

VAMDC

Breaking News

<http://www.vamdc.eu> (.org)

Carlo Maria Zwölf, Nicolas Moreau, Yaye Awa Ba,
Marie-Lise Dubernet, *on behalf of VAMDC consortium.*

Partners

FRANCE

Observatoire de Paris
 Université de Bordeaux
 Université Paul Sabatier (Toulouse)
 Université de Bourgogne (Dijon)
 Université de Champagne-Ardenne (Reims)
 Université Joseph Fourier (Grenoble)

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)

EUROPE

University of Cambridge (UK)
 University College London (UK)
 Uppsala Universitet (Sweden)
 Open University (UK)
 Universitaet Wien (Austria)
 Universitaet zu Koeln (Germany)
 Istituto Nazionale di Astrofisica (Italy)
 Queen's University Belfast (UK)
 Atomic and Molecular Data Unit (IAEA, Austria)
 Astronomska Opseratorija (Serbia)

ASIA-PACIFIC

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

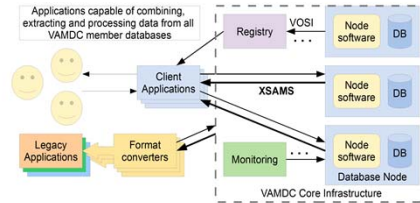
USA

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

University of South Africa, South Africa

How is VAMDC technically organised ?

- VAMDC may be seen as a *grid* architecture for sharing and distribute *cloud* data (**from 27 databases**)



- Communications (data serializations) are based on 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)
 - Node Software for implementation of databases within VAMDC
 - JAVA Libraries 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
- Monitoring of services (observatoire de paris)

What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

- Query all registered databases via the Portal (www.portal.eu) or other portals
 - Visualisation of Data
 - Download of Data
 - *Overview of portal redesign. (Carlo Maria Zwölf)*
- Standalone Work with Software:
 - Query databases
 - Mix heterogeneous databases
 - Download
 - *Example of Standalone XSAMS Multi Processor (Nicolas Moreau)*
 - *Example of SPECTCOL software (Yaye Awa Ba)*
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- Use of our libraries in user applications in order to access the VAMDC registered databases

Portal Evolution

Virtual Atomic and Molecular Data Centre

Dozen of conferences and tutorials were made

- tutorial.vamdc.eu
- (list at <http://voparis-twiki.obspm.fr/wiki/bin/view/VAMDC/ScientificWorkshopsTutorials>)
- **Collected feedbacks**
 - Portal is hard to use for inexperienced users.
 - It may exist ambiguity between user comprehension and portal actions.
- We redesigned the portal focusing on user experience (especially beginners)
 - No ambiguity about the actions to perform and the generated request.
 - Few a priori knowledge needed.
- Let us point out some of the introduced modification →

The portal (Before, ex for collisions)

Virtual Atomic and Molecular Data Centre

[The current portal query interface](#)

The redesigned portal (ex for collisions)

Virtual Atomic and Molecular Data Centre

Choose a request type

Request VAMDC

- For collisional Process
- For radiative Process
- By Species

Validate choices and continue

Define collision type

Please, choose the type of collision:

- Without reaction (Elastic and Inelastic)
- With reaction

Process Name: Choose between proposed processes

Process Code: Non editable code of chosen process

Process description: Non editable description of the chosen process

Validate choices and continue

The redesigned portal (ex for collisions)

Virtual Atomic and Molecular Data Centre

Define collision configuration

Please enter the number of reactants and products you would like to specify. Their combination will define the set of collisions for your query.

Number of Reactant(s)

Number of Product(s)

Validate choices and continue

The redesigned portal (ex for collisions)

Virtual Atomic and Molecular Data Centre

Definition of Reactant N°1

Select Reactant Type

Atom

Atom Symbol	<input type="text" value="Symbol"/>
Mass Number	From <input type="text" value="InfValue"/> to <input type="text" value="SupValue"/>
Nuclear Charge	From <input type="text" value="InfValue"/> to <input type="text" value="SupValue"/>
Ion Charge	From <input type="text" value="InfValue"/> to <input type="text" value="SupValue"/>
InChIKey	<input type="text" value="Non editable keyValue"/>
State energy	From <input type="text" value="InfValue"/> to <input type="text" value="SupValue"/> <input type="text" value="1/cm"/>

State energy equivalent to the range XX to YY 1/cm.

The redesigned portal (ex for collisions)

Virtual Atomic and Molecular Data Centre

Collision choice

Your request could be on the following combination of collisions, please choose those you are interested in:

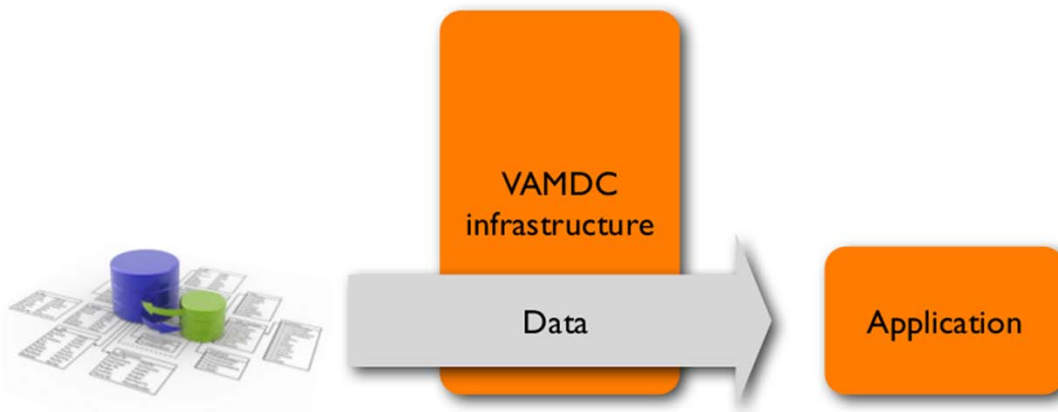
- Select all**
- (Reactant1, Reactant2, Reactant3) → (Product1 and Product2)
- (Reactant1, Reactant2, Reactant3) → (Product1)
- (Reactant1, Reactant2, Reactant3) → (Product2)
- (Reactant1, Reactant2) → (Product1 and Product2)
- (Reactant1, Reactant2) → (Product1)
- (Reactant1, Reactant2) → (Product2)
- (Reactant1, Reactant3) → (Product1 and Product2)
- (Reactant1, Reactant3) → (Product1)
- (Reactant1, Reactant3) → (Product2)
- (Reactant2, Reactant3) → (Product1 and Product2)
- (Reactant2, Reactant3) → (Product1)
- (Reactant2, Reactant3) → (Product2)

