Soutenance de thèse

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Excitation and fragmentation of C_nN^+ (n=1-3) molecules in collisions with He atoms at intermediate velocity; fundamental aspects and application to astrochemistry.

This thesis studies the aftermath of collision between singly positively charged Nitrogenated carbon species C_nN^+ (n = 0,1,2,3) and neutral Helium atom at a velocity of 2.25 au. At this velocity, close to the velocity of outer electrons in atoms and molecules, several electronic processes take place and are near their maximum of probability such as ionisation (single, double, triple), electronic excitation and electron capture (single and double). We looked at their cross sections and how their evolution with the molecule size. Following the collision the molecule can fragment, which leads to another interesting aspect, the fragmentation branching ratios.

The next step was to use a theoretical model to simulate the collision. We used Independent Atom and Electron (IAE) model coupled with Classical Trajectory Monte Carlo (CTMC) method to calculate the desired cross sections. A general good agreement was obtained, with the exception of double electron capture.

The model could also predict, through the calculation of the species internal energy, the fragmentation branching ratios of cations C_nN^+ after electronic excitation. Also, the branching ratios were used to construct semi-empirical Breakdown Curves (BDCs), which are internal energy dependent dissociation branching ratios specific to each molecule, type, size and charge. With those, we could recommend products branching ratios to be used for various processes of astrochemical interest. The products branching ratios will be made available for a wider network of researchers under the international Kinetic Database for Astrochemistry (KIDA).

Vendredi 28 septembre 2018 à 14 h
Amphithéâtre du bât 520 (3ème étage)
Université Paris-Sud, 91405 Orsay Cedex

La soutenance sera suivie d'un pot auquel vous êtes chaleureusement conviés.