

## MO 2: Collisions, Energy Transfer

Time: Monday 14:00–15:45

Location: F 142

MO 2.1 Mo 14:00 F 142

**Stereodynamics of  $O(^3P) + H_2$  at  $E_{rel} = 0.5 - 1.0$  eV** — ●VICTOR WEI-KEH WU — Victor Basic Research Laboratory e.V. Gadderbaumer-Str. 22, D-33602 Bielefeld, Germany — Department of Chemical and Materials Engineering, National Kaohsiung University of Applied Sciences, 80782 Kaohsiung, Taiwan

QCT calculation of  $O(^3P) + H_2$  at  $E_{rel} = 0.5, 0.75$  and  $1.0$  eV on the lowest electronically adiabatic PES  $1^3A''$  (GLDP) of Kuppermann et al. has been done. Distr.  $P(\vartheta_r)$  of polar angles between the rel. velocity  $k$  of the reactant and rotational angular momentum vector  $j'$  of the product, distr.  $P(\varphi_r)$  of azimuthal as well as dihedral angles correlating  $k - k' - j'$ , 3-dim. distr.  $P(\vartheta_r, \varphi_r)$ , and PDDCSs (polarization-dependent differential cross sections) dependent upon the scattering angle  $\vartheta_t$  between the rel. velocity  $k$  of the reactant and  $k'$  of OH at three energies are presented and discussed. OH with the rotational angular momentum vector  $j'$  preferentially aligned perpendicularly to  $k$ . The smaller the relative scattering energy of the two reactants is, the stronger is the alignment of OH at  $\vartheta_r = 90^\circ$ . Distr.  $P(\varphi_r)$  becomes sharper when the scattering energy decreases. The  $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$  showed that most of OH are scattered into the backward hemisphere  $\vartheta_t \geq 90^\circ$ . Distr.  $P(\varphi_r)$  becomes sharper when  $E_{rel}$  decreases, and OH are scattered at  $\vartheta_r = 90^\circ$  and  $\varphi_r = 271^\circ$ . Curve  $(2\pi/\sigma)(d\sigma_{02}/d\omega_t)$  dependent upon  $\vartheta_t$ , which is proportional to the alignment moment  $\langle P_k(\cos\vartheta_t) \rangle$ , shows that  $j'$  of the scattered OH becomes stronger and stronger aligned when the collision energy decreases. Financial aids from group 1101 of DCP, CAS, and VBR are acknowledged.

MO 2.2 Mo 14:15 F 142

**Strong field effects in an ion molecule reaction** — ●SEBASTIAN TRIPPEL<sup>1</sup>, MARTIN STEI<sup>1</sup>, RICO OTTO<sup>1</sup>, THORSTEN BEST<sup>1</sup>, MATTHIAS WEIDEMÜLLER<sup>2</sup>, and ROLAND WESTER<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — <sup>2</sup>Physikalisches Institut, Universität Heidelberg, Albert-Überle-Str. 3-5, 69120 Heidelberg

Steric effects are known to play a role in chemical reactions involving non spherical reaction partners. In case of neutral-neutral reactions these effect were investigated by orienting molecules in static electric fields. For ion-molecule reactions the situation is slightly more awkward, since the electric field not only orients the molecules but also changes the trajectory of the ion. In contrast strong light fields, provided by pulsed lasers, could reveal a doorway to overcome this problem due to their capability to align molecules in free space [1]. We accomplish alignment due to the interaction of the fast oscillating electric field of the laser pulse with the induced dipole moment of the molecule. Nano second laser pulses allow to adiabatically transform the molecules into the space fixed state. This talk will present the status of our analysis on the reaction of  $Cl^-$  with  $CH_3I$  in strong laser fields up to  $2 \cdot 10^{11} W/cm^2$ .

[1] H. Stapelfeldt and T. Seideman, *Rev. Mod. Phys.* **75**, 543 (2003)

MO 2.3 Mo 14:30 F 142

**Full two-electron description of  $H_2$  molecules in antiproton collisions** — ●ARMIN LÜHR and ALEJANDRO SAENZ — Institut für Physik, AG Moderne Optik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin

A peculiarity in quantum mechanics is the fact that in the case of hydrogen most experimental efforts were done for *molecules* while the theoretical description concentrates mainly on *atomic* hydrogen. This is in particular true for collisions involving low-energy antiprotons. The obvious discrepancy originates experimentally from the reactivity of atomic hydrogen and theoretically from the complexity of the full description of the molecular systems including, e.g., two correlated electrons as well as rotational and vibrational degrees of freedom.