Before implementation → Youtube Demo (on the vamdc channel) for getting community advices and feedback (<http://www.youtube.com/channel/UCg66E2aJbNzQraBVVh3D4Yw>)

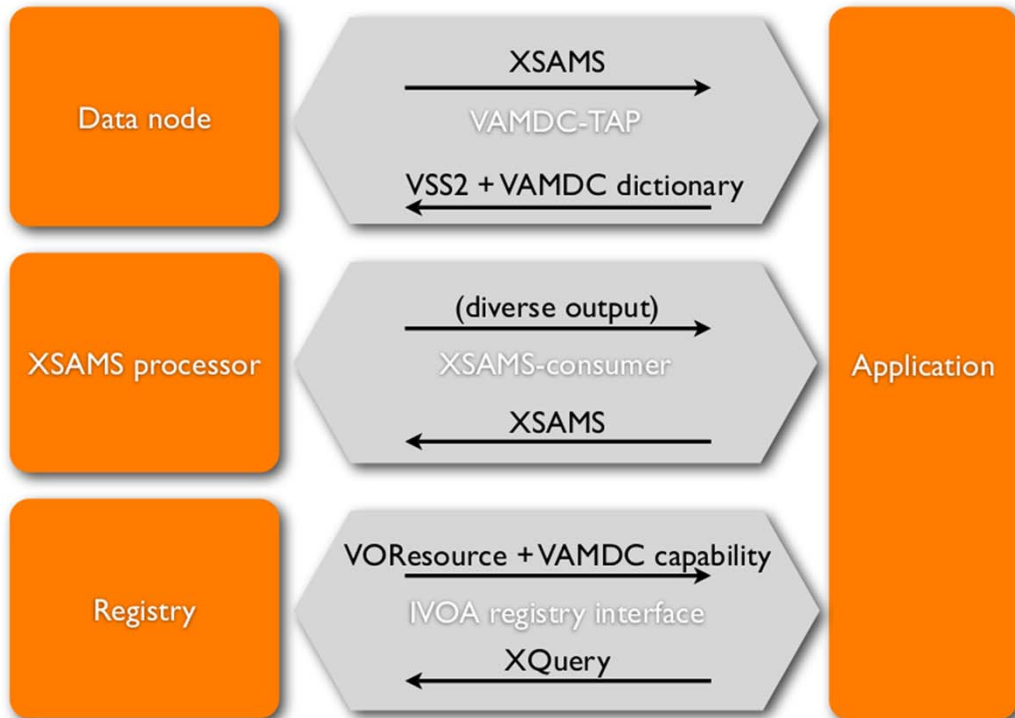
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- L'infrastructure VAMDC est une couche intermédiaire entre les bases de données et les applications
- VAMDC ne fournit ni ne modifie ces bases ou ces applications
- L'infrastructure impose un ensemble de standards afin de rendre le toutinteropérable



- Objectif : simplifier l'utilisation de fichier XSAMS par une transformation en des formats reconnus par des applications existantes
- Possibilité de conversion en CSV, XML (VOTable), HTML,...
- Ils sont accessibles depuis le portail sous forme de services webs
- Services standardisés : http://www.vamdc.org/documents/xsams-processor_v12.07.pdf

Les processors

- Un processor peut prendre de 1 à n fichiers en entrée

- Il va effectuer diverses actions :
 - conversion de format
 - fusion de fichiers

- Utilisation de XSLT pour les transformations

- Pour les futurs services :
 - un template de service est disponible, avec la gestion des entrées et des sorties et une interface web d'interrogation
 - seul le XSL est à modifier

- Les différentes communautés d'utilisateurs peuvent développer leurs services dédiés : VAMDC les inclura dans ses registries et son portail.

Les processors

- 4 processors sont disponibles :
 - Bibtex : crée un fichier bibtex à partir des des références
 - Tableview : Crée un tableau HTML avec les données
 - Xsams to SME : Crée un fichier au format SME (Spectroscopy Made Easy, <http://www.stsci.edu/~valenti/sme.html>)
 - Xsams Atomic data to HTML : Crée une page HTML avec des fonctionnalités de conversion et SAMP



1: Query Execution

Done

Modify query Stop waiting Save query

select * where ((AtomSymbol = 'He'))

Comments

3: Results Conversion (select in table below)

BibTeX from XSAMS
 Table views of XSAMS
 Xsams2SME
 Atomicxsams2HTML

Process

XSAMS processor displaying atomic data in a xsams file as an html array. The generated page provide some data extraction functions.

