VAMDC
Virtual Atomic and Molecular Data Centre
http://www.vamdc.eu (.org)

Coordinator: M.L. Dubernet[1,2]

on behalf of the VAMDC Consortium

[1]LUTH, UMR CNRS 8102,Observatoire de Paris

[2]LPMAA, UMR CNRS 7092, Université Pierre et Marie Curie

Agenda

- General Overview of VAMDC Program
  - Partners
  - Objectives
  - Program of Work
- Infrastructure
- Mid-Term Achievements
  - Release of Standards
  - Release of Softwares
  - Implementation
  - Portal

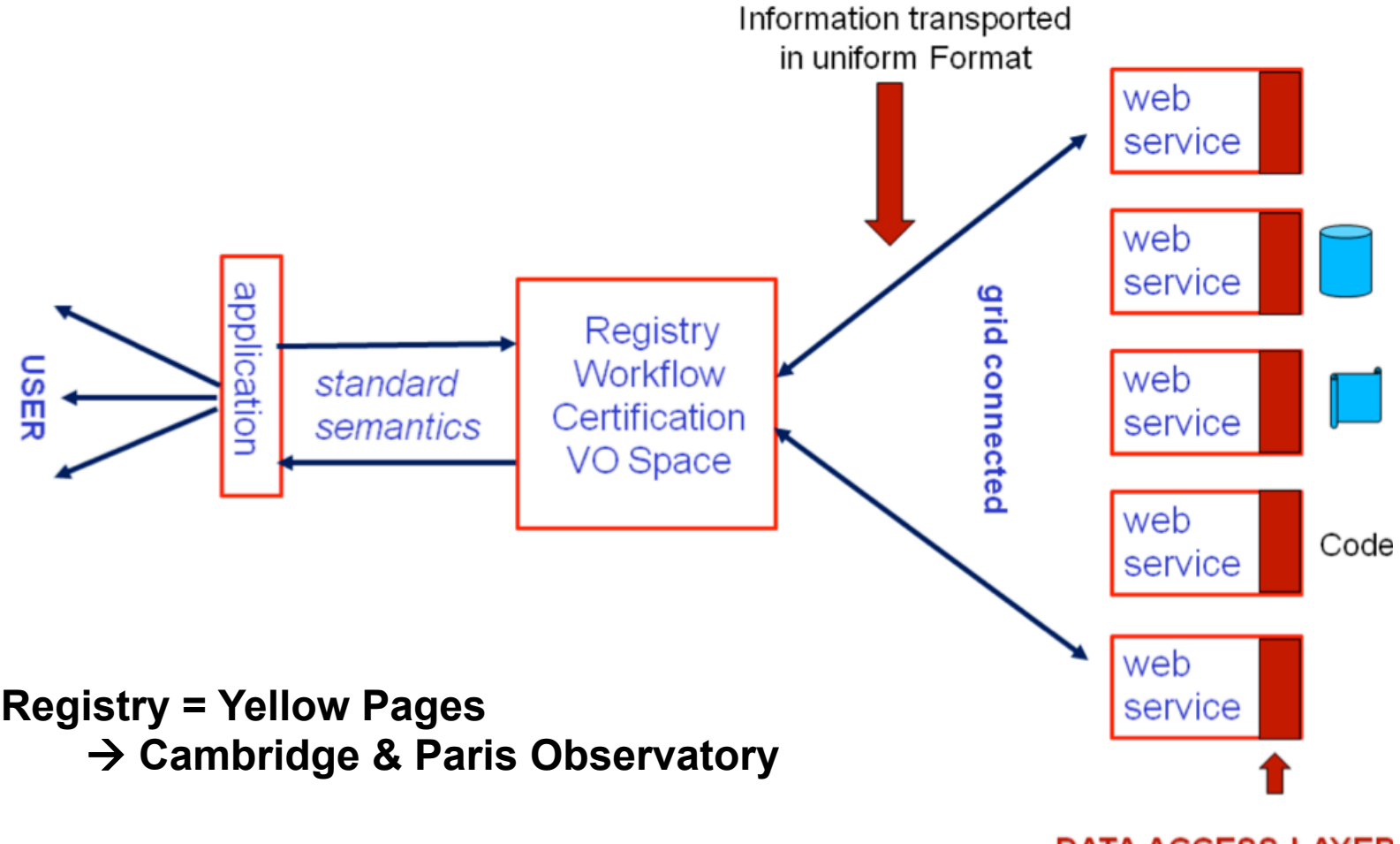
VAMDC in a nutshell

- International collaboration between groups involved in the generation, evaluation, and use of atomic and molecular data (A&M data).
- Aims: creating a well-documented interoperable interface to existing A&M data resources.
- Funded by EU-FP7 E-Science Infrastructures programme, started July 2009, until end 2012.
- Consortium: 15 partner institutes from six EU and three non-EU countries + external partners –

VAMDC in a nutshell

- 26 Different Departments and about 108 people: about 68 Full Time Equivalent for 42 months
- Connecting Europe to Russia, Central Europe, South America, North America → Aim at worldwide connection
- Connecting Different Fields of Producers of Atomic and Molecular Physics and Chemistry
- Connecting A.& M. Producers to A. & M. Users
- Connecting to Research/E-Infrastructures: Euro-VO (IVOA), Europlanet, HELIO

Schematic diagram of the VAMDC infrastructure



Registry = Yellow Pages
→ Cambridge & Paris Observatory

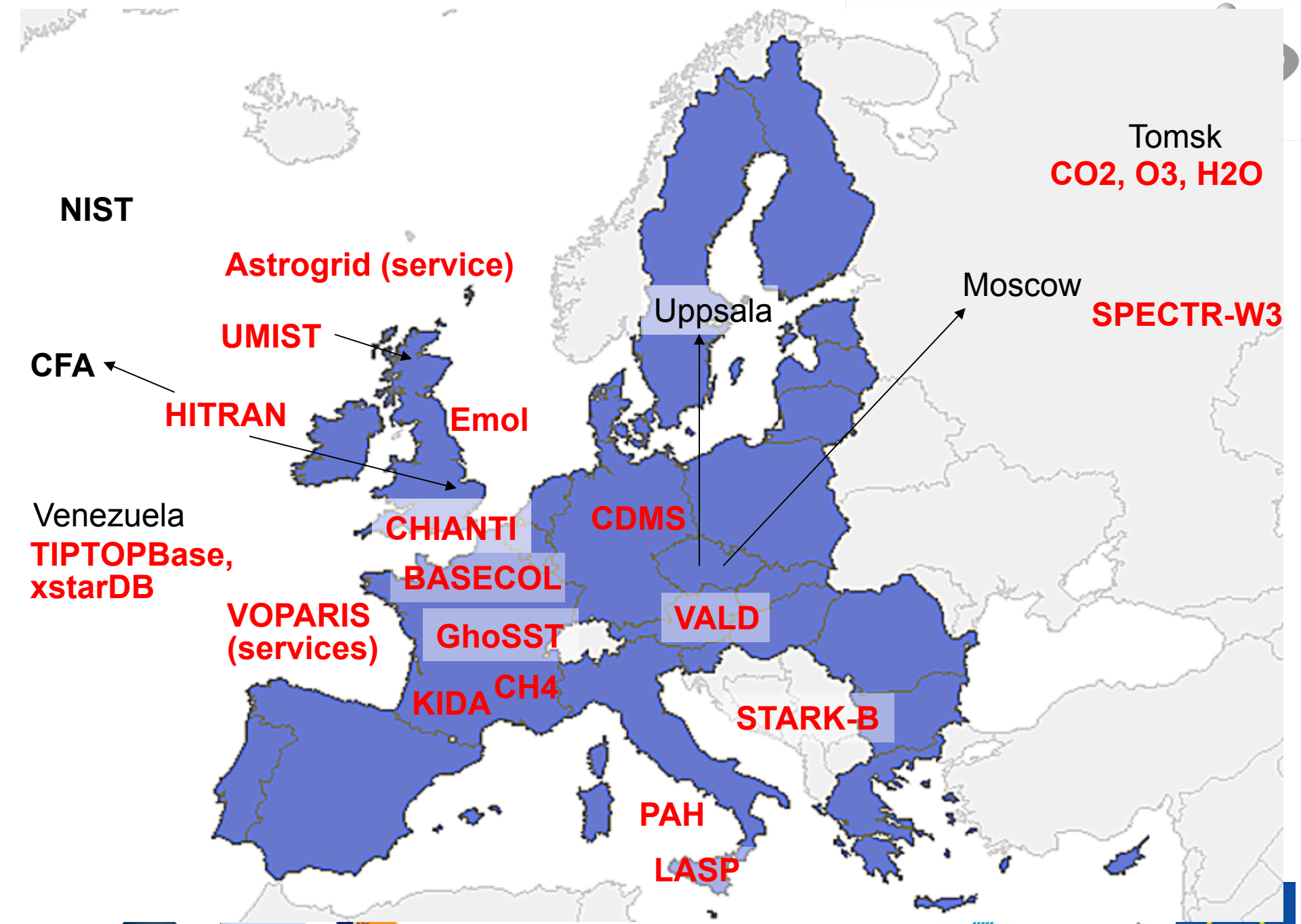
Core databases

- Developed and maintained at partner institutes, about 17 (+2) databases
- Atomic data for astrophysics – 6 databases (+2)
- Molecular data – 9 databases
- Solid Spectroscopy data – 2 databases

+ 2 Technological Nodes

Institute of Astronomy: Cambridge University

VO-Paris Data Center: Paris Observatory (WP1, WP5, WP6, WP8) – Diffusion – Stockage – GRID – Copy of Registry – VAMDC Portal – Databases such as BASECOL, Stark-B, TipTopBase


NIST
Astrogrid (service)
UMIST
CFA
HITRAN
Emol
Venezuela
TIPTOPBase,
xstarDB
VOPARIS
(services)
CHIANTI
BASECOL
GhoSST
KIDA
CH4
CDMS
VALD
STARK-B
PAH
LASP
Uppsala
Moscow
SPECTR-W3
Tomsk
CO2, O3, H2O

Basecol Database (basecol.obspm.fr)
Paris Observatory

Collaboration: Bordeaux, Besançon, Grenoble, Madrid, Durham

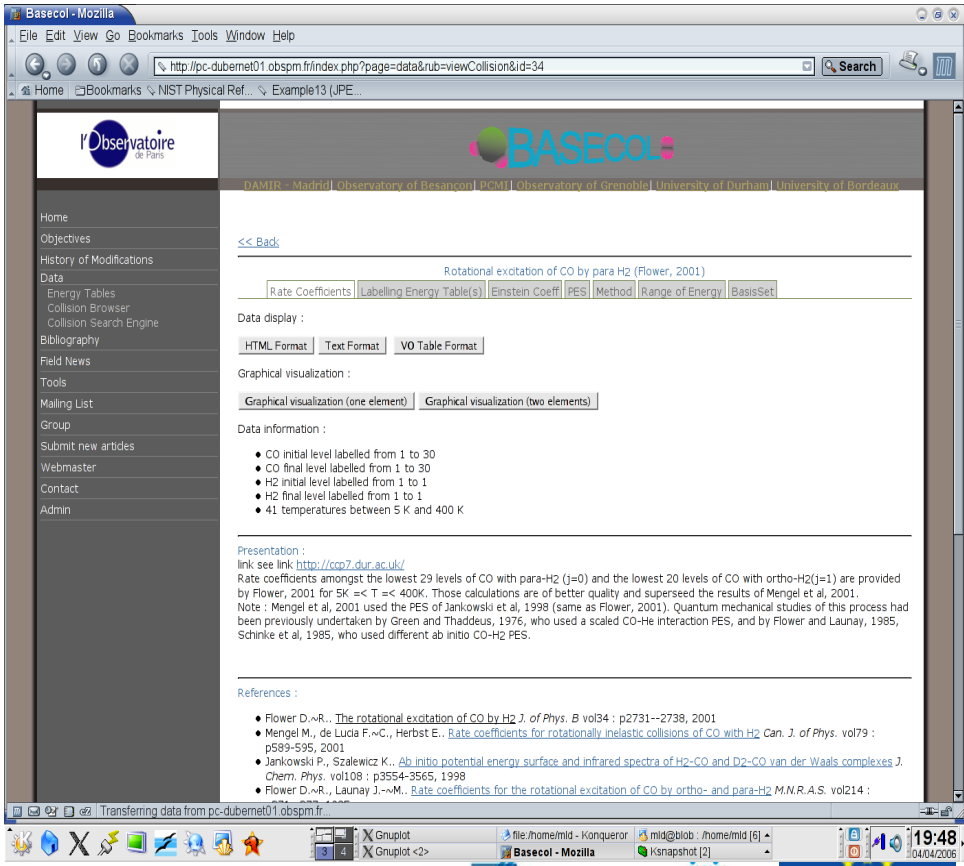
P.I. = ML Dubernet

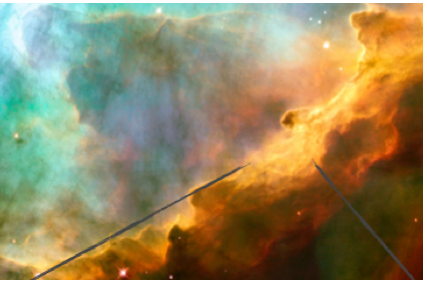
Linked to CDMS and JPL

Astrophysical Applications

Published (de)-excitation rate coefficients

- Rotational (fine, hyperfine), Ro-vib., Vib.
- Currently: 47 Target molecules; Perturbers : electrons, He, H, H_2
- 130 collisional systems
- Fully documented and referenced (759 ref.)
- Fitting coefficients, visualisation tools
- Energy levels, Einstein coefficients, QN
- Fully checked and evaluated





GhoSST

Observatory of Grenoble (B. Schmitt)

http://ghosst.obs.ujf-grenoble.fr

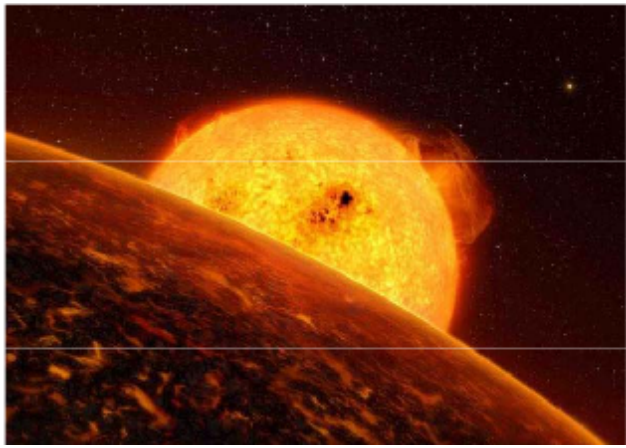
- GhoSST (Grenoble astrophysics and planetology Solid Spectroscopy and Thermodynamics,) database service, offers spectroscopic laboratory data on molecular and atomic solids from the near UV to the far-infrared.
- Solid Spectroscopy Data Model
- **ISM and Planetology Applications**

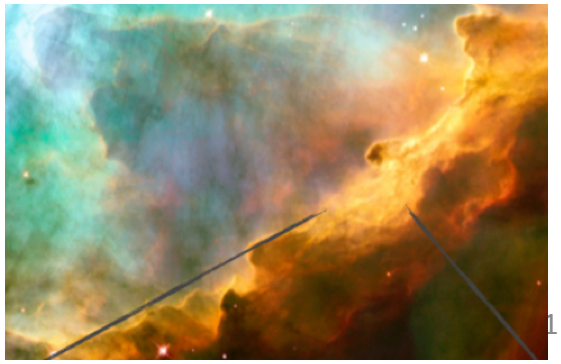
KIDA

Observatory of Bordeaux (V. Wakelam)

http://kida.obs.u-bordeaux1.fr

- KIDA - KInetic Database for Astrochemistry contains data on chemical reactions used in the modelling of the chemistry in the interstellar medium and in planetary atmospheres
- **ISM and Planetology Applications**

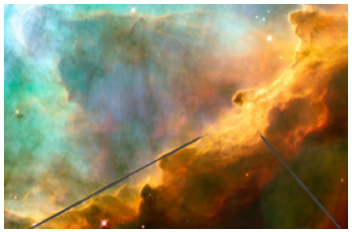


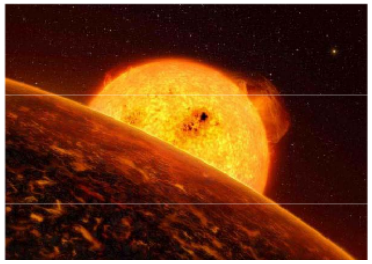


PAH

Observatory of Cagliari (G. Mulas) and « ex-CESR » (C. Joblin)

http://astrochemisty.ca.astro.it/database/





- PAHs (Polycyclic Aromatic Hydrocarbon) and carbon clusters spectral database provides a number of properties for a sample of presently about 60 species in four charge states: anion, neutral, cation and dication.
- The properties include general energetic such as electron affinity and ionisation energies, static polarizability, permanent dipole moment, van der Waals coefficients, symmetry, multiplicity, and optimised geometry of the ground electronic state; harmonic vibrational analyses, i. e. normal modes, their frequencies and IR activities; and vertical electronic photoabsorption cross-sections and complex frequency-dependent electronic polarisabilities in the linear regime.
- **ISM and Planetology Application**

Stark-B

- This is a database of the theoretical widths and shifts of isolated lines of atoms and ions due to collisions with charged perturbers, obtained within the impact approximation.
- This database is devoted to modelling and spectroscopic diagnostics of stellar atmospheres and envelopes. In addition, it is also relevant to laboratory plasmas, laser equipment and technological plasmas. The database is currently developed in Paris, and a mirror is planned in Belgrade
- **Astronomical Observatory of Belgrade (S. Dimitrijević) and Paris Observatory (S. Sahal-Bréchot, N.)**

TIPTOPBASE, OPSERVER

C. Mendoza (IVIC), N. Nunez (CPTM) in collaboration with Paris Observatory (C. Zeippen, F. Delahaye, N. Moreau)

TIPTOPbase located at the Centre de Données astronomiques de Strasbourg, France contains:

- **TOPbase** (http://cdsweb.u-strasbg.fr/topbase/topbase.html), listing atomic data computed in the Opacity Project, namely LS-coupling energy levels, gf-values and photoionization cross sections for light elements ($Z \leq 26$) of astrophysical interest.
- **TIPbase** (http://cdsweb.u-strasbg.fr/tipbase/home.html). Intermediate-coupling energy levels, A-values and electron impact excitation cross sections and rates for astrophysical applications ($Z \leq 28$), computed by the IRON Project.

Opserver, located at the Ohio Supercomputer Center, USA, (http://opacities.osc.edu/), a remote, interactive server for the computation of mean opacities for stellar modelling using the monochromatic opacities computed by the Opacity Project.

