VAMDC Interoperability

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

Nicolas Moreau

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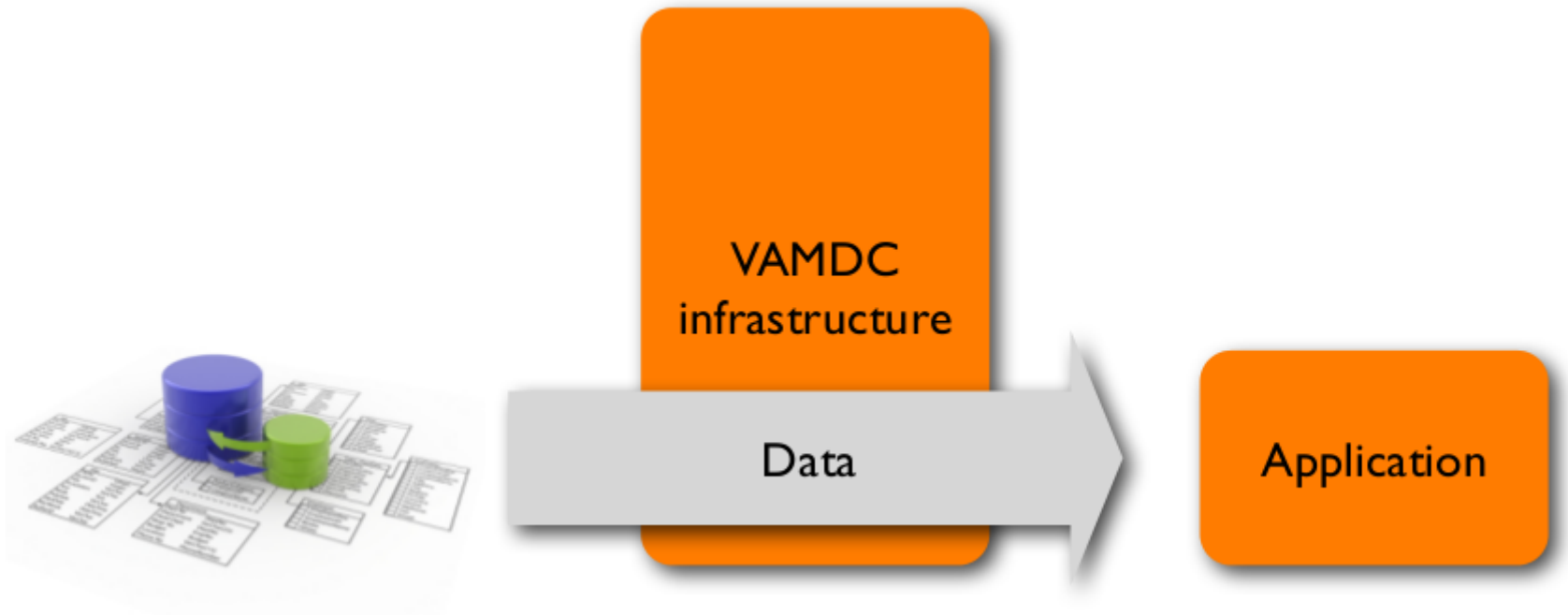
VAMDC
Virtual Atomic and Molecular Data Centre

