

How collisional rate coefficients contribute to investigating the journey of molecules in space

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Astrochemistry tries to unveil the origin and evolution of molecular complexity in space [1]. From molecular clouds to comets, molecular species serve as diagnostic tools, offering insights into the evolution of astrophysical objects and the emergence of life on Earth. By analysing molecular spectra captured by telescopes, we can infer the physical conditions—such as temperature, density, and molecular abundances—of these environments, shedding light on their origins and futures.

However, the analysis of molecular spectra is often performed under the Local Thermodynamic Equilibrium (LTE) approximation, which is not expected to hold in most astrophysical media. Relying solely on the LTE approach raises two critical issues: **(1) uncertainties in molecular line intensities can hinder the detection of new species**, and **(2) poorly constrained physical conditions limit our understanding of the physics and chemistry within these media**. To overcome these limitations, non-LTE radiative transfer models should be employed. However, these models require collisional rate coefficients, which are available for only a fraction of the molecules detected so far.

Such studies are highly interdisciplinary by nature. They require the use of quantum chemistry methods to compute the potential energy surface (PES) of the system (Figure 1.a.), scattering approaches to compute the collisional rate coefficients based on the PES (Figure 1.b), astronomy to capture the molecular spectra, and radiative transfer modeling to determine the physical conditions of the media using the new collisional data and comparing the results with the observations (Figure 1.c.).

In this presentation, I will focus on the methods and challenges involved in determining collisional rate coefficients for astrophysical applications. I will present the full quantum approaches we used to determine these coefficients for the CCS-He system and all its isotopologues [1,2]. These results led to a re-estimation of CCS abundances, and thus to a re-evaluation of its formation process before star formation [3]. I will also introduce statistical approaches, an alternative method employed for the study of molecules in comets [4,5]. This approach led to excellent results and shows great promise, particularly in cometary science where only five molecules can currently be accurately modelled.

By providing sets of collisional data, we enable the robust determination of molecular abundances, gaining valuable insights not only into the formation pathways of these molecules but also into the origins of our Solar System.

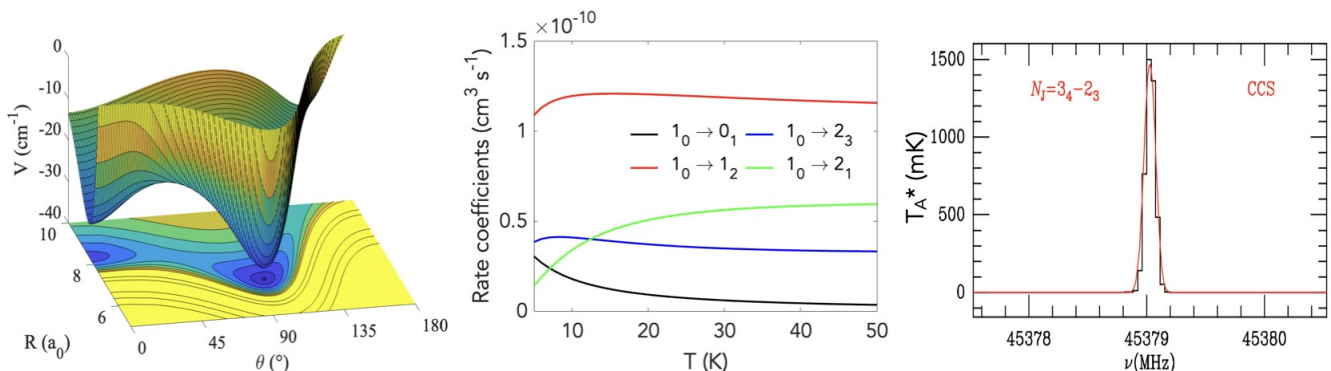


Figure 1: (a) Potential energy surface of the CCS-He system, (b) Collisional rate coefficients of the CCS-He system, (c) Molecular spectra of CCS captured in TMC-1

[1] A. Godard Palluet & F. Lique (2023).

[2] A. Godard Palluet & F. Lique (2024).

[3] R. Fuenteta et al., A&A 702, A23 (2025)

[4] A. Godard Palluet, R. Dawes; E. Quintas-Sánchez, A. Batista-Planas, F. Lique, J. of Chem. Phys. Comm. 162, 241101 (2025)

[5] A. Godard Palluet, J. Klos, D. Kedziera, F. Lique, A&A 707, A55 (2026)

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