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Development of collisional data base for elementary processes of electron scattering by atoms and molecules

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ABSTRACT

We present a progress report on the development of the Belgrade electron/molecule data base which is hosted by The Institute of Physics, University of Belgrade and The Astronomical Observatory Belgrade. The data base has been developed under the standards of Virtual Atomic Molecular Data Centre (VAMDC) project which provides a common portal for several European data bases that maintain atomic and molecular data. The Belgrade data base (BEAMDB) covers collisional data of electron interactions with atoms and molecules in the form of differential (DCS) and integrated cross sections as well as energy loss spectra. The final goal of BEAMDB becoming both a node within the VAMDC consortium and within the radiation damage RADAM data base has been achieved.

1. Introduction

Curating, maintaining and distributing the large amounts of atomic and molecular (A&M) data that is produced from fundamental experiments and calculations is now widely recognised to be a necessity for the modern research community. There are many disparate communities which would benefit from such data collections including those engaged in astrophysical and atmospheric physics [1], plasma science and technology (with its applications to the plasma processing [2] or lighting [3] industries), biomedicine/biophysics and to other fundamental and applied research disciplines such as spectroscopy or surface science [4].

Such communities expect to be able to search for A&M data through a computerised and networked web-based infrastructure, e.g., a newly formed EU consortium (developed through a COST Action MP1002) is creating the RADAM (RAdiation DAMage) database [5] in order to provide A&M data to the radiation chemistry community. The idea of the RADAM database is to provide access to relevant data which spans from elementary processes through to multi-scale and biological effect processes such that those developing models and radiotherapy tools can have access to current state of the art data. The importance of such data is highlighted by its use in the development of models of particle therapy that start from track structure and end by predicting cellular damage; such models are the basis of treatment planning [6]. In order to determine such track structures and to model the role of low energy electrons and positrons in biologically relevant media it is necessary to have a full set of cross sections that govern the elementary interactions along the track [7]. In addition, there is a necessity for predicting radiation induced DNA damage due to multi-scale processes or thermo-mechanical effects caused by the passage of charged particles such as heavy ions that are propagating through the tissue [8]. The present Belgrade data base (BEAMDB) is addressing a part of these needs being centred on electron collisions by molecular species and more specifically on biomolecules or molecules of biological relevance. Thus the newly created Belgrade database is oriented towards those researchers searching for state of the art collisional data.

Current data bases that cover the field of atomic and molecular physics can be distinguished between those that maintain mainly bibliographic data about the published work on atomic processes

