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VIRTUAL ATOMIC AND MOLECULAR DATA CENTER (VAMDC) AND STARK-B DATABASE

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Abstract: Virtual Atomic and Molecular Data Center (VAMDC) is an European FP7 project with aims to build a flexible and interoperable e-science environment based interface to the existing Atomic and Molecular data. The VAMDC will be built upon the expertise of existing Atomic and Molecular databases, data producers and service providers with the specific aim of creating an infrastructure that is easily tuned to the requirements of a wide variety of users in academic, governmental, industrial or public communities. In VAMDC will enter also STARK-B database, containing Stark broadening parameters for a large number of lines, obtained by the semiclassical perturbation method during more than 30 years of collaboration of authors of this work (MSD and SSB) and their co-workers. In this contribution we will review the VAMDC project, STARK-B database and discuss the benefits of both for the corresponding data users.

1. VIRTUAL OBSERVATORIES AND SERBIAN VIRTUAL OBSERVATORY

For various applications in astrophysics, atmospheric physics, fusion, environmental sciences, combustion chemistry, and in industrial applications from plasmas and lasers to lighting, a reliable, critically selected set of atomic and

molecular data is needed. However, the available data present in literature and databases are presented in different, non-standardized ways, so that their adequate exploitation is often difficult.

The need for a large amount of atomic and molecular data is in particular stimulated by the development of satellite astronomy, providing a huge amount of high quality astronomical spectra. This development produced an information avalanche and leaded to the creation of huge data collections as e. g. IUE and HST archive, or Sloan Digital Sky Survey SDSS, containing spectra of ~ 230 million objects.

In order to solve the problem of analysis and mining of such amount of data, the idea of Virtual Observatory was formulated at the end of 2000. It was realized as the FP5 project Astrophysical Virtual Observatory – AVO, the origin of European Virtual Observatory - EURO-VO (http://www.euro-vo.org), who started in 2001.

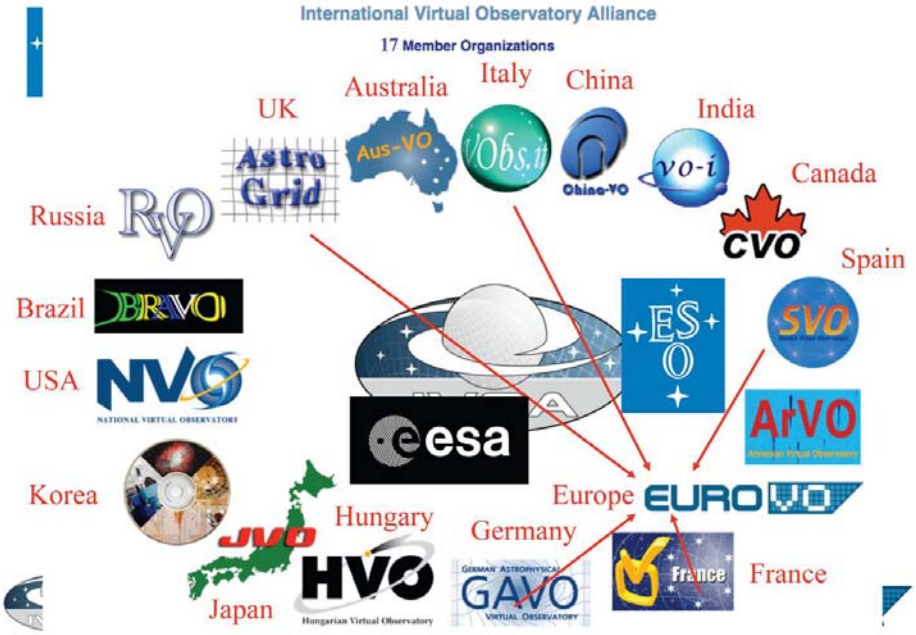


Fig. 1. International Virtual Observatory Alliance.

In order to coordinate the international collaboration in this field and develop and adopt the needed corresponding standards, International Virtual Observatory Alliance (IVOA, http://www.ivoa. net) was formed in June of 2002.

