VAMDC

Virtual Atomic and Molecular Data Centre

Science Use Cases and the Consortium

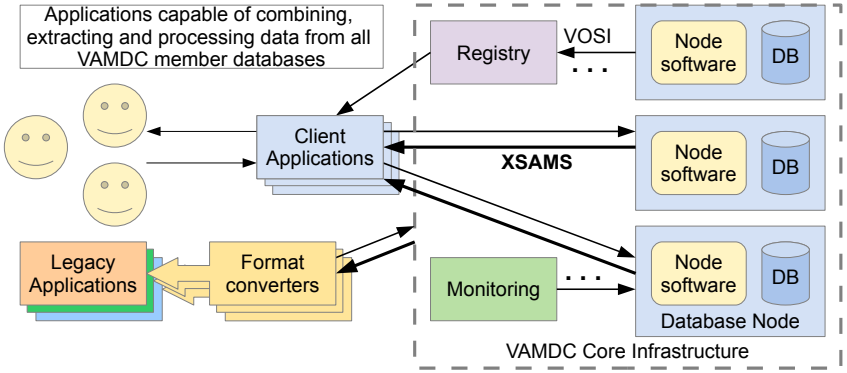
http://www.vamdc.eu

M.L. Dubernet[1], Y.A. Ba[1], N. Moreau[1], C.M. Zwölf[1]

And VAMDC Collaboration

[1]Paris Observatory, LERMA, VO-PDC

How is VAMDC e-infrastructure organised ?



- A set of standards (www.vamdc.eu/standards)
  - Data exchange Protocols, Data Description
  - Standard vocabulary for all exchanges, including for registration of ressources
- A set of software (www.vamdc.eu/software)
  - Node Software for implementation of databases within VAMDC
  - JAVA Librairies for the same purpose and to be used in user applications in order to access our databases and to handle the data
  - Software to check the outputs of databases within VAMDC
  - User software for the interstellar medium (will be extended) → SPECTCOL
  - Software Modules in different languages aimed at accessing infrastructure
- Documentation and on-line support system (www.vamdc.eu)
- Monitoring of services

Who has participated ?

EUROPE

Observatoire Astronomique (M. Dimitrijevic, Belgrade, Serbia)
Observatoire de Cagliari-INAF (G. Mulas, Italy)
Observatoire de Catania-INAF (G. Leto, Italy)
Observatoire de Paris (M.L. Dubernet et al)
Open University (N. Mason, UK)
Queen's University Belfast (T. Millar, UK)
University College London (J. Tennyson, UK)
University Joseph Fourier (B. Schmitt, Grenoble)
University of Bordeaux (V. Wakelam, Bordeaux)
University of Bourgogne (V. Boudon, Dijon)
University of Cambridge (N. Walton, UK)
University of Champagne-Ardenne (V. Tyuterev, Reims)
University of Cologne (S. Schlemmer, G.)
University of Uppsala (N. Piskunov, Sweden)
CNRS (France)
Universitaet Wien (Austria)
Université Paul Sabatier (Toulouse)
Atomic and Molecular Data Unit (IAEA, Austria)

Africa

University of South Africa, South Africa

RUSSIA

Institute of Spectroscopy RAS
Institute of Atmospheric Optics
Institute for Astronomy RAS
Russian Federal Nuclear Center- All-Russian Institute of Technical Physics

South America

Corporacion Parque tecnologico de Merida (IVIC)
Universidade Federal do Paraná (Brazil)

ASIA-PACIFIC

Tata Institute for Fundamental Research, India
Korea Atomic Energy Reserch Institute, South Korea
Australian National University
Flinders University (Australia)
National Institute for Fusion Science (Japan)

USA

NIST
The Harvard-Smithsonian Center for Astrophysics
Jet Propulsion Laboratory from NASA, CALTECH

VAMDC consortium

SUP VAMDC

Home | About Us | Services | News

You are here > About Us > **Databases**

ABOUT US

Presentation

Partners
France
UK
Germany
Sweden
Austria
Italy
Russia
USA
Australia
India
Korea
South Africa

Databases
France
UK
Germany
Sweden
Russia
Italy
USA

Logo

ECaSDa – Ethene Calculated Spectroscopic Database
Calculated data of ethylene (12C2H4). The data on ethylene contain the vibration-rotation energy levels, line positions
http://vamdc.univ-reims.fr/PHP/ethylene.php

Read more

Logo

VAMDC species-DB
This Database contains all the species and its VAMDC-Species Ids which are used by VAMDC
star.pst.qub.ac.uk/vamdc/inchiservice/db/

Read more

KIDA
The KInetic Database for Astrochemistry (KIDA) is a database of chemical reactions used in chemical models for astrophysical environments such as the interstellar medium and planetary atmospheres.
kida.obs.u-bordeaux1.fr/

Read more

Logo

Water internet Accessible Distributed Information System
Database containing information on water spectras, notably data on H216O, HDO, D2O, H217O and H218O
wadis.saga.iao.ru/

Read more

e-infrastructure

Databases	Type of A&M Data	Partners	Application's Fields
VALD	Atomic Linelists	Uppsalla, Vienna, Moscow – N. Piskunov	Stellar - GAIA
CHIANTI	Atomic Linelists and collisions	Cambridge (UK)+MSSL/UCL – H. Mason, G. Rixon	Solar Physics
Spectr-W3	Atomic Linelists and Collisions	Russia (RFNC VNIITF) – P. Loboda	Solar/Stellar Physics + Fusion
STARK-B	Atomic LineShifts/Broadening with charged perturbers	Observatory of Belgrade (Serbia) + Observatory of Paris (LERMA) – M. Dimitrijevic/S. Sahal-Bréchot	Stellar Physics + Plasmas
TIPBASE, TopBase	Atomic Linelists and Collisions from Opacity Project and IRON Project	Observatory of Paris (LERMA) + CTPM (Venezuela) + CDS (Strasbourg, Fce) – C. Zeippen/C. Mendoza/F. Delahaye	Stellar Physics
CDMS	Molecular Linelists (mm, Sub-mm)	Cologne (Germany) – S. Schlemmer	ISM + Earth
JPL	Molecular Linelists (mm, Sub-mm)	Pasadena (USA) + Cologne (Germany) – B. Drouin	ISM + Earth
SMPO	O_3 linelists	Reims (France)+ Tomsk (Russia) – V. Tyuterev	Earth – Exo-Planets
MeCaSDa	Linelists **CH_4**	Dijon (France) – V. Boudon	Earth, Planets, Exo-

Databases	Type of A&M Data	Partners	Application's Fields
HITRAN	Molecular Linelists and Broadening Coefficients	Harvard (USA) + UCL – L. Rothman+ J. Tennyson	Earth, Planets, Exo-Planets
CDSD	CO_2 Linelists	IAO, Tomsk – V. Perevalov	Earth, Planets, Brown Dwarfs
W@SIS	Water Information System	IAO, Tomsk – A. Fazliev+ UCL (J. Tennyson)	Earth and Planets
KIDA	Kinetic Data	Bordeaux (France) – V. Wakelam	ISM - Planetology
UdfA	Kinetic Data (ex-UMIST)	Belfast (UK) – T. Millar	ISM - Planetology
GhoSST	Solid Spectroscopy Data	Grenoble (France) – B. Schmitt	Planetology, ISM
LASP	Solid Spectroscopy Data	Obs. of Catania – G. Leto	Planetology, ISM
BASECOL	Low Energy Molecular Collisions	Observatory of Paris – M.L. Dubernet	ISM
PAH	PAH Theoretical Data and soon experimental Data	Observatory of Cagliari (Italy) – IRAP (Toulouse, France) – G. Mulas+C. Joblin	ISM and Planets

Databases	Type of A&M Data	Partners	Application's Fields
Lund DB	Experimental Data for transitions and lifetimes	Lund University	Stellar
RADAM	Database for Radiation damage of molecules of biological interest induced by ion collisions: cross sections and fragmentation yields	GANIL - FRANCE	Biology – radiation Damage
IDEABD	Dissociative electron attachment upon interaction of low energy electrons with molecules.	Innsbrück	Radiation Damage
ECaSDa	Ethene Calculated LInelists	Reims – L. Daumont	Earth and Planets
ALADDIN2	Sub-Set of IAEA ALADDIN : atomic collisions	IAEA - Vienna	Plasmas
DESIRE	Spectroscopy of Rare Earth Element	Belgium	Plasmas - Etching
SESAME	Electronic Spectra of atoms and molecules	Paris Obs. – E. Roueff	ISM - Stellar

What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

- **Query all registered databases via the Portal (www.portal.eu) or orther portals**
  - **Visualisation of Data**
  - **Download of Data**
  - **(Maintenance/Upgrade: M. Doronin, N. Moreau)**

- Standalone Work with Software:
  - Query databases
  - Mix heterogeneous databases
  - Download
  - → *Example of SPECTCOL software (Y.A. Ba)*

