

## First steps with the VAMDC web-portal

The VAMDC web-portal is the best place for new users to approach the system. It is a web-site that allows you to query all the databases in VAMDC.

### Task 1: find the right portal

With a web browser <sup>1</sup>, go to the page <http://portal.vamdc.eu/> (<http://portal.vamdc.org/> is the same place). You will see a simple entry-page with links to three <sup>2</sup> separate portals. One is released for external users (such as yourself) and the others are for VAMDC testing. Follow the links to all three portals and compare the results.

**Expected results:** the "development" portal asks for a password which you do not have. This portal is not available at all to end users. The others show you nearly identical welcome pages like this:



The number of available databases differs between the portals: the test versions have more. This reflects the fact that the different portals *lead to different versions of the VAMDC system* with different data linked in. For consistency of results, make sure that you always use the released version of the portal. <sup>3</sup> All the subsequent tasks assume that you use the released portal.

### Task 2: investigate the available databases

On the welcome page of the portal, find the link to the list of databases. Note the descriptions of the kinds of data on that page and explore the links to the longer descriptions. Identify the databases that specialise in molecular spectroscopy.

**Relevant section of user guide:**  
<http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PortalUserGuide#VAMDCDatabases>

**Expected results:** the list of databases looks something like this:

Name	Description
<a href="#">Cologne Database for Molecular Spectroscopy (CDMS)</a>	The Cologne Database for Molecular Spectroscopy (CDMS) contains a catalog of radio frequency and microwave to far-infrared spectral lines of atomic and molecular species in interstellar and circumstellar environments. The catalog is continuously updated.
<a href="#">MeCaSDa - Methane Calculated Spectroscopic Database</a>	Calculated line lists for methane (12CH <sub>4</sub> , 13CH <sub>4</sub> and 13CH <sub>3</sub> D). The data on methane contain the vibration-rotation energy levels, line positions and line intensities in the range 100-1000 cm <sup>-1</sup> .
<a href="#">VALD (atoms)</a>	The Vienna Atomic Line Database (VALD) is a collection of atomic line parameters (wavelengths, transition energies and quantum numbers, oscillator strengths, Landé factors) representation of the atomic data in VALD3.
<a href="#">OACT-LASP Database</a>	Laboratoire d'Astrophysique Spatiale (Clermont-LASP for short) has been active in Clermont starting from the eighties. The eldest of the group, after some training at the Physics Department of the University of Clermont-Ferrand, has been active in the Physics Department of the University of Clermont-Ferrand. Since then and thanks to several funding agencies (Conseil National des Recherches, Italian CNR, Ministero dell'Istruzione, dell'Università e della Ricerca, etc.) the Observatory has grown. Today Clermont-LASP means a group of 6 people with permanent position plus some students and post-docs for the deposition of ice films, ion and Lyman-alpha irradiation experiments, many spectrometers in the range from 190 nm up to 2000 nm, and also raman spectrographs.
<a href="#">BASECOL - VAMDC-TAP interface</a>	This database, called BASECOL, is devoted to collisional ro-vibrational excitation of molecules by colliders such as atom, ion, molecule or electron. It is supervised by an internal team of experts in order to ensure the continuity and the quality of the database.
<a href="#">TOPbase - VAMDC-TAP interface</a>	TOPbase lists LS-coupling energy levels, g-factors and photoionization cross sections for astrophysically abundant ions (Z=1-14, Z=16-18, Z=20, Z=28) computed in the O shell.
<a href="#">Theoretical spectral database of polycyclic aromatic hydrocarbons</a>	The Cagliari/Toulouse PAH database is a collection of theoretical spectroscopic data about Polycyclic Aromatic Hydrocarbons and carbon clusters. It provides basic geometric and spectroscopic data. It is maintained by the Astrochemistry group at INAF-Observatory of Cagliari and the Institut de Recherche en Astrophysique et Planétologie in Toulouse.

These databases deal with molecular spectroscopy: CDMS, MeCaSDa, OACT-LASP, Cagliari/Toulouse PAH, S&MPO, ECaSDa, CDSD, WADIS, HITRAN. Note that you have to follow the per-database links to find this out for some of the entries.

