trap frequency, damping constant, temperature, cloud size and number of molecules loaded depend on the key parameters. I will also present simulations which help to interpret the experimental results. This MOT is extremely robust and a solid foundation for further investigations, including transferring to an optical molasses to further cool below the Doppler limit, loading the molecules into a magnetic trap, and demonstrating coherent control of the molecular quantum states. These techniques will enable the next generation of cold and ultracold molecule experiments carrying out precision measurements to test fundamental physics, studying collisions and sympathetic cooling, or loading molecules into optical tweezer traps for quantum simulation.

Resonant charge exchange as an ion cooling mechanism

Sourav Dutta\textsuperscript{1} and S. A. Rangwala

Raman Research Institute, C. V. Raman Avenue, Sadashivanagar, Bangalore 560080, India

Of the numerous methods to cool trapped ions, laser cooling and collisional cooling with neutrals and ions are most widely used. In hybrid trap experiments, which simultaneously overlap trapped ions with trapped atoms, ion-atom collisions are the subject of study. A primary goal of hybrid trap studies is the realization of ultracold, trapped ion-atom mixtures where s-wave, elastic ion-atom collisions dominate\textsuperscript{1}. However, even at these energies other inelastic processes are accessible. In the case where the trapped ionic species is the singly ionized core of the co-trapped atomic species, resonant charge exchange (RCE) collisions are expected to occur. Operationally in this process, the ion and atom exchange an electron and therefore swap identities. This process is resonant because the electron can hop from the atom to the ion with no change in the internal energies of the colliding pair. Across the entire range of collision energies, the cross section for RCE is lower than elastic collision, rendering the experimental measurement of RCE challenging. The pursuit is nevertheless both interesting and important since this relatively rare RCE event has a huge impact on the efficiency of ion cooling.

We report experimental results on how the RCE mechanism can be used to efficiently cool ions at the expense of trapped atoms. That the RCE mechanism exists has been discussed in earlier experiments\textsuperscript{2}, albeit with laser cooled ions, and that RCE could cool ions has also been discussed\textsuperscript{3} but an unambiguous experiment demonstrating ion cooling by RCE is yet to be realized. Here we report a two species experiment and measure the ion cooling of Cs\textsuperscript{+} in the presence of a Cs MOT, where both RCE and elastic collisions are active, and separately, in the presence of a Rb MOT, where the RCE mechanism is inactive. The very efficient cooling of the ion when RCE is allowed is studied in detail and its efficiency as a cooling mechanism is determined relative to elastic collisions\textsuperscript{4}. This result has very important implications on the study of ion mobility\textsuperscript{5,6} and ions as impurities in ultracold dilute gases.


\textsuperscript{1} Department of Physics, Indian Institute of Science Education and Research, Bhopal – 462066, India.
Progress towards the next-generation eEDM measurement with trapped molecular ions

Yuval Shagam, William B. Cairncross, Daniel N. Gresh, Tanya Roussy, Yan Zhou, Kia Boon Ng, Jeffrey Meyers, Kevin Boyce, Jun Ye, Eric A. Cornell

JILA, NIST and University of Colorado, and Department of Physics, University of Colorado, Boulder, CO 80309

The first measurement of the electron’s electric dipole moment (eEDM) with HfF+ molecular ions has produced a value consistent with zero with an uncertainty of $1.3 \times 10^{-28}$ e*cm [1]. Pushing the upper bound further may reveal physics beyond the standard model. The next generation experiment will aim to increase the statistics that dominated the uncertainty despite the 360 hours of data taken [1]. The increased volume and field uniformity, will enable the interrogation of much larger numbers of ions with increased coherence times due to higher polarizing fields. We will present a recently employed rotational laser cooling scheme of the molecular ions that has led to a twofold increase in signal without compromising the coherence time. We will discuss the progress towards the improved measurement, including new methods of counting ions which will be needed to address the larger anticipated signal.

Determination of the Cs-Yb interspecies scattering lengths via 2-photon photoassociation

Alex Guttridge, Matthew D Frye, Jeremy M Hutson, Simon L Cornish

Joint Quantum Centre (JQC) Durham – Newcastle, Durham University, Durham, DH1 3LE, UK

John J McFerran

School of Physics, University of Western Australia, 6009 Crawley, Australia

Photoassociation is the association of two free atoms into a molecule by light resonant with a bound vibrational level of the molecule. It has been widely used to create ultracold molecules and as a sensitive probe of the molecular potential at long range. We present measurements of the CsYb ground state potential using 2-photon photoassociation of an ultracold mixture of Cs and Yb atoms\textsuperscript{1-3}. Comparison between photoassociation measurements and quantum scattering calculations allows the precise determination of the interspecies scattering lengths for all isotopic combinations. The extracted values are in good agreement with previous measurements using thermalisation of the two atomic species\textsuperscript{4}.

Accurate knowledge of the CsYb interaction potential will allow prediction of the positions of novel interspecies Feshbach resonances between an alkali-metal atom and a closed-shell atom \textsuperscript{5-7}. Magnetoassociation across such a Feshbach resonance, followed by STIRAP to the ro-vibrational ground state will allow the production of ultracold heteronuclear $^2\Sigma$ molecules possessing a magnetic dipole moment as well as an electric dipole moment. These molecules have a huge array of applications in quantum simulation\textsuperscript{8}, ultracold chemistry\textsuperscript{9} and as probes of fundamental physics\textsuperscript{10}.

Observation of excited quadrupole-bound states in cold deprotonated 4-cyanophenol anion

Guo-Zhu Zhu, Yuan Liu, Lai-Sheng Wang

Department of Chemistry, Brown University, Providence, RI 02906

Molecules with critical dipole moment of 2.5 D can bind an excess electron in a diffuse orbital, forming dipole-bound anions. With vanishing dipole moments but large quadrupole moments, molecules can bind an electron to form quadrupole-bound anions. However, few quadrupole-bound anions have been observed experimentally. Here, we report a photodetachment and high-resolution photoelectron imaging study of cold deprotonated 4-cyanophenol anions, which are expected to support excited quadrupole-bound states (QBS). The photodetachment spectrum reveals an excited QBS with a binding energy of 20 cm⁻¹ below the detachment threshold of 24927 cm⁻¹. Seventeen above-threshold excited vibrational levels of the QBS are observed as resonances in the photodetachment spectrum. By tuning the detachment laser to the above-threshold vibrational resonances, highly non-Franck-Condon photoelectron spectra are obtained due to autodetachment from the excited vibrational levels of the QBS. The perfect agreements of relative peak position and intensity presented in the non-resonant photoelectron spectrum and the photodetachment spectrum confirm the weakly bound nature of the extra electron in the QBS. The simulation of rotational profile yields a rotational temperature of 30-35 K. Surprisingly, excitation to the below-threshold vibrational ground state of the QBS shows well-defined two-photon photoelectron peaks at very low kinetic energies. These peaks, which have the appearance of vibrational hot bands, are probably due to fast fluorescent decay from the stationary ground QBS vibrational level to excited vibrational levels of the anion in its ground electronic state, followed by photodetachment with a second photon.
Ultracold atom-ion systems in spatially separated traps

Onyango Stephen Okeyo¹, Fabio Revuelta²,³, Alejandro Saenz¹

¹AG Moderne Optik, Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany
²Grupo de Sistemas Complejos, E.T.S.I.A.A.B., Universidad Politécnica de Madrid, Avda. Puerta de Hierro 2-4, 28040 Madrid, Spain
³Instituto de Ciencias Matemáticas (ICMAT), c/ Nicolás Cabrera 13-15, Cantoblanco, 28049 Madrid, Spain

Over the last years, several different systems have been studied as promising candidates for quantum simulation and quantum computation¹, such as photonic systems, ultracold atomic clouds, ionic setups or quantum dots, among others.

Single trapped ions are arguably the best controlled single particle quantum system. However, scaling them to large numbers remains a challenge due to the strong Coulombic repulsion. Contrary, ultracold systems formed by neutral alkaline atoms can be easily scaled up to thousands or millions of particles. Thus, the construction of mixed systems formed by ultracold neutral atoms and ions may exploit the advantages of both individual setups because of their complementary properties.

In this work², we present a numerical method for describing a hybrid system of an ultracold neutral atom and a single ion confined in spatially separated three dimensional trapping potentials. The interaction between the neutral atom and the ion is modeled using realistic Born-Oppenheimer potential curves obtained from ab initio quantum chemistry calculations. An application of the approach to the hybrid atom-ion system of ⁷Li²⁺ isotope reveals the trap-induced resonances that manifest as avoided crossings between the molecular bound states and the unbound trap states as a function of the separation between the two traps.

² Onyango Stephen Okeyo, F. Revuelta, Alejandro Saenz, Ultracold atom-ion systems in spatially separated traps (in preparation).
Quasi-closed optical transitions in large closed-shell molecules.

