VAMDC
Virtual Atomic and Molecular Data Centre

http://www.vamdc.eu

M.L. Dubernet$^1$
And VAMDC Consortium Collaboration
$^1$Paris Observatory, LERMA
History

The VAMDC Consortium is a technical and political framework for sharing Atomic and Molecular data

Build upon 2 FP7 European funded Projects:

- **VAMDC: 2009-2012 with 25 different laboratories**
  - The baseline of the Infrastructure
- **SUP@VAMDC: 2012-2014 with 9 laboratories**
  - Building the political framework
  - Expanding towards other communities
- **Currently « VAMDC Consortium » is sustained**
  - Via its members in kind (and cash via self-financing and fees for those not maintaining resources)
  - Via a small starting budget of 60kEuros for 4 years
Consortium overview

The VAMDC consortium is:
- Built on a Memorandum of Understanding.
- Currently composed by 15 members who signed the MoU.
- Officially launched on November 1, 2014.

Board of Directors: Full members ➔ Decisions
Science and Technical Board: Full and Associated Members
- Propose evolutions and Maintain the VAMDC infrastructure

How to join us (accession documents)
- Memorandum of Understanding
- Internal Regulations
- Roadmap
HOW TO JOIN US

You might become a VAMDC Consortium Member under conditions set up in the Memorandum of Understanding, Articles 3.1 and 3.2. For further details and information, contact director[at]vamdc.eu.

MoU's Articles 3.1 and 3.2

3.1 VAMDC Consortium Full Members

- The VAMDC Consortium Full Members are institutions that hold physically a resource tagged « VAMDC », i.e. a database or a service registered in the “VAMDC” registries, or that maintain/update a documentation officially tagged « VAMDC ».

- Otherwise full members can be institutions paying annual membership fees set by the Board of Directors.

Full Members can participate in calls engaging the VAMDC infrastructure and can use the “VAMDC brand”. Accession to full member status is granted by the Board of Directors and an accession document is signed.

3.2 VAMDC Consortium Associated Members

The VAMDC Consortium Associated Members are institutions, scientific groups, SMEs, companies that collaborate with the members for the benefit of the « VAMDC resources » and that have been co-opted by a VAMDC Consortium Member.

Accession to the Associated Member status is granted by the Board of Directors and an accession document is signed.

3.3 Request for membership

Any request for membership will be subject to the following conditions:

- To fulfill Article 3.1 or 3.2

- To make the commitment to abide by the Articles of this Memorandum of Understanding and the regulations of the VAMDC Consortium

When deciding on request for membership the Board of Directors will not have to justify its decision, which will be without appeal.
INTERNAL REGULATIONS
The VAMDC Consortium Internal Regulations serve the purpose of detailing the implementation of identified articles of the VAMDC Consortium Memorandum of Understanding. The document can be downloaded here.

The Internal Regulations cover the following items:

- Definitions
- VAMDC Consortium Activities
- Rules of Engagement
- Governance structure
  - The Legal Representative (provision of Art. 4.1.1 of MoU)
  - The VAMDC Consortium Scientific and Technical Board
  - The VAMDC Consortium Administrative Committee
  - The VAMDC Consortium Legal Committee
- The « VAMDC » brand
- Financial Provisions
- Licences
- Core and non-core components of VAMDC e-infrastructure
- Terms and Conditions
  - Disclaimers
  - Policy Citation
- Dissemination
- Technical by Law
  - Introduction
  - Duties for data and/or service provider
Partners

15 full members today, 5-7 FM candidates

+ Associated Members candidates

Astronomski Opservatorija (Serbia, M. Dimitrijevic)
Observatory of Cagliari - INAF (Italy, G. Mulas)
Observatory of Catania – INAF (Italy, G. Leto)
Observatory of Paris (France, M.L. Dubernet)

Queen’s University Belfast (UK, T. Millar)
Open University (UK, N. Mason)
University of Cambridge (UK, N. Walton)
University College London (UK, J. Tennyson)
Uppsala Universitet (Sweden, N. Piskunov)
Universitaet zu Koeln (Germany, S. Schlemmer)
Université de Bordeaux (France, V. Wakelam)
Université de Bourgogne (Dijon, V. Boudon)
Université de Champagne-Ardenne (Reims, V. Tyuterev)
Université Joseph Fourier (Grenoble, B. Schmitt)
Université Paul Sabatier (Toulouse, C. Joblin)
Universitaet Wien (Austria)
Atomic and Molecular Data Unit (IAEA, B. Braams)