The information is structured around the set of distinct databases contributed to VAMDC by data providers. This structure appears throughout VAMDC: there is no single database for "spectroscopy".

You might see more molecular-spectroscopy databases than listed above. This reflects that fact that VAMDC is dynamic. Databases can be added to the system at any time. <sup>4</sup>

## Task 3: find some spectroscopic data

From the portal's welcome page, follow the link to the query page. Enter a query on wavelength, specifying a wavelength range of 5000 to 5010 Angstroms.<sup>5</sup> (Hint: constraints on spectral region are in the "processes" menu.) Observe how the other information on the page changes as you enter the search terms. Submit the search (hint: use the "find data button"; the "save query button isn't relevant here) and note the results; identify the databases that have data for this search.

**Relevant section of user guide:**  
<http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PortalUserGuide#Query>

**Expected results:** the query page looks like this before you submit the search:

The screenshot shows the VAMDC query interface. On the left, there are tabs for 'Species', 'Processes', 'Environment', and 'Advanced'. The 'Radiative' section has input fields for 'Wavelength' (5000 to 5010 Å), 'Equivalent Wavelength', 'Upper state energy', 'Lower state energy', 'Equivalent to', and 'Probability, A'. On the right, a 'Legend' lists various databases, with some highlighted in green, indicating they are available and understand the search term.

The list to the right of the search form is a list of databases registered in VAMDC. Those that are available<sup>6</sup> and which understand the search term are highlighted in green.

When you submit the search, the portal comes back quickly with a page that looks like this:

The screenshot shows the VAMDC query results page. At the top, there are buttons for 'Done', 'Modify query', 'Stop waiting', and 'Save query'. Below these, there is a 'Comments' section and a 'XSAMS processors' section with a progress bar. The main part of the page is a table with columns: Name, Response, Download, Species, States, Processes, and Radiative. The table lists various databases and their corresponding results.

Name	Response	Download	Species	States	Processes	Radiative
<input type="checkbox"/> VALD sub-set in Moscow (oba)	OK	<a href="#">XSAMS</a>	81	1157	701	701
<input type="checkbox"/> Water Internet Accessible Distributed Information System	OK	<a href="#">XSAMS</a>	1	561	601	601
<input type="checkbox"/> TOPPhase - VAMDC-TAP interface	OK	<a href="#">XSAMS</a>	70	619	353	353
<input type="checkbox"/> HITRAN-UCL resource	OK	<a href="#">XSAMS</a>	8	64	149	149
<input type="checkbox"/> Chianti	OK	<a href="#">XSAMS</a>	18	81	43	43
<input type="checkbox"/> Spectr-W3	OK	<a href="#">XSAMS</a>	9	28	13	13
<input type="checkbox"/> GSMA Reims SAMPO	OK	<a href="#">XSAMS</a>	0	0	5	5
<input type="checkbox"/> Stark-6	OK	<a href="#">XSAMS</a>	4	6	3	3
<input type="checkbox"/> VALD (atoms)	TRUNCATED (9%)	<a href="#">XSAMS</a>	78	10078	65459	65459
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	EMPTY		0	0	0	0
Carbon Dioxide Spectroscopic Database - 1000K	EMPTY		0	0	0	0
Carbon Dioxide Spectroscopic Database - 298K	EMPTY		0	0	0	0
McCaSda - Methane Calculated Spectroscopic Database	EMPTY		0	0	0	0
Lund laboratory spectroscopy database	EMPTY		0	0	0	0
ECaSDa - Ethene Calculated Spectroscopic Database	EMPTY		0	0	0	0

When you first see this page, the search is still in progress: there is a progress bar at the top of the page. The page updates as each database reports its results. The whole search should complete within one minute.

The main part of the page is a table of results for each database queried, listing the number of species, lines etc. found in the search. There should be one row for each of the databases highlighted in the query form: the search only includes the databases which the portal knows to understand the search term.<sup>7</sup>

The response column states "OK" or "EMPTY" or "TRUNCATED" or "FAIL" for each database searched. "OK" means data are available. "EMPTY" means that no data match the search term. "TRUNCATED" means that many data are available from the search and the database is declining to give you all of them in one go. You can either get the indicated percentage of the results, or refine your query to match fewer results (e.g. by reducing the spectral range, or by limiting to particular emitting species). "FAIL" means that something broke within the system: this is not your fault! You should report failures to VAMDC for correction.


