

MO 16: Collisions and Spectroscopy in He-Droplets

Time: Thursday 10:30–12:30

Location: V38.02

MO 16.1 Thu 10:30 V38.02

Energy transfer in the gas phase collision reaction of $\text{Cl}^- + \text{CH}_3\text{I}$ — ●MARKUS KOWALEWSKI and REGINA DE VIVIE-RIEDLE — Department Chemie, Ludwigs-Maximilians Universität München

The bimolecular substitution reaction of chloride and methyl iodine belongs to a fundamental class of chemical reactions. We are motivated by the experimental results of Mikosch et al. [1], which has some open questions. The collision reaction is simulated by solving the time dependent Schrödinger equation on ab initio potential energy surfaces. With the chosen reactive coordinates it is possible to reproduce the basic features of the immediate collision reaction. The energy transfer in the system is investigated and compared to the experimental results. From the new insight into the process, an intuitive concept of a dynamical barrier can be derived. Moreover the role of the spectator mode can be clarified.

[1] J. Mikosch, S. Trippel, C. Eichhorn, R. Otto, U. Lourderaj, J. X. Zhang, W. L. Hase, M. Weidemüller, R. Wester, *Science* **319**, 183 (2008).

MO 16.2 Thu 10:45 V38.02

Rotational Angular Momentum Polarisation of HF in $\text{H} + \text{FCl}(v=0-5, j=0-9) \rightarrow \text{HF} + \text{Cl}$ at 0.5-20 kcal/mol — ●VICTOR WEI-KEH WU — Group 1101, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 116023 Dalian, PRChina — Department of Chemical and Materials Engineering, National Kaohsiung University of Applied Sciences, 80782 Kaohsiung, Taiwan — Victor Basic Research Laboratory e. V. Gadderbaumer-Str. 22, D-33602 Bielefeld, Germany

Using QCT-PDDCS method, product alignment and orientation on PES of $1^2\text{A}'$ have been studied. HF alignment is found to be, (a) weaker at all collision energies, (b) vibrationally enhanced by the reactant FCl, but for case (c), rather insensitive to initially rotational excitation. The rot. vector of HF orientation pointing to either negative or positive direction of the y-axis in the c.m. frame, e.g. origin of the coordinate system, is enhanced by collision energies, while it becomes weaker at higher vib. ($v = 0-5$) or rot. ($j = 0, 3, 6, 9$) excitation levels. Effects of collision energies and of rot. excitation with 15 kcal/mol on the calculated PDDCSs are also shown and discussed. $p(\varphi_r)$ in the range of $0 \leq \varphi_r \leq 360^\circ$, and $p(\vartheta_r, \varphi_r)$ of $0 \leq \vartheta_r \leq 180^\circ$ and $0 \leq \varphi_r \leq 360^\circ$ at 0.5-20 kcal/mol have been presented. Results of PDDCSs of the HF alignment and orientation at these collision energies are not very strongly distinguishable. QCT-PDDCS code from K-L Han, Group 1101 of DICP, and financial aids by VBR in Bielefeld, Germany are acknowledged. Ref. 1. V.W.-K.Wu, M.-Y.Chung, and F.Kure(Ko), *JMS*. 983 (2010) 1; 2. V.W.-K.Wu, *PCCP*. 13 (2011) 9407.

MO 16.3 Thu 11:00 V38.02

Transfer ionization in swift D^+ on H_2 collisions - dependence of the electron emission on the internuclear distance — ●MARKUS WAITZ, HONG-KEUN KIM, JASMIN TITZE, MARKUS S. SCHÖFFLER, TILL JAHNKE, ACHIM CZASCH, LOTHAR PH. H. SCHMIDT, HORST SCHMIDT-BÖCKING, and REINHARD DÖRNER — Institut für Kernphysik, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany

Transfer ionization in swift (several a.u. velocity) ion helium collisions leads to a rich structure in the momentum distribution of the emitted electron. One part of the electrons is emitted in the forward direction, similar to single ionization. This might be associated with a two step process, where two independent interactions of the projectile with either electron leads to capture of one and ionization of the second one. There is however also a strong distinct peak of backward emitted electrons. The underlying mechanism is single capture accompanied by a shake off of the second electron. Here we report on the first experimental observation of transfer ionization on molecular hydrogen. The momentum distribution of the measured electron shows a clear subdivision into forward and backward emission. In addition, we find a surprising dependence of electron emission on the internuclear distance. The forward part of the electron momentum distribution gives higher values for perpendicular orientation of the molecule with respect to the incident beam direction. The SO part does not show this dependence. As a result, the ratio between forward and backward

emission changes with internuclear distance.

MO 16.4 Thu 11:15 V38.02

Collision cross sections of state selected OH + NO — ●MORITZ KIRSTE, XINGAN WANG, HANS 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 experimental 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. The advantages of such an approach are the control over the external and internal degrees of freedom e.g. a tunable collision energy, a narrow energy spread and a selected quantum state. We will discuss our results on the inelastic scattering of state selected $\text{OH}(X^2\Pi_{3/2}, J=3/2, f)$ radicals with hexapole state-selected $\text{NO}(X^2\Pi_{1/2}, J=1/2, f)$ radicals, as a function of the collision energy. Excitation functions of four rotational excited channels have been measured and will be presented.

