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New database for collisional excitation/ ionization processes of astrophysical interest

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Abstract. In this paper, ACol database for the collisional processes in atom and Rydberg atom collisions is described. Database (DB) is hosted and is a part of the Serbian Virtual Observatory (SerVO) and VAMDC project. The database contains the rate coefficients for excitation and ionization collisional processes in hydrogen, helium and alkali plasmas. The ACol dataset could help with the investigation and modeling of laboratory low temperature plasmas as well as weakly ionized layers in various atmospheres and cosmic objects.

Key words: Atomic data – Modeling – Astrophysical plasma – Line profile – Planetary geochemistry – AGN

1. Introduction

Atomic and molecular (A&M) data and databases Sahal-Bréchot et al. (2014); Marinković et al. (2017); Albert et al. (2020) have become essential for diagnostics and development of models and simulations of complex physical processes and for the interpretation of data provided by measurements e.g. in laboratory and astrophysical plasmas (Christensen-Dalsgaard et al., 1996; Fontenla et al., 2009; Srećković et al., 2017; Hauschildt & Baron, 2010; Husser et al., 2013). Diagnostics and development of models and simulations of low temperature laboratory and astrophysical plasmas (LTPs) requires usage of accurate A&M data, both experimental and theoretical Jevremović et al. (2020); Albert et al. (2020).

It is shown Adamovich et al. (2017, 2022) that such data is very important in the development of plasmas as an enabling technology for a vast range of fields associated with modern society. From technological perspective, this often means heterogeneous e-ecosystem, consisting of different datasets and formats and various programming frameworks synchronized to work together, such as in VAMDC (vamdc.org) project efforts (Dubernet et al., 2016). Access to large amounts of A&M data is now required by the plasma community, and VAMDC provides 30+ nodes, several of them containing recommended data relevant to modeling LTPs.

The A&M community revealed a grown maturity in the process of curating (i.e. collecting, categorizing, archiving and distributing) dynamical data relevant to the kinetic modeling of LTPs, moving from the cold gas approximation to the state-to-state approach, in the perspective of deepening the knowledge on elementary processes involving both electron and heavy species collisions (Marinković et al., 2017; Srećković et al., 2018; Adamovich et al., 2022).

In this contribution, ACol database for heavy particle collisions i.e. for the collisional processes in atom and Rydberg atom collisions is described. Database is hosted and is a part of the Serbian Virtual Observatory (SerVO). It contains the rate coefficients for excitation and ionization collisional processes in hydrogen, helium and alkali plasmas. ACol database (DB) is in the development phase. The dataset could help with the investigation and modeling of laboratory low temperature plasmas as well as weakly ionized layers in various atmospheres and cosmic objects (Srećković et al., 2014; Klyucharev et al., 2007; Ignjatović et al., 2019).

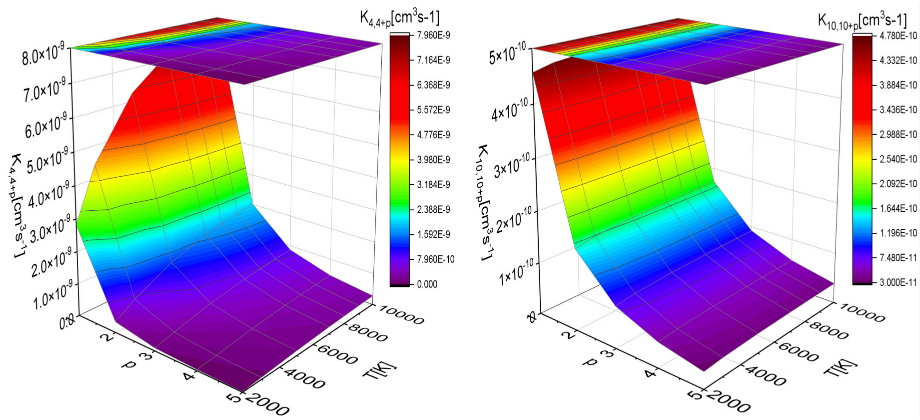

Figure 1. Left: Rate coefficients $K_{4;4+p}(T)$ for the excitation processes H*(n) + H => H*(n=n+p) + H in hydrogen plasmas (n=4, $1 \leq p \leq 5$, A=H in Eq.(2)). Right: Rate coefficients $K_{10;10+p}(T)$ for excitation processes H*(n) + H => H*(n=n+p) + H in hydrogen plasmas (n=10, $1 \leq p \leq 5$, A=H in Eq.(2)).