At this point, no data have actually been extracted from the databases. Only counts of things have been collected. Therefore the search is relatively quick, even when huge volumes of data match the search terms. Actually getting the data is the next task.

## Task 4: view the data found in a search

View the search results from the previous task are fine for this task). Select the Chianti results from the table (hint; use the checkbox at the start of the Chianti row), and no others, and send them to the "XSAMS processor" called "Table views of XSAMS" for viewing results as tables. Investigate the available information on the states and lines.

**Relevant section of user guide:**  
[http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PortalUserGuide#XSAMS\\_Processors](http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PortalUserGuide#XSAMS_Processors)

**Expected results:** The processor gives you a page, opening in a new tab or window of the browser, looking like this:

 **State-list view of XSAMS**

(Switch to view of [radiative transitions](#) or [collisions](#))

chianti-2013-07-21-16-2-57 : select \* where (RadTransWavelength >= 5000.0 AND RadTransWavelength <= 5010.0)

[Show table in CSV format](#)

Species	State	Energy
Fe <sup>9+</sup>	Schianti-10009026: 3s2 3p4 3d — [Ne] 3s <sup>2</sup> 3p <sup>4</sup> 3d <sup>1</sup> 4F <sub>3,5</sub>	422785.0 1/cm
Fe <sup>13+</sup>	Schianti-109013026: 3p 3d2 — [Ne] 3p <sup>1</sup> 3d <sup>2</sup> 4D <sub>3,5</sub>	1469476.0 1/cm
Fe <sup>13+</sup>	Schianti-115013026: 3p 3d2 — [Ne] 3p <sup>1</sup> 3d <sup>2</sup> 3P <sub>0,5</sub>	1489445.0 1/cm
Ne <sup>5+</sup>	Schianti-123005010: 2s 2p 4p — [He] 2s <sup>1</sup> 2p <sup>1</sup> 4p <sup>1</sup> 4S <sub>1,5</sub>	1119423.0 1/cm
Al <sup>+</sup>	Schianti-16001013: 3s 4p — [Ne] 3s <sup>1</sup> 4p <sup>1</sup> 3P <sub>1,0</sub>	105441.5 1/cm
Fe <sup>9+</sup>	Schianti-16009026: 3s2 3p4 3d — [Ne] 3s <sup>2</sup> 3p <sup>4</sup> 3d <sup>1</sup> 4P <sub>1,3</sub>	445204.0 1/cm
Fe <sup>+</sup>	Schianti-17001026: 2p5 3d6 4s2 — [Mg] 2p <sup>5</sup> 3d <sup>6</sup> 4s <sup>2</sup> 3d <sup>6</sup> 4s <sup>1</sup> 4p <sup>1</sup> 4D <sub>3,5</sub>	5779179.9 1/cm
Fe <sup>23+</sup>	Schianti-17023026: 1s2 5p — 1s <sup>2</sup> 5p <sup>1</sup> 1s <sup>2</sup> 5p <sup>1</sup> 2P <sub>0,5</sub>	13957516.0 1/cm
Fe <sup>10+</sup>	Schianti-181010026: 3s2 3p2 3d2 — [Ne] 3s <sup>2</sup> 3p <sup>2</sup> 3d <sup>2</sup> 1P <sub>1,0</sub>	1029001.0 1/cm
Fe <sup>9+</sup>	Schianti-19009026: 3s2 3p4 3d — [Ne] 3s <sup>2</sup> 3p <sup>4</sup> 3d <sup>1</sup> 4P <sub>2,5</sub>	442760.0 1/cm

The "XSAMS processors" are services associated with the portal <sup>8</sup> that transform the results from VAMDC's common, machine-readable format (XSAMS) into other forms. This particular processor tries to display in the browser "all" <sup>9</sup> the data and metadata.

