Online Atomic and Molecular Databases

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(24th Meeting of the A+M Data Centres)

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Summary

- **VAMDC** – connecting diverse databases through a common query interface and data exchange standard

- **HITRAN** – a database of molecular spectroscopic properties implemented as an online service with a relational backend

- **ExoMol** – methods for the storage and manipulation of large data sets

- **QuantemolDB** – Data on plasma processes implemented as an online service with user interaction

- **Challenges and future directions** for atomic and molecular databases

VAMDC

- VAMDC = Virtual Atomic and Molecular Data Centre
- http://vamdc.eu/
- EU FP7-funded 5-year project to build a consortium of research institutes and lay down a framework of standards for the interchange of atomic and molecular (AM) data:
  - VSS2: an SQL-like query language
  - XSAMS: an XML schema for storing and transmitting AM data.
  - VAMDC portal: an online resource for simultaneously querying multiple databases.

VAMDC

VSS2 Query Language

- Based on a subset of SQL (Structured Query Language)
- Used as a parameter to a “GET” query in a URL, e.g.

```
http://www.example.com/?query=SELECT States WHERE
StoichiometricFormula=“CO2”
```

- Defines “keywords” for types of data (returnables) and search parameters (restrictables)

VAMDC

XSAMS

- An XML-based format: a valid XSAMS document must conform to the XSAMS Schema
- Data from different databases can be compared, aggregated, etc.
- Data provenance: Requires data to have **units** and **sources** (for citation)
- Encourages specification of errors and uncertainties: data integrity

VAMDC

XSAMS

- Standard overseen by the IAEA (Atomic and Molecular Data Division)
- Verbose (because it's XML) ...
- .... but compresses well (typically 40x)
- "self-describing"
- "self-validating" (to some extent)

VAMDC

XSAMS

- Example XSAMS snippet: the self-describing XSAMS format helps verify quantum number assignments, e.g. 16O17O:

```
<hundb:QNs>
   <hundb:ElecStateLabel>X</hundb:ElecStateLabel>
   <hundb:Lambda>0</hundb:Lambda>
   <hundb:S>1.0</hundb:S>
   <hundb:v>0</hundb:v>
   <hundb:J>32.0</hundb:J>
   <hundb:N>32</hundb:N>
   <hundb:F nuclearSpinRef="O2">29.5</hundb:F>
</hundb:QNs>
```

Validation, e.g.

$v \geq 0$,

$N \geq \Lambda$,

$|N\text{-}S| \leq J \leq N\text{+}S$

$|J\text{-}I| \leq F \leq J\text{+}I$ ($I = 5/2$ for ^{17}O, identified as "O2")

VAMDC

Other VAMDC standards

- Standards for identifying species - i.e. specific **isotopes** of atoms or ions; specific **isotopologues** of molecules
- InChI = *IUPAC International Chemical Identifier*, e.g. $^{13}C^{16}O_2$ is:

`InChI=1S/CO2/c2-1-3/i1+1`

- The InChIKey is a 27-character hash on the species' InChI identifier: this InChI becomes

`CURLTUGMZLYLDI-OUBTZVSYSA-N`

- Allows **unambiguous** and **unique** identification of species

VAMDC

Other VAMDC standards

- Services exist (within VAMDC and on the wider www e.g. *ChemSpider*, *OpenBabel*) to translate between chemical identifier formats: e.g. for CO2:
  - SMILES: `C(=O)=O`
  - InChI: `InChI=1S/CO2/c2-1-3`
  - InChIKey: `CURLTUGMZLYLDI-UHFFFAOYSA-N`
  - CAS Registry Number: `124-38-9`
  - CML
  - …

VAMDC

Data Permanence

- Many databases simply replace old data with new
- Old data is therefore “lost”
- Can be impossible to reproduce results using old data
- VAMDC standards allow the use of the “`ValidOn`” keyword
- Old data can be “expired” but not deleted or replaced

VAMDC

VAMDC Portal

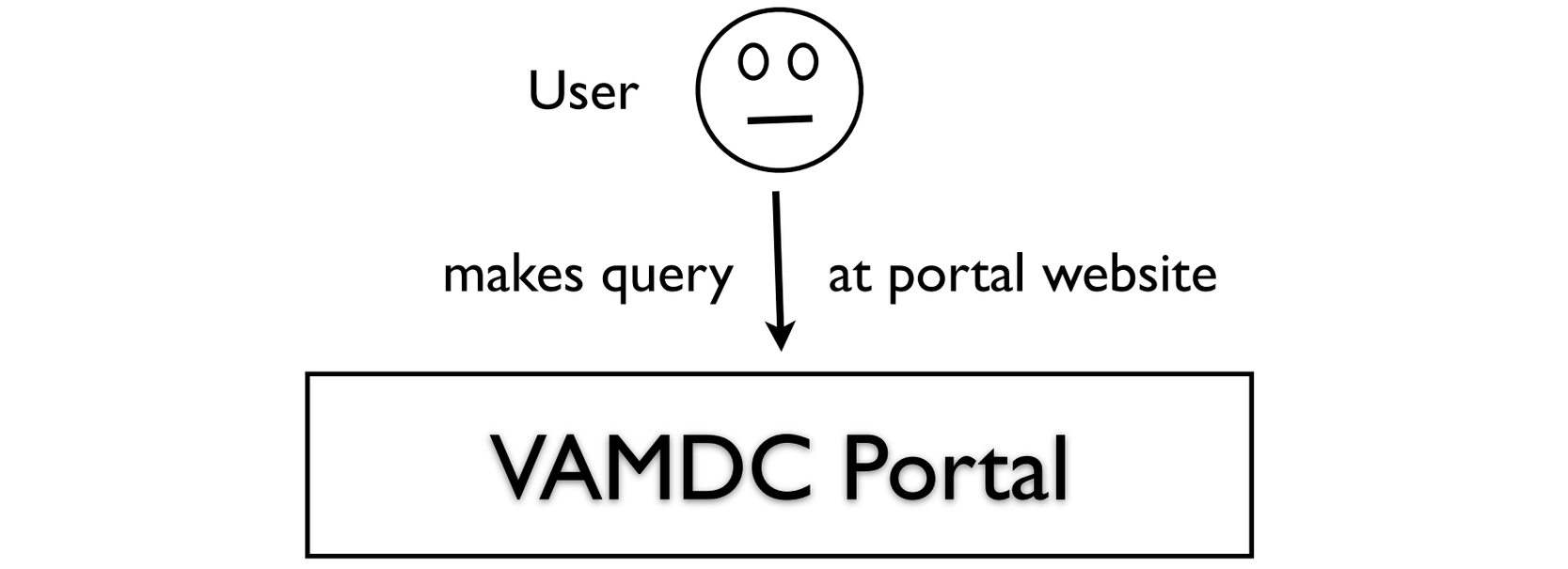
- The VAMDC portal (portal.vamdc.org/) links *nodes* to allow simultaneous querying of databases.
- A VAMDC database node is an online service which:
  - Can understand the VAMDC query language, VSS2
  - Will return data in valid XSAMS format
  - Is listed with the *VAMDC registry*