Timur A. Isaev, Sergey G. Semenov

Petersburg Nuclear Physics Institute, National Research Center “Kurchatov Institute”, Gatchina, 188300, Russia

The method of direct (Doppler&Sisyphus) molecular cooling (DMC) with lasers has recently attracted the increasing attention from the spectroscopic community. Particularly, considerable progress was achieved for cooling and trapping of the diatomic molecules in magneto-optical traps\textsuperscript{1}. One of the very attractive features of DMC is that such a technique can also be applied to polyatomic species\textsuperscript{2,3}. As the numbers of polyatomic species (and their fragments obtained by e.g. photodissociation) is effectively infinite, the DMC method can be in principle considered as a candidate for universal method of obtaining the arbitrary cold samples. To prove the universality of DMC method that would be highly desirable to demonstrate a multitude of examples of molecules having diverse chemical and/or spectroscopic properties and at the same time amenable for direct laser cooling. In such a context considerable interest present closed shell polyatomic molecules which can be routinely obtained in gas phase or in molecular beams.

In our previous article\textsuperscript{2} we outlined the scheme for identifying the polyatomic molecules with one (valence) electron over the closed shells, which molecules are expected to possess quasi-closed cooling transitions allowing efficient photon cycling and thus consequent Doppler&Sisyphus cooling. This takes place when valence electron undergoes transition between (mainly) non-bonding orbitals upon electronic excitation. For closed-shell molecules situation is expected to be more complicated. Nevertheless, there exist some classes of large closed-shell polyatomic molecules possessing rigid structure, which are weakly influenced by charge rearrangement in valence region. In our report we discuss the molecule 4a-aza-4b-boraphenanthrene\textsuperscript{4} as an example of such molecule and outline possible principles for identifying other closed-shell molecules possessing quasi-closed optical transitions.

The authors acknowledge financial support from RFBR grant 16-02-01064.

Intrabeam Scattering for Ultracold Collisions

Chandika Amarasinghe and Arthur G. Suits

Department of Chemistry, University of Missouri, Columbia MO 65202

Ultracold collisions, largely governed by quantum phenomena, have emerged as a unique opportunity to study quantum mechanical effects in chemical systems under precisely controlled conditions. Although laser cooling and trapping techniques adapted from AMO physics are making major contributions in this area, molecular beam methods remain a powerful means to probe chemistry in this novel realm with high flux. In these experiments, rather than trapping and cooling the reactants to low temperatures, low collision energies are achieved in the moving frame by reducing their relative kinetic energy. Merged beam techniques in particular have shown such methods can be used to great effect to study cold and ultracold chemistry, as many pioneering studies have recently demonstrated.

Building on these ideas, we have proposed and demonstrated a novel method to probe cold and ultracold chemistry by utilizing a single molecular beam. This technique possesses the advantage of reduced complexity and easy adaptation for a broad range of systems for low energy collisions. The velocity difference of different species in the same beam, the beam slippage, is exploited for achieving cold collisions in a single beam. With this approach, we have attained collisional energies as low as 2 mK with a 100% RMS spread. To achieve precise control of the relative velocity and to narrow the velocity spread we implemented a dual-slit chopper that can separately fix the velocities of the two species at the interaction region. Key to the double-slit system is a velocity chirp applied to the short molecular beam pulse using a pulsed discharge. Relative velocities of 7-10 ± 1.1 m/s are realized for l-changing collisions occurring between Xe Rydberg atoms and Xe ground state atoms. In this system, the collision energies are tunable between 125 mK to 275 mK with a root-mean-square deviation of ~18%.
Molecule detection using an optical cavity

Rahul Sawant
Raman Research Institute, C. V. Raman Avenue, Sadashivanagar, Bangalore 560080, India
and
Joint Quantum Centre (JQC) Durham-Newcastle, Department of Physics, Durham University, South Road, Durham DH1 3LE, United Kingdom

Olivier Dulieu
Laboratoire Aimé Cotton, CNRS, Université Paris-Sud, ENS Cachan, Université Paris-Saclay, Orsay Cedex 91405, France

S. A. Rangwala
Raman Research Institute, C. V. Raman Avenue, Sadashivanagar, Bangalore 560080, India

Significant effort is geared towards developing techniques to create long-lived molecules at ultracold temperatures, particularly in their rovibrational ground state, and to detect them efficiently\(^1\). In most experiments, detection is destructive and requires multiple cycles of system preparation and detection\(^2\). There is a tremendous advantage to be gained in the development of a non-destructive technique to detect state selected, ultracold molecules. For such a technique the objective would be to preserve the state of the largest number of molecules in the interrogated ensemble, post interrogation. Such a technique will enable repeated interrogation of the same molecular ensemble, build experimental statistics and enable the tracking of the dynamics of the molecular ensemble.

In this work, we theoretically explore non-destructive detection of ultra-cold molecules by using a Fabry-Perot cavity as a tool for this detection process. Specifically, we consider vacuum Rabi splitting (VRS), electromagnetically induced transparency (EIT) and transient response of cavity light when the molecules are interacting with a Fabry-Pérot cavity mode, as a means for non-destructive detection. We demonstrate the use of collective strong coupling for detection of molecules with many participating energy levels. We identify the parameters that are required for the detection of molecules in the cavity EIT configuration. The theoretical analysis of these processes is parametrized with realistic values of both, the molecule and the cavity. For each process, we quantify the state occupancy of the molecules interacting with the cavity and determine to what extent the population does not change during a detection cycle. Our analysis shows that it is indeed possible to detect state prepared molecule ensembles with a cavity, in a manner that should contribute to the ease of experimentation enormously.


High accuracy relativistic investigations of BaF in preparation for the experiment to measure eEDM.

A. Borschevsky\(^1\), Y. Hao\(^1\), P. A. B. Haase\(^1\), E. Eliav\(^2\), M. Ilias\(^3\), and the eEDM collaboration: P. Aggarwal\(^1\), R. Bethlem\(^4\), K. Esajas\(^1\), S. Hoekstra\(^1\), K. Jungmann\(^1\), T. Meijknecht\(^1\), M. Mooij\(^4\), R. Timmermans\(^1\), W. Ubachs\(^4\), L. Willmann\(^1\), and A. Zappara\(^1\)

\(^1\) Van Swinderen Institute, University of Groningen, 9747 Groningen, The Netherlands
\(^2\) School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel
\(^3\) Matej Bel University, Department of Chemistry, SK-97400 Banska Bystrica, Slovakia
\(^4\) Department of Physics and Astronomy, VU University Amsterdam, 1081 HV Amsterdam

Molecules are promising candidates for search for physical phenomena beyond the Standard model due to their rich spectra and various enhancement effects\(^1\). In particular, search for the electric dipole of the electron (eEDM) in recent years has focused on heavy diatomic molecules\(^2\). In the recently established collaboration in Groningen, we are currently preparing for an experiment to measure eEDM using a slow beam of BaF molecules in the $^2\Sigma$ ground state, aiming at an improved sensitivity of $5 \times 10^{-30}$ e·cm.

Theoretical predictions of various properties of the investigated molecule are important for planning the measurements and for interpreting the results of the experiment.

Here we present high accuracy theoretical calculations of the molecular parameters of ground and excited states of BaF, which are needed for planning its laser cooling. The spectroscopic constants and the Franck Condon Factors were calculated using the relativistic Fock space coupled cluster method (FSCC) and the permanent dipole moments and transition dipole moments between the different states were obtained within the multireference configuration interaction (MRCI) approach. Similar calculations were performed for the lighter homologues of BaF, CaF and SrF. We also present calculations of the effective electric field of BaF, $E_{\text{eff}}$, which is needed to extract the magnitude of (or the limit on) the electron dipole moment from the measurements. These calculations were performed using the relativistic single reference coupled cluster approach (CCSD(T)) within the finite field scheme. An analysis of the influence of various computational factors (basis set, correlation method, treatment of relativity and others) on the obtained $E_{\text{eff}}$ will be provided, along with the recommended value.

\(^1\) V. A. Dzuba and V. V. Flambaum, Parity Violation and Electric Dipole moment in atoms and molecules, Int. J. Mod. Phys. E \textbf{21}, 1230010 (2012)
Cryogenically cooled beams of bio-nanoparticles

Amit K. Samanta¹, Armando Estillore¹, Nils Roth¹,², Muhamed Amin¹, Vijay Singh¹,², Lena Worbs¹,², Nicolai Pohlmann¹, Daniel A. Horke¹,², and J. Küpper¹,²,³

¹ Center for Free-Electron Laser Science, DESY, Hamburg, Germany
² Center for Ultrafast Imaging, Universität Hamburg, Hamburg, Germany
³ Department of Physics, Universität Hamburg, Hamburg, Germany

Single-particle diffractive imaging (SPI) is emerging as a new structural-biology technique at x-ray free-electron lasers (XFELs). However, one of the primary bottlenecks in realizing SPI is the efficient delivery of isolated, reproducible target particles into the x-ray focus. Here, we present novel approaches for the production of cold and high-density beams of biological nanoparticles, such as viruses, designed for use in XFEL experiments.

