Title:	Elementary gas phase ion-molecule reactions: Their dynamics and chemical kinetics.
Student:	Guillem Zafra Valero
Date:	January 2020
Supervisor/s:	Dr. Antonio Aguilar Navarro Dr. Josep M <sup>a</sup> Lucas Alcorta Departament of Materials Science and Chemistry Physics

In this work, a kinetic and dynamic study of the reaction between an ion and a neutral molecule is performed. These reactions are of great interest in the field of the ionosphere and to interstellar chemistry.

The purpose of the work is to determine the total reactive cross-section and its dependence on the kinetic energy and finally obtain the thermal constant for each reaction channel and for different concentrations of the ion.

Methane reacts with argon and helium ions under single collision conditions. A certain kinetic energy is given to the ions and the formation of the different products is quantified for a range of energies.

The experiment is performed using a radio frequency guided ion beam apparatus (RF-GIB), where the primary gas ions (Ar<sup>+</sup>, He<sup>+</sup>) are ionized and directed to an octupole, which acts as reaction cell, where they collide with the methane molecules. The formed products are collected and detected by a quadrupolar mass spectrometer. To ensure unique collision conditions, the system is kept in a high vacuum level.

Atoms and molecules have an energy distribution that fits a Gaussian function. A linear relationship is observed between the reagent concentration and the signal obtained by the product confirming reactions under single collision conditions.

It is noted that Langevin's capture model describes charge transfer reactions better than those where there is an atom rearrangement. The yield of the reactions is greater for more exothermic reactions, with the exception of the formation of the CH<sub>4</sub><sup>+</sup> ion, since it has a significant Jahn-Teller distortion that could probably disfavour the reaction.