I. Infrastructure overview
II. XSAMS format
III. XSAMS Processors
IV. Web portal

SEVENTH FRAMEWORK PROGRAMME
e-infrastructure

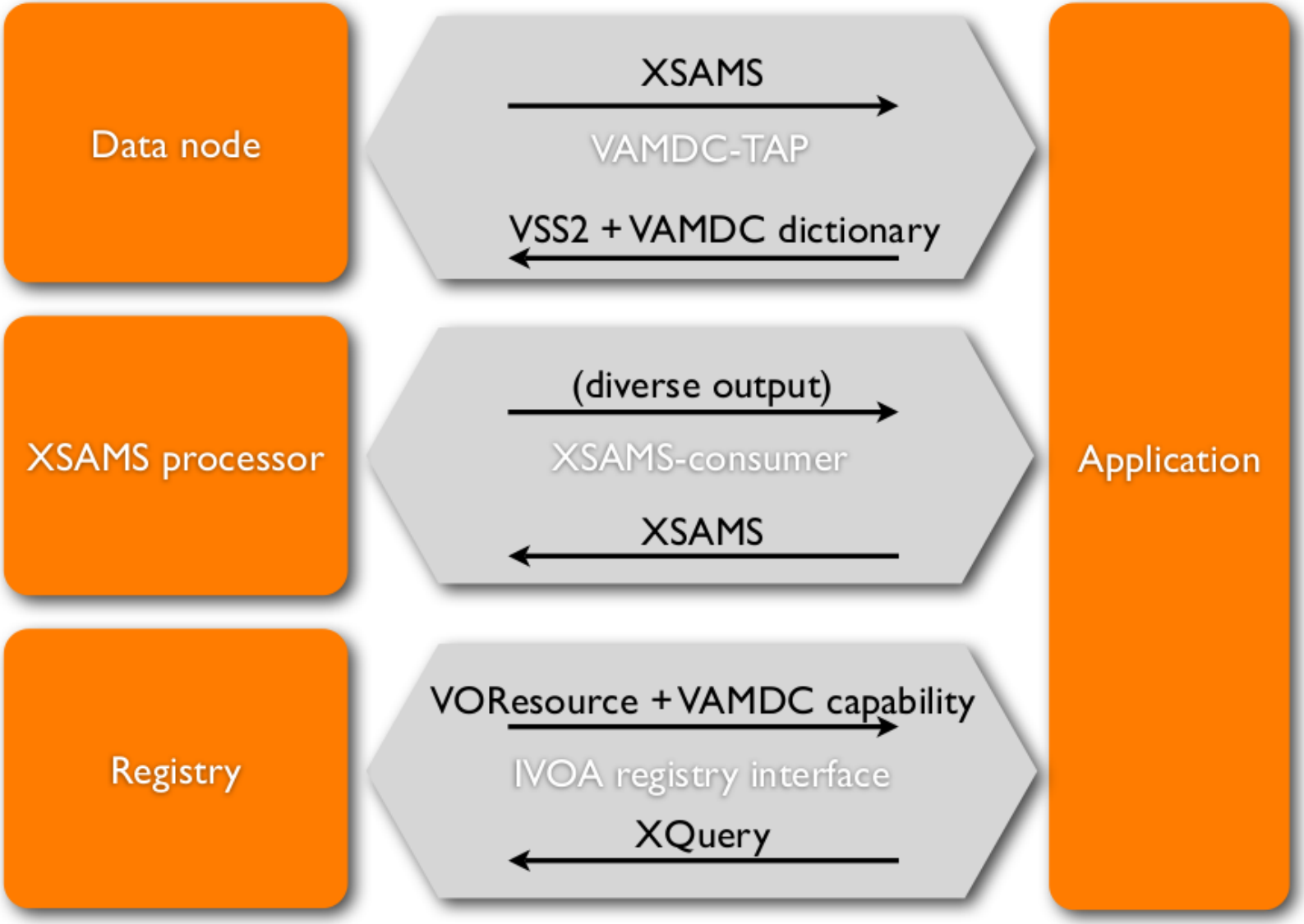
Infrastructure role



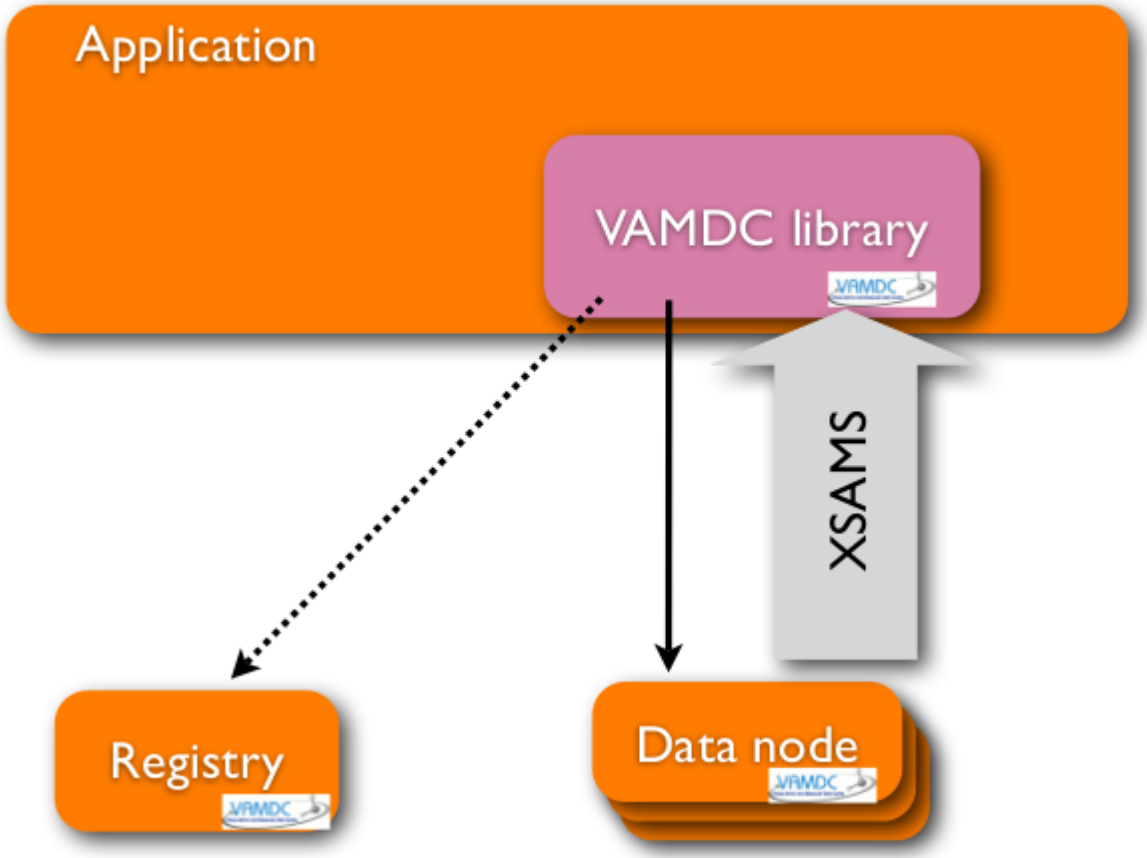
The VAMDC infrastructure is an intermediary layer to access databases from applications in a standardized way.

VAMDC provides softwares to achieve interoperability

The core components and standards



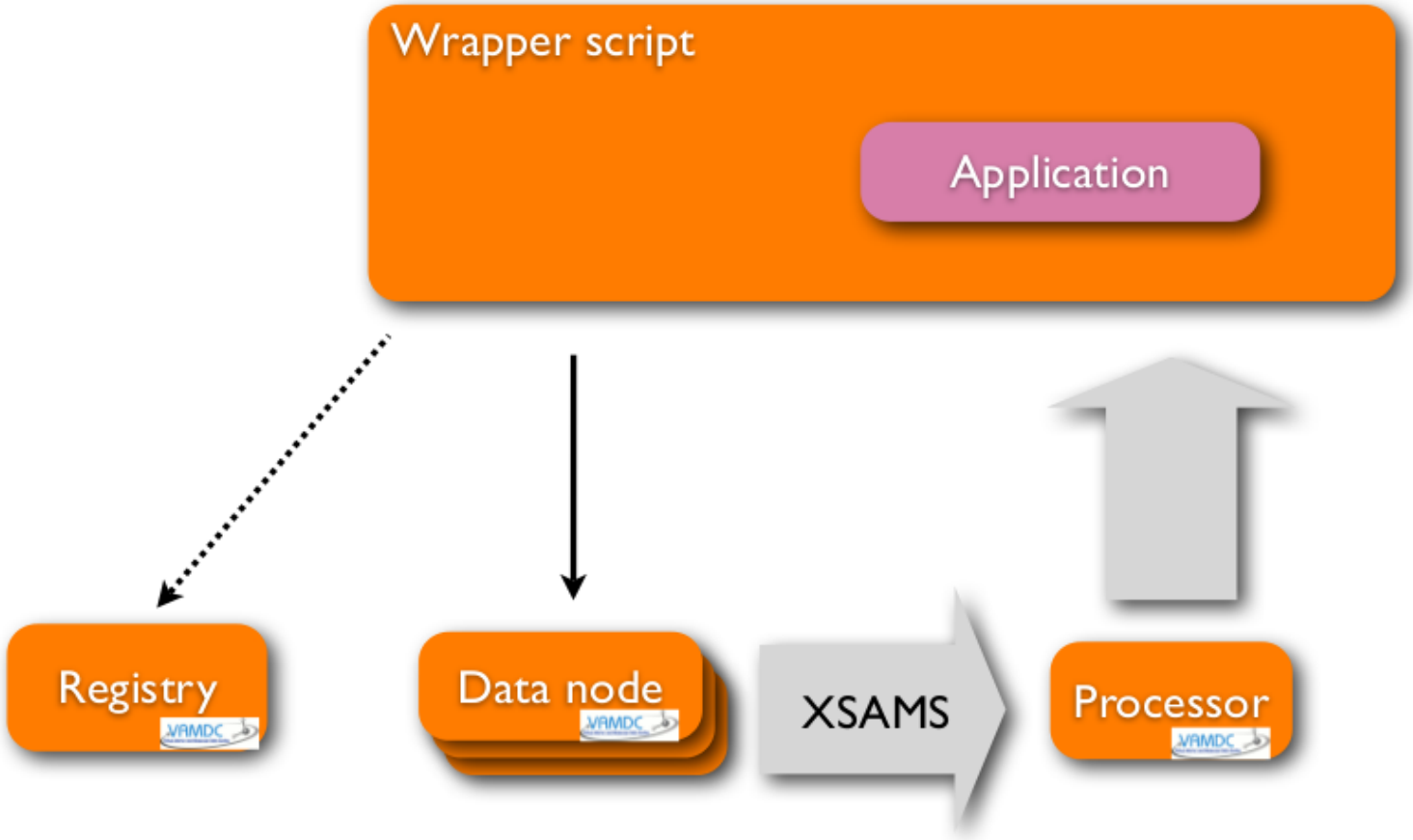
Adapted application



Some JAVA libraries have been developed to access the VAMDC infrastructure
Mainly to :