Isolated large nanoparticle-sized systems are produced in the gas phase using tightly focused liquid jets or electrospray ionization. The isolated nanoparticles are rapidly cooled down to cryogenic temperature using buffer-gas cooling. The produced cold nanoparticle beam can also be aerodynamically collimated to achieve higher density. Cryogenically-cooled nanoparticle beams are characterized using advanced particle-localization microscopy based on light scattering, which allows the full reconstruction of the transverse particle beam profile as well as the determination of absolute number densities.¹

Furthermore, we have developed a numerical simulation infrastructure that allows quantitative simulation of isolated particle trajectories from buffer gas cooling to aerodynamic focusing.² This allowed us to modify the buffer-gas-cooling-cell geometry and to build aerosol-injection systems optimized for specific particle sizes in order to produce the highest density particle beams. The produced cryogenically-cooled particle beams can subsequently be further manipulated and controlled using electric fields³ or using optical techniques, such as hollow-core vortex laser beams.⁴

Reactive scattering between metastable helium atoms and ultracold lithium atoms

Jonas Grzesiak\textsuperscript{1}, Simon Hofsaess\textsuperscript{1}, Vivien Behrendt\textsuperscript{1}, Frank Stienkemeier\textsuperscript{1}, Marcel Mudrich\textsuperscript{2}, and Katrin Dulitz\textsuperscript{1}

\textsuperscript{1}Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str.3, 79104 Freiburg i.Br.
\textsuperscript{2}Department of Physics and Astronomy, Ny Munkegade 120, 8000 Aarhus C, DK

The experimental observation of quantum effects in Penning ionization reactions has recently attracted a lot of attention \textsuperscript{1}. Our goal is to study such processes in a quantum-state-controlled manner at low collision energies to study the influence of electron-spin polarization on the reaction rate. For this, we use an experimental setup, which is composed of a magneto-optical trap for ultracold lithium atoms and a discharge source for the production of supersonic beams of metastable helium atoms. In this contribution, we will present a novel detection scheme, which allows for the mass-selected detection of the ionic reaction products at improved energy resolution and we will discuss the influence of elastic collisions on the reaction rate measurements.

Dipole trap with polarized thulium atoms

V.V. Tsyganok\textsuperscript{1}, E.S. Kalganova\textsuperscript{1,3}, E.T. Davletov\textsuperscript{1}, V.A. Khlebnikov\textsuperscript{1}, I.S. Cojocaru\textsuperscript{1,2}, I.A. Luchnikov\textsuperscript{1}, D.A. Pershin\textsuperscript{1}, V.S. Bushmakin\textsuperscript{1}, V.N. Sorokin\textsuperscript{1,3}, A.V. Akimov\textsuperscript{1,2,3}

\textsuperscript{1}Russian Quantum Center, 100A Novaya str., Skolkovo, Moscow, 143025, Russia
\textsuperscript{2}Texas A&M University, 4242 TAMU, College Station, Texas, 77843, USA
\textsuperscript{3}PN Lebedev Institute RAS, Leninsky prospekt 53, Moscow, 119991, Russia

One of the possible ways to understand complex phenomena that occur in materials with strong interaction is quantum simulations. The main idea of that approach is to construct tunable Hamiltonian equal to one describing system to be simulated. Cold atoms trapped into the optical lattice are form suitable and powerful platform for these simulation because of huge flexibility in construction of potentials. And to have even the better control over interatomic interactions it was suggested to use rare-earth metals with high magnetic and orbital momentum in ground state.

Bose–Einstein condensation (BEC) of atoms are required for quantum modulations. BEC appears when atoms have phase density less than one. In our setup we planned to use evaporation cooling at dipole trap reloaded from magneto-optical trap. In that case, spin’s magnetic sublevels populations become important, since large number of populated magnetic sublevels decrease the atomic phase density. Polarization of the atomic ensemble could only survive collisions if storage magnetic field, minimizing energy of polarized state in applied\textsuperscript{1}. In this work we demonstrate our results on achieving highly polarized atomic cloud of thulium atom and analyze various mechanism of degradation of the polarization including magnetic field dependent deputizing collisions.


Expansion experiment: Compare expansion of dipole trap without and with magnetic gradient.
Slow molecular beams of heavy diatomic polar molecules
to probe T/CP violation

K. Esajas, P. Aggarwal, H. Bethlem, A. Borschevsky, P. Haase, Y. Hao, S. Hoekstra, K. Jungmann,
T. Meijknecht, M. Mooij, R. Timmermans, W. Ubachs, L. Willmann, A. Zapara

Van Swinderen Institute for Particle Physics and Gravity, University of Groningen
Groningen, The Netherlands

We utilize slow BaF molecules in their ground state for a precision measurement of the electron electric dipole moment (eEDM). Electric dipole moments of fundamental particles are very sensitive probes for T and with the CPT theorem CP symmetry violation beyond the standard model. CP violation effects are strongly enhanced in heavy diatomic polar molecules, making them excellently suited to test this symmetry. To measure with high precision we require slow intense molecular beams. We are constructing a cryogenic buffer gas source that will produce molecular beams with velocities around 180 m/s. We have constructed a 4.5 meter long Stark decelerator that we currently operate using SrF molecules. Combining the cryogenic source with the decelerator enables production of intense and slow (30 m/s) BaF molecular beams, resulting in low statistical uncertainty in the subsequent eEDM measurement. Currently the source is being commissioned and results of recent progress will be presented.
**Slowing heavy molecules in a Stark decelerator**

*Artem Zapara, Parul Aggarwal, Kevin Esajas, Steven Hoekstra*

*Van Swinderen Institute for Particle Physics and Gravity, University of Groningen, Groningen, The Netherlands*

In recent decades a range of methods for cooling and trapping of molecules have been developed, motivated by a vast variety of possible applications of low-temperature molecular samples. These applications include high-precision fundamental physics tests. The most prominent examples of such tests are searches for electron electric dipole moment, parity violation effects, and time variation of fundamental constants. Some molecules are sensitive probes of the Physics beyond the Standard Model, while the statistical sensitivity of the measurement is linearly proportional to the coherent interaction time. Compared to a fast beam, slow beams or trapped samples provide significantly larger interaction time. In our lab we have been developing methods to produce intense and slow beams of heavy molecules with a mass greater than 100 amu. Our setup consists of a 4.5 m long traveling-wave Stark decelerator which can capture a molecular beam with a forward speed up to 350 m/s and successively bring a fraction of it to lower velocities. The number of molecules being decelerated and final temperature attained depend upon their mass and internal structure. Recent results\(^1\) demonstrated a significant reduction of kinetic energy of a beam of SrF molecules, that are promising candidates for nuclear-spin-dependent parity violation. On this poster we will show the basic concepts and approaches that are being used for production of low-energy molecular samples, current status of the experiment with a detailed overview of deceleration stability, and progress towards the stopping of supersonic beam of SrF in a lab frame.

\(^1\) S.C. Mathavan, A. Zapara, Q. Esajas, S. Hoekstra “Deceleration of a supersonic beam of SrF molecules to 120 ms\(^{-1}\)” *Journal of Chemical Physics*, (2016), 17, 3709-3713.
Photodissociation Spectroscopy of Cold Nitrophenolate Anions

Leah G. Dodson¹, Wyatt Zagorec-Marks², Shuang Xu³, James E. T. Smith², J. Mathias Weber²

¹JILA and NIST, University of Colorado, Boulder, CO 80309
²JILA and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309
³JILA and Department of Physics, University of Colorado, Boulder, CO 80309

The phenolate chromophore is an important chromophore in many chemical applications. We investigated the impact of the presence of a nitro group on the phenolate ring, and of its position. The nitrophenolate anions were generated using electrospray ionization. The anions were trapped and cooled through collisions with cold He and/or D₂ buffer gas in a three-dimensional radiofrequency ion trap (Paul trap), with trap temperatures ranging from 25–300 K. We obtained the spectrum in the UV-visible region for para-, ortho-, and meta-nitrophenolate using photodissociation spectroscopy in vacuo, identifying the origin band of the lowest-energy electronic transition and assigning the spectrum using computational chemistry. The substitution position of the phenolate and nitro substituents has a marked effect on the electronic spectrum. Preparation of cold ions in vacuo was critical in enabling us to measure a vibrationally-resolved spectrum of the meta-nitrophenolate anion.
Using the Precession of Molecular Electric Dipole Moment to Detect Rotation

Xiaobing Deng, Yi Ke, Zhongkun Hu

MOE Key Laboratory of Fundamental Physical Quantities Measurements, School of Physics,
Huazhong University of Science and Technology, Wuhan 430074, People’s Republic of China

We will present a scheme to detect the rotation by using the precession of molecular electric dipole moment in a static electric field. The molecular electric dipole moments are polarized under the static electric field and a macroscopic nonzero electric polarization vector emerges in the molecular gas. Then, a resonant radio-frequency pulse electric field is applied to realize a 90° flip of the electric polarization vector of a particular rotational state. Afterwards the electric polarization vector will precess under the static electric field. The shift induced by inertial rotation in the precession frequency will be measured to deduce the angular velocity of the rotation. The fundamental sensitivity limit on rotation detection of this method is estimated to be at the level of $10^{-3} - 10^{-4}$ rad s$^{-1}$ Hz$^{-1/2}$. Our proposed scheme opens up an alternative avenue for rotation detection even though the sensitivity is not competitive with the state of the art.

