

# VAMDC

## Asynchronous requests with PDL in VAMDC Portal

*<http://portal.vamdc.eu/>*

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# The VAMDC Consortium

- A consortium of Institutes and Research Institutions that share a common technical and political framework for the distribution and curation of atomic and molecular data
- 15 full members
- Distribution, curation, access to atomic and molecular data
- Provides tools to look for and manipulates data

# The VAMDC Portal

- Main access point to look for data in VAMDC
- <http://portal.vamdc.eu>
- Queries VAMDC registry to get active databases
- 29 databases
- Uses VAMDC-TAP for requests
- Results are obtained in **XSAMS format** ( xml schema to describe atomic and molecular data )
- XSAMS files can be transformed to simplify data access

## Welcome to the VAMDC portal!

Currently we have 29 databases running and ready to serve you with the data.

Portal provides two search modes :

## 1. Guided search

[Home](#) [VAMDC databases](#) [Guided query](#) [Advanced query](#) [Saved queries](#) | [Info](#) [Feedback](#) [Login](#) [Register](#)

### Welcome to the VAMDC portal!

Currently we have 29 databases running and ready to serve you with the data.

# Looking for data : Guided query

Choose a request type ( [reset page](#) )

- For radiative process
- By species

Build a request  
step by step

# Looking for data : Guided query

Build a request  
step by step

**Choose a request type ( [reset page](#) )**

For radiative process  
 By species

**Define radiative configuration**

Wavelength  to  A

**Equivalent Wavelength** A

Choose the transition type

Transition from an energy range to another one  
 Transition to and from a given energy range  
 Any transition

# Looking for data : Guided query

Build a request  
step by step

**Choose a request type ( [reset page](#) )**

For radiative process  
 By species

---

**Define radiative configuration**

Wavelength   to   A ▼  
 Equivalent Wavelength A

Choose the transition type

Transition from an energy range to another one  
 Transition to and from a given energy range  
 Any transition

---

**Search by state energy**

Upper state energy   to   1/cm ▼  
 Equivalent to 1/cm

Lower state energy   to   1/cm ▼  
 Equivalent to 1/cm

Probability, A   to   1/s



# Looking for data : Guided query

Build a request  
step by step

**Choose a request type ( [reset page](#) )**

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 Equivalent to 1/cm

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 Equivalent to 1/cm

Probability, A   to   1/s

**Please, enter the number of species you wish to add**

Number of atoms 1 ▼

Number of molecules 0 ▼

Number of particles 0 ▼

Next ->

Submit query and find data

Portal provides two search modes :

## 2. Advanced search

[Home](#) [VAMDC databases](#) [Guided query](#) [Advanced query](#) [Saved queries](#) | [Info](#) [Feedback](#) [Login](#) [Register](#)

### Welcome to the VAMDC portal!

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Query by...

Species

Processes

Environment

**Advanced**

**Atom 1**
Clear Remove form

Atom symbol

Mass number  to

Nuclear charge  to

Ion charge  to

InChIKey

State energy  to  1/cm ▾

Equivalent to 1/cm

---

**Radiative**
Clear Remove form

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  1/s

Find data

### Legend

available, can answer

available, don't support query

unsupported keyword

- Belgrade electron/atom(molecule) database (BEAMDB)
- TFMeCaSDa - CF4 Calculated Spectroscopic Database
- Photodissociation - MolD database
- Chianti
- GSMA Reims S&MPO
- ECaSDa - Ethene Calculated Spectroscopic Database
- GhoSST
- SHeCaSDa - SF6 Calculated Spectroscopic Database
- Stark-b
- JPL database: VAMDC-TAP service
- HITRANonline
- VALD sub-set in Moscow (obs)
- RADAM - Ion Interactions
- MeCaSDa - Methane Calculated Spectroscopic Database
- VALD (atoms)
- VAMDC species-DB
- LXcat
- OACT - LASP Database
- TOPbase : VAMDC-TAP interface
- BASECOL: VAMDC-TAP interface
- UMIST Database for Astrochemistry
- IDEADB - Innsbruck Dissociative Electron Attachment Database
- TIPbase : VAMDC-TAP interface
- CDMS
- Carbon Dioxide Spectroscopic Databank 296K (VAMDC-TAP)
- SpEctroScopy of Atoms and Molecules
- Carbon Dioxide Spectroscopic Databank 1000K (VAMDC-TAP)
- Spectr-W3
- KIDA: VAMDC-TAP interface

Query by...