2: Results by node

Name	Convert	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
ALADDIN2	<input type="checkbox"/>	OK	XSAMS	137	0	2807	0	2807	0
VALD sub-set in Moscow (obs)	<input type="checkbox"/>	OK (17/12/2012 21:00)	XSAMS	2	1260	2080	2080	0	0
VALD (atoms)	<input type="checkbox"/>	OK (18/12/2012 00:00)	XSAMS	2	1260	2080	2080	0	0
KIDA: VAMDC-TAP interface	<input type="checkbox"/>	OK (14/01/2014 13:52)	XSAMS	2	0	858	0	858	0
TOPbase : VAMDC-TAP interface	<input checked="" type="checkbox"/>	OK	XSAMS	2	108	600	600	0	0
Chianti	<input type="checkbox"/>	OK	XSAMS	2	3026	255	255	0	0
TIPbase : VAMDC-TAP interface	<input type="checkbox"/>	OK	XSAMS	1	16	105	0	105	0
BASECOL: VAMDC-TAP interface	<input type="checkbox"/>	OK (01/06/2012 00:00)	XSAMS	1	0	69	0	69	0
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	<input type="checkbox"/>	OK (23/01/2014 17:03)	XSAMS	0	0	0	0	0	0
JPL database: VAMDC-TAP service	<input type="checkbox"/>	OK (23/01/2014 17:03)	XSAMS	0	0	0	0	0	0
VAMDC species-DB	<input type="checkbox"/>	OK	XSAMS	2	0	0	0	0	0
Spectr-W3	<input type="checkbox"/>	TRUNCATED (11/12/2013 19:00) (44%)	XSAMS	2	362	1042	1042	0	0
Stark-b	<input type="checkbox"/>	TRUNCATED (24%)	XSAMS	4	19	21	21	0	0
DESIRE database (Moscow mirror)	<input type="checkbox"/>	EMPTY		0	0	0	0	0	0
IDEADB - Innsbruck Dissociative Electron Attachment Database	<input type="checkbox"/>	EMPTY		0	0	0	0	0	0
RADAM - Ion Interactions	<input type="checkbox"/>	EMPTY		0	0	0	0	0	0



1: Query Execution

Done

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select * where ((AtomSymbol = 'He'))

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3: Results Conversion (select in table below)

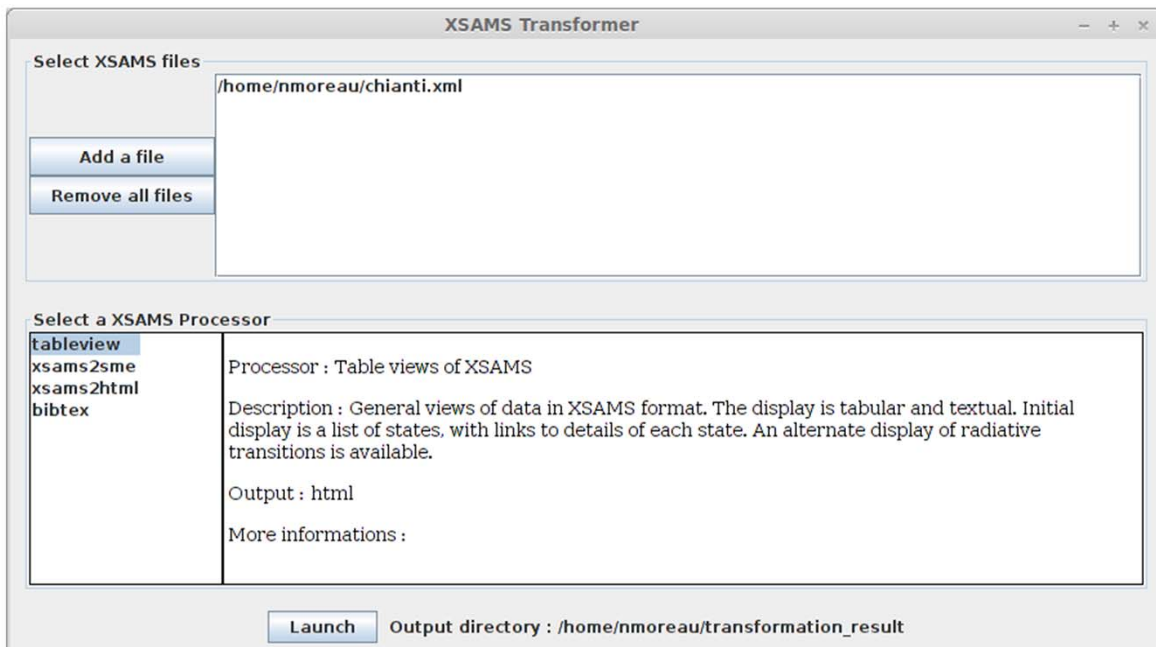
BibTeX from XSAMS
 Table views of XSAMS
 Atomix2XML
 Atomix2HTML

Process

XSAMS processor displaying atomic data in a xsams file as an html array. The generated page provide some data extraction functions.