Mobility Calculations of N\(^{+}(3P_J)\) Ions in Cooled Helium Gas

Lamia Aissaoui\(^1\), Peter Knowles\(^2\), Moncef Bouledroua\(^3\)

\(^1\)Physics Department, Batna 1 University, Algeria.
\(^2\)School of Chemistry, Cardiff University, Cardiff, United Kingdom.
\(^3\)Physics Department, Badji Mokhtar University, Annaba, Algeria.

Based on the recent ion mobility measurements, performed by Matoba et al., [1] and Sandreson et al., [2] with a mass-selected-ion-injected drift tube mass spectrometer, of ionic open-shell systems such as C\(^{+}\), N\(^{+}\) and O\(^{+}\) ions, evolving in a helium gas at very low temperatures (4.3 and 77 K), the results could not be explained at 4.3 K. The authors suggested to improve the calculations by using full quantum-mechanical transport cross sections and a higher-level kinetic theory of gas mobility.

On the light of the quantum-mechanical [3] and the classical [4] calculations of the ground and the metastable-excited C\(^{+}\) ion mobility in helium at temperatures 77 and 4.3 K, we have aimed to show the effect of the Spin-Orbit on the quantum-mechanical calculations of the N\(^{+}\) ions in a cooled buffer helium gas. For this reason, we use the interaction potentials corresponding to the ground state N\(^{+}(3P_J)\) ions which are performed with MOLPRO. Then we use the computed quantum-mechanical and classical transport cross sections in the Viehland gram-char Fortran code as to get the mobility of N\(^{+}(3P_J)\) ions at 4.3K and 77K helium gas temperatures.

A precision measurement of the electron’s Electric Dipole Moment using trapped molecular ions

Yan Zhou, William B. Cairncross, Daniel N. Gresh, Tanya S. Roussy, Yuval Shagam, Kia Boon Ng, Jeff Meyers, Kevin Boyce, Jun Ye, and Eric A. Cornell

JILA, NIST and University of Colorado, and Department of Physics, University of Colorado

Precision measurements of fundamental symmetries in low energy systems provide a complementary platform to high-energy colliders for exploring new physics beyond the Standard Model (SM). A more accurate value for the permanent electric dipole moment of the electron (eEDM, $d_e$), whether consistent with zero or otherwise, will have important implications for various extensions of the Standard Model. Precision metrology with trapped polarized molecular ions is challenging, partly due to complex interactions between molecular structure and trapping fields. However, trapping offers key advantages such as long coherence time and robust techniques to search for systematic effects. For example, by transferring from a static lab frame to a well-controlled rotating frame, many asynchronized perturbations are averaged out, and target signals can be extracted with high fidelity. We will present results of the first generation eEDM measurement using trapped $^{180}$Hf$^{19}$F$^+$ molecular ions. A long spin coherence time over 700 ms has been demonstrated, which facilitates the achievement of high sensitivity and stringent rejection of systematic errors. By accumulating 360 hours of electron spin resonance Ramsey spectra on $^3\Delta_1$ state, we determine $d_e = (0.9 \pm 7.7_{\text{stat}} \pm 1.7_{\text{syst}}) \times 10^{-29}$ e cm, resulting in an upper bound of $|d_e| < 1.3 \times 10^{-28}$ e cm (90% confidence) [Cairncross, W. B. et al., Phys. Rev. Lett. 119, 153001 (2017)]. This result confirms the current upper bound of $|d_e| < 9.3 \times 10^{-29}$ e cm [J. Baron et al., Science 343, 269 (2014)] in a completely different system.
Infrared Spectrum and Ring Opening Pathway of the Cyclobutyl Radical

Alaina R. Brown, Peter R. Franke, Gary E. Douberly

Department of Chemistry, University of Georgia, Athens, GA, 30602

Helium nanodroplet isolation (HENDI) is used to probe the infrared spectrum of cyclobutyl radical (\(\cdot\text{C}_4\text{H}_7\)), formed from the pyrolysis of cyclobutylmethyl nitrite (\(\text{C}_4\text{H}_7(\text{CH}_2)\text{ONO}\)). Rotational fine structure is partially resolved for five bands in the CH stretching region. A hybrid CCSD(T) force field with quadratic (cubic and quartic) force constants was computed with the ANO1 (ANO0) basis set. These results were used to simulate anharmonic frequencies in the 2800-3100 cm\(^{-1}\) region by VPT2+K simulations. Three bands in this region are purely harmonic in nature while the remainder derive intensity from highly coupled anharmonic states corresponding to CH\(_2\) bend overtones and combinations. As proposed by Schultz and co-workers,\(^1\) upon cyclobutyl ring opening, the 1-methylallyl radical is formed as well as 1,3-butadiene, given a sufficient pyrolysis temperature. Evidence of allylcarbinyl radical, another intermediate proposed along this path, is not observed.

\(^1\) Schultz, J.C.; Houle, F.A.; Beauchamp, J.L. “Photoelectron Spectroscopy of Isomeric \(\text{C}_4\text{H}_7\) Radicals. Implications for the Thermochemistry and Structures of the Radicals and Their Corresponding Carbonium Ions” Journal of the American Chemical Society, (1984), 106, 7336-7347.
Study of collision processes of different gases with trapped Methyl radicals

Manish Vashishta and Takamasa Momose

Department of Chemistry, University of British Columbia, Vancouver, Canada, V6T1Z1

We have demonstrated that a supersonic beam of methyl radicals (CH₃) in the ground rotational state has been slowed down to standstill with a magnetic molecular decelerator, and successfully captured spatially in an anti-Helmholtz magnetic trap for longer than 1 sec. The trapped CH₃ radicals have a mean translational temperature of about 200 mK with an estimated density of > 5.0 x 10⁷ cm⁻³. The methyl radical is an ideal system for the study of cold molecules not only because of its high reactivity at low temperatures, but also because further cooling below 1 mK is plausible via sympathetic cooling with ultracold atoms.

Introduction of different gases inside the trap region at temperature of 200 mK will have different collision dynamics because of their varying interaction potentials. We determine the collision cross section of these gases with the trapped methyl radicals by measuring the loss rate of Methyl radicals inside the trap. Our latest results will be discussed.

H$_6^+$ is generated in a supersonic expansion via pulsed electrical discharge of hydrogen. H$_n^+$ clusters are extracted into a reflectron time-of-flight mass spectrometer and probed with infrared photodissociation spectroscopy (IRPD) in the 2050 – 4600 cm$^{-1}$ region. H$_6^+$ was mass selected and found to have three distinct photodissociation channels by loss of one hydrogen atom, one hydrogen molecule or both. Each channel results in different spectra as a result of mode specific dissociation channels. The ground $^2$D$_{2d}$ state is 4 kcal/mol lower in energy than the $^2$C$_s$ state with a 7 kcal/mol barrier. We believe we are probing the D$_{2d}$ structure with the three H$_m^+$ (m=3,4,5) fragment channels as a result of rapid interconversion between the two states after IR photon absorption.
Contributed Abstracts: Poster Session 2
Stereodynamics of the Ne* \((^3P_2) + X (X = \text{Rg, N}_2)\) reactions

Junwen Zou, Sean D.S. Gordon, Silvia Tanteri, Andreas Osterwalder

Institute for Chemical Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

We have recently studied the stereodynamics of metastable Ne\((^3P_2)\) reacting with ground state atoms (Kr, Xe, Ar), as well as with the N\(_2\) molecule, in a crossed molecular beam experiment\(^1\).\(^2\) Because Ne\((^3P_2)\) is paramagnetic, it can be oriented by an external magnetic field, and the orientation has an influence on the branching ratio between Penning ionization and associative ionization. In the present study we investigated this reactivity as a function of the angle between the neon angular momentum and the relative velocity of the reactants, in a range of collision energies between 320 cm\(^{-1}\) and 500 cm\(^{-1}\). From these data we extract energy-dependent reactivities for states that differ only in \(\Omega\), the projection of the neon total angular momentum on the inter-particle axis. Results are explained by a model involving a long-range mechanism and a short-range interaction mechanism.


