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The MOL-D database VAMDC node for molecular collisional and radiative processes

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The MOL-D database is a collection of collisional data and a web service within the Virtual Atomic and Molecular Data Centre (VAMDC, http://www.vamdc.eu). In this paper we report on the current stage of MOL-D development. This database and web service/interface is intended for modeling stellar atmospheres, laboratory plasmas, technological plasmas etc. For example, the data for hydrogen are important for elaboration of atmosphere models of solar and near solar type stars and for radiative transport consideration as well as for the kinetics of stellar and other astrophysical plasmas. The helium data are of interest particularly for investigation of helium-rich white dwarf atmospheres. Stage 1 of the development was done at the end of 2014 when all the existing calculated data for photodissociation cross-sections of hydrogen H_2^+ and helium He_2^+ molecular ions and the corresponding averaged thermal photodissociation cross-sections had been processed and integrated into the database. We are now beginning Stage 2 of the development of MOL-D. At the moment we are including new cross-sections and rate coefficients for processes which involve species such as HeH^+, LiH^+, NaH^+, SiH^+ that are important for exploring the interstellar medium as well as for the early universe chemistry and for modeling stellar and solar atmospheres.

Keywords: Atomic processes – stellar atmospheres, databases, spectral line profiles

1 MOL-D database

Many fields in astronomy, physics, and industry depend on databases for atomic, molecular interaction processes. A reliable exchange of such data has become crucial for decades. In this context, we are developing the MOL-D database. The MOL-D database is a collection of cross-sections and rate coefficients for specific collisional

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processes (Vujčić et al., 2015). It can be accessed via the website of Serbian Virtual Observatory* (SerVO, Jevremović et al. (2009)) or as a web service which is part of the Virtual Atomic and Molecular Data Center† (VAMDC (Dubernet et al., 2016)) e-infrastructure.

The database contains photodissociation cross-sections for the individual ro-vibrational states of the diatomic molecular ions and rate coefficients for the atom–Rydberg atom chemi-ionization and inverse electron–ion–atom chemi-recombination processes. A graphical interface is provided at "Homepage" (Fig. 1): first, the consumer clicks on the wished molecular ion in the dropdown menu. Next, with a few clicks, the user chooses the individual cross section and/or average thermal cross section. The web interface offers access to data for photodissociation (bound-free) cross-sections of hydrogen H_2^+ and helium He_2^+ molecular ions as well as the corresponding averaged thermal photodissociation cross-sections for the requested wavelength and temperature (see for e.g. Fig. 1).