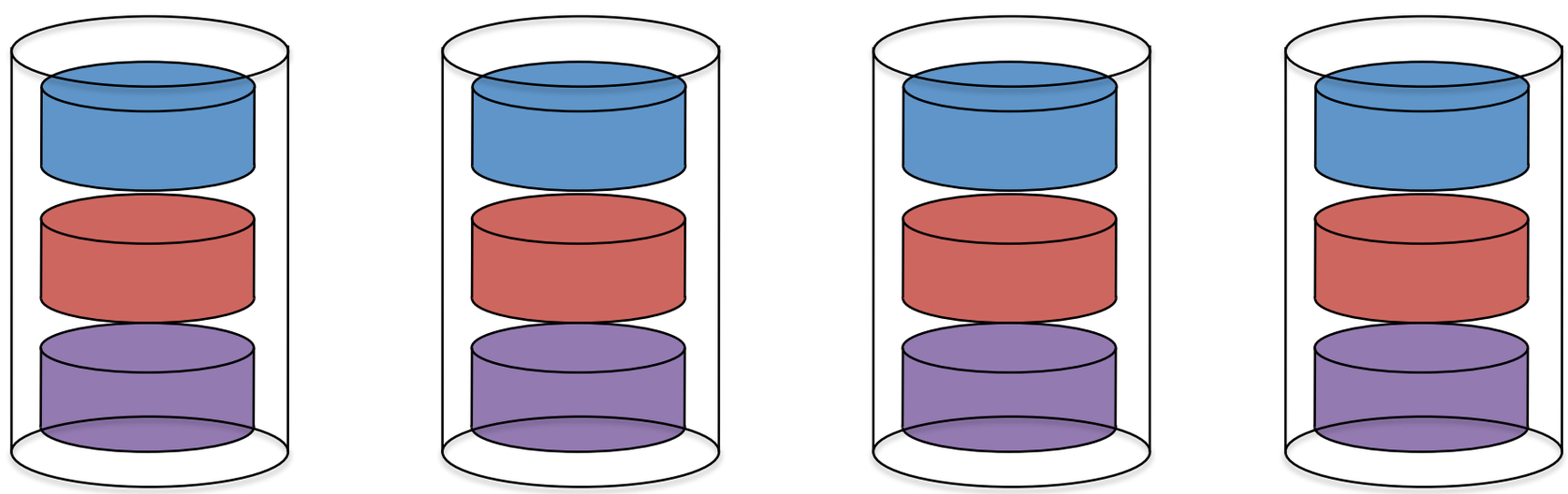
VAMDC

VAMDC Portal

- Some VAMDC database nodes:
  - **VALD** - a major database of atomic and small-molecule spectroscopic line parameters (focus: astronomy and astrophysics)
  - **HITRAN** - the major database of molecular spectroscopic line parameters for planetary atmospheres
  - **BASECOL** - database of atomic and molecular collisional cross sections
  - **CDMS / JPL** - microwave/ FIR line parameters for interstellar spectroscopy
  - **KIDA** - astrochemical kinetic database

