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RADIATIVE AND COLLISIONAL ATOMIC/MOLECULAR DATA FOR ASTROPHYSICS

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Abstract. The main aim of this article is to introduce the data management and services of the MOLecular Dissociation (MolD) database, which consists of user friendly and productive cross-correlation service, and data sharing interface based on international standards and protocols. MolD is a web service within the Serbian virtual observatory (SerVO) and node within Virtual Atomic and Molecular Data Center (VAMDC). MolD is an atomic and molecular (A&M) database devoted to the modelling of astrophysical plasmas. Data are important for the modeling of stellar and solar atmospheres, exploring of the interstellar medium as well as for the early Universe chemistry investigation. In this contribution, we present our ongoing work and plans for the future.

1. INTRODUCTION

Nowadays, the atomic and molecular (A&M) data are especially important for simulations/calculations in the field of astrophysics modeling. For example A&M data are needed for development of atmosphere models of solar and near solar type stars and for radiative transport investigations. Modern codes for stellar atmosphere modelling, like e.g. PHOENIX (see e.g. Hauschildt & Baron 2010) require the knowledge of atomic data, so that the access to such atomic data, via online databases become very important. Recently, in Marinković et al. (2017a) it has been highlighted the importance of atomic processes for the understanding of observations in coma, the tenuous atmosphere and on the surface of 67P/Churyumov-Gerasimenko during Rosetta mission. It has been shown the need for closer interactions and joint projects between the cometary, electron communities and IT software specialists.

On the other hand, the produced data volumes in nowadays astronomical sky surveys can range from several terabytes to petabytes and will increase even faster.

In some cases such as campaigns, surveys may generate terabytes of data per day (Brunner et al. 2001). The sky with billions of stars, galaxies, quasars, and other objects is being surveyed, detected and measured with an incredible level of details. As a consequence, the status of data-oriented science, research methods, algorithms, and techniques become very important (Brescia & Longo 2013). This has led to integration of computer science, physics, statistics, astrophysics on operative processing, scientific exploitation of such large data sets and developing state-of-the-art infrastructures such as the Virtual Observatories (VO). VO is a platform for launching astronomical investigations. It provides access to huge data banks, software systems with user-friendly interfaces for data processing, analysis, visualization and etc. (Borne 2013).

In this contribution, we give an overview of the motivations, current stage, and technological principles of A&M MolD database within Virtual Observatories.

Figure 1: The home page of the VAMDC consortium, SerVO and MolD database.

2. MOLD DATABASE, SERVO AND VAMDC

MolD database is a collection of cross-sections and rate coefficients for specific collisional processes (see e.g. Vujčić et al. 2015 or Srećković et al. 2017a). It can be accessed via http://servo.aob.rs/mold/ of Serbian Virtual Observatory (SerVO) or accessed as a web service http://portal.vamdc.eu/ which is part of the Virtual Atomic and Molecular Data Center (VAMDC), (see Fig.1).

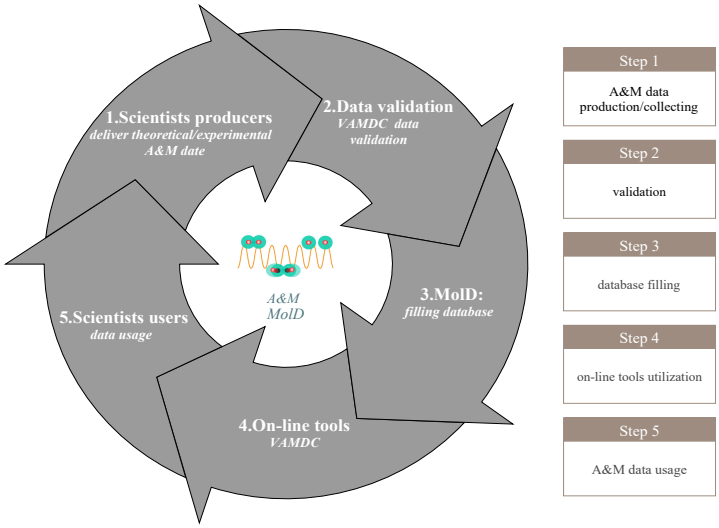

Figure 2: A&M data workflow.

The web interface offers access to data for photodissociation cross-sections of specific molecular ions (see Tab 1.) as well as the corresponding averaged thermal photodissociation cross-sections for hydrogen H_2^+ and helium He_2^+ molecular ions for the requested wavelength and temperature.

VAMDC is an international consortium which has built a well documented, secure, flexible interoperable e-science platform permitting an automated exchange of atomic and molecular data (Dubernet et al. 2016). VAMDC started as EU FP7 e-infrastructure project of developing communication between different A&M databases and providing a common portal for accessing all registered data. VAMDC e-infrastructure defines protocols for retrieving remote data as well as format for representing these data. The ultimate goal is interoperability of the data along various distributed nodes.