- Include new databases or data in the infrastructure

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

VAMDC Portal

portal.vamdc.eu/vamdc_portal_test/query.seam

Most Visited | Latest Headlines | Apple | Wikipédia | Google Maps | SourceForge.net ... | XSAMS – Browse... | VAMDC Infrastr... | reStructuredTex... | VAMDC/Standar... | Bookmarks

VAMDC Virtual Atomic and Molecular Data Centre

Portal User Guide

Home | VAMDC databases | Query | Saved queries | Info | Known issues | Login | Register

Query by...
- Species
- Processes
- Environment
- Advanced

Molecules Clear Remove

Chemical name: CO

Stoichiometric formula

Structural formula

Spin isomer

InChIKey

Methylene Glycol
Methyl alcohol
Methylic alcohol
Wood alcohol
Carbon oxide (CO2)
CO2
Dricold
Carbon oxide (CO)
CO
Acido cloridrico
Acido bromidrico
COS
Polyoxymethylene glycols

Find data | Save query

Legend
available, can answer
available, don't support query
unsupported keyword

- Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- ICB Dijon Methane
- VALD (atoms)
- Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)
- BASECOL: VAMDC-TAP interface
- TOPbase : VAMDC-TAP interface
- Theoretical spectral database of polycyclic aromatic hydrocarbons
- Chianti
- TIPbase : VAMDC-TAP interface
- GSMA Reims S&MPO
- GSMA Reims Ethylene
- TAP-XSAMS for GhoSST database
- Lund laboratory spectroscopy database
- Stark-b
- Spectr-W3
- Water internet Accessible Distributed Information System
- HITRAN-UCL resource
- VALD sub-set in Moscow (obs)
- KIDA: VAMDC-TAP interface

Only possible through SPECIES Database based on InchiKey and VAMDC Identifier

XSAMS Processor Services independant of Portal: can have your own on portal

1 : Query Execution

Done

Modify query | Stop waiting | Save query

select * where ((InchiKey IN ('UGFAIRIUMAVXCW-RGIGPVFXSA-N','UGFAIRIUMAVXCW-ZDOIIHCHSA-N','UGFAIRIUMAVXCW-HQMMCQRPSA-N','UGFAIRIUMAVXCW-VQEHIDDOSA-N','UGFAIRIUMAVXCW-UHFFFAOYSA-N','UGFAIRIUMAVXCW-OUBTZVSYSA-N')))

Comments

3 : Results Conversion (select in table below)

- BibTeX from XSAMS
- Table views of XSAMS
- Xsams2SME
- Atomicxsams2HTML
- Molecular Spectroscopy XSAMS to HTML
- XSAMS multiplexor

Process

XSAMS processor converting a XSAMS file containing molecular spectroscopy data into a HTML file

2 : Results by node

Name	Convert	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
HITRAN-UCL resource	☐	OK	XSAMS	6	1947	4477	4477	0	0
KIDA: VAMDC-TAP interface	☐	OK (14/10/2014 15:28)	XSAMS	1	0	540	0	540	0
UMIST Database for Astrochemistry	☐	OK	XSAMS	223	0	408	0	408	0
BASECOL: VAMDC-TAP interface	☐	OK (01/06/2012 00:00)	XSAMS	6	0	11	0	11	0
VAMDC species-DB	☐	OK	XSAMS	6	0	0	0	0	0
Belgrade electron/atom(molecule) database (BEAMDB)	☐	OK	XSAMS	0	0	0	0	0	0
SpEctroScopy of Atoms and Molecules	☐	TRUNCATED (43%)	XSAMS	1	1565	2000	2000	0	0
CDMS	☑	TRUNCATED (09/09/2014 16:36) (1%)	XSAMS	7	1059	1592	1592	0	0
Water internet Accessible Distributed Information System	☐	TRUNCATED (06/12/2012 18:00) (9%)	XSAMS	2	405	1000	1000	0	0
JPL database: VAMDC-TAP service	☐	TRUNCATED (05/09/2013 15:54) (1%)	XSAMS	4	265	261	261	0	0
DESIRE database (Moscow mirror)		EMPTY		0	0	0	0	0	0
IDEADB - Innsbruck Dissociative Electron Attachment		EMPTY		0	0	0	0	0	0

For molecular spectroscopy

Menu

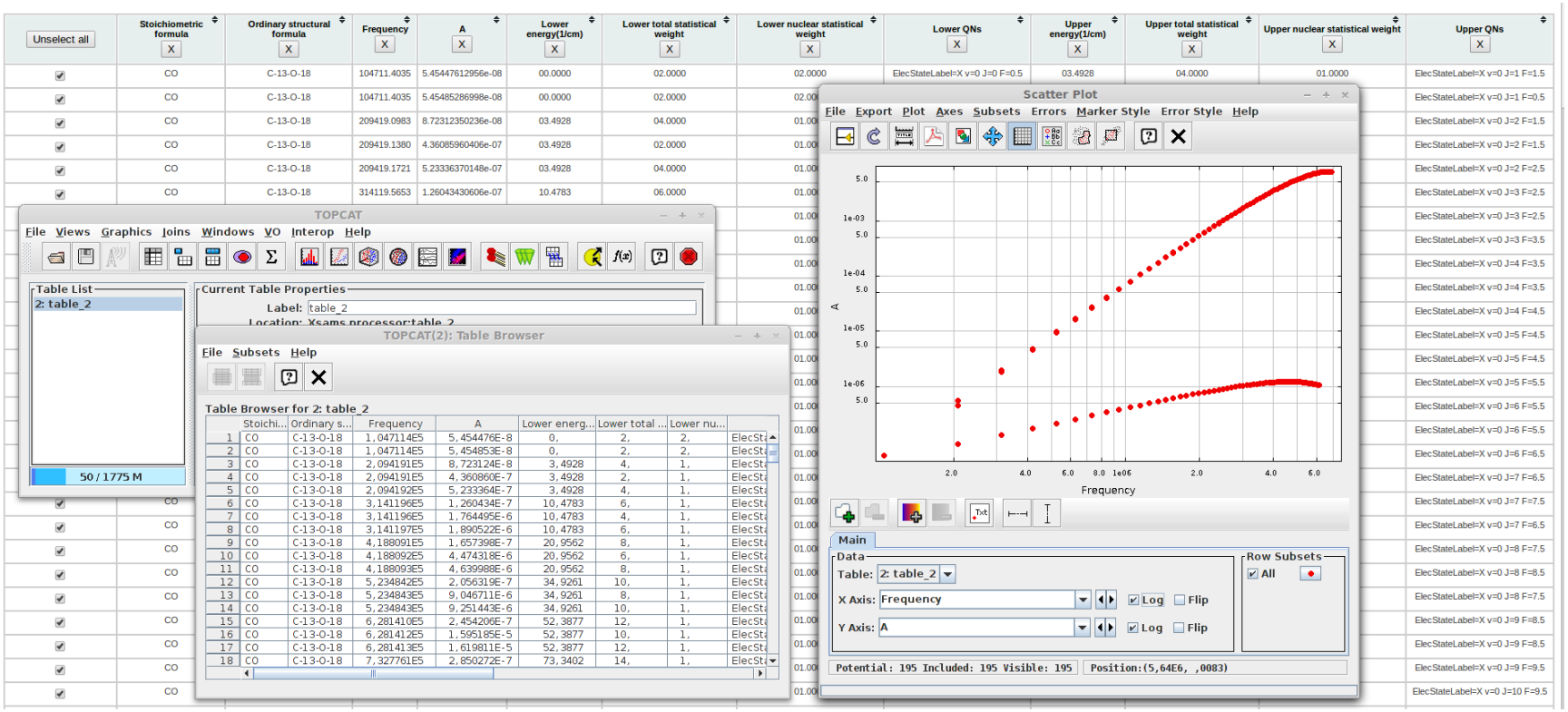
- Export as CSV
- Export as JSON
- Export as VOTable
- Send with samp
- Reset page