University of South Africa (D. Smits)

Institute for Astronomy RAS (T. Ryabchikova)
Institute of Atmospheric Optics (V. Perevalov)
Institute of Spectroscopy RAS (A. Ryabtsev)
& RFNC (P. Loboda)

NIST (Y. Ralchenko, C. Gonzalez)
The Harvard-Smithsonian Center for Astrophysics (L. Rothman)
Jet Propulsion Laboratory from NASA, CALTECH (B. Drouin)

Universidade Federal do Paraná (Brazil, M. Fujimoto)
Corporacion Parque tecnologico de Merida (IVIC, C. Mendoza)

Tata Institute for Fundamental Research (India, E Krishnakumar)
Korea Atomic Energy Reserch Institute (South Korea, Y. Rhee)
Australian National University Flinders University (Australia, M. Brunger)
National Institute for Fusion Science (Japan, NIFS, I. Murakami)
Other People

(MLD apologizes for missing some names)

- Sweden: T. Marquart, E. Stempels, U. Heiter (Uppsala)
- UK: C. Hill, K. Benson (UCL), G. Rixon, G. del Zanna, H. Mason (Cambridge), A. Markwick (UMIST QUB)
- Germany: C. Endres
- Serbia: D. Jevremovic (AOB Belgrade)
- Russia: Y. Pakhomov (INASAN), A. Fazliev (Tomsk), S. Gagarin (RFTN)
- Italy: G. Malloci, A. Saba (INAF Cagliari)
- France: P. Gratier (Bordeaux), T. Louge, C. Vastel, J.M. Glorian, E. Caux, A. Walters, L. Pitchford (Toulouse), R. Surleau, new Ing. X (Dijon), L. Daumont, M. Rotger (Reims), D. Albert (Grenoble), N. Moreau, Y.A. Ba, C.M. Zwölf, F. Delahaye, D. Egret, S. Sahal-Bréchot, E. Roueff, C. Zeippen, M. Doronin (left) (Obs de Paris)
About us
<table>
<thead>
<tr>
<th>Databases</th>
<th>Type of A&amp;M Data</th>
<th>Partners</th>
<th>Application’s Fields</th>
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<td>Stellar - GAIA</td>
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<td>Russia (RFNC VNIITF ) – P. Loboda</td>
<td>Solar/Stellar Physics + Fusion</td>
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<td>Observatory of Belgrade (Serbia) + Observatory of Paris (LERMA) – M. Dimitrijevic/S. Sahal-Bréchot</td>
<td>Stellar Physics + Plasmas</td>
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<td>Biology – radiation Damage</td>
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<td>Plasmas - Etching</td>
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<td>2 other nodes of RADAM</td>
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How is VAMDC technically organised?

- A set of standards (www.vamdc.eu/standards)
  - Data exchange Protocols, Data Description
  - Standard vocabulary for all exchanges, including for registration of resources

- A set of software (www.vamdc.eu/software)

- Documentation and on-line support system (www.vamdc.eu)
- Monitoring of services
VAMDC aims to be an interoperable e-infrastructure that provides the international research community with access to a broad range of atomic and molecular (A&M) data compiled within a set of A&M databases accessible through the provision of a single portal and of user software. Furthermore VAMDC aims to provide A&M data providers and compilers with a large dissemination platform for their work.
What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

- Query all registered databases via the Portal ([www.portal.eu](http://www.portal.eu)) or other portals
  - Visualisation of Data
  - Download of Data

- Standalone Work with Software:
  - Query databases & Mix heterogeneous databases
  - Example of SPECTCOL software

- Use of our libraries in user applications in order to access the VAMDC registered databases

- Include new databases or data in the infrastructure
What can we currently do with VAMDC?

Portal User Guide
Tutorials For Portal

RESEARCH SERVICES

Access to Data
VAMDC Research Portal
RADAM Portal

Software
SPECTCOL
SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal
TAPValidator
Java NodeSoftware
Python NodeSoftware
Libraries
Virtual machines for node building

Documents
Standards
Science use cases
Tutorials
See our videos
FAQ

TUTORIALS
We provide different tutorial addressed both to data providers and final users.
Follow the links below for further information on each item of the following list:

