(Quantum-)Statistical approaches for reactions and excitation of interstellar ions

Jérôme Loreau

KU Leuven, Department of Chemistry

3001 Leuven, Belgium

In order to model environments that are not at local thermodynamic equilibrium, such as those that commonly arise in astrophysical media or in the experimental study of cold and controlled chemistry, it is critical to be able to compute quantum-state-resolved rate coefficients for the excitation and reactions of ions induced by collisions with neutral atoms or molecules. State-to-state rate coefficients are notoriously difficult to obtain by means of quantum-mechanical approaches, and many approximate methods have been developed over the years. Here, I will focus on a statistical approach based on ab initio potential energy surfaces inspired by the statistical adiabatic channel method [1]. Through a few examples highlighting its advantages and drawbacks [2,3], I will show that this method is particularly adapted the study of ion-molecule reactions.

[1] J. Loreau, F. Lique, and A. Faure, *Ap. J. Letters* 853, L5 (2018).

[2] J. Loreau, A. Faure, and F. Lique, *J. Chem. Phys.* 148, 244308 (2018).

[3] M. Konings, B. Desrousseaux, F. Lique, and J. Loreau, *J. Chem. Phys.* 155, 104302 (2021).