




## **NEWS: VAMDC Annual Meeting**

To be held at the Campus of the University of Vienna, Austria,  
from 21-24 February, 2012

Please find details on our meeting page:

<http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PmCycleThree>

### In this issue:

-  What is VAMDC?
-  How to get involved
-  Participating institutions

**VAMDC** aims at building an interoperable e-infrastructure for the exchange of atomic and molecular data. VAMDC is a complex project involving 15 administrative partners representing 24 teams from 6 European Union member states, Serbia, the Russian Federation and Venezuela. It embraces on the one hand scientists from a wide spectrum of disciplines in atomic and molecular (AM) physics with a strong coupling to the users of their AM data (astrochemistry, atmospheric physics, plasmas) and on the other hand scientists and engineers from the ICT community used to deal with deploying interoperable e-infrastructure.

VAMDC is supported by the EU in the framework of the FP7 "Research Infrastructures - INFRA-2008-1.2.2 - Scientific Data Infrastructures" initiative. It started on the 1st of July 2009 for a duration of 42 months.

**How to get involved:** If you are interested to get involved into the VAMDC project, please contact the Project coordinator Marie-Lise Dubernet: [marie-lise.dubernet-tuckey@upmc.fr](mailto:marie-lise.dubernet-tuckey@upmc.fr)

## General research interest of the teams involved in VAMDC and their specific VAMDC related activities:

### (1) Centre National de Recherche Scientifique (CNRS)

**LPMAA**, UMR CNRS 7092, Université Pierre et Marie Curie  
(Partner of VO-Paris Data Center, Observatoire de Paris)

The research activities of LPMAA traditionally focus on molecular physics and its applications for the study of the terrestrial atmosphere and on the understanding of molecular processes in astrophysical environments (comets, planets, interstellar medium). Our expertise ranges from experimental and theoretical studies (IR and UV spectrometry, mass spectrometry, cryogenic surfaces, spectral analysis to measurement campaigns (ground and balloon based remote sensing of the troposphere and the stratosphere). With the coordinator of the VAMDC, LPMAA is now involved in theoretical calculations of ro-vibrational de-excitation rate coefficients for application to interstellar, circumstellar and cometary atmospheres, of line broadening coefficients for application to planetary and earth atmospheres.

**LUTH**, UMR CNRS 8102, Observatoire de Paris, Université Paris Diderot.

(Partner of VO-Paris Data Center, Observatoire de Paris)

LUTH emphasizes on intensive numerical simulations and interdisciplinarity, two determining aspects of modern research activity in astrophysics. LUTH is strongly implied in the development of the virtual observatory in different domains: VO-Theory, Molecular Physics, High Energy Astrophysics and Exoplanets. These virtual observatories are one of the strategic priorities of Paris Observatory. Services developed at LUTH cover: simulations of the physics of the interstellar medium, large scales simulations in cosmology, molecular data for the spectroscopy in the UV, high energy spectra, exoplanet encyclopedia. Members of LUTH participating to these VO services are often implied both in the development of the services and in the development of the VO standards at international level. LUTH has been involved in Virtual Observatory activities linked to atomic and molecular data.

The VAMDC P.I. belongs both to LPMAA and to LUTH (Observatoire de Paris) and the LPMAA/LUTH team lead the administration and the coordination of the VAMDC consortium. The VAMDC activities range from dissemination activities, development of XSAMS standards, development of publishing software to development of client software to handle XSAMS files. In addition the BASECOL database has been chosen as one of the test cases for VAMDC implementation and has been deployed as a fully functional and standard-compliant VAMDC node. Finally the team currently edits and maintains the different documentations linked to standards and to description of the infrastructure. The team maintains and updates the VAMDC website.

