Collaborating with VAMDC

Guy Rixon

RADAM database workshop, Caen, October 2013

Original use-case

Standard
query protocol

Standard
data-format

Energy-level matching

Model atmosphere calculations

More use cases...

- Composite spectrum for molecule
- Combine parameters for atomic lines
- Compare observation with theory
- Compare separate calculations of same levels
- Same modelling code uses multiple DBs
- New applications work with all DBs
- Self-describing format for data
- Bibliography of data sources
- etc...

Synthesis of parts

VALD CDMS

HITRAN CHIANTI

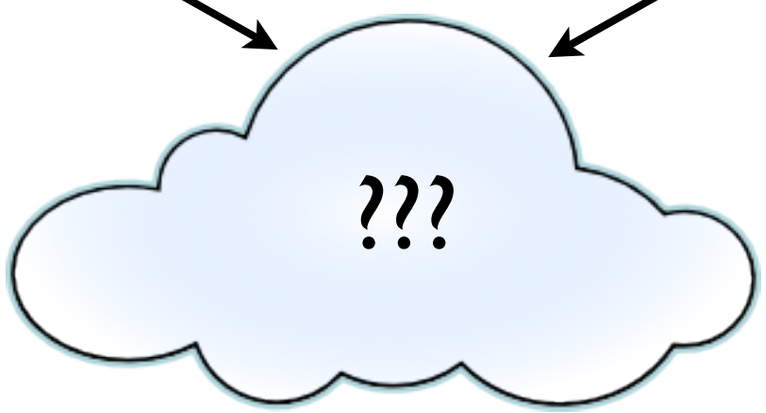
BASECOL

Existing databases

Web-service protocols

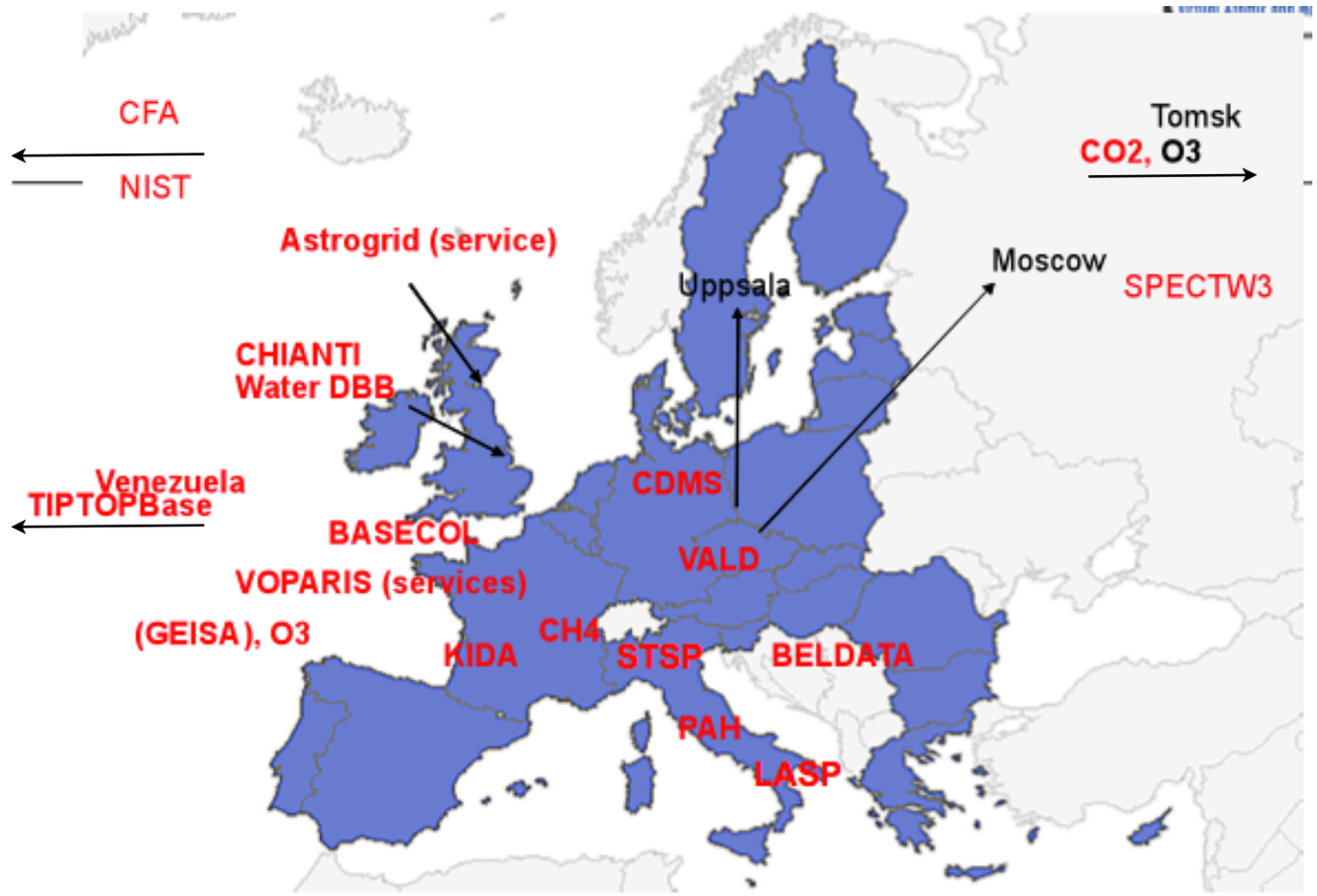
IAEA

XSAMS data-format

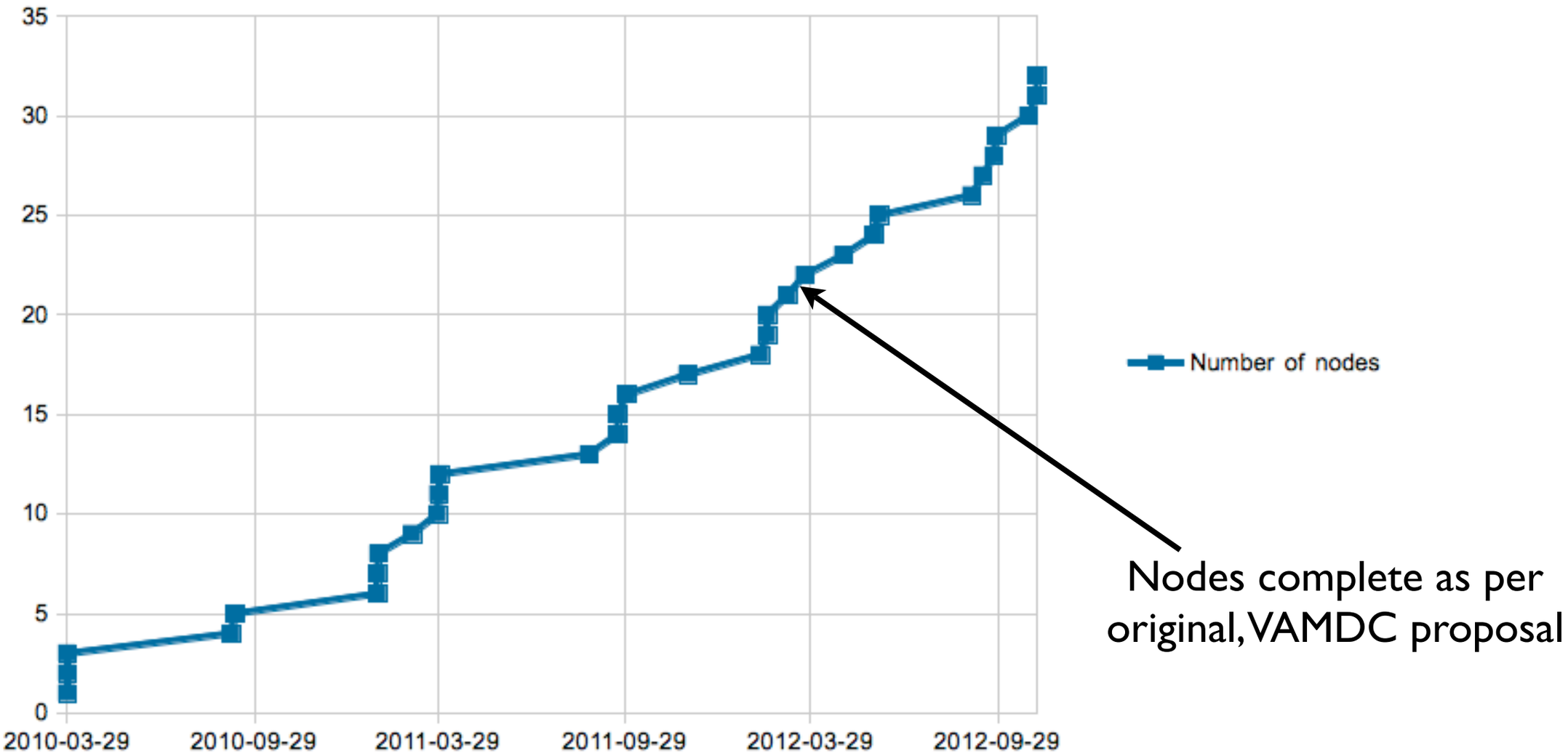


Original VAMDC project

- EU FP7 funding, 2009-2012
- 15 partners, 21 institutions
- 7 EU countries
- + Russian Federation
- + Venezula
- ~22 databases proposed initially

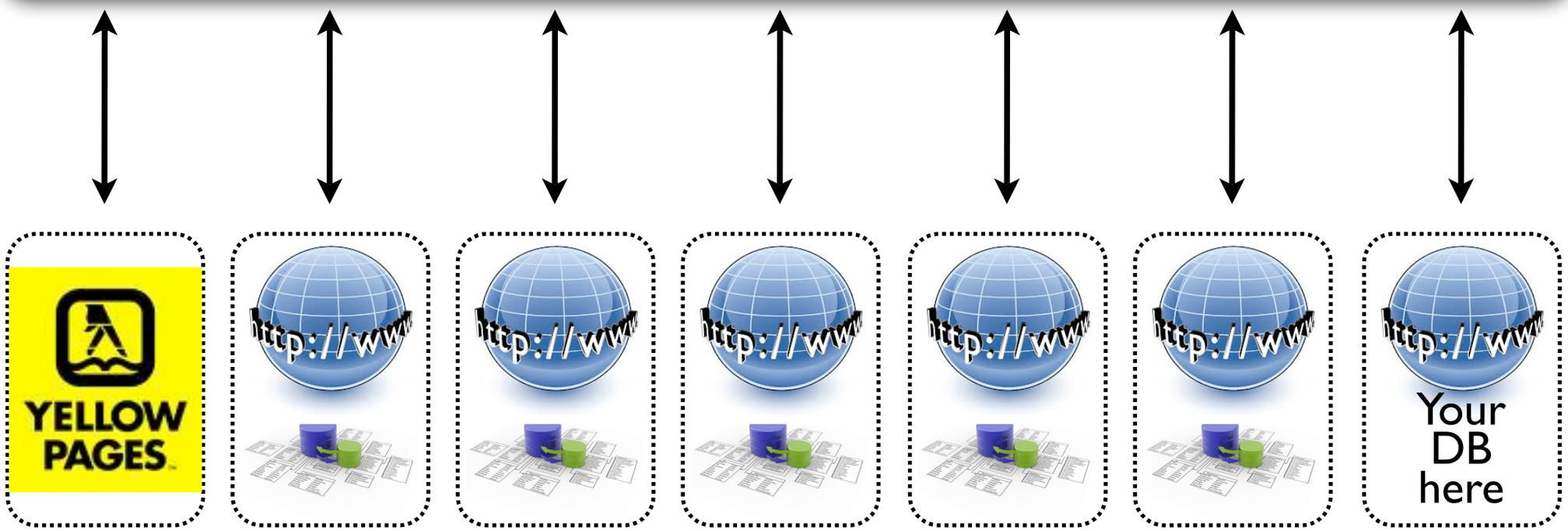


Database growth



A flock of databases

Science application



VAMDC data nodes

For list of databases see:

http://portal.vamdc.eu/vamdc_portal_test/nodes.seam

VAMDC
Virtual Atomic and Molecular Data Centre

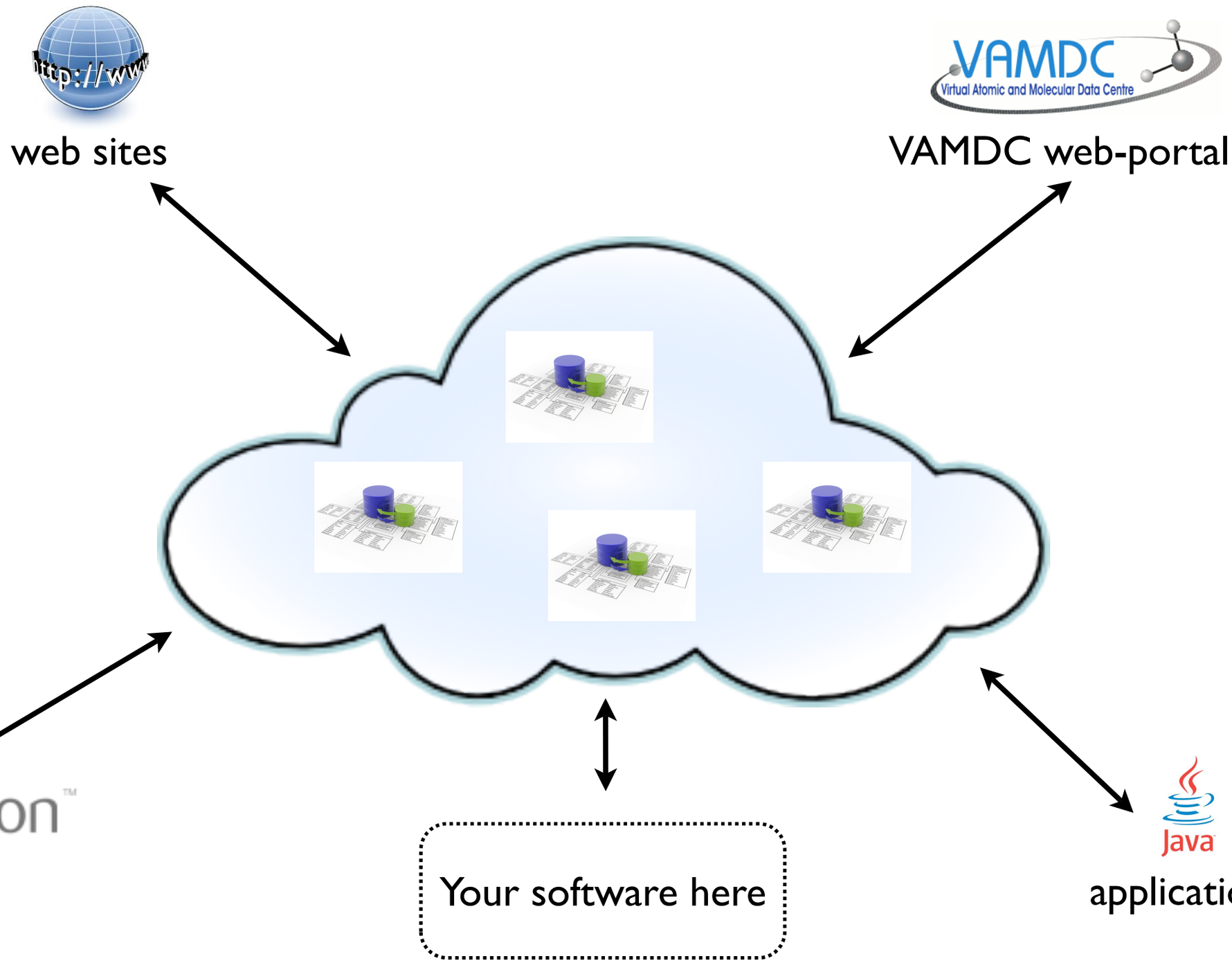
Home VAMDC databases Query Saved queries | Info Known issues Login Register

