

Collisional excitation of interstellar reactive molecules: towards a new statistical approach

B. Desrousseaux¹, J. Loreau², F. Lique¹

¹ Normandie Univ, UNILEHAVRE, UMR 6294 CNRS, LOMC, 76600 Le Havre, France

² KU Leuven, Department of Chemistry, 3001 Heverlee, Belgium

Our main knowledge about interstellar environments relies on molecular spectra. In such environments, the density is usually low and the frequency of collisions not large enough to maintain a local thermodynamical equilibrium (LTE). It is then necessary to take into account both collisional and radiative processes in order to properly interpret molecular spectra. State-to-state rate coefficients describing the collisional (de)excitation of interstellar species with the main collisional partners (H_2 , H, He) are then essential. As for now, full quantum time-independent close-coupling calculations is the method of choice to obtain accurate collisional rate coefficients at typically low interstellar temperatures (< 100 K). However, in the case of reactive systems, i.e. open-shell molecules and ions that can undergo a reaction with the most dominant interstellar species H or H_2 , this method is impractical due to its memory and CPU requirements. As a result, reliable collisional data is missing for many detected reactive molecules of key importance in astrochemistry (NH , OH^+ , CH^+ , HCl^+ , H_2O^+ , ...), preventing a proper determination of their abundance.

Here, we present a new approach based on the statistical adiabatic channel model (SACM) to compute collisional rate coefficients in the case of reactive molecules. This efficient approach allows the determination of the rate coefficients with an accuracy meeting the needs of astrophysical applications while overcoming the memory and CPU limitations of the close-coupling method. This new approach was successfully validated on light triatomic systems for which full quantum time-independent close-coupling results were available such as $CH^+ - H$ and $SH^+ - H$. The present statistical method should be considered as a useful alternative to prohibitive close-coupling calculations in order to provide the astrophysical community with accurate collisional data.