- Species
- Processes
- Environment
- Advanced

Molecule 1 Clear Remove form «

Chemical name

Stoichiometric formula

Structural formula

Spin isomer

Standard InChIKey

Carbon |

- Carbon
- Dicarbon
- Carbon ion
- Tetracarbon
- Carbon atom
- Carbon anion
- Carbon Cation
- Carbon dioxide
- Carbon monoxide
- Tetracarbon ion
- Carbonyl Sulfide
- Carbonyl sulphide
- Carbonyl Fluoride
- Dicarbon monoxide

Find data

**Legend**

available, can answer

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Only possible through SPECIES Database based on InchiKey and VAMDC Identifier

# Results visualization

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

**1 : Query Execution**

Done

Modify query Stop waiting Save query

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

Comments

**3 : Results Conversion (entries starting with \*\* are recommended)**

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

Process

**2 : Results by node**

Name	Convert	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
Chianti	<input checked="" type="checkbox"/>	OK (13/04/2012 02:00)	<a href="#">XSAMS</a>	9	7035	2080	2080	0	0
TIPbase : VAMDC-TAP interface	<input type="checkbox"/>	OK (13/04/2012 00:00)	<a href="#">XSAMS</a>	2	4	3	0	3	0
VAMDC species-DB	<input type="checkbox"/>	OK	<a href="#">XSAMS</a>	11	0	0	0	0	0
Belgrade electron/atom(molecule) database (BEAMDB)	<input type="checkbox"/>	OK	<a href="#">XSAMS</a>	0	0	0	0	0	0
VALD (atoms)	<input type="checkbox"/>	TRUNCATED (18/12/2012 00:00) (1%)	<a href="#">XSAMS</a>	0	0	7018411	7018411	0	0
Spectr-W3	<input type="checkbox"/>	TRUNCATED (11/12/2013 19:00) (13%)	<a href="#">XSAMS</a>	3	581	999	999	0	0
Stark-b	<input type="checkbox"/>	TRUNCATED (11/02/2014 00:00) (50%)	<a href="#">XSAMS</a>	4	15	16	16	0	0
JPL database: VAMDC-TAP service	<input type="checkbox"/>	TRUNCATED (04/02/2015 14:28) (1%)	<a href="#">XSAMS</a>	0	0	0	0	0	0

Menu

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

## Sources

Id	Title	Origin	Authors	Year	Link
BTopbase-19	Atomic data for opacity calculations. VII - Energy levels, f values and photoionisation cross sections for He-like ions	journal : Journal of Physics B Atomic Molecular Physics ( Vol : 20 , Page Begin : 6457 , Page End : 6476 )	Fernley, J. A.; Seaton, M. J.; Taylor, K. T.;	1987	<a href="http://cdsads.u-strasbg.fr/abs/1987JPhB...20.6457F">http://cdsads.u-strasbg.fr/abs/1987JPhB...20.6457F</a>
BTopbase-26		journal : unpublished	Seaton, M. J.;	1995	<a href="http://xsams-processors.obspm.fr/applyXSL/atomicxsams2html/result/1023">http://xsams-processors.obspm.fr/applyXSL/atomicxsams2html/result/1023</a>