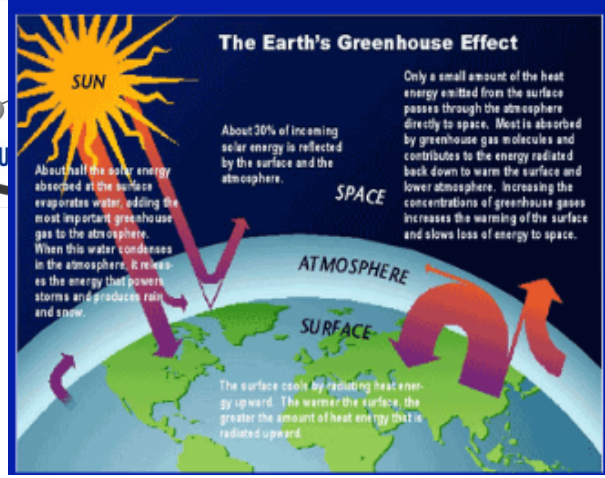
Stellar Physics

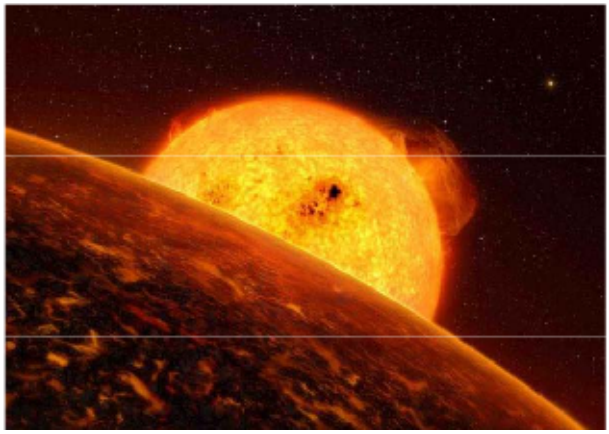
S&MPO AND Ethylene

- Spectroscopy & Molecular Properties of Ozone) relational database (http://ozone. iao.ru and http://ozone.univ-reims.fr/) contains spectral line parameters for the ozone molecule, experimental UV cross-sections, information on ozone's molecular properties, updated reference lists classified by type as well as programs and extended facilities for user applications.
- **Earth, Exo-Planet ?**
- **IAO-Tomsk (V. Perevalov) and University of Reims (V. Tyuterev)**

CH_4 Database

Institut Carnot de Bourgogne (V. Boudon)





- Database of line parameters for the three isotopologues of methane ($^{12}CH_4$, $^{13}CH_4$ and CH_3D) with positions, intensities, lineshape parameters from FIR to Visible
- Methane is a major greenhouse pollutant on Earth and an important constituent of many astrophysical bodies (giant planets, Titan, dwarf planets, brown dwarfs, methane stars, exoplanets).
- Modelling methane absorption over a wide spectral range is essential to retrieve methane vertical profiles, minor species abundances and surface propertie.

User Communities

- Atmospheric Science
  - input for complex terrestrial atmosphere/climate models, determination of concentrations and radiative transport of about 100 species, e.g. water
- Astrophysics, Astrochemistry and Planetary Science
  - great need for reliable A&M data because of extraordinary range of physical conditions
- Plasma Technologies
  - plasma-assisted materials processing or surface modification, e.g. manufacture of semi-conductor chips. A&M data needed for modeling chemically active plasmas.

User Communities cont'd

- Lighting
  - A&M databases needed for development of future light sources – new working gas species, e.g. Xe, and metal alloys such as InSb (Indium antimonide)
- Fusion Energy Research
  - design and operation of vital fusion device systems require large amounts of A&M collisional and spectroscopic data
- Radiation Science
  - radiotherapy models exploring damage of DNA by radiation need A&M data, e.g. electron collisions with DNA components and other biomolecules

Work packages – Management and Networking Activities

1. Project Management
   - financial control, reporting to EU, web site, wiki
   - appointing Strategic Advisory Board (external experts) and interacting with it
2. Scientific/Technical Coordination
   - project planning and progress monitoring
   - work package leader meetings
   - interaction with external projects, e.g. IVOA, EuroPlanet, HELIO
3. Dissemination and Training
   - interface of VAMDC to wider community of producers and users of data
   - organization of one annual "VAMDC meeting" and 2−3 scientific workshops per year, development of tutorials

Work packages – Joint Research Activities

6. Interoperability
   - extension of data model and XML schema (XSAMS), e.g. different description of molecular states, description of line shapes, Solid Spectroscopy
   - creation of dictionaries, definition of access protocols and query languages, definition of registry structure
7. Publishing Tools
   - developing tools and formulating procedures to include new atomic and molecular data into VAMDC

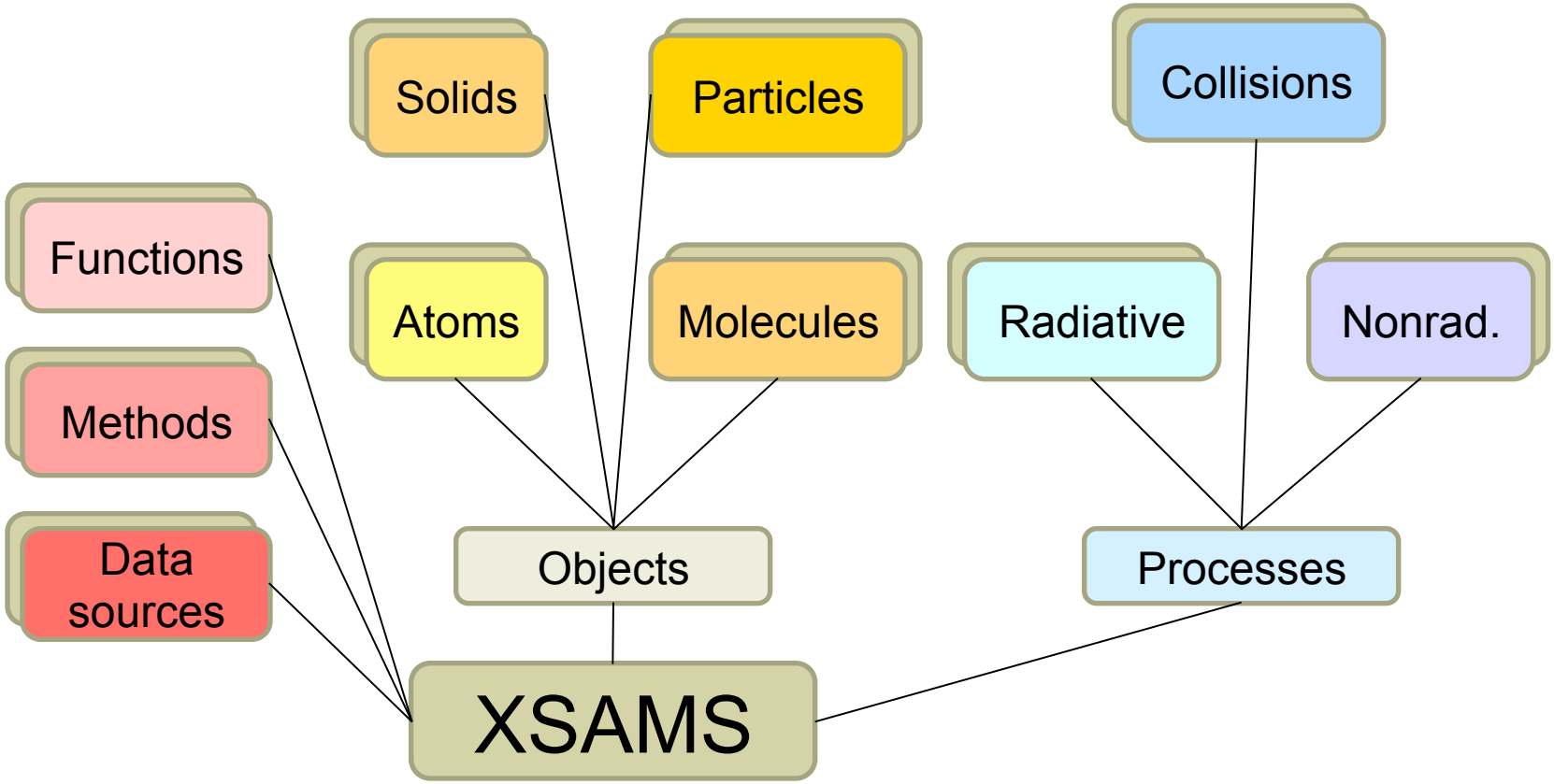
Interoperability

- Common data model – XSAMS
- XML Schema for Atoms Molecules and Solids
  - Quantum states, radiative transitions, collisional processes, etc.: broad range of A&M data
  - Easily transformed into other formats
- Original IAEA initiative
  - Development now at VAMDC

XSAMS/VAMDC Development Group

- IAEA, Austria
  - *Bas Braams*
  - *D. Humbert*
- Observatory Paris[1]/ LPMAA[2], France
  - *[1,2]M.L. Dubernet*
  - *[1]E. Roueff, N. Moreau*
  - *[2]M. Doronin*
- Oak Ridge Nat. Lab, USA
  - D.R. Schultz
- VNIITF, Russia
  - S. Gagarin
  - P.A. Loboda
- NIST, USA
  - *Yu. Ralchenko*
- UCL, UK
  - *J. Tennyson, C.Hill*
- Uppsala Univ., Sweden
  - *N. Piskunov*

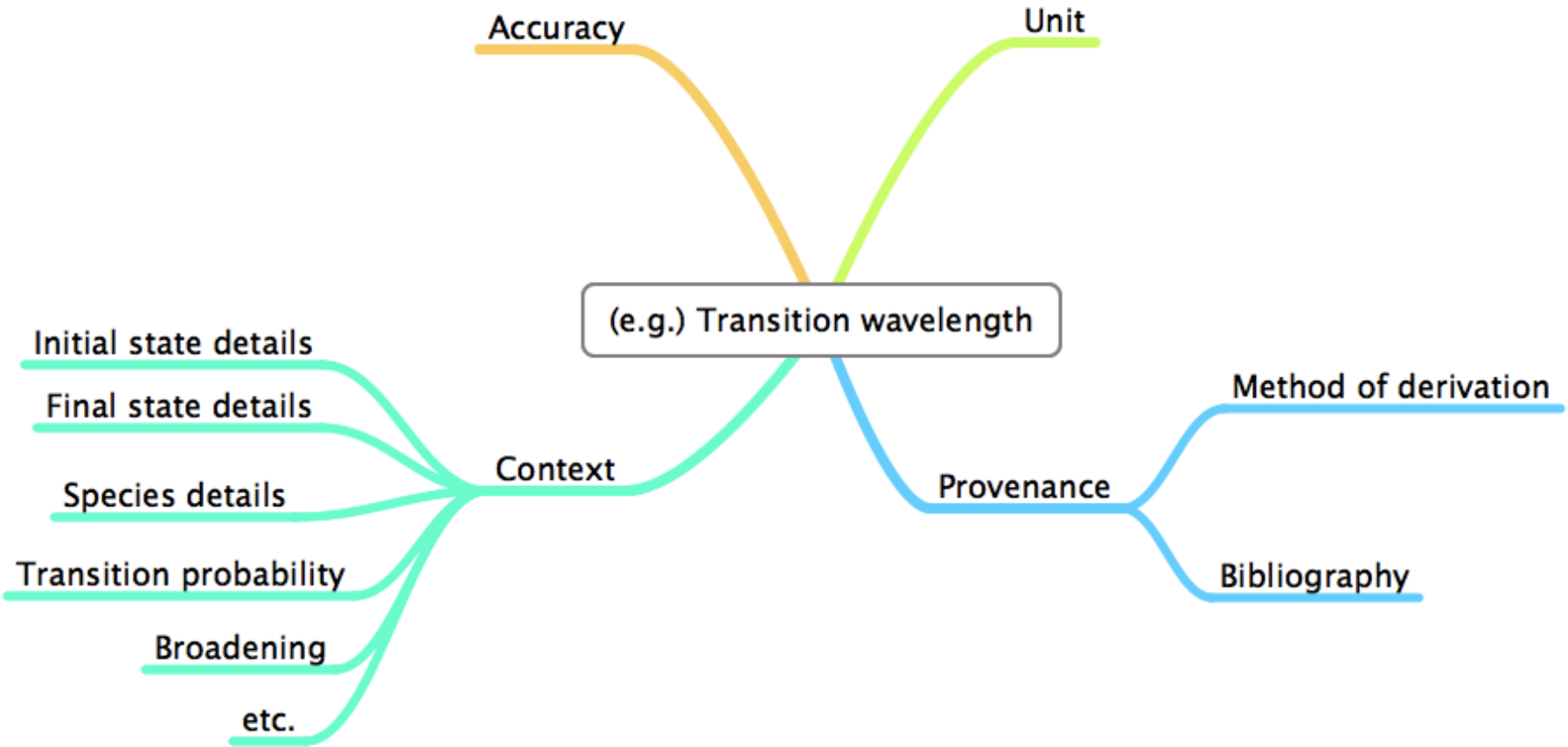
XSAMS tree


Solids
Particles
Collisions
Functions
Atoms
Molecules
Radiative
Nonrad.
Methods
Data sources
Objects
Processes
XSAMS

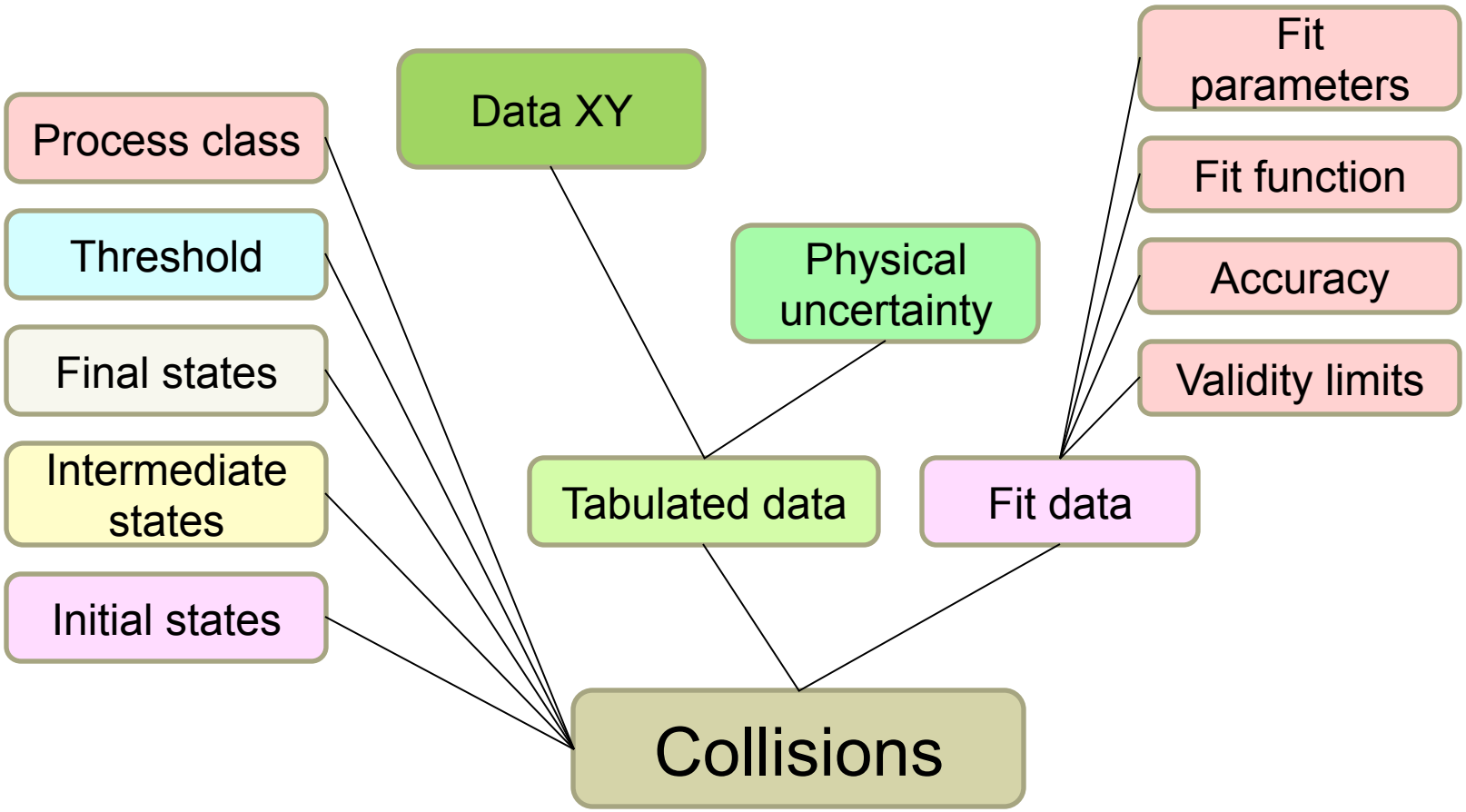
XSAMS: data sources

- May include:
  - **Authors**
  - **Production date**
  - **Source category**
    - Journal
    - Database
    - Private communication
    - Book
    - Report
    - …
- Universal Resource Identifier
- Digital Object Identifier
- Editors
- Publisher
- City
- Comments (any other relevant information)

Traceability of data origins: a must!


Accuracy
Unit
(e.g.) Transition wavelength
Initial state details
Final state details
Species details
Transition probability
Broadening
etc.
Context
Provenance
Method of derivation
Bibliography

XSAMS: collisions



Development of a Solid Spectroscopy Data Model (SSDM) and GhoSST DB

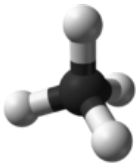
GhoSST

"Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics" database service

Bernard Schmitt, Damien Albert
and the SSDM Expert group*

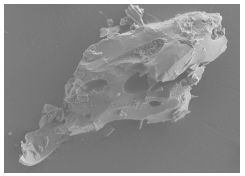
Institut de Planétologie et Astrophysique de Grenoble (former LPG), CNRS / UJF

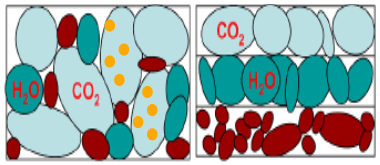
Solid Spectroscopy DM General Structure



SPECIES

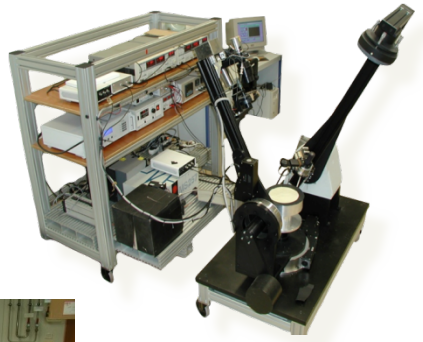
MATTERS

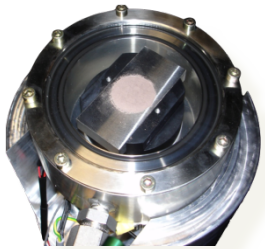




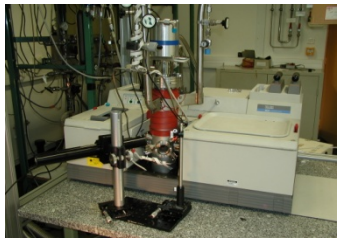
SAMPLE

INSTRUMENT



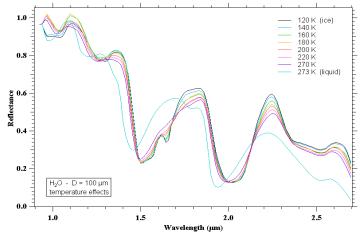


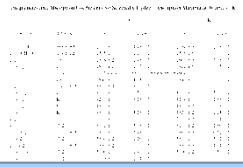
EXPERIMENT



BAND LIST

SPECTRA





JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 103, NO. E11, PAGES 25,809–25,822, OCTOBER 25, 1998

The temperature-dependent near-infrared absorption spectrum of hexagonal H_2O ice

W. M. Grundy[1] and B. Schmitt

CNRS/Laboratoire de Glaciologie et Géophysique de l'Environnement, Grenoble, France

Abstract. Transmission spectra were measured between 1.9 and 2.7 μm for monocrystalline samples of hexagonal water ice at temperatures between 20 and 270 K. Samples were crystallized from liquid water within closed cells, with thicknesses ranging from 100 μm to 1.0 cm. The absorption spectrum of ice changes with temperature in several ways. With higher temperature, the shapes of absorption bands become more smoothed, the strengths of some absorption bands decrease, the absorption in continuum wavelengths increases, and the band centers of some absorption bands shift to shorter wavelengths. In this paper we present the new absorption coefficient spectra along with an examination of the different temperature effects. These data should prove eminently valuable for analysis of near-infrared reflectance spectra of low-temperature icy surfaces, such as those of cold solar system objects, Asteroid Belt objects, Pluto and Charon, comet nuclei, and terrestrial snow- and ice-covered regions. The data should also be valuable for radiative transfer in clouds of ice particles in the atmospheres of planets.

