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Collisional data for the study of laboratory and space plasmas

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Abstract. This paper highlights the importance of collisional processes in astrophysical environments, including the interstellar medium, planetary atmospheres, and laboratory studies. We emphasize the critical roles of heavy-particle ionization and dissociative recombination, underscoring the need for accurate cross-section data. Our research focuses on calculations of cross sections and rate coefficients needed for modeling. We also discuss future research directions.

Key words: atomic and molecular datasets – laboratory and astrophysical plasma – collisional peocesses – astrochemistry – modeling

1. Introduction

We are living in an era of big data, where unprecedented volumes of information demand reduction and analysis on scales far beyond human capability (Škoda & Adam, 2020; Garofalo et al., 2017). This has driven the adoption of artificial intelligence (AI) and machine learning (ML). Effective interpretation also requires complementary datasets for example, spectroscopic data for telescope spectra or collisional data for plasma modeling (Ivezić et al., 2017; Sen et al., 2022; Srećković et al., 2017; Srećković et al., 2018). As a result, growing emphasis is placed on systematic collections of atomic and molecular data, including collisional and photo-absorption studies, some now produced or refined with AI/ML methods (Anirudh et al., 2023; Trieschmann et al., 2023).

The need for reliable datasets has long been recognized, leading to the creation of dedicated databases. A notable example is the Virtual Atomic and Molecular Data Centre (VAMDC) Albert et al. (2020), which pioneered distributed databases accessible through a unified portal, initially for astronomy. Some initiatives like Europlanet related to testing and research in laboratories should also be mentioned here. Europlanet has a special program called Europlanet 2024 Research Infrastructure. It provides transnational access to unique labs where scientists can simulate planetary conditions.

This paper highlights challenges in collisional data collection and modeling fundamental to both astrophysical environments (e.g., interstellar medium, planetary atmospheres) and laboratory plasmas. A schematic presentation illustrating the connections between collisional processes, astrophysical environment modeling, and laboratory investigations is shown in Figure 1.

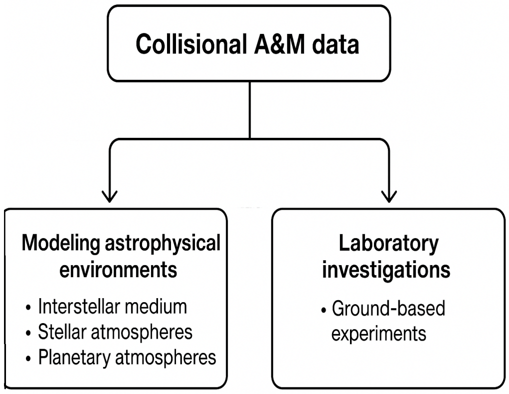

Figure 1. Schematic presentation with connection of collisional processes and modeling astrophysical environments and laboratory investigations.

Planetary atmospheres are generally weakly ionized gases, where ionization originates from diverse sources such as galactic cosmic rays, solar UV radiation, magnetospheric particles, and radioactive decay (Atreya, 1999). One of the most striking manifestations of atmospheric electrification is lightning, a transient high-current discharge that can act as a natural particle accelerator and has been observed not only on Earth but also on Jupiter, Saturn, and possibly other planets. In addition, electron impact ionization and related collisional processes, including associative ionization, chemi-ionization, and photoionization, play a central role in governing the conductivity and discharge phenomena of both terrestrial and extraterrestrial atmospheres (see e.g. Fox et al., 2008; Yair et al., 2008).

2. Collisional processes

2.1. Heavy particle ionization

Exciting an atom into a *Rydberg state* with a high principal quantum number n makes it highly sensitive to inelastic thermal collisions, which may lead to ionization. This process, known as *chemi-ionization* (CI), can proceed through different channels depending on the reaction outcome:

$$B^*(n) + B \;\rightarrow\; B + B^+ + e, \tag{1}$$

i.e. non-associative ionization and

$$B^*(n) + B \;\rightarrow\; B_2^+ + e, \tag{2}$$

known as associative ionization.

In these expressions, B represents atoms in the ground state, B^+ the corresponding ions, $B^*(n)$ Rydberg atoms with $n \gg 1$, B_2^+ molecular ions in the ground electronic state, and e the free electron.