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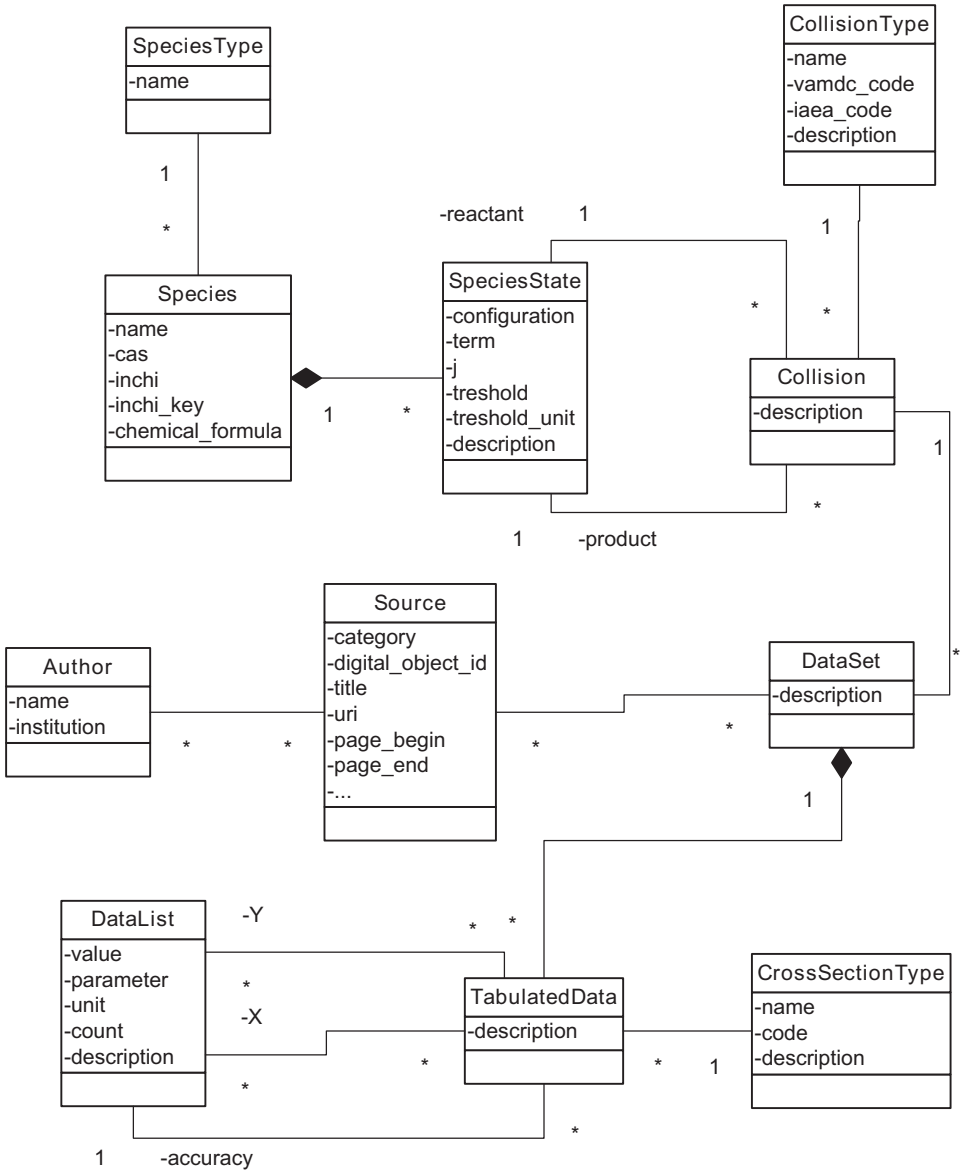

Fig. 1. The data model of BEAMDB, the Belgrade electron/molecule database, with entities and attributes. The relationships of one-to-one, one-to-many and many-to-many are shown.

(such as NIST bibliographic database on Atomic Transition Probabilities [9]) and those that maintain actual data sets of evaluated and recommended values [10]. A new era of data accessibility opened with the idea of the Virtual Atomic and Molecular Data Centre (VAMDC) [11] 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 the called "xsams" xml files (XML Schema for Atomics & Molecular Spectroscopy [12]). VAMDC now provides a scientific data e-infrastructure enabling easy access to atomic and molecular data [13].

While there is a vast amount of structural and transition data in the current VAMDC data bases, the number of collisional data bases is currently rather small. Our goal is to make a functional data base that will 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. In addition 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 since these may be important for direct comparison with theory and useful in determining 'total' energy transfer into a medium. The aim of BEAMDB was to create a specialised node within VAMDC consortium and RADAM database and this goal has been achieved.

2. The Belgrade database (BEAMDB)

The first ideas for developing a Belgrade data base came through a combination of the research interests of those involved in the development of expert and information systems and those producing A&M data in Belgrade. It was realised that the establishment of such an A&M database would both facilitate data analysis and ensure the long term curation of 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 [14]. This relational data model was then developed and ultimately implemented.

