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Molecular ion reaction rates for planetary atmospheres and the interstellar medium

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Abstract. Planetary systems are formed in dense interstellar clouds where chemistry is driven by complex ion–molecule processes. To improve astrochemical models, we present theoretically calculated datasets of cross sections and rate coefficients for important molecular ions under astrophysical conditions. The results provide a dataset relevant to protoplanetary disks and laboratory plasmas, and support the development of a user-friendly platform for data dissemination within the Virtual Atomic and Molecular Data Center (VAMDC) and the Serbian Virtual Observatory (SerVO).

Key words: databases – molecules – collisions – astrochemistry – modeling – planets – atmosphere

1. Introduction

Planetary systems originate from dense clouds of interstellar gas and dust, where gravitational forces interplay with thermal pressure, turbulence, and magnetic fields to drive collapse and disk formation (van Dishoeck et al., 2023; Walsh et al., 2012). To interpret the complex chemistry observed in these environments, astrochemical models - rooted in interstellar medium (ISM) chemistry while evolving into diverse transformations - are employed to refine our understanding of planetary formation processes. These models are supported by advances in astrochemical databases such as UMIST (Millar et al., 2024), KIDA (Wakelam et al., 2024), and the A&M VAMDC initiative (Albert et al., 2020), which enhance the accuracy of reaction rate coefficients (see Fig.1). A critical aspect of these models involves examining reaction rates that reveal the presence and behavior of various molecular species, particularly small molecular ions (Öberg et al., 2023; Bae et al., 2022). Consequently, it is important to investigate not only radiative processes but also non-radiative mechanisms, such as electron-driven reactions including dissociative recombination.

Observations, including those from ALMA, of ions such as N_2H^+ provide insights into midplane conditions within protoplanetary disks-regions where planetesimals are believed to form. Additional ions, such as NS^+, may also influence ion-driven chemistry, contribute to cooling processes, and impact the physical and chemical evolution of star-forming regions.