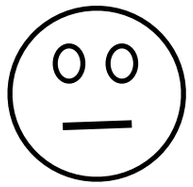
VAMDC Portal

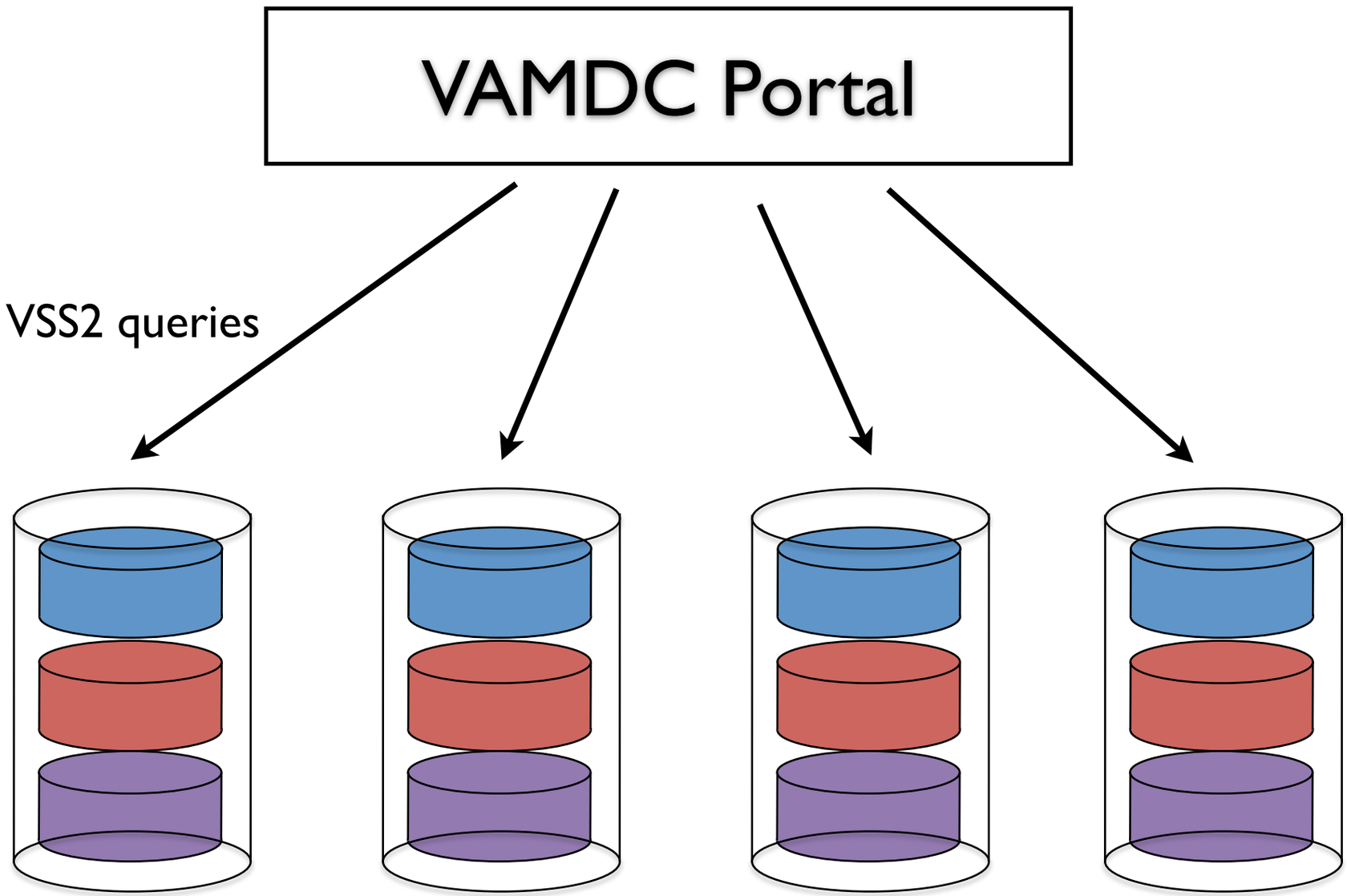




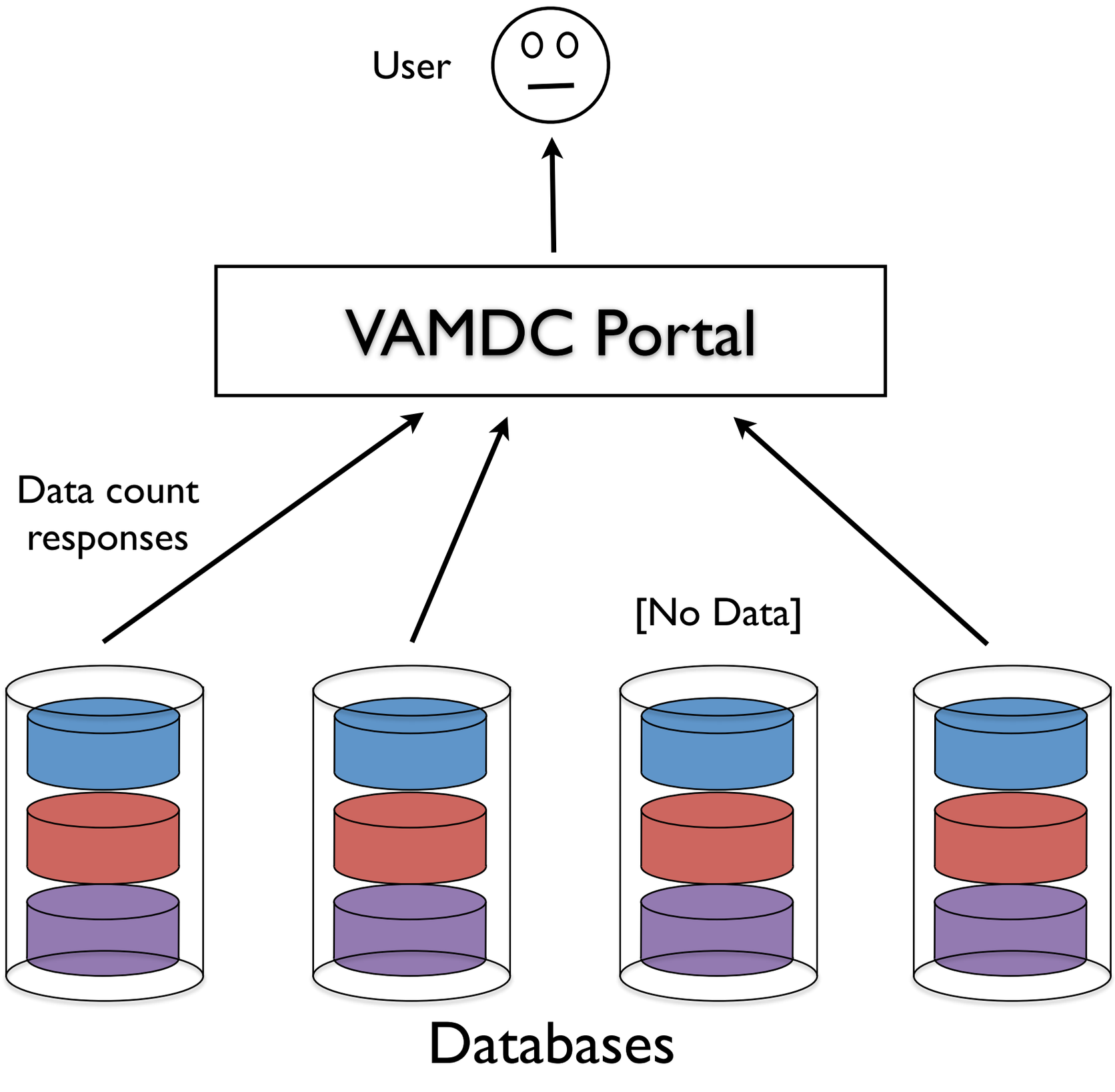
Databases

VAMDC Portal

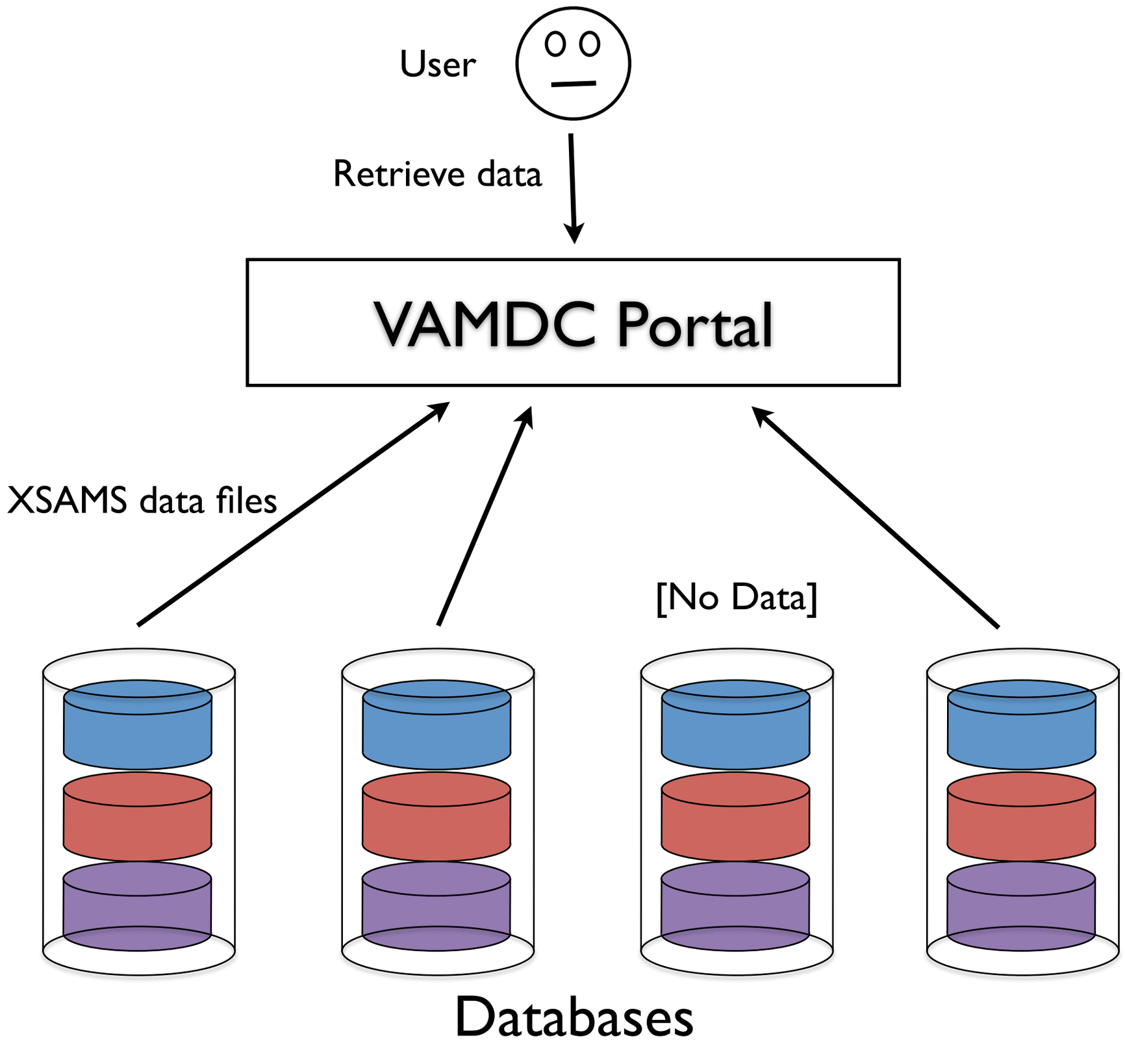
User 



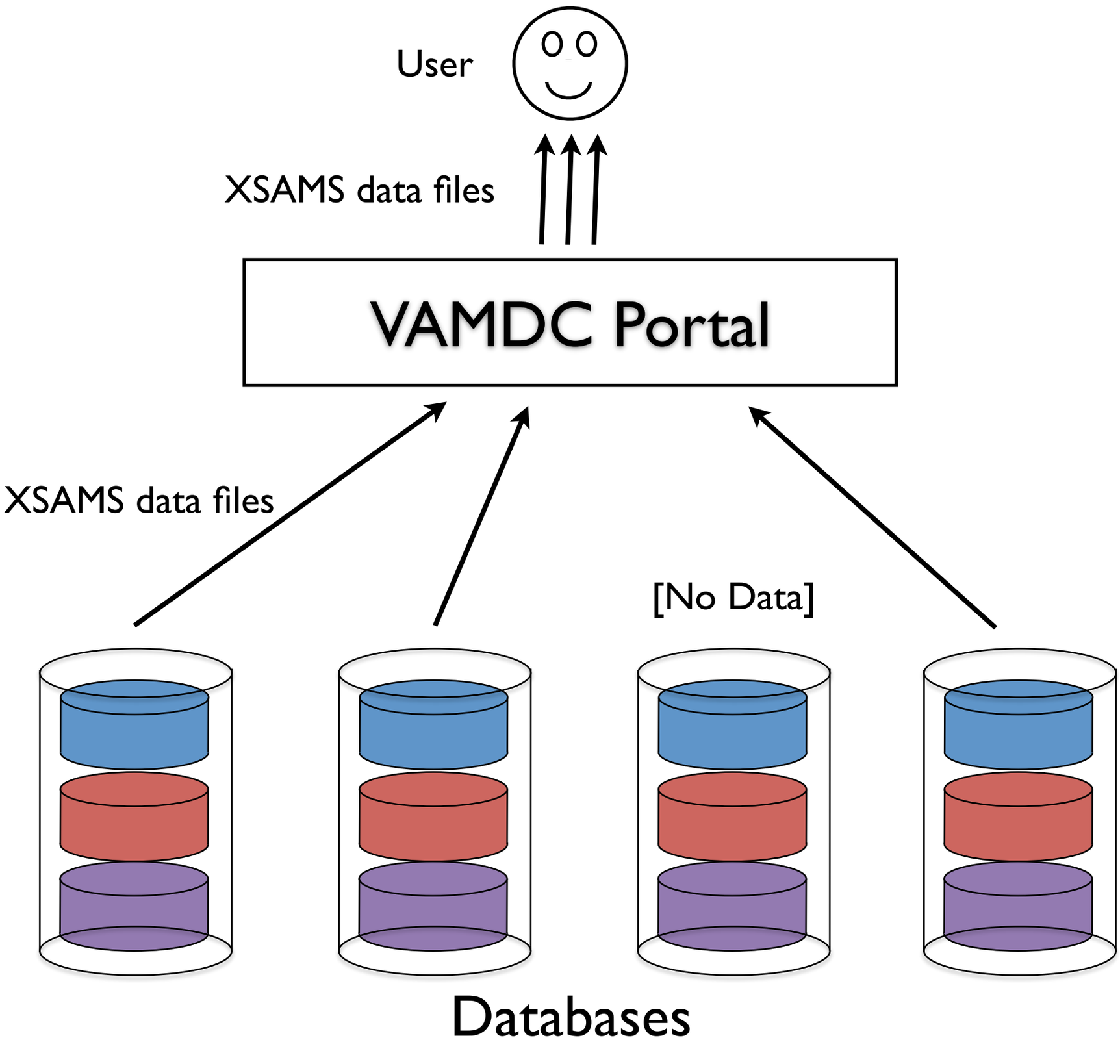
VAMDC Portal



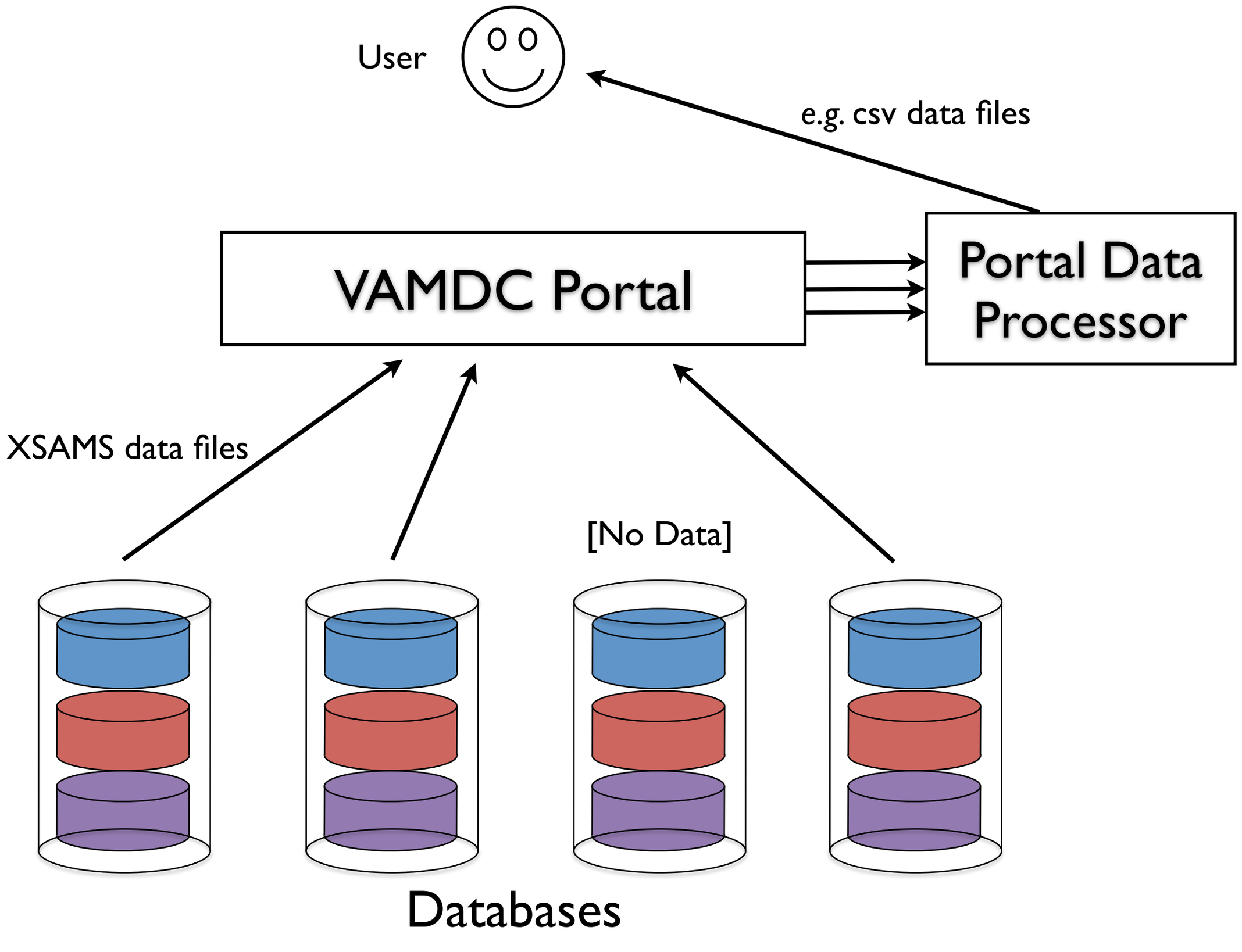
VAMDC Portal



VAMDC Portal



VAMDC Portal



VAMDC Portal

VAMDC
Virtual Atomic and Molecular Data Centre

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

Query by...

- Species
- Processes
- Environment
- Advanced

Molecules Clear Remove «

Chemical name	Carbon Monoxide
Stoichiometric formula	CO
Structural formula	CO
Spin isomer	
Standard InChIKey	UGFAIRIUMAVXCW-UHFFFAOYSA-N

Select All None Search by stoichiometric formula if no inchikey is selected.

Formula	InChIKey
☑ (12C)(16O)	UGFAIRIUMAVXCW-UHFFFAOYSA-N
☐ (13C)(16O)	UGFAIRIUMAVXCW-OUBTZVSYSA-N
☐ (12C)(18O)	UGFAIRIUMAVXCW-HQMMCQRPSA-N
☐ (12C)(17O)	UGFAIRIUMAVXCW-VQEHIDDOSA-N
☐ (13C)(18O)	UGFAIRIUMAVXCW-RGIGPVFXSA-N
☐ (13C)(17O)	UGFAIRIUMAVXCW-ZDOIIHCHSA-N

Find data | Save query

Legend

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

- Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- MeCaSDa - Methane Calculated Spectroscopic Database
- VALD (atoms)
- OACT - LASP Database
- BASECOL: VAMDC-TAP interface
- TOPbase : VAMDC-TAP interface
- Theoretical spectral database of polycyclic aromatic hydrocarbons
- IDEADB - Innsbruck Dissociative Electron Attachment Database
- Chianti
- TIPbase : VAMDC-TAP interface
- GSMA Reims S&MPO
- ECaSDa - Ethene Calculated Spectroscopic Database
- Carbon Dioxide Spectroscopic Databank - 296K
- GhoSST
- Carbon Dioxide Spectroscopic Databank - 1000K
- 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

VAMDC Portal

VAMDC
Virtual Atomic and Molecular Data Centre

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

Done

Modify query | Stop waiting | Save query

select * where (RadTransWavelength >= 42999.99999999999 AND RadTransWavelength <= 49999.99999999999) AND ((InchiKey = 'UGFAIRIUMAVXCW-UHFFFAOYSA-N'))