- General page for Tutorials
- You produce/collection atomic and molecular data and want to include them into VAMDC
  - Outline
  - Self-Study Course
- How to use the VAMDC Portal
  - User Guide for the Portal
  - First Steps with the VAMDC Portal
  - Extracting Data from query results with the viewers
- How to use VAMDC software
  - Spectcol – Readmore
  - Specview – Readmore
  - PDL-VAMDC – Readmore
  - The XSAMS file format and TAP Validator application (mainly for the data providers)
  - Python Scripting
  - Using VAMDC Java libraries
  - You want to check XSAMS files, TAPValidator – ReadMore
### Query Execution

1. **Modify query**
2. **Stop waiting**
3. **Save query**

#### Comments

```
select * where ((AtomSymbol = 'Ti'))
```

### Results Conversion (entries starting with ** are recommended)

- **BibTeX from XSAMS**
- **Table views of XSAMS**
- **Atomicxsams2HTML**
- **XSAMS multiplexor**
- **Collisional data XSAMS to HTML**
- **Xsams2SME**

### Results by node

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<th>Name</th>
<th>Convert</th>
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<th>Download</th>
<th>Species</th>
<th>States</th>
<th>Processes</th>
<th>Radiative</th>
<th>Collisions</th>
<th>Non Radiative</th>
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XSAMS Processor Services independant of Portal: can have your own on portal
## For atomic and molecular spectroscopy

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<td>3s 3p</td>
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<td></td>
</tr>
</tbody>
</table>
Data are sent to TOPCAT VO tool
Full compatibility with Virtual Observatory Tools

OUR NEW VISUALISATION on PORTAL
Visualisation Collisions

Results from VAMDC node

Rate Coefficients of Rotational de-excitation of CO by para-HS$_2$S ($j=0$), 5K < T < 70K - 6 levels (Wernli et al., 2006)

<table>
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<th>Rate Coefficients</th>
<th>Unselect all</th>
<th>I1</th>
<th>I2</th>
<th>F1</th>
<th>F2</th>
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<td>3.18E-11</td>
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<td>2: Rotational excitation of CO by ortho-HS$_2$S (Flower, 2001)</td>
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<td>1</td>
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<td>4: Rotational de-excitation of CO by H for 5K &lt; T &lt; 100K (Balakrishnan &amp; al., 2002)</td>
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<td>2</td>
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<td>5: Vibrational de-excitation of CO by H (Balakrishnan &amp; al., 2002)</td>
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<td>6: Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini &amp; al., 2002)</td>
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<td>1</td>
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<tr>
<td>7: Vibrational de-excitation of CO by He (Cecchi-Pestellini &amp; al., 2002)</td>
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<td>3</td>
<td>1</td>
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<td>5.9E-12</td>
</tr>
</tbody>
</table>

IAU– VAMDC - 05/08/2015
What is the portal / What it is not

- Portal gives a visibility on the content of all the databases
- A single way to query all databases
- A single way to visualise the data
  - A single format description for quantities and quantum numbers
- Cannot perform the specific services that some databases might provide
  - Portal might be a first step towards finding the data
Work currently in progress

- Beginner mode: a guided way to query
- Processors (visualisation of data)
  - Improve association of processors/database
  - Add new processors, i.e. KIDA/UdfA databases
- Systematic quality check of all outputs of databases
- Timestamp on the datasets
- Identification of the datasets via DOI
  - Versioning of Data
  - Citation of Datasets
- Limitation on size of files retrieved from DB
  - Asynchronous mode that allows download of more data
  - Political restrictions imposed by the DB owners
- Link to Evaluation/Validation Groups: Data Quality
What can we currently do with VAMDC?

**Virtual Atomic and Molecular Data Centre**

- Query all registered databases via the Portal ([www.portal.eu](http://www.portal.eu)) or other portals
  - Visualisation of Data
  - Download of Data

- Standalone Work with Software:
  - Query databases & Mix heterogeneous databases
    - *Example of SPECTCOL software*

- Use of our libraries in user applications in order to access the VAMDC registered databases

- Include new databases or data in the infrastructure
SPECTCOL is a graphical tool implemented in Java. It allows to manipulate and combine spectroscopic and collisional data coming from the databases (BASECOL, CDMS, HITRAN, JPL, ...) using VAMDC technology.

XSAMS (XML Schema for Atoms, Molecules and Solids) is the VAMDC data format and SPECTCOL is able to manipulate and provides methods to convert these data into other formats (CSV, RADEX, LTE ...).

For any question or feedback use the forum link [here](#).