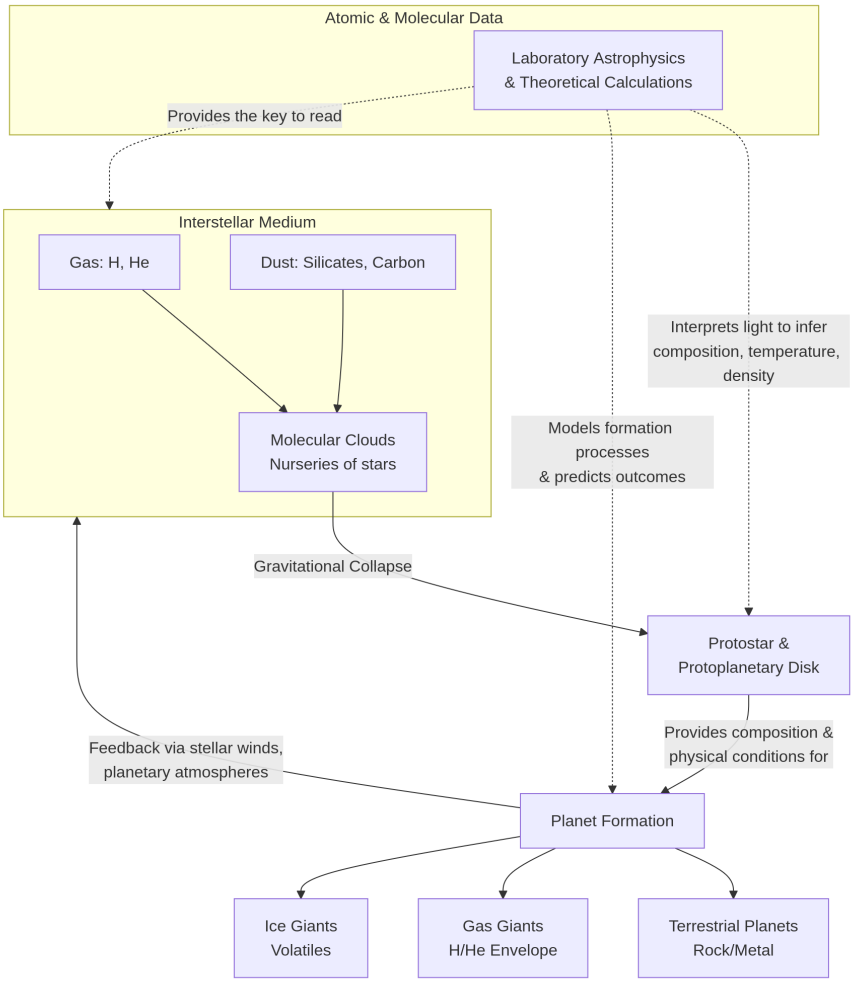

Figure 1. A&M data and its astro importance.

Accurate molecular ion data are essential for modeling astrophysical environments, from protoplanetary disks to planetary atmospheres. Recent studies of dissociative recombination and resonance structures in NS+ systems provide benchmarks for cation chemistry (Hassaine et al., 2024; Iacob et al., 2022). From a theoretical perspective, solvable potential models such as relativistic pseudo-Gaussian oscillators extend the family of exactly or approximately tractable systems, offering valuable tools for understanding confinement and spectral properties in hydrogen-like and molecular systems (Iacob, 2010; Iacob et al., 2019; Pop et al., 2021)

This paper aims to conduct theoretical studies involving the calculation, comparison, and analysis of cross sections and rate coefficients for molecular ions such as H_2^+, SiH^+, He_2^+, HeH^+, etc. under astrophysically relevant conditions. The intended outcome is a comprehensive dataset applicable to astrochemical environments as well as laboratory plasmas. Moreover, we aim to contribute to the broader scientific infrastructure by developing a user-friendly, extensible, and searchable e-platform for data dissemination and integration-aligned with existing frameworks such as VAMDC (Dubernet et al., 2024).

2. Data and databases

The databases are important for modeling laboratory and stellar plasmas, as well as for studies of planet formation. The Belgrade databases include astrophysically relevant data. The Belgrade database ACol provides collisional data, while the MolD database contains photodissociation cross sections for individual rovibrational states of diatomic molecular ions.

The Belgrade nodes provide unique datasets and specialized spectroscopic data, that are not fully covered by international repositories, thereby offering complementary resources for molecular collision and astrophysical research. This complementarity emphasizes the nodes' value in filling data gaps and supporting precise modeling in astrophysics and chemical physics.

2.1. SerVO

The SerVO (`http://servo.aob.rs`) hosts the Belgrade radiative and collisional nodes MolD and ACol of the Virtual Atomic and Molecular Data Centre (VAMDC) (Albert et al., 2020). The databases MolD (`http://servo.aob.rs/mold`) and ACol (`http://servo.aob.rs/acol`) include astrophysically relevant data. Furthermore, the data and its analysis demonstrate their interdisciplinary character and applications, such as in physics, astrophysics, and chemistry. One can see on the left side of the SerVO web page are links to BG Nodes (MolD, ACol). In the middle are links to the photo plate archive as well as new information related to scientific meetings, etc.

The MolD and ACol Belgrade A&M databases have been linked with the VAMDC project (`http://vamdc.eu`) since their early phases of development