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Name	Convert	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
ALADDIN2	<input type="checkbox"/>	OK	XSAMS	137	0	2807	0	2807	0
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KIDA: VAMDC-TAP interface	<input type="checkbox"/>	OK (14/01/2014 13:52)	XSAMS	2	0	858	0	858	0
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TIPbase : VAMDC-TAP interface	<input type="checkbox"/>	OK	XSAMS	1	16	105	0	105	0
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Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	<input type="checkbox"/>	OK (23/01/2014 17:03)	XSAMS	0	0	0	0	0	0
JPL database: VAMDC-TAP service	<input type="checkbox"/>	OK (23/01/2014 17:03)	XSAMS	0	0	0	0	0	0
VAMDC species-DB	<input type="checkbox"/>	OK	XSAMS	2	0	0	0	0	0
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Stark-b	<input type="checkbox"/>	TRUNCATED (24%)	XSAMS	4	19	21	21	0	0
DESIRE database (Moscow mirror)	<input type="checkbox"/>	EMPTY		0	0	0	0	0	0
IDEADB - Innsbruck Dissociative Electron Attachment Database	<input type="checkbox"/>	EMPTY		0	0	0	0	0	0
RADAM - Ion Interactions	<input type="checkbox"/>	EMPTY		0	0	0	0	0	0



The screenshot shows a Java application window titled "XSAMS Transformer". It has two main sections:

- Select XSAMS files:** A text box contains the file path `/home/nmoreau/chianti.xml`. Below it are buttons for "Add a file" and "Remove all files".
- Select a XSAMS Processor:** A list of processors is shown on the left: `tableview` (highlighted), `xsams2sme`, `xsams2html`, and `bibtex`. The right side displays details for the selected processor:
 - Processor : Table views of XSAMS
 - Description : General views of data in XSAMS format. The display is tabular and textual. Initial display is a list of states, with links to details of each state. An alternate display of radiative transitions is available.
 - Output : html
 - More informations :

At the bottom, there is a "Launch" button and the text "Output directory : /home/nmoreau/transformation_result".

Exemple de conversions

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Spectcol

GUI Tool to Query/Manipulate Spectroscopic and Collisional Data
(Download : <http://www.vamdc.eu/software>)

• Handles VAMDC-XSAMS files from different databases

• Merging of spectroscopic and collisional data

• Display spectroscopic and collisional data: Species, Energy Tables, Frequencies, Einstein Coefficient, Partition function, sources, Rate Coefficients

Spectcol : The Main Panel with Complex Query in Transition Tab

SPECTCOL-45

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: Wavelength: to A
 Equivalent Wavelength: A
 Molecular species InChIKey: Upper state energy: to 1/cm
 Equivalent to: 1/cm
 Molecular stoichiometric formula: Lower state energy: to 1/cm
 Equivalent to: 1/cm
 Ion charge: Probability, A: to
 Atomic symbol: Submit query Cancel
 Particle name:

Transitions

	comment	source	structural formula	stoichiometric fo...	spin	InChI key
1	31502-v1:C-13-O-18; \$v=0\$	CDMS 2014-01-2...	C-13-O-18	CO		UGFAIRIUMAVXC...
2	28503-v1:CO; \$v=0\$	CDMS 2014-01-2...	CO	CO		UGFAIRIUMAVXC...
3	28512-v1*CO; \$v=1,2,3\$	CDMS 2014-01-2...	CO	CO		UGFAIRIUMAVXC...
4	30503-v1:C-13-O-17; \$v=0\$	CDMS 2014-01-2...	C-13-O-17	CO		UGFAIRIUMAVXC...
5	29501-v2*C-13-O; \$v=0\$	CDMS 2014-01-2...	C-13-O	CO		UGFAIRIUMAVXC...
6	30502-v1:CO-18; \$v=0\$	CDMS 2014-01-2...	CO-18	CO		UGFAIRIUMAVXC...

Collisions

	comment	source	target stru...	target sto...	target spin	target inCh...	collider stru...	collider sto...	collider spin	collider inCh...
1	Rotational de-excitation of CO by para-H ₂ 2 ₁ (J=0, S _K < T...	BASECOL 2...	CO	CO		UGFAIRIUM...H ₂ 2 ₁	H2	para		UFHFLECO...
2	Rotational excitation of CO by ortho-H ₂ 2 ₁ (Flower, 2001)	BASECOL 2...	CO	CO		UGFAIRIUM...H ₂ 2 ₁	H2	ortho		UFHFLECO...
3	Rotational excitation of CO by para H ₂ 2 ₁ (Flower, 2001)	BASECOL 2...	CO	CO		UGFAIRIUM...H ₂ 2 ₁	H2	para		UFHFLECO...
4	Rotational de-excitation of CO by H for S _K < T=1.00K (Bala...	BASECOL 2...	CO	CO		UGFAIRIUM...H	H			YZCKVEUG...
5	Vibrational de-excitation of CO by H (Balakrishnan & al. 20...	BASECOL 2...	CO	CO		UGFAIRIUM...H	H			YZCKVEUG...
6	Rotational de-excitation of CO (v=0) by He (Cecchi-Pestelli...	BASECOL 2...	CO	CO		UGFAIRIUM...HE	HE			SWQJQJGL...
7	Vibrational de-excitation of CO by He (Cecchi-Pestelli & al...	BASECOL 2...	CO	CO		UGFAIRIUM...HE	HE			SWQJQJGL...
8	Rotational de-excitation of CO by H for 100K < T < 3000K (B...	BASECOL 2...	CO	CO		UGFAIRIUM...H	H			YZCKVEUG...
9	Rotational de-excitation of CO by ortho-H ₂ 2 ₁ (J=1, S _K < T...	BASECOL 2...	CO	CO		UGFAIRIUM...H ₂ 2 ₁	H2	ortho		UFHFLECO...
10	Rotational de-excitation of CO by para-H ₂ 2 ₁ (J=0, 1K < T...	BASECOL 2...	CO	CO		UGFAIRIUM...H ₂ 2 ₁	H2	para		UFHFLECO...
11	Rotational de-excitation of CO by ortho-H ₂ 2 ₁ (J=1, 1K < T...	BASECOL 2...	CO	CO		UGFAIRIUM...H ₂ 2 ₁	H2	ortho		UFHFLECO...