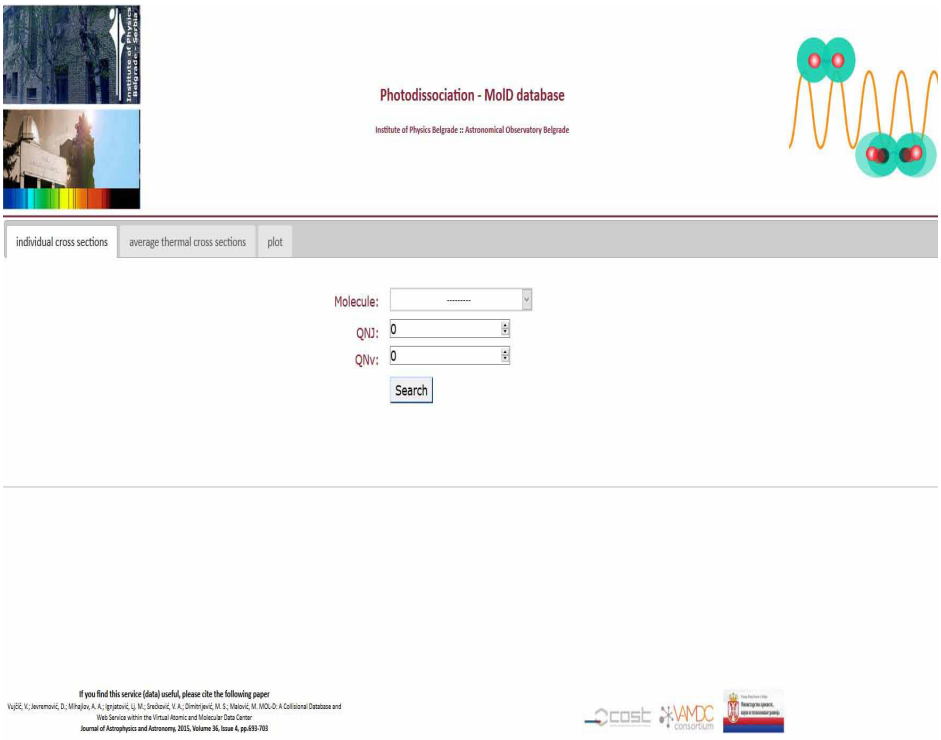


Figure 1 Access to the data: the graphical interface.

The consumer can also make a query for the data plot of the corresponding averaged thermal photodissociation cross-sections in the domain of wavelengths at requested temperature (see Fig. 2). The data can be downloaded in ASCII format.

*http://servo.aob.rs/mold/
†http://portal.vamdc.eu/

Stage 2: At this moment, MOL-D is at stage 2 of the development. We are including new cross-section and rate coefficients data for processes which involve species such as MgH^+, HeH^+, LiH^+, NaH^+, SiH^+ which are important for the experimental plasma physics as well as for exploring the interstellar medium, the early Universe chemistry and for modeling different stellar and solar atmospheres (Srećković et al. (2014); Ignjatović et al. (2014); Vujčić et al. (2015)). We are planning incremental inclusion of data from our papers concerning atomic and molecular processes important for modeling different stellar atmospheres and laboratory plasmas as they become published. Along with database updates, we intend to develop new web utilities and interfaces for SerVO MOL-D website.

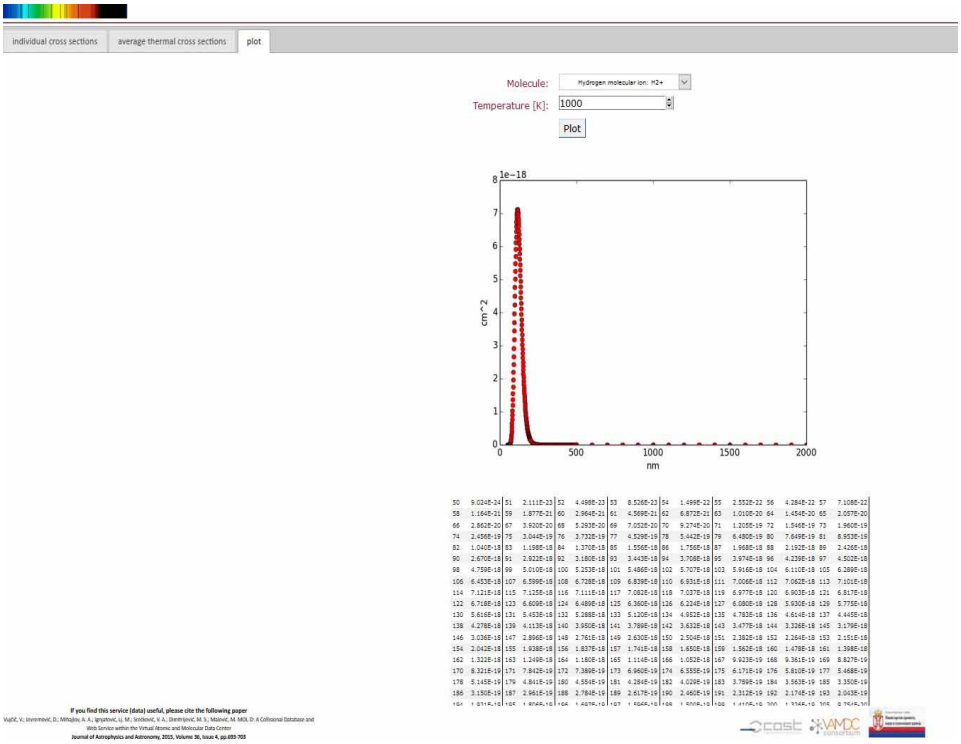


Figure 2 Example of results of a query. Case of average thermal photodissociation cross-section plot for H_2^+ molecular ion in the wide range of wavelengths from $\lambda = 50$ nm to $\lambda = 2000$ nm, and for the specified temperature.