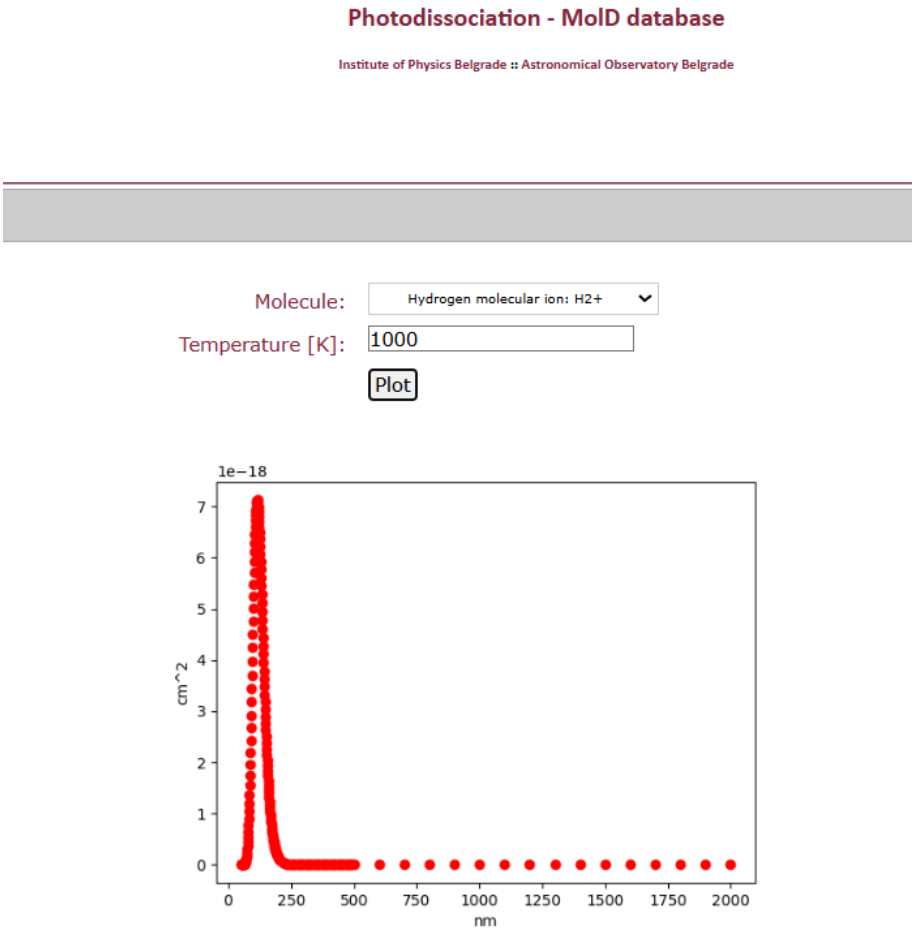

Figure 2. Snapshot of the MolD database (`http://servo.aob.rs/mold`): Photodissociation of the H_2^+ molecular ion for selected parameters. The SerVO (`http://servo.aob.rs`) hosts the Belgrade radiative and collisional nodes MolD

(see e.g. Vujčič et al., 2015). The VAMDC project Albert et al. (2020) intends to bring together numerous current databases under a common standard, creating a centralized platform for accessing atomic and molecular data. Users can download A&M data in a consistent format using the XML Schema for Atoms, Molecules, and Solids (XSAMS) (Jevremović et al., 2020; Albert et al., 2020; Marinković et al., 2017). Technically, the data models were updated to effortlessly transition to the VAMDC's tree-structured serialization schema,

XSAMS. All databases are stored on a MariaDB server (an open-source relational database management system based on MySQL) and backed up on a regular basis.

The Belgrade nodes of the VAMDC offer practical accessibility for external researchers through standardized web services and user-friendly query tools. These platforms execute queries locally and transmit data in the VAMDC-specified XSAMS format, ensuring compatibility with VAMDC standards. The web interfaces allow researchers to perform searches and retrieve data without complex programming, and while detailed API documentation is explicitly provided, adherence to VAMDC standards enables programmatic access using standard protocols.