PUBLICATIONS

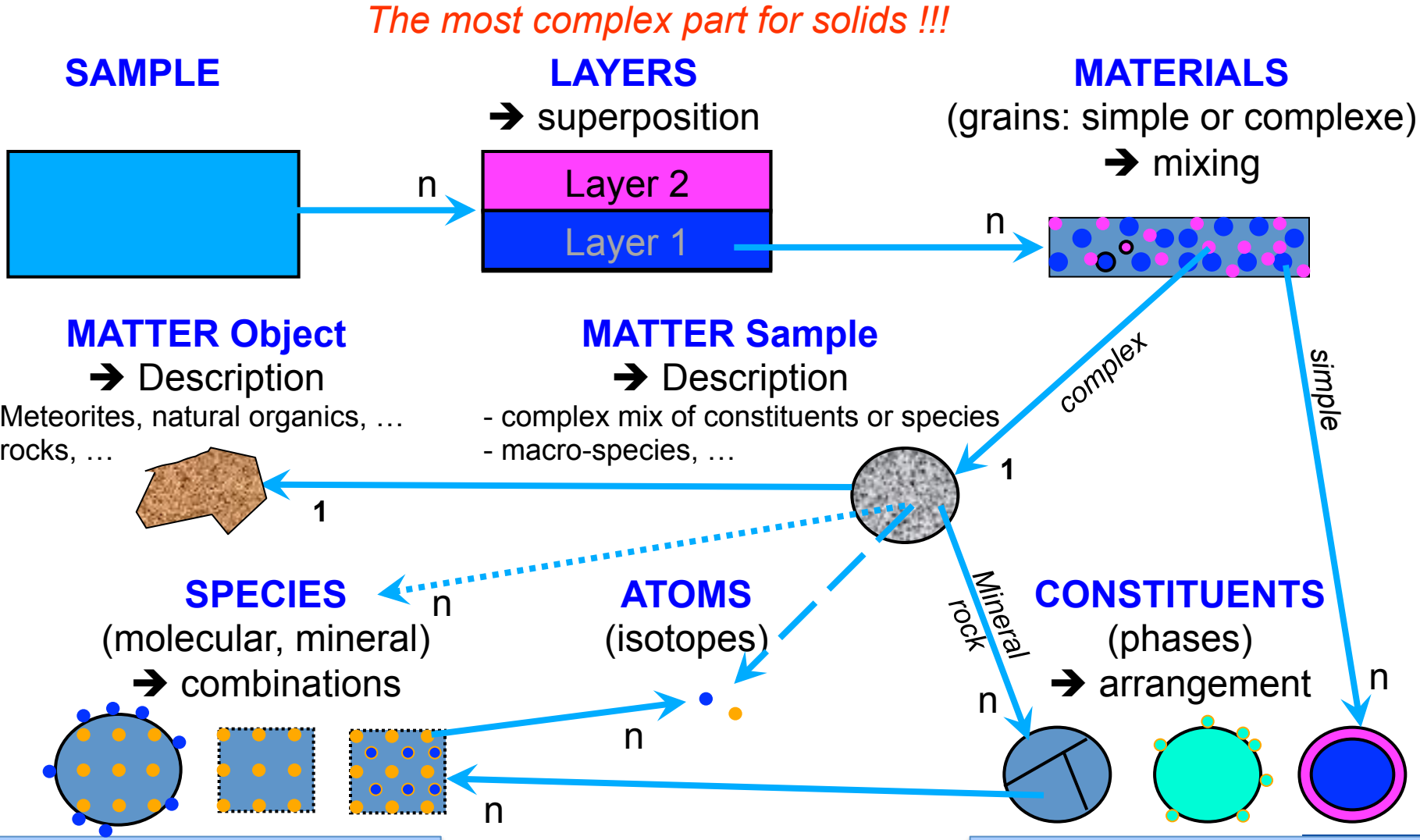
Virtual Observatory Paris Data Centre

infrastructure

SEVENTH FRAMEWORK PROGRAMME

Sample description

The most complex part for solids !!!



VAMDC Standards

http://vamdc.org/documents/standards/

VAMDC
Virtual Atomic and Molecular Data Centre

Documenting VAMDC standards

On the pages listed below you will find the specifications of standards currently used by the VAMDC. The next official release of standards is scheduled for July 2011.

Data access protocol, query language and dictionaries

- Data access protocol [v 11.05] [r 11.05]
- Query language [v 11.05] [r 11.05]
- Dictionaries [v 11.05] [r 11.05]

Data model

- VAMDC-XSAMS reference guide [v 0.2] [r 11.05]
- VAMDC-XSAMS changelog [v 0.2] [r 11.05]

- VAMDC-XSAMS schema files are available for download below.
- VAMDC-XSAMS schema documentation can be viewed in the browser or downloaded from below.
- Case-By-Case schema documentation can be viewed in the browser or downloaded from below.

Registry

Table Of Contents

Next topic

Data access protocol [v 11.05] [r 11.05]

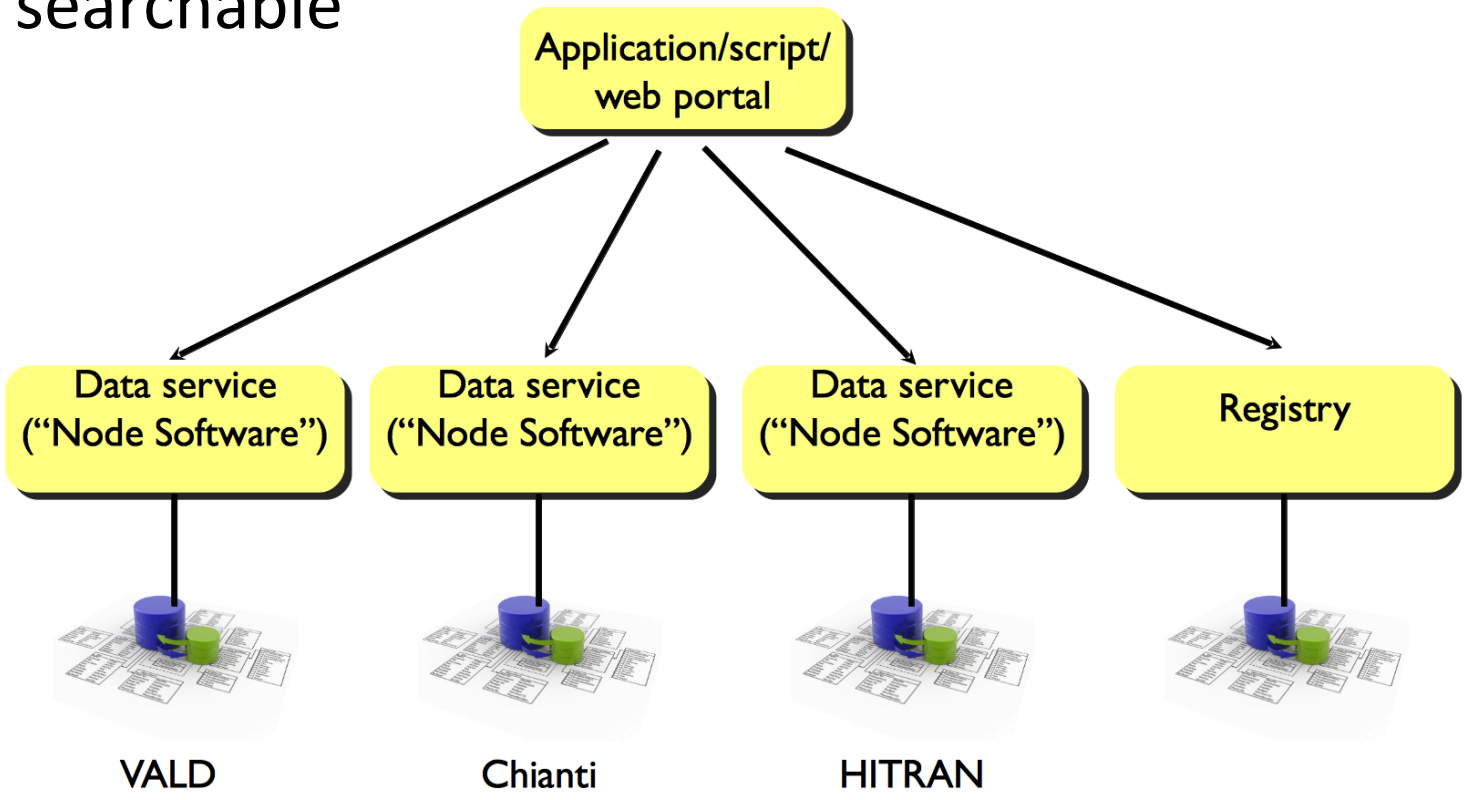
Quick search

Go

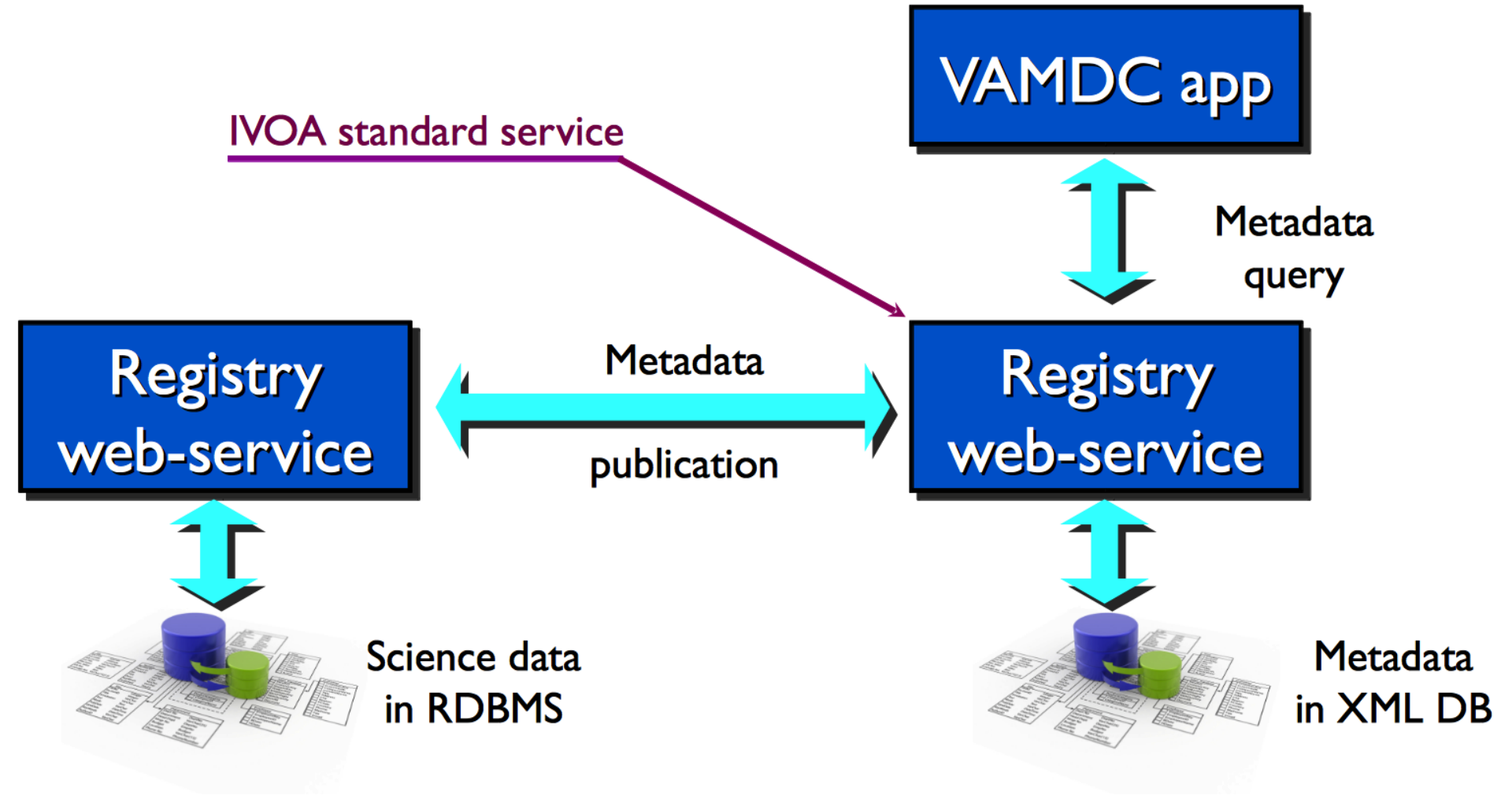
Enter search terms or a module, class or function name.

Deployment Strategy

- All data on the WWW
- Databases stay at their producers' sites
- All data searchable

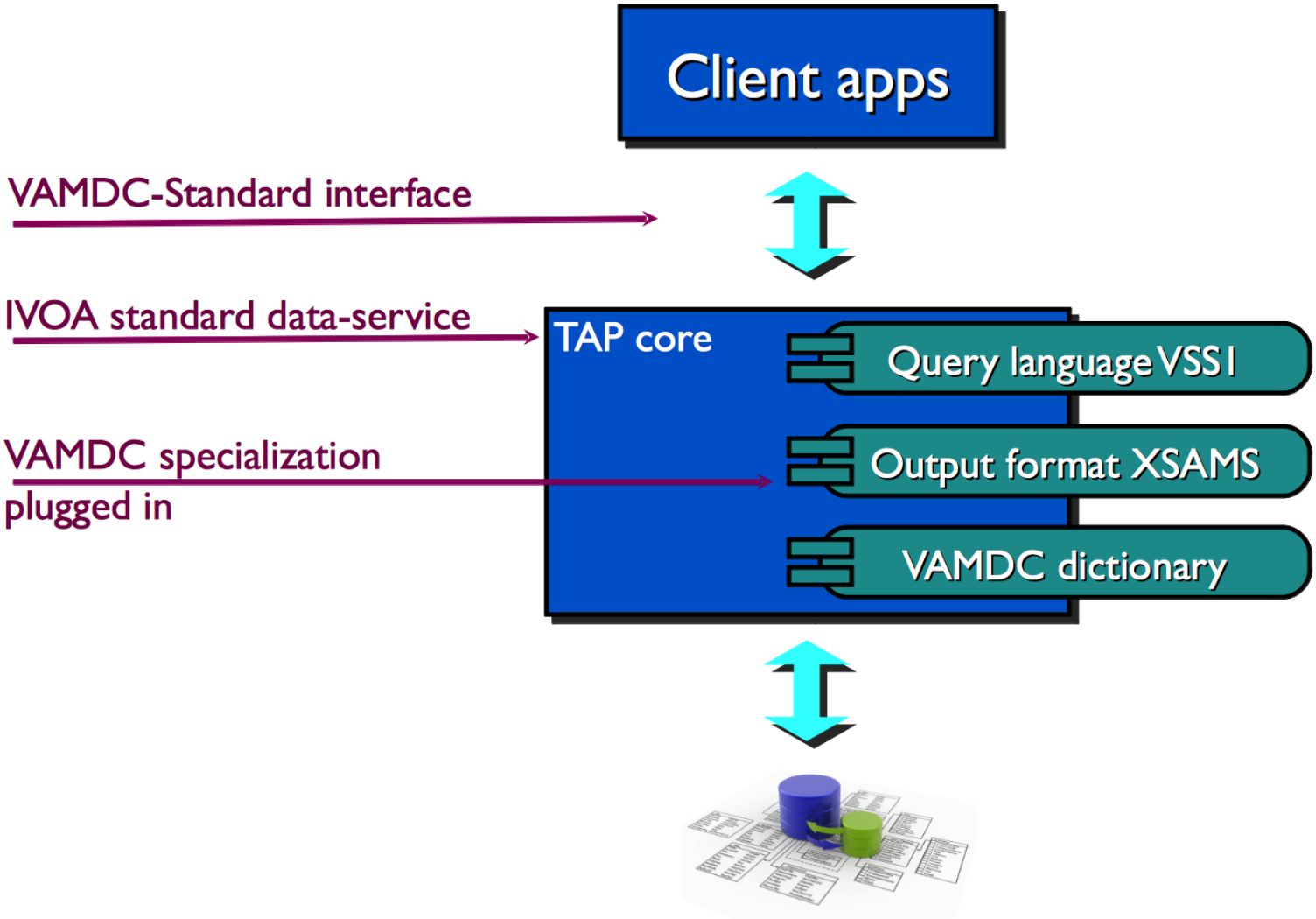


VAMDC Registry based on IVOA Registry Std



Data Access: TAP-XSAMS

Based on TAP standard



TAP-XSAMS

http://www.vamdc.eu/documents/standards/dataAccessProtocol/vamdctap.html

The VAMDC variant of the Table Access Protocol (TAP)

Many data-sets in VAMDC include information that can be rendered in the VAMDC-XSAMS data model. Data in that common model could be transformed to and from a table model which uses the same columns for all data-sets. If all the data-sets had this table model as part of the schemata of their databases, then a SQL query to that model would work on all data-sets, and the results could be written in a common format.

VAMDC-TAP is a protocol for data-access services that provide the common table model matching VAMDC-XSAMS and which can return the results of queries in VAMDC-XSAMS. VAMDC-TAP services accept queries in a restricted form of SQL (VSS1: VAMDC SQL Sub-set #1) and return results in VAMDC-XSAMS or in certain tabular formats. Implementations of VAMDC-TAP map queries from the common table-model to the actual schemata of their databases.