The first page of results tabulate the atomic states. From here you can look at details of each state, or switch to a view of lines or collisions; from those pages, you can get details of individual lines and collisions. <sup>10</sup>

Now try to send the data to the processor called "Atomicxsams2HTML".

**Expected results:** The processor gives you a page, opening in a new tab or window of the browser, looking like this:

Reset page

Show As Csv

Send with samp

Unselect all	Spec ion	Wavelength(Å)	A	Weighted Oscillator Strength	Lower state description	Lower energy(1/cm)	Lower statistical weight	Lower parity	Lower total angular momentum	Upper state description	Upper energy(1/cm)	Upper statistical weight	Upper parity	Upper total angular momentum
<input checked="" type="checkbox"/>	Al 2	5009.9800	8822.0000	0000.0001	3p2	85481.4000	05.0000	even	2.0	3s 4p	105441.5000	03.0000	odd	1.0
<input checked="" type="checkbox"/>	Ca 13	5003.5000	0178.6000		2s 2p5	618280.0000	05.0000	odd	2.0	2s 2p5	638266.0000	03.0000	odd	1.0
<input checked="" type="checkbox"/>	Ca 13	5007.3500	0000.0016		2s2 2p3 3d	3789959.0000	07.0000	odd	3.0	2s2 2p3 3d	3828150.0000	11.0000	odd	5.0
<input checked="" type="checkbox"/>	Ca 2	5002.8700	23570000.0000	0000.3538	3p6 5p	60533.0000	02.0000	odd	0.5	3p6 6d	80521.5000	04.0000	even	1.5
<input checked="" type="checkbox"/>	Fe 10	5006.2600	0000.6356		3s2 3p4 3d	422785.0000	08.0000	even	3.5	3s2 3p4 3d	442760.0000	06.0000	even	2.5
<input checked="" type="checkbox"/>	Fe 10	5007.0100	0000.5278		3s2 3p4 3d	425232.0000	02.0000	even	0.5	3s2 3p4 3d	446204.0000	04.0000	even	1.5
<input checked="" type="checkbox"/>	Fe 11	5000.2500	0000.0000		3s2 3p2 3d2	1053166.0000	09.0000	even	4.0	3s2 3p2 3d2	1073165.0000	03.0000	even	1.0
<input checked="" type="checkbox"/>	Fe 11	5000.5000	0000.0000		3s 3p3 3d2	1155548.0000	05.0000	odd	2.0	3s 3p3 3d2	1175548.0000	09.0000	odd	4.0

This page provides several useful features. It possible to hide/show lines and columns in the table and to sort lines. Then you can display all selected data as a csv text. Try to display the available data for Ca 13 ion as csv ( you can remove columns containing no data ).