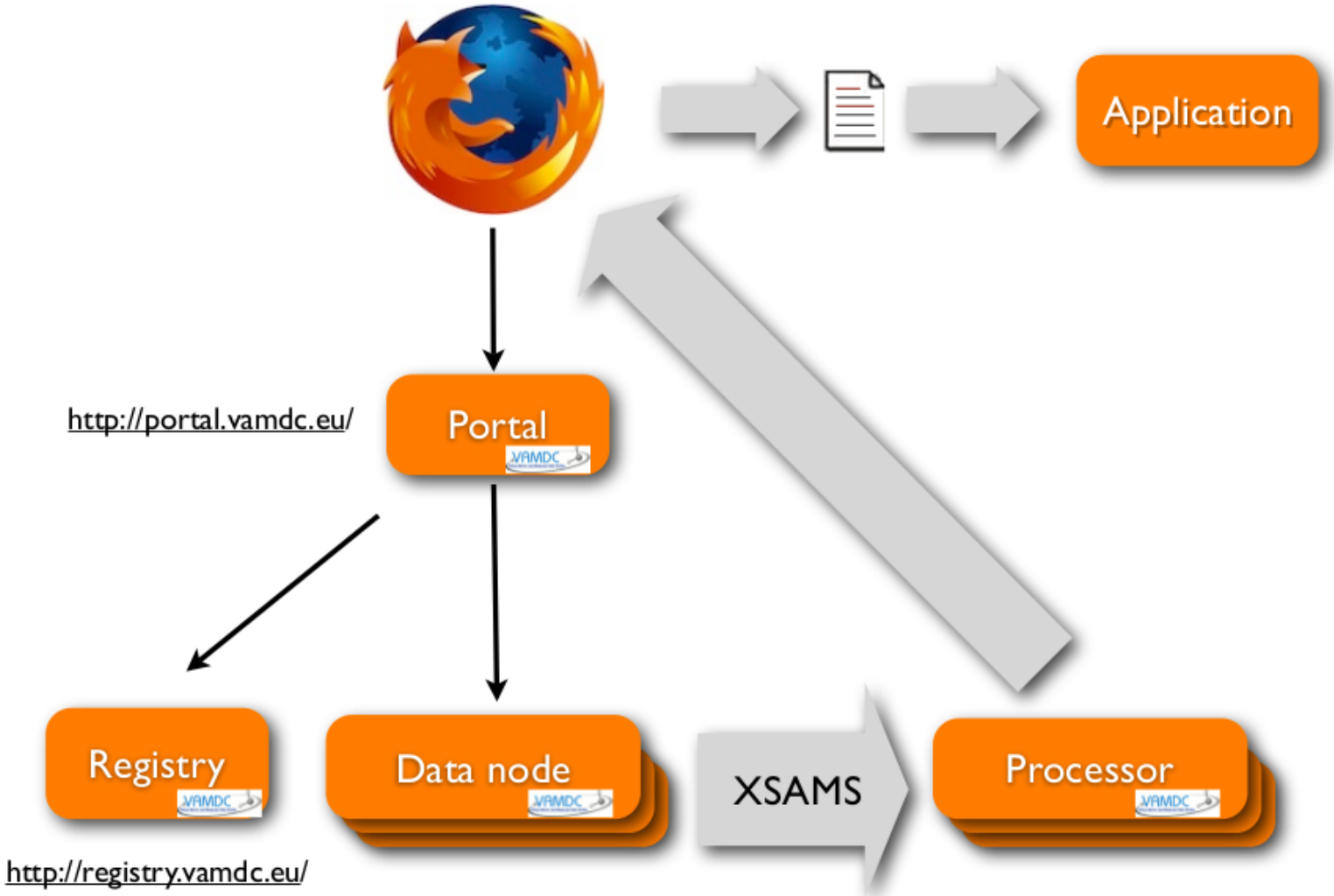
- Query the registry
- Parse XSAMS files
- Build VAMDC-TAP requests

Wrapped application



It is possible to use VAMDC facilities within an existing code by writing a wrapper script, which can be a simple shell script or a small program in, e.g., Python.
All VAMDC services can be called easily from scripts.

Portal, nodes & processors



= “infrastructure”

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XSAMS goals

- XSAMS stands for XML Schema for Atomic, Molecular and Solid data

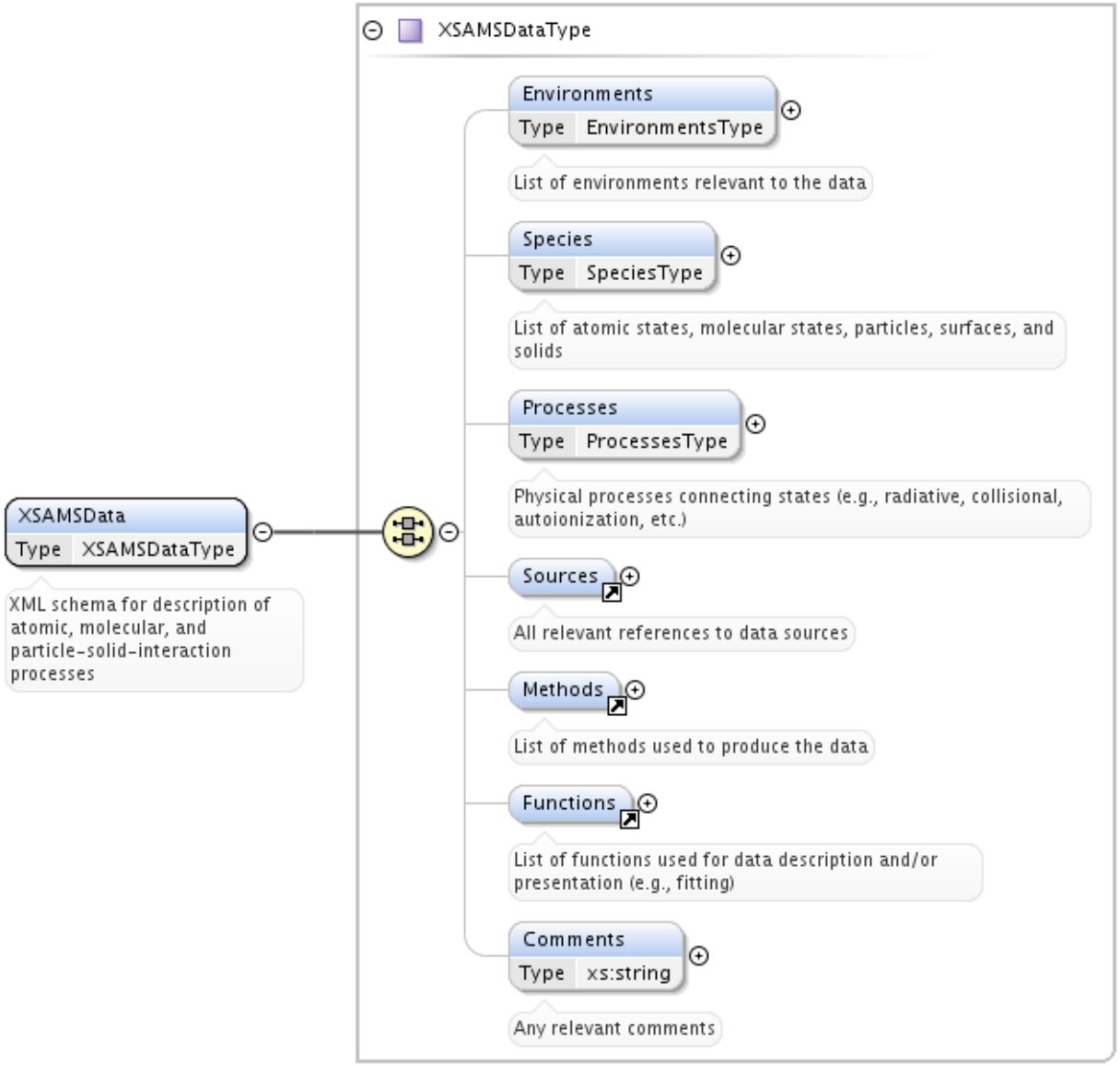
- A common format was necessary because VAMDC includes databases providers from very different fields (atomic, molecular and solid spectroscopy)