Clear Sources Energy table Einstein coef. Partition func. Export Group by hand Group by species


Display of partition function Table



Energy level (E)	Degeneracy (g)
0	1
1	3
2	5
3	7
4	9
5	11
6	13
7	15
8	17
9	19
10	21
11	23
12	25
13	27
14	29
15	31
16	33
17	35
18	37
19	39
20	41
21	43
22	45
23	47
24	49
25	51
26	53
27	55
28	57
29	59
30	61
31	63
32	65
33	67
34	69
35	71
36	73
37	75
38	77
39	79
40	81
41	83
42	85
43	87
44	89
45	91
46	93
47	95
48	97
49	99
50	101
51	103
52	105
53	107
54	109
55	111
56	113
57	115
58	117
59	119
60	121
61	123
62	125
63	127
64	129
65	131
66	133
67	135
68	137
69	139
70	141
71	143
72	145
73	147
74	149
75	151
76	153
77	155
78	157
79	159
80	161
81	163
82	165
83	167
84	169
85	171
86	173
87	175
88	177
89	179
90	181
91	183
92	185
93	187
94	189
95	191
96	193
97	195
98	197
99	199
100	201

Display of scaled Rate coefficients and Collision

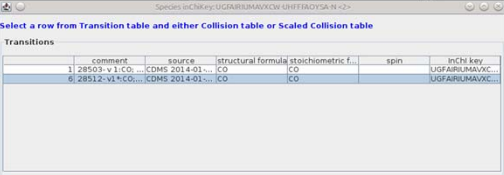
Scaled rate coefficients - Factor = 1.2 - Rotational de-excitation of CO (v=0) by He, 2002

Transition	Rate coefficient (k)
1-0(0-0)	1.2000000000000000e+00
1-0(1-0)	1.2000000000000000e+00
1-0(2-0)	1.2000000000000000e+00
1-0(3-0)	1.2000000000000000e+00
1-0(4-0)	1.2000000000000000e+00
1-0(5-0)	1.2000000000000000e+00
1-0(6-0)	1.2000000000000000e+00
1-0(7-0)	1.2000000000000000e+00
1-0(8-0)	1.2000000000000000e+00
1-0(9-0)	1.2000000000000000e+00
1-0(10-0)	1.2000000000000000e+00
1-0(11-0)	1.2000000000000000e+00
1-0(12-0)	1.2000000000000000e+00
1-0(13-0)	1.2000000000000000e+00
1-0(14-0)	1.2000000000000000e+00
1-0(15-0)	1.2000000000000000e+00
1-0(16-0)	1.2000000000000000e+00
1-0(17-0)	1.2000000000000000e+00
1-0(18-0)	1.2000000000000000e+00
1-0(19-0)	1.2000000000000000e+00
1-0(20-0)	1.2000000000000000e+00
1-0(21-0)	1.2000000000000000e+00
1-0(22-0)	1.2000000000000000e+00
1-0(23-0)	1.2000000000000000e+00
1-0(24-0)	1.2000000000000000e+00
1-0(25-0)	1.2000000000000000e+00
1-0(26-0)	1.2000000000000000e+00
1-0(27-0)	1.2000000000000000e+00
1-0(28-0)	1.2000000000000000e+00
1-0(29-0)	1.2000000000000000e+00
1-0(30-0)	1.2000000000000000e+00
1-0(31-0)	1.2000000000000000e+00
1-0(32-0)	1.2000000000000000e+00
1-0(33-0)	1.2000000000000000e+00
1-0(34-0)	1.2000000000000000e+00
1-0(35-0)	1.2000000000000000e+00
1-0(36-0)	1.2000000000000000e+00
1-0(37-0)	1.2000000000000000e+00
1-0(38-0)	1.2000000000000000e+00
1-0(39-0)	1.2000000000000000e+00
1-0(40-0)	1.2000000000000000e+00
1-0(41-0)	1.2000000000000000e+00
1-0(42-0)	1.2000000000000000e+00
1-0(43-0)	1.2000000000000000e+00
1-0(44-0)	1.2000000000000000e+00
1-0(45-0)	1.2000000000000000e+00
1-0(46-0)	1.2000000000000000e+00
1-0(47-0)	1.2000000000000000e+00
1-0(48-0)	1.2000000000000000e+00
1-0(49-0)	1.2000000000000000e+00
1-0(50-0)	1.2000000000000000e+00
1-0(51-0)	1.2000000000000000e+00
1-0(52-0)	1.2000000000000000e+00
1-0(53-0)	1.2000000000000000e+00
1-0(54-0)	1.2000000000000000e+00
1-0(55-0)	1.2000000000000000e+00
1-0(56-0)	1.2000000000000000e+00
1-0(57-0)	1.2000000000000000e+00
1-0(58-0)	1.2000000000000000e+00
1-0(59-0)	1.2000000000000000e+00
1-0(60-0)	1.2000000000000000e+00
1-0(61-0)	1.2000000000000000e+00
1-0(62-0)	1.2000000000000000e+00
1-0(63-0)	1.2000000000000000e+00
1-0(64-0)	1.2000000000000000e+00
1-0(65-0)	1.2000000000000000e+00
1-0(66-0)	1.2000000000000000e+00
1-0(67-0)	1.2000000000000000e+00
1-0(68-0)	1.2000000000000000e+00
1-0(69-0)	1.2000000000000000e+00
1-0(70-0)	1.2000000000000000e+00
1-0(71-0)	1.2000000000000000e+00
1-0(72-0)	1.2000000000000000e+00
1-0(73-0)	1.2000000000000000e+00
1-0(74-0)	1.2000000000000000e+00
1-0(75-0)	1.2000000000000000e+00
1-0(76-0)	1.2000000000000000e+00
1-0(77-0)	1.2000000000000000e+00
1-0(78-0)	1.2000000000000000e+00
1-0(79-0)	1.2000000000000000e+00
1-0(80-0)	1.2000000000000000e+00
1-0(81-0)	1.2000000000000000e+00
1-0(82-0)	1.2000000000000000e+00
1-0(83-0)	1.2000000000000000e+00
1-0(84-0)	1.2000000000000000e+00
1-0(85-0)	1.2000000000000000e+00
1-0(86-0)	1.2000000000000000e+00
1-0(87-0)	1.2000000000000000e+00
1-0(88-0)	1.2000000000000000e+00
1-0(89-0)	1.2000000000000000e+00
1-0(90-0)	1.2000000000000000e+00
1-0(91-0)	1.2000000000000000e+00
1-0(92-0)	1.2000000000000000e+00
1-0(93-0)	1.2000000000000000e+00
1-0(94-0)	1.2000000000000000e+00
1-0(95-0)	1.2000000000000000e+00
1-0(96-0)	1.2000000000000000e+00
1-0(97-0)	1.2000000000000000e+00
1-0(98-0)	1.2000000000000000e+00
1-0(99-0)	1.2000000000000000e+00
1-0(100-0)	1.2000000000000000e+00