MO 16.5 Thu 11:30 V38.02

Study on the pyridine aggregation in helium nanodroplets — ●PABLO NIETO, TORSTEN POERSCHKE, DANIEL HABIG, GERHARD SCHWAAB, and MARTINA HAVENITH — Department of Physical Chemistry II, Ruhr-University, 44780 Bochum, Germany

Pyridine crystals show the unusual property of isotopic polymorphism. Experimentally it has been observed that deuterated pyridine crystals exist in two phases while pyridine does not show a phase transition [1]. Therefore, although isotopic substitution is the smallest possible modification of a molecule it greatly affects the stability of pyridine crystals. A possible experimental approach in order to understand this striking effect might be the study of pyridine aggregation for small clusters. By embedding the clusters in helium nanodroplets the aggregates can be stabilized and studied by means of Infrared Depletion Spectroscopy.

Pyridine small clusters were identified in the C-H asymmetric vibration region ($3000-3100 \text{ cm}^{-1}$) using this method. The number of molecules of the clusters responsible of the different bands were identified by means of pickup curves measurements as well as mass sensitive detection of the clusters. Investigations with stark field measurements will be also discussed.

[1] S. Crawford *et al.*, *Angew. Chem. Int. Ed.*, 48, 755 (2009)

MO 16.6 Thu 11:45 V38.02

Time-Of-Flight and Velocity-Map-Imaging-Spectroscopy of Rubidium-doped Helium Nanodroplets — ●AMON SIEG¹, LUTZ FECHNER², BARBARA GRÜNER¹, MARCEL MUDRICH¹, and FRANK STIENKEMEIER¹ — ¹Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany — ²Max-Planck-Institut für Kernphysik, 69029 Heidelberg, Germany

Helium nanodroplets provide an ideal matrix for spectroscopy of embedded atoms and molecules due to the low temperature conditions (0.4 K) and extremely weak interactions with the dopants. In our experiments we ionize rubidium atoms attached to helium nanodroplets via resonant 2-photon-ionization. With our time-of-flight mass spectrometer we are able to discriminate between neat Rb^+ ions and RbHe_n^+ -exciplexes ($n=1,2$) which are formed upon excitation. The mass-resolved excitation spectra are in agreement with a pseudodiatomic model which treats the dopant atom as one and the whole helium droplet as the other atom of a diatomic molecule. From velocity-map-images (VMI) of photoelectrons and ions we extract energies and angular distributions which give detailed insight into the desorption process of excited Rb and RbHe_n off the droplets.

MO 16.7 Thu 12:00 V38.02

Photoionization dynamics of rubidium atoms attached to helium nanodroplets with amplified femtosecond laser pulses — ●BARBARA GRÜNER, MANUEL ROMETSCH, FRANK STIENKEMEIER, and MARCEL MUDRICH — Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

Photoionization of alkali-doped helium nanodroplets with femtosecond laser pulses entails complex dynamics which strongly depends on

the laser pulse intensity. Low laser intensities allow for investigating the desorption process of the alkali atom off the surface of the helium droplet and may induce exciplex formation, depending on the excitation wavelength [1,2]. At high pulse intensities the ionization of the dopant atoms induces the ignition of a nanoplasma that resonantly couples to the laser field [3]. However, this has not been studied, so far, for dopants residing at the surface of the droplets. We present first experiments on the photoionization dynamics of alkali-doped He nanodroplets using an amplified femtosecond laser.

[1] Krishnan et al., Phys. Rev. Lett. 107, 173402 (2011)

[2] Droppelmann, et al. Phys.Rev.Lett. 93, 023402 (2004)

[3] Mudrich et al., Phys. Rev. Lett. 100, 023401 (2008)

MO 16.8 Thu 12:15 V38.02

Investigation of Organic Molecules (PTCDA, Phthalocyanines and Porphyrines) in Helium Nanodroplets or on Neon Clusters — ●MARKUS MÜLLER, MATTHIEU DVORAK, SEBASTIAN MÜLLER, LUKAS SCHÄFER, FABIAN HOHNLOSER, and

FRANK STIENKEMEIER — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str.3, 79104 Freiburg

Organic molecules either used as organic semiconductors (PTCDA) or as dyes in organic solar cells like copper phthalocyanine (CuPc) gain high interest in their optoelectronic properties. To reveal the electronic structure of these molecules we utilize Helium Nanodroplet Isolation (HENDI) Spectroscopy, a well established method to characterize single molecules but also molecular complexes inside a cold (370mK) and weak interacting surrounding.

Laser Induced Fluorescence (LIF) excitation and emission spectra provide insight into the vibrational structure of the electronic ground state and the first electronically excited state. We present (LIF) absorption and fluorescence emission spectra of various organic molecules and complexes of them attached to helium nanodroplets. Furthermore, measurements with neon clusters have been performed in order to study the effect of the different cryogenic environment (line shifts and line broadening).