Sources

Id	Title	Origin	Authors	Year	Link
BCDMS-176		journal : Astrophys. J. (Vol : 582 , Page Begin : 262 , Page End : 268)	Klapper, G.; Surin, L.; Lewen, F.; Müller, H. S. P.; Pak, I.; Winnewisser, G.;	2003	
BCDMS-177		journal : Phys. Chem. Chem. Phys. (Vol : 4 , Page Begin : 3575)	Cazzoli, G.; Dore, L.; Puzzarini, C.; Beninati, S.;	2002	
BCDMS-178		journal : Astrophys. J. Suppl. (Vol : 95 , Page Begin : 535)	Goorvitch, D.;	1994	
BCDMS-331		journal : J. Mol. Spectrosc. (Vol : 201 , Page Begin : 124)	Klapper, G.; Lewen, F.; Gendriesch, R.; Belov, S. P.; Winnewisser, G.;	2000	
BCDMS-332		journal : J. Mol. Spectrosc. (Vol : 143 , Page Begin : 304)	Zink, L. R.; Natale, P.; Pavone, F. S.; Prevedelli, M.; Evenson, K. M.; Inguscio, M.;	1990	
BCDMS-333		journal : Astrophys. J. (Vol : 611 , Page Begin : 615 , Page End : 620)	Cazzoli, G.; Puzzarini, C.; Lpinov, A. V.;	2004	
BCDMS-344		journal : Z. Naturforsch. (Vol : 55a , Page Begin : 441)	Klapper, G.; Lewen, F.; Belov, S. P.; Winnewisser, G.;	2000	
BCDMS-345		journal : J. Mol. Spectrosc. (Vol : 98 , Page Begin : 64)	Guelachvili, G.; De Villeneuve, G.; arrenq, R.; Urban, W.; Verges, J.;	1983	
BCDMS-921		journal : Astron. Astrophys. (Vol : 497 , Page Begin : 927 , Page End : 930)	Gendriesch, R.; Lewen, F.; Klapper, G.; Menten, K. M.; Winnewisser, G.; Coxon, J. A.; Müller, H. S. P.;	2009	
BCDMS-1919		journal : J. Mol. Spectrosc. (Vol : 174 , Page Begin : 606 , Page End : 612)	Belov, S.P.; Lewen, F.; Klaus, T.; Winnewisser, G.;	1995	
BCDMS-1920		private communication : 52nd Okazaki Conference, Okazaki, Japan	Evenson, K. M.;	1995	
BCDMS-1921		database : CDMS database	Müller, H. S. P.; Endres, C. P.; Schlemmer, S.; Stutzki, J.;	2012	

Results from CDMS VAMDC node

Unselect all	Chemical name X	Stoichiometric formula X	Ordinary structural formula X	Frequency X	Frequency reference X	A X	Lower energy(1/cm) X	Lower total statistical weight X	Lower nuclear statistical weight X	Lower QNs X	Upper energy(1/cm) X	Upper total statistical weight X	Upper nuclear statistical weight X	Upper QNs X
☑	Carbon Monoxide	CO	C-13-O-18	104711.4035	BCDMS-344	0000.0000	00.0000	02.0000	02.0000	ElecStateLabel=X v=0 J=0 F=0.5	03.4928	04.0000	01.0000	ElecStateLabe v=0 J=1 F=1
☑	Carbon Monoxide	CO	C-13-O-18	104711.4035	BCDMS-344	0000.0000	00.0000	02.0000	02.0000	ElecStateLabel=X v=0 J=0 F=0.5	03.4928	02.0000	01.0000	ElecStateLabe v=0 J=1 F=0
☑	Carbon Monoxide	CO	C-13-O-17	107288.5500	BCDMS-176	0000.0000	00.0000	06.0000	01.0000	ElecStateLabel=X v=0 J=0 F=2.5	03.5788	08.0000	01.0000	ElecStateLabe v=0 J=1 F=3
☑	Carbon Monoxide	CO	C-13-O-17	107288.5500	BCDMS-176	0000.0000	00.0000	06.0000	01.0000	ElecStateLabel=X v=0 J=0 F=2.5	03.5788	04.0000	01.0000	ElecStateLabe v=0 J=1 F=1
☑	Carbon Monoxide	CO	C-13-O-17	107289.6500	BCDMS-176	0000.0000	00.0000	06.0000	01.0000	ElecStateLabel=X v=0 J=0 F=2.5	03.5788	06.0000	01.0000	ElecStateLabe v=0 J=1 F=2
☑	Carbon Monoxide	CO	CO-18	109782.1734	BCDMS-1435	0000.0000	00.0000	01.0000	01.0000	ElecStateLabel=X v=0 J=0	03.6619	03.0000	01.0000	ElecStateLabe v=0 J=1
☑	Carbon Monoxide	CO	C-13-O	110201.3216	BCDMS-333	0000.0000	00.0000	02.0000	01.0000	ElecStateLabel=X v=0 J=0 F=0.5	03.6759	02.0000	01.0000	ElecStateLabe v=0 J=1 F=0



Data are sent to TOPCAT VO tool

Full compatibility with Virtual Observatory Tools

What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

- Query all registered databases via the Portal (www.portal.eu) or orther portals
  - Visualisation of Data
  - Download of Data
- Standalone Work with Software:
  - Query databases
  - Mix heterogeneous databases
  - Download
  - → *Example of SPECTCOL software*
- Include new databases or data in the infrastructure
- Use of our libraries in user applications in order to access the VAMDC registered databases

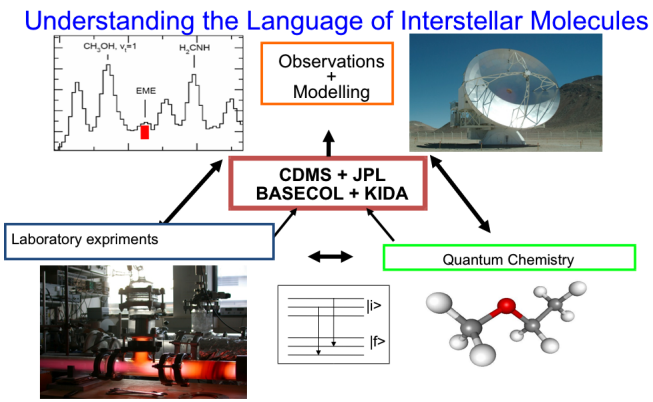
Provide to users GUI to solve specific users problems

SPECTCOL Tool: www.vamdc.eu/software

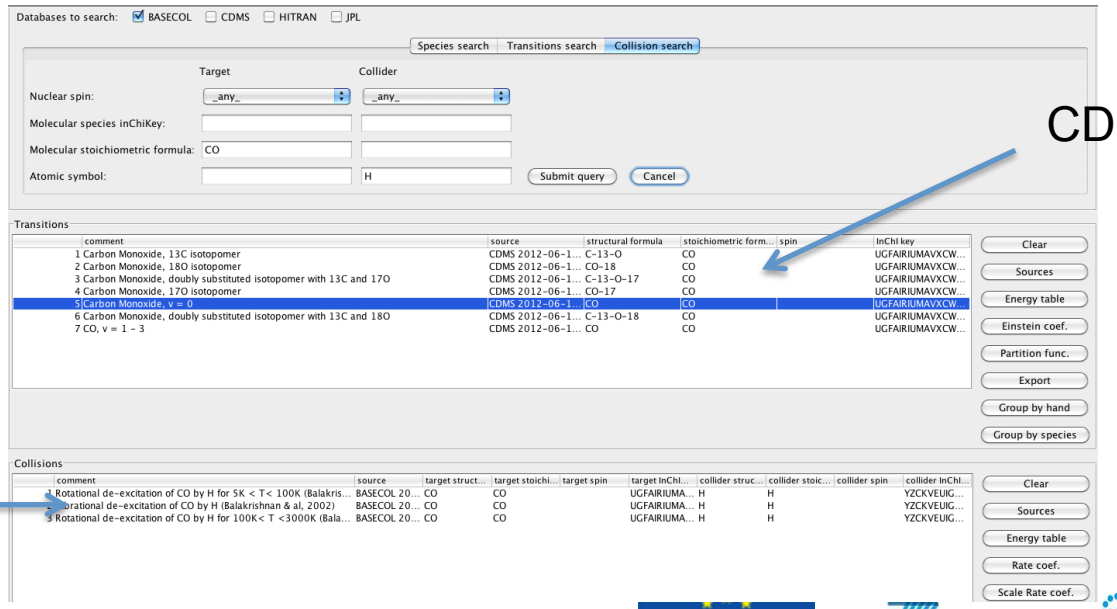
Current developer: Y.A. Ba, LERMA;

Tested&feedbacks by/from CASSIS Team (IRAP) and P. Schlike's Team (Koeln)

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



Courtesy of Stephan Schlemmer



CDMS

BASECOL

Import data from file

Browse... File path: collisions transitions Import

Search VAMDC databases

Databases to search: BASECOL CDMS HITRAN JPL

Species search | Transitions search | Collision search

Nuclear spin: _any_

Molecular species InChiKey:

Molecular stoichiometric formula: CO

Ion charge:

Atomic symbol:

Particle name:

Wavelength to A

Equivalent Wavelength A

Upper state energy: to 1/cm

Equivalent to 1/cm

Lower state energy: to 1/cm

Equivalent to 1/cm

Probability, A: to

Submit query Cancel

Transitions

	comment	source	structural formula	stoichiometric for...	spin
1	29501- v2*:C-13-O; $v=0$	CDMS 2014-10-...	C-13-O	CO	
2	30503- v 1:C-13-O-17; $v=0$	CDMS 2014-10-...	C-13-O-17	CO	
3	28503- v 1:CO; $v=0$	CDMS 2014-10-...	CO	CO	
4	31502- v 1:C-13-O-18; $v=0$	CDMS 2014-10-...	C-13-O-18	CO	
5	28512- v1*:CO; $v=1,2,3$	CDMS 2014-10-...	CO	CO	
6	30502- v 1:CO-18; $v=0$	CDMS 2014-10-...	CO-18	CO	
7	29503- v 1:CO-17; $v=0$	CDMS 2014-10-...	CO-17	CO	

Category	Source Name	Year	Authors	Title	Volu...	Digit...	Page...
JOURNAL	Z. Naturforsch.	2000	Klapper, G., Lewen, F., Belov, S. P., Winnewisser, G.		55a	10.1...	441
JOURNAL	J. Mol. Spectrosc.	1983	Guelachvili, G., De Villeneuve, G., arrenq, R., Urban, W., Verges, J.		98	10.1...	64
JOURNAL	Astrophys. J. Suppl.	1994	Goorvitch, D.		95	10.1...	535

```
@article{BCDMS-345,
author = "Guelachvili, G., De Villeneuve, G., arrenq, R., Urban, W., Verges, J.",
title = "",
journal = "J. Mol. Spectrosc.",
year = "1983",
volume = "98",
pages = "64"
}
```

Clear

Sources

Energy table

Einstein coef.