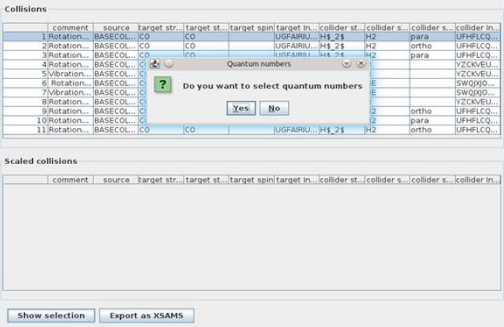
Merging heterogeneous data (implies selection of QN)



Transitions

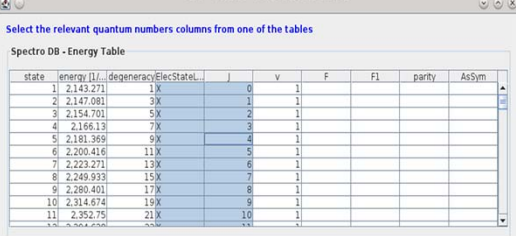
comment	source	structural formula	stoichiometric f.	spin	inchi key
1	28503-VI*CO...	CO	CO		UGFARJUMAVXC...
6	28512-VI*CO...	CO	CO		UGFARJUMAVXC...

Select QNs to keep in the schema



Collisions

comment	source	target str.	target st.	target spin	target in.	collider st.	collider s.	collider in.
1	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	para	UPHFLLCQ...
2	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	ortho	UPHFLLCQ...
3	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	para	UPHFLLCQ...
4	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	para	UPHFLLCQ...
5	Vibration...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	para	UPHFLLCQ...
6	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	ortho	UPHFLLCQ...
7	Vibration...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	ortho	UPHFLLCQ...
8	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	ortho	UPHFLLCQ...
9	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	ortho	UPHFLLCQ...
10	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	ortho	UPHFLLCQ...
11	Rotation...	BASECOL	CO	CO	UGFARJUMAVXC...	H2	ortho	UPHFLLCQ...





Select the relevant quantum numbers columns from one of the tables


Spectro DB - Energy Table

state	energy (J)	degeneracy	ElecState...	J	v	F	Fl	parity	AsSym
1	2,143.271	1X		0	1				
2	2,147.081	3X		1	1				
3	2,154.701	5X		2	1				
4	2,166.13	7X		3	1				
5	2,181.369	9X		4	1				
6	2,200.416	11X		5	1				
7	2,223.271	13X		6	1				
8	2,249.933	15X		7	1				
9	2,280.401	17X		8	1				
10	2,314.674	19X		9	1				
11	2,352.75	21X		10	1				
12	2,394.624	23X		11	1				

The merging is based on and possible because of **XSAMS**







Spectcol with New Output Formats

The screenshot displays the Spectcol software interface with several data tables and an export menu. The tables include:

- Rate coefficients:** A table with columns for transition (T1, T2), frequency (F1, F2), and rate coefficients at various temperatures (5.0, 10.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0).
- Einstein coefficients:** A table with columns for upper level, lower level, frequency (MHz), Einstein coefficient, log(intensity), uncertainty, and upper degeneracy.
- Collider state energy and quantum numbers:** A table with columns for state, energy (J/c), degeneracy, ElecState, J, v, F, F1, parity, and Asym.
- Partition function with CDMS degeneracy:** A table with columns for T (K) and Q.

At the bottom, there is an **Export** section with checkboxes for:

- energy
- rate coefficients
- Einstein coefficients
- collider energy
- partition function

 A **save as ASCII** button is also present.

Combination of Spectroscopic and collisional Data

Output format

Spectcol for Education

The screenshot displays the Spectcol software interface. On the left, a table lists energy levels for the $28503-v\ 1:CO; \$v=0\$$ state. The table includes columns for state, energy, degree of freedom, electronic state, angular momentum (J), vibrational quantum number (v), parity, and symmetry. On the right, the 'EnergyApp' window contains controls for 'Energy levels' (Min and Max energy level) and 'Quantum Numbers' (Select Qn: ElecStateLabel, J, v). Below these controls is an 'Energy diagram' graph showing energy levels in $1/cm$ versus energy in $1/cm$. The graph shows a series of energy levels starting from 0 and increasing to approximately 15,000 $1/cm$.