Name	Description	Maintainer	Status
Theoretical spectral database of polycyclic aromatic hydrocarbons	The Cagliari/Toulouse PAH database is a collection of theoretical spectroscopic data about Polycyclic Aromatic Hydrocarbons and carbon clusters. It provides basic geometric characteristics, energetics, harmonic analyses and electronic photoabsorption data. It is maintained by the Astrochemistry group at INAF-Observatory of Cagliari and the Institut de Recherche en Astrophysique et PlanÃ©tologie in Toulouse.	gmulas@oa-cagliari.inaf.it	OK
Chianti	Chianti consists of a critically evaluated set of up-to-date atomic data, together with user-friendly programs written in Interactive Data Language (IDL), to analyse the spectra from astrophysical plasmas. The VAMDC interface presents just the data from the Chianti-v7 release.	gtr@ast.cam.ac.uk	OK
GSMA Reims S&MPO	Calculated line lists for ozone (16O3, 16O18O16O and 18O3). The data on methane contain the vibration-rotation energy levels, line positions and line strengths in the range from 0 to 8000 cm-1.	ylb@iao.ru, vladimir.tyuterev@univ-reims.fr	OK
ECaSDa - Ethene Calculated Spectroscopic Database	Calculated data of ethylene (12C2H4). The data on ethylene contain the vibration-rotation energy levels, line positions and line intensities in the range from 500 to 7500 cm-1	ludovic.daumont@univ-reims.fr, maud.rotger@univ-reims.fr	OK
GhoSST	The GhoSST database ("Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics" database service) provides laboratory data on spectra (from UV to FIR) of natural and synthetic solids (ices, molecular solids, minerals, salts, inorganic materials, organic materials, meteorites, adsorbed molecules, hydrated solids,?) of space sciences, Earth sciences and astrophysical interest. It is completed with band list data (NIR to FIR) on molecular solids and adsorbed/hydratation molecules. The GhoSST data come from laboratory experiments performed since 1989 at IPAG (and formerly at LGGE and LPG) with different spectroscopy techniques (transmission, bidirectional reflection, micro-spectroscopy, ATR, Raman, Fluorescence, ...).	damien.albert@obs.ujf-grenoble.fr	OK
Lund laboratory spectroscopy	Experimental data for transitions and lifetimes	hampus@astro.lu.se	OK

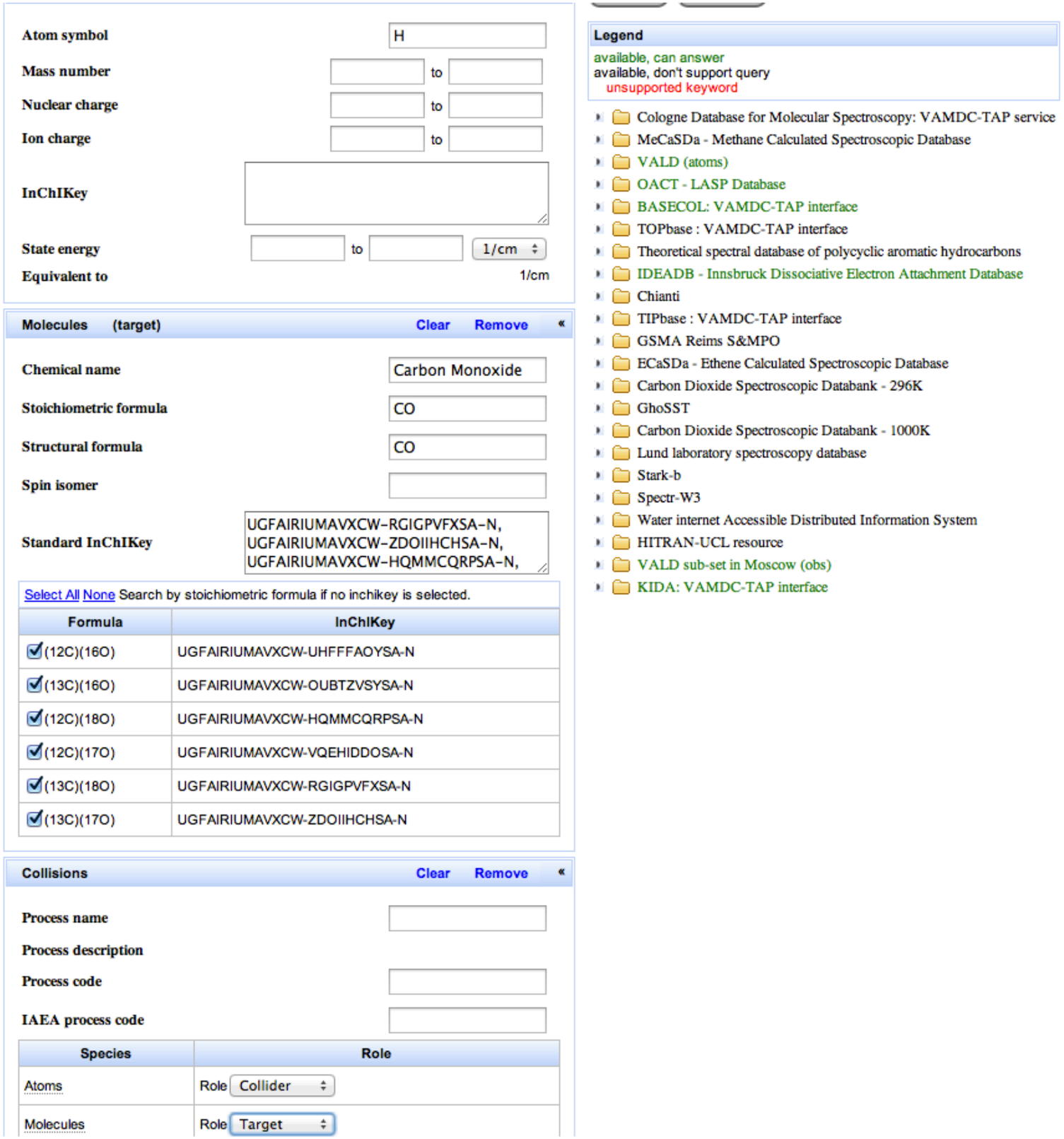
DBs relevant to RADAM

- IDEADB
- RADAM template database, Caen
- BASECOL?
- Kinetic Database for Astrochemistry (KIDA)?
- ALADDIN-2 (IEAE)?
- UMIST Database for Astrochemistry (UDfA)?
- Various electron-molecule data to come from India, Korea, Japan?