- Standard for exchange of atomic, molecular and particle-surface-interaction (AMPSI) data

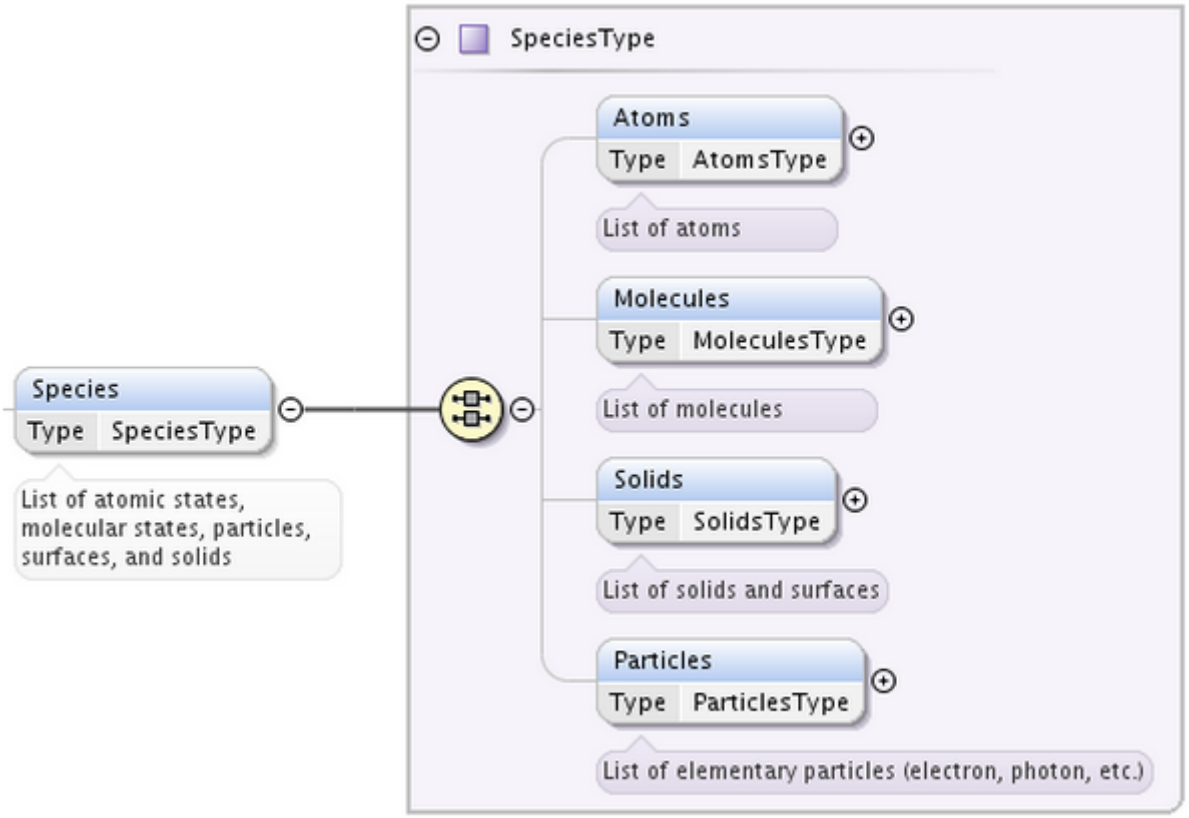
- Informations concerning sources and generation of the data must be provided

- Correctness or applicability of the data is left to the producer responsibility