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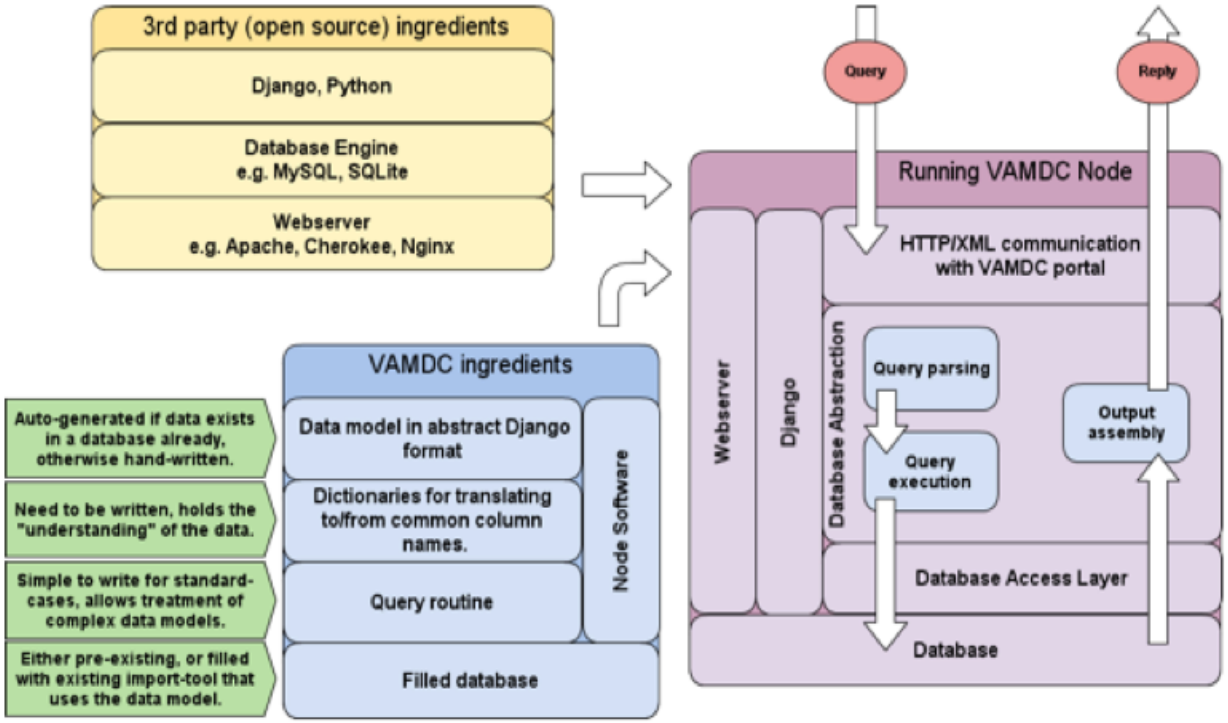
Previous topic

Step by Step Guides

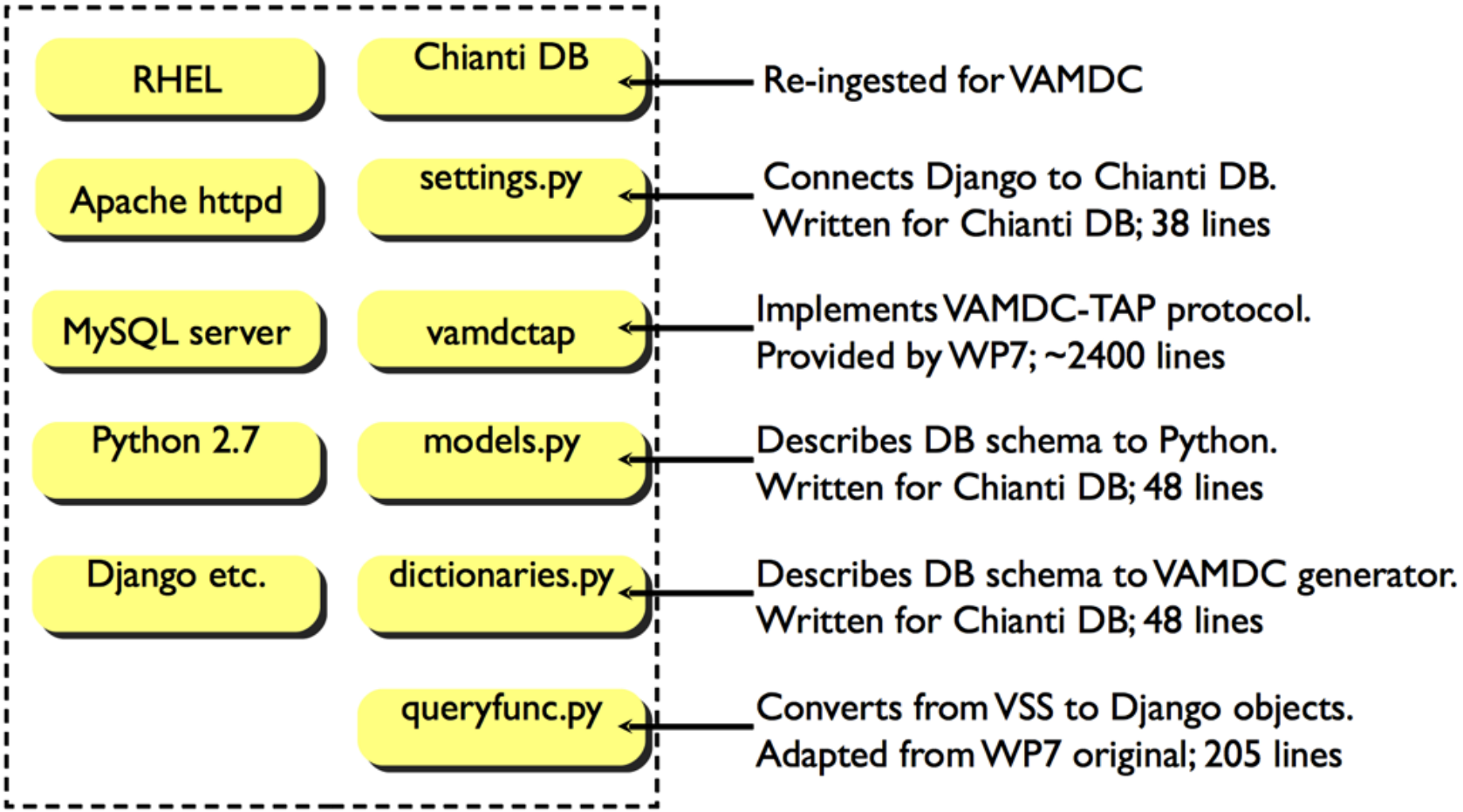
Step by step guide to a new VAMDC node

Let's have a look at the structural diagram from the *Introduction* once more:



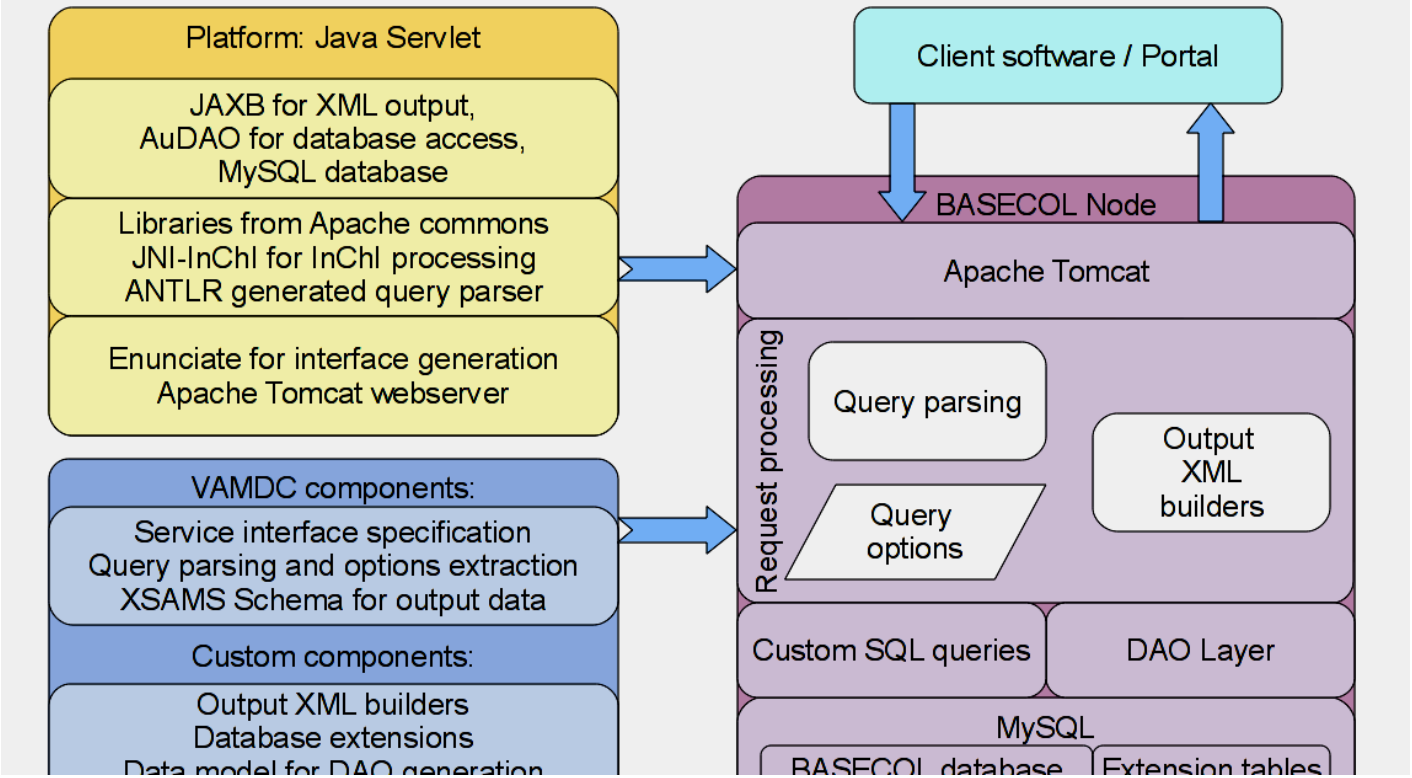
If you have followed the instructions of the page on *Software prerequisits and installation*, you are done with the yellow box in the figure. This page will tell you first how to configure and write the few code bits that your node needs before running (blue box), and then how to deploy the node and make it run as shown in the violet box.

Deployment stack at Data Node: an example with CHIANTI



VAMDC-BASECOL Java interface

M. Doronin, Paris



Comprehensive Deployment

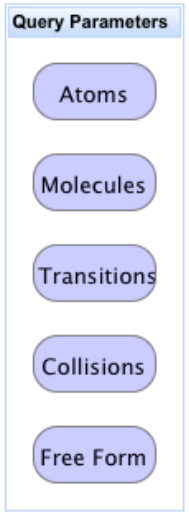
important early task to include most AM data

Data	Site	Software
VALD	Uppsala	WP7-Python
Chianti	Cambridge/MSSL	WP7-Python
CDMS	Koeln	WP7-Python
BASECOL	CNRS-LPMAA-LUTH	WP7-Java
KIDA	CNRS-LAB	WP7-Java
STSP/GhoSST	CNRS-LPG/IPAG	Custom
TipTopBase	CNRS - LERMA	WP7-Python
UDfA	QUB	WP7-Python
Lund	Uppsala	WP7-Python
Spectr-W3	VNIITF	WP7-Python
S&MPO	CNRS-GSMA	WP7-Python
CDSD	IAO	WP7-Python
HITRAN	UCL	WP7-Python
Methane lines	CNRS-ICB	WP7-Python
Ethylene	CNRS-GSMA	WP7-Python

VAMDC Virtual Atomic and Molecular Data Centre

VAMDC PORTAL

VAMDC Portal | Home | XSAMS Query Builder | Query Log

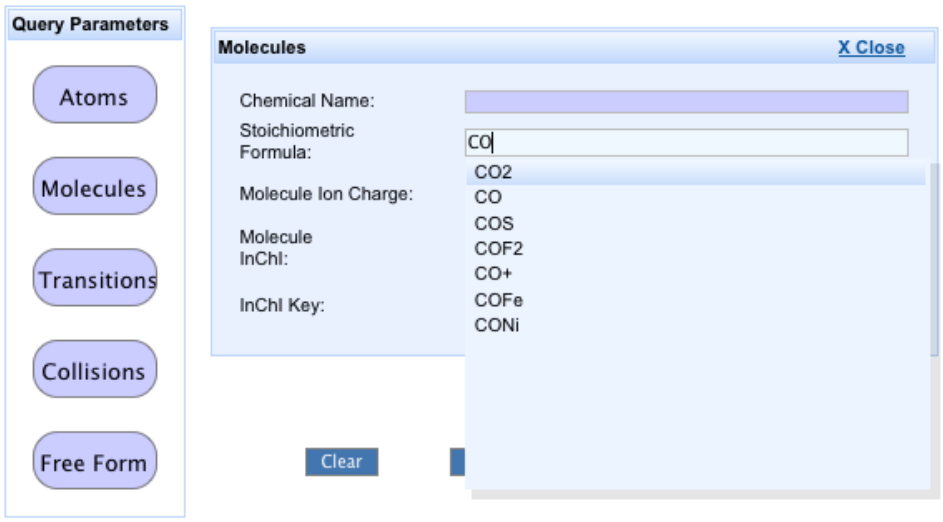


Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey moleculestoichiometricformula moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength atomsymbol

Common way of specifying a data extract
Standard web-service parameters
Common query language
Common dictionary of terms

VAMDC
Virtual Atomic and Molecular Data Centre

VAMDC Portal | Home | XSAMS Query Builder | Query Log



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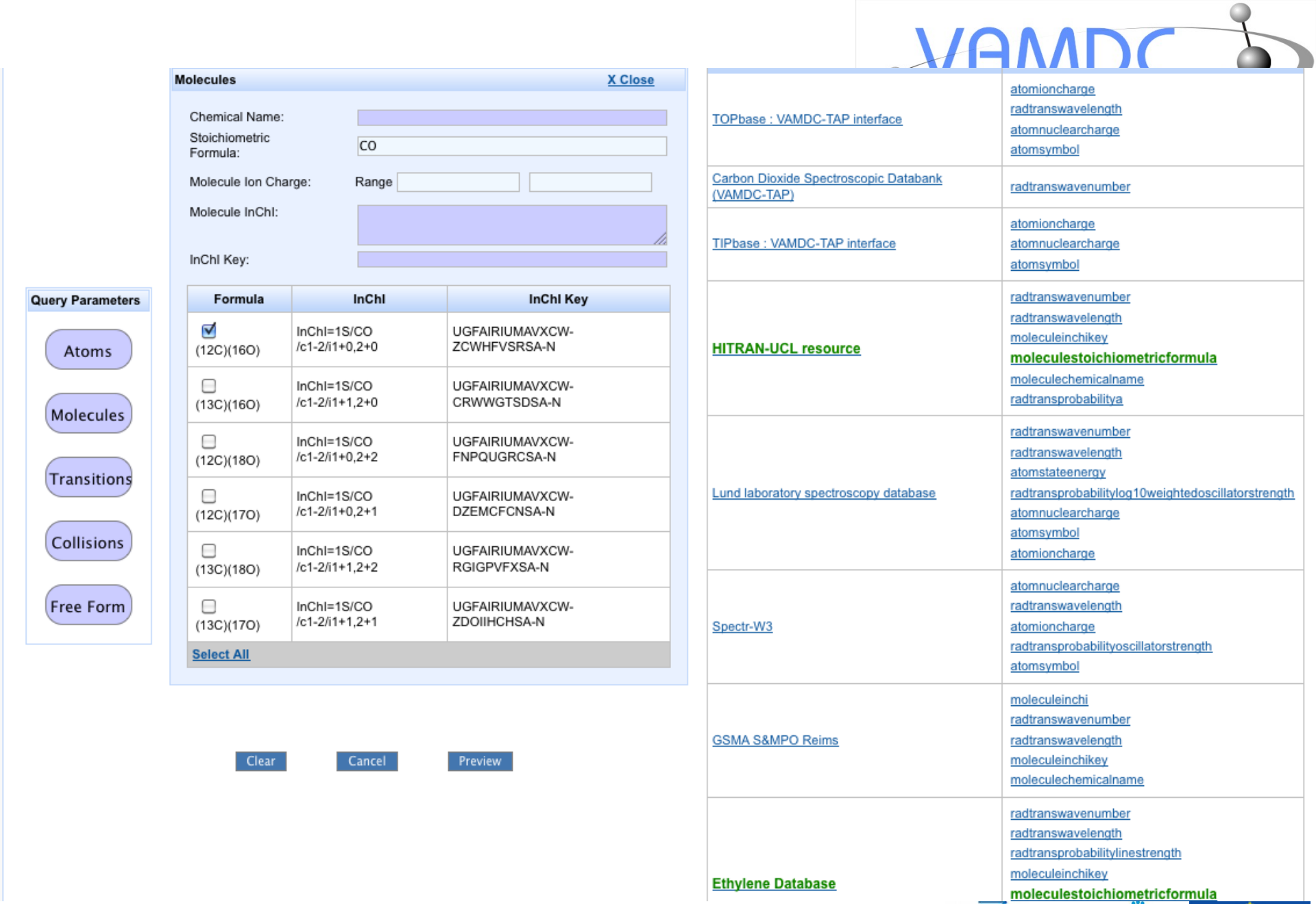
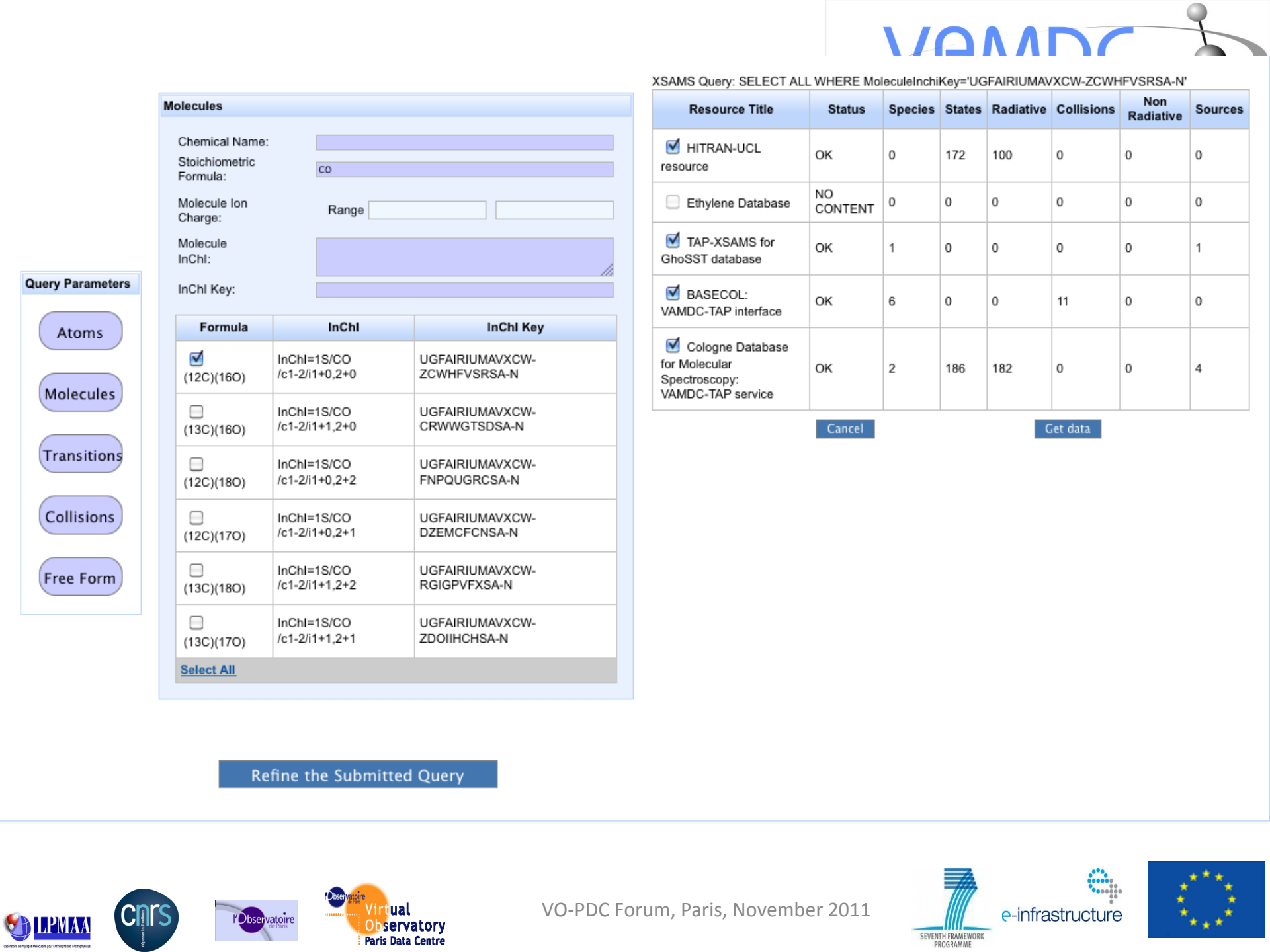
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength



TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength atomsymbol
GSMA S&MPO Reims	moleculeinchi radtranswavenumber radtranswavelength moleculeinchikey moleculechemicalname
Ethylene Database	radtranswavenumber radtranswavelength radtransprobabilitylinestrength moleculeinchikey **moleculestoichiometricformula**


Molecules
Chemical Name:
Stoichiometric Formula:
CO
Molecule Ion Charge:
Range
Molecule InChI:
InChI Key:
Formula
InChI
InChI Key
(12C)(16O)
InChI=1S/CO /c1-2/i1+0,2+0
UGFAIRIUMAVXCW-ZCWHFVSRSA-N
(13C)(16O)
InChI=1S/CO /c1-2/i1+1,2+0
UGFAIRIUMAVXCW-CRWWGTSDSA-N
(12C)(18O)
InChI=1S/CO /c1-2/i1+0,2+2
UGFAIRIUMAVXCW-FNPQUGRCSA-N
(12C)(17O)
InChI=1S/CO /c1-2/i1+0,2+1
UGFAIRIUMAVXCW-DZEMCFCNSA-N
(13C)(18O)
InChI=1S/CO /c1-2/i1+1,2+2
UGFAIRIUMAVXCW-RGIGPVFXSA-N
(13C)(17O)
InChI=1S/CO /c1-2/i1+1,2+1
UGFAIRIUMAVXCW-ZDOIIHCHSA-N
Select All
Query Parameters
Atoms
Molecules
Transitions
Collisions
Free Form
XSAMS Query: SELECT ALL WHERE MoleculeInchiKey='UGFAIRIUMAVXCW-ZCWHFVSRSA-N'
Resource Title
Status
Species
States
Radiative
Collisions
Non Radiative
Sources
HITRAN-UCL resource
OK
0
172
100
0
0
0
Ethylene Database
NO CONTENT
0
0
0
0
0
0
TAP-XSAMS for GhoSST database
OK
1
0
0
0
0
1
BASECOL: VAMDC-TAP interface
OK
6
0
0
11
0
0
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
OK
2
186
182
0
0
4
Cancel
Get data
Refine the Submitted Query

Query results: atomic and molecular states

(Switch to display of radiative transitions.)