Quantum technologies for the spectroscopy of single trapped nitrogen ions

Gregor Hegi, Kaveh Najafian, Mudit Sinhal, Ziv Meir, Stefan Willitsch

Department of Chemistry, University of Basel, Basel, Switzerland

The application of quantum techniques to the spectroscopy of single trapped particles has enabled the determination of atomic properties at unprecedented levels of precision. “Quantum-logic spectroscopy” (QLS) has enabled the next generation of atomic clocks and new precision tests of fundamental physical theories. Here, we extend the scope of quantum techniques to spectroscopically probe single molecular nitrogen ions. We are currently establishing a toolbox for the efficient non-destructive interrogation of single nitrogen ions by coupling to a single atomic ion using the shared motion in the RF-trap. These developments will pave the way for precise spectroscopic measurements of molecular nitrogen ions with applications as a molecular clock, as a highly precise frequency standard in the mid-IR domain and for precision tests of fundamental concepts, e.g., a possible time variation of the electron-to-proton mass ratio.

**Ab initio investigation of reactive collision involving hydrated hydroxide anion OH(H₂O)ₙ (n=1-4) clusters**

M. Kas*, J. Loreau, J. Liévin and N. Vaeck

Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, Brussels, Belgium. *milakas@ulb.ac.be

The structure and spectra of hydrated hydroxide anions have been extensively studied by both theoretical and experimental methods. There are only few studies concerning their reactivity. Associative detachment reactions are usually the most probable reactive channel when dealing with anions. The rate strongly depends on the accessibility of the so called autodetachment region of the potential energy surface (PES), i.e the region where the anion PES is embedded in the electronic continuum (E_{anion}<E_{neutral}). The OH-anion is currently under investigation in the context of cold collision: He+OH [1] and Rb+OH [2]. In the second case, loss have been observed and attributed to the AD reaction [2]. Simple Langevin based model seem to corroborate the experimental observations [3]. One of the possibility to reduce loss from AD reaction is to use hydrated hydroxides. In fact a rather old experiment in which room temperature collisions between hydrated hydroxide and H atoms have been studied, shows that the AD rate decreases for increasing hydration number [4].

In the present study, we show our preliminary results on the structure and electroaffinity (as vertical electronic detachment) of the hydrated hydroxide clusters and discuss the implication for photodetachment spectroscopy in the context of sympathetic cooling experiments. In addition we investigate the interaction between the different clusters with H and Rb atoms: optimized geometry, dissociation energy, electroaffinity and cuts of the potential energy hypersurfaces. Finally, we discuss some reaction path and their products and emphasis on the differences between H and Rb.

NO Evaporative Cooling in the $^2\Pi_{3/2}$ State

Lucie D. Augustovičová$^{1,2}$, John L. Bohn$^1$

$^1$JILA, NIST, and Department of Physics, University of Colorado, Boulder, CO 80309-0440

$^2$Charles University, Faculty of Mathematics and Physics, Department of Chemical Physics and Optics, Ke Karlovu 3, CZ-12116 Prague 2, Czech Republic

We investigate scattering of $^{14}$NO molecules in the $^2\Pi_{3/2}$ state that collide at ultracold-cold temperatures and are under the influence of an electric and magnetic field. It is found that evaporative cooling is viable only for collision energies $E_c$ no lower than $\sim 100$ mK which is similar to a result obtained for NO in the $^2\Pi_{1/2}$ state.$^1$

Without an influence of external magnetic field the ratio of elastic to inelastic rates is highly unfavorable and does not exceed 100 at $E_c = 100$ mK even when unrealistically high electric field is applied.

Magnetic field of few thousand Gauss is necessary for effective cooling, the suppression of inelastic rate can be then controlled by additional electric field that is in accordance with the phenomenon found for the $^2\Pi_{1/2}$ state.

Relaxation of highly rotationally excited $H_2$ in cold and ultracold $H_2 + H_2$ collisions

Yier Wan$^1$, Benhui Yang$^1$, P. C. Stancil$^1$, N. Balakrishnan$^2$, R. C Forrey$^3$

$^1$Department of Physics and Astronomy, Center for Simulational Physics, The University of Georgia, Athens, GA 30602
$^2$Department of Chemistry, University of Nevada, Las Vegas, NV 89154
$^3$Department of Physics, Penn State University, Berks Campus, Reading, PA 19610

Quenching of highly rotationally excited $H_2$ due to $H_2$ collisions are theoretically investigated over a wide range of energies, extending from the ultracold limit to the superthermal region. Cross sections at low temperatures for quenching from all rotational states of $H_2$, including those highly excited ones with $j$ up to 31, are presented using accurate quantum mechanical calculations along with the most recent published potential energy surface for the $H_2 + H_2$ complex calculated by Patkowski et al. (2008)$^1$. We found discrepancies for several low-lying initial rotational levels in rotational de-excitation cross sections at around 1 K compared with previous calculations. It is noted that multiple resonances are observed arising from single $J$ resolved partial wave and only even values of the total angular momentum quantum number $J$ are allowed for $para - H_2 + para - H_2$ collisions. It is shown that in the presence of inelastic scattering, zero energy elastic and inelastic scattering can be characterized by a complex scattering length. Real and imaginary components of the complex scattering length are presented as a function of initial quantum number. It is noted that the real part decreases very slowly with increasing rotational excitation, while the imaginary part, which is related directly to the total inelastic scattering cross section, can be extrapolated using an exponential energy gap fit.

$^1$Patkowski, K., Cencek, W., Jankowski, P., Szalewicz, K., Mehl, J. B., Garberoglio, G., Harvey, A. H., 2008, JChPh,129, 094304
Precision spectroscopy on OH

Arthur Fast,1 John E. Furneaux,1,2 Samuel A. Meek1

1Max Planck Institute for Biophysical Chemistry, 37077 Göttingen, Germany
2Department of Physics and Astronomy, University of Oklahoma, Norman, OK 73019, USA

Measurements of vibrational transitions in small molecules can be used as a sensitive test for a possible time variation of the electron-proton mass ratio.1 While the relative sensitivity to a mass ratio change is not as large as in rotational or tunneling transitions,2 the absolute change of a vibrational frequency can be much larger. The ultimate sensitivity limit of any such measurement is given by the coherent interaction time, which for OH, can be greatly extended by slowing the molecules to low velocity using a Stark decelerator. Since the interaction time affects the absolute frequency uncertainty, larger absolute shifts can be more sensitive to a mass ratio variation, but at the same time, reaching the same level of sensitivity places higher demands on the frequency stability of the spectroscopy laser.

Over the last few years, we have been constructing a precision laser system with the eventual goal of measuring two-photon $v' = 2 \leftrightarrow v'' = 0$ transitions in $X^2\Pi OH$ with a relative accuracy of $10^{-14}$. The primary short-term reference for this system is a narrow-linewidth continuous-wave Nd:YAG laser, which is stabilized to an iodine transition using saturated absorption spectroscopy.4 The two degrees of freedom of an optical frequency comb, based on a mode-locked Ti:Sapphire laser, are stabilized using optical beat notes between the 1064- and 532-nm harmonics of the Nd:YAG laser and the nearest respective comb modes; this effectively transfers the stability of the iodine reference onto the comb. Spectroscopy lasers are then stabilized to the comb using optical beat notes. Long-term stability is achieved by monitoring the repetition rate of the comb relative to a rubidium oscillator and a global navigation satellite system receiver.

As a first test of this laser system, we have recorded spectra of $A^2\Sigma^+, v' = 0 \leftrightarrow X^2\Pi_{3/2}, v'' = 0, J'' = 3/2$ transitions in $^{16}$OH and $^{16}$OD. The absolute optical frequencies of the transitions in $^{16}$OH have been determined with an uncertainty of less than 100 kHz ($10^{-10}$ relative precision), and a precision of 100–200 kHz is expected for the transitions in $^{16}$OD. These measurements have enabled us to determine the $^{16}$OH $A^2\Sigma^+, v' = 0$ band origin with three orders of magnitude higher precision and the rotational constant with two orders of magnitude higher precision than previously possible.5 While the analysis is still ongoing, similar improvements are expected in the corresponding constants of $^{16}$OD. In contrast to the previous best values for the absolute frequencies, which were typically off by about 100 MHz, our new measurements are easily accurate enough to enable tuning a narrow-linewidth continuous-wave laser to a transition without the need for scanning.

Centrifuge deceleration and electrostatic trapping of buffer gas cooled molecules

Manuel Koller, Thomas Gantner, Xing Wu ø, Martin Zeppenfeld, Gerhard Rempe

Max-Planck-Institute of Quantum Optics, Garching, 85748 Germany

By combining cryogenic buffer gas cooling and centrifuge deceleration we recently demonstrated a record high flux exceeding $10^{10}$s$^{-1}$ and densities up to $10^9$cm$^{-3}$ of cold polar molecules at kinetic energies corresponding to less than 1K. This allowed us to observe cold dipolar collisions between polar molecules within an electric quadrupole guide. The dipolar nature of these collisions leads to large observed cross sections ($>10^{-12}$cm$^2$) with theoretically modeled elastic and inelastic collisional loss rates agreeing with the experimental findings. The low absolute velocity enables the straightforward loading of molecules into an electrostatic microstructured trap. In addition, the implementation of optoelectrical Sisyphus cooling in such a trap facilitates approaching the ultracold temperature regime where the observation of scattering resonances could become possible. Thus more detailed collision studies as well as measuring thermalization rates for various molecular species should become feasible.

