Collisional studies of heavy molecules observed in comets

Comets – Time Capsule

Comets formed together with our Solar system. Those rocky object are covered by an icy envelope made from frozen molecules. As a comet approaches the Sun, its ice shell begins to dissolve causing sublimation of the molecules. In that way is formed the comet's tail, also called its atmosphere. By studying these molecules, we are able to determine the conditions prevailing during the formation of the planets of our solar system. With better understanding of the evolution of the young Solar System, we can attempt to answer questions such as: how did life emerge on our Earth? How did our Solar System actually form? How to look for life in space? We are carrying on investigation on the beginning of the Solar System through astronomical observations. To accurately describe observations, we need theoretical model of the comet's atmosphere. That requires calculations of collisions between different molecules present in the cometary atmosphere. Unfortunately, for the most commonly observed molecules, such as **hydrogen sulfide (H_2S)**, **formaldehyde (H_2CO)** or **formic acid (HCOOH)**, this collisional data does not exist. **Therefore, the motivation of this project, is to provide the first collisional data** of the most frequently observed molecules in comets: **H_2S, H_2CO and HCOOH in collision with water (H2O), and carbon monoxide (CO).**

Analysis of observations

Comets are among the few astronomical objects we can study *in situ*. Despite some successful missions, they remain rare because each of them is extremely expensive, and require very long preparation, as well as execution. Therefore, the main source of information about molecules in comets are astronomical observations. Most molecules are discovered in the infrared and radio range, using telescopes such as Atacama Large Millimeter Array (ALMA) and James Webb Space Telescope (JWST). In this spectral range we observe rotational and rovibrational transitions. **Therefore, for this project, calculations** for H_2S, H_2CO, and HCOOH will focus only on rotational transitions.

Research Methodology

The lack of collisional data can be explained by extreme cost of calculation. Collisional calculations require a huge amount of memory and computational time. These days we observe the exponential increase in computational power. Yet, as of today, collisional calculations using the exact quantum method are still limited to small 3-4 atomic molecules with light partners such as H, He and H_2. Unfortunately, in the case of comets, we have to deal with more complex molecules and heavier partners (H_2O and CO). Thus, using quantum methods to calculate such complex systems is impossible. In 2018 Jerome Loreau, Francois Lique and Alexandre Faure, proposed to use a statistical method (SACM) in non-reactive scattering calculations. The advantage of this method is that it significantly reduces the cost of calculations. They tested this method on several systems and compared their results to those obtained with exact quantum calculations. Result of this comparison showed that for low temperatures (which is the case of comets) agreement between these two methods is very good. Using this new method, we can study much more complex systems (like the ones of cometary interest), which would otherwise be impossible to calculate. **Therefore,** I will apply the new SACM method to the collisional calculations of the systems proposed in this project.

Expected results

We will apply the results of our calculations to the analysis observations of comets. **The new results will allow, for the first time, to perform an accurate analysis of the observations and derive accurate temperatures, densities, etc. This analysis may be remarkably helpful in solving** some puzzles of the primary conditions of our Solar System and the origin of life.