Experimental and Theoretical Studies of the Isotope Exchange Reaction: $\text{D} + \text{H}_3^+ \rightarrow \text{H}_2\text{D}^+ + \text{H}^+$

Daniel Wolf Savin, Kyle P. Bowen, Pierre-Michel Hillenbrand, Columbia University, Jacques Lievin, Université Libre de Bruxelles, Xavier Urbain, Université catholique de Louvain — H$_2$D$^+$ is an important chemical tracer of the evolution of protostellar cores. Accurate thermal rate coefficients for the reactions that generate this ion are critical for reliably understanding the star formation process. Here we present laboratory measurements of the titular reaction. Astrochemical models currently rely on rate coefficients from classical (Langevin) or semi-classical methods for this reaction. Fully quantum-mechanical calculations are beyond current computational capabilities. Laboratory studies are the most tractable means of providing the needed data. For our studies we used our novel dual-source, merged fast-beams apparatus, which enables us to study reactions of neutral atoms and molecular ions. Co-propagating beams allow us to measure cross sections as a function of collision energy. We then convolve these results with a Maxwell-Boltzmann distribution to generate thermal rate coefficients. High level quantum $ab$ $initio$ calculations have been used to model the reaction energy profile and the shape of the potential energy barrier, allowing an evaluation of the tunneling effects. Here we present our experimental and theoretical results for this reaction and discuss some of the astrochemical implications.

1This work is supported, in part, by the NSF Division of Astronomical Sciences, the German Research Foundation, and Fonds de la Recherche Scientifique-FNRS