Many UIs


http://www
web sites
VAMDC
Virtual Atomic and Molecular Data Centre
VAMDC web-portal
python
scripts
Your software here
Java
applications

VAMDC web portal: query



VAMDC web-portal: results

Done

Modify query | Stop waiting | Save query

select * where (RadTransWavelength >= 5000.0 AND RadTransWavelength <= 5010.0)

Comments

XSAMS processors

- BibTeX from XSAMS
- Table views of XSAMS
- Xsams2SME

Process

Name	Response	Download	Species	States	Processes	Radiative
VALD sub-set in Moscow (obs)	OK	XSAMS	81	1157	701	701
Water internet Accessible Distributed Information System	OK	XSAMS	1	591	601	601
TOPbase : VAMDC-TAP interface	OK	XSAMS	70	619	353	353
HITRAN-UCL resource	OK	XSAMS	8	64	149	149
Chianti	OK	XSAMS	18	81	43	43
Spectr-W3	OK	XSAMS	9	26	13	13
GSMA Reims S&MPO	OK	XSAMS	0	0	5	5
Stark-b	OK	XSAMS	4	6	3	3
VALD (atoms)	TRUNCATED (9%)	XSAMS	78	10076	65459	65459
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	EMPTY		0	0	0	0
Carbon Dioxide Spectroscopic Databank - 1000K	EMPTY		0	0	0	0
Carbon Dioxide Spectroscopic Databank - 296K	EMPTY		0	0	0	0
MeCaSDa - 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

VAMDC web-portal: display

Data for single collision

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

- 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)	(cm3/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