Partition func.

Export

Group by hand

Group by species

CDMS

BASECOL

Databases to search: ☑ BASECOL ☐ CDMS ☐ HITRAN ☐ JPL

Species search | Transitions search | Collision search

	Target	Collider
Nuclear spin:	_any_	_any_
Molecular species inChiKey:		
Molecular stoichiometric formula:	CO	
Atomic symbol:		H

Submit query | Cancel

Transitions

	comment	source	structural formula	stoichiometric form...	spin
1	Carbon Monoxide, 13C isotopomer	CDMS 2012-06-1...	C-13-O	CO	
2	Carbon Monoxide, 18O isotopomer	CDMS 2012-06-1...	CO-18	CO	
3	Carbon Monoxide, doubly substituted isotopomer with 13C and 17O	CDMS 2012-06-1...	C-13-O-17	CO	
4	Carbon Monoxide, 17O isotopomer	CDMS 2012-06-1...	CO-17	CO	
5	Carbon Monoxide, v = 0	CDMS 2012-06-1...	CO	CO	
6	Carbon Monoxide, doubly substituted isotopomer with 13C and 18O	CDMS 2012-06-1...	C-13-O-18	CO	
7	CO, v = 1 - 3	CDMS 2012-06-1...	CO	CO	

Collisions

	comment	source	target struct...	target stoichi...	target spin	target InChI...	collider struc...	collider
1	Rotational de-excitation of CO by H for 5K < T< 100K (Balakris...	BASECOL 20...	CO	CO		UGFAIRIUMA...	H	H
2	Vibrational de-excitation of CO by H (Balakrishnan & al, 2002)	BASECOL 20...	CO	CO		UGFAIRIUMA...	H	H
3	Rotational de-excitation of CO by H for 100K< T <3000K (Bala...	BASECOL 20...	CO	CO		UGFAIRIUMA...	H	H

Clear

Sources

Energy table

Einstein coef.

Partition func.

Export

Group by hand

Group by species

Spectro and Collisions are combined

State energy and quantum numbers

state	energy [1/cm]	J	v	F	F1	parity	r	AsSym
1	0	0	0					
2	3.845	1	0					
3	11.535	2	0					
4	23.069	3	0					
5	38.448	4	0					
6	57.67	5	0					
7	80.735	6	0					
8	107.642	7	0					
9	138.39	8	0					
10	172.978	9	0					
11	211.404	10	0					

Rate coefficients

I1	I2	F1	F2	5.0	10.0	20.0	40.0	60.0	80.0	100.0	200.0	300.0	500.0
2	1	1	1	3.4E-11	3.2E-11	3E-11	2.8E-11	2.7E-11	2.6E-11	2.6E-11	2.5E-11	2.5E-11	2.6E-11
3	1	1	1	1.3E-11	1.3E-11	1.2E-11	1.1E-11	1.1E-11	1.1E-11	1.1E-11	1.4E-11	1.6E-11	1.9E-11
3	1	2	1	4.2E-11	4.5E-11	4.5E-11	4.6E-11	4.7E-11	4.8E-11	4.9E-11	5E-11	5.2E-11	5.7E-11
4	1	1	1	6.2E-12	6.6E-12	7.2E-12	8.5E-12	9.5E-12	1E-11	1.1E-11	1.2E-11	1.3E-11	1.4E-11
4	1	2	1	2.3E-11	2.2E-11	2E-11	1.8E-11	1.8E-11	1.8E-11	1.9E-11	2.2E-11	2.6E-11	3.2E-11
4	1	3	1	4.6E-11	4.9E-11	5E-11	5.1E-11	5.2E-11	5.3E-11	5.4E-11	5.8E-11	6.1E-11	6.8E-11
5	1	1	1	1.8E-12	1.9E-12	1.9E-12	2E-12	2.1E-12	2.1E-12	2.2E-12	2.6E-12	3.1E-12	4E-12
5	1	2	1	1.3E-11	1.4E-11	1.5E-11	1.7E-11	1.8E-11	2E-11	2.1E-11	2.4E-11	2.7E-11	3.1E-11
5	1	3	1	2.7E-11	2.7E-11	2.4E-11	2.2E-11	2.2E-11	2.2E-11	2.3E-11	2.7E-11	3.1E-11	3.7E-11
5	1	4	1	5.3E-11	5.4E-11	5.4E-11	5.4E-11	5.4E-11	5.5E-11	5.6E-11	6E-11	6.4E-11	7.1E-11
6	1	1	1	1.4E-12	1.5E-12	1.8E-12	2.4E-12	2.9E-12	3.3E-12	3.7E-12	4.9E-12	5.6E-12	6.8E-12

Einstein coefficients

lower level	upper level	frequency [MHz]	Einstein coefficient [1/cm]	log(intensity) [unitless]	uncertainty	upper state degeneracy
1	2	115,271.202	7.20378864479E-8	-5.01		3
2	3	230,538	6.91079000503E-7	-4.12		5
3	4	345,795.99	2.49670085538E-6	-3.612		7
4	5	461,040.768	6.12668117242E-6	-3.266		9
5	6	576,267.931	1.22134274135E-5	-3.012		11
6	7	691,473.076	2.13750692698E-5	-2.819		13
7	8	806,651.801	3.42239824576E-5	-2.672		15
8	9	921,799.704	5.13419191151E-5	-2.559		17
9	10	1,036,912.385	7.33007011041E-5	-2.475		19
10	11	1,151,985.443	1.00638923207E-4	-2.416		21
11	12	1,267,014.482	1.33903406762E-4	-2.377		23

Collider state energy and quantum numbers

state	energy[1/cm]	parity	J	F	M	Kappa	term type	l	S	j	S2	K
1	0	0					LS	0	0			

Help

ZCWHFV...
ZCWHFV...

nChl key
GLNCZE...
GLNCZE...

Clear
Sources
Energy table
Einstein coef.
Export
Group by species

Clear
Sources
Energy table
Rate coef.
Export

and saved in customized outputs

Export

* ☐ energy ☐ rate coefficients ☐ Einstein coefficients ☐ collider energy ☐ partition function save as ASCII

* save as RADEX save as XSAMS

```
!Molecule
CO
!MASS
28.0
!Number of Energy Level
7
!LEVEL + ENERGY(CM^-1) + WEIGHT + QUANTUM NOS.  ElecStateLabel_J_v
    1           0.0    1    X_0_0
    2      3.845033    3    X_1_0
    3     11.534953    5    X_2_0
    4     23.069466    7    X_3_0
    5     38.448131    9    X_4_0
    6      57.67036   11    X_5_0
    7     80.735419   13    X_6_0
!NUMBER OF RADIATIVE TRANSITIONS
6
!TRANS + UP + LOW + EINSTEINA(s^-1) + FREQ(GHz) + E_up(K)
    1     2     1   7.2036e-8      115.2712018       5.532
    2     3     2   6.9106e-7      230.5380000      16.597
    3     4     3   2.4966e-6      345.7959899      33.193
    4     5     4   6.1265e-6      461.0407682      55.321
    5     6     5   1.2213e-5      576.2679305      82.979
    6     7     6   2.1375e-5      691.4730763     116.166
!NUMBER OF COLLISION PARTNERS
1
!COLLISIONS BETWEEN
6 CO-HE,  Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini & al, 2002)
!NUMBER OF COLLISIONAL TRANSITIONS
105
!NUMBER OF COLLISION TEMPERATURES
10
!COLLISION TEMPERATURES
    5.0 10.0    20.0    40.0    60.0    80.0    100.0   200.0   300.0   500.0
!TRANS + UP + LOW + RATE COEFFS(cm^3 s^-1)
    1     2     1   3.4e-11   3.2e-11     3e-11   2.8e-11   2.7e-11   2.6e-11   2.6e-11   2.5e-11   2.5e-11   2.6e-11
    2     3     1   1.3e-11   1.3e-11   1.2e-11   1.1e-11   1.1e-11   1.1e-11   1.1e-11   1.4e-11   1.6e-11   1.9e-11
    3     3     2   4.2e-11   4.5e-11   4.5e-11   4.6e-11   4.7e-11   4.8e-11   4.9e-11     5e-11   5.2e-11   5.7e-11
    4     4     1   6.2e-12   6.6e-12   7.2e-12   8.5e-12   9.5e-12     1e-11   1.1e-11   1.2e-11   1.3e-11   1.4e-11
    5     4     2   2.3e-11   2.2e-11     2e-11   1.8e-11   1.8e-11   1.8e-11   1.9e-11   2.2e-11   2.6e-11   3.2e-11
```