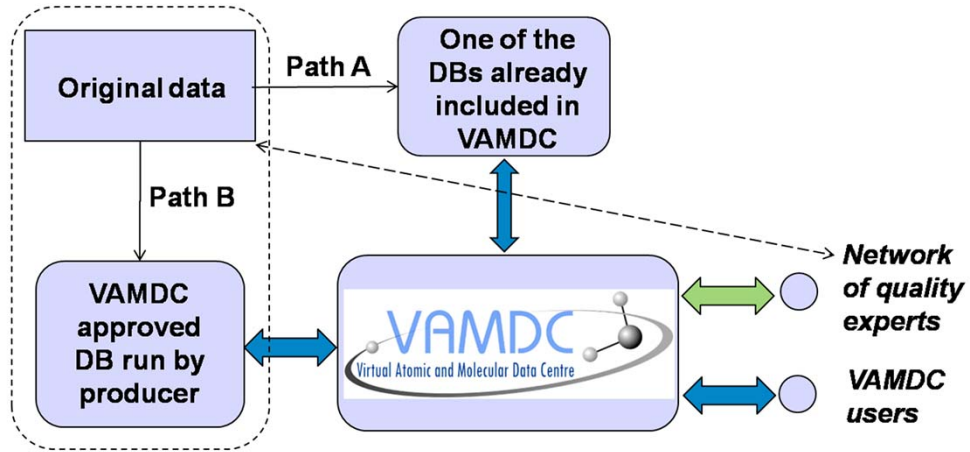
state	ener...	dege...	Elec...	J	v	F	F1	parity	AsSym
1	0.0	1X		0	0				
2	3.84...	3X		1	0				
3	11.5...	5X		2	0				
4	23.0...	7X		3	0				
5	38.4...	9X		4	0				
6	57.6...	11X		5	0				
7	80.7...	13X		6	0				
8	107...	15X		7	0				
9	138...	17X		8	0				
10	172...	19X		9	0				
11	211...	21X		10	0				
12	253...	23X		11	0				
13	299...	25X		12	0				
14	349...	27X		13	0				
15	403...	29X		14	0				
16	461...	31X		15	0				
17	522...	33X		16	0				
18	587...	35X		17	0				
19	656...	37X		18	0				
20	729...	39X		19	0				
21	806...	41X		20	0				
22	886...	43X		21	0				
23	971...	45X		22	0				
24	105...	47X		23	0				
25	115...	49X		24	0				
26	124...	51X		25	0				
27	134...	53X		26	0				

What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

- Query all registered databases via the Portal (www.portal.eu) or other portals
 - Visualisation of Data
 - Download of Data
 - *Overview of portal redesign. (Carlo Maria Zwölf)*
- Standalone Work with Software:
 - Query databases
 - Mix heterogeneous databases
 - Download
 - *Example of Standalone XSAMS Multi Processor (Nicolas Moreau)*
 - *Example of SPECTCOL software (Yaye Awa Ba)*
- Include new processors and/or applications on the portal.
- **Include new databases or data in the infrastructure**
- Use of our libraries in user applications in order to access the VAMDC registered databases

Include your data within VAMDC



What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

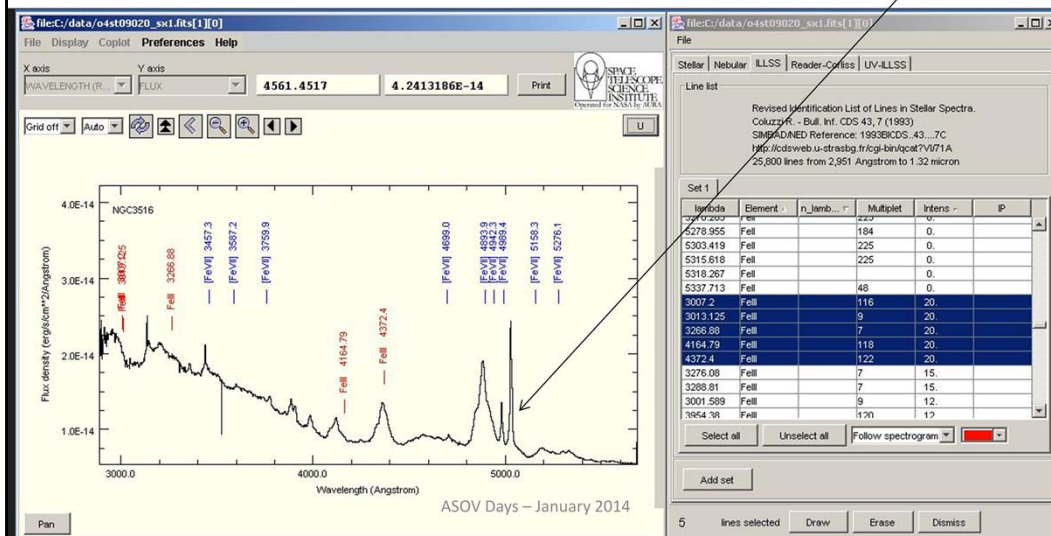
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Accessing VAMDC from User's Tool Specview Software



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

SSAP VO



BASS2000
Solar Survey Archive

327 MHz
Alpha
H3

Previous day OK Next day

Enter a date: Ex: 28/3/2001, 28.3.1, 28-3-01, YYYYMMDD or YYMMDD

en | fr My Selection

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- Latest observations
- Latest movies
- Long term archive
- News

QUERY

- For observations
- For specific content
- For solar features
- For synoptic maps
- HELIOS features cat.