The present data base follows the VAMDC data model which defines A&M processes in domain of three classes: radiative,

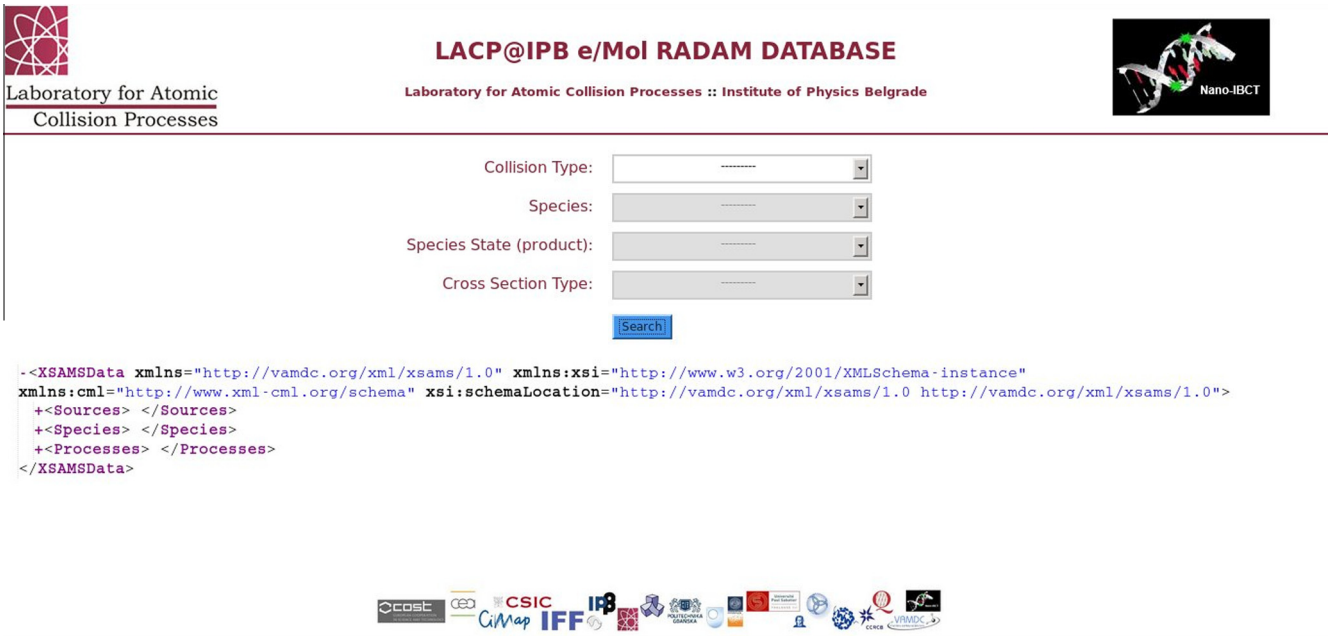

Fig. 2. A screen shot of the BEAMDB database at Belgrade server station.

non-radiative and collisional. BEAMDB follows the protocols defined for presentation of data for collisional processes. In collisions there are always a reactant and a product. In the case of BEAMDB one of the reactants and one of the products is an electron. The target in the reactant side could be either an atom or a molecule but it is always assumed to be in the ground level state. For molecules it is assumed that the target is in an ensemble of rotationally excited states that corresponds to the molecule being in thermal equilibrium at the temperature that is evidenced under the entity of 'environment temperature'. The product after the interaction with an electron can be either in the ground state (elastic scattering) or in an excited state, at present only electronic state excitations are included but also other types of inelastic processes (e.g., vibrational excitation or ionisation) can easily be added as database develops.

The data model of the Belgrade electron/molecule data base (BEAMDB) is shown in Fig. 1 in which the relationships between entities of one-to-one and one-to-many are shown. The principle adopted for data storage is that only those data that have been previously published and so have been subject to a formal refereeing procedure, should be included. This principle follows from discussion amongst A&M community and is a consensus of the views of the data providers, who measure and calculate these A&M data. For such reasons the sources of the data are therefore included in the data base with all their crucial entities (authors, journal, volume, pages, doi, Bibtex). Atoms and molecules are covered by the entity 'Species' and are characterised by their state i.e., 'SpeciesState' entity. The data itself are organised within 'DataSets' which include 'TabulatedData' of cross sections or spectroscopic data.