Collisions with data sets

PBASC48t2T1c1C1

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

M.-L. Dubernet 2013; N. Balakrishnan et al. 2002

rateCoefficient

Table (CSV): Rate coefficients

PBASC48t3T1c1C1

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

M.-L. Dubernet 2013; N. Balakrishnan et al. 2002

rateCoefficient

Table (CSV): Rate coefficients

PBASC48t3T2c1C1

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

M.-L. Dubernet 2013; N. Balakrishnan et al. 2002

rateCoefficient

Table (CSV): Rate coefficients

PBASC48t4T1c1C1

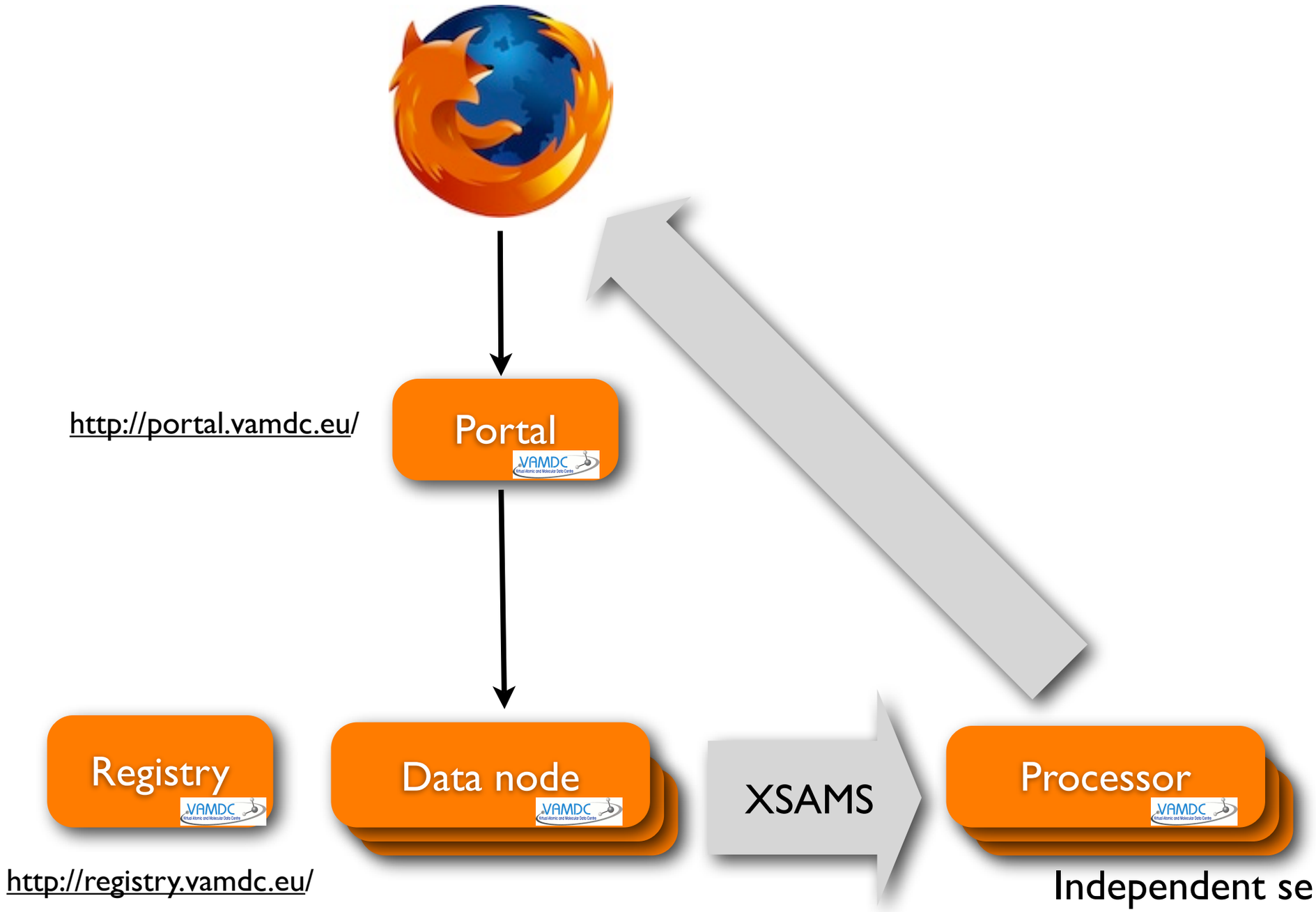
$CO + {}^1H \rightarrow CO + {}^1H$

M.-L. Dubernet 2013; N. Balakrishnan et al. 2002

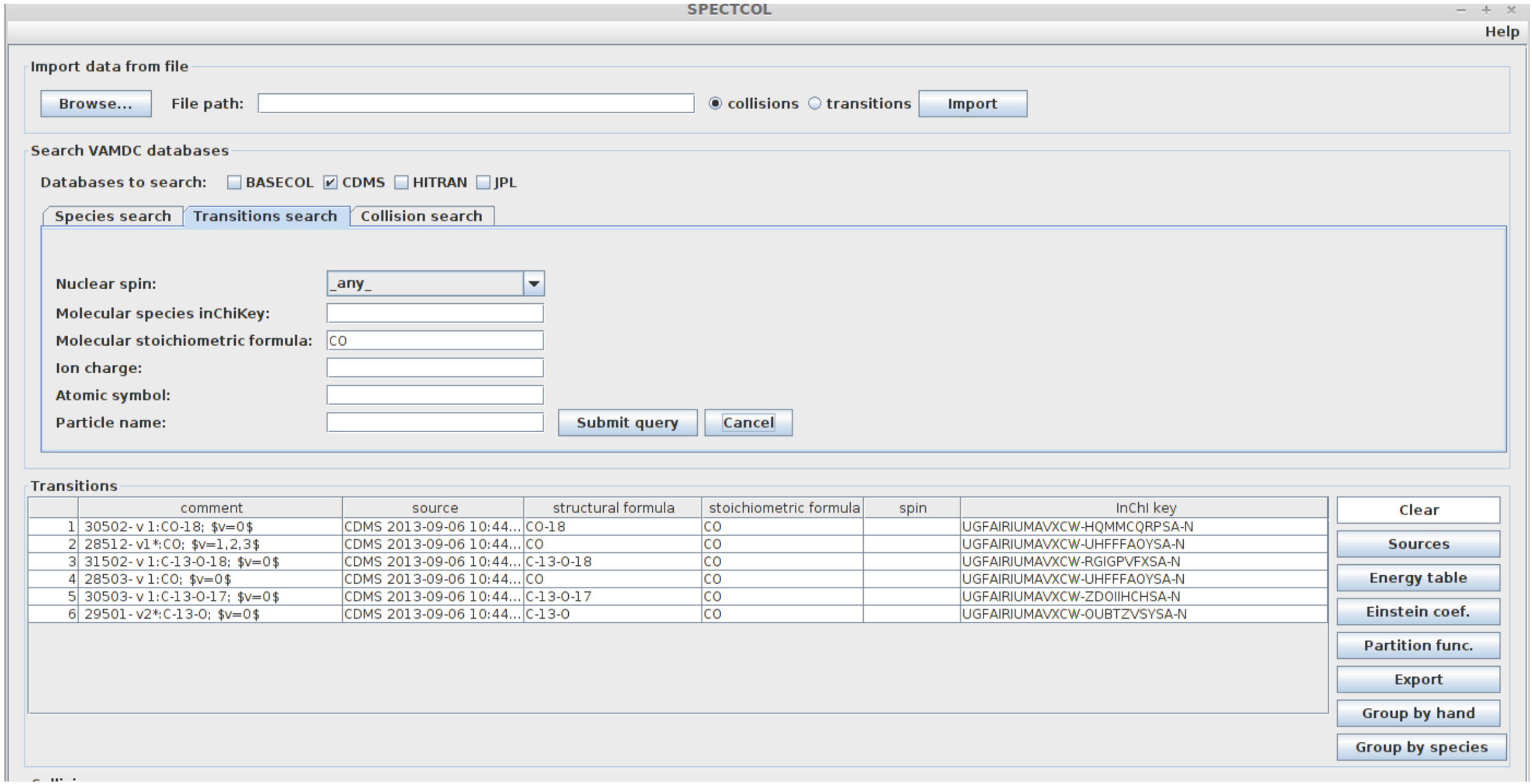
