MO 25: Molecular Collisions and Kinetics

Time: Thursday 14:30–15:15 Location: P 105

MO 25.1 Thu 14:30 P 105

Mutual neutralization reactions in a cryogenic ion trap — •Maximilian Märk, Michael Hauck, Robert Wild, and Roland Wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

While there are many studies on ion-neutral reactions at low temperatures, mutual neutralization (MN) reactions are still experimentally poorly understood. However, these anion-cation reactions play a crucial role in the astrochemical models of interstellar clouds [T. J. Millar *et al.*, Chem. Rev. 117, (2017)]. In the literature the majority of these reactions are assigned the same rate coefficient, which is an approximation [N. S. Shuman *et al.*, J. Phys.: Conf. Ser. 300 (2011)]. We will address this gap by measuring MN reactions for abundant ions in interstellar space. To achieve this, we will utilize our cryogenic 16-pole wire trap, which is designed to create a relatively flat potential with steep walls [M. Nötzold *et al.*, Phys. Rev. A, 106 (2022)]. The wires of the trap are driven with an RF voltage to contain the ions radially. A DC voltage is usually applied to endcap electrodes for axial confinement, but this only works for one charge polarity at a time. To perform MN reactions, we will also drive the axial confinement using an RF voltage. The large expected cross section due to the attractive Coulomb potential will be offset by the low densities in the ion trap. Therefore, long storage times are essential. Our group has already demonstrated long trapping lifetimes for three-body reaction studies [C. Lochmann *et al.*, J. Phys. Chem. A, 127 (2023)]. Our measurements will provide much-needed data for astrochemical models.

MO 25.2 Thu 14:45 P 105

Gas phase redox stability of the molecular ruby [Cr(ddpd)2]3+ and related complexes — •Boris Heeb, Jana Eck, and Jennifer Meyer — RPTU Kaiserslautern-Landau, Fachbereich Chemie und Landesforschungszentrum OPTIMAS, Kaiserslautern, Germany

Chromium(III) complexes, also known as molecular rubies, exhibit particularly good luminescence properties.[1,2] Studies on gas phase stability of these compounds are rare to date. For this reason, the stability of the chromium complexes $[Cr(ddpd)_2]^{3+}$ (ddpd=N,N′-dimethyl-N,N′-dipyridin-2-ylpyridine-2,6-diamine), $[Cr(bpmp)_2]^{3+}$ (bpmp=2,6-bis(2-pyridylmethyl)pyridine), and $[Cr(tpeF)_2]^{3+}$ (tpeF=singly fluorinated 1,1,1-tris(pyrid-2-yl)ethane) with the corresponding reduced forms were examined in the gas phase through collision-induced dissociation. The experiments were performed on an electrospray ionization quadrupole mass spectrometer with in-situ reduction. Quantum chemical calculations suggest that $[Cr(ddpd)_2]^{3+}$ undergoes a metal-centered transition upon photoexcitation, whereas $[Cr(tpe)_2]^{3+}$ undergoes a ligand-centered transition.[3] However, fragmentation patterns of the reduced complexes show strong similarities, whereas the triply-charged complexes show different fragmentation behavior. In contrast, a different pattern can be observed for $[Cr(bpmp)_2]^{3+}$, which is assigned a mixed behaviour in condensed phase.

[1] W. R. Kitzmann et al., *Dalton Trans.* **2022**, *51*, 6519-6525. [2] F. Reichenauer et al., *J. Am. Chem. Soc.* **2021**, *143*, 11843-11855. [3] S. Otto et al., *Angew. Chem. Int. Ed.* **2015**, *54*, 11572-11576.

MO 25.3 Thu 15:00 P 105

Investigating electron and proton transfer reactions with velocity map imaging — •Viviane C. Schmidt, Dasarath Swaraj, Jerin Judy, Fabio Zappa, and Roland Wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

Crossed-beam apparatuses employing velocity map imaging (VMI) techniques are versatile tools to study ion-neutral collisions. Here, it is possible to either directly measure or infer the kinematics of all reactants and products, enabling a detailed look into underlying reaction mechanisms. These include the transfer of charge, either in the form of an electron or a proton, from one species to the other.

Two prototypical systems will be discussed here. The first reaction is the electron transfer between Ar^+ and N_2 studied at the newly-commissioned crossed-beam apparatus at Innsbruck University [1]. Here, it was possible to measure the reaction pathway into the N_2^+ vibrational ground state at low collision energies. It showed clear signatures of complex-mediated dynamics.

The second reaction is the proton transfer between HeH^+ and H_2. Here, a special focus is placed on the influence of rotational excitation of the charged reactant. For this project, a technical upgrade of a second crossed-beam set-up at Innsbruck University is ongoing. The current status as well as next steps will be presented.

[1] D. Swaraj *et al.*, in preparation