Specie	Ion charge	State energy	Description	Quantum numbers	More information
Carbon Monoxide - CO		0.0 1/cm		Label=X^1\Sigma^+, v=0, J=0, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		3.845033 1/cm		Label=X^1\Sigma^+, v=0, J=1, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		11.534953 1/cm		Label=X^1\Sigma^+, v=0, J=2, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		23.069466 1/cm		Label=X^1\Sigma^+, v=0, J=3, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		38.448131 1/cm		Label=X^1\Sigma^+, v=0, J=4, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		57.67036 1/cm		Label=X^1\Sigma^+, v=0, J=5, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		80.735419 1/cm		Label=X^1\Sigma^+, v=0, J=6, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		107.642427 1/cm		Label=X^1\Sigma^+, v=0, J=7, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		138.390355 1/cm		Label=X^1\Sigma^+, v=0, J=8, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		172.978029 1/cm		Label=X^1\Sigma^+, v=0, J=9, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		211.404127 1/cm		Label=X^1\Sigma^+, v=0, J=10, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		253.667181 1/cm		Label=X^1\Sigma^+, v=0, J=11, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		299.765576 1/cm		Label=X^1\Sigma^+, v=0, J=12, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		349.69755 1/cm		Label=X^1\Sigma^+, v=0, J=13, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		403.461194 1/cm		Label=X^1\Sigma^+, v=0, J=14, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		461.054454 1/cm		Label=X^1\Sigma^+, v=0, J=15, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		522.475129 1/cm		Label=X^1\Sigma^+, v=0, J=16, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		587.720871 1/cm		Label=X^1\Sigma^+, v=0, J=17, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		656.789186 1/cm		Label=X^1\Sigma^+, v=0, J=18, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		729.677434 1/cm		Label=X^1\Sigma^+, v=0, J=19, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		806.382828 1/cm		Label=X^1\Sigma^+, v=0, J=20, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		886.902435 1/cm		Label=X^1\Sigma^+, v=0, J=21, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		971.233178 1/cm		Label=X^1\Sigma^+, v=0, J=22, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1059.371831 1/cm		Label=X^1\Sigma^+, v=0, J=23, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1151.315024 1/cm		Label=X^1\Sigma^+, v=0, J=24, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1247.059241 1/cm		Label=X^1\Sigma^+, v=0, J=25, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1346.60082 1/cm		Label=X^1\Sigma^+, v=0, J=26, F1=, F2=, parity=, symmetry=	Detail

Available data for selected state

Specie

Structural formula: CO

Stoichiometric formula: CO

Molecule name: Carbon Monoxide

InChI: 1S/CO/c1-2/i1+0,2+0 (UGFAIRIUMAVXCW-ZCWHFVSRSA-N)

State

State description:

State energy above ground state: 38.448131 1/cm

Total statistical weight: 9

Quantum description of state as closed-shell, diatomic molecule: Label=X^1\Sigma^+, v=0, J=4, F1=, F2=, parity=, symmetry=

Closed-shell, diatomic molecules

- case prefix: dcs
- case ID: 1

`ElecStateLabel`

XML Element
`dcs:ElecStateLabel`

Description
`ElecStateLabel` is a label identifying the electronic state: X, A, a, B, etc..

Attributes
None

Restrictions
string

v

XML Element
`dcs:v`

Description
v is the vibrational quantum number.

Attributes
None

Restrictions
non-negative integer

J

XML Element
`dcs:J`

Query results: radiative transitions

(Switch to display of states.)

Specie	Ion charge	λ/ν/n/E	Probability	Initial state	Final state
Carbon Monoxide - CO		ν=115271.2021 MHz	A=7.20378864479e-08 1/cm $\log_{10}$gf=-5.0105	- 0.0 1/cm	- 3.845033 1/cm
Carbon Monoxide - CO		ν=230538.0 MHz	A=6.91079000503e-07 1/cm $\log_{10}$gf=-4.1197	- 3.845033 1/cm	- 11.534953 1/cm
Carbon Monoxide - CO		ν=345795.9899 MHz	A=2.49670085538e-06 1/cm $\log_{10}$gf=-3.6118	- 11.534953 1/cm	- 23.069466 1/cm
Carbon Monoxide - CO		ν=461040.7681 MHz	A=6.12668117242e-06 1/cm $\log_{10}$gf=-3.2657	- 23.069466 1/cm	- 38.448131 1/cm
Carbon Monoxide - CO		ν=576267.931 MHz	A=1.22134274135e-05 1/cm $\log_{10}$gf=-3.0118	- 38.448131 1/cm	- 57.67036 1/cm
Carbon Monoxide - CO		ν=691473.076 MHz	A=2.13750692698e-05 1/cm $\log_{10}$gf=-2.8193	- 57.67036 1/cm	- 80.735419 1/cm
Carbon Monoxide - CO		ν=806651.8008 MHz	A=3.42239824576e-05 1/cm $\log_{10}$gf=-2.6716	- 80.735419 1/cm	- 107.642427 1/cm
Carbon Monoxide - CO		ν=921799.7039 MHz	A=5.13419191151e-05 1/cm $\log_{10}$gf=-2.559	- 107.642427 1/cm	- 138.390355 1/cm
Carbon Monoxide - CO		ν=1036912.3846 MHz	A=7.33007011041e-05 1/cm $\log_{10}$gf=-2.4751	- 138.390355 1/cm	- 172.978029 1/cm
Carbon Monoxide - CO		ν=1151985.4434 MHz	A=0.000100638923207 1/cm $\log_{10}$gf=-2.4156	- 172.978029 1/cm	- 211.404127 1/cm
Carbon Monoxide - CO		ν=1267014.4817 MHz	A=0.000133903406762 1/cm $\log_{10}$gf=-2.3773	- 211.404127 1/cm	- 253.667181 1/cm
Carbon Monoxide - CO		ν=1381995.1022 MHz	A=0.000173532853014 1/cm $\log_{10}$gf=-2.3581	- 253.667181 1/cm	- 299.765576 1/cm
Carbon Monoxide - CO		ν=1496922.9091 MHz	A=0.000220040322442 1/cm $\log_{10}$gf=-2.3561	- 299.765576 1/cm	- 349.69755 1/cm
Carbon Monoxide - CO		ν=1611793.5079 MHz	A=0.00027390476357 1/cm $\log_{10}$gf=-2.3699	- 349.69755 1/cm	- 403.461194 1/cm
Carbon Monoxide - CO		ν=1726602.5057 MHz	A=0.000335356678509 1/cm $\log_{10}$gf=-2.3987	- 403.461194 1/cm	- 461.054454 1/cm
Carbon Monoxide - CO		ν=1841345.5116 MHz	A=0.000404993044566 1/cm $\log_{10}$gf=-2.4413	- 461.054454 1/cm	- 522.475129 1/cm
Carbon Monoxide - CO		ν=1956018.1363 MHz	A=0.000482878531678 1/cm $\log_{10}$gf=-2.4973	- 522.475129 1/cm	- 587.720871 1/cm
Carbon Monoxide - CO		ν=2070615.9924 MHz	A=0.000569495347659 1/cm $\log_{10}$gf=-2.5659	- 587.720871 1/cm	- 656.789186 1/cm
Carbon Monoxide - CO		ν=2185134.6949 MHz	A=0.000664985100589 1/cm $\log_{10}$gf=-2.6467	- 656.789186 1/cm	- 729.677434 1/cm
Carbon Monoxide - CO		ν=2299569.8609 MHz	A=0.000769499240577 1/cm $\log_{10}$gf=-2.7393	- 729.677434 1/cm	- 806.382828 1/cm
Carbon Monoxide - CO		ν=2413917.1097 MHz	A=0.000883246473397 1/cm $\log_{10}$gf=-2.8433	- 806.382828 1/cm	- 886.902435 1/cm

VAMDC Portal Home XSAMS Query Builder Query Log

Query Parameters

Atoms

Molecules

Transitions

Collisions

Free Form

Atoms X Close

Atomic (elemental) symbol:

Atom Inchi:

Atom Inchi Key:

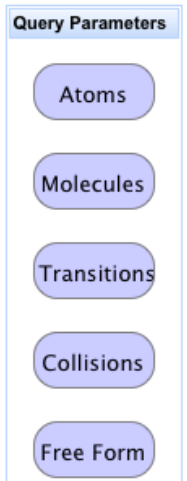
Atom Mass Number: Range

Atom Ion Charge: Range

Atom Nuclear Charge: Range

Clear Cancel Preview

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey moleculestoichiometricformula moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength



Transitions X Close

RadTransWavelength: From / To / Units Å

RadTransFrequency: From / To / Units Hz

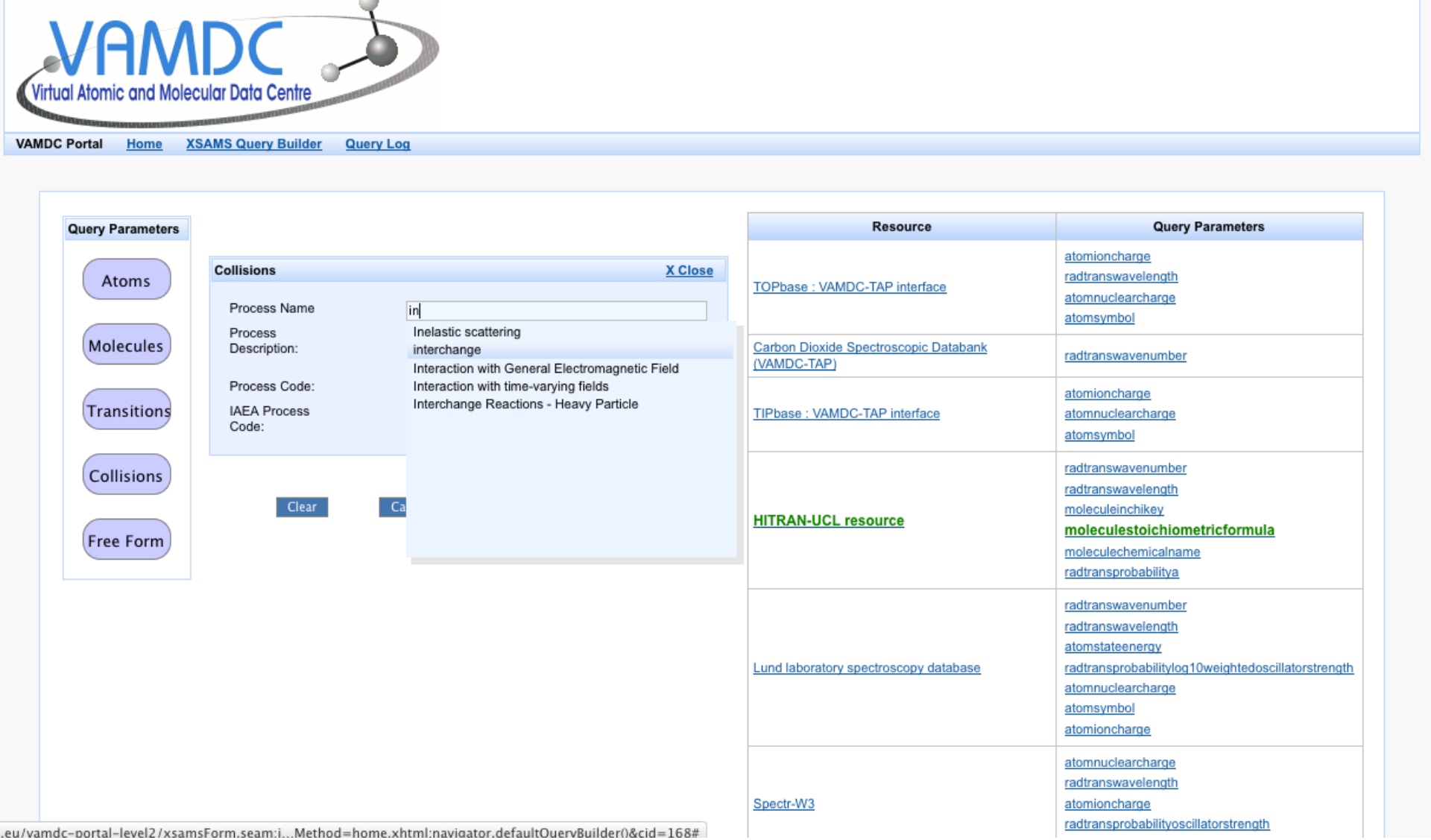
RadTransEnergy: From / To / Units eV

RadTransWavenumber: From / To / Units 1/cm

Initial State Energy: From / To / Units eV

RadTransProbabilityA: From / To / Units 1/s

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey moleculestoichiometricformula moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength atomsymbol
GSMA S&MPO Reims	moleculeinchi radtranswavenumber radtranswavelength moleculeinchikey moleculechemicalname

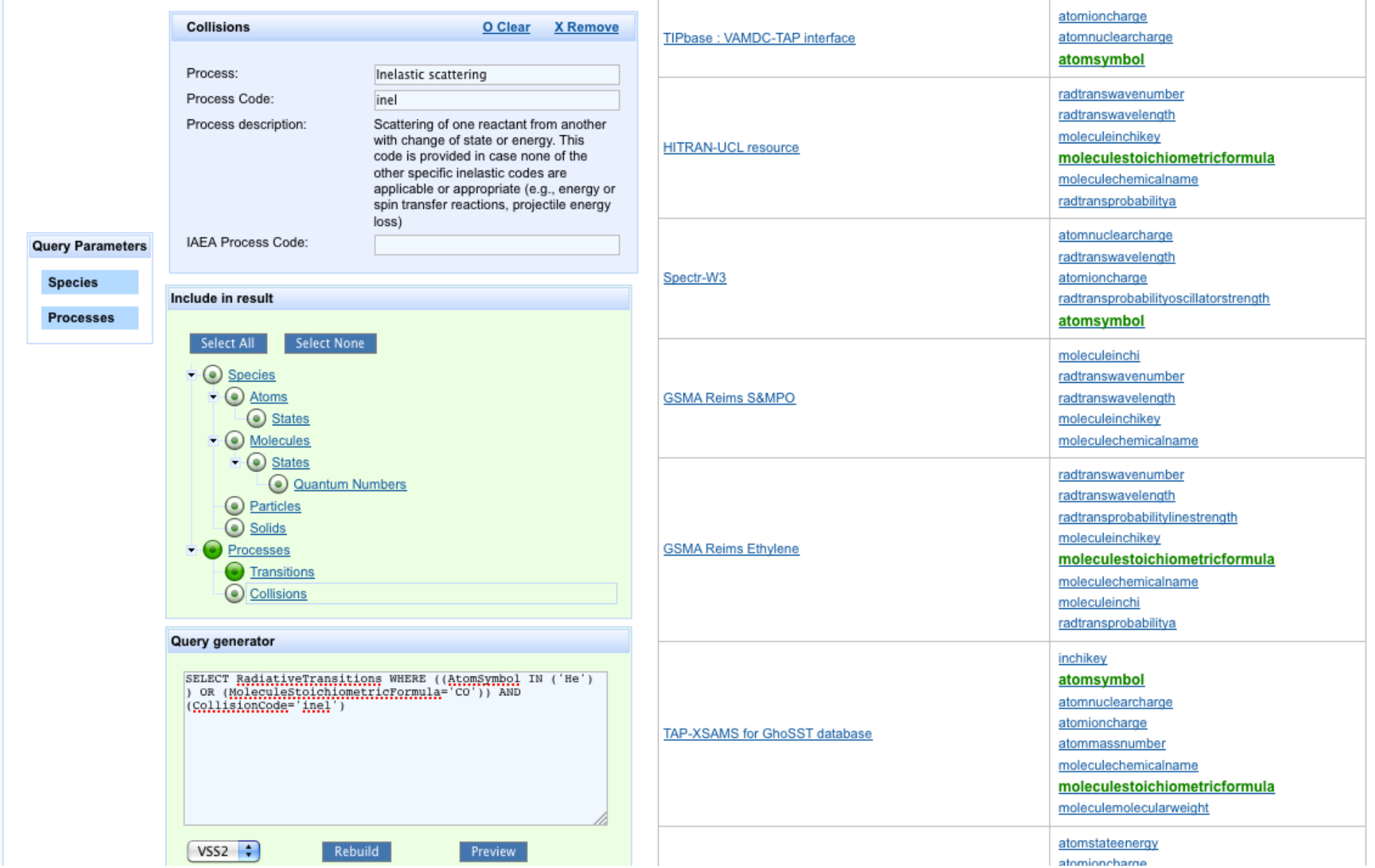


Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength

VSS2 : Level-3

Resource	Query Parameters
BASECOL: development VAMDC-TAP interface	atomsymbol collisioncode inchikey moleculeinchikey moleculestoichiometricformula moleculestateenergy moleculestatenuclearspinisomer sourceyear temperature
KIDA: VAMDC-TAP interface	moleculeioncharge moleculechemicalname moleculeinchi moleculeinchikey moleculeioncharge moleculestoichiometricformula atomsymbol
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
	radtranswavenumber

Resource	Query Parameters
BASECOL: development VAMDC-TAP interface	**atomsymbol** collisioncode inchikey moleculeinchikey **moleculestoichiometricformula** moleculestateenergy moleculestatenuclearspinisomer sourceyear temperature
KIDA: VAMDC-TAP interface	moleculeioncharge moleculechemicalname moleculeinchi moleculeinchikey moleculeioncharge **moleculestoichiometricformula** **atomsymbol**
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge **atomsymbol**
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge **atomsymbol**
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength **atomsymbol**