ø Current address: Department of Physics, Yale University, New Haven, CT 06511, USA; Department of Physics, Harvard University, Cambridge, MA 02138, USA
High precision spectroscopy of electrically trapped cold formaldehyde

Martin Ibrügger, Alexander Prehn, Maximilian Löw, Martin Zeppenfeld, Gerhard Rempe

Max Planck Institute of Quantum Optics, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Due to their rich internal structure ultracold molecules are ideal systems for the investigation of fundamental physics. Thus they are perfect candidates for measuring a variation of physical constants such as the proton-electron mass ratio and the fine structure constant. High internal electric fields also make them well suited for measuring the electron's electric dipole moment. These types of precision experiments call for trapping to increase interrogation times, as is being done for atomic optical clocks. However, for neutral polyatomic molecules, there are few to none experiments where spectroscopy is performed on cooled and trapped ensembles. We now use optoelectrical Sisyphus cooling\(^1\) to prepare up to \(3 \times 10^5\) molecules of formaldehyde (H\(_2\)CO) at submillikelvin temperatures\(^2\). The molecules are cooled and stored in an electric trap\(^3\) providing a box-like potential with a tunable and homogeneous offset field. Good control over the internal state of the molecules allows us to prepare them with a purity of over 80\% in a single rotational state by optical pumping\(^4\). This setup provides an ideal environment to perform precision spectroscopy.

Here we present microwave spectroscopy of trapped formaldehyde on a magic transition between rotational levels \(J=4\) and \(J=5\) with a splitting of 364 GHz. Stark broadening gives transition widths on the order of MHz, however, by tuning the homogeneous electric field of the trap appropriately it can essentially be eliminated. We achieve Doppler limited linewidths down to 3.8 kHz corresponding to a precision below \(10^{-8}\). In our experiment we have even colder molecules readily available, and by applying this technique measurements with unprecedented precision for polyatomic molecules seem feasible.


Benchmarking a stimulated force for molecular beams with Rb atoms

Xueping Long¹, Andrew Jayich², Scarlett Yu¹, Wesley C. Campbell¹

¹Department of Physics & Astronomy, University of California, Los Angeles, Los Angeles, CA 90095
²Department of Physics, University of California, Santa Barbara, Santa Barbara, CA 93106

The rich internal structures of molecules make ultracold molecules attractive candidates for sensitive probe of fundamental physics, but for the same reason they are hard to decelerate, cool and trap, as the many possible spontaneous emission paths limit the ability to optically decelerate molecules to trappable speed. We demonstrate a stimulated force solution to this problem using pulses generated from a mode-locked laser. A molecular beam can be first excited by a counter-propagating “pump” pulse, then driven back to the initial ground state by a co-propagating “dump” pulse via stimulated emission. The delay between the pump and dump pulse is set to be shorter than the excited state lifetimes in order to limit decays to dark states. We report results of our benchmarking this stimulated force by accelerating a cold sample of neutral Rb atoms.
Precision Infrared Spectroscopy in a Molecular Beam Experiment

Matin Kaufmann, Guido Fuchs, Thomas Büchling, Daniel Witsch, Alexander Breier, Thomas Giesen

Experimentalphysik V, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

With frequency combs having become available for the infrared regime, a new generation of precision spectrometers has been made possible. Combining the high power, wide range tunability, and narrow line width of OPO systems with the possibility to accurately determine their frequency via a frequency comb, spectrometers with a sub MHz accuracy are built.\(^1\) By locking the OPOs to the frequency comb their frequencies can be stabilized to an even higher accuracy and their phases can be controlled, which opens the way to new possible experiments.

We are building a precision spectroscopy molecular beam setup, where two narrow linewidth OPOs are stabilized and phase-locked with an infrared frequency comb and used as light sources. The molecular beam is generated in a supersonic expansion of a pulsed nozzle and doped by e.g. laser evaporation. With this setup, several different experiments are feasible, for instance cavity ring-down spectroscopy or two-photon sub-Doppler spectroscopy. These experiments allow for a wide range of applications, for instance this setup is perfectly suited for accurate measurements of gas-phase molecules and molecular clusters. As a different application, we explore the interaction of light with chiral molecules. The phase control of all light sources will be used to differentiate between enantiomers and induce transitions between these. In an effort to push the limits of precision spectroscopy, this setup might reach an accuracy high enough to detect the energy difference between enantiomers caused by the parity violation.

Infrared Laser Spectroscopy of the Mass-selected Protonated CO Dimer

Daniel Leicht\textsuperscript{a}, Gary E. Douberly\textsuperscript{a}, Masashi Tsuge\textsuperscript{b}, Daniel T. Mauney\textsuperscript{a}, J. Philipp Wagner\textsuperscript{a}, David C. McDonald II\textsuperscript{a}, Yuan-Pern Lee\textsuperscript{b}, Michael A. Duncan\textsuperscript{a}

\textsuperscript{a}Department of Chemistry, University of Georgia, Athens, GA 30602, USA
\textsuperscript{b}Department of Applied Chemistry, National Chiao Tung University, Taiwan

Protonated CO dimers are produced in a pulsed discharge supersonic expansion of a gas mixture of CO, hydrogen, and argon. The ions are pulse-extracted into a reflectron time-of-flight mass spectrometer, where they are analyzed and mass-selected. In the turning region of the reflectron, the ions are overlapped with an infrared laser beam and their vibrational spectrum is recorded by photo-dissociation of the argon-tagged species. The infrared spectra of the H and D isotopologues were recorded in the wavelength region 500 – 3500 cm\textsuperscript{-1}. Several bands are observed for both isotopologues. Computational studies at the CCSD(T)/ANO1 level of theory analyze the geometries, energetics, and anharmonic frequencies of six stable isomers and their argon-tagged variants. Surprisingly, the comparison of the experimental data with the \textit{ab initio} predictions suggests that the most stable isomer, the proton-bound dimer, is not formed in our experiment. Instead, one higher energy isomer is formed, which lies 5.9 kcal/mol higher in energy than the global minimum.
Cold Trapped Atom-ion System Studies in an Hybrid Trap

Zhubing Jia, Jyothi Saraladevi, Kisra N. Egodapitiya

Department of Electrical and Computer Engineering, Duke University, Durham, NC 27708

The cold trapped atom-ion systems can be used to explore a variety of cold collisions, including elastic\(^1\), charge exchange\(^2\), ultra-cold molecular ions production\(^3\), and quenching of internal states in molecular ions\(^4\). Here we developed an apparatus to observe the interactions between cold trapped atoms and ions. To do this, we implemented an atom trap (magneto-optical trap) and a linear Paul trap with their centers coincide so that cold trapped potassium atoms and calcium ions (Ca\(^+\)) can interact. A high-resolution time-of-flight mass spectrometer and a fluorescence detection scheme are used to observe the interaction process, and to detect as well as identify the reaction products.


Infrared Spectra of Propene in Helium Nanodroplets and Solid \textit{para}-Hydrogen Matrices

Gregory T. Pullen\textsuperscript{1}, Peter R. Franke\textsuperscript{1}, Gary E. Douberly\textsuperscript{1}, Yuan-Pern Lee\textsuperscript{2,3}

\textsuperscript{1}Department of Chemistry, University of Georgia, Athens, GA 30602
\textsuperscript{2}Department of Applied Chemistry, National Chiao Tung University, Taiwan
\textsuperscript{3}Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

We report the infrared spectra of propene in the C-H stretching region measured in helium nanodroplets (HENDI) at 0.4 K and solid \textit{para}-hydrogen (\textit{p}-H\textsubscript{2}) matrices at 3.2 K, in order to probe the effects of the matrix host environments on the experimental spectra. Propene is an ideal test molecule to study these matrix effects, due to the many anharmonic resonance polyads present in the C-H stretching region of the spectrum. We observe a 4 – 5 cm\textsuperscript{-1} on average red-shift of the bands in \textit{p}-H\textsubscript{2} relative to HENDI. Moreover, the choice of matrix environment influences the positions and intensity ratios of transitions within each resonance polyad, leading to qualitatively different spectra. To better understand the nuances involved, simulations were performed that capture the important resonance interactions in a VPT2+K effective Hamiltonian. Certain elements of the Hamiltonian were adjusted to model the impact that different matrix environments have on the anharmonic couplings. In addition, propene reacted with hydrogen atoms \textit{via} electron bombardment of a \textit{p}-H\textsubscript{2} matrix during sample deposition, producing propyl radicals. \textit{i}-Propyl radicals were produced in greater proportion than \textit{n}-propyl radicals, indicating that for hydrogen addition to the double bond, the rate of addition to the terminal carbon (\textit{i}-propyl) is faster than the rate of addition to the center carbon (\textit{n}-propyl). Because the barriers for addition are approximately 700 cm\textsuperscript{-1} – 1500 cm\textsuperscript{-1} (1000 K – 2000 K), the only available mechanism for reaction in the \textit{p}-H\textsubscript{2} matrix (3.2 K) is tunneling. \textit{Ab initio} calculations were used to compute the tunneling probabilities for the formation of the \textit{n}-propyl and \textit{i}-propyl radicals. The rate of addition to the terminal carbon (\textit{i}-propyl) was calculated to be faster, in agreement with experiment.
The Ethyl + O₂ Reaction in Helium Nanodroplets: Infrared Spectroscopy of the Ethylperoxy Radical