**Expected results:** The page content is updated with the selected data displayed as text

Reset page

Show As Csv

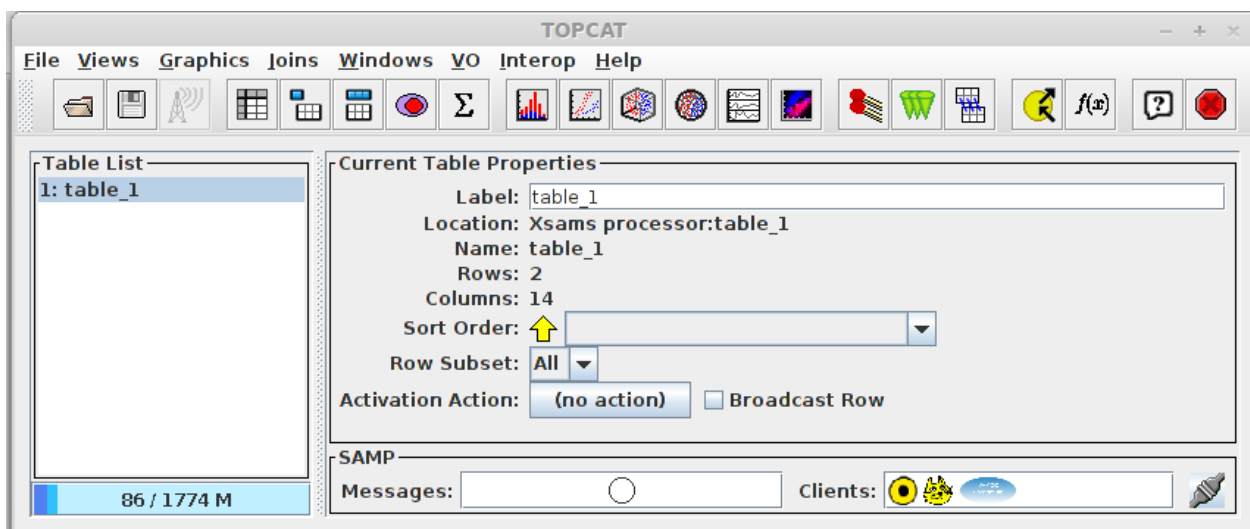
Send with samp

#,Spec Ion,Wavelength(Å),A,Weighted Oscillator Strength,Lower state description,Lower energy(1/cm),Lower statistical weight,Lower parity,Lower total angular momentum,Upper state description,Upper energy(1/cm),Upper statistical weight,Upper parity,Upper total angular momentum  
Ca 13,5003.5000,0178.6000,,2s 2p5,618280.0000,05.0000,odd,2,0,2s 2p5,638266.0000,03.0000,odd,1,0  
Ca 13,5007.3500,0000.0016,,2s2 2p3 3d,3789959.0000,07.0000,odd,3,0,2s2 2p3 3d,3828150.0000,11.0000,odd,5,0

Select all	Spec ion	Wavelength(Å)	A	Weighted Oscillator Strength	Lower state description	Lower energy(1/cm)	Lower statistical weight	Lower parity	Lower total angular momentum	Upper state description	Upper energy(1/cm)	Upper statistical weight	Upper parity	Upper total angular momentum
<input type="checkbox"/>	Al 2	5009.9800	8822.0000	0000.0001	3p2	85481.4000	05.0000	even	2.0	3s 4p	105441.5000	03.0000	odd	1.0
<input checked="" type="checkbox"/>	Ca 13	5003.5000	0178.6000		2s 2p5	618280.0000	05.0000	odd	2.0	2s 2p5	638266.0000	03.0000	odd	1.0
<input checked="" type="checkbox"/>	Ca 13	5007.3500	0000.0016		2s2 2p3 3d	3789959.0000	07.0000	odd	3.0	2s2 2p3 3d	3828150.0000	11.0000	odd	5.0
<input type="checkbox"/>	Ca 2	5002.8700	23570000.0000	0000.3538	3p6 5p	60533.0000	02.0000	odd	0.5	3p6 6d	80521.5000	04.0000	even	1.5

The last fonctionnality provided by the page is the possibility to send data from this html table to another application thanks to the Simple Application Message Protocol (Samp) **Standard page:** <http://www.ivoa.net/documents/SAMP/>

This is a protocol from the International Virtual Observatory Alliance allowing data exchange between applications. Launch the "Topcat" application. At startup, Topcat automatically launches a Samp Hub that will listen to messages from other applications. Click on the "Send with samp" button. A warning message will appear, you can click "Yes". All selected lines will be sent to Topcat which provides a great set of data manipulation features.



	Spec Ion	Wavelength(A)	A	Weight...	Lower state ...	Lower energy...	Lower st...	Lower ...	Lower tot...	Upper state ...	Upper energy...	Upper sta...	Upper ...	Upper to...
1	Ca 13	5003,5	178,6		2s 2p5	6,182800E5	5,	odd	2,	2s 2p5	6,382660E5	3,	odd	1,
2	Ca 13	5007,35	0,0016		2s2 2p3 3d	3,798959E6	7,	odd	3,	2s2 2p3 3d	3,828150E6	11,	odd	5,

## Task 5: find some data on atom-molecule collisions

Go to the query page of the portal. Enter a search where the target is a carbon monoxide molecule (all isotopologues) and the collider is a hydrogen atom (hint: you need to enter the two reactants from the species menu and then assign the roles from the processes/collisions menu; you don't need to specify any code for the kind of collision). Submit the query and from the results, select and view the Basecol results and then the Kida results.