Comments

XSAMS processors

- BibTeX from XSAMS
- Table views of XSAMS
- Xsams2SME

Process

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
Water internet Accessible Distributed Information System	OK	XSAMS	1	201	627	627	0	0
HITRAN-UCL resource	OK	XSAMS	1	82	189	189	0	0
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	EMPTY		0	0	0	0	0	0
Carbon Dioxide Spectroscopic Databank - 1000K	EMPTY		0	0	0	0	0	0
Carbon Dioxide Spectroscopic Databank - 296K	EMPTY		0	0	0	0	0	0
MeCaSDa - Methane Calculated Spectroscopic Database	EMPTY		0	0	0	0	0	0
ECaSDa - Ethene Calculated Spectroscopic Database	EMPTY		0	0	0	0	0	0
GSMA Reims S&MPO	EMPTY		0	0	0	0	0	0
VALD sub-set in Moscow (obs)	EMPTY		0	0	0	0	0	0
VALD (atoms)	EMPTY		0	0	0	0	0	0

VAMDC Portal

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Virtual Atomic and Molecular Data Centre

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

Done

Modify query | Stop waiting | Save query

select * where (RadTransWavelength >= 42999.99999999999 AND RadTransWavelength <= 49999.99999999999) AND ((InchiKey = 'UGFAIRIUMAVXCW-UHFFFAOYSA-N'))

Comments

XSAMS processors

- BibTeX from XSAMS
- Table views of XSAMS
- Xsams2SME

Process | Result

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.

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
Water Internet Accessible Distributed Information System	OK	XSAMS	1	201	627	627	0	0
HITRAN-UCL resource	OK	XSAMS	1	82	189	189	0	0
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	EMPTY		0	0	0	0	0	0
Carbon Dioxide Spectroscopic Databank - 1000K	EMPTY		0	0	0	0	0	0
Carbon Dioxide Spectroscopic Databank - 296K	EMPTY		0	0	0	0	0	0
MeCaSDa - Methane Calculated Spectroscopic Database	EMPTY		0	0	0	0	0	0
ECaSDa - Ethene Calculated Spectroscopic Database	EMPTY		0	0	0	0	0	0
GSMA Reims S&MPO	EMPTY		0	0	0	0	0	0
VALD sub-set in Moscow (obs)	EMPTY		0	0	0	0	0	0
VALD (atoms)	EMPTY		0	0	0	0	0	0

VAMDC Portal

Line-list view of XSAMS

(Switch to view of states or collisions)

Assume* all wavelengths are in vacuum and Convert to air (at IAU STP).