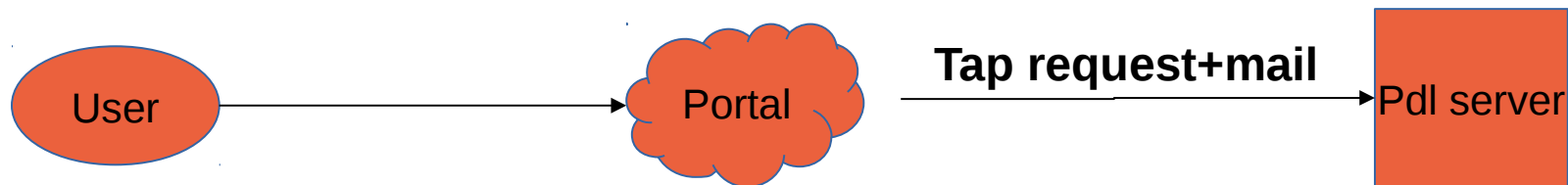
## Results from Topbase VAMDC node

<input type="checkbox"/> Unselect all	Spec Ion <input checked="" type="checkbox"/> X	Wavelength(A) <input checked="" type="checkbox"/> X	A <input checked="" type="checkbox"/> X	Weighted Oscillator Strength <input checked="" type="checkbox"/> X	Lower state source <input checked="" type="checkbox"/> X	Lower energy(Ry) <input checked="" type="checkbox"/> X	Lower ionization(Ry) <input checked="" type="checkbox"/> X	Lower statistical weight <input checked="" type="checkbox"/> X	Lower parity <input checked="" type="checkbox"/> X	Lower configuration <input checked="" type="checkbox"/> X	Lower coupling <input checked="" type="checkbox"/> X	Upper state source <input checked="" type="checkbox"/> X	Upper energy(Ry) <input checked="" type="checkbox"/> X	Upper ionization(Ry) <input checked="" type="checkbox"/> X	Upper statistical weight <input checked="" type="checkbox"/> X	Upper parity <input checked="" type="checkbox"/> X	Upper configuration <input checked="" type="checkbox"/> X	Upper coupling <input checked="" type="checkbox"/> X
<input checked="" type="checkbox"/>	He 2	303.797315958	20043477020.3	0.832	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.0	1.0	6	odd	2p	L=1 S=0.5 Multiplicity=2
<input checked="" type="checkbox"/>	He 2	256.328953298	5346620510.16	0.158	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.555556	0.444444	6	odd	3p	L=1 S=0.5 Multiplicity=2
<input checked="" type="checkbox"/>	He 2	243.037852766	2183221280.01	0.058	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.75	0.25	6	odd	4p	L=1 S=0.5 Multiplicity=2
<input checked="" type="checkbox"/>	He 2	237.341653092	1101219463.61	0.0279	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.84	0.16	6	odd	5p	L=1 S=0.5 Multiplicity=2
<input checked="" type="checkbox"/>	He 2	234.357922757	631513908.254	0.0156	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.888889	0.111111	6	odd	6p	L=1 S=0.5 Multiplicity=2
<input checked="" type="checkbox"/>	He 2	232.59481688	395770867.642	0.00963	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.9183674	0.0816326	6	odd	7p	L=1 S=0.5 Multiplicity=2
<input checked="" type="checkbox"/>	He 2	231.464621682	264355160.481	0.00637	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.9375	0.0625	6	odd	8p	L=1 S=0.5 Multiplicity=2
<input checked="" type="checkbox"/>	He 2	230.696085868	185072066.972	0.00443	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.9506173	0.0493827	6	odd	9p	L=1 S=0.5 Multiplicity=2
<input checked="" type="checkbox"/>	He 2	230.149481786	134741888.818	0.00321	<a href="#">BTopbase-26</a>	0.0	4.0	2	even	1s	L=0 S=0.5 Multiplicity=2	<a href="#">BTopbase-26</a>	3.96	0.04	6	odd	10p	L=1 S=0.5 Multiplicity=2

# Asynchronous requests

- The returned files are truncated above a certain volume limit (decided by data provider)
  - For policy reason
  - For technical reasons (execution time, volume)
- We need to allow the possibility to retrieve very large files (when this is allowed by the provider)
- We chose PDL because :
  - it was very fast to develop an asynchronous web service and to interface it with the VAMDC portal.
  - it provides a convenient way for job monitoring, based on the existing PDL framework

# Asynchronous requests



- Available in Advanced query interface
- Parameters sent to PDL server :
  - Tap request
  - User email address for monitoring