## **VO-PARIS Data Centre**, UMS CNRS 2201, Observatoire de Paris

VO-PARIS Data Center is a federative infrastructure linked to the Departments and the Computer Centre of Paris Observatory and to LPMAA from Université Pierre et Marie Curie. It is strongly involved in Virtual Observatory activities covering many disciplines in astrophysics, molecular physics, solar physics, etc. The Computer Center of VOPARIS Data Centre has a staff of 4 engineer with an infrastructure including computing power linked to the EGEE grid, storage facilities and servers.

The Computer Center of VO-Paris Data Center is in charge of monitoring the infrastructure, of providing access to the EGEE GRID, of providing duplication services and long term preservation of data.

## **LERMA**, UMR CNRS 8112, Observatoire de Paris.

The LERMA is an interdisciplinary laboratory covering astrophysical observations and modelling of stars, the interstellar medium and galaxies, theoretical and experimental atomic, molecular and plasma physics, the primordial universe and gravitation, hyper-frequency radiometry and the remote sensing of atmospheres and planetary surfaces. The laboratory is also involved in the Planck, Herschel and Alma projects. The LERMA team contributes to the Stark-B database with the Observatory of Belgrade and to TIPTOPbase with IVIC (Venezuela).

## **LAB**, UMR CNRS 5804, Observatoire de Bordeaux

Laboratoire d'Astrophysique de Bordeaux is part of the Observatoire Aquitain des Sciences de l'Univers, which groups several laboratories involved in astronomical and Earth sciences. LAB is part of several international astrophysical projects such as ALMA and is currently developing a strong expertise in astrochemistry. The LAB team is the leader of the Kinetic Database for Astrochemistry (KIDA) and contributes to the definition of standards for chemical reactions.

## **ICB**, UMR CNRS 5209, Université de Bourgogne

The Molecular Spectroscopy and Applications group of the Institut Carnot de Bourgogne is the world leader in the analysis of high-resolution spectra of methane ( $^{12}\text{CH}_4$ ,  $^{13}\text{CH}_4$  and  $\text{CH}_3\text{D}$ ). Methane is a major greenhouse pollutant on Earth and an important constituent of many astrophysical bodies (giant planets, Titan, dwarf planets, brown dwarfs, methane stars, exoplanets). Modelling methane absorption over a wide spectral range is essential to retrieve methane vertical profiles, minor species abundances and surface properties. It is thus of primary importance for the study of these objects to constitute a highly reliable and consistent database of line parameters extending for the far infrared to the visible region. Within VAMDC the ICB team will provide a data base of line parameters for these three isotopologues (positions, intensities, lineshape parameters).

## **GSMA**, UMR CNRS 6089, Université de Champagne-Ardenne

The Group of Molecular and Atmospheric Spectroscopy (GSMA) is the world recognized leader in the analysis and theoretical modelling of high-resolution spectra of ozone. The group has the unique experimental equipment for recording long-path Fourier transform spectra (FTS) in the infra-red and visible range, which over years has been used for producing very accurate data on line positions, intensities and line shape parameters for isotopologues of water, ozone, H<sub>2</sub>S, SO<sub>2</sub>, methane, CO<sub>2</sub>, acetylene, ethylene and other molecules. These parameters are used as reference data in various databanks for atmospheric and astrophysical applications.

Within VAMDC the GSMA team will provide access to Ozone and Ethylene Databases in collaboration with IAO, Tomsk, Russia.

## **CESR**, Toulouse

The Toulouse team is strongly involved in the study of the physics and chemistry of interstellar matter: gas and dust. This is an interdisciplinary team that provides expertise in molecular physics and solid properties. Their role in VAMDC is to contribute to the definition of standards and help in the transfer of databases to VAMDC format. There is an important connection with the PAH database in Cagliari but there are also links with the Cologne molecular database (CDMS) and the GhoSST database on solids.