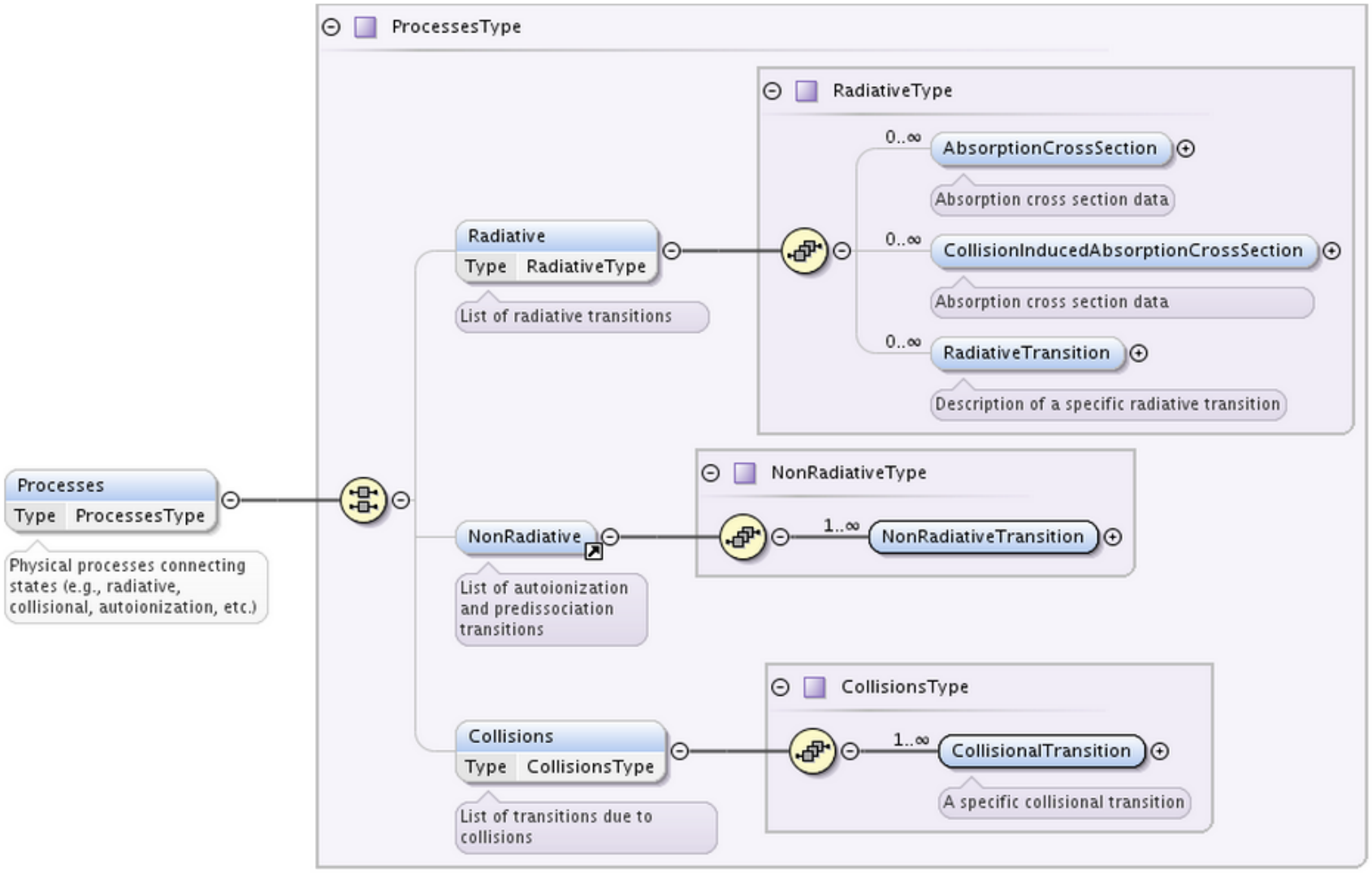
XSAMS structure : root element



XSAMS structure : species element



XSAMS structure : processes element



Data presentation II

```
<RadiativeTransition id="Pchianti-R277588">
    <EnergyWavelength>
        <Wavelength methodRef="Mchianti-EXP">
            <Value units="A">5005.51</Value>
        </Wavelength>
        <Wavelength methodRef="Mchianti-THEO">
            <Value units="A">5037.84</Value>
        </Wavelength>
    </EnergyWavelength>
    <UpperStateRef>Schianti-4014026</UpperStateRef>
    <LowerStateRef>Schianti-2014026</LowerStateRef>
    <SpeciesRef>Xchianti-14026</SpeciesRef>
    <Probability>
        <TransitionProbabilityA>
            <Value units="1/s">0.008762</Value>
        </TransitionProbabilityA>
    </Probability>
</RadiativeTransition>
```

Experimental wavelength

Theoritical wavelength

Reference to lower and upper states

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XSAMS Processors

- Web services applying transformations to one or more input files giving one output file as a result

- Two goals :
  - Simplifying XSAMS format usage through a transformation into other formats
  - Combining/Comparing files (for example level identification between databases)

- Existing processors use XSL stylesheets to transform XSAMS files (not a requirement)

- They are accessible from the VAMDC portal

- They are standardized :
http://www.vamdc.org/documents/xsams-processor_v12.07.pdf

- They provide a simple web interface to upload XSAMS files but can be called directly from scripts

- Parameters :
    - GET/POST : url (one or more, leading to the XSAMS file)
    - POST : upload (one or more, contains the document itself)

- The job receives an ID that is used to identify it, the newly created document then stays available on the server with this id

Current Processors (1/2)

- Bibtex : extracts references informations from a XSAMS document and returns them as a Bibtex file

- XSAMS to SME : converts XSAMS file to SME compatible file (Spectroscopy Made Easy (SME) is IDL software and a compiled external library that fits an observed high-resolution stellar spectrum with a synthetic spectrum to determine stellar parameters)

- Table view : presents XSAMS document as an HTML table

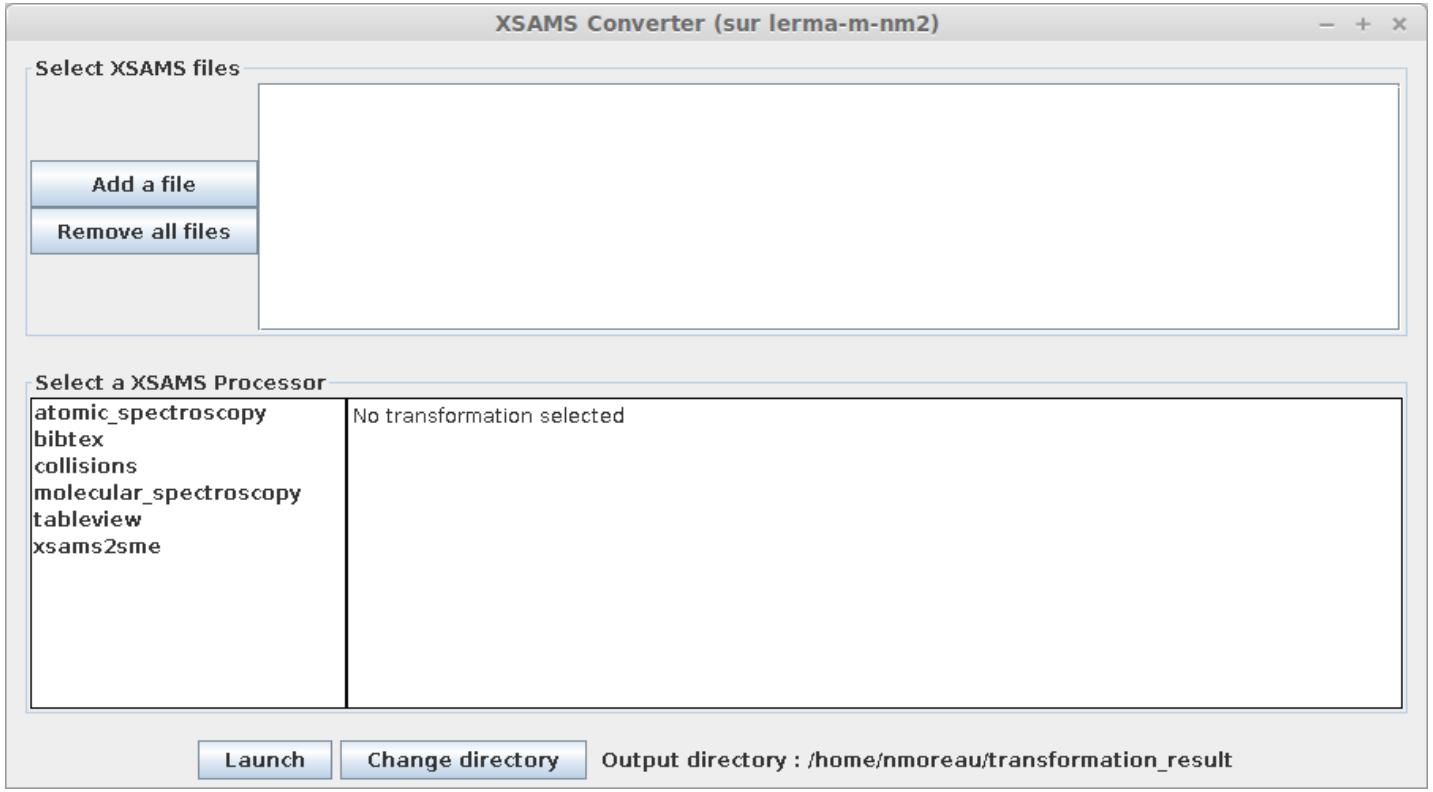
Current Processors (2/2)