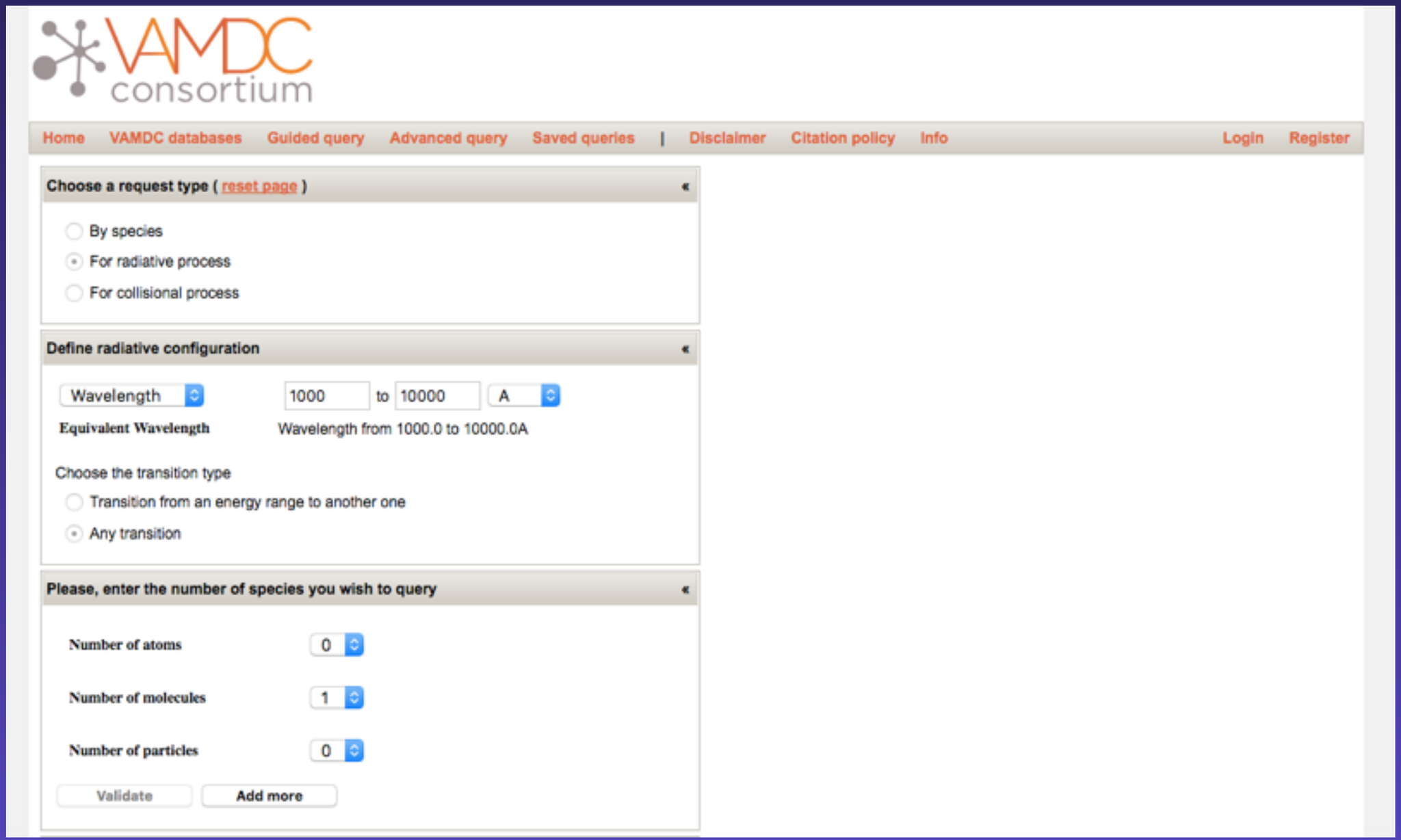
Assume all wavelengths are in air (at IAU STP) and Convert to vacuum .

Show table in CSV format

Species	λ/ν/n/E	Probability	Upper state	Lower state	Broadening/shifting
(12C)(16O)	n=2002.115 1/cm	A=28.85	5582.0901 1/cm — X $v = 2$ $J = 26$	3579.9751 1/cm — X $v = 1$ $J = 27$	Detail
(12C)(16O)	n=2003.6679 1/cm	A=14.46	4027.0394 1/cm — X $v = 1$ $J = 31$	2023.3715 1/cm — X $v = 0$ $J = 32$	Detail
(12C)(16O)	n=2006.7836 1/cm	A=29.08	5484.3687 1/cm — X $v = 2$ $J = 25$	3477.5851 1/cm — X $v = 1$ $J = 26$	Detail
(12C)(16O)	n=2008.5254 1/cm	A=14.57	3909.6562 1/cm — X $v = 1$ $J = 30$	1901.1308 1/cm — X $v = 0$ $J = 31$	Detail
(12C)(16O)	n=2011.4211 1/cm	A=29.29	5390.3747 1/cm — X $v = 2$ $J = 24$	3378.9536 1/cm — X $v = 1$ $J = 25$	Detail
(12C)(16O)	n=2013.3524 1/cm	A=14.68	3796.0148 1/cm — X $v = 1$ $J = 29$	1782.6624 1/cm — X $v = 0$ $J = 30$	Detail
(12C)(16O)	n=2016.0272 1/cm	A=29.51	5300.1117 1/cm — X $v = 2$ $J = 23$	3284.0845 1/cm — X $v = 1$ $J = 24$	Detail
(12C)(16O)	n=2018.1488 1/cm	A=14.79	3686.1197 1/cm — X $v = 1$ $J = 28$	1667.9709 1/cm — X $v = 0$ $J = 29$	Detail
(12C)(16O)	n=2020.6018 1/cm	A=29.73	5213.5832 1/cm — X $v = 2$ $J = 22$	3192.9814 1/cm — X $v = 1$ $J = 23$	Detail
(12C)(16O)	n=2022.9144 1/cm	A=14.9	3579.9751 1/cm — X $v = 1$ $J = 27$	1557.0607 1/cm — X $v = 0$ $J = 28$	Detail
(12C)(16O)	n=2025.1447 1/cm	A=29.95	5130.7926 1/cm — X $v = 2$ $J = 21$	3105.6479 1/cm — X $v = 1$ $J = 22$	Detail
(12C)(16O)	n=2027.6491 1/cm	A=15.02	3477.585 1/cm — X $v = 1$ $J = 26$	1449.9359 1/cm — X $v = 0$ $J = 27$	Detail

VAMDC

Guided Queries



VAMDC

Guided Queries

VAMDC consortium

Home | VAMDC databases | Guided query | Advanced query | Saved queries | Disclaimer | Citation policy | Info | Login | Register

Query Execution

Done

Modify query | Stop waiting | Save query

Comments

Your request

```
select * where (RadTransWavelength >= 1000.0 AND
RadTransWavelength <= 10000.0) AND ((InchiKey =
'UGFAIRIUMAVXCW-UHFFFAOYSA-N'))
```