**Relevant section of user guide:**  
<http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PortalUserGuide#Query>

**Expected results:** the completed search-form looks like this:

Atoms (collider)

Clear

Remove

Find data

Save query

Atom symbol

H

Mass number

Nuclear charge

Ion charge

InChIKey

State energy

Equivalent to

1/cm

Molecules (target)

Clear

Remove

Chemical name

Carbon Monoxide

Stoichiometric formula

CO

Structural formula

CO

Spin isomer

Standard InChIKey

UGFAIRUMAVXQW-RGIGPVFXSA-N  
UGFAIRUMAVXQW-ZDQIHCHSA-N  
UGFAIRUMAVXQW-HQMMCCQPSA-N

Select All None

Search by stoichiometric formula if no inchikey is selected.

Formula

InChIKey

☒

(12C)(16O)

UGFAIRUMAVXQW-UHFFFAOYSA-N

☒

(13C)(16O)

UGFAIRUMAVXQW-DUBTZBYSA-N

☒

(12C)(18O)

UGFAIRUMAVXQW-HQMMCCQPSA-N

☒

(12C)(17O)

UGFAIRUMAVXQW-VQEHGDOOSA-N

☒

(13C)(18O)

UGFAIRUMAVXQW-RGIGPVFXSA-N

☒

(13C)(17O)

UGFAIRUMAVXQW-ZDQIHCHSA-N

Collisions

Clear

Remove

Process name

Process description

Process code

IAEA process code

Species

Role

Atoms

Role

Collider

Molecules

Role

Target

Legend

available, can answer

available, don't support query

unsupported keyword

Cologne Database for Molecular Spectroscopy: VAMDC-TAP service

McAfee - Methane Calculated Spectroscopic Database

VALD (atoms)

OACT - LASP Database

BASECOL: VAMDC-TAP interface

TOPbase - VAMDC-TAP interface

Theoretical spectral database of polycyclic aromatic hydrocarbons

IEAD18 - Ionsbruck Dissociative Electron Attachment Database

Chianti

TPbase - VAMDC-TAP interface

GSMA Reims S&MPO

ECASDs - Ethene Calculated Spectroscopic Database

Carbon Dioxide Spectroscopic Database - 290K

GbaSST

Carbon Dioxide Spectroscopic Database - 1000K

Land laboratory spectroscopy database

Stark-9

Spect-W3

Water Internet Accessible Distributed Information System


HITRAN-2016

VALD sub-set in Moscow (obs)

KIDA: VAMDC-TAP interface

As you enter the identity of the molecule, the portal suggest a list of possible matches. When you select one of the matches, the portal then suggests a list of isotopologues for that molecule. You can select all isotopologues or a sub-set. <sup>11</sup>

In the data viewer, you should look at the collisions list and from there, the information for a single collision. You will find, for Basecol, a table of rate coefficients, like this:


**Data for single collision**


$$\text{CO} + {}^1\text{H} \rightarrow \text{CO} + {}^1\text{H}$$

- M.-L. Dubernet, BASECOL database, , 2013
- N. Balakrishnan, M. Yan and A. Dalgarno, *Quantum-Mechanical Study of Rotational and Vibrational Transitions in CO Induced by H Atoms*, *apj*, **568**, 443-447, 2002

**rateCoefficient**

(K)	(cm <sup>3</sup> /s)
5.0	1.78E-10
10.0	1.93E-10
20.0	2.02E-10
30.0	2.09E-10
40.0	2.15E-10
50.0	2.2E-10
60.0	2.25E-10
70.0	2.28E-10
80.0	2.32E-10
90.0	2.34E-10
100.0	2.37E-10

or, for Kida, alegbraic fits to the rate coefficients like this:


**Data for single collision**

$$\text{COH} + {}^4\text{He}^+ \rightarrow \text{CO} + \text{HHe}$$

**rateCoefficient**

- unspecified, OSU, , 2009

$$\alpha \cdot (T/300)^{\beta} \cdot e^{-\gamma \cdot (T/300)}$$

(in Fortran) where:
 

- T (K; valid from 10.0 to 280.0) Temperature
- alpha = 6.9E-10
- beta = -0.5
- gamma = 0.0