- Atomic XSAMS to HTML : presents atomic spectroscopy data as an HTML table with sort functions and SAMP functionnalities (selected content is converted into votable and sent to Topcat for example)

- Molecular XSAMS to HTML : presents molecular spectroscopy data as an HTML table with sort functions and SAMP functionnalities

- Collisional XSAMS to HTML : presents collisional data as an HTML table with sort functions and SAMP functionnalities

Standalone Processor application



- Java application executing processors locally
- Does not require a network connection
- Provide both a GUI and a CLI so that it can be used in scripts
- Execute the XSL stylesheets on one or more input files

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Web portal

- Url : portal.vamdc.eu
- Main access point to look for data
- Currently gives an access to 30 databases
- Provides a web interface to build requests

Welcome to the VAMDC portal!

Currently we have 30 databases running and ready to serve you with the data.

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

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Available databases

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Name	Description	Maintainer	Status	Availables species
Belgrade electron/atom(molecule) database (BEAMDB)	Electron interaction cross-sections for elastic scattering, electron excitation, ionization and total scattering.	bratislav.marinkovic@ipb.ac.rs	OK	Show
TFMeCaSDa - CF4 Calculated Spectroscopic Database	Calculated line lists for carbon tetrafluoride (12CF4). The data on CF4 contain the vibration-rotation energy levels, line positions and line intensities in the range from 500 to 1500 cm-1.	Vincent.Boudon@u-bourgogne.fr	OK	Show
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	Show
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	Show
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	Show
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	Show
SHeCaSDa - SF6 Calculated Spectroscopic Database	Calculated line lists for sulfur hexafluoride (32SF6, 33SF6, 34SF6). The data on SF6 contain the vibration-rotation energy levels, line positions and line intensities in the range from 200 to 3000 cm-1.	Vincent.Boudon@u-bourgogne.fr	OK	Show
Stark-b	Database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation	sylvie.sahal-brechot@obspm.fr	OK	Show
JPL database: VAMDC-TAP service	The JPL database contains a catalog of radio frequency and microwave to far-infrared spectral lines of atomic and molecular species that (may) occur in the interstellar or circumstellar medium or in planetary atmospheres. The catalog is continuously updated. THIS IS JUST FOR DEVELOPMENT	endres@ph1.uni-koeln.de	OK	Show
HITRAN-UCL resource	The HITRAN database - truncated version for beta testing, from http://www.cfa.harvard.edu/HITRAN/	christian.hill@ucl.ac.uk	OK	Show
VALD sub-set in Moscow (obs)	The part of Vienna Atomic Line Database (VALD) with accurate wavelength and energy levels. It also provides laboratory and calculated transition probabilities, Lande factors and broadening parameters. It is used for line identification and spectral synthesis.	pakhomov@inasan.ru	OK	Show
RADAM - Ion Interactions	Database for Radiation damage of molecules of biological interest induced by ion collisions: cross sections and fragmentation yields.	domaracka@ganil.fr	OK	Show
ALADDIN2	A subset of the IAEA ALADDIN database for testing its implementation as a VAMDC node.	christian.hill@ucl.ac.uk	OK	Show
MeCaSDa - Methane Calculated Spectroscopic Database	Calculated line lists for methane (12CH4, 13CH4 and 12CH3D). The data on methane contain the vibration-rotation energy levels, line positions and line intensities in the range from 0 to 6200 cm-1.	Vincent.Boudon@u-bourgogne.fr	OK	Show
VALD (atoms)	The Vienna Atomic Line Database (VALD) is a collection of atomic line parameters (wavelengths, transition energies and quantum numbers, oscillator strengths, Lande factors, radiative and collisional broadening). This resource is the VAMDC-TAP representation of the atomic data in VALD3.	thomas.marquart@fysast.uu.se	OK	Show
VAMDC species-DB	This Database contains all the species and its VAMDC-Species Ids which are used by VAMDC.	endres@ph1.uni-koeln.de	OK	Show

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Available species in Cologne Database for Molecular Spectroscopy

CDMS species

Go to molecules

Atoms				
Element symbol	**Nuclear charge**	**Ion charge**	**InChI**	**InChIKey**
Al	13	0	1/Al	XAGFODPZIPBFFR-UHFFFAOYNA-N (Search in NIST database)
C	6	0	1S/C	OKTJSMMVPCPJKN-UHFFFAOYSA-N (Search in NIST database)
C	6	0	1S/C/i1+1	OKTJSMMVPCPJKN-OUBTZVSYSA-N (Search in NIST database)
C	6	1	1S/C/q+1	GKDCRJWYAGBLFY-UHFFFAOYSA-N (Search in NIST database)
C	6	1	1S/C/q+1/i1+1	GKDCRJWYAGBLFY-OUBTZVSYSA-N (Search in NIST database)
Fe	26	0	1/Fe	XEEYBQQBJWHFJM-UHFFFAOYNA-N (Search in NIST database)
Fe	26	1	1/Fe/q+1	WZGNVVUXVXNNOX-UHFFFAOYNA-N (Search in NIST database)
N	7	1	1S/N/q+1	DELRCXTYJVVNEW-UHFFFAOYSA-N (Search in NIST database)
O	8	0	1S/O	QVGXLLKOCUKJST-UHFFFAOYSA-N (Search in NIST database)
S	16	0	1S/S	NINIDFKCEFEMDL-UHFFFAOYSA-N (Search in NIST database)
Si	14	0	1S/Si	XUIMIQQOPSSXEZ-UHFFFAOYSA-N (Search in NIST database)
Si	14	1	1S/Si/q+1	FSLGCYNKXXIWGJ-UHFFFAOYSA-N (Search in NIST database)