What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

- Query all registered databases via the Portal (www.portal.eu) or orther portals
  - Visualisation of Data
  - Download of Data

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

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

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

RESEARCH SERVICES

Access to Data
VAMDC Research Portal

Users/Developers
Software
SPECTCOL
SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal

Developers
Standards
Libraries
Tutorials
FAQ

TUTORIALS

We provide different tutorial addressed both to data providers and final users. These could be founded at the link: http://tutorial.vamdc.eu

(This page will be modified after the reorganization of tutorials website)

VAMDC-tutorials 1.0 documentation »

VAMDC tutorials ¶

Contents:

What can we currently do with VAMDC?

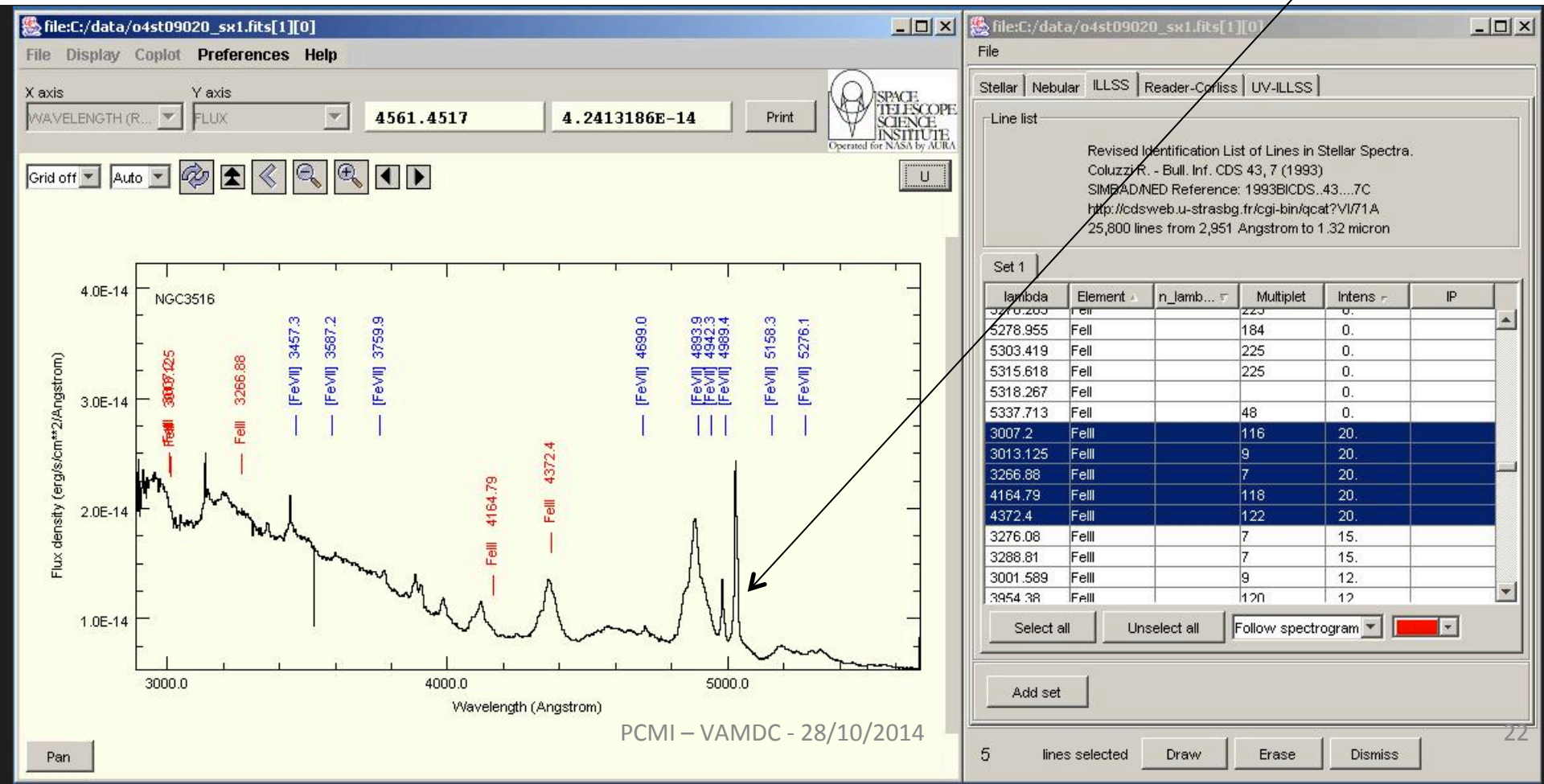
Virtual Atomic and Molecular Data Centre

- Query all registered databases via the Portal (www.portal.eu) or orther portals
  - Visualisation of Data
  - Download of Data
- Standalone Work with Software:
  - Query databases
  - Mix heterogeneous databases
  - Download
  - → *Example of SPECTCOL software*
- Include new databases or data in the infrastructure
- **Use of our libraries in user applications in order to access the VAMDC registered databases**

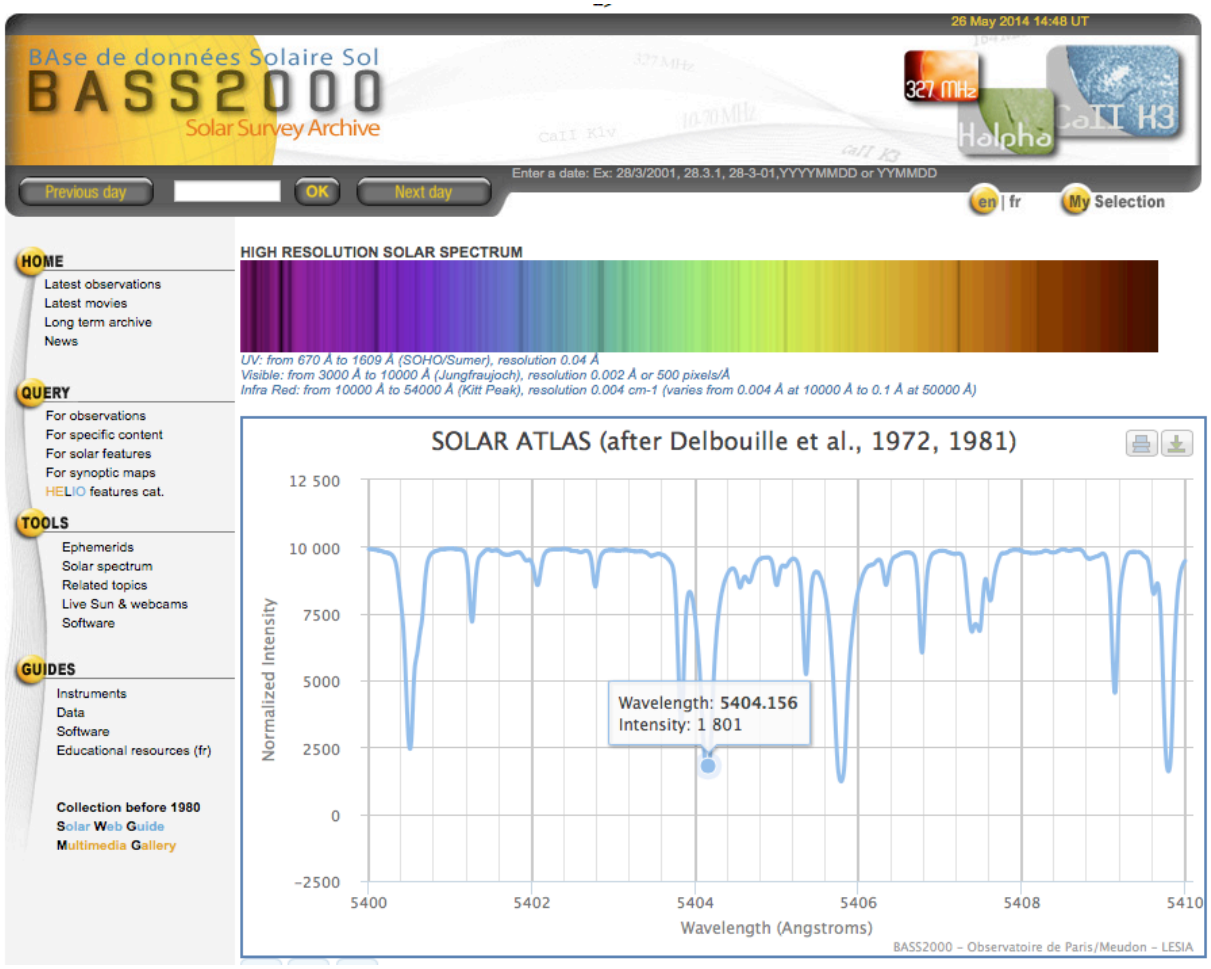
Accessing VAMDC from User's Tool Specview Software