Serbia entered in such activities by creating SerVO - Serbian virtual observatory (http://servo.aob.rs/~darko), funded through the project TR13022 by Ministry of Science and Technological Development of Republic of Serbia (Jevremović et al., 2009, 2012). After establishing SerVO, our objective is to join

IVOA, if possibly on the interoperability meeting in Nara, Japan, 7-11 of December 2010, and the EuroVO. Our plan is also to establish SerVO data Center for digitizing, archiving and publishing in VO format photo-plates (Tsvetkova et al., 2009) and other data produced at Belgrade Astronomical Observatory and to develop tools for visualization of the corresponding data. Two of us (MSD-SSB) work on the development of STARK-B - Stark broadening data base containing, as the first step, our results for Stark broadening parameter determination obtained within the semiclassical perturbation approach, in VAMDC and VO compatible format. A mirror site of this database will be a part of SerVO. Also, within the frame of SerVO will be a mirror site for DSED (Darthmouth Stellar Evolution Database, Dotter et al., 2007, 2008) in the context of VO.

2. VAMDC – VIRTUAL ATOMIC AND MOLECULAR DATA CENTER

The need for an efficacious and adequate search and mining for available atomic and molecular data, highly fragmented and provided in different non standardized formats, which was an obstacle for their suitable use, leaded to the VAMDC idea. In order to make the search of atomic and molecular data efficacious, we need the search engines that must look "everywhere" for the needed A&M dat and to create an accessible and interoperable e-infrastructure.

This is in fact the main objective of Virtual Atomic and Molecular Data Center (VAMDC – Dubernet et al., 2010), a FP7 funded project which started on July 1st 2009 with budget of 2.9 MEuros over 42 months. The above mentioned objectives will be achieved by upgrading and integrating European (and wider) A&M database services and catering for the needs of variety of data users in science, research and development, and industry. In order to establish a better communication between data producers, data users and databases developers, one of the important VAMDC aims is also the creation of a forum for discussion of the corresponding subjects, as well as to organize the training of potential users in European Research Area and wider.

The VAMDC can be understood as a publisher infrastructure (Fig. 2), which will deploy yellow pages (registries) in order to find resources, design user applications, build data access layers above databases to provide unified outputs from these databases, and connect its infrastructure to the grid.

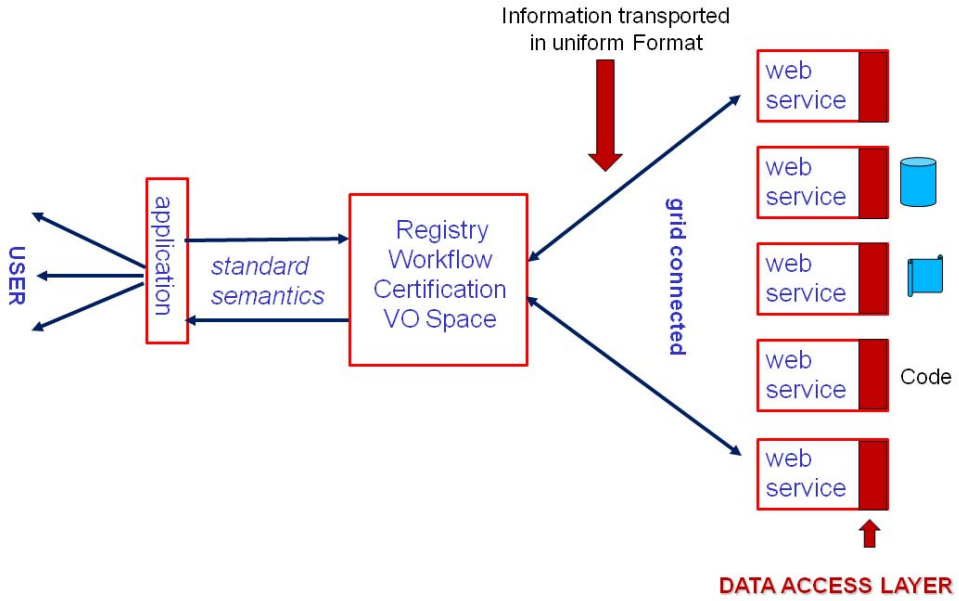
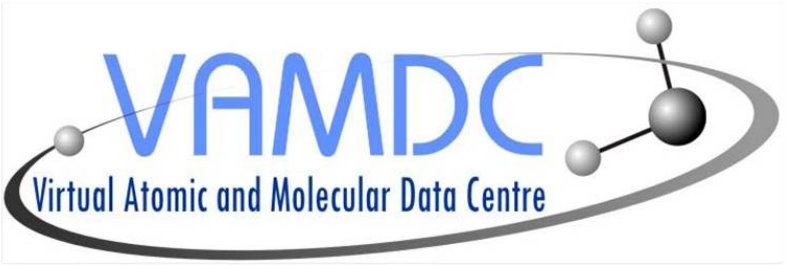


Fig. 2. Schematic diagram of the VAMDC infrastructure; note that it is a distributed system.