Project "Serbian Virtual Observatory" was funded in year 2008 (see Jevremović et al. 2009). This project was funded as technological developement project. The main goals of this project were digitization and publishing of old photo plates in Virtual Observatory, development of BelData, Stark broadening database (it became StarkB database), contribution to Darthmouth Stellar Evolution Database and collection of other Serbian data. Idea was that all these would be accessible at http://servo.aob.rs. Today, many services are currently running on the SerVO. The Belgrade nodes of VAMDC are hosted by SerVO and presently consists of two databases BEAMDB (http://servo.aob.rs/emol) (Marinković et al. 2015) and MolD (http://servo.aob.rs/mold) (Srećković et al. 2017b, Marinković et al. 2017b).

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      0.513610E-19 0.481166E-19 0.127658E-19 0.276956E-21 0.143429E-19 0.483756E-19
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Figure 3: Data set is represented in XSAMS (Extensible Markup Language (XML) Schema for Atoms, Molecules and Solids) format for He_2^+ photo-dissociation cross-sections for the individual ro-vibrational state.

2. 1. LEVEL 3 RELEASE

At the end of 2017 MolD is in the *stage 3* of development (Srećković et al. 2017a). At this moment, the database includes cross-section data for processes which involve species such as H_2^+, He_2^+, MgH^+, HeH^+, LiH^+, NaH^+ as can be seen in Tab. 1. These processes are important for exploring of the interstellar medium, the early Universe chemistry as well as the modeling of different stellar and solar atmospheres (see Srećković et al. 2014, Coppola et al. 2016). Currently we are including new cross-sections and rate coefficients data for processes which involve species such as SiH^+, Na_2^+, Li_2^+ which are important for the exploring of the geo-cosmical plasmas (Klycharev et al. 2007).

Table 1: Summary of species and states included in Belgrade MolD database as of October 2017. Additional data will successively be added.

Molecules					
Stoichiometric formula	Node	Types of reaction	States	InChI	InChIKey
H_2^+	MolD	photo-dissociation	424	1S/H2/h1H/q+1	ZZIJOQHRUPVPQC-UHFFFAOYSA-N
He_2^+	MolD	photo-dissociation	834	1S/He2/c1-2/q+1	ZAJTYDXIUNGESO-UHFFFAOYSA-N
HeH^+	MolD	photo-dissociation	150	1S/HHe/h1H/q+1	HSFAAVLNFOAYQX-UHFFFAOYSA-N
LiH^+	MolD	photo-dissociation	60	1S/Li.H/q+1	HSOYNNFNUCWPIZ-UHFFFAOYSA-N
MgH^+	MolD	photo-dissociation	600	1S/Mg.H/q+1	LMAKMUADRKEOEM-UHFFFAOYSA-N
NaH^+	MolD	photo-dissociation	50	1S/Na.H/q+1	FYDBACYJBJQTSN-UHFFFAOYSA-N

Our plans are incremental inclusion of data from our papers concerning A&M processes important for modeling different stellar atmospheres and laboratory plasmas as they become published (see Fig 2. for data workflow). Together with database updates, we intend to develop new services as well as new web interface of MolD on SerVO.

2. 2. SERVICES, DATABASE DESCRIPTION AND STRUCTURE

The principal structure of the Belgrade MOL-D database is shown schematically in Fig. 4 using UML (Unified Modelling Language) notation.

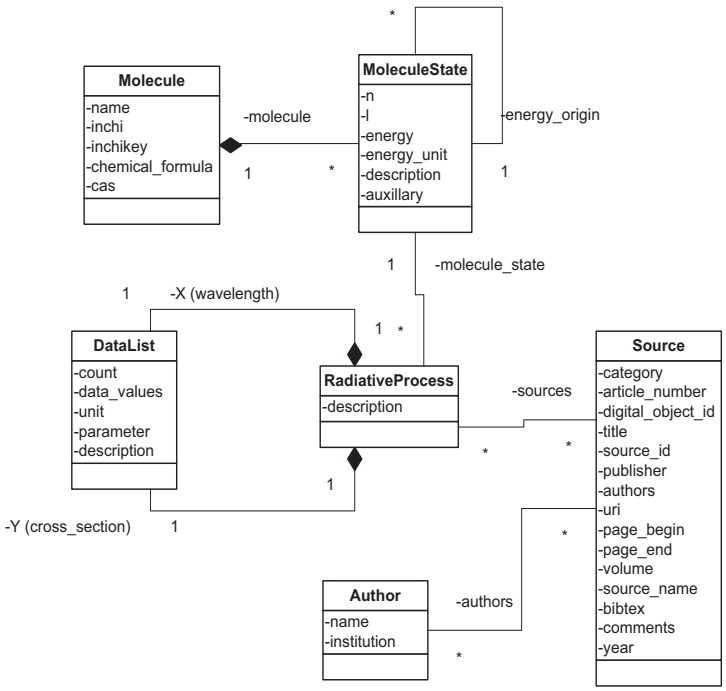

Figure 4: Static structure of the MolD database. Relationships between entities are shown by connected lines with designated cardinalities ('1' and '*' denote one and many, respectively), i.e. a molecule can have multiple states.

