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# Charge transfer of polyatomic molecules in ion-atom hybrid traps: Stereodynamics in the millikelvin regime

In the framework of ultra-cold chemistry, where reactions can be studied in well-defined quantum states, collisional phenomena between cations and neutral atoms are still not fully understood. Widely used semi-classical capture models, such as the one of Langevin [1], fail in some cases in predicting correctly rate constants associated to the charge transfer between two such species. The discrepancies between these models and experiment usually indicate that the detailed shape of the relevant potential energy surfaces (PES) at short ion-atom distance are determining in the reaction dynamics [2].

Ion-atom hybrid trap experiments capable of handling molecular ions and atoms at temperatures in the millikelvin regime allow for measuring charge transfer reaction rate constants with precision. We present here the results for the collision between the prototypical triatomic ion $N_2H^+$ and Rb which also display a deviation from semi-classical models. The focus of this presentation is the exploration of the PESs involved in the $N_2H^+$ + Rb reaction, carried out with multiconfigurational *ab initio* electronic structure methods, through which we identify the main reasons for such a deviation [3]. Namely, the charge transfer is limited to certain configurations of the polyatomic system and it occurs via deformation of $N_2H^+$. This work hence reveals the onset of anisotropic and polyatomic effects that were absent in the atomic and diatomic molecular ions studied so far in a similar context [2], highlighting the importance of stereodynamics in cold molecular-ion collisions.

[1] G. Gioumousis and D. P. Stevenson, *J. Chem. Phys.* **29**, 294-299 (1958)
[2] A. Dörfler, P. Eberle, D. Koner, M. Tomza, M. Meuwly and S. Willitsch, *Nat. Comm.* **10**, 5429 (2019)
[3] A. Voute, A. Dörfler, L. Wiesenfeld, O. Dulieu, F. Gatti, D. Peláez and S. Willitsch, (2023), [*under review*]

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