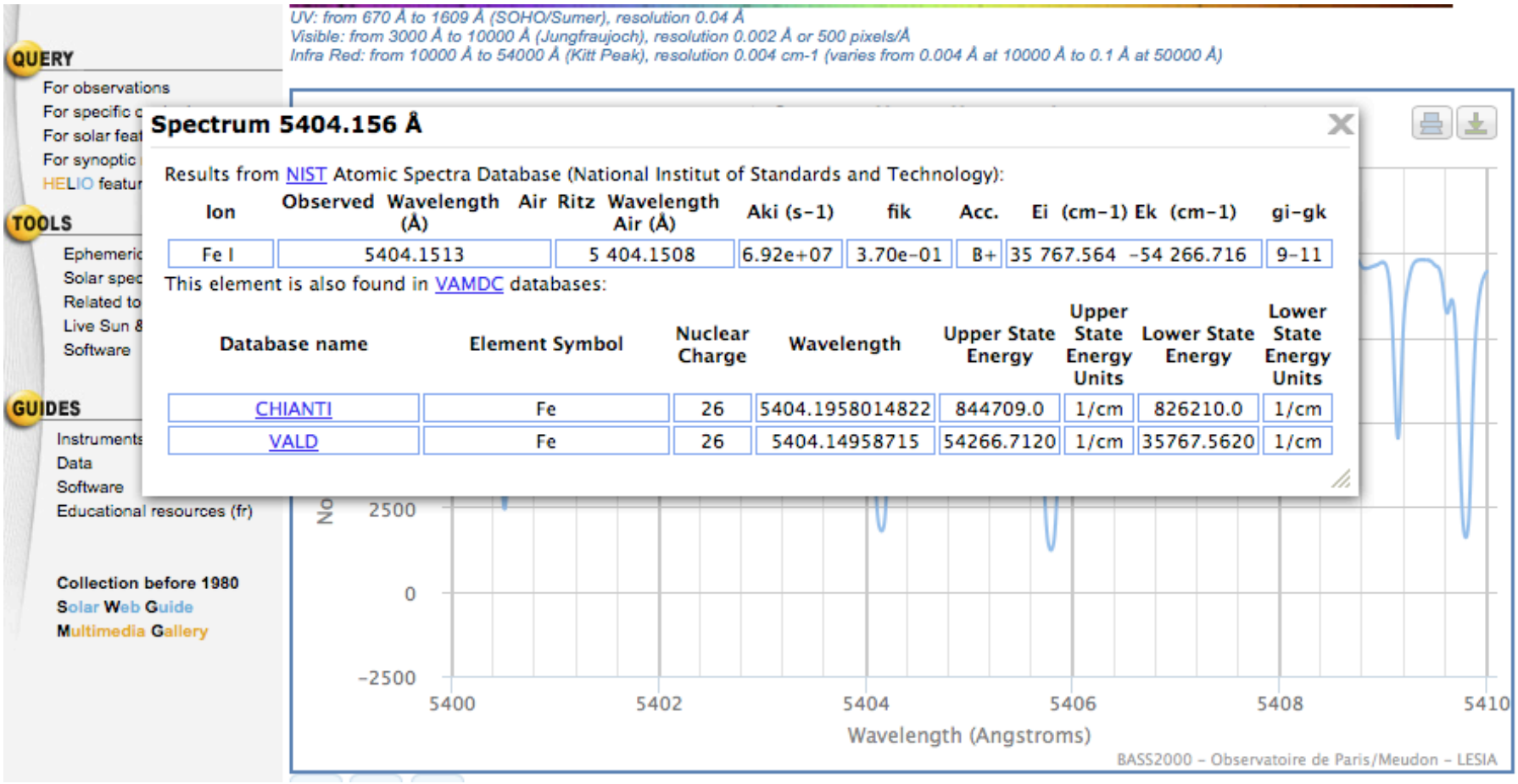
- Specview is a java tool for 1-D spectra visualization
  www.stsci.edu/institute/software_hardware/specview/ (I. Busko)

SSAP VO



LESIA, Observatoire de Paris, J. Aboudarham
Support from VAMDC: N. Moreau, LERMA

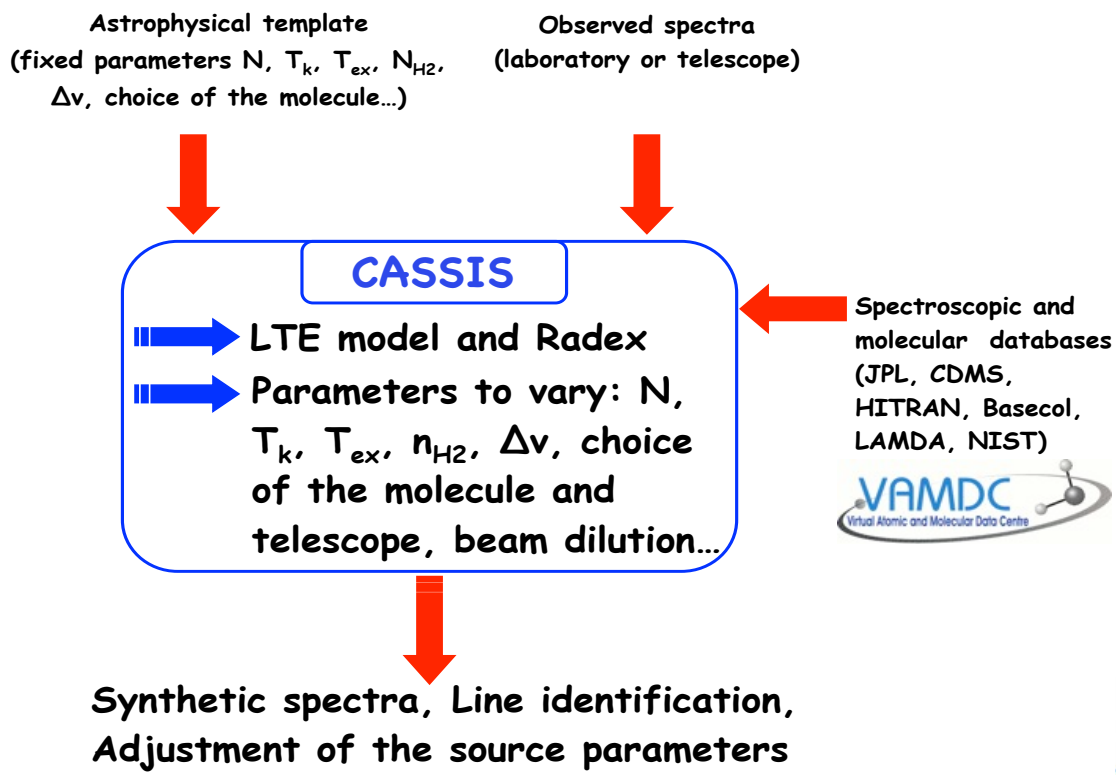



UV: from 670 Å to 1609 Å (SOHO/Sumer), resolution 0.04 Å
Visible: from 3000 Å to 10000 Å (Jungfraujoch), resolution 0.002 Å or 500 pixels/Å
Infra Red: from 10000 Å to 54000 Å (Kitt Peak), resolution 0.004 cm-1 (varies from 0.004 Å at 10000 Å to 0.1 Å at 50000 Å)
QUERY
For observations
TOOLS
Ephemeric
Solar spec
Related to
Live Sun &
Software
GUIDES
Instruments
Data
Software
Educational resources (fr)
Collection before 1980
Solar Web Guide
Multimedia Gallery
Spectrum 5404.156 Å
Results from NIST Atomic Spectra Database (National Institut of Standards and Technology):
Ion | Observed Wavelength (Å) | Air Ritz Wavelength Air (Å) | Aki (s-1) | fik | Acc. | Ei (cm-1) | Ek (cm-1) | gi-gk
Fe I | 5404.1513 | 5 404.1508 | 6.92e+07 | 3.70e-01 | B+ | 35 767.564 | -54 266.716 | 9-11
This element is also found in VAMDC databases:
Database name | Element Symbol | Nuclear Charge | Wavelength | Upper State Energy | Upper State Energy Units | Lower State Energy | Lower State Energy Units
CHIANTI | Fe | 26 | 5404.1958014822 | 844709.0 | 1/cm | 826210.0 | 1/cm
VALD | Fe | 26 | 5404.14958715 | 54266.7120 | 1/cm | 35767.5620 | 1/cm
2500
0
-2500
5400
5402
5404
5406
5408
5410
Wavelength (Angstroms)
BASS2000 - Observatoire de Paris/Meudon - LESIA