MolD services are compatible with VAMDC standards and act as a VAMDC "node" (for the list of nodes, see http://www.vamdc.org/structure/ databases/).

Access to the MolD data is possible in several ways:

- Via standalone applications which support VAMDC-TAP (Table Access Protocol) for data access and transformation to VAMDC-XSAMS.
- via AJAX (Asynchronous JavaScript and XML)-enabled web interface[1].

[1] http://servo.aob.rs/mold

- Via VAMDC portal[2], with query to 32 databases across the European scientific institutes.

All queries return data in XSAMS (XML Schema for Atoms, Molecules and Solids) format (see Fig. 3). The XSAMS schema provides a framework for a structured presentation of atomic, molecular, and particle-solid-interaction data in an XML file. Underlying application is written in Django, a Python web framework and represents a customization and extension of VAMDCs NodeSoftware (Marinković et al. 2017a). Additional on-site utilities include:

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

AJAX enabled queries and visualizations.

3. CONCLUDING REMARKS AND FUTURE DEVELOPMENT

A&M databases have become essential for the stellar modeling and for the interpretation of data provided by observations and laboratory measurements. As a consequence the full exploitation of such data is crucial. Therefore the further development of MolD database within SerVO and VAMDC is our main task.

The next step of development i.e. the stage four of MolD development will be the implementation of possibility to fit the tabulated data, before a major upgrade of the MolD database.

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References

Borne, K.: 2013, in *Virtual observatories, data mining and astroinformatics in Planets, Stars and Stellar Systems*, **2**, 404443, Wiley.

Brunner, R., Djorgovski, S. G., Prince, T. & Szalay, A.: 2001, in *Massive Datasets in Astronomy in Handbook of Massive Data Sets*, J. Abello et al., eds., Boston: Kluwer, 931.

Brescia, M. & Longo, G.: 2013, *Nucl Instrum Methods Phys Res A*, **720**, 92.

Coppola, C. M., Mizzi, G., Bruno, D. et al.: 2016, *Mon. Not. R. Astron. Soc*, **457**, 3732.

[2]http://portal.vamdc.eu

Dubernet, Marie-Lise, et al.: 2016, *J. Phys. B*, **49**, 7, 074003.
Hauschildt, P. H., Baron, E. A.: 2010, *Astron. Astrophys.* , **509**, A36.
Jevremović, D. et al.: 2009, *New Astron. Rev.*, **53**, 7, 222-226.
Klyucharev, A. N., Bezuglov, N. N., Matveev, A. A., Mihajlov, A. A., Ignjatović, L. M. & Dimitrijević, M. S.: 2007, *New Astron. Rev.*, **51**, 7, 547-562.
Marinković, B. P. et al.: 2015, *Nucl. Instr. Meth. Phys. Res. B*, **354**, 90-95.
Marinković, B. P., Bredehoft, J. H., Vujčić, V., Jevremović, D. & Mason, N. J.: 2017a, *Preprints*, doi:10.20944/preprints201709.0107.v2.
Marinković, B. P., Jevremović, D., Srećković, V. A., Vujčić, V., Ignjatović, Lj. M., Dimitrijević, M. S. & Mason, N. J.: 2017b, *Eur. Phys. J. D*, **71**, 6, 158.
Srećković, V. A., Mihajlov, A. A., Ignjatović, L. M. & Dimitrijević, M. S.: 2014, *Adv. Space. Res.*, **54**, 1264-1271.
Srećković, V. A., Ignjatović, Lj. M., Jevremović, D., Vujčić, V. & Dimitrijević, M. S.: 2017a, *Atoms*, **5**, 3, 31.
Srećković, V. A., Jevremović, D., Vujčić, V., Ignjatović, Lj. M., Milovanović, N., Erkapić, S. & Dimitrijević, M. S.: 2017b, *Proceedings of IAU*, **325**, 393-396.
Vujčić, V., Jevremović, D., Mihajlov, A. A., Ignjatović, Lj. M., Srećković, V. A., Dimitrijević, M. S. and Malović, M.: 2015 *J. Astrophys. Astron.*, **36**, 693703.