European Virtual Atomic Data Centre - VAMDC

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Abstract
The Virtual Atomic and Molecular Data Centre (http://www.vamdc.eu, VAMDC) is an European Union funded FP7 project aiming to build a secure, documented, flexible and interoperable e-science environment-based interface to existing atomic and molecular data. It will also provide a forum for training potential users and dissemination of expertise worldwide. This review describes the VAMDC project and its objectives.

1. Introduction
Reliable atomic and molecular data are of critical importance for different applications in astrophysics, atmospheric physics, fusion, environmental sciences, combustion chemistry, and in industrial applications from plasmas and lasers to lighting. Resources of such data are highly fragmented, presented in different, non-standardized ways, available through a variety of highly specialized and often poorly documented interfaces, so that their full exploitation is limited, which make difficulties in many research fields like for example the understanding the chemistry of Solar system and of the wider universe, the study of the terrestrial atmosphere, the development of the fusion research, lasers etc.

The development of powerful computers stimulates the development of atomic data on a large scale. The modelling of stellar atmospheres and of the stellar interiors needs extensive sets of atomic data, including collisional broadening. For example, the PHOENIX computer code [1] developed for stellar modelling includes a database containing more than $10^7$ atomic, ionic and molecular spectral lines.

The development of satellite astronomy, providing a huge amount of high quality astronomical spectra produced an information avalanche and led to the creation of huge data collections as e. g. IUE and HST archive. For example Sloan Digital Sky Survey SDSS, contains spectra of ~ 230 million objects. The problem is how to analyse such amount of data?

The idea of Virtual Observatory was formulated at the end of 2000, and from 2001 the FP5 project Astrophysical Virtual Observatory – AVO was the basis for creation of European Virtual Observatory - EURO-VO (http://www.euro-vo.org).
Virtual observatories today combine research in different areas of astrophysics (some of which are fairly new): multi-wavelength astrophysics, archival research, survey astronomy, temporal astronomy, theory and simulations (comparisons with observations) and information technology, digital detectors, massive data storage, the Internet, data representation standards.

In order to facilitate the international coordination and collaboration necessary for the development and deployment of the tools, systems and organizational structures necessary to enable the international utilization of astronomical archives as an integrated and interoperating virtual observatory, International Virtual Observatory Alliance (IVOA, http://www.ivoa.net) was formed in June of 2002. So the work of the IVOA mainly focuses on the development of standards.

SerVO - Serbian virtual observatory (http://www.servo.aob.rs/~darko) is a project whose funding was approved through a grant TR13022 from Ministry of Science and Technological Development of Republic of Serbia [2]. The project objectives are: a) Establishing SerVO and join the EuroVO and IVOA; b) Establishing SerVO data Center for digitizing, archiving and publishing in VO format photo-plates [3] and other astronomical data produced at Belgrade Astronomical Observatory; c) Development of tools for visualization of data; d) Publishing, together with Observatoire de Paris, STARK-B - Stark broadening data base containing as the first step Stark broadening parameters obtained within the semiclassical perturbation approach by two of us (MSD-SSB) in VO compatible format; e) Make a mirror site for DSED (Dartmouth Stellar Evolution Database [4,5] in the context of VO.

2. VAMDC – Virtual Atomic and Molecular Data Centre

In order to enable an efficacious and convenient search for available atomic and molecular data and their adequate use, we should try to solve existing problems in A&M data community, preventing productive search and data mining, which led to the VAMDC Idea. Main of such problems are: a) Lack of standards and common guidelines; b) Interoperability problem. c) Data exchange problem. Namely data exchange is often informal, via e-mails, ASCII files… without a standardization; d) Overlapping of efforts; e) Need of hiring computer engineers since the majority of developers are Astronomers, Physicists, Chemists; f) Data identification problem - XML schemata keys not only for data exchange but also for data identification; g) Need for a critical evaluation of data.

