27th Summer School and International Symposium on the Physics of Ionized Gases

August 26-29, 2014, Belgrade, Serbia

CONTRIBUTED PAPERS

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ABSTRACTS OF INVITED LECTURES, TOPICAL INVITED LECTURES, PROGRESS REPORTS AND WORKSHOP LECTURES

Editors:
Dragana Marić
Aleksandar R. Milosavljević
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Institute of Physics, Belgrade
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BELGRADE ELECTRON/MOLECULE DATABASE COMPATIBLE WITH VAMDC PROJECT

Bratislav P. Marinković[1,3], Veljko Vujčić[2,4], Stefan Đorđević[3], Stefan Ivanović[3], Dara B. Marinković[4], Darko Jevremović[2] and Nigel J. Mason[5]

[1] *Institute of Physics, University of Belgrade, Pregrevica 118, P.O.Box 68, 11080 Belgrade, Serbia*
[2]*Astronomical Observatory, Volgina 7, P.O.Box 74 11060 Belgrade, Serbia*
[3]*School of Electrical and Computer Engineering of Applied Studies, Vojvode Stepe 283, 11000 Belgrade, Serbia*
[4]*Faculty of Organizational Sciences, University of Belgrade, Jove Ilića 154, 11000 Belgrade, Serbia*
[5]*The Open University, Department of Physical Sciences, Walton Hall, Milton Keynes, MK7 6AA, United Kingdom*

Abstract. We present the progress report on the development of Belgrade electron/molecule data base which is hosted by The Institute of Physics, University of Belgrade. The data base has been developed under the standards of VAMDC project which provides a common portal for several European data bases that maintain atomic and molecular data. Belgrade data base covers collisional data of electron interactions with atoms and molecules in the form of differential (DCS) and integral (QINT, QMT, QVIS) cross sections as well as energy loss spectra. The final goal is to become a node within the VAMDC consortium and to integrate into the wider scope of radiation damage RADAM data base.

1. INTRODUCTION

Providing, maintaining and distributing the atomic and molecular data that comes from fundamental experiments and calculations based on different levels of sophistication of theoretical insights in atomic particle world, nowadays is a quest of computerized and networked society. There are so many communities which would benefit from such collections, let us just mention several ones from astrophysical and atmospheric physics [1], plasma (with all applications to industry like plasma processing [2] or lighting [3]), biomedicine/biophysics to other fundamental and applied research disciplines like spectroscopy or surface science [4]. Among data bases that cover the field of atomic and molecular physics one can distinguish those that maintain mainly bibliographic data about the published work on atomic processes (like NIST bibliographic database on Atomic Transition Probabilities [5]) or that maintain

actual data sets or evaluated and recommended values [6]. A new era of data accessibility opened with the idea of Virtual Atomic and Molecular Data Centre VAMDC [7] that creates a common portal for different data bases in the field which use the same data protocol for exchanging and representing data in the format of so called “xsams” xml files. VAMDC now provides a scientific data e-infrastructure enabling easy access to atomic and molecular data [8].

While the vast of structural and transition data are present in the current VAMDC consortium data bases, the number of collisional data bases is rather small. Our goal is to make a functional data base that would maintain data on electron/atom and molecule interactions. These data are in the form of differential and integral cross sections for elastic scattering and electronic excitation processes. Also, energy loss spectra as relative intensities of scattered electrons versus electron energy loss at the fixed impact electron energy and scattering angle are stored in the present data base.

2. BELGRADE DATABASE

The first ideas of development of Belgrade data base came with the research interests on expert and information systems that would facilitate data analysis and maintenance of the measured sets of data in electron atom/molecule interactions. The process model was defined and further developed from the context level to several hierarchical levels each of them represented by the data flow diagram [9]. Also, the relational data model was implemented and developed up to the level of recognition of all the entities.

The present data base follows the part of VAMDC data model that concerns with the collisions. Namely, processes that are under the scope of VAMDC are divided in three classes: radiative, non-radiative and collisional. In collisions there are always a reactant and a product side. In the case of our data base one of the reactants and one of the products is electron. The target in the reactant side could be either atom or molecule but it is always in the ground level state. The product after the interaction with electron could be either in the ground state, when we are talking about elastic scattering, or in the excited state, up to now only electronic state excitations are covered but also other types of inelastic processes could be easily included.