## **IPAG (formerly LPG)**, Observatoire de Grenoble

The Planeto team at Institut de Planétologie et Astrophysique de Grenoble (IPAG, formerly LPG) is strongly involved in laboratory simulations and analyses of various types of solids of planetary and astrophysical interests: ices, minerals, extraterrestrial and synthetic organic matter. It mainly uses different visible and infrared spectroscopy techniques (transmission, bidirectional reflection, microscopy, Raman, Fluorescence), among other instruments, to study their optical properties as well as their composition, chemistry and thermodynamical properties.

These data are used to interpret spectroscopic and imaging spectroscopy data gathered by instruments onboard space missions (NIMS on Galileo, DISR+VIMS on Cassini, OMEGA on Mars Express, VIRTIS on Rosetta, ...).

Its activities within the VAMDC programme is to develop a European Solid Spectroscopy Data Model (SSDM) accurately describing the solid samples, the experiments, the spectra and their products for a wide range of natural and synthetic solid materials of planetary and astrophysical interests and to implement this data model in a distributable database structure: GhoSST.

## (2) The Chancellor, Masters and Scholars of the University of Cambridge (CMSUC)

The VAMDC team at the University of Cambridge consists of team members in two laboratories: The Institute of Astronomy (IoA), and the Department of Applied Mathematics and Theoretical Physics (DAMTP). The team at the IoA is focussing on the technical development of the VAMDC infrastructure. The IoA software engineers are primarily overseeing the VAMDC architecture, deploying the VAMDC services, and developing the user portal. Further, the IoA team organise the technical management of the project. The IoA team have been using their experience of developing distributed computing systems, through involvement in projects such as the Virtual Observatory and Open Grid Forum, and applying this in the development of VAMDC. Staff at the IoA are also involved in the next ESA space astronomy mission, the Gaia satellite. Atomic and Molecular data will be used in the analysis and interpretation of some of the data from Gaia, and access via the VAMDC infrastructure is now being considered. VAMDC will also be used as a tool for use by young researchers, and in this context will be demonstrated at a GREAT (Gaia Research for European Astronomy Research – <http://www-great-esf.eu>) training school.

The VAMDC team at DAMTP provides scientific input to VAMDC and ensure the availability of the CHIANTI database through the VAMDC service infrastructure. CHIANTI is a well-established atomic database for ions of astrophysical importance. Combined with IDL spectroscopic diagnostic programs, it is used in the analysis of optically thin collisionally-ionised plasmas (it is the reference database in solar physics). The CHIANTI package contains atomic structure data (experimental and calculated wavelengths and radiative data), and rates for electron and proton collisions. The data are obtained from published literature, sometimes supplemented by the CHIANTI group calculations. They are regularly assessed and updated every year or so. References to the original sources are supplied and each version is described in a journal paper.

The VAMDC team contact at the IoA is Nicholas Walton ([naw@ast.cam.ac.uk](mailto:naw@ast.cam.ac.uk)) whilst Helen Mason ([H.E.Mason@damtp.cam.ac.uk](mailto:H.E.Mason@damtp.cam.ac.uk)) leads the VAMDC staff within DAMTP.

## (3) University College London (UCL)

Contributions to VAMDC from University College London are by the Department of Physics and Astronomy and the Mullard Space Science Laboratory (MSSL). The team in Physics and Astronomy, led by Jonathan Tennyson has interests in the development of techniques based on first principle quantum mechanical methods for study of the structure, spectra and collision properties of molecules and how these methods can be applied in several areas including astrophysics, atmospheric physics and technological plasmas. The team based at MSSL, led by Len Culhane, has interests in solar physics and virtual observatories, having been heavily involved in the development and deployment of the AstroGrid Virtual Observatory services and the EC-supported Heliophysics Integrated Observatory (HELIO). Thus they will be

strongly concerned with ensuring access to VAMDC for the Solar Physics and Heliospheric communities and for those working in the Space Weather applications field. VAMDC effort at both sites plays to their key strengths and interests.