2. The collisional processes

ACol database contains calculated data for excitation and ionization processes in heavy particle collisions. In other words, the database consists of collisional ionization

$$A^*(n) + A \Rightarrow e + \begin{cases} A_2^+, \\ A + A^+, \end{cases} \tag{1}$$

and excitation

$$A^*(n) + A \Rightarrow A^*(n' = n + p) + A \tag{2}$$

data. Here A are atoms and their ions in the ground states, $A^*(n)$ is the Rydberg atom (RA), and A_2^+ their molecular ions.

2.1. DRM

The data are obtained within the DRM i.e., the collisional reactions have been treated by the so-called dipole resonant mechanism (DRM). In this characterization, the processes are caused by the dipole part of the electrostatic interaction between the outer highly excited i.e. Rydberg electron and the inner (ion-atom) system. This method is especially effective when used with the so-called decay approximation. A detailed description can be found in paper of Mihajlov and coworkers (Mihajlov et al., 2011; Mihajlov et al., 2012; Srećković et al., 2018).

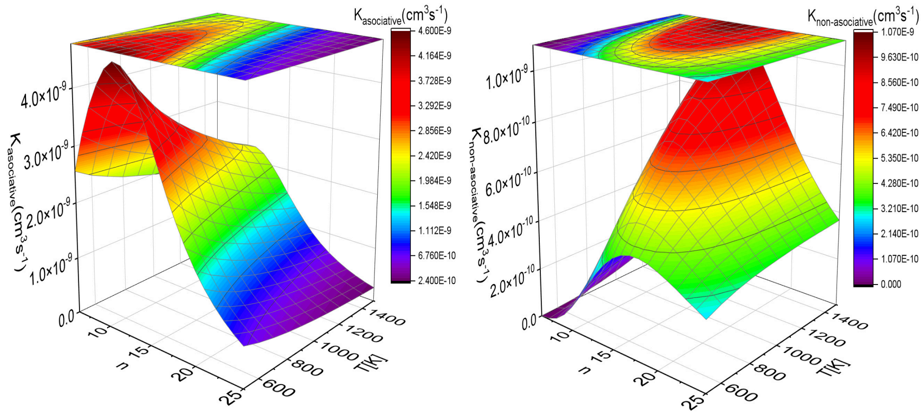

Figure 2. Left: Rate coefficient $Ka(n;T)$ for ionization collisional processes Eq.(1a) in potassium plasmas. Associative channel; Right: Rate coefficient $Kb(n;T)$ for ionization collisional processes Eq.(1b) in potassium plasmas. Non-associative channel

2.2. The obtained quantities

In the process of ACol DB creation, we collected needed data, made a corresponding model and we calculated rate coefficients. For the calculations, we developed sophisticated model for corresponding collision processes. We determined theoretically - calculated cross-sections and rate coefficients for the ionization and excitation processes for hydrogen, helium and alkali plasmas, for conditions of interest of laboratory/astrophysical LTPs.

The figures 1 and 2 show heavy species collisions - rate coefficients from the calculations we carried out (see e.g. Mihajlov et al. (2011); Srećković et al. (2018)).

Validation is also a crucial step in the development of databases (Srećković et al., 2017). For instance, measurements of the rate coefficients of associative ionization in collisions of metastable atoms necessitate meeting several technical challenges as noted in the literature (Boyd & Josyula, 2021). Perhaps the biggest challenge of these measurements is isolating the associative ionization in atomic collisions (Adamovich et al., 2022)

3. Software and Data

We wrote data model (shown in Fig 3) for our new atomic collisional data node (ACol) as a subset of XSAMS (XML Schema for Atoms, Molecules and Solids - `https://vamdc-standards.readthedocs.io/en/latest/dataModel/vamdcxsams/structure.html`) to set up a new VAMDC node for the LTP data that could be useful for the laboratory and astrophysical community. After translating data model into Django-Python models class, we generated a MySQL (MariaDB) database with object-relational mapping to tables. We converted data from a textual source to the database. We customly fit software for this new VAMDC node, according to the NodeSoftware project (`https://github.com/VAMDC/NodeSoftware`).