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

- Util
- Query editor
- Request
- Comments
- Asynchronous request

**Atom 1** Clear Remove form «

Atom symbol

Mass number  to

Nuclear charge  to

Ion charge  to

to  1/cm ▾

1/cm

**Radiative** Clear Remove form «

Wavelength ▾  to  A ▾

Equivalent Wavelength Wavelength from 0.0 to 15000.0A

Upper state energy  to  1/cm ▾

Equivalent to 1/cm

Lower state energy  to  1/cm ▾

Equivalent to 1/cm

Probability, A  to  1/s

**Asynchronous request** Clear Remove form «

Email

Find data

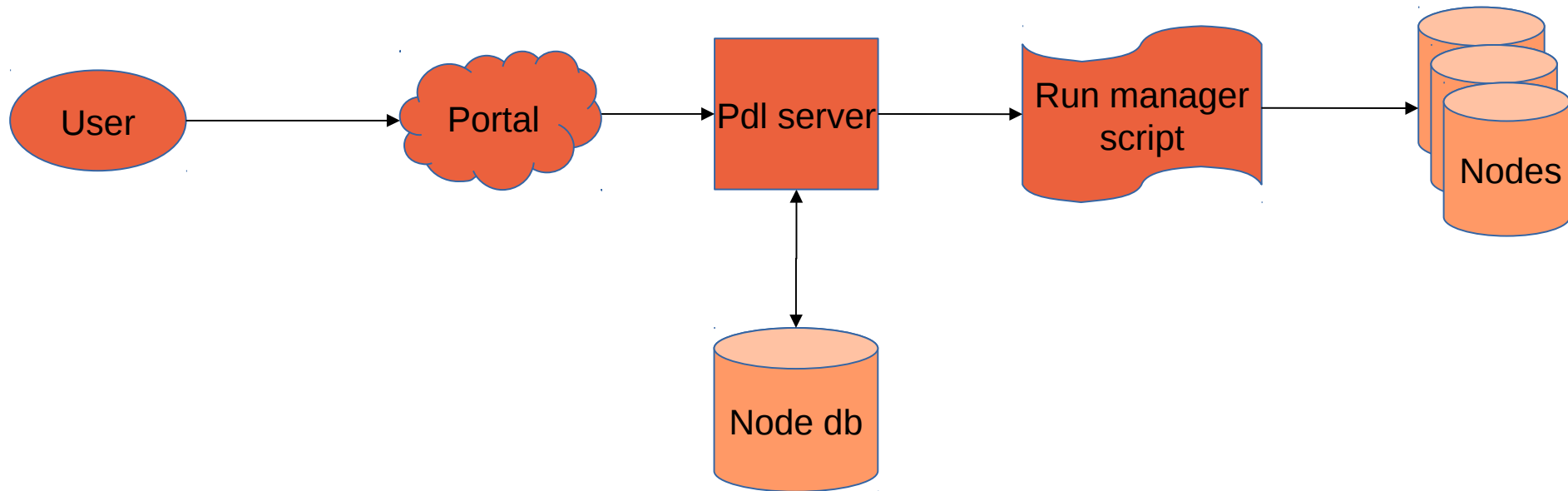
Find data

## Legend

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

- BASECOL: VAMDC-TAP interface
- OACT - LASP Database - N1207
- Theoretical spectral database of polycyclic aromatic hydrocarbons
- Chianti
- GSMA Reims S&MPO
- TOPbase : VAMDC-TAP interface (12.07 version)
- ECaSDa - Ethene Calculated Spectroscopic Database
- TAP-XSAMS for GhoSST database
- Carbon Dioxide Spectroscopic Databank 4000K (VAMDC-TAP)
- Lund laboratory spectroscopy database
- Stark-b
- JPL database: VAMDC-TAP service
- CDMS: VAMDC-TAP service (xsams 1.0)
- HITRANonline resource
- RADAM database: Innsbruck Dissociative Electron Attachment Database
- VALD sub-set in Moscow (obs)
- Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- MeCaSDa - Methane Calculated Spectroscopic Database
- Carbon Dioxide Spectroscopic Databank 1000K (VAMDC-TAP)
- VALD (atoms)
- VamdcSpeciesDB-Tap Service (xsams 1.0)
- LXcat
- OACT - LASP Database
- TOPbase : VAMDC-TAP interface
- Theoretical spectral database of polycyclic aromatic hydrocarbons
- TIPbase : VAMDC-TAP interface (12.07 version)
- DESIRE database (Moscow mirror)

# Asynchronous requests



- PDL Server has its own node DB
- Nodes are modified to return full content
- Informations will be in registry
- Request sent to a script that executes them
- All results returned in an compressed archive file

# Asynchronous requests

- User receives a mail when he creates a request and when it has been completed
- He/She can access a monitoring web interface (developped with GWT) :
  - Status of request
  - Download results
  - Delete request and results

# Asynchronous requests

## PDL Service

Job list for user nicolas.moreau@obspm.fr

Job Id	Job Phase	Demand Date	End Date
1	finished	2015/05/27 16:49:47	2015/05/27 16:54:02

⏪ ⏩ 1-1 of 1 ⏪ ⏩

Detail for the selected Job (Id=1)

Delete this job

VamdcFileResult:<http://vm-euhoutestc62.obspm.fr/vamdc/output/1.xsams.zip>

Parameter Name	Parameter Value
query	select * where ((AtomSymbol = 'He'))

⏪ ⏩ 1-1 of 1 ⏪ ⏩

- Results are kept in cache for 30 days, then deleted

# Conclusion

- Some evolutions are planned :
  - Look for collisional data in guided interface
  - A new CSS closer to the VAMDC website one
- Some new processors
- For any question/suggestion related to the portal :  
[nicolas.moreau@obspm.fr](mailto:nicolas.moreau@obspm.fr)
- For any question/suggestion related to PDL :  
[carlo-maria.zwolf@obspm.fr](mailto:carlo-maria.zwolf@obspm.fr)