Results by node

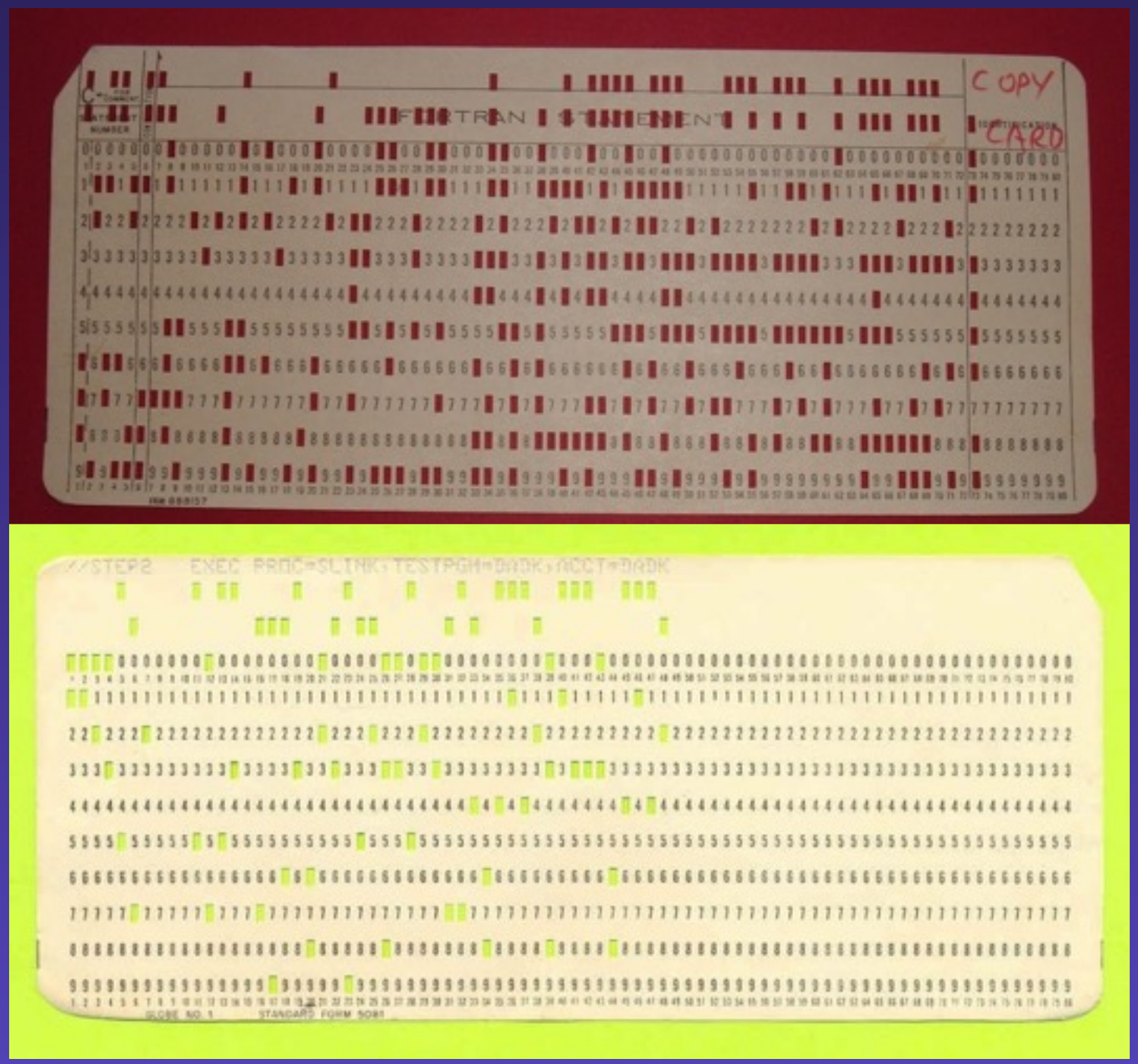
Name	View data	Response	Last database update	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
HITRANonline	-- Choose display --	OK	Not available	XSAMS file	1	74	172	172	0	0
GSMA Reims S&MPO	-- Choose display --	OK	Not available	XSAMS file	0	0	5	5	0	0
SpEctroScopy of Atoms and Molecules	-- Choose display --	TRUNCATED (43% of data returned)	30/01/2017 00:00	XSAMS file	1	1564	2000	2000	0	0
JPL database: VAMDC-TAP service		EMPTY	03/09/2017 14:01		0	0	0	0	0	0
TOPbase : VAMDC-TAP interface		EMPTY	13/06/2016 00:00		0	0	0	0	0	0

HITRAN

- A database of molecular spectroscopic data for atmospheric applications (climate modelling, remote sensing, etc.)
- Initiated by the US Air Force in the 1960s
- 5,000,000+ lines, 100 MB+ of cross sections
- Increasingly used for planetary atmospheres
- Now an provided by a web service, HITRAN*online*
- Also acts as a VAMDC node

HITRAN

Evolution: 1960s / 1970s



HITRAN

Evolution: 2004 – 2015

```
...
 21 2291.946330 4.940E-29 3.414E-02.06820.086 3595.59060.78-.007000      4 0 0 02      2 1 1 03              Q 32f     4455501221 1 1 1 4    65.0   65.0
 21 2291.947360 1.660E-28 3.650E+02.06980.093 5204.94610.780.000400      0 4 4 21      0 4 4 11              R 24f     4455501221 1 1 1 4    51.0   49.0
 21 2291.953028 4.614E-27 2.522E+00.06610.073 3633.90910.760.000000      0 4 4 11      0 4 4 01              Q 49f     454550 2 2 1 1 1 0*   99.0   99.0
 23 2291.957370 6.450E-27 1.504E+02.08930.123 2501.49690.750.000000      2 0 0 13      2 0 0 03              R  1e     455550 2 2 1 1 1 0     5.0    3.0
 21 2291.959750 4.980E-28 4.906E-01.06920.091 3634.14400.78-.007000      2 1 1 12      2 1 1 02              Q 27e     4455501221 1 1 1 4    55.0   55.0
 22 2291.967650 4.920E-28 1.880E+02.06030.060 4140.44010.66-.007100      1 1 1 11      1 1 1 01              R 73e     4455501221 1 1 1 4   298.0  294.0
 21 2291.974450 3.600E-29 1.790E+02.06660.075 5496.45810.77-.004490      0 7 7 11      0 7 7 01              R 45e     4455501221 1 1 1 4    93.0   91.0
 21 2291.977720 5.480E-28 8.715E-04.06820.086 2345.92090.78-.007000      3 0 0 01      1 1 1 02              Q 32f     4455501221 1 1 1 4    65.0   65.0
 21 2291.986760 1.620E-27 1.084E+00.07280.100 3473.12120.74-.007000      2 1 1 12      2 1 1 02              Q 18f     4455501221 1 1 1 4    37.0   37.0
 27 2291.987280 4.040E-30 1.946E+02.06640.074 3386.79000.77-.004430      0 4 4 11      0 4 4 01              R 46e     4355501221 1 1 1 4    95.0   93.0
 21 2291.946330 4.940E-29 3.414E-02.06820.086 3595.59060.78-.007000      4 0 0 02      2 1 1 03              Q 32f     4455501221 1 1 1 4    65.0   65.0
 21 2291.947360 1.660E-28 3.650E+02.06980.093 5204.94610.780.000400      0 4 4 21      0 4 4 11              R 24f     4455501221 1 1 1 4    51.0   49.0
 21 2291.953028 4.614E-27 2.522E+00.06610.073 3633.90910.760.000000      0 4 4 11      0 4 4 01              Q 49f     454550 2 2 1 1 1 0*   99.0   99.0
 23 2291.957370 6.450E-27 1.504E+02.08930.123 2501.49690.750.000000      2 0 0 13      2 0 0 03              R  1e     455550 2 2 1 1 1 0     5.0    3.0
 21 2291.959750 4.980E-28 4.906E-01.06920.091 3634.14400.78-.007000      2 1 1 12      2 1 1 02              Q 27e     4455501221 1 1 1 4    55.0   55.0
 22 2291.967650 4.920E-28 1.880E+02.06030.060 4140.44010.66-.007100      1 1 1 11      1 1 1 01              R 73e     4455501221 1 1 1 4   298.0  294.0
 21 2291.946330 4.940E-29 3.414E-02.06820.086 3595.59060.78-.007000      4 0 0 02      2 1 1 03              Q 32f     4455501221 1 1 1 4    65.0   65.0
 21 2291.947360 1.660E-28 3.650E+02.06980.093 5204.94610.780.000400      0 4 4 21      0 4 4 11              R 24f     4455501221 1 1 1 4    51.0   49.0
 21 2291.953028 4.614E-27 2.522E+00.06610.073 3633.90910.760.000000      0 4 4 11      0 4 4 01              Q 49f     454550 2 2 1 1 1 0*   99.0   99.0
 23 2291.957370 6.450E-27 1.504E+02.08930.123 2501.49690.750.000000      2 0 0 13      2 0 0 03              R  1e     455550 2 2 1 1 1 0     5.0    3.0
 21 2291.959750 4.980E-28 4.906E-01.06920.091 3634.14400.78-.007000      2 1 1 12      2 1 1 02              Q 27e     4455501221 1 1 1 4    55.0   55.0
 22 2291.967650 4.920E-28 1.880E+02.06030.060 4140.44010.66-.007100      1 1 1 11      1 1 1 01              R 73e     4455501221 1 1 1 4   298.0  294.0
 21 2291.974450 3.600E-29 1.790E+02.06660.075 5496.45810.77-.004490      0 7 7 11      0 7 7 01              R 45e     4455501221 1 1 1 4    93.0   91.0
 21 2291.977720 5.480E-28 8.715E-04.06820.086 2345.92090.78-.007000      3 0 0 01      1 1 1 02              Q 32f     4455501221 1 1 1 4    65.0   65.0
 21 2291.986760 1.620E-27 1.084E+00.07280.100 3473.12120.74-.007000      2 1 1 12      2 1 1 02              Q 18f     4455501221 1 1 1 4    37.0   37.0
 27 2291.987280 4.040E-30 1.946E+02.06640.074 3386.79000.77-.004430      0 4 4 11      0 4 4 01              R 46e     4355501221 1 1 1 4    95.0   93.0
 21 2291.974450 3.600E-29 1.790E+02.06660.075 5496.45810.77-.004490      0 7 7 11      0 7 7 01              R 45e     4455501221 1 1 1 4    93.0   91.0
 21 2291.977720 5.480E-28 8.715E-04.06820.086 2345.92090.78-.007000      3 0 0 01      1 1 1 02              Q 32f     4455501221 1 1 1 4    65.0   65.0
 21 2291.986760 1.620E-27 1.084E+00.07280.100 3473.12120.74-.007000      2 1 1 12      2 1 1 02              Q 18f     4455501221 1 1 1 4    37.0   37.0
 27 2291.987280 4.040E-30 1.946E+02.06640.074 3386.79000.77-.004430      0 4 4 11      0 4 4 01              R 46e     4355501221 1 1 1 4    95.0   93.0
...
```

