

MO 13: Collisions & Energy Transfer

Time: Wednesday 11:00–13:00

Location: PH/SR106

Invited Talk

MO 13.1 Wed 11:00 PH/SR106

Cryo-stored ion beams for studying neutral production in molecular fragmentation — ●ANDREAS WOLF — Max-Planck-Institut für Kernphysik, Heidelberg

Reactive and unimolecular fragmentation are powerful tools for probing molecular composition, structure, potential surfaces and internal dynamics. Energetic ion beams are unique in offering access to the neutral fragments, which can be efficiently detected and kinematically analyzed in coincidence measurements. In the cryogenic ion storage ring CSR [1], molecular ion beams accelerated by up to 300 kV circulate in a low-temperature and low-pressure environment suppressing collisional and radiative background interactions, while the molecules are excited or fragmented by velocity-tuned merged particle beams (electrons or atoms) or by lasers. The CSR energy is particularly suited for calorimetric single-particle fragment detection [2]. Studies on the neutral fragmentation, ranging to direct fragment-mass detection and kinetic energy release measurements, will become feasible for a wide range of complex singly-charged species, including (de-)protonated compounds, radical ions and ionic clusters. We will present the experimental method and discuss the options for complex molecules, considering in particular the interface to ion beam generation and to fragmentation detection methods. – See presentations at this meeting by [1] R. von Hahn et al. and [2] L. Gamer et al. in the session on Ion Storage Rings, Fachverband Masenspektrometrie.

MO 13.2 Wed 11:30 PH/SR106

Imaging the influence of vibrational excitation in ion-molecule reactions — ●MARTIN STEI¹, EDUARDO CARRASCO¹, ALEXANDER DÖRFLER², MARTIN KAINZ¹, JENNIFER MEYER¹, and ROLAND WESTER¹ — ¹Institute for Ion Physics and Applied Physics, University of Innsbruck, 6020 Innsbruck, Austria — ²now at: Department of Chemistry, University of Basel, 4056 Basel, Switzerland

We study the dynamics of ion-molecule reactions by kinematically complete velocity map imaging in a crossed-beam setup [1]. One major focus of our research is reactions of halide anions with methylhalides, a model system for nucleophilic substitution (S_N2) reactions [2]. An open question is how vibrational excitation of the reactant molecules would influence these reaction.

Here, we report on reactions of F^- and Cl^- with vibrationally excited CH_3I in the CH_3 symmetric stretch (ν_1) mode. This excitation is provided by rotationally selective excitation of the $^0R(3)$ line with a narrowband dye laser and probed by REMPI.

For F^- we find an enhancement of the rate of the proton transfer channel for the excited vibrational state. We will discuss the implications of our findings for the S_N2 channel.

[1] R. Wester, Phys. Chem. Chem. Phys. 16, 396 (2014) [2] J. Xie, R. Otto, J. Mikosch, J. Zhang, R. Wester, and W. L. Hase, Acct. Chem. Res. 47, 2960 (2014)

MO 13.3 Wed 11:45 PH/SR106

Dissociative Recombination measurements of SH^+ — ●ARNO BECKER¹, CHRISTIAN DOMESLE¹, WOLF GEPPERT², CLAUDE KRANTZ¹, OLDŘICH NOVOTNÝ^{1,3}, DANIEL SAVIN³, DIRK SCHWALM^{1,4}, BIAN YANG⁵, and ANDREAS WOLF¹ — ¹Max-Planck-Institut für Kernphysik, Heidelberg — ²Stockholm University, Stockholm, Sweden — ³Columbia Astrophysics Laboratory, New York, USA — ⁴Weizmann Institute of Science, Rehovot, Israel — ⁵Chinese Academy of Sciences, Lanzhou, PRC

Astrophysicists observe trace molecules to investigate the properties of interstellar medium. SH^+ is believed to be a very efficient probe for energetic interstellar environments, such as shocked gas. To interpret the observations, however, the models need reliable experimental data on dissociative recombination (DR) of SH^+ .

To this end we have experimentally investigated DR of SH^+ at the Test Storage Ring (TSR) of the Max Planck Institute for Nuclear Physics in Heidelberg, Germany. An SH^+ beam was merged with a cold electron beam produced by a photo-cathode. Utilizing an energy sensitive Si detector, recombination rate coefficients were determined for collision energies ranging from sub-meV up to 6 eV, covering kinetic temperatures down to 10 K. Moreover, we have determined branching ratios for various product excitation states utilizing a position sensitive microchannel plate detector. Here, we have employed a novel

approach requiring detection of only one fragmentation partner. The method will be a valuable tool for analyzing imaging data of the heavier molecules to be stored in the upcoming Cryogenic Storage Ring (CSR).