Peter R. Franke and Gary E. Douberly

Department of Chemistry, University of Georgia, Athens, GA 30602

Helium-solvated ethylperoxy radicals (CH₃CH₂OO•) are formed via the in situ reaction between ethyl radicals and electronic ground state O₂. The reactants are captured sequentially through the droplet pick-up technique. Helium droplets are doped with ethyl radical via pyrolysis of di-tert-amyl peroxide or diethyl sulfone in an effusive, low-pressure source. A mid-infrared spectrum of ethylperoxy is recorded with species-selective droplet beam depletion spectroscopy. Spectral assignments in the CH stretching region are made via comparisons to second-order vibrational perturbation theory with resonances (VPT2+K) based on coupled-cluster quartic force fields. Gauche and trans conformers are predicted to be nearly isoenergetic; however, the spectrum indicates that one dominant conformer is present. Indeed, in several previous studies in our group, where chemical reactions were conducted inside droplets, only a single conformer of the product was observed. Exploration of the ethylperoxy potential energy surface, particularly along the CCOO torsional and CO stretching coordinates, motivates an explanation that is based upon an adiabatic funneling mechanism that leads to the exclusive production of one conformer. The slower torsional degree of freedom is cooled more rapidly than the higher frequency stretching and bending coordinates owing to the stronger coupling between the torsional modes and the collective modes of the helium droplet. The reactants are cooled into the torsional well that stabilizes first during their approach on the PES.
Measuring trap dynamics of cold OH molecules

John M. Gray, Yomay Shyur, Jason A. Bossert, H. J. Lewandowski

JILA and Department of Physics, University of Colorado, Boulder, Colorado 80309-0440, USA

Electrostatically trapped OH molecules can be used for studies of molecular interactions and precision spectroscopy. Characterizing the energy distribution of the trapped molecules is important for such studies. Using a recently identified resonance enhanced multi-photon ionization (REMPI) scheme,1 we detect OH molecules at different locations in the trap to experimentally determine the density distribution of molecules.2 These measurements are used to measure trap dynamics while loading the trap and determine the energy distribution at long times. This method can also be used to characterize different trap loss mechanisms. The lifetime of molecules in the trap can be limited by non-adiabatic transitions to untrapped and weakly trapped states. Adding a uniform magnetic field to a quadrupole electrostatic trap has been predicted to suppress these losses.3 We examine this loss mechanism and how it affects the distribution of molecules in our trap.

Hybrid trapping of cold molecules and cold molecular ions

Dominik Haas, Claudio von Planta, Christian Mangeng, Dongdong Zhang, Stefan Willitsch

Department of Chemistry, University of Basel, Basel, Switzerland

Hybrid systems of cold atoms and ions have been studied intensively in recent years. The simultaneous trapping of atoms with ions has opened up new possibilities for the investigation of interactions between the two species and has greatly contributed to the understanding of collisional and chemical processes at low temperatures.1,2,3

Here, we report on progress towards the development of an advanced cryogenic hybrid trapping technique which aims at trapping neutral molecules and molecular ions simultaneously. A translationally cold package of neutral molecules ($T_{\text{trans}} > 1 \text{ mK}$) is produced by means of Stark deceleration.4 During the last deceleration stage, the molecular package is loaded into a magnetic trap, which is incorporated into an RF ion trap and where molecular ions are sympathetically cooled by their interaction with laser-cooled atomic ions. The hybrid trap environment is cryogenically shielded from ambient black body radiation to prolong the trapping lifetime. The superposition of cold neutral molecules with molecular ions allows for quantum-state selective investigations of elastic, inelastic and reactive collisions of completely molecular systems at very low translational energies.

We present the experimental implementation of the hybrid trap including the cryogenic trap design. The coupling of the hybrid trap to the Stark decelerator, the design of the experiment and the loading efficiency of molecules into the trap have been numerically optimized employing the NOMAD5 direct search algorithm on Monte-Carlo trajectory simulations of the particles. The Stark decelerator has been optimised for operation at low final velocities6 using new high-density radical-beam sources.7 First results for the trapping of OH radicals in the hybrid trap are presented.

5 M.A. Abramson, C. Audet, G. Couture, J. E. Dennis, Jr., S. Le Digabel, C. Tribes, The NOMAD project, https://www.gerad.ca/nomad/
CPT tests with the anti-hydrogen molecular ion

Edmund G. Myers

Department of Physics, Florida State University, Tallahassee, FL 32306

High precision radio-frequency, microwave and infra-red spectroscopic measurements of the anti-hydrogen molecular ion (H₂⁻), compared with its normal matter counterpart, can provide direct tests of the CPT theorem¹. The fractional precision that can be achieved with such measurements can potentially exceed that from comparing anti-protons with protons or anti-hydrogen with hydrogen. Schemes are outlined for measurements on a single H₂⁻ ion in a Penning trap, that use non-destructive state identification by measuring the cyclotron frequency² and positron spin-flip frequency³, and also methods for creating an H₂⁻ ion and initializing its quantum state.

¹ Myers, E.G. “CPT tests with the antihydrogen molecular ion”, arXiv:1802.01514v1
The Reaction of the Oxygen Cations with HD at Low Temperature

Petr Dohnal, Thuy D. Tran, Artem Kovalenko, Serhiy Rednyk, Štěpán Roučka, Radek Plašil, Juraj Glosík

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

The reaction of O$^+$ with HD was studied in the temperature range of 15 – 200 K using 22-pole radiofrequency ion trap$^1$. Two reaction channels were observed:

$$
O^+ + HD \xrightarrow{k_{OH}} OH^+ + D, \quad (1)
$$

$$
O^+ + HD \xrightarrow{k_{OD}} OD^+ + H, \quad (2)
$$

where $k_{OH}$ and $k_{OD}$ are corresponding rate coefficients for each channel and their sum is the total rate coefficient $k = k_{OH} + k_{OD}$. The rate coefficients were evaluated from the measured dependences of the number of primary and product ions in the trap on trapping time. The preliminary results show that the isotopic branching ratio $k_{OH}/k$ is close to 0.5 in the probed temperature range. To the best of our knowledge, this is the first study on O$^+$ + HD reaction including its branching ratios performed for temperatures lower than 93 K$^{2,3,4}$, i.e. at conditions relevant for chemistry of interstellar medium. Further details will be discussed at the conference.

Acknowledgements. We thank the Technical University of Chemnitz and the DFG for lending us the 22-pole ion trap instrument and professor Dieter Gerlich for discussion. This work is partly supported by Czech Science Foundation projects GACR 17-19459S, 17-18067S and 17-08803S and by GAUK Grant No. 1584217 and 1168216.

Experimental upgrades to measure the electron’s electric dipole moment using YbF molecules


Centre for Cold Matter, The Blackett Laboratory, Imperial College London

The existence of a permanent electric dipole moment (EDM) of the electron is intimately related to the violation of time-reversal symmetry in nature, and to the observed matter-antimatter asymmetry in the universe. The Standard Model of particle physics predicts an upper limit to the electron EDM that is far below current experimental sensitivities1 (|de| < 10^-38 e cm). However, modern extensions to the Standard Model predict electron EDM values in the range^2 |de| \sim 10^{-27} – 10^{-30} e cm. The current generation of experiments that utilize cold molecules^3,4 and molecular ions^5 are precise enough to measure this. The current upper limit to the electron EDM^4 is |de| < 9.4 \times 10^{-29} e cm.

We report improvements made to increase the sensitivity of an interferometry experiment to measure the electron EDM using ytterbium fluoride (YbF) molecules. This is done by improving the signal we detect by two orders of magnitude, through a combination of better initial state preparation and detection. We have also improved our control and measurement of spurious magnetic fields inside the experiment^6. These factors will allow us to measure de at the 10^{-29} e cm level.