This database is a natural extension of VAMDC software which provides infrastructure for implementing atomic and molecular data as a web service. VAMDC software is implemented in Django, a Python-based web framework which offers forward and reverse database generation, automatised object-relational mapping, loose coupling of software modules, automatic administrative interface, extensible templating system and other advanced features. The relational database of choice is MySQL, the web server is Nginx and Python application server is Gunicorn, hosted on a Linux machine.

VAMDC software requires customisation in terms of writing data models, mapping fields in the database to keywords in VAMDC dictionaries and adapting query functions to connect the xml generator with the database. Dictionaries are lists of names which identify certain type of data, key-value pairs that indicate which attributes could be used in filtering the data on user's end ("restrictables") and what kind of data can be returned from the database end ("returnables").

In cases where the generator does not support desired xml output out-of-the-box, it can be overridden. For the BEAMDB node, we had to provide 3-dimensional data structure represented with two *X* axes and one *Y* axis. Such data structure is supported in xsams schema but not implemented in VAMDC generator, which expects single *X* and *Y* axes. For such specific needs, VAMDC software allows writing a function named *XML*() on the specific entity in the model that needs alteration. In this way, a generator is bypassed and desired custom output can be controlled by the node owner which adds flexibility and removes potential bottleneck in software development.

Access to the data is possible via Table Access Protocol (TAP), a Virtual Observatory standard of a web service or via AJAX-enabled web interface (http://servo.aob.rs/emol/). Relying on JQuery (a javascript framework) libraries, the web interface allows asynchronous access to database which enhances the dynamic nature of the application. Both queries return data in xsams format.

3. Data sets

A screen shot of BEAMDB Database at Belgrade server station is shown in Fig. 2. Since the intention of the authors was to easily identify what kind of electron collisional data could be retrieved, the front page of BEAMDB is created in such manner that it consists of simple and small number (four) combo-boxes. Within the field entity entitled 'Collision Type' one can choose between 'Elastic' and 'Electronic Excitation' or 'Energy-loss Spectrum' and 'Total Scattering'. One also can select under the entity 'Species' all available atomic and molecular targets that are currently maintained in the data base. After selecting one of the targets, automatically the