**rateCoefficient**

- Woon, D. E. and Herbst, E., *Quantum Chemical Predictions of the Properties of Known and Postulated Neutral Interstellar Molecules*, *apjs*, **185**, 273-288, 2009

$$\alpha \cdot (T/300)^{\beta} \cdot e^{-\gamma \cdot (T/300)}$$

(in Fortran) where:
 

- T (K; valid from 10.0 to 800.0) Temperature
- alpha = 0.333 branching ratio
- beta = 1.99E-9
- gamma = 3.58

Whereas spectroscopic data from VAMDC can be well represented in one row of a table per line, the collision data have one or more complete 2D data-sets per collision. Kida includes alternate functions for the rate coefficient from different sources.

## Task 6: downloading the data

Execute a search in the portal (the results from any of the previous tasks will suit). Download the results in XSAMS format and inspect them.

Relevant	section	of	user	guide:
<a href="http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PortalUserGuide#Query_results_table">http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PortalUserGuide#Query_results_table</a>				

**Expected results:** the downloaded data are in XSAMS format, which is a dialect of XML. If you look at the XSAM file in a text editor, the start looks like this:

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?><XSAMSData xmlns="http://vamdc.org/xml/xsams/0.3"
xmlns:cml="http://www.xml-cml.org/schema" xmlns:asymcs="http://vamdc.org/xml/xsams/0.3/cases/asymcs"
xmlns:asytnc="http://vamdc.org/xml/xsams/0.3/cases/asytnc" xmlns:atc="http://vamdc.org/xml/xsams/0.3/cases/atc"
xmlns:gms="http://vamdc.org/xml/xsams/0.3/cases/gms" xmlns:hunda="http://vamdc.org/xml/xsams/0.3/cases/hunda"
xmlns:hundb="http://vamdc.org/xml/xsams/0.3/cases/hundb" xmlns:lpcs="http://vamdc.org/xml/xsams/0.3/cases/lpcs"
xmlns:lpoc="http://vamdc.org/xml/xsams/0.3/cases/lpos" xmlns:lptcs="http://vamdc.org/xml/xsams/0.3/cases/ltpcs"
xmlns:ltpos="http://vamdc.org/xml/xsams/0.3/cases/ltpos" xmlns:nltcs="http://vamdc.org/xml/xsams/0.3/cases/nltcs"
xmlns:nltos="http://vamdc.org/xml/xsams/0.3/cases/nltos" xmlns:sphcas="http://vamdc.org/xml/xsams/0.3/cases/sphcas"
xmlns:sphos="http://vamdc.org/xml/xsams/0.3/cases/sphos"
xmlns:stcas="http://vamdc.org/xml/xsams/0.3/cases/stcs"><Species><Atoms><Atom><ChemicalElement><NuclearCharge></NuclearCharge><ElementSymbol>H</ElementSymbol>
```

which is not particularly readable. With line breaks added, it looks like this:

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<XSAMSData xmlns="http://vamdc.org/xml/xsams/0.3" xmlns:cml="http://www.xml-cml.org/schema"
  xmlns:asymcs="http://vamdc.org/xml/xsams/0.3/cases/asymcs"
  xmlns:asymos="http://vamdc.org/xml/xsams/0.3/cases/asymos"
  xmlns:dcsc="http://vamdc.org/xml/xsams/0.3/cases/dcs"
  xmlns:gen="http://vamdc.org/xml/xsams/0.3/cases/gen"
  xmlns:hunda="http://vamdc.org/xml/xsams/0.3/cases/hunda"
  xmlns:hundb="http://vamdc.org/xml/xsams/0.3/cases/hundb"
  xmlns:lpcc="http://vamdc.org/xml/xsams/0.3/cases/lpcs"
  xmlns:lpoc="http://vamdc.org/xml/xsams/0.3/cases/lpos"
  xmlns:ltcc="http://vamdc.org/xml/xsams/0.3/cases/ltcs"
  xmlns:ltoc="http://vamdc.org/xml/xsams/0.3/cases/ltos"
  xmlns:nlcc="http://vamdc.org/xml/xsams/0.3/cases/nltcs"
  xmlns:nlto="http://vamdc.org/xml/xsams/0.3/cases/nltos"
  xmlns:sphcc="http://vamdc.org/xml/xsams/0.3/cases/sphcs"
  xmlns:sphoc="http://vamdc.org/xml/xsams/0.3/cases/sphos"
  xmlns:stcc="http://vamdc.org/xml/xsams/0.3/cases/stcs">
  <Species>
    <Atoms>
      <Atom>
        <ChemicalElement>
          <NuclearCharge>1</NuclearCharge>
          <ElementSymbol>H</ElementSymbol>
        </ChemicalElement>
        <Isotope>
          <IsotopeParameters>
            <MassNumber>1</MassNumber>
            <Mass>
              <Value units="amu">1.00783</Value>
            </Mass>
          </IsotopeParameters>
          <Ion speciesID="XBAS8">
            <IonCharge>0</IonCharge>
            <AtomicState stateID="SBASET57-1">
              <Comments>Energy level of H (no structure)</Comments>
              <SourceRef>BBAS0</SourceRef>
              <AtomicNumericalData>
                <StateEnergy>
                  <Value units="1/cm">0.0</Value>
                </StateEnergy>
              </AtomicNumericalData>
              <AtomicQuantumNumbers>
                <TotalAngularMomentum>0.0</TotalAngularMomentum>
              </AtomicQuantumNumbers>
            </AtomicState>
          </Ion>
        </Isotope>
      </Atom>
    </Atoms>
    <AtomicComposition>
      <Component>
        <Term>
          <LS>
```

```

        <L>
          <Value>0</Value>
          <Symbol>L</Symbol>
        </L>
        <S>0.0</S>
      </LS>
    </Term>
  </Component>
</AtomicComposition>
</AtomicState>
<InChIKey>YZCKVEUIGOORGS-UHFFFAOYSA-N</InChIKey>
</Ion>
</Isotope>
</Atom>
</Atoms>
...