CASSIS Software

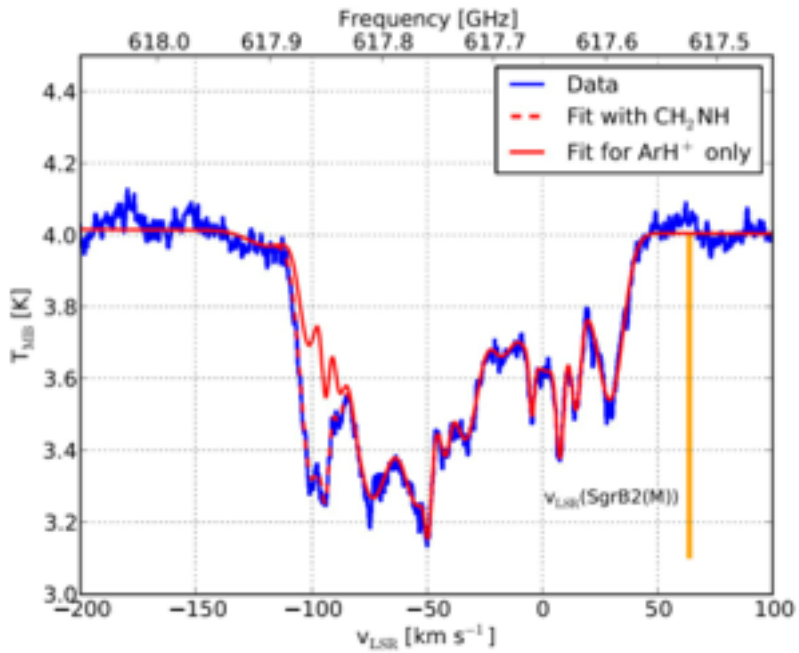
M. Boiziot, S. Bottinelli, E. Caux, J.M. Glorian, C. Vastel, IRAP, VO-GSO
Y. A. Ba, VAMDC Support, LERMA2, VO-PDC

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 flow chart below:



myXCLASS for CASA

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



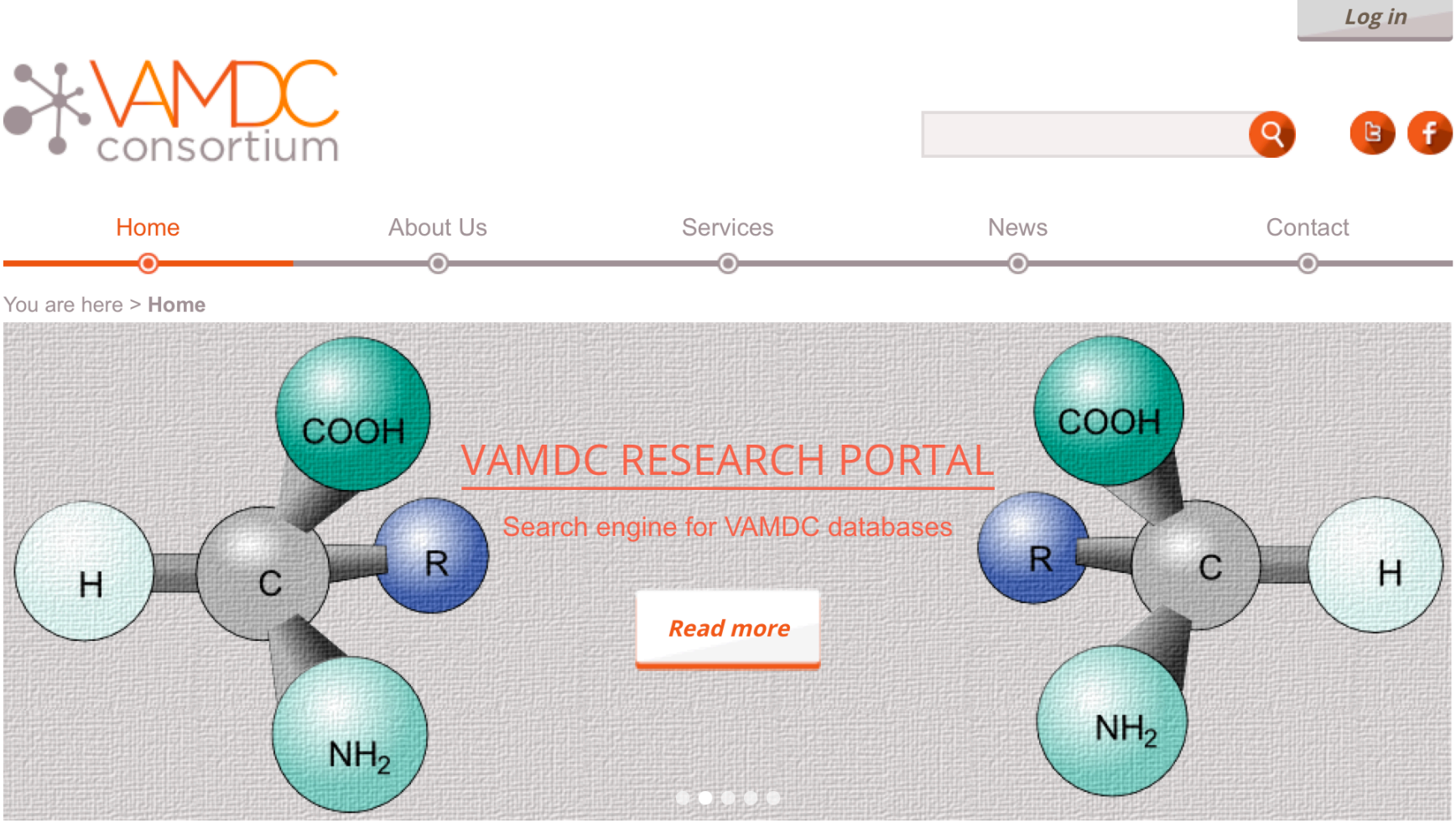
Schilke et al., ArXiv e-prints, 1403.7902 (2014)

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

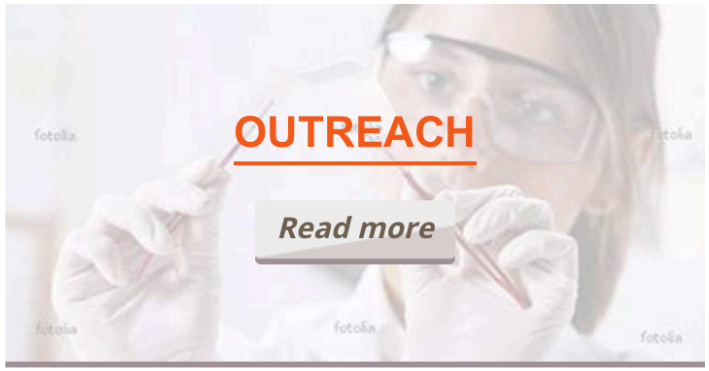
VAMDC Products

- **Support =**
  - **Send mail to** support@vamdc.eu
  - Go to vamdc.eu/usersupport
  - Tutorial (different types)
- Portal = http://portal.vamdc.eu
- Software and Librairies = http://vamdc.eu/software
- Standards = http://vamdc.eu/standards
- Tutorials = http://tutorial.vamdc.eu
- Forums = http://forum.vamdc.org



VAMDC Consortium Website's Maintenance/Upgrades: Y.A. Ba, LERMA

Services



ACCESS TO THE FORUM

Exchange ideas, Ask questions, Find answers

Read more

or

Access to the forum

MORE INFORMATION?

You have questions? You want to participate in our projects?

Contact us

Success stories

RESEARCH

VAMDC has successfully brought new possibilities to Research.

Read more

EDUCATION

Participate/Propose Activities so that we can record our success stories. For now read about our Research Success Stories.