Go to atoms

Molecules						
Stoichiometric formula	**Ordinary structural formula**	**Chemical name**	**Ion charge**	**Molecular weight**	**InChI**	**InChIKey**
AlC2H	AlCCH	Aliminum acetylide		52	1/C2H.Al/c1-2;/h1H;/rC2HAl/c1-2-3/h1H	NPKICPBOXPXYSD-OKROMESVNA-N (Search in NIST database)
AlCN	AlNC	Aluminum monoisocyanide		53	1/CN.Al/c1-2;/rCAlN/c1-3-2	HWKFKJIIRKPLHF-FRUVTJLNNA-N (Search in NIST database)
AlCN	AlCN	Aluminum monocyanide		53	1/CN.Al/c1-2;/rCAlN/c2-1-3	HWKFKJIIRKPLHF-ZZXBCICDNA-N (Search in NIST database)
AlH	AlH	Aluminum monohydride		28	1/Al.H/rAlH/h1H	SPRIOUNJHPCKPV-OBKUDOBONA-N (Search in NIST database)
AlS	AlS	Aluminum monosulfide		59	1/Al.S/rAlS/c1-2	SLWLWUJHXQUDJS-DRDSLJIGNA-N (Search in NIST database)
ArH+	ArH+	Argon hydride cation		41	1S/ArH/h1H/q+1	TVQSUVFYDVJWLI-UHFFFAOYSA-N (Search in NIST database)
ArH+	ArD+	Argon hydride cation		42	1S/ArH/h1H/q+1/i1D	TVQSUVFYDVJWLI-MICDWDOJSA-N (Search in NIST database)

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

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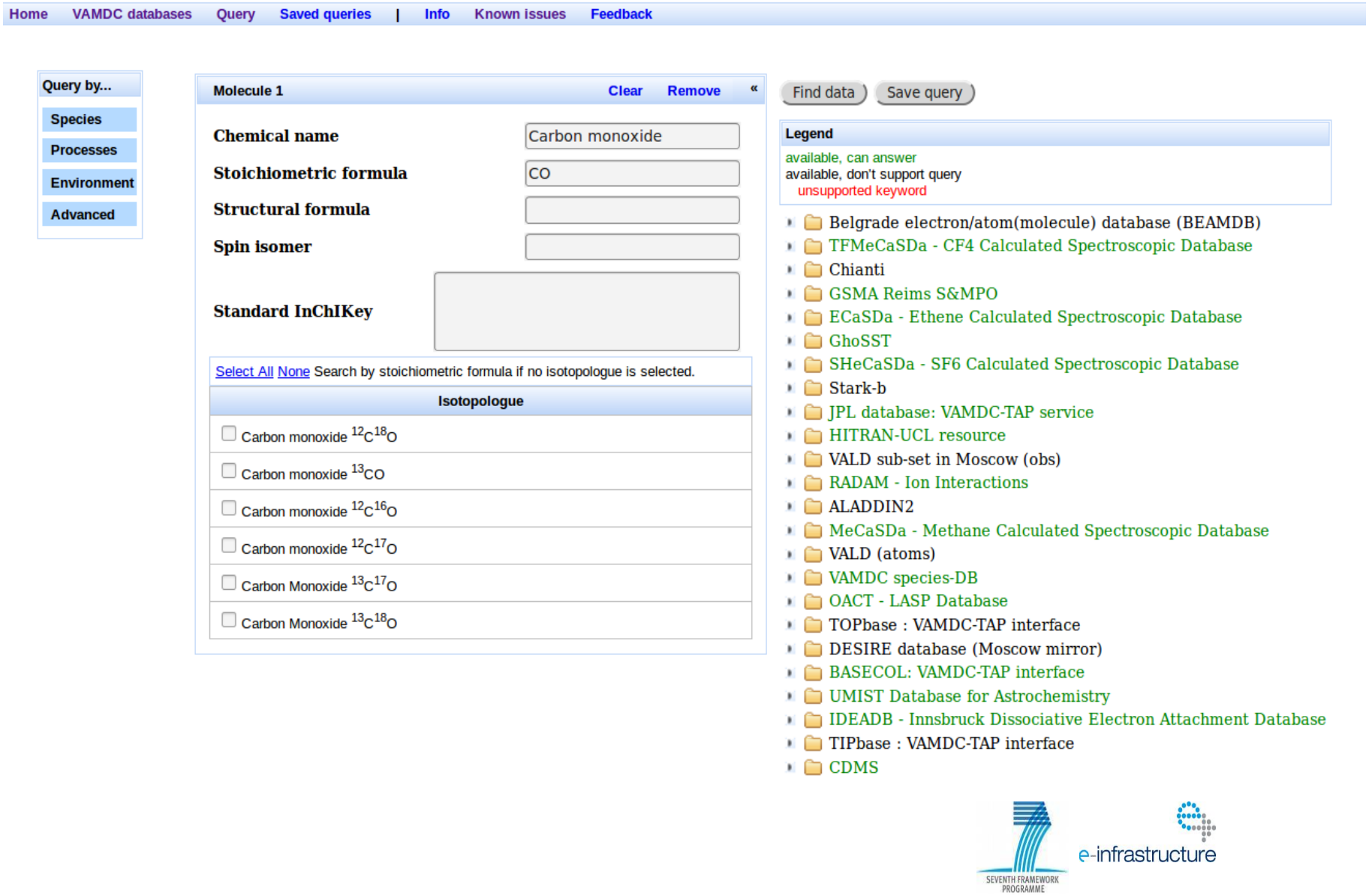
Building a query



Query result

1 : Query Execution

Done

Modify query | Stop waiting | Save query

select * where ((InchiKey IN ('UGFAIRIUMAVXCW-RGIGPVFXSA-N','UGFAIRIUMAVXCW-ZDOIIHCHSA-N','UGFAIRIUMAVXCW-HQMMCQRPSA-N','UGFAIRIUMAVXCW-VQEHIDDOSA-N','UGFAIRIUMAVXCW-UHFFFAOYSA-N','UGFAIRIUMAVXCW-OUBTZVSYSA-N')))

Comments

3 : Results Conversion (select in table below)

- BibTeX from XSAMS
- Table views of XSAMS
- Xsams2SME
- Atomicxsams2HTML
- Molecular Spectroscopy XSAMS to HTML