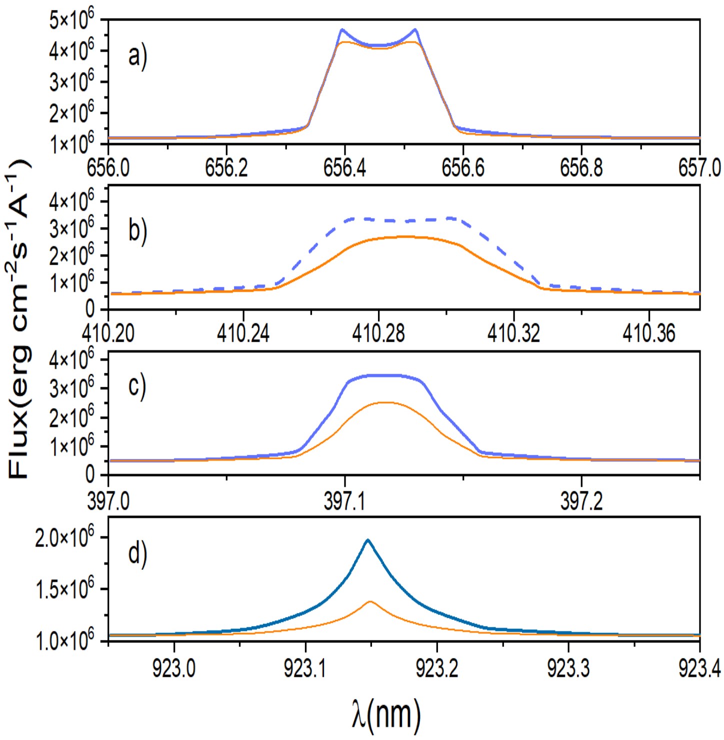

Figure 2. Profiles of hydrogen lines (a) Hα, (b) Hδ, (c) Hϵ, and (d) Paϵ in the atmospheres of late-type (M) stars. The blue curves correspond to profiles without CI processes, while the yellow curves include the contribution of CI processes.

These collisional CI mechanisms significantly affect the ionization balance and excited-state populations in weakly ionized laboratory plasmas (Ignjatović et al., 2019; Mihajlov et al., 2016; Hörnquist et al., 2023; Falcinelli et al., 2021). In astrophysical contexts, the processes (1) and (2), such as those involving hydrogen, are particularly important (Gnedin et al., 2009; Barklem, 2007). Results from Srećković et al. (2022) demonstrate that CI reactions can strongly modify the optical properties of the solar photosphere compared to electron–atom impact ionization, and therefore must be included in non-local thermodynamic equilibrium (non-LTE) modeling of the solar atmosphere (see e.g. Fig. 2).

Furthermore, atom-Rydberg atom CI processes have been proposed as useful tools for modeling and diagnosing dense, partially ionized regions in the broad-line regions (BLRs) of active galactic nuclei (AGN) (Srećković et al., 2018). Srećković et al. (2020) showed that when neutral hydrogen densities exceed 10^{12} cm^{-3}, CI reactions dominate over electron-atom collisions, thus exerting a major influence on the optical properties of these regions.

The associative channel of CI has also been suggested to contribute to the formation of molecular ions in interstellar gas (Dalgarno & Black, 1976). To model interstellar cloud chemistry, reliable cross sections and rate coefficients for such processes are required. Studies on helium, lithium, and alkali atoms Klyucharev et al. (2007); Srećković et al. (2018); Srećković et al. (2023) have further connected CI to astrophysical and planetary phenomena, including Io's atmosphere, Li-rich stars, and various geo-cosmical plasmas.

Finally, excitation and de-excitation in atom–Rydberg atom collisions can impact the efficiency of the ionization processes (1) and (2) (Barklem, 2007; Dimitrijević et al., 2020, 2021; Srećković et al., 2023). Such effects are especially relevant for the solar photosphere, the interstellar medium, DB-type white dwarf atmospheres, and AGN BLRs.

2.2. Electron driven collisional processes

Over recent decades, computational methods have become central to studying the dynamics and interactions of molecules embedded in larger structures (Reis et al., 2022; Iacob, 2020; Pop et al., 2021). Despite their massive scale, interstellar clouds remain poorly understood as confined systems. Deep within molecular clouds, molecules are shielded from photodissociation and photoionization by absorption and scattering of interstellar radiation (Puzzarini & Barone, 2020; Guerrero-Méndez et al., 2023). To model such environments, it is essential to consider not only radiative but also collisional processes, especially electron-driven reactions involving molecular ions such as dissociation.