HITRAN

Evolution: 2015 – Present

HITRAN*online*

Login | Register

Home | Data Access | Documentation | Conferences | Links | About

The HITRAN Database

HITRAN is an acronym for *hi*gh-resolution *trans*mission molecular absorption database. HITRAN is a compilation of spectroscopic parameters that a variety of computer codes use to predict and simulate the transmission and emission of light in the atmosphere.

News

Articles describing HITRAN*online*, HAPI and new line shape representations

Video tutorial for using HITRAN*online*. Recording from 10.26.2015 webinar

All inquiries can now be made to HITRAN's support team at *info@hitran.org!*

Database Updates

Update of ν_9 and ν_8 band regions and addition of data for $\nu_6+\nu_8$ band region of diacetylene (C_4H_2)

Global update of the CO linelist, including addition of new bands up to the sixth overtone. Broadening and shift by CO_2, H_2 and He is also included for the first time.

Update of the line list for the principal isotopologue of ozone ($^{16}O_3$)

HITRAN

HITRANonline

- Web browser-based application with a relational database backend (MySQL) for searching the HITRAN database.

- www.hitran.org

- Features:
  - User management (security, accounting, profiles)
  - Per-user, customisable output formats
  - Species metadata (partition sums, masses, …)
  - Interactive charts (for cross sections)
  - Acts as a VAMDC database node

ExoMol

- *Ab initio* calculated molecular line lists for high-temperature spectroscopic applications:
  - Flames
  - Cool stars
  - Exoplanet atmospheres

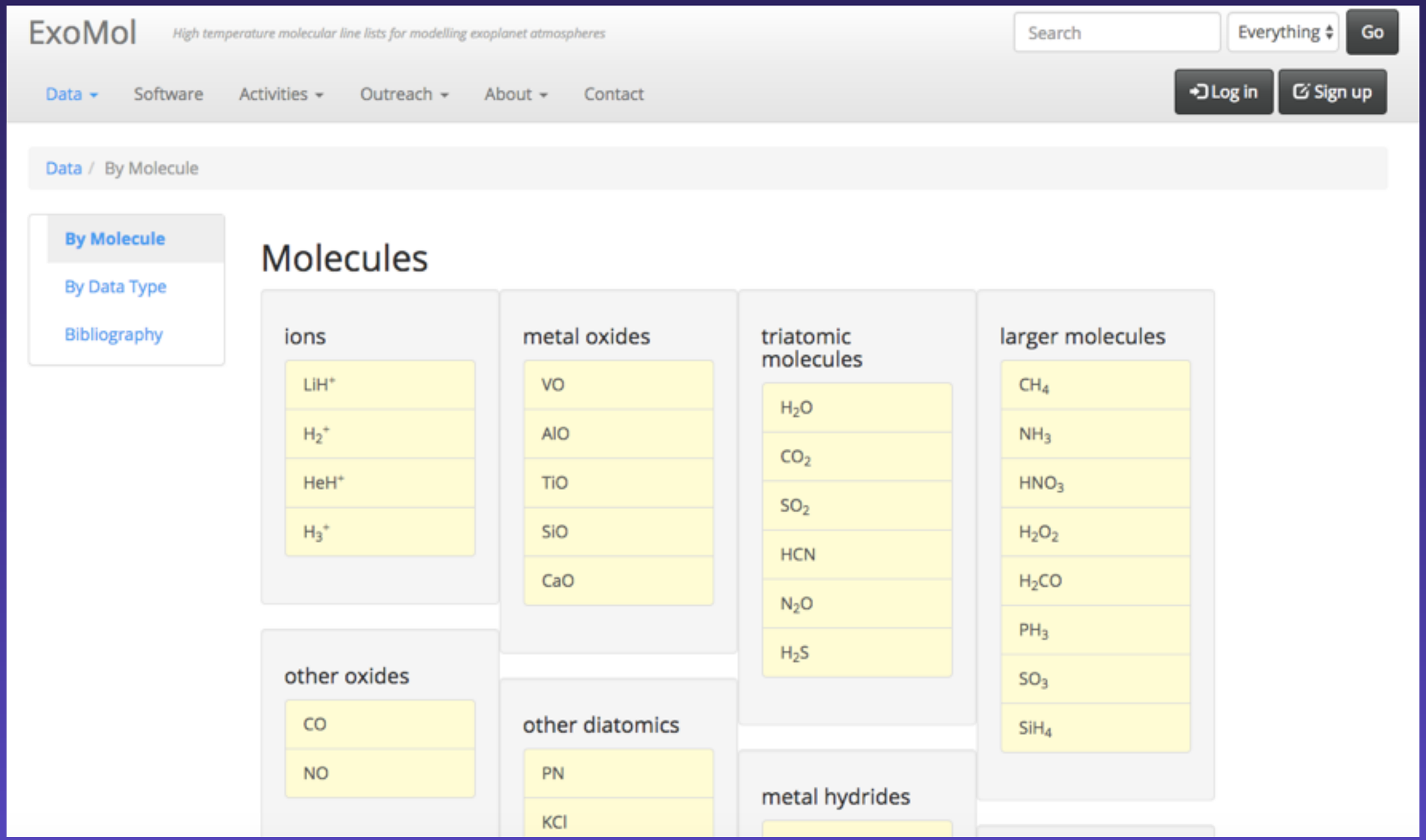
- ERC-funded, 5-year project at UCL (PI: Jonathan Tennyson)
- ~50 molecules in all major isotopologues
- Line positions (cm^{-1}) and Einstein *A*-coefficients

ExoMol

- Larger molecules have a *huge* number of transitions (e.g. CH_4 10^{10} lines in *preliminary* form)
- At elevated temperature opacity due to all transitions must be included
- Too much data for a RDBMS, so:
  - Separate states and transitions into **separate files**
  - Break large transitions files into **spectral regions**
  - Provide **software tools** for conversion to other formats (e.g. HITRAN)
  - Provide online services for the calculation of *p*- and *T*-dependent **absorption cross sections**

ExoMol

exomol.com



ExoMol

exomol.com

- Free-to-use, no sign-up required
- Search by **molecule / isotopologue** or
- Search by **data type** (species energies, line lists, partition functions, cooling functions, spectroscopic model, *ab initio* calculation details, pressure-broadening coefficients, etc.)
- **Bibliographic database** of published journal articles relating to small molecules

QuantemolDB

quantemoldb.com

- Comprehensive database of data relating to low-temperature plasmas:
  - Energy-dependent collisional cross sections
  - Arrhenius-like parameters
  - Sticking coefficients for surface processes
  - Surface reaction probabilities
  - …
- Relational database backend with a user-friendly web-based frontend

QuantemolDB

- Flexible data model allows for
  - Generic parameter data
  - Generic tabular data
  - Bibliographic references
    - Building “Chemistries” of related reactions / collisions
- Software libraries provide tools for:
  - Identifying and providing metadata on species and their quantum states
  - Manipulating the units of physical quantities

QuantemolDB

QDB plasma chemistry

SPECIES REACTIONS CHEMISTRIES CONTACT ABOUT GOLD

christian LOG OUT

Quantemol-DB

Trusted chemistries for plasma research.