The group in Physics and Astronomy is working towards a SQL based version of the HITRAN database and will thus make significant contributions to establishing the XSAMS standard, developing the VAMDC node software, and providing advice on long term survivability through their experience with Quantemol software and the ExoMol project. Based on their Astrogrid experience, the group at MSSL is focussing on the VAMDC infrastructure through the development of the VAMDC registry, Taverna workflow plugins and the deployment and maintenance of key services such as the production versions of the Chianti and HITRAN databases and the production VAMDC registry. The Chianti data base in particular is intensively used by the Solar Physics community and the MSSL group has substantial experience of its application in solar spectroscopy.

#### (4) Open University (OU)

The Open University supports a range of research appropriate for VAMDC including one of the UK's and Europe's largest planetary and space science research groups, a thriving astronomy group and a recently established atomic, molecular and plasma physics (AMP) group that aims to provide fundamental data for inclusion in the VAMDC databases. In particular the AMP group performs both experimental and theoretical studies of electron scattering and coordinates several EU and international research collaborations exploring the role of electron collisions in applied areas including astrochemistry, atmospheric science, radiation damage and plasma technology. The OU also has many years experience in assembling spectroscopic databases in particular assembling VUV spectra for 100 molecules, data that is widely used in atmospheric chemistry. This database has recently been extended to condensed phase spectra for astrochemical ices data that is being used to interpret recent observations of reflection spectra of Kuiper belt objects and the Saturnian moons.

Accordingly the OU provides the conduit for communicating both the aims and results of the VAMDC e-infrastructure. Dissemination activities are aimed at VAMDC's users, the wider European science community, European industrial stakeholders and policy makers. It is intended to provide an attractive platform to exchange and present results, develop new ideas and to network with other data providers and e-infrastructures. This is to be accomplished by being represented at other appropriate conferences and hosting a series of targeted topical workshops and teaching tutorials. Links with several other database providers have been established and presentations made at suitable meetings (these are recorded on the VAMDC website). Such dissemination is coordinated by the Communication and Training Committee (CTC) which is chaired by the OU.

## (5) Universität Wien (UNIVIE)

Both researchers from the Institute for Astronomy and the Institute of Mathematics of the University of Vienna (UNIVIE) work for its VAMDC node. Research fields at the Institute for Astronomy for which VAMDC is particularly important include stellar spectroscopy, the modelling of stellar atmospheres, as well as asteroseismology, among others. At the Institute of Mathematics, a large software package for the numerical simulation of astrophysical flows is developed which is used to construct numerical models for stellar astrophysics. In all these fields, opacity data from atomic and molecular spectroscopy is a crucial input quantity. The Institute of Astronomy at UNIVIE is also the site where the development of the Vienna Atomic Line Data Base (VALD) by an international research team began who later on brought the further evolution of VALD to partner sites at Uppsala University (UU) and INASAN. All three development sites of VALD have become partners of the VAMDC consortium.

An important part of work for VAMDC at UNIVIE is dissemination and training to communicate the capabilities of the growing VAMDC infrastructure to the European scientific community and beyond it (work package chaired by the OU node of VAMDC). Editing the VAMDC Newsletter and organizing VAMDC related conferences is part of these activities. Other contributions to VAMDC include work required for building up the electronic infrastructure (registries) and for the integration of the VALD data base into the VAMDC framework.

## (6) Uppsala Universitet (UU)

The VAMDC team at Uppsala University specializes in the spectroscopy of stars and their environments. Our research is related to the physics of planetary systems and stars, the interactions between stars and planetary systems, and stars as building blocks of galaxies. Methods developed or advanced at UU are spectral synthesis including deviations from local thermodynamic equilibrium, Doppler imaging, 1D opacity sampling atmosphere modelling, and 3D radiation hydrodynamics simulations. We are applying these techniques to the detailed analysis of individual objects as well as to parameter estimations for large samples of stars from massive surveys, such as the Gaia space mission. All of the above relies heavily on the availability of accurate and complete atomic and molecular data. Thus, VAMDC-UU is one of the main drivers behind VALD – a major collection of A&M data in the UV, optical, and IR region for cool and intermediate temperatures and low/intermediate densities. Astronomers at UU are also carrying out ab initio calculations of collisional effects on line shapes.

