Influence of the collision Energy on the Reaction Rate of the ${\rm D_2}^+$ + ${\rm H_2O}$ Ion-Molecule Reaction near 0 K

D. Schlander¹, R. Hahn¹, V. Zhelyazkova¹, F. Merkt¹*

¹Departement Chemie und Angewandte Biowissenschaften, ETH Zürich, 8093, Switzerland

lon-molecule reactions are important reactions in atmospheric chemistry, astrophysics, and plasma physics.^[1] Reliable values for the reaction rates are key to modelling the relevant reaction networks. This poster focusses on the reactions of water with D_2^+ at the low temperatures in the range of 0-50 K of interstellar molecular clouds.^[1-2] For technical reasons D_2^+ is instead of H_2^+ .

Because ions are easily accelerated by (stray) electric fields, high Rydberg states ($n \approx 30$, $v^+=0$, $N^+=0$) are utilised as proxies for the ionic reaction partner, because the Rydberg-electron does not significantly affect the reaction but shields it from electric fields.^[3-4] We use a merged-beam approach featuring a Rydberg-Stark deflector and decelerator to access the collision-energy range below $k_B \cdot 10$ K. The molecular beam of water is characterised.

The reaction rates are modelled with an adiabatic capture model inspired by earlier work in Refs. [5-7] which is constructed by modifying the Langevin model with the rotational-state-specific energy of the neutral molecules in the field of the ion.^[5-8] For Maxwell-Boltzmann rotational-state distributions below 100 K the model predicts an increase of the reaction-rate constant at low collision energies.

[1] B. A. McGuire, O. Asvany, S. Brünken, S. Schlemmer, *Nat. Rev. Phys.*, **2020**, 2, 402-410.

[2] E. Herbst, Annu. Rev. Phys. Chem., 1995, 46, 27-53.

[3] P. Allmendinger, J. Deiglmayr, O. Schullian, K. Höveler, J. A. Agner, H. Schmutz, F. Merkt, *ChemPhysChem*, **2016**, 17, 3596.

[4] F. B. V. Martins, V. Zhelyazkova, C. Seiler, F. Merkt, New J. Phys., 2021, 23, 095011.

[5] J. Troe, Chem. Phys., **1987**, 87, 2773-2780.

[6] D. C. Clary, Mol. Phys., 1985, 54, 605-618.

[7] J. Troe, J. Chem. Phys., **1996**, 105, 6249-6262.

[8] V. Zhelyazkova, F. B. V. Martins, J. A. Agner, H. Schmutz, F. Merkt, *Phys. Chem. Chem. Phys.*, **2021**, 23, 21606.