rateCoefficient

Table (CSV): Rate coefficients

Portal, nodes & processors



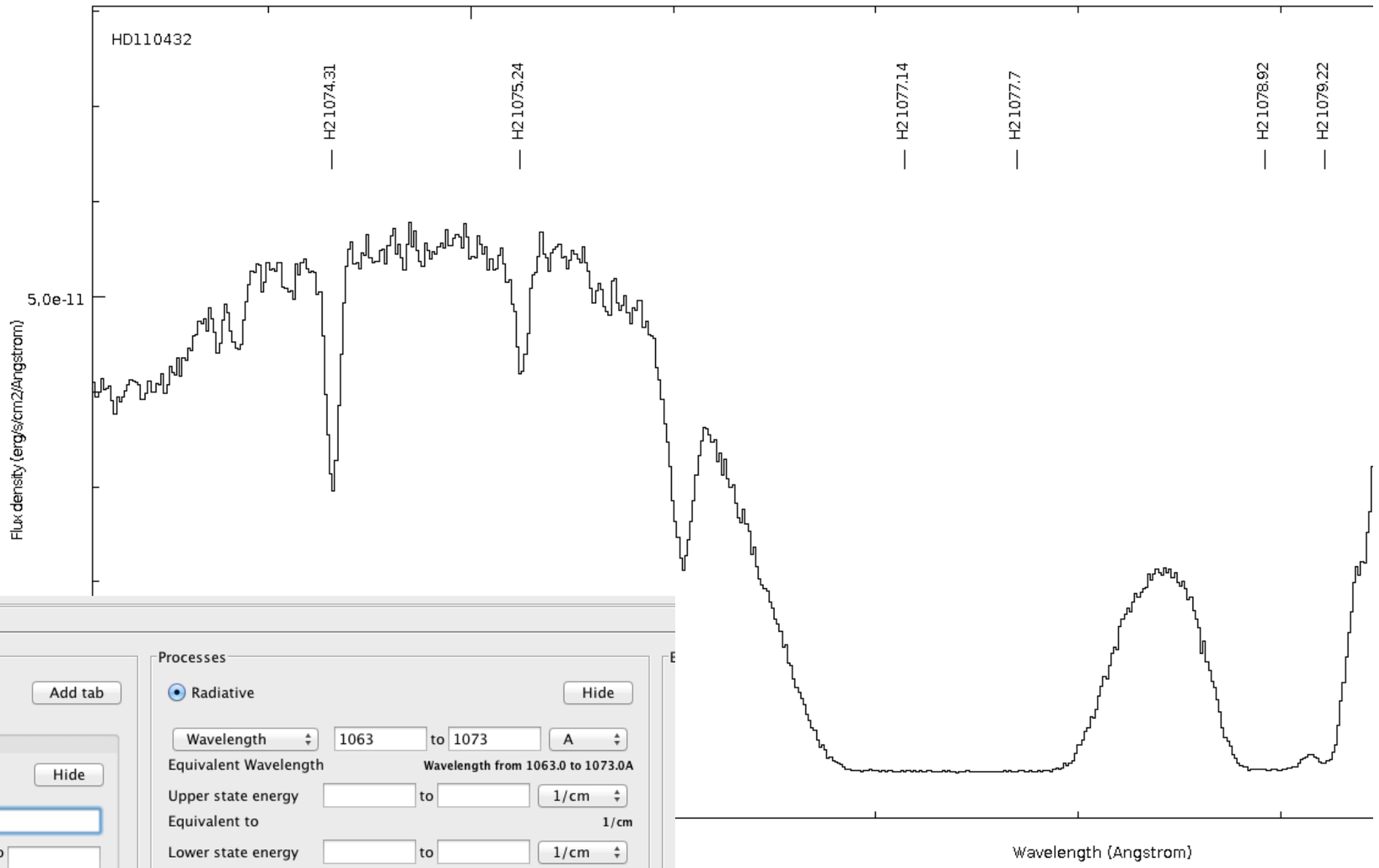
SpectCol application

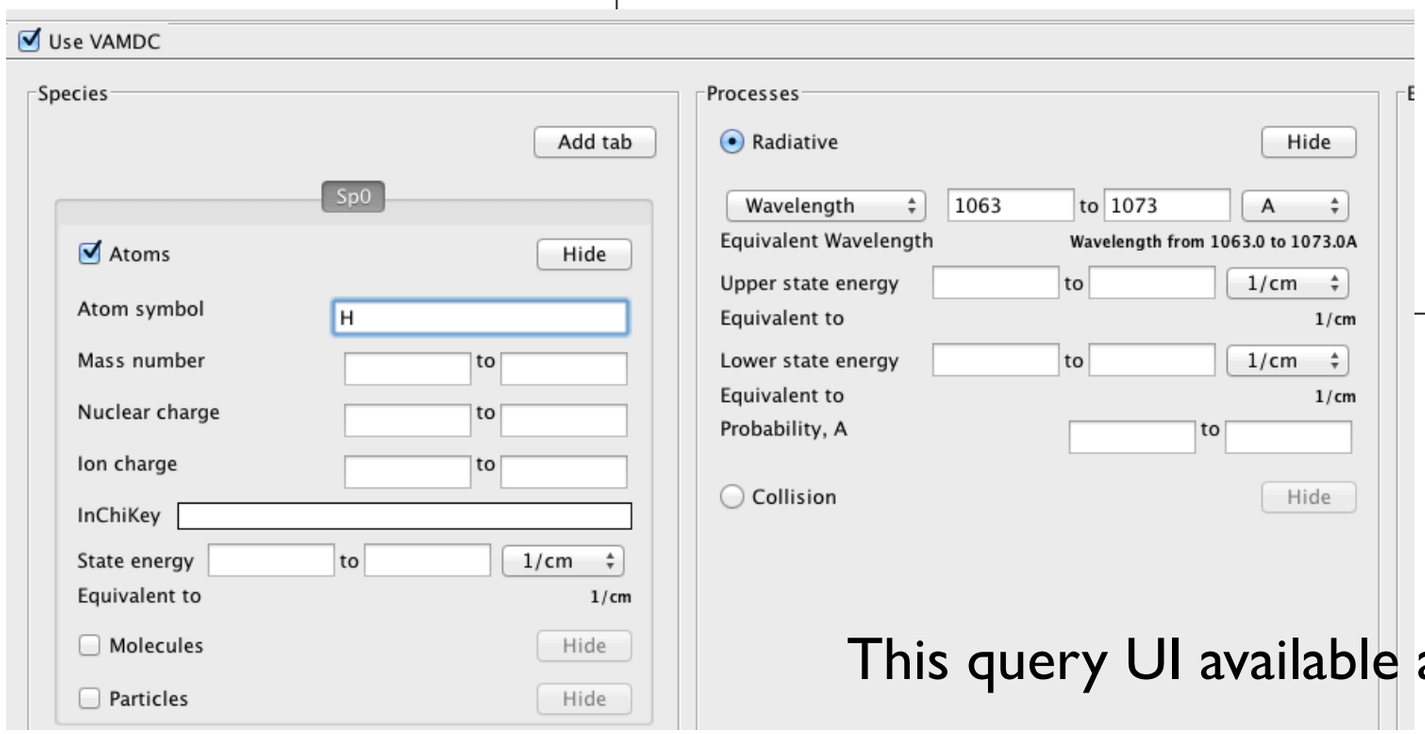


Implements the original use case for matching spectroscopic and collisional data

Specview application

Line IDs for astronomy: VAMDC data added to existing application





This query UI available as a Java library

SUP@VAMDC: successor project

- Further EU funding, 2012-2014
- 6 of 15 original VAMDC partners involved
- New partners in India, Korea, South Africa
- External partners in USA, Brazil, Australia, Japan, Austria
- Most nodes connected from outside the project
- Focused on **support** for users, data-providers