Credits:
M.L. Dubernet, Y.A. Ba, L. Nenadovic, M. Doronin

BSD Licence, @VAMDC Copyright

Scientific Use Case
Provide to users GUI to solve specific users problems

SPECTCOL Tool: Y.A. Ba (Obs Paris, LERMA)

Understanding the Language of Interstellar Molecules

Non-LTE Analysis of Spectra requires Combined spectroscopic And collision Data

CDMS

BASECOL

Courtesy of Stephan Schlemmer

IAU–VAMDC - 05/08/2015
Spectro and Collisions are combined and saved in customized outputs

Next Version:
Same query as portal
Find all DB
Send Data to TopCat for visualisation
What can we currently do with VAMDC?

**Virtual Atomic and Molecular Data Centre**

- Query all registered databases via the Portal ([www.portal.eu](http://www.portal.eu)) or other portals
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- Include new databases or data in the infrastructure
Specview is a tool for 1-D spectral visualization and analysis of astronomical spectrograms. It is written in Java thus can be run anywhere Java is supported. Specview is capable of reading all the Hubble Space Telescope spectral data formats, as well as data from several other instruments (such as IUE, FUSE, ISO, FORS and SDSS), preview spectra from MAST, and data from generic FITS and ASCII tables. It can also read data from Virtual Observatory servers, and read and write spectrogram data in Virtual Observatory SED format. It can also read files in the SPC Galactic format used in the chemistry field.

Specview can overplot spectral line identifications taken from a variety of line lists, including user-supplied lists. Its linelists’ query form has been modified to include the VAMDC Query Module, called QueryBuilder, thus providing the full capability of querying the VAMDC databases. In particular it allows to select finely the observed species and properties of linelists. Currently about 20 spectroscopic databases are inter-connected through VAMDC and accessible through VAMDC software and libraries.
Accessing VAMDC from User’s Tool
Specview Software
LESIA, Observatoire de Paris, J. Aboudarham
Support from VAMDC: N. Moreau, LERMA
The CASSIS (Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques) software has been developed by CESR/IRAP since 2005. All information about it can be found on a dedicated website: http://cassis.irap.omp.eu. The functionalities are represented in the flowchart below:

- **Astrophysical template** (fixed parameters $N$, $T_k$, $T_{ex}$, $N_{H_2}$, $\Delta v$, choice of the molecule...)
- **Observed spectra** (laboratory or telescope)
- **CASSIS**
  - LTE model and Radex
  - Parameters to vary: $N$, $T_k$, $T_{ex}$, $n_{H_2}$, $\Delta v$, choice of the molecule and telescope, beam dilution...
- **Synthetic spectra, Line identification, Adjustment of the source parameters**
- **Spectroscopic and molecular databases** (JPL, CDMS, HITRAN, Basecol, LAMDA, NIST)
myXCLASS for CASA

C. Endres (VAMDC Support), T. Möller, P. Schilke, University of Cologne

VAMDC has supported the development of a toolbox (1) for the Common Astronomy Software Applications package (CASA) in order to include access to its databases. The toolbox contains the myXCLASS program, which is used to model astronomical spectra by solving the radiative transfer equation for an isothermal object in one dimension, whereas the finite source size and dust attenuation are considered as well.

(1) http://www.astro.uni-koeln.de/projects/schilke/myXCLASSInterface

Schilke et al., ArXiv e-prints, 1403.7902 (2014)
What can we currently do with **VAMDC**?

**Virtual Atomic and Molecular Data Centre**

- Query all registered databases via the Portal ([www.portal.eu](http://www.portal.eu)) or other portals
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  - Download of Data

- Standalone Work with Software:
  - Query databases & Mix heterogeneous databases
  - *Example of SPECTCOL software*

- Use of our libraries in user applications in order to access the VAMDC registered databases

- **Include new databases or data in the infrastructure**
Include your data in VAMDC

Include your data in existing Database connected to VAMDC
- Contact the DB manager directly
- Contact VAMDC Support: support@vamdc.eu

Create a new DB to be connected to VAMDC
- Contact a node in order to include your DB at their node
- Contact VAMDC Support: support@vamdc.eu
  - To include at an existing node
  - To create a new node
Tutorials For Data Producers

RESEARCH SERVICES

TUTORIALS
We provide different tutorial addressed both to data providers and final users.
Follow the links below for further information on each item of the following list:

- General page for Tutorials

- You produce/collect atomic and molecular data and want to include them into VAMDC
  - Outline
  - Self-Study Course

- How to use the VAMDC Portal
  - User Guide for the Portal
  - First Steps with the VAMDC Portal
  - Extracting Data from query results with the viewers