SEARCH

LATEST NEWS

10 Aug 2017
We are moving! >

28 Jul 2017
We will see you at ISPC! >

10 Jul 2017
AVS 17th International Conference on Atomic Layer Deposition (ALD 2017) >

02 Jun 2017
New NF3/O2/Ar chemistry added to QDB! >

02 Jun 2017
Nitrogen Trifluoride (NF3) Cross Section Calculated and Confirmed >

Current Status

12545 Reaction data sets

LEARN MORE »

Website by Quantemol

QuantemolDB

QDB plasma chemistry | SPECIES | REACTIONS | CHEMISTRIES | CONTACT | ABOUT | GOLD | christian | LOG OUT

REACTIONS / SEARCH

SEARCH
DATA SOURCES
UPLOAD
PROCESSES
API

Reactions Search

CO2 | SEARCH

Reactants | Products

33 reactions found for reactants matching CO2.

To compare up to 5 reaction cross sections, click on the icon in the table below to add it to the "Selected Cross Sections" clipboard. All data sets for each reaction will be displayed.

SELECTED CROSS SECTIONS

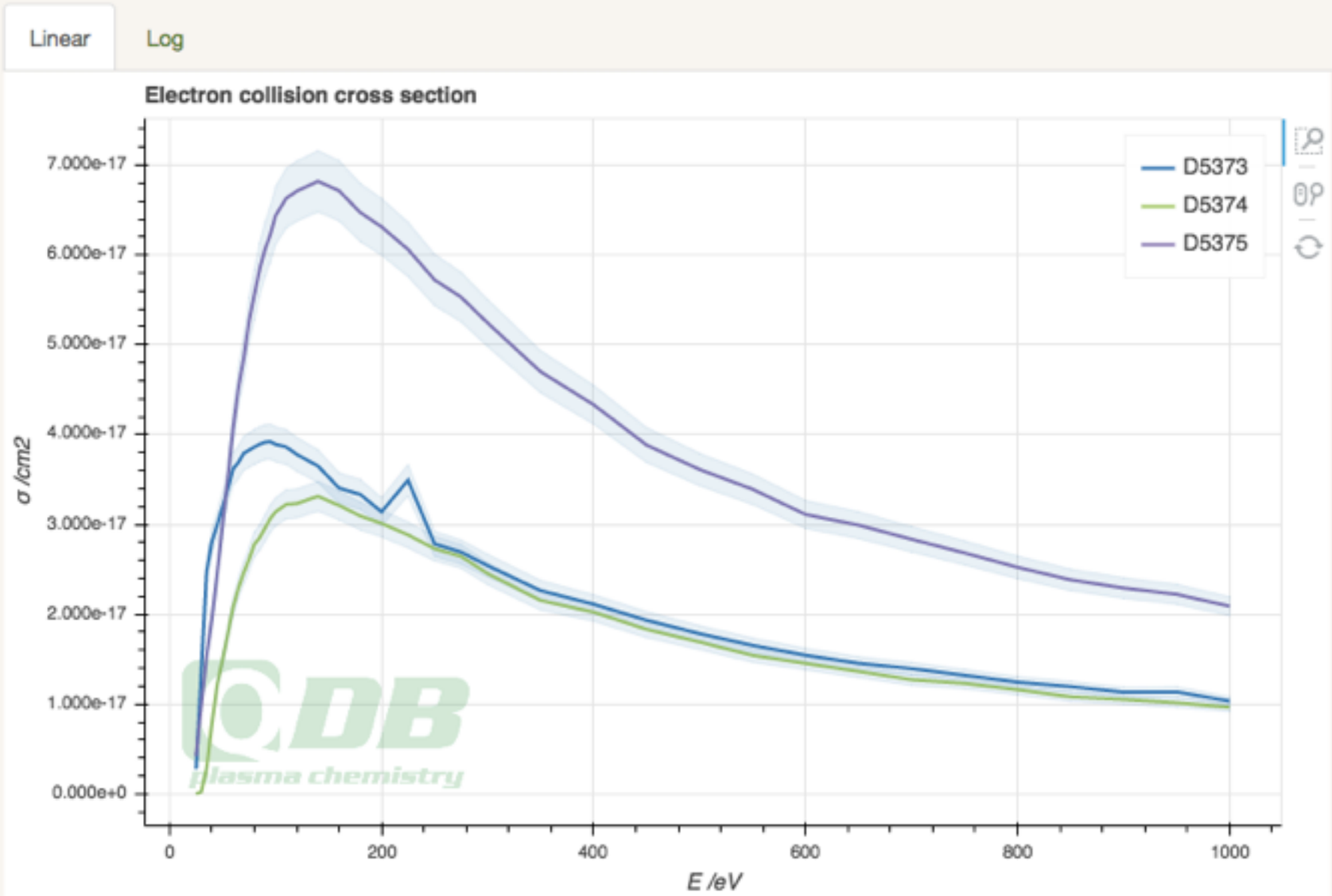
———

COMPARE

Species
CO_2
CO_2 [v=1]
CO_2 [v=2]
CO_2 [v=3]
CO_2 [v=4]
CO_2 [v=5]
CO_2 [v=6]
CO_2 [v=7]
CO_2 [v=8]
CO_2 [1*]
CO_2 [2*]
$\Sigma\{CO_2\}$
CO_2 [v=*]

	Reaction	Process	Data available: Cross section	Data available: Rate constant data
	$e^- + CO_2 \rightarrow e^- + e^- + CO_2^+$	EIN	—	—
✓	$e^- + CO_2 \rightarrow O^- + CO$	EDA	✓	—
	$CO_2 + CO^+ \rightarrow CO_2^+ + CO$	HIR	—	✓
	$e^- + CO_2 \rightarrow e^- + O + CO$	EDS	—	✓
✓	$e^- + CO_2 \rightarrow e^- + CO_2$ [v=1]	EVX	✓	—
✓	$e^- + CO_2 \rightarrow e^- + CO_2$ [v=2]	EVX	✓	—
✓	$e^- + CO_2 \rightarrow e^- + CO_2$ [v=3]	EVX	✓	—
✓	$e^- + CO_2 \rightarrow e^- + CO_2$ [v=4]	EVX	✓	—
✓	$e^- + CO_2 \rightarrow e^- + CO_2$ [v=5]	EVX	✓	—
✓	$e^- + CO_2 \rightarrow e^- + CO_2$ [v=6]	EVX	✓	—
✓	$e^- + CO_2 \rightarrow e^- + CO_2$ [v=7]	EVX	✓	—
✓	$e^- + CO_2 \rightarrow e^- + CO_2$ [v=8]	EVX	✓	—

QuantemolDB



Datasets

D5373:	$e^- + CO_2 \rightarrow e^- + e^- + O + CO^+$	B383: Y. Itikawa, "Cross Sections for Elect...
D5374:	$e^- + CO_2 \rightarrow e^- + e^- + O_2 + C^+$	B383: Y. Itikawa, "Cross Sections for Elect...
D5375:	$e^- + CO_2 \rightarrow e^- + e^- + O^+ + CO$	B383: Y. Itikawa, "Cross Sections for Elect...

QuantemolDB

- Flexible data model allows for
  - Generic parameter data
  - Generic tabular data
  - Bibliographic references
    - Building “Chemistries” of related reactions / collisions
- Software libraries provide tools for:
  - Identifying and providing metadata on species and their quantum states
  - Manipulating the units of physical quantities

QuantemolDB

- Complex demands for user-management:
  - AAA (Authentication, Authorization, Accounting)
  - Some users can **upload data**:
    - Such contributions must be validated, logged and attributed
    - Incoming data must have the correct format and physical units
    - Security concerns
- Users can **evaluate data**
- Use of the **API** (next slide) requires a *key* (token)

QuantemolDB

API

- quantemoldb.com exposes an API for the automated retrieval of data by software applications
- Data is returned in one of several formats specified by a keyword as part of the API request
- Entire Chemistries can be downloaded ready-made or constructed by specifying the species involved, e.g.

```
https://www.quantemoldb.com/reactions/api/?key=XXXX-XXXX-XXXX-XXXX&qsymbols=AR,AR^,H,AR2^
```

Challenges for AM databases

- Sustainability is a problem for any non-commercial database (= €,$,£,¥,₩)
- Security concerns and database / server maintenance
- A database cannot be sustainable unless it is easy to upload data to it (even if only by its administrators or their proxies)
- The problem of a common query language and output format across a wide range of applications has still not been solved

Future Directions

- A lightweight, generic relational database model for AM data?
- Software tools for conversion between different data formats
- Data attribution through simple identifiers (DOI or similar)
- Time stamping and versioning
- Distributed database hosting?
  - Subscription-based?
  - Blockchain technology? (Ethereum?)

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