In Figure 3 is presented a class diagram for the ACol node (logical model).

The result is a new VAMDC node, hosted on Serbian virtual observatory `http://servo.aob.rs/acol/`. Establishing this database/node might be important for diagnostics and modeling of LTPs which are used for the modeling astrophysical and laboratory plasmas. The node is in debug phase and will need some time to be officially included to VAMDC portal (`https://portal.vamdc.eu/vamdc_portal/home.seam`). Tap query already is available as a web service (also via TAPValidator). Capabilities listed at `http://servo.aob.rs/acol/tap/capabilities`; sample query: `servo.aob.rs/acol/tap/sync?LANG=VSS2&REQUEST=doQuery&FORMAT=XSAMS&QUERY=select+*`. Also, we will host queries locally on the website which also deliver data in XSAMS format defined by the VAMDC (servo.aob.rs/acol/).

4. Summary

Based on the foregoing, it can be inferred that examined collisional excitation/ionization processes and data in ACol DB could play a important role in the

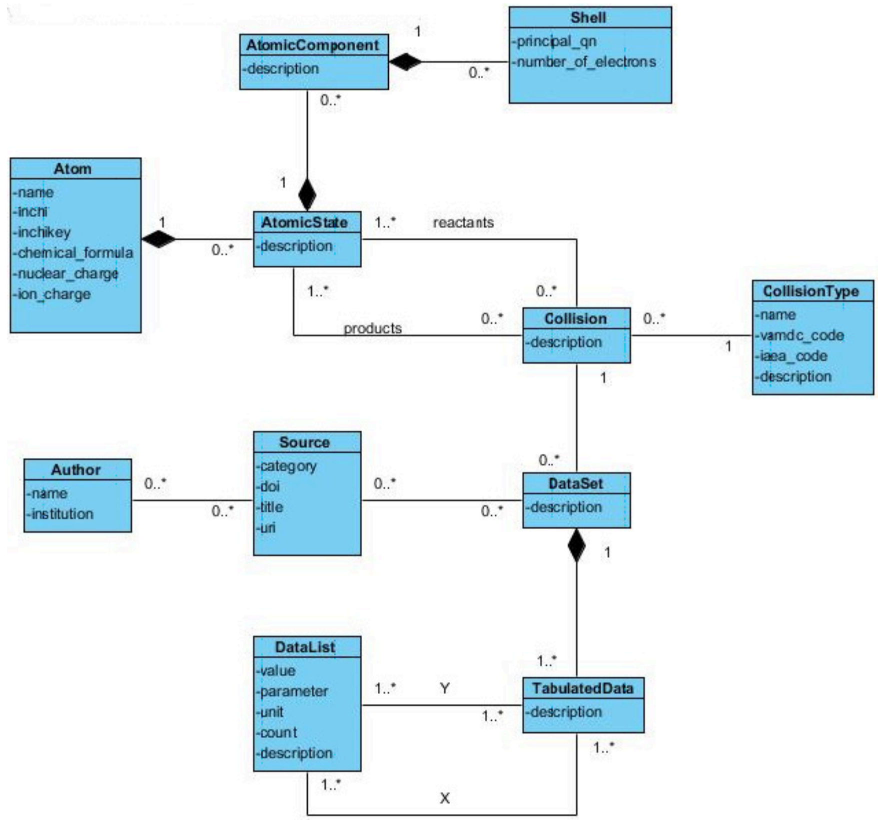

Figure 3. Class diagram for the ACol node (logical model)

spectral exploration of many astrophysical environments and laboratory LTPs (Wilson et al., 2002; Klyucharev et al., 2007; Ignjatović et al., 2019; Adamovich et al., 2022) although it is in the development i.e. debug stage. Due to their rapid expansion in the modern world, services like atomic databases and astronomical virtual observatories must continue to be developed and offered. This is the rationale behind SerVO's and VAMDC's ACol continued database development.

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