In the VAMDC project, the UU team is responsible for the development of the Publishing Tools – software packages which enable data producers to include more A&M data into the VAMDC infrastructure. This involves data conversion from and to various formats, implementing the VAMDC standards for querying and data transfer, as well as instruction documents. The VALD database has been chosen as one of the test cases for VAMDC implementation and has been deployed as a fully functional and standard-compliant VAMDC node. In addition, UU team members are

also active in the development of the standards themselves and the common VAMDC user interface.

### (7) Universität zu Köln (KÖLN)

The VAMDC team at the University of Cologne is specializing in molecular physics and is part of the I. Physikalisches Institut whose focus is astrophysics. It hosts the Cologne Data Base for Molecular Spectroscopy (CDMS) which provides a wealth of spectroscopy data for the millimetre and sub-mm wavelength regime for many years.

In order to support the VAMDC activities, the CDMS has now been transformed from an ascii-file based DB into a mysql database with an appropriate infrastructure (database structure, data import, data access, etc.) supporting the XSAMS schema.

CDMS has been chosen by the VAMDC network as one of the test cases. Thus the improvement of the XSAMS schema and the development of the surrounding infrastructure, namely a common (<http://vamdc.fysast.uu.se:8888/doc/index.html>) interface to process users queries and to generate data output is actively supported. This new framework gives access to the CDMS via a common query interface

(<http://casx019-zone1.ast.cam.ac.uk/vamdc-demo-portal/>). The CDMS also supports the DSA-catalogue infrastructure and thus associated tools such as VO-Desktop.

### (8) Istituto Nazionale di Astrofisica (INAF)

Istituto Nazionale di Astrofisica (INAF) includes 2 legal entities (Osservatorio Astronomico di Cagliari – OAC and Osservatorio Astrofisico di Catania – OACT) with distinct roles.

The astrochemistry group at INAF-OAC studies the physics and chemistry of the interstellar medium, combining state of the art computational models and a multi-wavelength observational approach. Since 2003, in collaboration with Dr C. Joblin at CESR Toulouse, the astrochemistry group has been building a database of the computed spectral properties of a large number of polycyclic aromatic hydrocarbons, available at <http://astrochemistry.oa-cagliari.inaf.it/database>. This group is recognised as one of the international leaders in the field of interstellar PAHs. The participation of this group to VAMDC involves the integration of their database in VAMDC and the development of automated tools to make it a straightforward task for data producers to add their results to VAMDC, either using their database or creating a new one.

The group LASP (Laboratory for Experimental Astrophysics) at INAF-OACT has been mainly devoted to experimental studies of the chemical and physical modifications induced by fast ions on targets of astrophysical relevance (frozen gases, silicates, carbonaceous materials). The LASP Database (<http://web.ct.astro.it/weblab/>) provides (a) infrared (IR) spectra of molecules in the solid phase (10-100 K) both pure species and their mixtures before and after processing with energetic ions (30-200 keV) and UV photons (10.2 eV); (b) IR optical

constants of molecules in the solid phase as well as optical constants of frozen molecules after processing with energetic ions (30-200 keV); (c) band strengths (A values) of the most relevant IR absorption bands; (d) density values of frozen samples. The participation of this group in VAMDC involves the integration of their database into VAMDC.