Collisions
O Clear
X Remove
Process:
Inelastic scattering
Process Code:
inel
Process description:
Scattering of one reactant from another with change of state or energy. This code is provided in case none of the other specific inelastic codes are applicable or appropriate (e.g., energy or spin transfer reactions, projectile energy loss)
IAEA Process Code:
Query Parameters
Species
Processes
Include in result
Select All
Select None
Species
Atoms
States
Molecules
States
Quantum Numbers
Particles
Solids
Processes
Transitions
Collisions
Query generator
SELECT RadiativeTransitions WHERE ((AtomSymbol IN ('He')
) OR (MoleculeStoichiometricFormula='CO')) AND
(CollisionCode='inel')
VSS2
Rebuild
Preview
TIPbase : VAMDC-TAP interface
atomioncharge
atomnuclearcharge
atomsymbol
HITRAN-UCL resource
radtranswavenumber
radtranswavelength
moleculeinchikey
moleculestoichiometricformula
moleculechemicalname
radtransprobabilitya
Spectr-W3
atomnuclearcharge
radtranswavelength
atomioncharge
radtransprobabilityoscillatorstrength
atomsymbol
GSMA Reims S&MPO
moleculeinchi
radtranswavenumber
radtranswavelength
moleculeinchikey
moleculechemicalname
GSMA Reims Ethylene
radtranswavenumber
radtranswavelength
radtransprobabilitylinestrength
moleculeinchikey
moleculestoichiometricformula
moleculechemicalname
moleculeinchi
radtransprobabilitya
TAP-XSAMS for GhoSST database
inchikey
atomsymbol
atomnuclearcharge
atomioncharge
atommassnumber
moleculechemicalname
moleculestoichiometricformula
moleculemolecularweight
atomstateenergy

VAMDC Portal Home XSAMS Query Builder Query Log

Atoms

Atomic (elemental) symbol: He
Atom Inchi:
Atom Inchi Key:
Atom Mass Number: Range
Atom Ion Charge: Range
Atom Nuclear Charge: Range
VSS2 Prefix: prefix index 2

Molecules

Chemical Name:
Stoichiometric Formula: CO
Molecule InChI:
Molecule InChI Key:
VSS2 Prefix: prefix index 1

Collisions

Process: Inelastic scattering
Process Code: inel

Resource Title	Direct download	Status	Species	States	Radiative	Collisions	Non Radiative	Sources
☑ BASECOL: development VAMDC-TAP interface	download	OK	7	0	0	59	0	0
☑ BASECOL: VAMDC-TAP interface	download	OK	7	0	0	59	0	0

Get data

VAMDC Portal Home XSAMS Query Builder Query Log

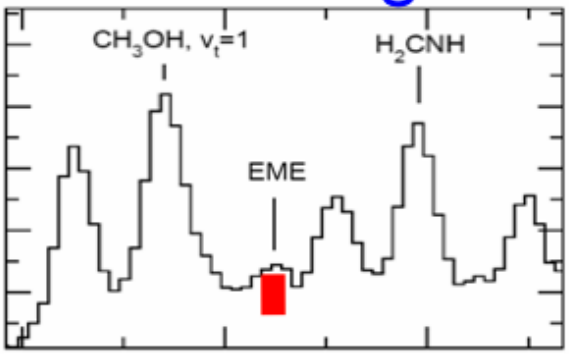
Query	Resource	
SELECT RadiativeTransitions WHERE ((AtomSymbol IN ('He')) OR (MoleculeStoichiometricFormula='CO')) AND (CollisionCode='inel')	http://batz.lpma.jussieu.fr:8080/tapservice/TAP/sync?REQUEST=doQuery&LANG=VSS2&FORMAT=XSAMS&QUERY=SELECT+RadiativeTransitions+WHERE+%28%28AtomSymbol+IN+%28%27He%27%29+%29+OR+%28MoleculeStoichiometricFormula%3D%27CO%27%29%29+AND+%28CollisionCode%3D%27inel%27%29	Executing

OK

Resource Title	Direct download	Status	Species	States	Radiative	Collisions	Non Radiative	Sources
☐ BASECOL: development VAMDC-TAP interface	download	OK	7	0	0	59	0	0
☑ BASECOL: VAMDC-TAP interface	download	OK	7	0	0	59	0	0

Get data

Understanding the Language of Interstellar Molecules

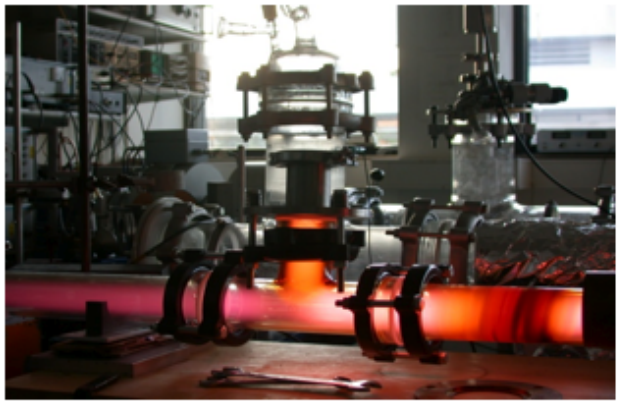


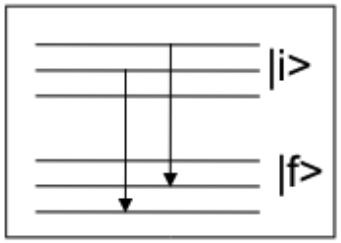
Observations
+
Modelling

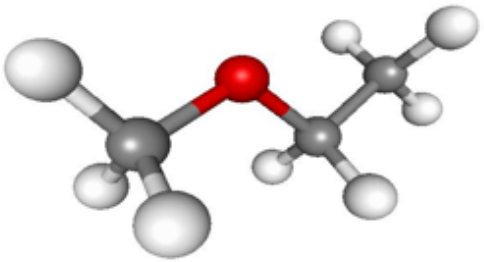
CDMS + JPL
BASECOL + KIDA

Laboratory expriments

Quantum Chemistry







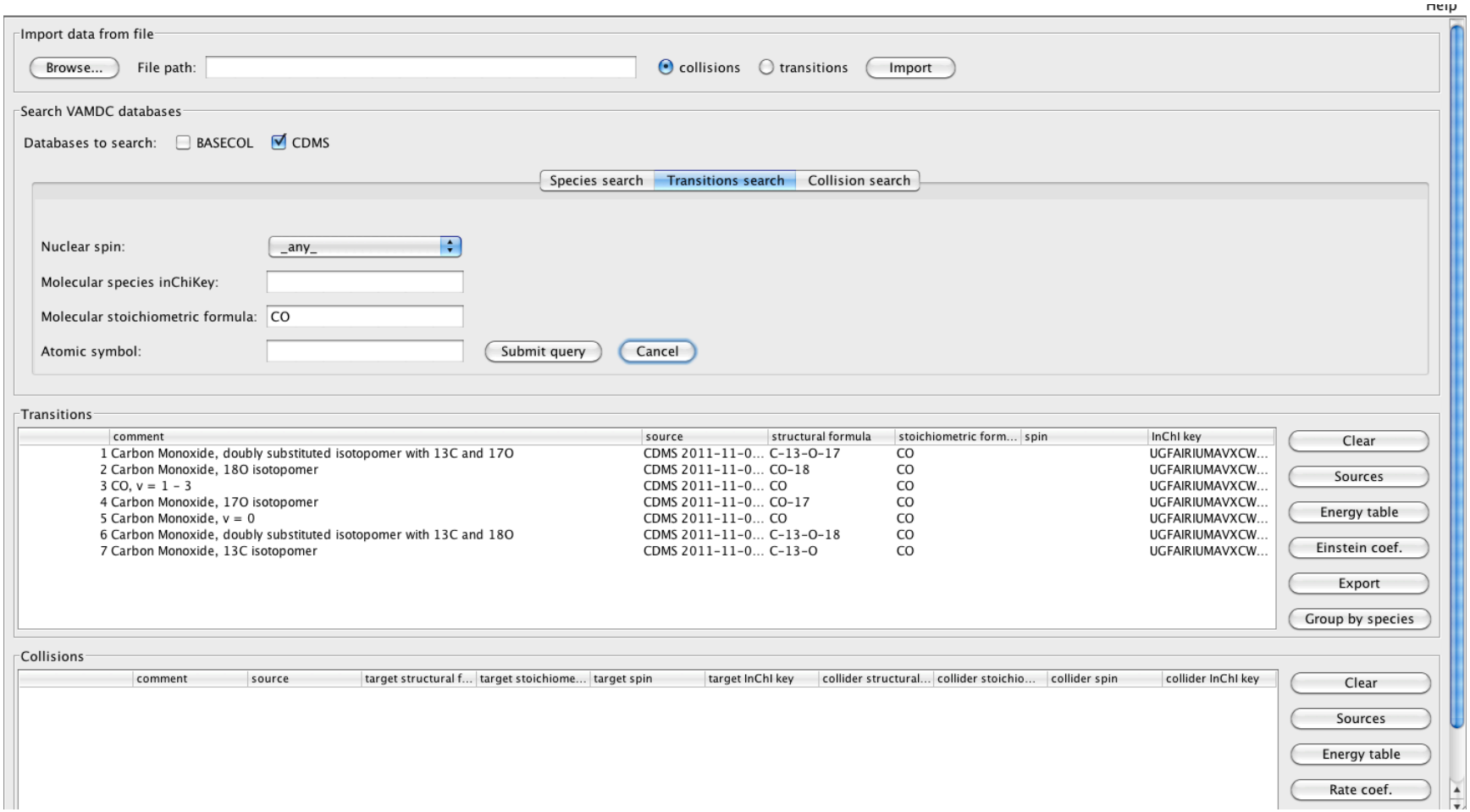
Courtesy of Stephan Schlemmer

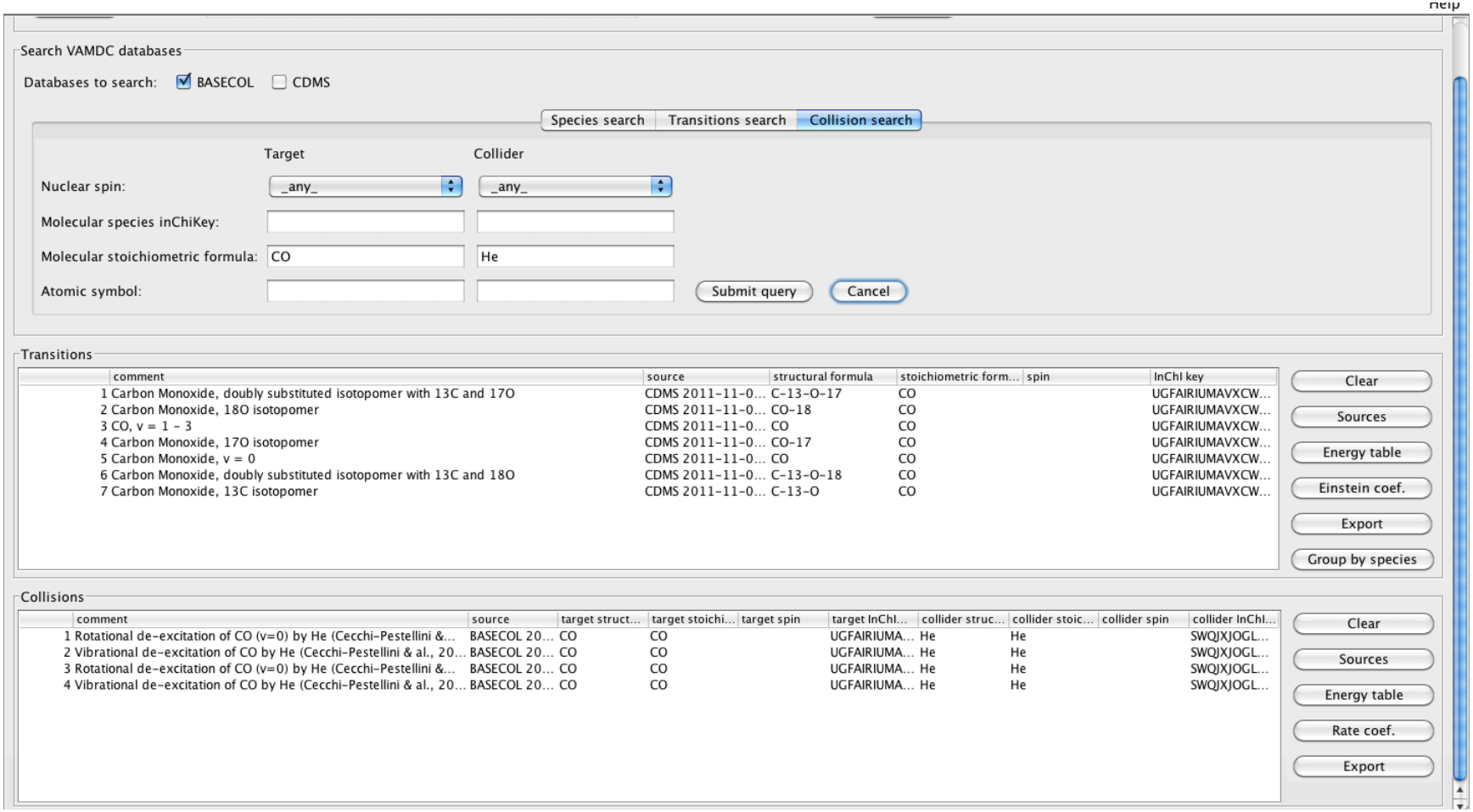
Work packages – Joint Research Activities

8. New mining and Integration Tools
   - tools for manipulation of data, e.g. cross-matching data from different databases
   - advanced data mining services: data access work flows targeted at specific user groups, e.g. solar physics, astrochemistry

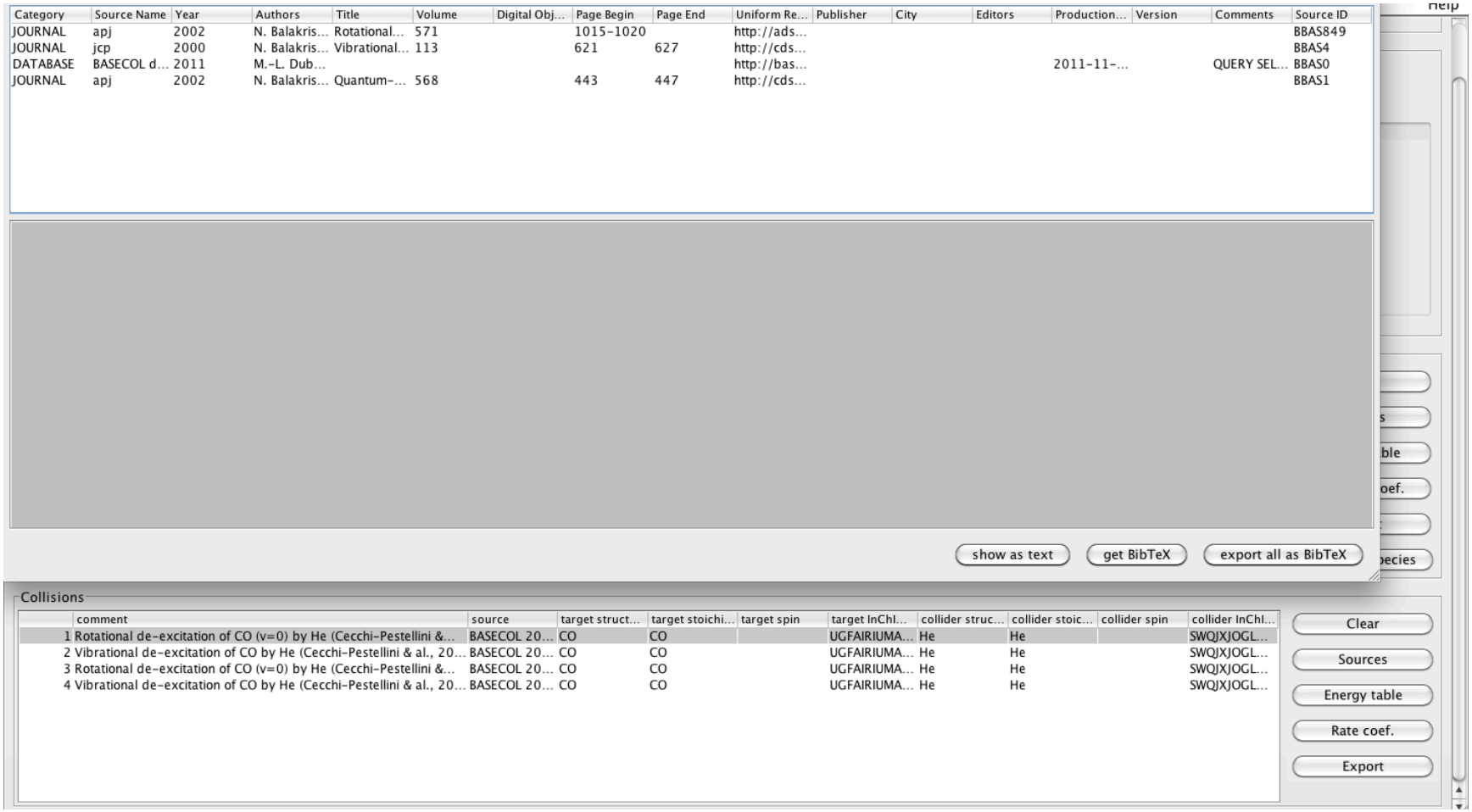
SPECTCOL Tool

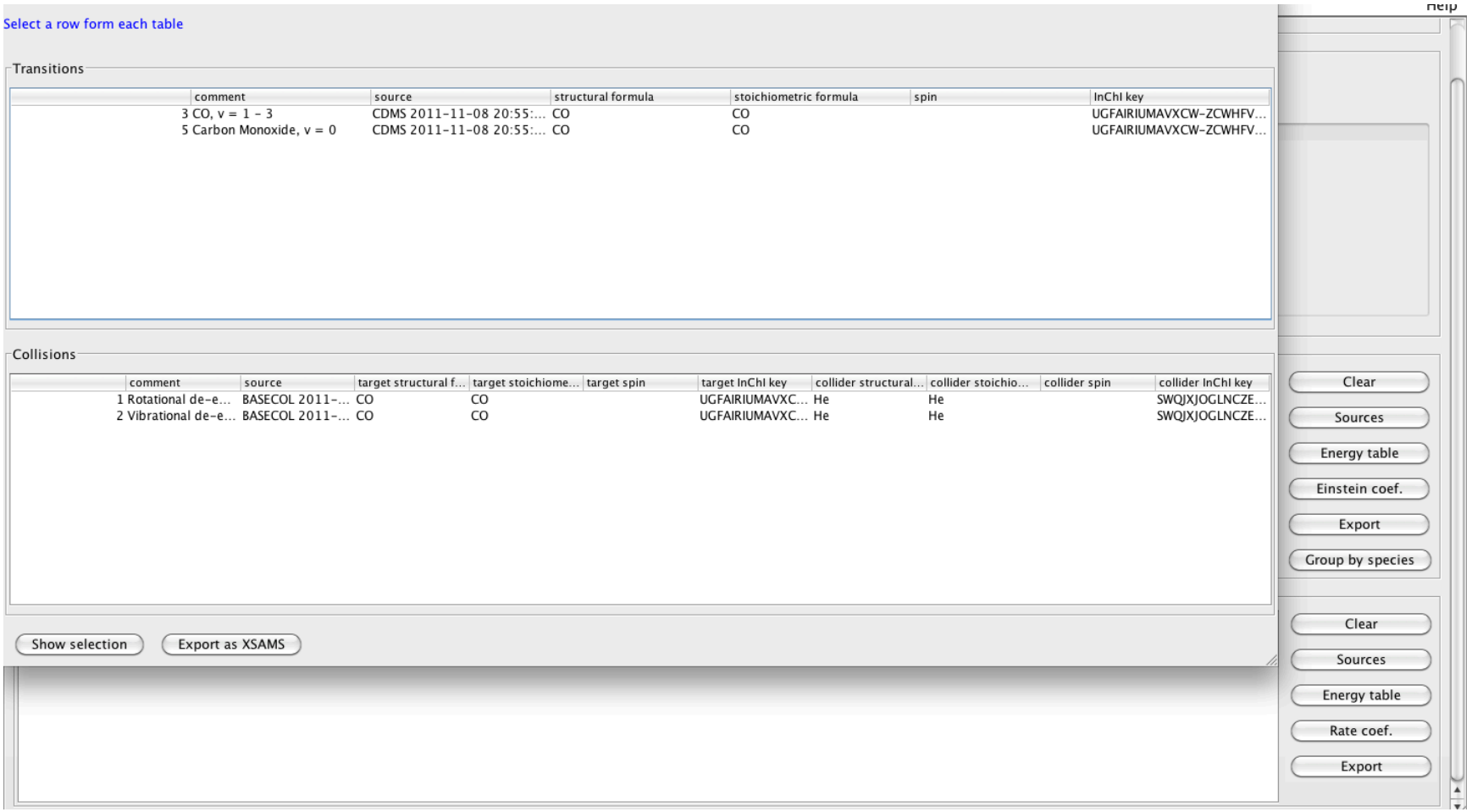
- Handles
  - VAMDC-XSAMS files from different databases
  - Matching and Cross-Federation of Spectroscopic data and Collisional Data From Different Databases
- Spectroscopic Data
  - Species, Energy Tables, Frequencies, Einstein Coefficients (CDMS for now), Sources
- Collisional Data
  - Species, Energy Tables (not the same), Rate Coefficients