For the first time, a full two-electron two-center description of the  $H_2$  molecule has been implemented in a nonperturbative time-dependent calculation of antiproton collisions [1]. Close-coupling calculations are performed using a spectral expansion of the scattering wave function in eigenstates of the  $H_2$  molecule. The approach allows for the study of arbitrary molecular orientations and different internuclear distances. Besides a comparison of ionization cross sections to experimental data the obtained results are also contrasted to the outcome of a recent ap-

proach which employed two simple one-electron model potentials [2]. Thereby, the importance of two-electron effects and different orientations is demonstrated

[1] A. Lühr and A. Saenz, *Phys. Rev. A* **80** (2009)

[2] A. Lühr and A. Saenz, *Phys. Rev. A* **78**, 032708 (2008)

MO 2.4 Mo 14:45 F 142

**Three Dimensional Imaging of the Charge Transfer Reaction  $Ar^+ + N_2 \rightarrow Ar + N_2^+$**  — ●MARTIN STEI<sup>1</sup>, SEBASTIAN TRIPPEL<sup>1</sup>, JAMES COX<sup>1</sup>, RICO OTTO<sup>1</sup>, THORSTEN BEST<sup>1</sup>, MATTHIAS WEIDEMÜLLER<sup>2</sup>, and ROLAND WESTER<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — <sup>2</sup>Physikalisches Institut, Universität Heidelberg, Albert-Überle-Str. 3-5, 69120 Heidelberg

In our group we have developed a crossed-beam imaging experiment to carry out kinematically complete studies of ion-molecule-reactions [1]. Here we report on the upgrade of our velocity map imaging spectrometer to three dimensional detection by including a time-of-flight measurement with a photomultiplier.

With this improved setup we have investigated the charge transfer reaction  $Ar^+ + N_2 \rightarrow Ar + N_2^+$ . Relative cross-sections and angular distributions of  $N_2^+$  in different vibrational modes have been studied as a function of collision energies between 0.3 and 2 eV. Unlike earlier investigations of this reaction [2][3], our results are in quite good agreement with recent theoretical predictions by Candori et al [4].

[1] J. Mikosch *et al.*, *Science* **319**, 183 (2008)

[2] K. Birkinshaw *et al.*, *Chem. Phys.* **113**, 149-158 (1987)

[3] J. Mikosch *et al.*, *Phys. Chem. Chem. Phys.* **8**, 2990-2999 (2006)

[4] R. Candori *et al.*, *J. Chem. Phys.* **115**, 8888-8898 (2001)

MO 2.5 Mo 15:00 F 142

**Isomers in Space - Dissociative Recombination of  $^2HCN^2H^+$**  — ●MARIO B. MENDES<sup>1</sup>, HENRIK BUHR<sup>2,1</sup>, OLDŘICH NOVOTNÝ<sup>1</sup>, MAX H. BERG<sup>1</sup>, DENNIS BING<sup>1</sup>, MICHAEL FROESE<sup>1</sup>, MANFRED GRIESER<sup>1</sup>, BRANDON JORDON-THADEN<sup>1</sup>, CLAUDE KRANTZ<sup>1</sup>, STEFFEN NOVOTNY<sup>1</sup>, DMITRY A. ORLOV<sup>1</sup>, ANNEMIEKE PETRIGNANI<sup>1</sup>, JULIA STÜTZEL<sup>1</sup>, ODED HEBER<sup>2</sup>, MICHAEL L. RAPPAPORT<sup>2</sup>, DIRK SCHWALM<sup>2,1</sup>, DANIEL ZAJFMAN<sup>2</sup>, and ANDREAS WOLF<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Kernphysik, Heidelberg, Germany — <sup>2</sup>Faculty of Physics, Weizmann Institute of Science, Rehovot, Israel

Hydrogen cyanide (HCN) and its energetically higher lying isomer hydrogen isocyanide (HNC) play an important role in the chemistry of dense molecular clouds within the interstellar medium. Despite the fact that HNC is less stable than HCN, its abundance is of the same order of magnitude. In order to explain this unusual abundance ratio, it has been proposed that both isomers are formed with the same efficiency in dissociative electron-ion recombination of  $HCNH^+$ . Although this hypothesis has been discussed for more than 35 years now, there is still no convincing experimental evidence.