This means that at present, every time the same A&M database is used for a new application, the output has to be adapted. For example if we want to develop automatic tools for the visualisation of simulations of planetary, stellar or the interstellar medium spectra, this will require automatic access to different A&M databases, cross-matching the retrieved data as well as checking the quality of data. For such a purpose there is no actually a coherent and sufficiently general infrastructure to perform such tasks.

Additionally, if we want to enable an efficacious search for A&M data, we have a need for the:
- Creation of search engines that must look “everywhere" in order to map A&M Universe;
- An accessible and interoperable e-infrastructure for A&M data.

Very useful will be also the creation of a forum of data producers, data users and databases developers, as well as the training of potential users in European Research Area and wider.

All above mentioned problems will address Virtual Atomic and Molecular Data Centre (VAMDC – [6]), a FP7 founded project which started on July 1 2009 with budget of 2.9 MEuros over 42 months. Its aim is to build accessible and interoperable e-infrastructure for atomic and molecular data 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.

The VAMDC will build a secure, documented, flexible, easily accessible and interoperable e-infrastructure for A&M data that on the one hand can directly extract data from the existing depositories, while on the other hand be sufficiently flexible to be tuned to the needs of a wide variety of users from academic, governmental, industrial communities or by the general public.

The starting points are infrastructure and capabilities developed by EURO-VO (Virtual Observatory) EGEE (Enabling Grids for E-sciencE) and Astrogrid and a series of network and service
activities will be organized in order to establish self-sustainable computational and data mining services. It has the specific aim of creating an infrastructure.

The VAMDC can be understood as a publisher infrastructure. The VAMDC will deploy yellow pages (registries) in order to find resources, design user applications in order to meet the user needs, build data access layers above databases to provide unified outputs from these databases, care about asynchronous queries with workflows and the storage of large quantity of data with VO space, and connect its infrastructure to the grid.

![VAMDC logo](image)

VAMDC
Virtual Atomic and Molecular Data Centre

In fulfilling these aims, the VAMDC project will organise a series of Networking Activities specifically aimed at engaging data providers, coordinating activities among existing database providers, ascertaining and responding to the needs of different user communities and providing training and awareness of the VAMDC across the international A&M community and communities of other users.

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, Italy, 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) Astronomiska Observatoriet - 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 main users of VAMDC facilities will be Astronomy, Plasma science, Atmospheric Science Radiation science and Fusion community as well as Industries using technological plasmas and Lightning industry.
3. Databases

The core of the VAMDC e-infrastructure is the databases upon which it is based. The actual (the number will change) databases are shortly described below.

VALD database [7] of atomic data for analysis of radiation from astrophysical objects, developed and maintained by researchers at 7 European institutes, is created in 1995 in Vienna. The main nodes are in Vienna, Uppsala and Moscow, where are the three mirror sites. VALD contains a vast collection of spectral line parameters (central wavelengths, energy levels, statistical weights, transition probabilities, line broadening parameters) for all chemical elements of astronomical importance (http://vald.astro.univie.ac.at/).

CHIANTI [8] is an atomic database for spectroscopic diagnostics of astrophysical plasmas. Created in 1997, it contains critically evaluated set of up-to-date atomic data for the analysis of optically thin collisionally ionised astrophysical plasmas and is the preferred reference database in solar physics. It lists experimental and calculated wavelengths, radiative data and rates for electron and proton collisions (http://sohowww.nascom.nasa.gov/solarsoft, http://www.damtp.cam.ac.uk/user/astro/chianti/).

EMol Database [9], at the Open University in Milton Keynes, contains a comprehensive listing of critically evaluated and regularly updated measured and calculated cross sections for electron interactions with molecular systems. It is of interest for the plasma industry, and for the disciplines of discharge physics, fusion, aeronomy and radiation chemistry. It also offers a suite of semi-empirical theoretical methods so that cross sections may be evaluated for targets for which 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 in the frequency range 0-10 THz, i.e. 0-340 cm⁻¹. The CDMS is cross correlated with its US counterpart, the JPL Jet Propulsion Laboratory Submillimeter Catalogue (http://spec.jpl.nasa.gov/) [10].