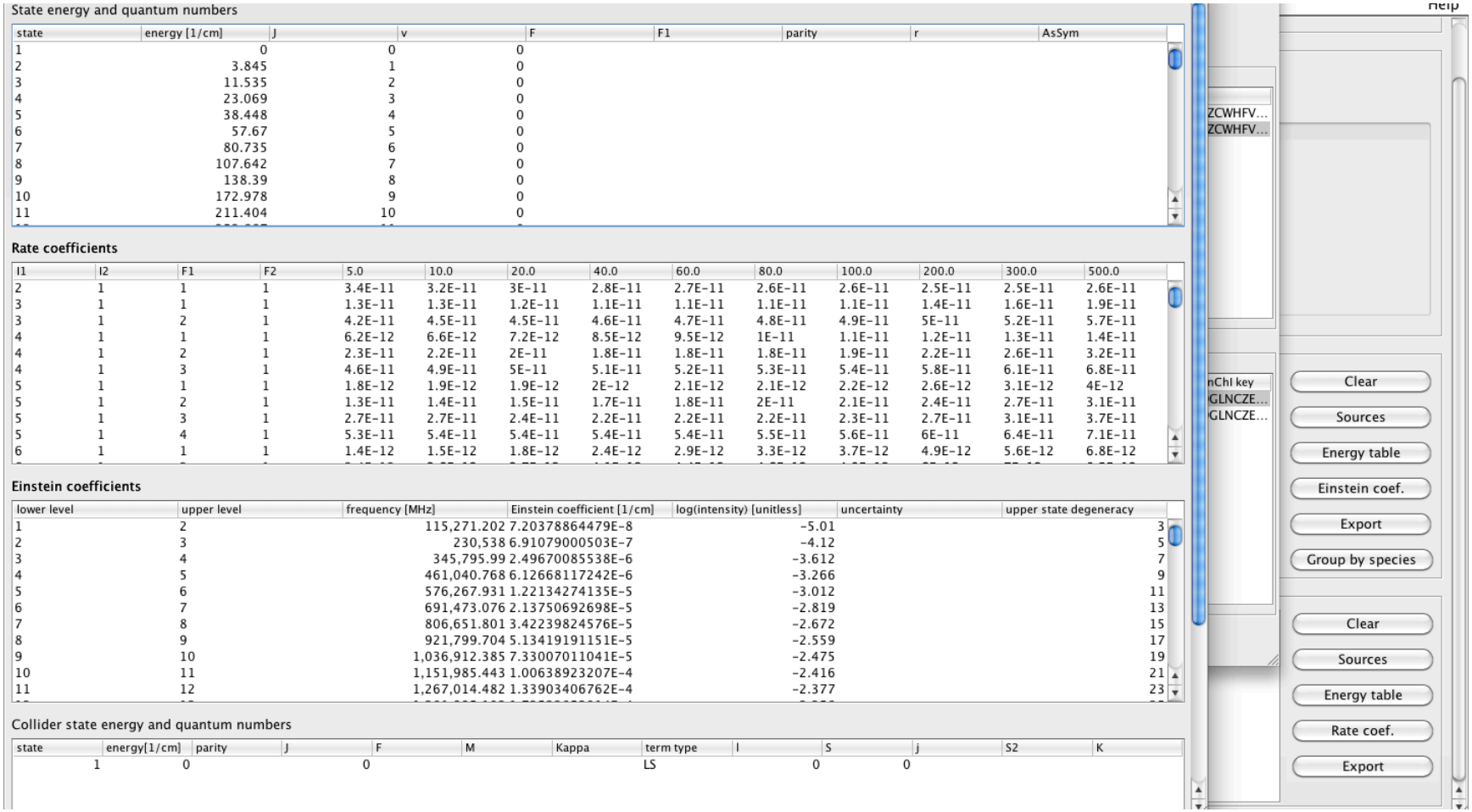

Help
Import data from file
Browse...
File path:
collisions
transitions
Import
Search VAMDC databases
Databases to search:
BASECOL
CDMS
Species search
Transitions search
Collision search
Nuclear spin:
any
Molecular species inChiKey:
Molecular stoichiometric formula:
CO
Atomic symbol:
Submit query
Cancel
Transitions
comment
source
structural formula
stoichiometric form...
spin
InChI key
1 Carbon Monoxide, doubly substituted isotopomer with 13C and 17O
CDMS 2011-11-0... C-13-O-17
CO
UGFAIRIUMAVXCW...
2 Carbon Monoxide, 18O isotopomer
CDMS 2011-11-0... CO-18
CO
UGFAIRIUMAVXCW...
3 CO, v = 1 - 3
CDMS 2011-11-0... CO
CO
UGFAIRIUMAVXCW...
4 Carbon Monoxide, 17O isotopomer
CDMS 2011-11-0... CO-17
CO
UGFAIRIUMAVXCW...
5 Carbon Monoxide, v = 0
CDMS 2011-11-0... CO
CO
UGFAIRIUMAVXCW...
6 Carbon Monoxide, doubly substituted isotopomer with 13C and 18O
CDMS 2011-11-0... C-13-O-18
CO
UGFAIRIUMAVXCW...
7 Carbon Monoxide, 13C isotopomer
CDMS 2011-11-0... C-13-O
CO
UGFAIRIUMAVXCW...
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Collisions
comment
source
target structural f...
target stoichiome...
target spin
target InChI key
collider structural...
collider stoichio...
collider spin
collider InChI key
Clear
Sources
Energy table
Rate coef.


Help
Search VAMDC databases
Databases to search: BASECOL CDMS
Species search
Transitions search
Collision search
Target
Collider
Nuclear spin:
any
any
Molecular species inChiKey:
Molecular stoichiometric formula:
CO
He
Atomic symbol:
Submit query
Cancel
Transitions
comment
source
structural formula
stoichiometric form...
spin
InChI key
1 Carbon Monoxide, doubly substituted isotopomer with 13C and 17O
CDMS 2011-11-0... C-13-O-17
CO
UGFAIRIUMAVXCW...
2 Carbon Monoxide, 18O isotopomer
CDMS 2011-11-0... CO-18
CO
UGFAIRIUMAVXCW...
3 CO, v = 1 - 3
CDMS 2011-11-0... CO
CO
UGFAIRIUMAVXCW...
4 Carbon Monoxide, 17O isotopomer
CDMS 2011-11-0... CO-17
CO
UGFAIRIUMAVXCW...
5 Carbon Monoxide, v = 0
CDMS 2011-11-0... CO
CO
UGFAIRIUMAVXCW...
6 Carbon Monoxide, doubly substituted isotopomer with 13C and 18O
CDMS 2011-11-0... C-13-O-18
CO
UGFAIRIUMAVXCW...
7 Carbon Monoxide, 13C isotopomer
CDMS 2011-11-0... C-13-O
CO
UGFAIRIUMAVXCW...
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Collisions
comment
source
target struct...
target stoichi...
target spin
target InChI...
collider struc...
collider stoic...
collider spin
collider InChI...
1 Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini &...
BASECOL 20...
CO
CO
UGFAIRIUMA...
He
He
SWQJXJOGL...
2 Vibrational de-excitation of CO by He (Cecchi-Pestellini & al., 20...
BASECOL 20...
CO
CO
UGFAIRIUMA...
He
He
SWQJXJOGL...
3 Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini &...
BASECOL 20...
CO
CO
UGFAIRIUMA...
He
He
SWQJXJOGL...
4 Vibrational de-excitation of CO by He (Cecchi-Pestellini & al., 20...
BASECOL 20...
CO
CO
UGFAIRIUMA...
He
He
SWQJXJOGL...
Clear
Sources
Energy table
Rate coef.
Export

VAMDC
Virtual Atomic and Molecular Data Centre




Select a row form each table
Transitions
comment
source
structural formula
stoichiometric formula
spin
InChI key
3 CO, v = 1 - 3
CDMS 2011-11-08 20:55:...
CO
CO
UGFAIRIUMAVXCW-ZCWHFV...
5 Carbon Monoxide, v = 0
CDMS 2011-11-08 20:55:...
CO
CO
UGFAIRIUMAVXCW-ZCWHFV...
Collisions
comment
source
target structural f...
target stoichiome...
target spin
target InChI key
collider structural...
collider stoichio...
collider spin
collider InChI key
1 Rotational de-e...
BASECOL 2011-...
CO
CO
UGFAIRIUMAVXC...
He
He
SWQJXJOGLNCZE...
2 Vibrational de-e...
BASECOL 2011-...
CO
CO
UGFAIRIUMAVXC...
He
He
SWQJXJOGLNCZE...
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Show selection
Export as XSAMS
Clear
Sources
Energy table
Rate coef.
Export



State energy and quantum numbers

state	energy [1/cm]	J	v	F	F1	parity	r	AsSym
1	0	0	0					
2	3.845	1	0					
3	11.535	2	0					
4	23.069	3	0					
5	38.448	4	0					
6	57.67	5	0					
7	80.735	6	0					
8	107.642	7	0					
9	138.39	8	0					
10	172.978	9	0					
11	211.404	10	0					

Rate coefficients

I1	I2	F1	F2	5.0	10.0	20.0	40.0	60.0	80.0	100.0	200.0	300.0	500.0
2	1	1	1	3.4E-11	3.2E-11	3E-11	2.8E-11	2.7E-11	2.6E-11	2.6E-11	2.5E-11	2.5E-11	2.6E-11
3	1	1	1	1.3E-11	1.3E-11	1.2E-11	1.1E-11	1.1E-11	1.1E-11	1.1E-11	1.4E-11	1.6E-11	1.9E-11
3	1	2	1	4.2E-11	4.5E-11	4.5E-11	4.6E-11	4.7E-11	4.8E-11	4.9E-11	5E-11	5.2E-11	5.7E-11
4	1	1	1	6.2E-12	6.6E-12	7.2E-12	8.5E-12	9.5E-12	1E-11	1.1E-11	1.2E-11	1.3E-11	1.4E-11
4	1	2	1	2.3E-11	2.2E-11	2E-11	1.8E-11	1.8E-11	1.8E-11	1.9E-11	2.2E-11	2.6E-11	3.2E-11
4	1	3	1	4.6E-11	4.9E-11	5E-11	5.1E-11	5.2E-11	5.3E-11	5.4E-11	5.8E-11	6.1E-11	6.8E-11
5	1	1	1	1.8E-12	1.9E-12	1.9E-12	2E-12	2.1E-12	2.1E-12	2.2E-12	2.6E-12	3.1E-12	4E-12
5	1	2	1	1.3E-11	1.4E-11	1.5E-11	1.7E-11	1.8E-11	2E-11	2.1E-11	2.4E-11	2.7E-11	3.1E-11
5	1	3	1	2.7E-11	2.7E-11	2.4E-11	2.2E-11	2.2E-11	2.2E-11	2.3E-11	2.7E-11	3.1E-11	3.7E-11
5	1	4	1	5.3E-11	5.4E-11	5.4E-11	5.4E-11	5.4E-11	5.5E-11	5.6E-11	6E-11	6.4E-11	7.1E-11
6	1	1	1	1.4E-12	1.5E-12	1.8E-12	2.4E-12	2.9E-12	3.3E-12	3.7E-12	4.9E-12	5.6E-12	6.8E-12

Einstein coefficients

lower level	upper level	frequency [MHz]	Einstein coefficient [1/cm]	log(intensity) [unitless]	uncertainty	upper state degeneracy
1	2	115,271.202	7.20378864479E-8	-5.01		3
2	3	230,538	6.91079000503E-7	-4.12		5
3	4	345,795.99	2.49670085538E-6	-3.612		7
4	5	461,040.768	6.12668117242E-6	-3.266		9
5	6	576,267.931	1.22134274135E-5	-3.012		11
6	7	691,473.076	2.13750692698E-5	-2.819		13
7	8	806,651.801	3.42239824576E-5	-2.672		15
8	9	921,799.704	5.13419191151E-5	-2.559		17
9	10	1,036,912.385	7.33007011041E-5	-2.475		19
10	11	1,151,985.443	1.00638923207E-4	-2.416		21
11	12	1,267,014.482	1.33903406762E-4	-2.377		23

Collider state energy and quantum numbers

state	energy[1/cm]	parity	J	F	M	Kappa	term type	I	S	j	S2	K
1	0		0				LS	0	0			

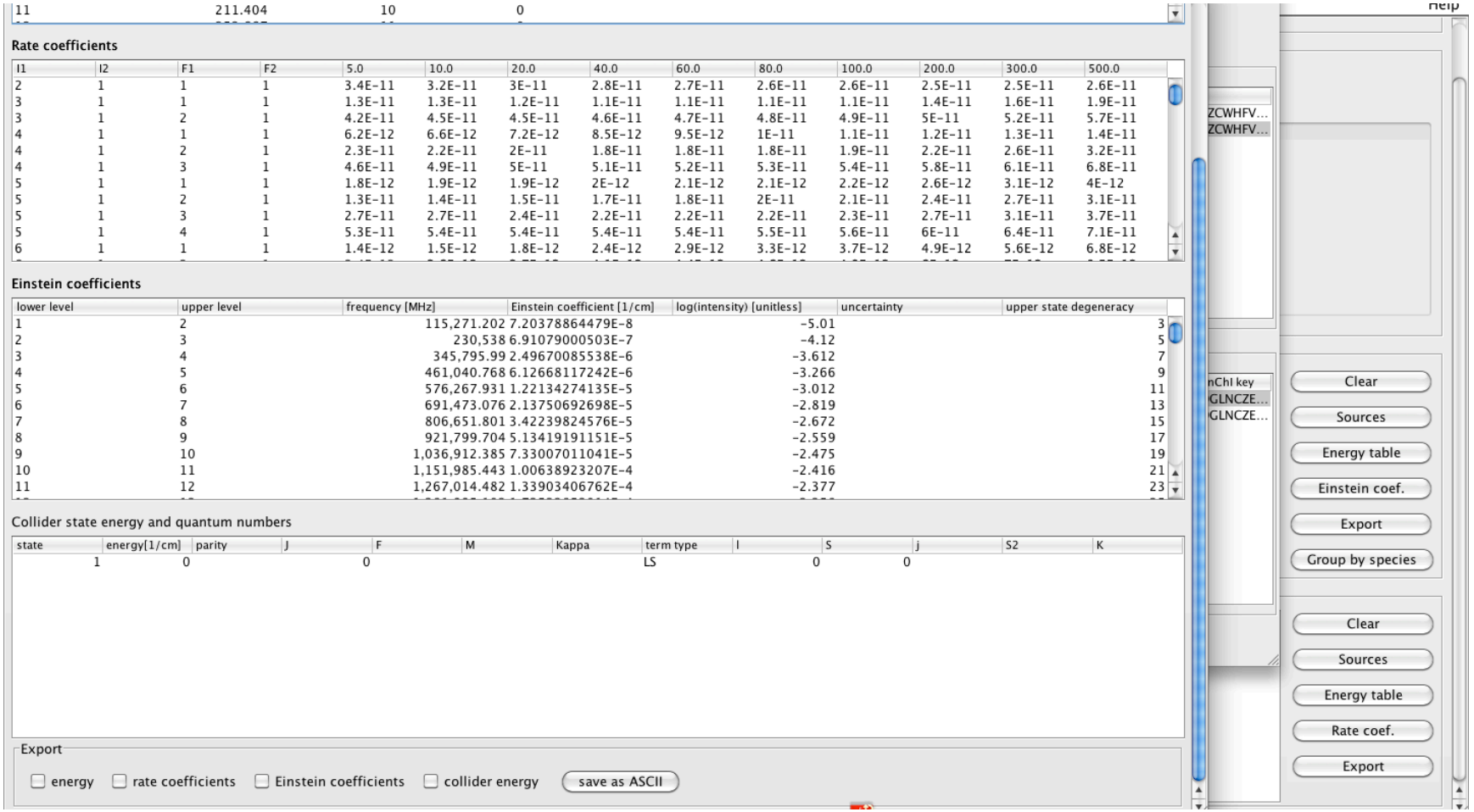
Help

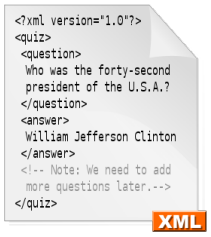
ZCWHFV...
ZCWHFV...

nChI key
GLNCZE...
GLNCZE...