MO 13.4 Wed 12:00 PH/SR106

Collective excitation in energetic proton collision with naphthalene — ●PREETI M MISHRA^{1,2}, JYOTI RAJPUT³, C P SAFVAN⁴, SARITA VIG¹, and UMESH KADHANE¹ — ¹Indian Institute of Space Science and Technology, Trivandrum-695547, India — ²Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany — ³University of Delhi, Delhi-110 007, India — ⁴Inter-University Accelerator Centre, Aruna Asaf Ali Marg, New Delhi-110 067, India

The structural and dynamical study for Polycyclic aromatic hydrocarbons (PAHs) is important in astrophysics as well as in medical science. Due to delocalized electrons, PAHs show collective excitation characterized by large oscillator strength which are difficult to isolate from other physical processes due to broader energy deposition in ion-molecule collision. The contribution of collective excitation is distinctly identified in ionization and evaporation processes (H, 2H, C₂H₂ loss) in proton (50-180 keV) collision experiments with gaseous naphthalene at IUAC, New Delhi using an electron cyclotron resonance ion source. The photoelectron spectroscopy with pyrene and fluorene showed that collective excitation is coupled to inner valence shell and hence a good amount of excitation energy goes in heating which leads to above evaporation process. In the direct ionization mode, two mechanisms are active in the collision process: large impact parameter plasmon excitation mode and closer encounters with higher amount of electronic energy loss leading to fragmentation, whereas the resonant electron capture process was found to be associated with less electronic energy loss.

MO 13.5 Wed 12:15 PH/SR106

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MO 13.6 Wed 12:30 PH/SR106

ICD in He droplets induced by electron-ion recombination — ●MARCEL MUDRICH¹, AARON LAFORGE¹, FRANK STIENKEMEIER¹, ROBERT MOSHAMMER², and THOMAS FENNEL³ — ¹Universität Freiburg — ²Universität Rostock — ³MPI für Kernphysik, Heidelberg

The photoionization dynamics of helium droplets irradiated by EUV light is studied using synchrotron radiation and photoelectron-photoion coincidence imaging spectroscopy. At photon energies > 46 eV, secondary processes such as elastic and inelastic electron-helium scattering become important. For large droplets (> 10⁶ atoms), an additional ionization channel dominates even over direct ionization – interatomic Coulombic decay (ICD) induced by electron impact excitation and electron-ion recombination. We present a combined experi-

mental and theoretical study of the dynamics of ionization of large He droplets at high photon energies.

MO 13.7 Wed 12:45 PH/SR106

Rotational Angular Momentum Polarisation of HCl and HF in $\text{H}+\text{FCl}(v=0-5, j=0-9)\rightarrow\text{HCl}+\text{F}$ and $\text{HF}+\text{Cl}$ at $E_{rel} = 0.5-20$ kcal/mol —

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QCT calculation with trajectories 100,000 for the title reactions on the DHTSN ground $1^2A'$ PES has been done. Having the early barrier patterns, both PESs with barrier heights 2.2 and 2.6 kcal/mol, at

(2.05, 1.75) and (1.9, 1.7) Å, respectively, can cause bent intermediate [HClF] and [HFCl] ca. 120° . Polar $p(\vartheta_r)$, azimuthal $p(\varphi_r)$, dihedral $p(\vartheta_r, \varphi_r)$ and PDDCS angular distr. of HCl and HF depend. upon $\text{FCl}(v, j)$ show, that both are at $\vartheta_r=90^\circ$ for all E_{rel} , v and j ; at $\varphi_r = 270^\circ$ and 90° , respectively, for $\text{FCl}(v=0-2, j=0-9)$ at $E_{rel} \approx 5$ kcal/mol; both at $\varphi_r = 270^\circ$ for $\text{FCl}(v=2-5, j=0-9)$ at $E_{rel} \approx 15$ kcal/mol; for $\text{FCl}(v=0-5, j=0-9)$ at $E_{rel} \approx 0.5-1$ kcal/mol around E_{th} is uncertain; both are scattered back- ($\vartheta_t=180^\circ$) and forwards (90°); both are strongly aligned at $E_{rel} < 1$ kcal/mol. Influence of E_{rel} becomes decisive at $E_{rel} \geq 5$ kcal/mol, independ. on v or j . Intergration of a higher PES might unnecessary. Support with QCT-PDDCS code by K-L. Han, Group 1101, and financial aids by DICP, CAS (KF-2013-01, KF-2014-01), and VBR in Bielefeld are acknowledged. **Ref.** V.W.-K. Wu, *PCCP*. 13 (2011) 9407; 14 (2012) 16784; *Chin.Phys.B*, 22 (2013) 103101-1-13.