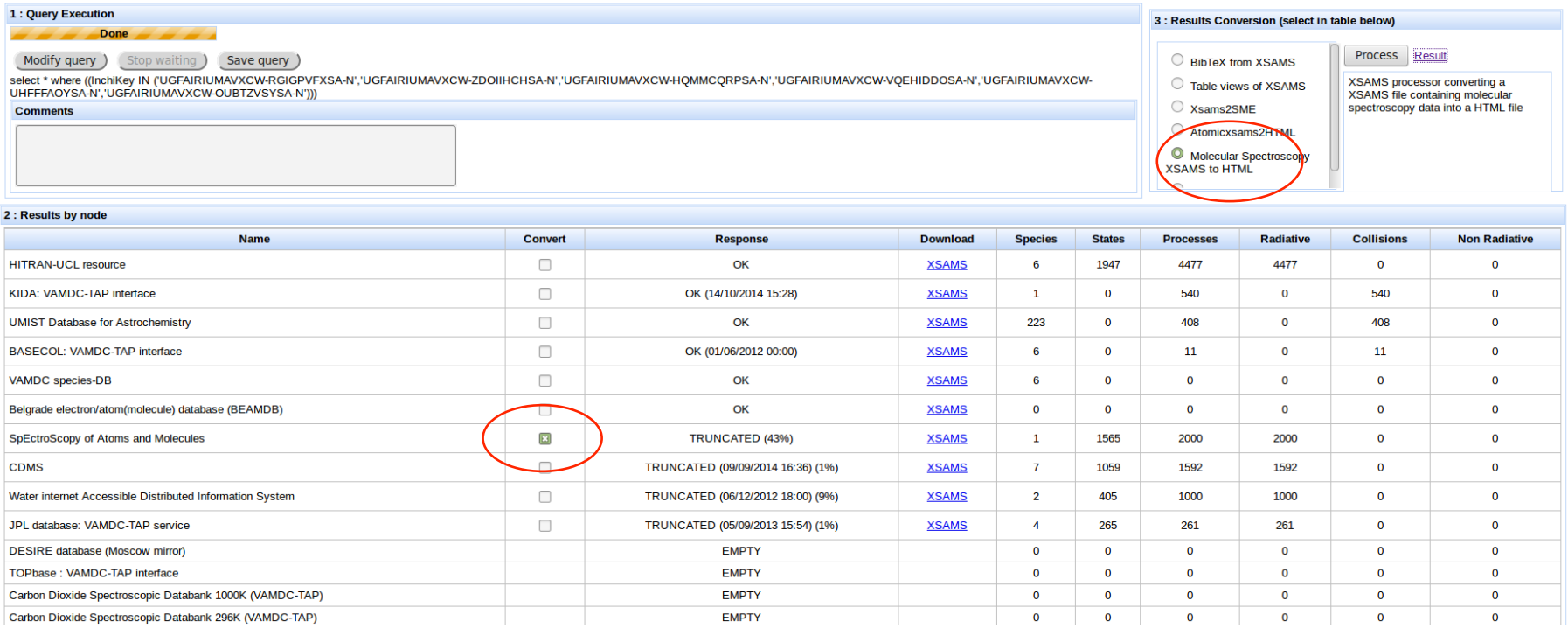
Process | Result

XSAMS processor converting a XSAMS file containing molecular spectroscopy data into a HTML file

2 : Results by node

Name	Convert	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
HITRAN-UCL resource	☐	OK	XSAMS	6	1947	4477	4477	0	0
KIDA: VAMDC-TAP interface	☐	OK (14/10/2014 15:28)	XSAMS	1	0	540	0	540	0
UMIST Database for Astrochemistry	☐	OK	XSAMS	223	0	408	0	408	0
BASECOL: VAMDC-TAP interface	☐	OK (01/06/2012 00:00)	XSAMS	6	0	11	0	11	0
VAMDC species-DB	☐	OK	XSAMS	6	0	0	0	0	0
Belgrade electron/atom(molecule) database (BEAMDB)	☐	OK	XSAMS	0	0	0	0	0	0
SpEctroScopy of Atoms and Molecules	☒	TRUNCATED (43%)	XSAMS	1	1565	2000	2000	0	0
CDMS	☐	TRUNCATED (09/09/2014 16:36) (1%)	XSAMS	7	1059	1592	1592	0	0
Water internet Accessible Distributed Information System	☐	TRUNCATED (06/12/2012 18:00) (9%)	XSAMS	2	405	1000	1000	0	0
JPL database: VAMDC-TAP service	☐	TRUNCATED (05/09/2013 15:54) (1%)	XSAMS	4	265	261	261	0	0
DESIRE database (Moscow mirror)		EMPTY		0	0	0	0	0	0
TOPbase : VAMDC-TAP interface		EMPTY		0	0	0	0	0	0
Carbon Dioxide Spectroscopic Databank 1000K (VAMDC-TAP)		EMPTY		0	0	0	0	0	0
Carbon Dioxide Spectroscopic Databank 296K (VAMDC-TAP)		EMPTY		0	0	0	0	0	0

Query result



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Done

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Carbon Dioxide Spectroscopic Databank 296K (VAMDC-TAP)		EMPTY		0	0	0	0	0	0

Query result

Menu

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

Sources

Id	Title	Origin	Authors	Year	Link
Bsesam-4		communication	Eidelsberg, M.; Roueff, E.;	2012	

Results from sesam VAMDC node

Unselect all	Stoichiometric formula X	Ordinary structural formula X	Wavelength(A) X	Transition reference X	Wavenumber X	Oscillator Strength X	Lower energy(1/cm) X	Lower total statistical weight X	Lower QNs X	Upper energy(1/cm) X	Upper total statistical weight X	Upper QNs X
	CO	CO	1323.0500	Bsesam-4	75582.8000	0000.0000	00.0000	01.0000	case:ElecStateLabel=X case:v=0 case:J=0	75582.8000	03.0000	case:ElecStateLabel=e case:elecRefl=- case:Lambda=0 case:S=1 case:v=12 case:J=1 case:N=0 case:SpinComponentLabel=1 case:kronigParity=e
	CO	CO	1323.0800	Bsesam-4	75581.4900	0000.0000	03.8450	03.0000	case:ElecStateLabel=X case:v=0 case:J=1	75584.8950	05.0000	case:ElecStateLabel=e case:elecRefl=- case:Lambda=0 case:S=1 case:v=12 case:J=2 case:N=1 case:SpinComponentLabel=1 case:kronigParity=e
	CO	CO	1323.1400	Bsesam-4	75578.5800	0000.0000	11.5350	05.0000	case:ElecStateLabel=X case:v=0 case:J=2	75589.1650	07.0000	case:ElecStateLabel=e case:elecRefl=- case:Lambda=0 case:S=1 case:v=12 case:J=3 case:N=2 case:SpinComponentLabel=1 case:kronigParity=e
	CO	CO	1323.2300	Bsesam-4	75572.5200	0000.0000	23.0695	07.0000	case:ElecStateLabel=X case:v=0 case:J=3	75595.5895	09.0000	case:ElecStateLabel=e case:elecRefl=- case:Lambda=0 case:S=1 case:v=12 case:J=4 case:N=3 case:SpinComponentLabel=1 case:kronigParity=e
	CO	CO	1323.3500	Bsesam-4	75566.3900	0000.0000	38.4481	09.0000	case:ElecStateLabel=X case:v=0 case:J=4	75604.1581	11.0000	case:ElecStateLabel=e case:elecRefl=- case:Lambda=0 case:S=1 case:v=12 case:J=5 case:N=4 case:SpinComponentLabel=1 case:kronigParity=e