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Laboratory for Atomic Collision Processes

Update of the BEAMDB database presented in the topical SPIG issue

BEAMDB and MOLD—Databases at the Serbian Virtual Observatory for Collisional and Radiative Processes

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BEAMDB and MOLD—Databases at the Serbian Virtual Observatory for Collisional and Radiative Processes

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BEAMDB AND MOLD – COLLISIONAL AND RADIATIVE DATABASES AT THE SERBIAN VIRTUAL OBSERVATORY

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Serbian virtual observatory (SerVO)

Abstract: We present a progress report of two atomic and molecular databases, BEAMDB and MolD, which are web services at the Serbian virtual observatory (SerVO) and nodes within the Virtual Atomic and Molecular Data Center (VAMDC). The Belgrade Electron/Atom(Molecule) Data Base (BEAMDB) provides collisional data for electron interactions with atoms and molecules. The MolD database contains photo-dissociation cross-sections for individual rovibrational states of diatomic molecular ions and rate coefficients for the chemi-ionisation/ recombinetion processes.

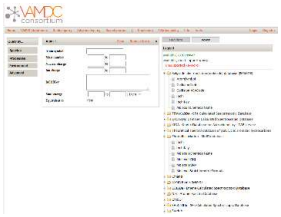
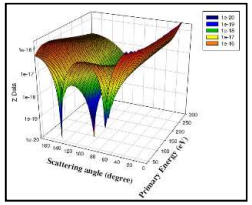


Figure 2. Virtual Atomic and Molecular Data Center (VAMDC) [5] portal query snapshot (http://www.portal.vamdc.eu).



Figures 3 Differential cross section surface

Introduction: Databases in atomic and molecular physics have become essential for develop of models and simulations of complex physical and chemical processes and for the interpretation of data provided by observations measurements e.g. in laboratory plasmas [1] and plasma chemistries and reactions in planetary atmospheres [2]. In order to solve the problem of analysis and mining of such large amounts of data, the creation of a Virtual Observatory and Virtual Data Center has been crucial [3 and refs. therein]. In this contribution we present a progress report of two atomic and molecular databases, BEAMDB and MolD, which are web services at the Serbian virtual observatory (SerVO) [4] and nodes within the Virtual Atomic and Molecular Data Center (VAMDC) [5].

This branch of science often entitled 'Data management' or 'Data mining' is undergoing rapid expansion snd development, however nowadays it is not enough for these databases to satisfy the standards of Virtual centers etc., but they have to deal with new challenges such as the input of large amounts of data i.e. Big Data. Thus we can expect major investment and activity in this field in the next decade.

MolD (http://servo.aob.rs/mold)

The MolD database has undergone three stages of development (9,10). The initial stage of development was completed at the end of 2014, when the service for all the photodissociation data for hydrogen H_2^+ and helium He_2^+ molecular ions was constructed together with the web interface and some utility programs. At the end of 2016 MolD completed the stage 2 of development when it added averaged thermal photodissociation cross-sections H_2^+ and helium He_2^+ molecular ions and new cross-section for processes which involve species such as diatomic molecular ions HX^+, where X=Mg, Li, Na. During 2017, MolD entered stage 3 of its development in which MolD includes cross-section data for processes which involve species such as MgH^+, HeH^+, LiH^+, NaH^+, H_3^+, He_2^+... The third stage also improved the design of the web interface and developed utility programs that allow online data visualization of a wide range of data. This phase of development was completed at the beginning of 2018. The database is currently in the phase of a major upgrade.

- XSAMS evolution to deal with Big Data (resources to be accessed by diverse client platforms across the network; generating and transferring data over a network without requiring human-to-human or human-to-computer; provide security and data quality; etc.)
- Python, Django updates
- Installing the Query Store on VAMDC node that should have a plan store for holding the execution plan information, and a runtime stats store for carrying on the execution statistics information.

Acknowledgements

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Figure 2. The home page of the SerVO [4].

The Belgrade Electron/ Atom(Molecule) Data Base (BEAMDB) (http://servo.aob.rs/emol)

The origins of BEAMDB database date from the early ideas of developing an Information System in Atomic Collision Physics [11] and at first it provided only cross sections for electron interactions with neutral atoms and molecules [12]. However the database has now been extended to cover electron spectra (energy-loss and threshold) and ionic species [3].

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