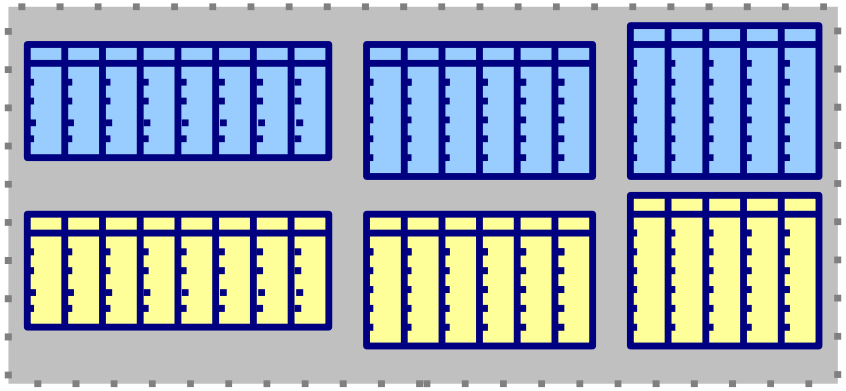
Clear
Sources
Energy table
Einstein coef.
Export
Group by species

Clear
Sources
Energy table
Rate coef.
Export

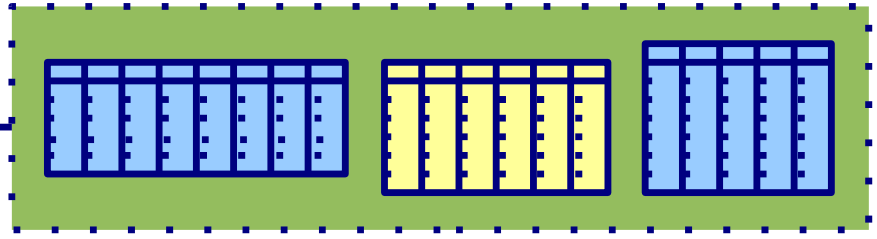

11 211.404 10 0
Rate coefficients
I1 I2 F1 F2 5.0 10.0 20.0 40.0 60.0 80.0 100.0 200.0 300.0 500.0
2 1 1 1 3.4E-11 3.2E-11 3E-11 2.8E-11 2.7E-11 2.6E-11 2.6E-11 2.5E-11 2.5E-11 2.6E-11
3 1 1 1 1.3E-11 1.3E-11 1.2E-11 1.1E-11 1.1E-11 1.1E-11 1.1E-11 1.4E-11 1.6E-11 1.9E-11
3 1 2 1 4.2E-11 4.5E-11 4.5E-11 4.6E-11 4.7E-11 4.8E-11 4.9E-11 5E-11 5.2E-11 5.7E-11
4 1 1 1 6.2E-12 6.6E-12 7.2E-12 8.5E-12 9.5E-12 1E-11 1.1E-11 1.2E-11 1.3E-11 1.4E-11
4 1 2 1 2.3E-11 2.2E-11 2E-11 1.8E-11 1.8E-11 1.8E-11 1.9E-11 2.2E-11 2.6E-11 3.2E-11
4 1 3 1 4.6E-11 4.9E-11 5E-11 5.1E-11 5.2E-11 5.3E-11 5.4E-11 5.8E-11 6.1E-11 6.8E-11
5 1 1 1 1.8E-12 1.9E-12 1.9E-12 2E-12 2.1E-12 2.1E-12 2.2E-12 2.6E-12 3.1E-12 4E-12
5 1 2 1 1.3E-11 1.4E-11 1.5E-11 1.7E-11 1.8E-11 2E-11 2.1E-11 2.4E-11 2.7E-11 3.1E-11
5 1 3 1 2.7E-11 2.7E-11 2.4E-11 2.2E-11 2.2E-11 2.2E-11 2.3E-11 2.7E-11 3.1E-11 3.7E-11
5 1 4 1 5.3E-11 5.4E-11 5.4E-11 5.4E-11 5.4E-11 5.5E-11 5.6E-11 6E-11 6.4E-11 7.1E-11
6 1 1 1 1.4E-12 1.5E-12 1.8E-12 2.4E-12 2.9E-12 3.3E-12 3.7E-12 4.9E-12 5.6E-12 6.8E-12
Einstein coefficients
lower level upper level frequency [MHz] Einstein coefficient [1/cm] log(intensity) [unitless] uncertainty upper state degeneracy
1 2 115,271.202 7.20378864479E-8 -5.01 3
2 3 230,538 6.91079000503E-7 -4.12 5
3 4 345,795.99 2.49670085538E-6 -3.612 7
4 5 461,040.768 6.12668117242E-6 -3.266 9
5 6 576,267.931 1.22134274135E-5 -3.012 11
6 7 691,473.076 2.13750692698E-5 -2.819 13
7 8 806,651.801 3.42239824576E-5 -2.672 15
8 9 921,799.704 5.13419191151E-5 -2.559 17
9 10 1,036,912.385 7.33007011041E-5 -2.475 19
10 11 1,151,985.443 1.00638923207E-4 -2.416 21
11 12 1,267,014.482 1.33903406762E-4 -2.377 23
Collider state energy and quantum numbers
state energy[1/cm] parity J F M Kappa term type I S j S2 K
1 0 0 LS 0 0
Export
energy
rate coefficients
Einstein coefficients
collider energy
save as ASCII
Help
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Clear
Sources
Energy table
Rate coef.
Export



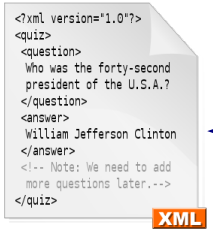
extract **equivalent** data from different sources



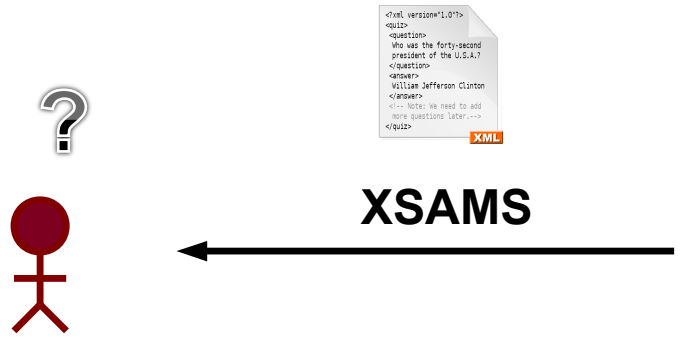
select sections of interest



generate new file form selected data



User's perspective



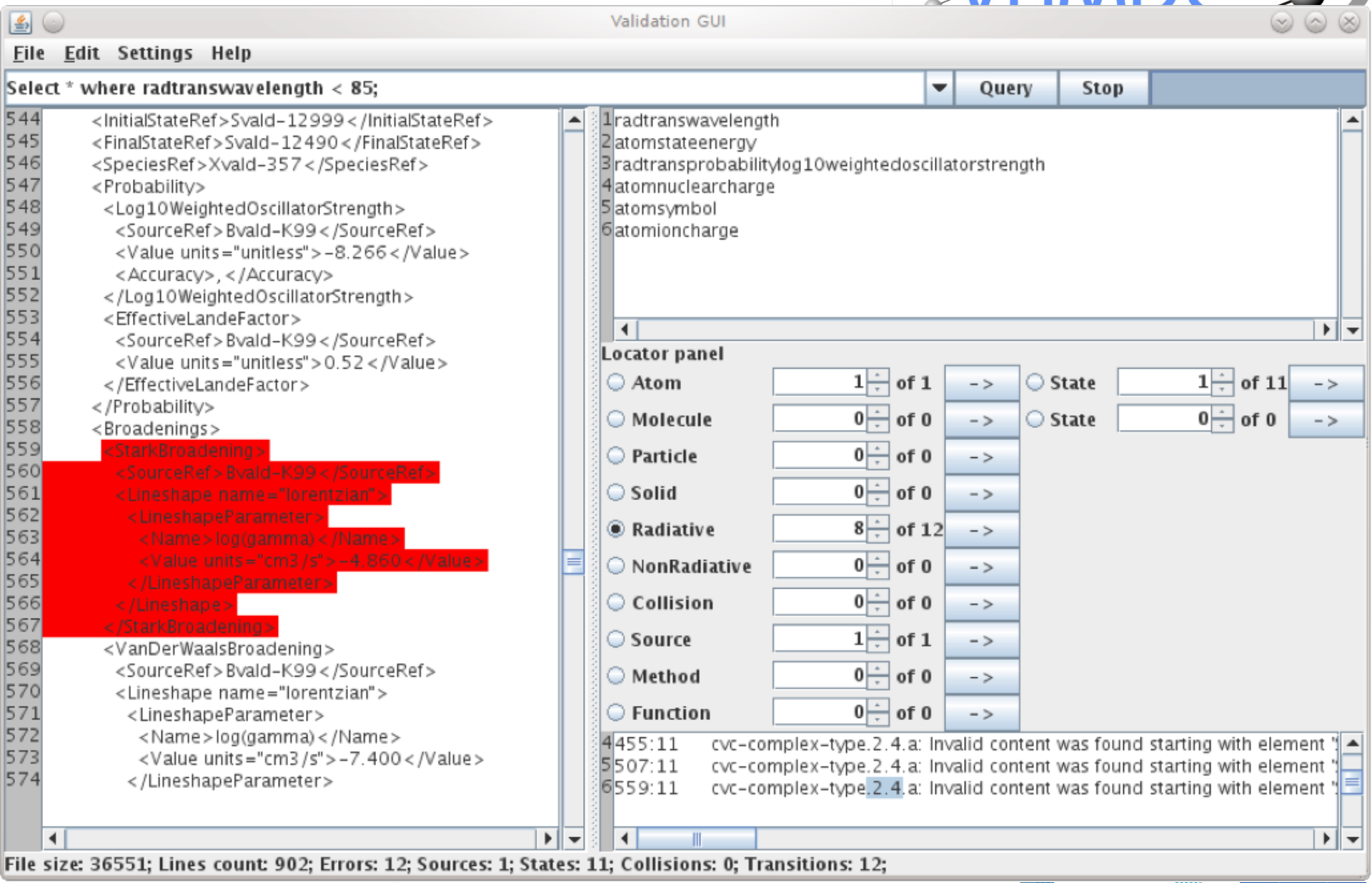
XSAMS → custom format → existing code

XSAMS → graphical display

TAPValidator

M. Doronin (LPMAA)

- Designed to validate XSAMS documents against the XML schema
- Existing node validation and testing
- Simplify development of new nodes using the Java node software (and Python)
- Suitable for monitoring task due to command-line mode


Validation GUI
File Edit Settings Help
Select * where radtranswavelength < 85;
Query
Stop
<InitialStateRef>Svald-12999</InitialStateRef>
<FinalStateRef>Svald-12490</FinalStateRef>
<SpeciesRef>Xvald-357</SpeciesRef>
<Probability>
<Log10WeightedOscillatorStrength>
<SourceRef>Bvald-K99</SourceRef>
<Value units="unitless">-8.266</Value>
<Accuracy>,</Accuracy>
</Log10WeightedOscillatorStrength>
<EffectiveLandeFactor>
<SourceRef>Bvald-K99</SourceRef>
<Value units="unitless">0.52</Value>
</EffectiveLandeFactor>
</Probability>
<Broadenings>
<StarkBroadening>
<SourceRef>Bvald-K99</SourceRef>
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<LineshapeParameter>
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</LineshapeParameter>
</Lineshape>
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<VanDerWaalsBroadening>
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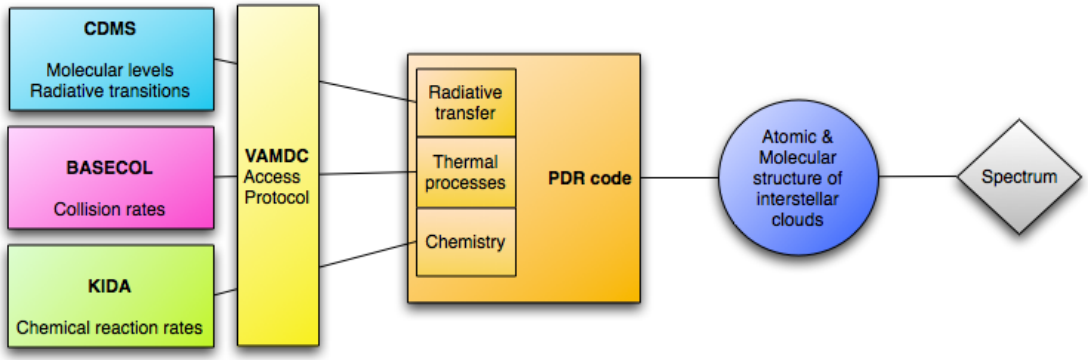
<LineshapeParameter>
<Name>log(gamma)</Name>
<Value units="cm3/s">-7.400</Value>
</LineshapeParameter>
radtranswavelength
atomstateenergy
radtransprobabilitylog10weightedoscillatorstrength
atomnuclearcharge
atomsymbol
atomioncharge
Locator panel
Atom 1 of 1 ->
Molecule 0 of 0 ->
Particle 0 of 0 ->
Solid 0 of 0 ->
Radiative 8 of 12 ->
NonRadiative 0 of 0 ->
Collision 0 of 0 ->
Source 1 of 1 ->
Method 0 of 0 ->
Function 0 of 0 ->
State 1 of 11 ->
State 0 of 0 ->
455:11 cvc-complex-type.2.4.a: Invalid content was found starting with element
507:11 cvc-complex-type.2.4.a: Invalid content was found starting with element
559:11 cvc-complex-type.2.4.a: Invalid content was found starting with element
File size: 36551; Lines count: 902; Errors: 12; Sources: 1; States: 11; Collisions: 0; Transitions: 12;

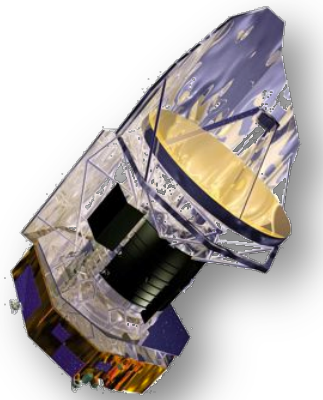
They require atomic and molecular data :
- Atomic and molecular levels
- Radiative transitions (Einstein coefficients, life time, …)
- Collision rates with major partners (H, H_2, electrons, He)
- Chemical reaction rates

Need complete data sets

Meudon PDR code
- Thousands chemical reactions
- Computation of line intensities (from UV to sub mm) for tens of species
- 30 000 UV H2 lines
- 318 H_2 ro-vib. levels in the ground elect. level

Interpretation of new instruments require to treat in detail more and more species





F. Le Petit

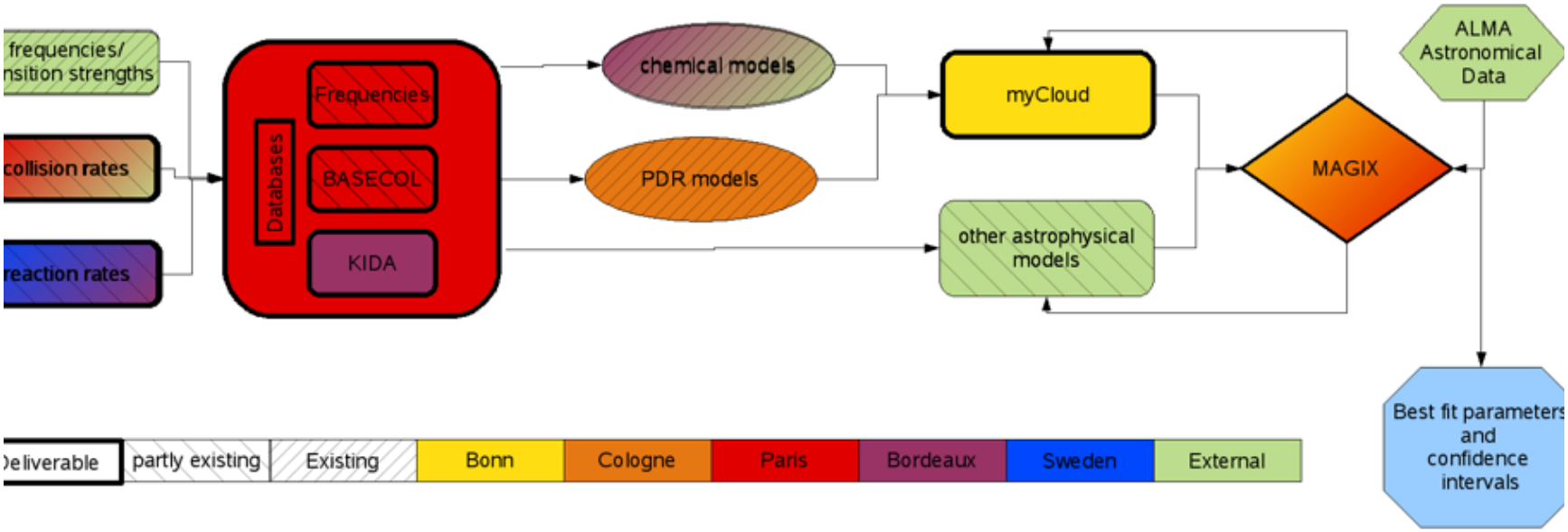
VAMDC infrastructure can be used to
- discover easily data
- build complete sets of data
- get data in standard format

=> Simplify the development of such codes

CATS Project – ASTRONET –
P. Schilke (Univ. Of Cologne)

VAMDC
Virtual Atomic and Molecular Data Centre

Coherent set of Astrophysical Tools for Astrophysics



Other Astro - Impact

- Connect to ARC (ALMA)
  - Talk on the 28th
  - Inclusion of VAMDC technology in IRAM Software
- Connect to CASSIS (Software developed for Herschel/ HIFI) – Toulouse (IRAP)

VAMDC - Achievements

- All databases able to answer queries and send back information in standardized format
- Portal From which you can query any VAMDC databases
- Standalone Tools to query VAMDC databases and manipulate retrieved files
  - Example of cross-matching of spectroscopic and collisional data in order to produce combined sets directly usuable in astrophysical tools

VAMDC Main Contributors to Infrastructure

- Central e-infrastructure: A. Akram, M.L. Dubernet, M. Doronin, C. Endres, C. Hill, T. Marquart, L. Nenadovic, N. Piskunov, G. Rixon, K. Smith
- VAMDC-XSAMS Group Current Activity : Y. Ralchenko, E. Roueff, J. Tennyson
- P.I. of Databases

Releases Level-n

- A level-n release is a combined release of:
  - standards for data access;
  - VAMDC nodes, each containing a database and web service following the standards;
  - a registry of the services;
  - a web portal as UI for the system;
  - software to prepare the databases and implement the web services.

- All releases include user support and training materials. Successive release-levels improve the sophistication and interoperability of the nodes. The L2 release is now supposed to be frozen.
- Intermediate Releases every 4 months

Focus of Year 3

- Consolidate Infrastructure (Upgrade of standards and software + Internal testing)
- Beta testing of Infrastructure
  - Node Software/Standards with New producers
  - Infrastructure : APEX/IRAM/PDR/CASSIS users (integration of our standards and procedures)
  - Portal, Cross-Federation software with User Panel
- Extend to external DB through call
- Prepare sustainability

Sustainability (I)

- **Extend VAMDC through answer to EU call (Political)**
  - 23rd November = 2 Yrs – 1ME max – Extend US, Brazil, India, Korea, South Africa, Australia – High Education – Schools - SMEs – Citizen-Scientists – International Coordination –
  - Obs Paris Coordination
- Inclusion VAMDC in **National Projects**
  - Part of the « Valorisation » of MAGI Labex (2e vague)
    - Molecules, Atoms, Grains Initiative for Space, Life, Environment
    - 35 UMR, 16 Universites, 6 Organismes/Ecoles
    - CNRS Coordination (INSU/INP) with Coordinator at LUTH
- Inclusion VAMDC in **SPACE EU CALL**
  - ASTRA Project = MIS (LUTH/GEPI) – Coord. Cambridge (23rd November)

Sustainability (II)

- Sustainability of central e-infrastructure
  - Standards, Related Software
  - Maintenance, Upgrade
  - Support to existing users and extension to new users
- Databases supported through their own fundings
- Political Coherence of VAMDC Consortium

Sustainability (III)

some answers ?

- Create a LEGAL ENTITY
  - Association under French Law able to be part of projects with core participants + associated members
- Make a Business Plan: Income
  - From states agencies/agencies/contracts/inclusion in research projects
  - From subscription of libraries (when states not part of the agreement) ? - quite unrealistic during the next few years
- Still necessity to have a **stable** core for Maintenance and Technology Transfer for the common infrastructure.

Open to Any Producers & Users **from June 2012**

- Open to Producers to include their data within VAMDC environment
  - In existing databases
  - Building their own database (Django publishing tools for example) and registrying it to VAMDC registries
- Open to users to include VAMDC developed software into their own applications
  - Licencing will allow any use
- All Softwares & Documentation From June 2012

at http://www.vamdc.eu (org)