Table 1
Data set represented in 'xsams' format for electron excitation of silver atom [15].

```
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                      </SourceRef>
                      <ProcessClass>
                        <UserDefinition>Electronic Excitation</UserDefinition>
                        <Code>exci</Code>
                        <IAEACode>EEX</IAEACode>
                      </ProcessClass>
                      <Reactant>
                        <SpeciesRef>XIPBemol-14</SpeciesRef>
                        <StateRef>SIPBemol-43</StateRef>
                      </Reactant>
                      <Reactant>
                        <SpeciesRef>XIPBemol-XElectron</SpeciesRef>
                      </Reactant>
                      <Product><SpeciesRef>XIPBemol-14</SpeciesRef>
                         <StateRef>SIPBemol-44</StateRef>
                      </Product>

                      <DataSets>
                      <DataSet dataDescription=''IPB(2012) Ag_2P DCS small angels''>
                      <TabulatedData>
                        <SourceRef>BIPBemol-NIMB279_53_2012_1-s2.0-S0168583X11010263-main_SDTosic_etal
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20 20 20 40 40 40 40 40 40 40 60 60 60 60 60 60 60 60 60 80 80 80 80 80 80 80 80 80 100 100 100 100 100 100 100</DataList></X>
                        <X units=''deg'' parameter=''angle''><DataList count=''57''>3 4 5 6 7 8 9 10 11 12 13 14 15 5 6 7 8 9 10 11 12 13 14 5 6 7
8 9 10 11 12 4 5 6 7 8 9 10 11 12 4 5 6 7 8 9 10 11 12 3 4 5 6 7 8 9 10</DataList></X>
                        <Y units=''m2/sr'' parameter=''DCS''>
                           <DataList count=''57''>52.9e-20 49.7e-20 46.5e-20 43.4e-20 40.3e-20 37.2e-20 34e-20 30.9e-20 28e-20 25.1e-20
22.6e-20 20.4e-20 18.7e-20 67.4e-20 57.9e-20 48.9e-20 40.7e-20 33.5e-20 27.4e-20 22.4e-20 18.4e-20 15.3e-20 13e-20 62e-20
46.5e-20 34.4e-20 25.4e-20 18.9e-20 14.3e-20 11.1e-20 8.9e-20 85e-20 55.7e-20 36.2e-20 23.6e-20 15.5e-20 10.4e-20 7.3e-20
5.3e-20 4.01e-20 64e-20 40e-20 25.6e-20 16.6e-20 10.9e-20 7.2e-20 4.8e-20 3.28e-20 2.34e-20 112e-20 57e-20 30.9e-20 18.1e-20
11.2e-20 7e-20 4.2e-20 1.95e-20</DataList>
                           <Accuracy relative=''false'' type=''statistical''>
                           <ErrorList count=''57''>6.6e-20 5.7e-20 5.1e-20 4.7e-20 4.3e-20 3.9e-20 3.5e-20 3.2e-20 2.9e-20 2.6e-20 2.3e-20
2.1e-20 1.9e-20 7.4e-20 6.2e-20 5.2e-20 4.2e-20 3.5e-20 2.8e-20 2.3e-20 1.9e-20 1.6e-20 1.4e-20 11e-20 7.8e-20 5.7e-20 4.3e-20
3.2e-20 2.5e-20 2e-20 1.6e-20 19e-20 12.3e-20 7.8e-20 5e-20 3.3e-20 2.2e-20 1.5e-20 1.1e-20 0.86e-20 18e-20 11e-20 6.7e-20
4.2e-20 2.8e-20 1.8e-20 1.2e-20 0.84e-20 0.6e-20 38e-20 18e-20 9.6e-20 5.5e-20 3.4e-20 2.1e-20 1.3e-20 0.59e-20</ErrorList>
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                      </DataSet>
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```

choice of 'Species State' can be selected. Finally, one may select 'Cross Section Type' that is of interest for a specific species and states and this includes differential (DCS) or other integrated cross sections (integral, Q_{INT}, momentum transfer, Q_{MT} and viscosity cross sections, Q_{VIS}).

The BEAMDB provides data in the 'xsams' xml format only. Providing the datasets in some other reader friendly formats is achieved through data portals, both VAMDC and RADAM, where the current data base is registered as a node. Both portals use specific data tools that converts 'xsams' data in either tabular form or graphical representation. One of the VAMDC consortium goals is to improve accessibility and presentation of data via standardised graphic interface. BEAMDB implement these tools as soon as they become available.