1 Roberts, B. L.; Marciano, W. J. Lepton Dipole Moments (World Scientific Publications,( 2010).
Density matrix renormalization group for the ground state of linear rotor chains

Dmitri Iouchtchenko, Martin Ganahl, Isaac De Vlugt, Tom Halverson, Pierre-Nicholas Roy

Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada, N2L 3G1

We demonstrate an application of the density matrix renormalization group (DMRG) to linear chains of linear rigid rotors. To make use of the symmetries of the Hamiltonian, we first derive an expression for the dipole-dipole interaction potential in terms of angular momentum ladder operators. The system under study is a model for a one-dimensional lattice of pinned linear molecules with permanent dipole moments that is sufficiently cold to be in its ground state. This can be implemented in an experiment in a number of ways, such as by placing the molecules in an optical lattice or by making a peapod of endofullerenes. We show that the von Neumann entropy of the ground state of this system suggests the presence of a second-order quantum phase transition.
Ultracold YbF molecules for measuring the electron's electric dipole moment


Centre for Cold Matter, Blackett Laboratory, Imperial College London, Prince Consort Road, London SW7 2AZ, UK

We are measuring the electron's electric dipole moment (eEDM) by observing the electric field induced spin precession of YbF molecules\(^1\). Theories that extend the Standard Model generally contain additional sources of charge conjugation and parity (CP) symmetry violation and predict an eEDM that is large enough to be measured by today's experiments. Recent measurements\(^{1,2,3}\) already strongly constrain some of these theories. Laser cooling of a beam of diatomic molecules was first demonstrated\(^4\) in 2010, and this new field promises a number of applications including cold chemistry, quantum simulations, quantum information, and precision measurements. A laser-cooled beam of YbF could increase the eEDM experiment's sensitivity by two orders of magnitude\(^5\). We recently demonstrated one-dimensional sub-Doppler transverse laser cooling of our YbF cryogenic buffer gas beam to below 100 \(\mu\)K, investigated the magnetically assisted and polarization gradient Sisyphus cooling mechanisms, and successfully modelled our experiment\(^5\).

A Molecular Zeeman Slowing Scheme

Maurice Petzold, Paul Kaebert, Mariia Stepanova, Mirco Siercke, Silke Ospelkaus

Institute for Quantum Optics, Leibniz University of Hanover, Welfengarten 1, 30167 Hannover

We report on our progress in implementing a novel scheme for slowing laser-coolable, buffer gas cooled molecules, reminiscent of Zeeman slowing. We show the results of our proof of principle experiment, realizing the scheme on the D1-line of $^{39}$K, and detail our progress on performing the experiment on molecules. From our theoretical simulations and our experimental results we expect the technique to outperform current slowing methods [1,2], and hope that the resulting large flux of trappable molecules will be the enhancement needed to produce large, ultra-cold ensembles of directly cooled molecules [3,4]. We also show our approach for the optimization of our buffer gas cell. We compare our first characterization data to computational fluid dynamic simulations to verify improvements in the cell geometry.

Steering Hydrogen Atom Diffusion Through Impurity-Doped Solid Parahydrogen

Robert J. Hinde

Department of Chemistry, University of Tennessee, Knoxville, TN 37996

Ultraviolet irradiation of solid parahydrogen (pH$_2$) matrices doped with suitable H atom precursor molecules generates H atoms in situ through a series of photoinitiated chemical reactions. These H atoms move through the matrix via a quantum diffusion process that involves the tunneling-mediated reaction H + H$_2$ = H$_2$ + H. The mobile H atoms may react chemically with other species that are also embedded in the pH$_2$ matrix; an investigation of the kinetics of these H-atom reactions provides us with information about reaction dynamics in the pH$_2$ matrix environment. Recent experimental studies$^{1,2}$ by David Anderson and coworkers at the University of Wyoming, our long-term collaborators, represent a rich source of temperature-dependent kinetic data for H-atom reactions in solid pH$_2$, and a detailed analysis of these experimental observations would help us understand the microscopic mechanism for these reactions.

Here we use quantum Monte Carlo simulations to investigate the energy landscape that mobile H atoms experience as they diffuse through an impurity-doped pH$_2$ matrix. Depending on the relative magnitudes of the long-range interactions of H–H$_2$ and H–impurity pairs, the presence of an impurity in the pH$_2$ matrix can create an effective, matrix-induced barrier to H + impurity reactions. Tunneling through this barrier could be the rate-determining step for some H-atom reactions in solid pH$_2$.


Electronic Ground State Switching upon Argon-Oxygen Bond Formation: The ArOH⁺ Molecular Ion

J. Philipp Wagner, David C. McDonald II, Michael A. Duncan

Department of Chemistry, University of Georgia, Athens, GA 30602

Although the OH⁺ cation is decidedly a triplet (³Σ⁻) being over 50 kcal mol⁻¹ more stable than the corresponding singlet (¹Δ), binding to an argon atom can reverse this situation. The singlet forms a strong donor-acceptor bond to the noble gas atom with a bond strength of 66.4 kcal mol⁻¹ at the CCSDT(Q)/CBS level of theory. This makes the singlet 3.9 kcal mol⁻¹ more stable than the most favorable triplet structure. In a cold molecular beam experiment we have prepared both, singlet and triplet, isomers of this molecular ion depending on the employed ion source. Photodissociation spectroscopy in combination with messenger atom tagging reveals that the two observed spin isomers exhibit completely different spectral signatures in the infrared and the O−H stretching fundamentals differ by about 900 cm⁻¹. These findings might encourage the search for a new potential interstellar noble gas molecule.
Cavity-Enhanced Direct Absorption Frequency Comb Spectroscopy of Cold Buckminsterfullerene

Marissa L. Weichman,¹ P. Bryan Changala,¹ Thinh Q. Bui,¹ Kana Iwakuni,¹ Justin Niedermeyer,¹ Kevin Lee,² Martin Fermann,² and Jun Ye¹

¹JILA, NIST and University of Colorado, Boulder, CO, USA
²Laser Research, IMRA AMERICA, Inc, Ann Arbor, MI, USA

Buckminsterfullerene (C₆₀) has been of great interest since its 1985 discovery.¹ The spectroscopy of C₆₀ has become especially relevant in the field of astrochemistry after its identification in the interstellar medium via its infrared (IR) emission spectrum.² Moreover, this system is of significant fundamental interest, being a rare example of icosahedral symmetry and a unique opportunity to study the bridge between few- and many-body quantum systems. However, no rotationally resolved gas phase spectrum of C₆₀ has yet been reported, in large part due to the difficulty of generating a vibrationally cold gas phase sample of sufficient number density.³

Here, we combine internal state cooling of gas-phase C₆₀ molecules with mid-IR cavity enhanced frequency comb spectroscopy,⁴ which has enabled the first direct probe of its internal rovibrational structure at the single quantum state level. Frequency comb light sources consist of thousands of discrete, evenly spaced, sharp frequency “teeth,” which inherently provide both broad bandwidth and high frequency resolution. The development of mid-IR combs has extended their utility to a frequency regime critical for molecular spectroscopy; here we use a comb centered at 8.5 µm generated by difference frequency mixing.⁵ The comb light is coupled into a high-finesse optical cavity containing the absorbing species. This configuration dramatically increases the path length of light through the sample, yielding highly sensitive absorption spectra which are then recorded with an FTIR spectrometer. Cold gas phase C₆₀ molecules are prepared by coupling the output of a 1000 K effusive oven to a cryogenic buffer gas cooling cell within the optical cavity.⁶,⁷

We report a preliminary direct absorption IR spectrum of the 1185 cm⁻¹ vibrational band of C₆₀, demonstrating successful vibrational cooling and observation of resolved rotational fine structure. We discuss ongoing experimental modifications to improve the collisional cooling efficiency and C₆₀ number density.

Towards laser cooling of AlF molecules

S. Truppe, S. Marx, H-C. Schewe, S. Kray, B. Sartakov*, G. Meijer

Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany
*Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, Russia

Direct laser cooling has been demonstrated for four diatomic molecules (SrF$^1$, YO$^2$, CaF$^{3,4}$ and YbF$^5$) and one polyatomic molecule (SrOH$^6$) so far. For all these molecules, the laser cooling transition is between a $^3\Sigma^+$ ground state and an electronically excited $^2\Pi_{1/2}$ state. For laser cooling to be feasible, the molecule must have a short-lived excited state that decays with very high probability to just one or a few vibrational levels of the ground state. Molecules with a $^1\Sigma^+$ ground state and a $^1\Pi$ excited state, such as AlF are particularly attractive candidates for laser cooling, though none have yet been cooled.$^7$

The excited $^3\Pi$ state of the AlF molecule has a lifetime of 2 ns permitting rapid photon scattering and a large capture velocity for a magneto-optical trap. The hyperfine structure in the ground state is smaller than the linewidth of the laser cooling transition, so that all hyperfine components are addressed without needing to apply sidebands to the lasers. The vibrational branching is expected to be exceedingly small, allowing $10^4$ photons to be scattered with a single laser. To slow a molecule from a speed of 140 m/s to standstill it needs to scatter about 3500 photons which corresponds to a stopping distance of approximately 5 mm.

The AlF molecule also possesses a spin-forbidden $X^1\Sigma^+ \rightarrow a^3\Pi$ transition which can be used to laser cool the molecules close to the recoil temperature of 3 µK. We present first results on high resolution optical, radio-frequency and microwave spectroscopy of the metastable $a^3\Pi$ state in AlF to determine its rotational, hyperfine and Zeeman levels and spectroscopic constants with high accuracy.

End

Photos Courtesy of Jennifer A. Douberly
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