TOOLS


- Ephemerids
- Solar spectrum
- Related topics
- Live Sun & webcams
- Software

GUIDES

- Instruments
- Data
- Software
- Educational resources (fr)

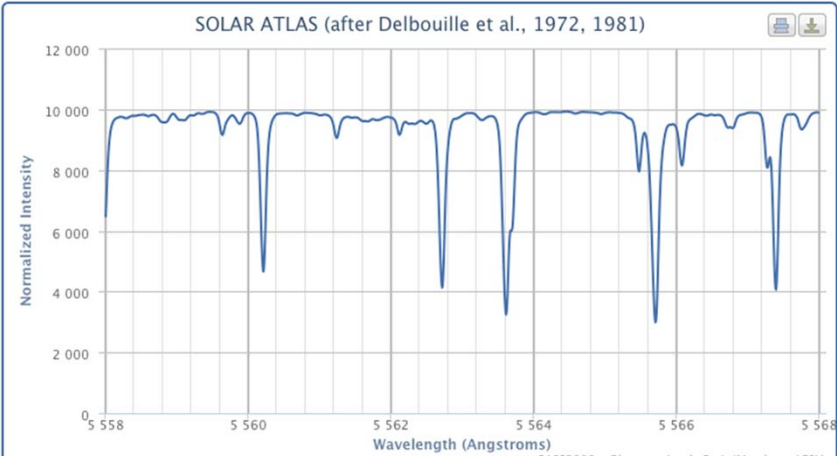
Collection before 1980
[Solar Web Guide](#)
[Multimedia Gallery](#)

HIGH RESOLUTION SOLAR SPECTRUM



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)

SOLAR ATLAS (after Delbouille et al., 1972, 1981)



Normalized Intensity

Wavelength (Angstroms)

BASS2000 - Observatoire de Paris/Meudon - LESIA

BASE DE DONNÉES SOLAIRE SOI
BASS2000
 Solar Survey Archive

327 MHz
 10-70 MHz
 Call K1V
 Call H3
 Helpha

Enter a date: Ex: 28/3/2001, 28.3.1, 28-3-01, YYYYMMDD or YYMMDD

Previous day OK Next day en | fr My Selection

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SOLAR ATLAS (after Delbouille et al., 1972, 1981)

12 000

Spectrum 5562.672 Å

Results from [NIST](#) (National Institut of Standards and Technology):

Ion	Observed Wavelength	Air (Å)	Ritz Wavelength Air (Å)	Aki (s-1) fik Acc.	Ei (cm-1)	Ek (cm-1)	gi-gk
Fe I	5562.7061		5 562.7052		35 767.564	-53 739.438	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	5562.9732121133	1219502.0	1/cm	1201531.0	1/cm

Database name	Element Symbol	Nuclear Charge	Wavelength	Upper State Energy	Upper State Energy Units	Lower State Energy	Lower State Energy Units
VALD	Fe	26	5560.209631067	53747.4960	1/cm	35767.5620	1/cm

VAMDC Products

- **Support =**
 - **Send mail to** support@vamdc.eu
 - Go to vamdc.eu/usersupport
 - Tutorial (different types)
- Portal = <http://portal.vamdc.eu>
- Software and Libraries = <http://vamdc.eu/software>
- Standards = <http://vamdc.eu/standards>
- Forums

Role of International Consortium

- Provide easy access to atomic and molecular data to the widest range of users
- Optimise time and work of users
- Be a vector of promotion for fundamental research in atomic and molecular physics
- Promote development of new scientific partnerships
- Be part of the future environment of research and education (help with answers to calls/promote pluri-disciplinarity/promote attractiveness of high education training)
- Develop industrial partnerships (know-how transfer, provide data, ..)
- Promote VAMDC and its partners



PROMOTION of research results of atomic and molecular
Physics and of their applications

Pôle Thématique National F-VAMDC

- Fait la promotion et anime la diffusion des données de physique atomique et moléculaire en France, en suivant la charte de qualité du consortium VAMDC (organisation de meetings, tutoriaux)
- A un avis consultatif sur les activités françaises vis-a-vis des instances françaises, cet avis étant donné par le collectif = c-a-d les membres de F-VAMDC
- Répond aux besoins des utilisateurs astrophysiques français ou se fait l'interlocuteur auprès de VAMDC des besoins de ces utilisateurs (chacun dans son domaine)
- S'appuie sur les centres d'expertise, son université, sa région, son institut CNRS au niveau des moyens humains et financiers
- Lieu d'échange pour les solutions techniques, Mutualisation des moyens est une possibilités
- Chaque membre de F-VAMDC maintient ses bases de données et ses services en suivant la charte VAMDC

- Chaque membre est individuellement membre de VAMDC International

From **International** to **Local** Organisations
Pôle Thématique National F-VAMDC

- OV-GSO (OSU Bordeaux + OSU Toulouse)
- OSU THETA
- Observatoire de Paris

- Avec des laboratoires associés qui ne sont pas dans des OSU
- Université de Lille
- Université de Champagne-Ardenne
- Autres

- Comité Pilotage: OSU, INSU, PN, P.I. Scientifiques des services, Responsable Technique (N. Moreau) et Coordinateur.
- Comité Utilisateur: les producteurs et les utilisateurs de données/standards/software/clients (chaque base a son propre comité utilisateur)

From **International** to **Local** Organisations
**Axe Physique Atomique et
Moléculaire à VO-PDC**

Responsable: C.M. Zwölf
Chef de Projet: N. Moreau
CDD IE SUP@VAMDC: Y.A. Ba

Services VAMDC*
P.I. ML Dubernet

Services
Physique Moléculaire
BASECOL* (M.L. Dubernet)
SESAM (E. Roueff)

Services Physique
Atomique
TipTopBase (F. Delahaye)
Stark-B (S. Sahal-Bréchet)