```

which is better but still not comfortable to read. XSAMS is VAMDC's exchange format for moving data between applications and it is not optimised for human viewing. (If you need to read it yourself, the XSAMS viewer from the earlier task of this exercise is your friend.) You might download the XSAMS if you have local software that reads the format; if you plan to upload the data to an on-line service that reads XSAM; or if you want to archive your search results in a self-describing form.

### Footnotes

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- 1 Any recent browser should work with VAMDC portal. You must have Javascript, but not Java, enabled in the browser; this is how most browsers are set by default.
  - 2 Depending on the state of development, there might be fewer than three portals. There will always be at least one, and normally at least two.
  - 3 When there is an unlocked portal for testing, you are free to use it. However, beware of changes in both the system software and the underlying data: this test system may be using newer versions of the databases.
  - 4 VAMDC sometimes gains major features such as new databases across system releases, but databases are more likely to be added to an already-released system.
  - 5 The default search term for spectral region is wavelength in Angstroms because many of the builders and early users of VAMDC are Astrophysicists. You can search on frequency, wavenumber or photon energy instead, if you wish, and you can use different units.
  - 6 "Registered" means that the database is known to VAMDC and usually accessible. "Available" means that the VAMDC node that gives access to the database is actually working at present.
  - 7 The exact query sent to each database is shown at the top of the results page, near the progress bar. It is sometimes useful to write this down for future reference, although we won't need that information in the current exercise.
  - 8 These services work with the portal but are not structurally part of it. This means that you can use them separately from the portal; but that is an advanced usage and not part of this exercise.



- 9 XSAMS is rich in metadata and flexible, so displaying all the information for every case is challenging. The current viewer doesn't get all of it, but is upgraded occasionally to be more complete. If you find that the display is missing something of importance to you, raise an issue with VAMDC support.
- 10 In the current example, the Chianti data-extract has line data but nothing on collisions (Chianti's excitation tables should show up here but sadly have not yet been added to the Chianti node.) The collisions page is reachable but contains an empty table.
- 11 This matching of identifies for species is done using a local database of species built into the portal, essentially a union of all the species known to all the VAMDC nodes. The content of that database is also available as a specialised VAMDC node that know of species but not lines or collisions. In advanced uses, you can query that database directly, but this trick is not explored in the current exercise.