BASECOL database [11] (http://basecol.obspm.fr) contains excitation rate coefficients for ro-vibrational excitation of molecules by electrons, He and H₂ and it is mainly used for the study of interstellar, circumstellar and cometary atmospheres.

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 [12] (http://www.udfa.net/), created [13] in 1991, 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. A preliminary version was released in June 2009 (http://kida.obs.u-bordeaux1.fr).

PAHs (Polycyclic Aromatic Hydrocarbon) and carbon clusters spectral database (http://astrochemistry.ca.astro.it/database/) in Cagliari, is developed by the CESR (Centre d'Etude Spatiale des Rayonnements/CNRS), and provides a number of properties for a sample of presently about 60 species in four charge states: anion, neutral, cation and dication [14]. The properties include general energetic such as electron affinity and ionisation energies, static polarizability, permanent dipole moment, van der Waals coefficients, symmetry, multiplicity, and optimised geometry of the ground electronic state; harmonic vibrational analyses, i.e. normal modes, their frequencies and IR activities; and vertical electronic photoabsorption cross-sections and complex frequency-dependent electronic polarisabilities in the linear regime.

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 for both pure species and their mixtures before and after processing with energetic ions and UV photons [15, 16, 17] (ii) IR
optical constants of molecules in the solid phase and after processing with energetic ions [18, 19]; (iii) band strengths of the IR absorption bands [20, 21]; and (iv) density values of frozen samples [21,22].

Spectr-W³ [23] atomic database (http://spectr-w3.snz.ru), created in 2002 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 [24] (http://cdsd.iao.ru and ftp://ftp.iao.ru/pub/CDSD-2008), containing calculated spectral line parameters for seven isotopologues of carbon dioxide.

S&MPO - Spectroscopy & Molecular Properties of Ozone) relational database [25] (http://ozone.iao.ru and http://ozone.univ-reims.fr/), developed in collaboration with the University of Reims, contains spectral line parameters for the ozone molecule, experimental UV cross-sections, information on ozone’s molecular properties, updated reference lists classified by type as well as programs and extended facilities for user applications.

"Spectroscopy of Atmospheric Gases" (http://spectra.iao.ru), containing the well-known databases such as HITRAN [25], GEISA [26] and HITEMP [27]. Both "Spectroscopy of Atmospheric Gases" and S&MPO have the programs for simulation of synthetic spectra from microwave to visible wavelengths.

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. W@DIS contains energy levels, transition positions and line intensities, and line profile characteristics.

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

TIPTOPbase [28] located at the Centre de Données astronomiques de Strasbourg, France (http://cdsweb.u-strasbg.fr/topbase/home.html), contains:

TOPbase (http://cdsweb.u-strasbg.fr/topbase/topbase.html), listing atomic data computed in the Opacity Projec, namely LS-coupling energy levels, gf-values and photoionization cross sections for light elements (Z ≤ 26) of astrophysical interest.

TIPbase (http://cdsweb.u-strasbg.fr/tipbase/home.html). Intermediate-coupling energy levels, A-values and electron impact excitation cross sections and rates for astrophysical applications (Z ≤ 28), computed by the IRON Project.

OPserver [29], 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 [30], used by the XSTAR code (http://heasarc.gsfc.nasa.gov/ docs/software/xstar/xstar.html) for modelling photoionised plasmas.

HITRAN - HIgh-resolution TRANsmission molecular absorption database [25] (http://www.cfa.harvard.edu/hitran/), used extensively by the atmospheric and planetology research communities. It lists individual line parameters for molecules in the gas phase (microwave through to the UV), photoabsorption cross-sections for many molecules, and refractive indices of several atmospheric aerosols.

GEISA - Gestion et Etude des Informations Spectroscopiques Atmosphériques (Management and Study of Atmospheric Spectroscopic Information) database [26] (http://ara.lmd.polytechnique.fr/index.php?page=geisa-2 or http://ether.ipls.jussieu.fr/etherTypo/?id=950) is a computer accessible
database system, designed to facilitate accurate and fast forward, calculations of atmospheric radiative transfer.