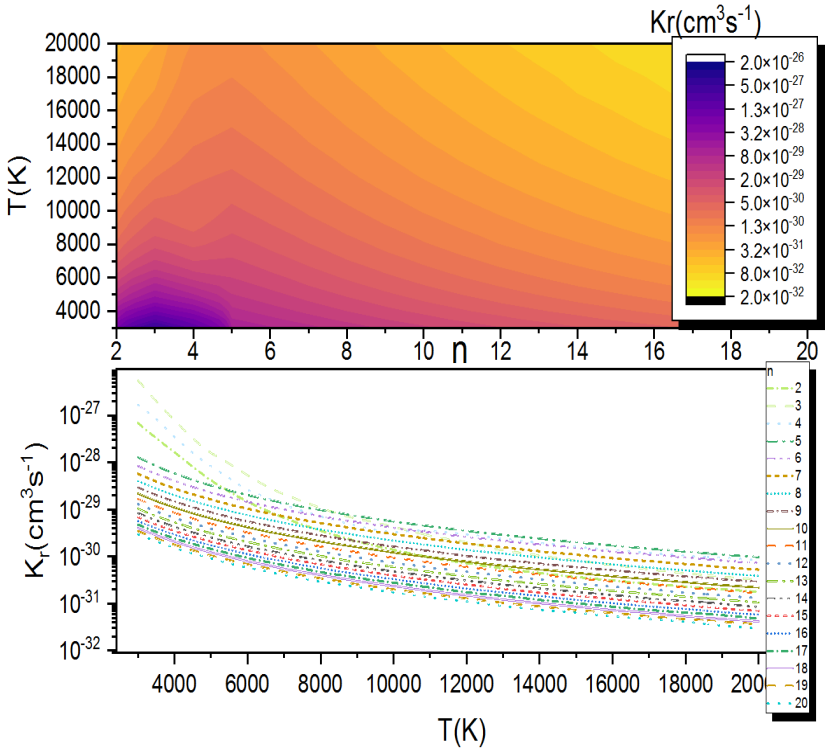

Figure 3. Figures created using data from the ACol database (http://servo.aob.rs/acol).

2.2. The MolD photodissociation database

The MolD database provides information on numerous molecular species and their excited states (see e.g. Srećković et al., 2017a; Vujčić et al., 2023). As a radiative database, it contains averaged thermal photodissociation cross sections as well as state-resolved data for the ro-vibrational levels of diatomic molecular ions (see Fig. 2).

The database has undergone several development phases and is maintained by the Astronomical Observatory in Belgrade. It is widely used in astronomy for investigating diverse astrophysical processes and modeling (Mihajlov et al., 2011; Srećković et al., 2014; Coppola et al., 2013), while its data also support studies of plasma chemistry and laboratory experiments (Srećković et al., 2021, 2022).

2.3. The ACol database for collisional processes

The ACol database provides cross sections and rate coefficients for collisional processes, including excitation, de-excitation, ionization, and recombination in hydrogen, helium, and alkali (see e.g. Srećković et al., 2022; Srećković et al., 2017b; Vujčić et al., 2023, and references therein). It represents the newest BG VAMDC node and is hosted by SerVO. Queries are processed locally, with results delivered in the VAMDC-standard XSAMS format through an AJAX-based interface. The database is applicable to laboratory studies as well as to modeling interstellar gas, weakly ionized atmospheric layers, and low-temperature plasmas. (see Fig. 3)

3. Summary

Emergence of planetary systems starts with the gravitational collapse of dense interstellar clouds, in a process where turbulence, pressure, and magnetic fields result in formation. Understanding the complex chemistry relies on astrochemical models, supported by specialized databases/data ecosystems such as UMIST, KIDA, and VAMDC, which provide essential reaction rate data. A key focus is the study of molecular ion reaction rates, including both radiative and electron-driven non-radiative processes like dissociative recombination.

In this work, we present an overview of the MolD and ACol databases - hosted within the VAMDC and SerVO frameworks - designed to support both astrophysical and laboratory research. Reliable maintenance and curation require not only adherence to established principles but also continuous alignment with rapid developments in information technology. Future improvements and standards should involve regular updates of Node software, including Python and Django, alongside enhancements to the web interface with AJAX-based queries, new visualizations, and additional extensions. Equally important is the expansion of datasets to include newly calculated or measured radiative and

collisional processes. Another direction is the integration of machine learning techniques to accelerate the prediction of atomic and molecular data, supported by ongoing efforts to prepare training and testing datasets for the development of advanced models. Although machine learning approaches can speed up data generation, their predictions may lack precision. Therefore, results obtained through such models should be interpreted with caution.

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