### (9) Queen's University Belfast (QUB)

The research interests of the Molecular Astrophysics group at Queen's University Belfast ([https://habu.pst.qub.ac.uk/groups/arcresearch/wiki/a0050/Molecular\\_astrophysics.html](https://habu.pst.qub.ac.uk/groups/arcresearch/wiki/a0050/Molecular_astrophysics.html)) are primarily concerned with the physical and chemical state, evolution and dynamics of the interstellar medium, in particular through studies of the molecular component of that medium. The current emphasis of the group is on the modelling of astrochemical processes in various environments (including dark, quiescent molecular clouds, carbon-rich circumstellar envelopes and protoplanetary discs), to build understanding of the molecular evolution of the universe from clouds of gas to stars and ultimately planets. More recently, we have been developing coupled physical and chemical models of exoplanet atmospheres. We have coupled our models with radiative transfer codes to predict the emergent line emission from our models for direct comparison with observations. Microwave observations of molecules in space allow us to test our models, refine theories and generate further knowledge about the physics and chemistry of space.

A database of fundamental chemical kinetic data has been developed: the UMIST Database for Astrochemistry (RATE06 – <http://www.udfa.net>). This contains a set of chemical reactions and associated rate coefficients for use in astrochemical modelling.

Queen's is involved in adapting the UMIST database for interaction with the VAMDC portal. In addition QUB is involved in the Dictionaries task of VAMDC, to facilitate the unique identification of resources - and in particular, common Molecule Identifiers.

### (10) Astronomska Opervatorija (AOB)

The Astronomical Observatory Belgrade (AOB) is a multidisciplinary institution, founded in 1887, and it is one of the oldest scientific institutions in Serbia. Scientific research carried out at the AOB closely followed the trends in the astronomical and astrophysical research of the XX century, from observations of minor planets, comets and double stars and determination of their orbits, stellar photometry, spectroscopy and polarimetry (mostly eruptive stars, cool supergiants and Be stars), spectrography of the Sun and monitoring of the large scale photospheric motions to modelling of line emission in a large variety of astrophysical plasma.

Today's scientific topic covered by the staff are: astrophysics of stars and the Sun. Astrophysical spectroscopy, spectroscopy of active galactic nuclei, astroinformatics, stellar and galactic systems, Interstellar and intergalactic matter, cosmology and astrobiology, dynamic astronomy and planetology, and history and philosophy of astronomy.

On AOB, the VAMDC node is the Group for Astrophysical Spectroscopy (Milan S. Dimitrijevic, Luka Ch. Popovic, Darko Jevremovic, Andjelka Kovacevic, Zoran Simic, Edi Bon and Nenad Milovanovic). The scientific interests of the members of the group are: influence of collisional processes on spectra of astrophysical, laboratory and technological plasmas, in particular theoretical determination of Stark broadening parameters of non hydrogenic atoms and ions, where together with the partners in LERMA (S. Sahal Brechot), we have one of the leading positions in Europe; physics and spectroscopy of active galactic nuclei, quasars, gravitational lenses and gamma-ray bursts, and astroinformatics with the aim to develop the Serbian Virtual Observatory and together with LERMA the STARK-B database as a part of VAMDC.

The role of the AOB Group for Astrophysical Spectroscopy is development, together with LERMA, of the STARK-B database for VAMDC, connection to the users of Stark broadening data, testing and producing Stark broadening data, connection to users working in the fields of stellar spectra and stellar atmospheres, connection to the Serbian Virtual Observatory, quality assurance and VAMDC regional node for Balkan countries, with organization of local tutorials.

### (11) Institute of Spectroscopy RAS (ISAN)

The department of atomic spectroscopy of the Institute for Spectroscopy of the Russian Academy of Sciences is involved in the experimental and theoretical study of energy structures of atoms and ions throughout the Periodic Table from the light elements such as boron to heavy elements of the palladium group which are necessary for astrophysics, for works on controlled thermo-nuclear synthesis, for the creation of vacuum ultra-violet and X-ray lasers, and also for the development of spectral diagnostics of high temperature plasma. More than 30000 spectral lines were identified in about 290 atomic and ionic spectra in roughly the last 40 years. The work is based on high resolution spectroscopic equipment and on the theoretical calculations of atomic spectra using a variety of theoretical approaches (Hartree-Fock, Dirac-Fock, orthogonal operator technique and others). A Database of Bibliography on Atomic Spectra (BIBL) has been created and maintained. It is accessible on line from the site <http://das101.isan.troitsk.ru/bibl.htm>