HITRAN, a high temperature extension to HITRAN [27] (To access the HITRAN data: ftp to cfa-
ftp.harvard.edu; user = anonymous; password = e-mail address). So far HITRAN contains data for water, CO₂, CO, NO and OH.

The external partner of VAMDC is NIST - National Institute of Standards and Technology, a major centre for atomic and molecular data compilation, which has developed a number of numerical and bibliographic atomic and molecular databases. Among others it hosts:

Atomic Spectra Database (http://physics.nist.gov/asd3) listing critically evaluated data on about 77,000 energy levels and 144,000 spectral lines from atoms and ions of 99 elements.

The Handbook of Atomic Spectroscopic Data [31] (http://physics.nist.gov/Handbook) listing energy levels and prominent spectral lines for neutral and singly ionised atoms.

The Spectral Data for the Chandra X-Ray Observatory database [32] (http://physics.nist.gov/chandra) presenting critically compiled wavelengths (20 A to 170 A), energy levels, line classifications, and transition probabilities for several astrophysically important elements.

SAHA, The NLTE plasma population kinetic modeling database containing theoretical data [33, 34]. (http://nlte.nist.gov/SAHA).

Three bibliographic databases providing references on atomic energy levels and spectra (http://physics.nist.gov/cgi-bin/ASBib1/ELevBib.cgi), transition probabilities (http://physics.nist.gov/ cgi-bin/ASBib1/TransProbBib.cgi) and spectral line shapes and line broadening (http://physics.nist.gov/cgi-bin/ASBib1/LineBroadBib.cgi).

4.STARK-B database

Our contribution to the VAMDC e-infrastructure is the STARK-B database (http://stark-b.obspm.fr) [35], a collaborative project between Laboratoire d’Etude du Rayonnement et de la matière en Astrophysique of the Observatoire de Paris-Meudon and the Astronomical Observatory of Belgrade. This is a database of the theoretical widths and shifts of isolated lines of atoms and ions due to collisions with charged perubers, obtained within the impact approximation. For the moment STARK-B contains results obtained using the semiclassical perturbation approach [36,37]. The corresponding computer code has been optimized and updated in Refs. [38, 39, 40] and following papers. For the review and all updates see e.g. Ref. [41].

This database is devoted to modelling and spectroscopic diagnostics of stellar atmospheres and envelopes. In addition, it is also relevant to laboratory plasmas, laser equipment and technological plasmas. The database is currently developed in Paris, and a mirror is planned in Belgrade. It is already on line though not yet complete. It is described in detail in Ref. [35].

The precursor of STARK-B as well as of SerVO was BELDATA and its main content was database on Stark broadening parameters. A history of BELDATA can be traced in Refs [42, 43, 44, 45, 46, 47].

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

We also have a close collaboration with Sylvie Sahal-Bréchot from Paris Observatory, Nebil Ben Nessib, Walid Mahmoudi, Rafik Hamdi, Haykel Elabidi, Besma Zmerli and Neila Larbi-Terzi from Tunisia, Magdalena Christova from Technical University of Sofia and Tanya Ryabchikova from Institute of Theoretical Astronomy in Moscow.

Initiatives like VAMDC are important for both producers of atomic and molecular data and stellar atmosphere modellers as one of prime users. VAMDC is an example of the global collaborations and innovations in e-science. It is expected to become one of major European cyber-infrastructures with a world wide impact.

Acknowledgments
A part of this work has been supported by VAMDC, funded under the “Combination of Collaborative Projects and Coordination and Support Actions” Funding Scheme of The Seventh Framework Program. Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure. Grant Agreement number: 239108. The authors are also grateful for the support provided by Ministry of Science and Development of Republic of Serbia through projects TR13022 “Serbian Virtual Observatory”, 146001 "Influence of collisional processes on astrophysical plasma spectra" and 146002 "Astrophysical Spectroscopy of Extragalactic Objects".

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