We studied the dissociative recombination of  $DCND^+$  in a storage ring experiment at the TSR, Heidelberg, using a new mass-sensitive fragment imaging detector. Surprisingly,  $DCN/DNC$  is mostly produced in vibrationally excited states, well above the isomerization barrier. The final branching ratios are fixed by radiative relaxation. This presents the formation of the two isomers in a new light, supporting the assumption that both of them are produced in this process.

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**Fragmentation of protonated water by low-energy electrons** — ●JULIA STÜTZEL<sup>1</sup>, HENRIK BUHR<sup>2,1</sup>, OLDŘICH NOVOTNÝ<sup>3,1</sup>, MAX H. BERG<sup>1</sup>, DENNIS BING<sup>1</sup>, MANFRED GRIESER<sup>1</sup>, BRANDON JORDON-THADEN<sup>1</sup>, JENS HOFFMANN<sup>1</sup>, CLAUDE KRANTZ<sup>1</sup>, MARIO MENDES<sup>1</sup>, STEFFEN NOVOTNY<sup>1</sup>, DMITRY A. ORLOV<sup>1</sup>, ANNEMIEKE PETRIGNANI<sup>1</sup>, ANDREY SHORNIKOV<sup>1</sup>, and ANDREAS WOLF<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany — <sup>2</sup>Department of Particle Physics, Weizmann Institute of Science, 76100 Rehovot, Israel — <sup>3</sup>Columbia Astrophysics Laboratory, 550 West 120th Street, MC 5247, New York, NY 10027, USA

Dissociative Recombination (DR) of  $H_3O^+$  with cold (few meV) electrons is believed to be the major source of water production in interstellar clouds. Momentum spectroscopy of collision products from

a stored  $D_3O^+$  ion beam merged with an intense cold electron beam showed a branching ratio of  $\sim 17\%$  for  $D_2O$  production, with at least half of these products internally excited by more than 4 eV. In addition, recent analysis of the Dalitz Plot of the dominant ( $\sim 71\%$ ) three-body dissociation channel  $D + D + OD$  indicates the intermediate formation of unstable water molecules above their dissociation barrier. The decay of the molecules on their way to the coincidence detector yields characteristic structures in the Dalitz geometry map. The significant internal excitation we found in the stored  $D_3O^+$  might be of importance for the occurrence of the observed two-step dissociation.

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**Scattering of state selected molecular beams** — ●MORITZ KIRSTE, LUDWIG SCHARFENBERG, HENRIK HAAK, CHRISTIAN SCHEWE, GERARD MEIJER, and SEBASTIAAN VAN DE MEERAKKER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland  
The crossed molecular beam technique is a mature and important ex-

perimental method to understand molecular interactions and molecular reaction dynamics. The Stark deceleration technique yields unprecedented control over both the internal and external degrees of freedom of polar molecules in a molecular beam. The combination of both techniques offers new possibilities in scattering experiments. In particular, crossed Stark-decelerated molecular beams allow detailed molecular scattering studies as a function of the collision energy, from low to high collision energies, and with a very high energy resolution. The success of any collision experiment critically depends on the number density, the state purity and the energy resolution i.e. the velocity distribution of the collision partners. We have developed a Stark decelerator that is operated using a unique decelerating scheme to provide a higher density of decelerated molecules, and we have developed a hexapole to focus and state select molecules. We will present our results on the scattering of beams of  $D_2$  and state selected  $OH(X^2\Pi_{3/2}, J=\frac{3}{2})$ , and our progress on the scattering of state selected beams of  $\dot{O}H(X^2\Pi_{3/2}, J=\frac{3}{2})$  and  $NO(X^2\Pi_{1/2}, J=\frac{1}{2})$ .