Coding support

- Class libraries for Java
- Module and small-app collection for Python
- Open-source licensing

Tutorials

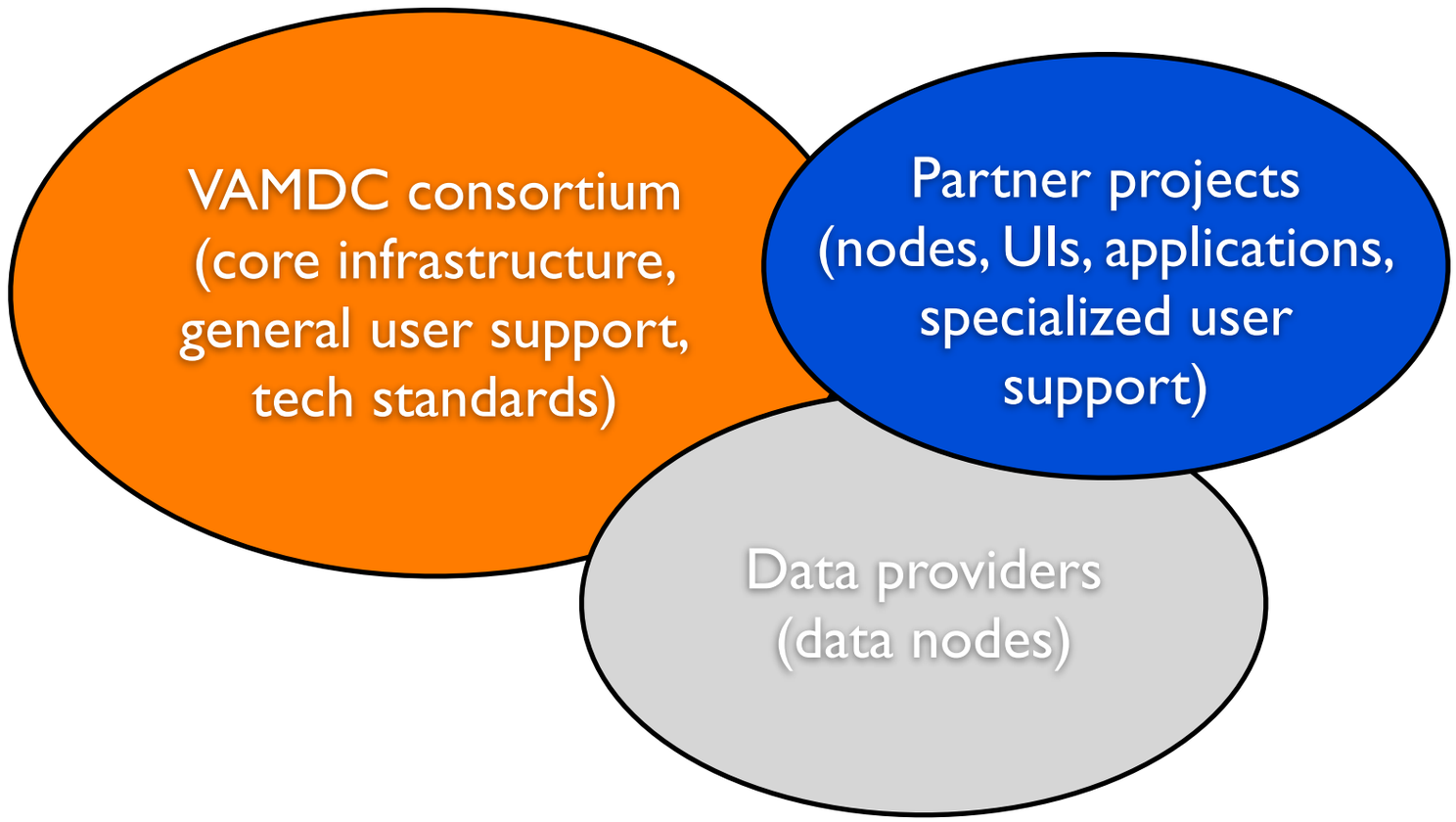
http://www.vamdc.eu/usersupport/tutorials

- Introductory papers
- Self-paced exercises
- Video guides
- Reference manuals

Support after SUP@VAMDC

- VAMDC consortium continues support:
  - consortium of universities signatory to a MOU;
  - contains the active members of the SUP@VAMDC project, plus some others;
  - maintains the infrastructure for users and node-operators;
  - separate MOU between consortium and that node operators;
  - node operators do not need to join the consortium to get support;
  - consortium will seek grants to continue the work;
  - consortium → legal entity; EU recognition as a body rather than an ephemeral collaboration.

Three-way cooperation



Summary

- Collaborate with VAMDC to get:
  - standards for distributed databases;
  - established network of services for same;
  - technical support;
  - user training.
- Collaborate by:
  - making data nodes and XSAMS processors;
  - making UIs for VAMDC services;
  - acknowledging VAMDC.
- Collaborate with:
  - VAMDC consortium;
  - currently supported by SUP@VAMDC project;
  - later established as legal entity with grant/subscription support.