VAMDC

Virtual Atomic and Molecular Data Centre

Fig. 3. VAMDC logo.

Project leader is Marie-Lise Dubernet from Observatoire de Paris and core consortium is made of 15 institutions with 24 scientific groups from France, Serbia, Russia, England, Austria, Italia, Germany, Sweden and Venezuela.

Partners in the Consortium of the Project are: 1) The coordinator, Centre National de Recherche Scientifique - CNRS (Université Pierre et Marie Curie, Paris; Observatoire de Paris; Université de Reims; Université Joseph Fourier de Grenoble, Université de Bordeaux 1: Université de Bourgogne, Dijon; Université Toulouse 3); 2) The Chancellor, Masters and Scholars of the University of Cambridge – CMSUC; 3) University College London – UCL; 4) Open University – OU (Milton Keynes, England); 5) Universitaet Wien - UNIVIE; 6) Uppsala Universitet – UU; 7) Universitaet zu Koeln – KOLN; 8) Istituto Nazionale di Astrofisica – INAF (Catania, Cagliari); 9) Queen's University Belfast – QUB; 10) Astronomska Opservatorija - AOB (Belgrade, Serbia); 11) Institute of Spectroscopy RAS – ISRAN (Troitsk, Russia); 12) Russian Federal Nuclear Center - All-Russian Institute of Technical Physics - RFNC-VNIITF (Snezhinsk, Chelyabinsk Region, Russia); 13) Institute of Atmospheric Optics - IAO (Tomsk, Russia); 14) Corporacion Parque tecnologico de Merida – IVIC (Merida, Venezuela); 15) Institute for Astronomy RAS - INASAN (Moscow, Russia).

External VAMDC partner is also NIST – National Institute for Standards and Technology in Washington.

The VAMDC facilities are dedicated to the various users in Astronomy, Plasma science, Atmospheric Science Radiation science and Fusion community as well as Industries using technological plasmas and Lightning industry

The basis of VAMDC e-infrastructure are the included databases upon which are actually:

VALD database (Kupka et al., 1999) of atomic data for analysis of radiation from astrophysical objects (http://vald.astro.univie.ac.at/).

CHIANTI (Dere et al., 2009), an atomic database for the analysis of optically thin collisionally ionised astrophysical plasmas. (http://sohowww.nascom.nasa.gov/solarsoft, http://www.damtp.cam.ac.uk/ user/astro/chianti/)

EMol Database, at the Open University in Milton Keynes (Mason, 2007), containing critically evaluated measured and calculated cross sections for electron interactions with molecular systems, and a suite of semi-empirical theoretical methods for the corresponding evaluation when there are currently no experimental data.

CDMS - Cologne Database for Molecular Spectroscopy (http://www.ph1.uni-koeln. de/ vorhersagen/) provides recommendations for spectroscopic transition frequencies and intensities for atoms and molecules of astronomical interest and for studying the Earth atmosphere. It is cross correlated with its US counterpart, the JPL Jet Propulsion Laboratory Submillimeter Catalogue (http://spec.jpl.nasa.gov/) (Müller et al., 2005).

BASECOL database (Dubernet et al., 2004) (http://basecol.obspm.fr) contains excitation rate coefficients for ro-vibrational excitation of molecules by electrons, He and H_2.

GhoSST (Grenoble astrophysics and planetology Solid Spectroscopy and Thermodynamics, http://ghosst.obs.ujf-grenoble.fr) database service, offers spectroscopic laboratory data on molecular and atomic solids and liquids from the near UV to the far-infrared.

UMIST - University of Manchester Institute of Science and Technology (UMIST) database for astrochemistry (Millar et al., 1991; Woodall et al., 2007) (http://www.udfa.net/), provides reaction rate data and related software for chemical kinetic modelling of astronomical regions.

KIDA - KInetic Database for Astrochemistry will contain data on chemical reactions used in the modelling of the chemistry in the interstellar medium and in planetary atmospheres (http://kida.obs.u-bordeaux1.fr).

PAHs (Polycyclic Aromatic Hydrocarbon) and carbon clusters spectral database (http://astrochemisty.ca.astro.it/database/) in Cagliari, developed in collaboration of CESR (Centre d'Etude Spatiale des Rayonnements) with CNRS (Malloci et al., 2007).

LASP (Laboratorio di Astrofisica Sperimentale) Database (http://web.ct.astro.it/weblab/ dbindex.html#dbindex) at the INAF (Istituto Nazionale di Astrofisica) - Catania Astrophysical Observatory, contains (i) infrared (IR) spectra of molecules in the solid phase (ii) IR optical constants of molecules in the solid phase and after processing with energetic ions; (iii) band strengths of the IR absorption bands ; and (iv) density values of frozen samples.