ISAN jointly with INASAN are searching, extracting, critically evaluating and preparing atomic parameters of spectral lines for the Vienna Atomic Line Database (VALD) which is part of VAMDC. The search is made using ISAN's Bibliography on the Atomic Spectra Database (BIBL). Extracted atomic data are evaluated using extensive atomic calculations and long-term experience in laboratory analyses of atomic spectra. A description of atomic transitions in VALD is converted to a unified format of VAMDC.

(12) **Russian Federal Nuclear Center- All-Russian Institute of Technical Physics** (RFNC-VNIITF)

The Spectr-W3 workgroup members are involved in research programmes in the domains of high-energy-density physics (HEDP) and computer science. Appropriate modelling of EUV and X-ray emission and absorption spectra of matter under extreme conditions of hot laboratory and astrophysical plasmas is an inherent feature of the HEDP research and, in turn, implies realistic description of atomic structure and spectral properties of various multielectron ions. The latter activities involve spectroscopic data calculations for multielectron ions and elaboration of atomic databases; development of theoretical models to calculate detailed Stark-broadened lineshapes; and development of theoretical models to calculate opacities of the multielectron-ion plasmas utilizing both the detailed and statistically averaged description of the bound-bound and bound-free transitions. The spectroscopic constituent of the effort, in particular, resulted in the creation of the Spectr-W3 information-reference system (<http://spectr-w3.snz.ru>). The node is located at the Centre for International Science and Technology Cooperation of RFNC-VNIITF and provides free round-the-clock access to the Spectr-W3 factual atomic database presenting experimental, calculated, and compiled data on ionization potentials, energy levels, wavelengths, radiation transition probabilities and oscillator strengths, and also parameters of analytical approximations of electron-collisional cross-sections and rates for atoms and ions. The Spectr-W3 project is being implemented under the long-term collaboration with the high-level experts of the Joint Institute for High Temperatures of Russian Academy of Sciences (JIHT RAS) and partial support of International Science and Technology Centre (ISTC, <http://www.istc.ru>). To date, the Spectr-W3 atomic database is still the largest factual database in the world, containing the information on spectral properties of multicharged ions (about 450,000 records).

(13) **Institute of Atmospheric Optics** (IAO)

V. E. Zuev Institute of Atmospheric Optics of the Siberian Branch of the Russian Academy of Sciences (IAO) has two types of activities appropriate for VAMDC including a generation of databases of the molecular spectral line parameters for the applications in atmospheric physics and astrophysics and elaboration of the information systems on molecular spectroscopy. The Laboratory of Theoretical Spectroscopy (LTS) of this institute is mainly a data producer. It elaborated several versions of the Carbone Dioxide Spectroscopic Databank (CDS, <ftp://ftp.iao.ru/pub/CDS-2008/>, <ftp://ftp.iao.ru/pub/CDS-4000/>) for atmospheric, astrophysical and industrial applications. Together with the Groupe de Spectroscopie Moleculaire et Atmospherique (GSMA) de Université de Reims et CNRS (France) it elaborated the information system Spectroscopy and Molecular Properties of Ozone (S&MPO, <http://smpo.iao.ru/>). The Integrated Information Systems Center (IISC) of IAO develops a distributed information systems on molecular spectroscopy containing the data on the states and transitions of a number of molecules. The work is performed in cooperation with the Institute of Applied Physics of the Russian Academy of Sciences (Nizhnii Novgorod) and Saint-Petersburg State University. The elaboration