- How to use VAMDC software
  - Spectcol – Readmore
  - Specview – Readmore
  - PDL-VAMDC – Readmore

- The XSAMS file format and TAP Validator application (mainly for the data providers)
  - Python Scripting
  - Using VAMDC Java libraries
  - You want to check XSAMS files, TAPValidator – ReadMore

ACCESS TO THE DATA
Access to VAMDC databases

ACCESS TO THE FORUM
Exchange ideas, Ask questions, Find answers

Read more
or
Access to the forum
RESEARCH SERVICES

Access to Data
VAMDC Research Portal
RADAM Portal

Software
SPECTCOL
SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal
TAPValidator
Java NodeSoftware
Python NodeSoftware
Libraries
Virtual machines for node building

Documents
Standards
Science use cases
Tutorials
See our videos
FAQ

STANDARDS

VAMDC standards are a set of norms, protocols, regulations which are the basis of the VAMDC-infrastructure operations.

Follow the links below for further information on each item of the following list:

- [VAMDC standards documentation page](#)
  - [VAMDC documentation and software versioning policy](#)
  - [Data access protocol, query language and dictionaries](#)
  - [Data model](#)
  - [Registry](#)
  - [Units](#)
  - [InChI Generation](#)
  - [XSAMS Processor service](#)

Official citation of VAMDC standards

The official citation of VAMDC standards is:

XSAMS tree: XML Schema for Atoms, Molecules and Solids
Case-by-Case Quantum Number Descriptions

1. des: Diatomic closed-shell molecules
2. hunda: Hund's case (a) diatomics
3. hundb: Hund's case (b) diatomics
4. ltc: Closed-shell, linear triatomic molecules
5. nltcs: Closed-shell, non-linear triatomics
6. sctes: Closed shell, symmetric-top molecules
7. lpcs: Closed-shell, linear polyatomic molecules
8. asymcs: Closed-shell, asymmetric top molecules
9. asymos: Open-shell, asymmetric top molecules
10. sphcs: Closed-shell, spherical-top molecules
11. sphpos: Open-shell, spherical-top molecules
12. ltos: Open-shell linear triatomic molecules
13. ltops: Open-shell, linear polyatomic molecules
14. nltos: Open-shell, non-linear triatomic
AtomicState

List of atomic states within an ion

Description
- An arbitrary label
- Numerical parameters describing an atomic state
- Discrete quantum numbers describing an atomic state
- Expansion of the wavefunction in a specific basis
Advantages of Inclusion in VAMDC

- Each Data is precisely described and referenced
  - Allows to check consistency of Databases
- Methodology to obtain data can be included

- Uniform query and visualisation
  - Similar Databases can be compared

- Allows visibility of small databases
- Allowed new paradigms for existing DB: CDMS, HITRAN
We provide on-line and face-to-face support

- To include your data and your databases
- To implement our « modules » in your software
- To use our software, our standards

- We can organize tutorials
- We can support visits for the purpose of implementation
- We have communications channels that are available to all
Can create WG for discussions on specific topics: data needs, data evaluation.

If critical mass and sufficient interest, official VAMDC WG can be created and have specific inputs from our Research Activities Website.
RESEARCH NEWS

Software

Standards

Publications

2014/09/01 - SPECTCOL 4th Release software
Version 12.07-r2

2013/12/01 - SPECTCOL 3rd release software
Version 12.07-r1

2011/05/27 - Standards 1st release standards
Version 11.05

EVENTS

Conferences
Research
Education
Industry
Outreach

Workshops
Research
Industry

Tutorials

2015/08/24 - 2015/08/28 - 24th Colloquium on High Resolution Molecular Spectroscopy
Conferences
The Twenty Fourth Colloquium on High Resolution Molecular Spectroscopy that will take place in Dijon, France, on August 24-28, 2015.

2015/08/03 - 2015/08/14 - XXIX General Assembly IAU 2015
Conferences
XXIX General Assembly IAU (http://astronomy2015.org), Hawaii, August 3-14, 2015

2015/06/15 - 2015/06/19 - VAMDC at spring 2015 Interop in Sexto
Conferences
The IVOA is an organisation aiming at creating interoperability standards to publish and exchange astronomical data. It will held a meeting in Sexten, Italy, between

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Partners blog
Populär Astronomi Blog in Swedish
See the blog

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Provide easy access to atomic and molecular data to the widest range of users
Strengthen links

VAMDC

EDUCATION

INDUSTRY

RESEARCH