In this paper we outline a MOL-D database that is based on the data generated and published by the authors of this text. We hope that, in time, MOL-D will be filled with measured/calculated data from sources all over the world.

2 Database technical description

The static UML model of MOL-D data structure is shown in Fig. 3. It depicts classes (entities) which describe concepts of data domain and their relationships along with cardinalities (degrees of relationships).

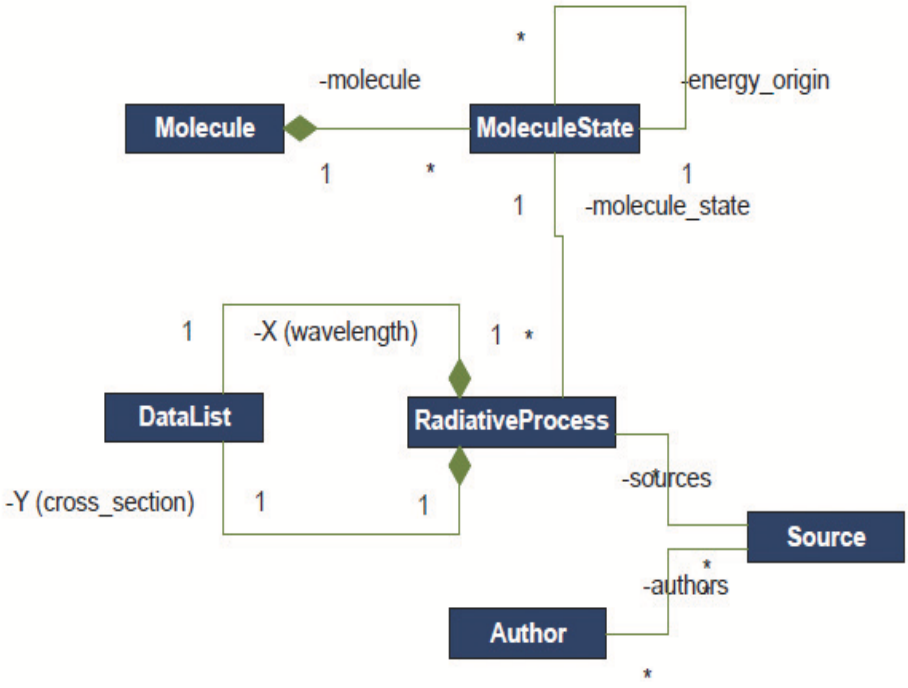


Figure 3 Schematic presentation. Static UML diagram of MOL-D application.

VAMDC e-infrastructure defines the protocols for retrieving remote data as well as the format for representing these data. The ultimate goal is interoperability of the data along various distributed nodes. The Belgrade MOL-D node can be accessed as a VAMDC standardized web service or as an AJAX-enabled web page (http://servo.aob.rs/mold). Both queries return data in XSAMS (XML Schema for Atoms, Molecules and Solids) format. The underlying application is written in Django, a Python web framework, and represents a customization and extension of VAMDC's NodeSoftware. Additional on-site utilities include:

1. data selection based on molecule name and QNJ/QNv numbers
2. average thermal cross-section calculation based on temperature for a specific molecule and wavelength
3. plotting average thermal cross-sections along available wavelengths for a given temperature.

3 Conclusions and further development

Atomic and molecular databases in today's science (physics, chemistry, astrophysics) have become essential for modeling and interpretation of data provided by observations and laboratory measurements (Srećković et al. (2014); Ignjatović et al. (2014); Marinković et al. (2015)).

Nowadays, very important resources of such data are dissipated, presented in different, non-standardized ways, available through a variety of highly specialized and often not very well documented interfaces. As a consequence the full exploitation and interconnection of all available data is limited. The free exchange of these data requires the definition of some standards and tools that help users and producers in this process. The continuation of such developments and services is crucial. This is the purpose of MOL-D database.

Our ambition is to update in the near future the current databases with new data as well as to include completely new databases into Belgrade VAMDC node.

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