MO 5: Miscellaneous

Time: Thursday 10:45–12:15 Location: H2

MO 5.1 Thu 10:45 H2

Dissociative recombination of OH^+ at the Cryogenic Storage Ring — •Ábel Kálosi[1,2], Klaus Blaum[2], Lisa Gamer[2], Manfred Grieser[2], Robert von Hahn[2], Leonard W. Isberner[2,3], Julia I. Jäger[2], Holger Kreckel[2], Daniel Paul[2], Daniel W. Savin[1], Viviane C. Schmidt[2], Andreas Wolf[2], and Oldřich Novotný[2] — [1]Columbia Astrophysics Laboratory, Columbia University, New York, 10027 New York, USA — [2]Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — [3]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

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

MO 5.2 Thu 11:00 H2

Electron recombination of rotationally cold CH^+ molecules — •Daniel Paul[1,2], Manfred Grieser[1], Robert von Hahn[1], Ábel Kálosi[1,2], Claude Krantz[1], Holger Kreckel[1], Damian Müll[1], Daniel W. Savin[2], Patrick Wilhelm[1], Andreas Wolf[1], and Oldřich Novotný[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg, Germany — [2]Columbia Astrophysics Laboratory, Columbia University, New York, NY, USA

Molecular cations in the interstellar medium (ISM) are used to trace the properties of interstellar clouds, out of which stars and planets form. These cations can be destroyed by dissociative recombination (DR) with free electrons. Since calculations of this reaction are challenging, and thus often do not match experimental results, laboratory studies of DR are needed to understand the molecular evolution in space.

We have studied the DR of CH^+, which is of particular interest for the interpretation of diffuse cloud observations. In the electrostatic cryogenic storage ring CSR, CH^+ ions in their lowest rovibrational states can be stored for DR experiments under conditions relevant for the diffuse ISM. Using merged ion and electron beams in the CSR electron cooler, low energy (meV) collisions can be studied, corresponding to temperatures on the order of 10 K. We report on experimental DR rate coefficient results for the CH^+ rovibrational ground state ($v = 0, J = 0$). In addition, final state branching ratios and angular fragmentation characteristics give a hint for a yet undiscovered dissociative CH state.

MO 5.3 Thu 11:15 H2

Optical Properties of Simple Diamondoid Cations and Their Astrochemical Relevance — •Parker B. Crandall, Robert G. Radloff, Jan Weissflog, Marko Förstel, and Otto Dopfer — Technische Universität Berlin, Berlin, Germany

Diamondoids are a class of highly stable, aliphatic cycloalkanes arranged into cage-like structures by sp^3 hybridization of the carbon atoms. Similarities between the IR spectra of diamondoids and unidentified infrared emission bands seen in the spectra of young stars with circumstellar disks were found.[1,2] It is also suggested that the radical cations of these molecules, which are predicted to absorb in the IR-UV/VIS range,[3] might be responsible for features in the diffuse interstellar bands. However, the optical spectra of these cations have not been measured experimentally until recently. Here, we present the first optical spectrum of the diamantane radical cation in the gas phase at $5K$ by trapping in a cryogenic 22-pole ion trap and compare it to the recently reported spectrum of the adamantane radical cation ($C_{10}H_{16}^+$).[4] Both spectra reveal broad features in the gas phase, which is attributed to significant lifetime broadening and/or Franck-Condon congestion. Geometric changes due to Jahn-Teller distortion and the astrophysical implications of these ions will also be discussed.