Read more

EVENTS

VAMDC participates to organises conferences, workshops, tutorials

See our events

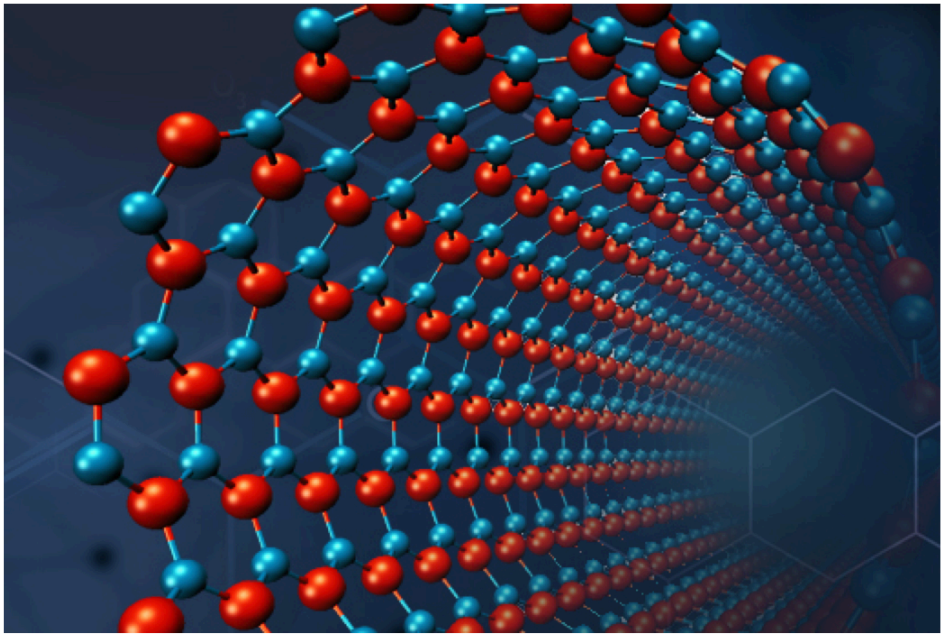
RESEARCH SERVICES

Access to Data
VAMDC Research Portal

Users/Developers
Software
SPECTCOL
SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal

Developers
Standards
Libraries
Tutorials
FAQ

SERVICES [RESEARCH]



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.

VAMDC infrastructure was established to provide a service to the wider

ACCESS TO THE DATA

Access to VAMDC databases

Access to the data

ACCESS TO THE FORUM

Exchange ideas, Ask questions, Find answers

Read more

or

Access to the forum

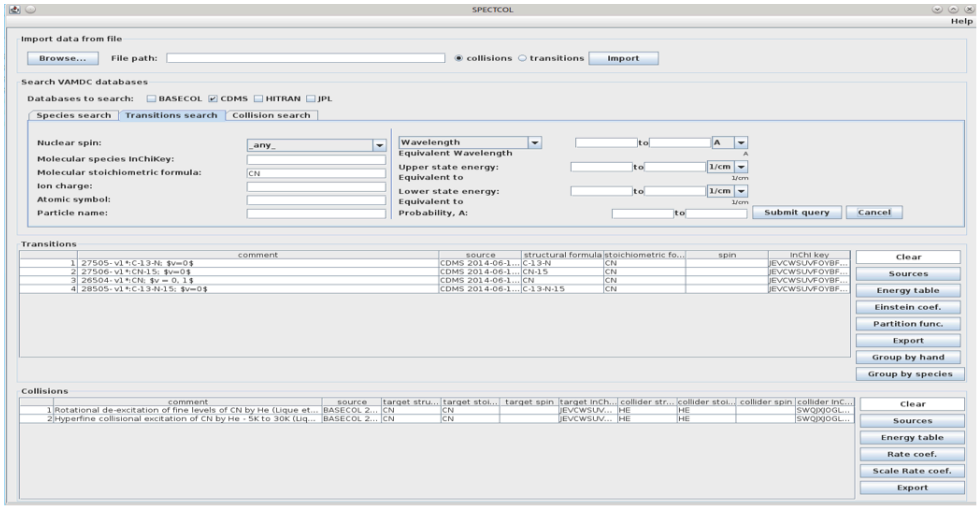
RESEARCH SERVICES

Access to Data
VAMDC Research Portal

Users/Developers
Software
SPECTCOL
SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal

Developers
Standards
Libraries
Tutorials
FAQ

SPECTCOL



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.

Scientific Use Case

Tutorial

Version History

ACCESS TO THE DATA

Access to VAMDC databases

Access to the data

ACCESS TO THE FORUM

Exchange ideas, Ask questions, Find answers

Read more

or

Access to the forum

VAMDC consortium

Files to download

Spectcol Jar File v12.07-r2
Download

SPECTCOL user guide documentation v12.07-r1
Download

Technical information of SPECTCOL tool
Download

VAMDC Virtual Atomic and Molecular Data Centre

SUP VAMDC

Home | About Us | Servi

You are here > **Register**

REGISTER

You are*	Researcher
Your field*	Astrophysics
Choose a Username*	
Structure	
Country	
Last Name	
First Name	
Email*	
Website	
Phone Number	

Register

*Required field

VAMDC
Virtual Atomic and Molecular Data Centre

forum.vamdc.org
Forums of VAMDC project

Board index

A&M Data Producers

NEWTOPIC ★ | Search this forum... | Search

TOPICS

BASECOL
by awa » Thu Oct 16, 2014 1:47 pm

View unanswered posts • View active topics

FORUM

A&M Data Producers
Exchange ideas, Ask questions, Find answers or

A&M Scientist Users
Exchange ideas, Ask questions, Find answers

VAMDC Education
Exchange ideas, Ask questions, Find answers or

Industry
Exchange ideas, Ask questions, Find answers or

Public Outreach
Exchange ideas, Ask questions, Find answers or

A&M Scientist Users

NEWTOPIC ★ | Search this forum... | Search

TOPICS

SPECTCOL
by awa » Thu Oct 16, 2014 1:54 pm

VAMDC Portal discussion and feedback
by misdoro » Mon Nov 25, 2013 4:06 pm

Advantages of Inclusion in VAMDC

- Users can easily access and transform data
- Each Data is referenced
- Methodology to obtain data can be included
- Data can be visualised easily
- Similar Databases can be compared easily
  - Improves quality for modeling

- Support is provided by VAMDC Team

Political and technical organization

C.M. Zwölf
LERMA

Evaluation Validation WG

International Collaboration WG

Board of directors

Scientific
and technical board

New DB

R&D

Monitoring

Training Support

User WG

Technical quality WG

French Partic.
N. Moreau
Y.A. Ba

- Inclusion of new Databases / Data providers
  - If new data are fully compatible→ link with Training & Support WG.
  - If data are not compatible → link with R&D WG
- R&D
  - Evolution of standard and software for meeting community needs
- Monitoring:
  - Maintenance and monitoring of all the element of the infrastructure

Political and technical organization

Evaluation Validation WG

International Collaboration WG

Board of directors

Scientific
and technical board

New DB

R&D

Monitoring

Training Support

User WG

Technical quality WG

- Creates and maintains supports and training materials
- Organize tutorials
- Work with Technical Operational WG and User WG
  - For building tutorials on up-to date products and features
  - For meeting the need of the user community

French Partic.
N. Moreau
Y.A. Ba
C.M. Zwölf

Political and technical organization

Evaluation Validation WG

International Collaboration WG

Board of directors

Scientific
and technical board

New DB

R&D

Monitoring

Training Support

User WG

Technical quality WG

- Interface between the consortium and the user communities
- VAMDC users are both
  - End-users: Research, Education, Industry, Outreach
  - Data providers
- Gather needs from community and relay them to Technical Operational WG and to Training/Support WG.

Political and technical organization

Evaluation Validation WG

International Collaboration WG

Board of directors

Scientific
and technical board

New DB

R&D

Monitoring

Training Support

User WG

Technical quality WG

- Defines
  - quality procedures, rules and good practices
  - duties required from data providers
  - Procedures for publishing new software
  - Key performance indicator for evaluating the infrastructure
- Administer collaborative tools for technical management (e.g. Redmine)

C.M. Zwölf
LERMA

Political and technical organization

Evaluation Validation WG

International Collaboration WG

Board of directors

Scientific
and technical board

New DB

R&D

Monitoring

Training Support

User WG

Technical quality WG

- Defines
  - Scientific evaluation of datasets contained into the infrastructure
- Works
  - Via connection to other networks that asses A+M data

Memorandum of Understanding

- Full members (holding a VAMDC Resource)
  - **15 Members from 1rst of November 2014 (EU+Russia)**
  - **Accession (by end of 2014)**
    - **Atomic & Molecular Physics Division of India (for several institutes), India**
    - **NIST Atomic Division, Gaithersburg, USA**
    - **JPL, B. Drouin, Caltech, USA**
    - **HITRAN, L. Rothman, CfA, USA**
  - Right of Vote, Have free upgrade and training
  - Can use « VAMDC brand» to apply for grant
  - Must have a VAMDC resource or pay Membership Fee
- Board of Directors, Scientific and Technical Board
- Working Groups
  - Standards, Software, Evaluation of Data
  - **User Communities Groups**
  - **Education**, Outreach, Industry

Strengthen links