Spectr-W^3 (Faenov et al., 2002) atomic database (http://spectr-w3.snz.ru), created in collaboration between the Russian Federal Nuclear Centre All-Russian Institute of Technical Physics (RFNC VNIITF - Snezhinsk, Chelyabinsk Region, Russia) and the Institute for High Energy Densities of the Joint Institute for High Temperatures of the Russian Academy of Sciences (IHED JIHT RAS - Moscow). It lists experimental, calculated, and compiled data on ionization potentials, energy levels, wavelengths, radiation transition probabilities and oscillator strengths, and also parameters for analytic approximations for electron-collision cross-sections and rates for atoms and ions.

The V.E. Zuev Institute of Atmospheric Optics (IAO) in Tomsk (http://www.iao.ru/) hosts the following databases:

CDSD - The Carbon Dioxide Spectroscopic Databank (Perevalov and Tashkun, 2008) (http://cdsd.iao.ru and ftp://ftp.iao.ru/pub/CDSD-2008).

S&MPO - Spectroscopy & Molecular Properties of Ozone) relational database (Rothman et al., 2009) (http://ozone. iao.ru and http://ozone.univ-reims.fr/), developed in collaboration with the University of Reims.

"Spectroscopy of Atmospheric Gases" (http://spectra.iao.ru), containing HITRAN (Rothman et al., 2009) , GEISA (Jacquinet-Husson et al., 2008) and HITEMP (Rothman et al., 2010) databases.

W@DIS – Water Internet @ccessible Distributed Information System (http://wadis.saga.iao.ru) lists experimental water-vapour spectroscopy data from the literature and calculated line lists.

Databases under the management of Corporacion Parque tecnologico de Merida – IVIC (Instituto Venezoelano de Investigaciones Scientificas) and CeCalCULA (Centro Nacional de Cálculo Científico de la Universidad de Los Andes).

TIPTOPbase (Cunto et al., 1993) located at the Centre de Données astronomiques de Strasbourg, France (http://cdsweb.u-strasbg.fr/topbase/home.html), contains:

TOPbase: Atomic data computed in the Opacity Project, namely LS-coupling energy levels, gf-values and photo ionization cross sections for light elements ($Z \leq 26$) of astrophysical interest.

TIPbase: Intermediate-coupling energy levels, A-values and electron impact excitation cross sections and rates for astrophysical applications ($Z \leq 28$), computed by the IRON Project.

OPserver (Mendoza et al., 2007), located at the Ohio Supercomputer Center, USA, (http://opacities.osc.edu/), a remote, interactive server for the computation of mean opacities for stellar modelling using the monochromatic opacities computed by the Opacity Project.

Within VAMDC e-infrastructure are also:

XSTAR database (Bautista and Kallman, 2001), used by the XSTAR code (http://heasarc.gsfc.nasa.gov/ docs/software/ xstar/xstar.html) for modelling photo ionised plasmas.

HITRAN - HIgh-resolution TRANsmission molecular absorption database (Rothman et al., 2008) (http://www.cfa. harvard.edu/hitran/).

GEISA - Gestion et Etude des Informations Spectroscopiques Atmosphériques database (Jacquinet-Husson et al., 2008)
(http://ara.lmd.polytechnique.fr/index.php?page=geisa-2 or
http://ether.ipsl.jussieu. fr/etherTypo/ ?id=950) is a computer accessible database system, designed to facilitate accurate and fast forward, calculations of atmospheric radiative transfer.

HITEMP, a high temperature extension to HITRAN (Rothman et al., 2010) containing data for water, CO_2, CO, NO and OH.

3. STARK-B DATABASE

The STARK-B database (http://stark-b.obspm.fr) (Sahal-Bréchot, 2010), is created in collaboration between Laboratoire d'Etude du Rayonnement et de la matière en Astrophysique of the Observatoire de Paris-Meudon and the Astronomical Observatory of Belgrade, and it enters also in the VAMDC e-infrastructure. It contains the theoretical widths and shifts of isolated lines of atoms and ions due to collisions with charged perturbers, obtained within the impact approximation (Stark broadening). At this stage it contains results obtained

using the semiclassical perturbation approach (Sahal-Bréchot, 1969ab, for optimization of computer code and updates see e.g. Sahal-Bréchot, 2010; Dimitrijević, 1996).