Dissociative rate coefficients, defined as the change in molecular cation concentration over time, provide critical insight into the abundance of molecular ions. For instance, ions such as HeH^+, H_2^+, and He_2^+ have been detected in stellar media, with receiving particular attention due to its importance at relatively low temperatures (see e.g. Augustovičová et al., 2013; Guberman, 2012). The destruction of H_2^+ is a crucial step in the chemical network that leads to water formation in protoplanetary disks. The reactions that destroy H_2^+ actually

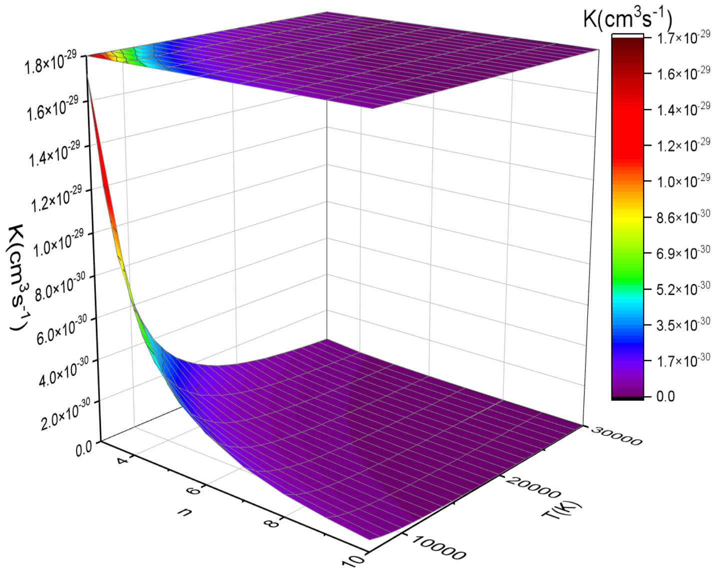

Figure 3. Three-dimensional plot of the dissociative rate coefficients for the He_2^+ system, based on data from the ACol database.

initiate the production of key intermediates such as OH^+, H_2O^+, and H_3O^+. The He_2^+ molecular ion has notable diagnostic value in astrophysics. It forms transiently under strong ionizing radiation and serves as a tracer of high-energy processes in environments such as protoplanetary disks and planetary atmospheres. Although short-lived and chemically inert, He_2^+ provides insight into the ionization state and radiation conditions that influence the evolution of these systems.

Access to reliable datasets and recommended values remains crucial for the modeling community (Marinković et al., 2017; Anirudh et al., 2023).

Dissociative recombination (DR), a dominant electron-driven destruction process, can be written as

$$e + M_2^+ \Longrightarrow M^*(n) + M, \tag{3}$$

where M and $M^*(n)$ are ground and Rydberg atoms, and M_2^+ is a molecular ion in its ground state.

These reactions are often explained through the dipole resonant mechanism, where the dipole component of the electron–ion interaction drives recombination, and may be analyzed using the decay approximation (Mihajlov et al., 2012). Figure 3 shows DR rate coefficients for He_2^+ from the ACol database, across $7000 \leq T \leq 30000$ K and $3 \leq n \leq 10$. The probability of DR increases with smaller n and lower T, confirming electron-driven collisions as a primary channel for Rydberg atom formation under such plasma conditions.

Since these processes influence both excited-state populations and free-electron densities, they also affect spectral line shapes, not only in molecular clouds and the interstellar medium but also in weakly ionized stellar atmospheres (Gnedin et al., 2009; Beuc & Pichler, 2020).

3. Summary

In this paper, we have highlighted the significance of collisional processes in the study of the astrophysical environments such as interstellar medium, planetary atmospheres, and laboratory experiments. We have emphasized the critical role of processes such as heavy-particle ionization and dissociative recombination, as well as the necessity for accurate cross-section data.

With regard to data resources, numerous comprehensive databases provide atomic and molecular information for spectroscopic studies of atmospheres and the interstellar medium like BASECOL, KIDA, etc. Despite the availability of these individual databases, we believe that the approach promoted by the VAMDC consortium, linking distributed databases through a single unified portal, represents the future standard for providing researchers with streamlined access to scientific data.

As a future step, we intend participation of ML models to produce i.e., to fast predict new A&M data. We are currently in the process of preparation for training and testing datasets for development of advanced models.

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