MO 20: Poster – Molecular Collisions and Kinetics

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

MO 20.1 Wed 17:00 Philo 1. OG

MOCCA: A molecule camera for the position and energy resolved detection of neutral molecule fragments — •N. Fiedler[1], A. Fleischmann[1], C. A. Jakob[2], D. Kreuzberger[1], A. Özkara[1], D. Hengstler[1], A. Reifenberger[1], L. Gastaldo[1], P. Martini[3], S. Rosén[3], H. Zettergren[3], O. Novotný[2], H. T. Schmidt[3], and C. Enss[1] — [1]Kirchhoff Institute for Physics, Heidelberg University — [2]Max Planck Institute for Nuclear Physics, Heidelberg — [3]Department of Physics, Stockholm University

The MOCCA detector is a high-resolution camera for neutral molecule fragments with kinetic energies in the keV range. It features several thousand pixels based on metallic magnetic calorimeters and is read out using SQUIDs. To reconstruct the kinematics of electron-ion and ion-ion reactions, MOCCA measures both the energy and the impact position of molecular fragments incident on the detector, even with multiple particles hitting the detector simultaneously. The latest fabricated version is currently being deployed at the Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics in Heidelberg, where molecular ions are stored and prepared in their rotational and vibrational ground states, allowing detailed studies of electron-ion interactions. We present plans for integrating the 11.5k-pixel MOCCA-Quattro detector system into the Double ElectroStatic Ion Ring ExpEriment (DESIREE) at Stockholm University, which enables mutual neutralization of ions at extremely small relative velocities. This will significantly enhance studies of neutralization processes in complex molecules prepared in their quantum ground state.

MO 20.2 Wed 17:00 Philo 1. OG

Insights into the activation of small molecules by transition metal ions — Marcel Meta, Maximilian Huber, •Maurice Birk, Martin Wedele, Boris Heeb, and Jennifer Meyer — RPTU Kaiserslautern-Landau, Fachbereich Chemie und Landesforschungszentrum OPTIMAS, Kaiserslautern, Germany

A model process for single atom catalysis can be the study of isolated transition metal ion molecule reactions in the gas phase [1,2]. Here, we present studies of the dynamics on the activation of small organic molecules by transition metal cations. Nominally spin-forbidden reactions proceed via intersystem crossing (ISC) in the presence of such metal cations. The impact of ISC on the dynamics is studied by collaborative effort combining experiment and theory.

We used crossed-beam velocity map imaging to measure differential cross sections for the activation of methane and carbon dioxide with different transition metal cations [3,4]. These reactions show dominantly indirect dynamics which is associated to the formation of a long-lived intermediate complex. In addition recent theoretical studies confirmed our observations regarding the reaction with Ta^+ and methane which revealed that the bottleneck of this reaction is ISC between the quintet and triplet states.

[1] D. K. Böhme, H. Schwarz, Angew. Chem. Int. Ed. 2005, 44, 2336; [2] H. Schwarz, Catal. Sci. Tech. 2017, 7, 4302; [3] M. Meta, Faraday Discuss. 2024, 251, 587; [4] M. Meta et al., J. Phys. Chem. Lett. 2023, 14, 24, 5524

MO 20.3 Wed 17:00 Philo 1. OG

Low-energy dynamics of the H_2^+(v = 2) + Ar reaction probed by velocity map imaging — •Jerin Judy, James K. Bateman, Dasarath Swaraj, Fabio Zappa, Viviane C. Schmidt, and Roland Wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

Crossed-beam experiments combined with the velocity map imaging (VMI) technique are a robust tool for obtaining energy- and angle-resolved differential cross sections [1]. Here, we report low-collision-energy studies on the reaction between H_2^+(v = 2) and Ar. The reactant ion, H_2^+, is produced predominantly in its second excited vibrational state using a (3+1) REMPI scheme. The reaction proceeds through two pathways-charge transfer and proton transfer-which we probe via Ar^+ and ArH^+, respectively. The charge transfer pathway exhibits a quasi-energy resonance between reactants and products. The velocity map images, together with the extracted product internal-energy and angular distributions, provide new detailed insights into the underlying reaction mechanisms.

[1] R. Wester, Phys. Chem. Chem. Phys. 16, 396 (2014).

MO 20.4 Wed 17:00 Philo 1. OG

Three-body reactions in cryogenic multipole traps — •Miriam Westermeier, •Gregor Rack, Michael Hauck, Sruthi Purushu Melath, Samuel J. M. White, Christian Sprenger, Robert Wild, Eric Endres, and Roland Wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

Three-body (3B) reactions are relevant for many different topics, such as atmospheric physics and cluster physics, especially at higher gas densities. As benchmarks for theoretical calculations, the 3B reaction of Ar^+ + Ar + Ar and of alkali-water complexes are studied. The versatility of cryogenic ion traps makes them suitable for studying these 3B reactions and their temperature dependence [1, 2]. In our group, 3B reactions are researched on two different setups, both containing a cryogenic multipole trap. One setup is equipped with an electrospray ionization (ESI) source and the other with a plasma source. ESI sources are efficient in the production of water clusters, allowing the study of 3B reactions of these cluster ions. The ESI setup is currently undergoing changes to make it suitable for the higher pressures needed for the 3B reactions. The plasma source allows for the ionization of atoms with high ionization energy, and the trap has been optimized to study reactions with very low reactions rates. The 3B reaction Ar^+ + Ar + Ar is studied on this setup and the recorded data shall be presented, together with an overview of the current experiments.

[1] S. Schlemmer *et al.*, J. Chem. Phys. **116**,11 (2002)
[2] R. Wild *et al.*, J. Phys. Chem. A **125**,39 (2021)