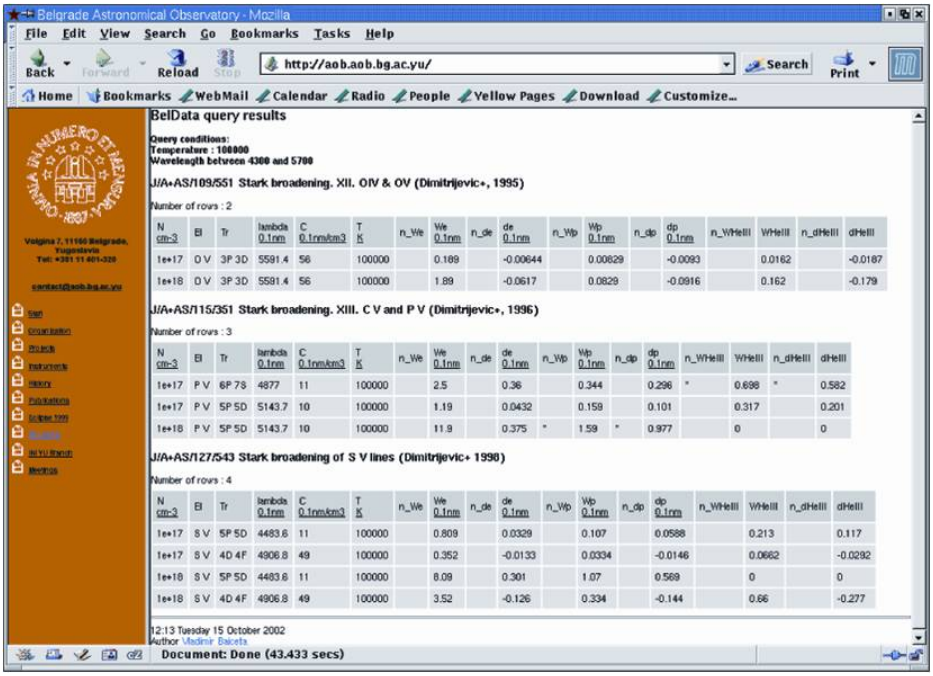


Fig. 4. Output from the old BELDATA database.

STARK-B may be useful for modelling and spectroscopic diagnostics of stellar atmospheres and envelopes, as well as for laboratory plasmas, analysis of laser produced plasma and laser equipment design and development, fusion plasma and technological plasmas. The database is currently developed in Paris, and a mirror site is planned in Belgrade, within the frame of SerVO. It is described in detail in Sahal-Bréchot (2010).

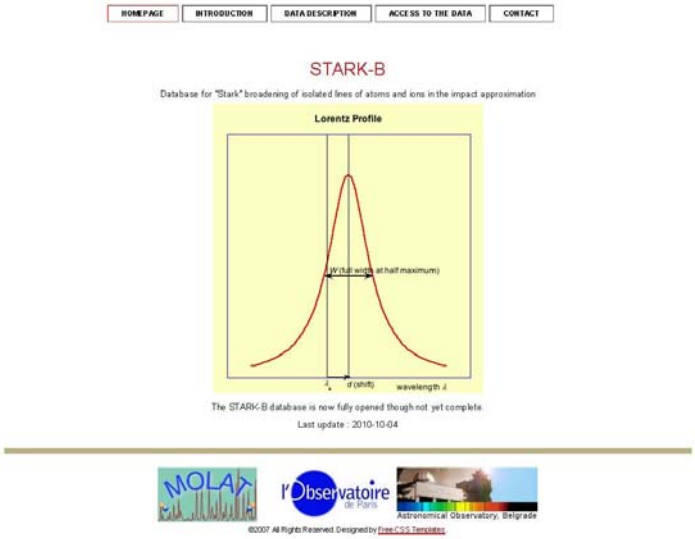


Fig. 5. The homepage of STARK-B.

On Belgrade Astronomical Observatory was created previously, as a precursor of STARK-B and SerVO, BELDATA database with Stark broadening parameters as its main content. A history of BELDATA can be traced in Popović et al. (1999ab), Milovanović et al. (2000ab), Dimitrijević et al. (2003) and, Dimitrijević and Popović (2006).

The participants of AOB (Astronomical Observatory – Belgrade) VAMDC Node are: Milan S. Dimitrijević, Luka Č. Popović, Andjelka Kovačević, Darko Jevremović, Zoran Simić, Edi Bon and Nenad Milovanović.

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Our ambition is that in the future, Group for Astrophysical spectroscopy and SerVO become a VAMDC regional center, in particular since it is expected that VAMDC, as an example of the global collaborations and innovations in e-science, will become one of major European cyber-infrastructures with a world wide impact.

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