of the information system W@DIS IS (<http://wadis.saga.iao.ru/>) was performed in cooperation with the IUPAC data group. The key features of these works are a collection of primary data of measurements performed during the last 75 years as well as the validity check of these data according to the formal criteria. The results of the collected data analysis are published in a form of OWL-ontologies. These ontologies are the catalogues that allow one to analyze published spectral data. At present the catalogues contain complete information on three molecules and its isotopologs (water, hydrogen sulfide, and carbon dioxide). Within the framework of the VAMDC project LTS will provide a unified access to its databases. According to the plans corrected during the first year of the project the IISC will provide VAMDC with the data quality control tool.

#### (14) Corporacion Parque tecnologico de Merida

##### Venezuelan node (CeCaLCULA/IVIC)

The Venezuelan VAMDC node has been involved in the migration of the following atomic databases to the SQL DBMS MySQL and in the development of the corresponding TAP/XSAMS interfaces: uaDB (<http://heasarc.gsfc.nasa.gov/uadb/>), TOPbase (<http://cdsweb.u-strasbg.fr/topbase/topbase.html>), and TIPbase (<http://cdsweb.u-strasbg.fr/tipbase/home.html>). We have also implemented operational registries of SOAP web services for several atomic database applications: XSTAR, TLUSTY200-SYNSPEC43-ROTIN3, AUTOSTRUCTURE, SELECT3, and DevinTheDevil, experimenting with various clients (command-line, web, Taverna workflows and SUDS python scripts). A comparison has been made of the SOAPLAB2 (<http://soaplab.sourceforge.net/soaplab2/>) and Astrogrid CEA server frameworks (<http://www.astrogrid.org/maven/docs/HEAD/applications/index.html>).

#### (15) Institute for Astronomy RAS (INASAN)

The scientists of INASAN are carrying out research in many different fields of astrophysics. Among the most important related to the VAMDC project are stellar atmosphere structure, stellar spectroscopy, and modelling of star formation. This dictates an interest for atomic and molecular data, in particular, transition probabilities for atomic and molecular lines, bound-free and free-free radiative cross-sections, impact cross-sections, and molecular reaction rates. Our astronomers need both kinds of data: accurate laboratory measured or calculated wavelengths, energy levels and transition probabilities for fine analysis of stellar and interstellar medium spectra (line profiles) as well as massive blocks of data for millions of predicted lines used in opacity calculations needed in different kinds of modelling, for example, calculating the stellar atmospheric structure. INASAN is related to the VAMDC project through the holding, supporting, and running of a mirror-site of Vienna Atomic Data Base (VALD) which is one of the main databases widely used by the spectroscopic community all over the world.

The INASAN team consists of two members. Tatiana Ryabchikova is one of the main experts for quality estimate in the atomic part of VALD. She makes a critical analysis of the new data appeared in the literature through the comparison of them with the data already included in VALD and with stellar spectra of extremely high quality through spectral synthesis. This is the last comparison which allows to fix errors in the laboratory measurements of atomic parameters. Then data are ranked according to their quality and the user gets the final tables of the best quality data. The final set of merged data constitutes the body of VALD which is being included in VAMDC. It is prepared in a form allowing an easy transformation to the accepted VAMDC standard XSAMS schema. This part was done by the members of the Uppsala team with the participation of another representative from INASAN, Yury Pakhomov, who is a system administrator of the Moscow VALD mirror-site. Yu. Pakhomov together with F. Kupka (UNIVIE) provided the full reference list for VALD entries in BibTex format (365 items in the current version) that is easily transformed to XSAMS format. INASAN team members were taking part in preparation of VALD for a 1<sup>st</sup> year Service Release demonstration in Paris. Yu. Pakhomov currently is working on the implementation of VALD selection tools into a MySQL database for subsequent use in various applications within the VAMDC infrastructure.

*edited by Theresa Lüftinger and Friedrich Kupka, August, 2011*