[1] O. Guillois et al., Astrophys. J. 1999, 521, L133
[2] O. Pirali et al., Astrophys. J. 2007, 661, 919
[3] M. Steglich et al., Astrophys. J. 2011, 729, 91
[4] P. B. Crandall et al., 2020, ApJL, 900, L20

MO 5.4 Thu 11:30 H2

Penning Electron Spectroscopy of Chiral Camphor Molecules Embedded in Helium Nanodroplets — •Subhendu De[1], S. Mandal[2], Sanket Sen[3], L. Ben Ltaief[1,4], Ram Gopal[5], R. Richter[6], M. Coreno[7], S. Turchini[7], D. Catone[7], N. Zema[7], M. Mudrich[1,4], V. Sharma[3], and S.R. Krishnan[1] — [1]QuCenDiEM group and Dept. of Physics, Indian Institute of Technology Madras, Chennai, India. — [2]Indian Institute of Science Education and Research, Pune, India. — [3]Indian Institute of Technology Hyderabad, Kandi, India. — [4]Department of Physics and Astronomy, Aarhus University, Aarhus C. — [5]Tata Institute of Fundamental Research, Hyderabad, Telangana, India. — [6]Elettra-Sincrotrone Trieste, Basovizza, Italy — [7]Istituto di Struttura della Materia - Consiglio Nazionale delle Ricerche (ISM-CNR), Trieste, Italy.

We performed Penning electron spectroscopy of chiral Camphor molecules embedded in cold sub-Kelvin He nanodroplets (~ 0.4 K). We have employed a velocity map imaging (VMI) spectrometer to measure kinetic energy spectra and angular distributions of photoelectrons in coincidence with photoions detected by the time-of-flight (ToF) technique. When photoexcited at $h\nu = 21.43$ eV , there is a significant transfer of excitation energy from the host atoms to the dopant molecules leading to the Penning ionization [1,2] of the dopant molecules. From, these spectra, we discern details of the excited states of fragment ions and photoelectron spectra associated with them.
[1] D. Buchta, et al. 2013 *J. Phys. Chem. A*, 117, 4394.
[2] L. Ben Ltaief et al. 2021 *J Low Temp Phys*, 202, 444-455.

MO 5.5 Thu 11:45 H2

Lifetime of AlF molecules in a dipole trap — •Weiqi Wang, Xiangyue Liu, and Jesús Pérez-Ríos — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

In this work, we construct a six-dimensional potential energy surface (PES) for AlF-AlF collisions based on high-level quantum chemistry method CCSD(T) (coupled-cluster with single and double and perturbative triple excitations) calculations. In addition, we employ machine learning techniques in the interpolative and extrapolative regime to describe the long-range interaction accurately. Finally, we compute the density of states of the complex and analyze its lifetime, and with it, the trapping losses of AlF in a dipole trap.

MO 5.6 Thu 12:00 H2

Combined IR/UV spectroscopic investigations on neutral isolated ion pairs in a molecular beam — •Pol Boden, Markus Gerhards, and Christoph Riehn — TU Kaiserslautern, Fachbereich Chemie and Research Center Optimas, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern

Investigations of neutral isolated ion pairs in the gas phase within the context of Stark effects constitute a still very new field. For these studies, molecular beam experiments combined with IR/UV-laser spectroscopic techniques are an ideal tool, yielding spectra of the free ion pairs which are not affected by any environmental effects, facilitating comparison with quantum chemical predictions. Within this context, the alkali salts (Li-Cs) of para-aminobenzoic acid (PABA) were studied in different electronic states (S_0 and D_0). PABA is a so-called push-pull system, showing rather unique electronic features, with the carboxylate group acting as electron density acceptor, while the amino group donates electron density to the aromatic ring. Hence, for the series of ion pairs, the influence of the reigning electric fields on the electronic behaviour of the distinct compounds can be investigated. More specifically, the often small but considerable IR- and UV-frequency shifts provoked by exchanging the alkali cation (e.g. Li to Na) were followed in detail. A clear correlation between the measured spectral shifts and the distance separating the coordinating alkali cation from the carboxylate anion, depending on the size of the alkali ion (increasing from Li to Cs), is observed and confirmed by quantum chemical calculations (DFT/B3LYP-D3(BJ)/def2-TZVP).