Data model of Belgrade electron/molecule data base with the entities and attributes is shown in Figure 1. Also, the relations between entities of one-to-one and one-to-many are shown. The principle adopted for data storage is that only those data that has been previously published and so had passed the refereeing procedure, should be maintained within the data base. For such reasons a part concerning the sources of data is present in the data base with all crucial entities (authors, journal, volume, pages, doi, Bibtex). Atoms and molecules are covered by the entity Species and are characterized by their state i.e. SpeciesState entity. Data itself are organized within Data Sets which include Tabulated data of cross sections or spectroscopic data.

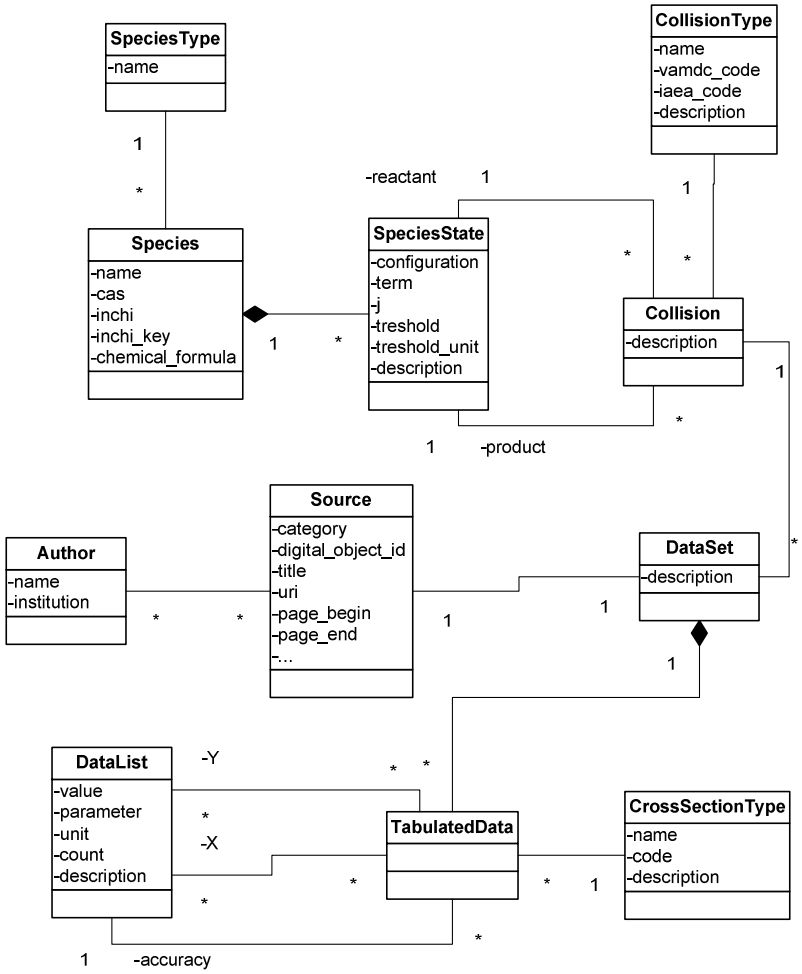

Figure 1. Data model of Belgrade electron/molecule database with entities and attributes. Relationships of one-to-one, one-to-many and many-to-many are shown.

Belgrade eMol database is generated with Django, a Python-based web framework, and runs under MySQL RDBMS. Application is hosted on a linux machine with Nginx as a web server and Gunicorn as app server. Access to data is possible via VAMDC-Tapservice protocol or via AJAX-enabled web interface (http://emol.ipb.ac.rs). Both queries return data in xsams format.

Connection and compatibility with VAMDC is established by written dictionary, TAP validator and xsams output form of data.

4. CONCLUSIONS AND PROSPECTS

The present Belgrade data base maintains electron/molecule interaction data published in the scientific literature and it contains unique set of data within VAMDC consortium. Its aim is also to facilitate the evaluation of data undertaken by the eMol board of experts that meets regularly and perform critical analysis of published electron/molecule data on specific molecular targets. Further more Belgrade data base is included in the wider scope of RADAM data base which covers specific needs of radiation community. RADAM data base has five distinctive sets of areas that cover complex processes met in radiation damage i.e. photon, ion, electron/positron interactions, multiscale processes and biological effects [10].

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