All data maintained within the BEAMDB data base are arranged in the form of strings, e.g., for the DCS sets of data there are two strings for the X axes ($X1$ – scattering angle and $X2$ – impact energy) and two strings for Y axes (values of DCS and an accompanied string with uncertainties). Examples of such data sets are those published for absolute differential cross sections for electron excitation of silver at small scattering angles [15] (see Table 1) or for elastic electron scattering from the formamide molecule [16].

An example of the visualisation of a data set that represents the differential cross section surface versus impact electron energy and scattering angle for elastic scattering from formamide [16] is shown in Fig. 3.

For integrated cross sections (Q_{INT}, Q_{MT}, Q_{VIS}) the data requires only one X axis (Impact Energy) while the Y axes displays both values and uncertainties. When Energy Loss spectra are presented then the X axis represents energy loss and Y axis represent counts that are obtained in the specific scan. An example of an energy loss spectrum is shown in Fig. 4 for 80 eV electrons scattered at the angle of 2° from the alanine molecule CH_3-CH(NH_2)-COOH [17,18].

4. Conclusions and prospects

The present Belgrade BEAMDB data base curates and displays electron/(atom)molecule interaction data published in the scien-

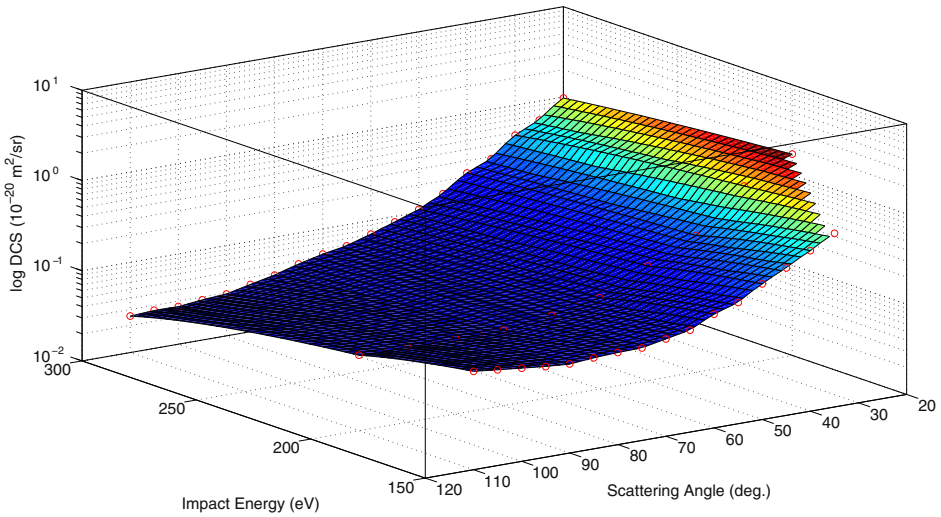

Fig. 3. Differential cross section (DCS) surface versus impact electron energy and scattering angle for elastic scattering from formamide. The DCS is in units of 10^{-20} m^2/srad, the impact energy is expressed in eV and the scattering angle in degrees. The data points are represented by open circles while the connecting lines are interpolated values.

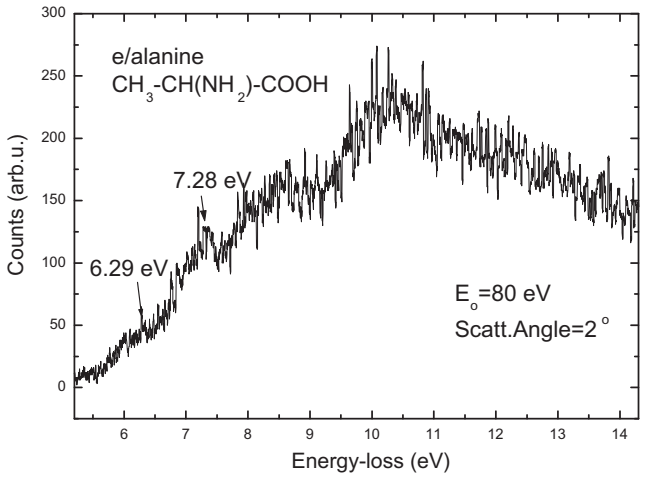

Fig. 4. An energy loss spectrum of 80 eV electrons scattered at the angle of 2° from alanine, CH_3-CH(NH_2)-COOH, molecule.

tific literature and contains a unique set of data within the VAMDC consortium. It is therefore contributing to the e-infrastructure that has been created the VAMDC project. The aim of this database is to be accessible to, and be used by, the wider scientific community and its accessibility through VAMDC will allow this.

Another aim of the BEAMDB database is to facilitate the evaluation of data undertaken by the Electron-Molecule Data Board (eMol-board), a team of experts that meets regularly and perform critical analysis of published electron/molecule data on specific molecular targets. The combination of data sets within this database and other databases that contain collisional data (e.g., [19]) with data reviews (e.g., [2,20]) will facilitate the task of eMol-board to provide recommended cross-section values and consider future data needs [13].

The BEAMDB is also included in the wider scope of RADAM data base which covers the specific needs of radiation community. The RADAM data base [21] has five distinctive areas that cover complex processes met in radiation damage i.e., photon, ion, electron/positron interactions, multi-scale processes and biological effects [5]. In future, the present electron interaction database may be used to make a clone database that would maintain the same structure but would curate positron interaction data sets.

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