VAMDC Interoperability

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

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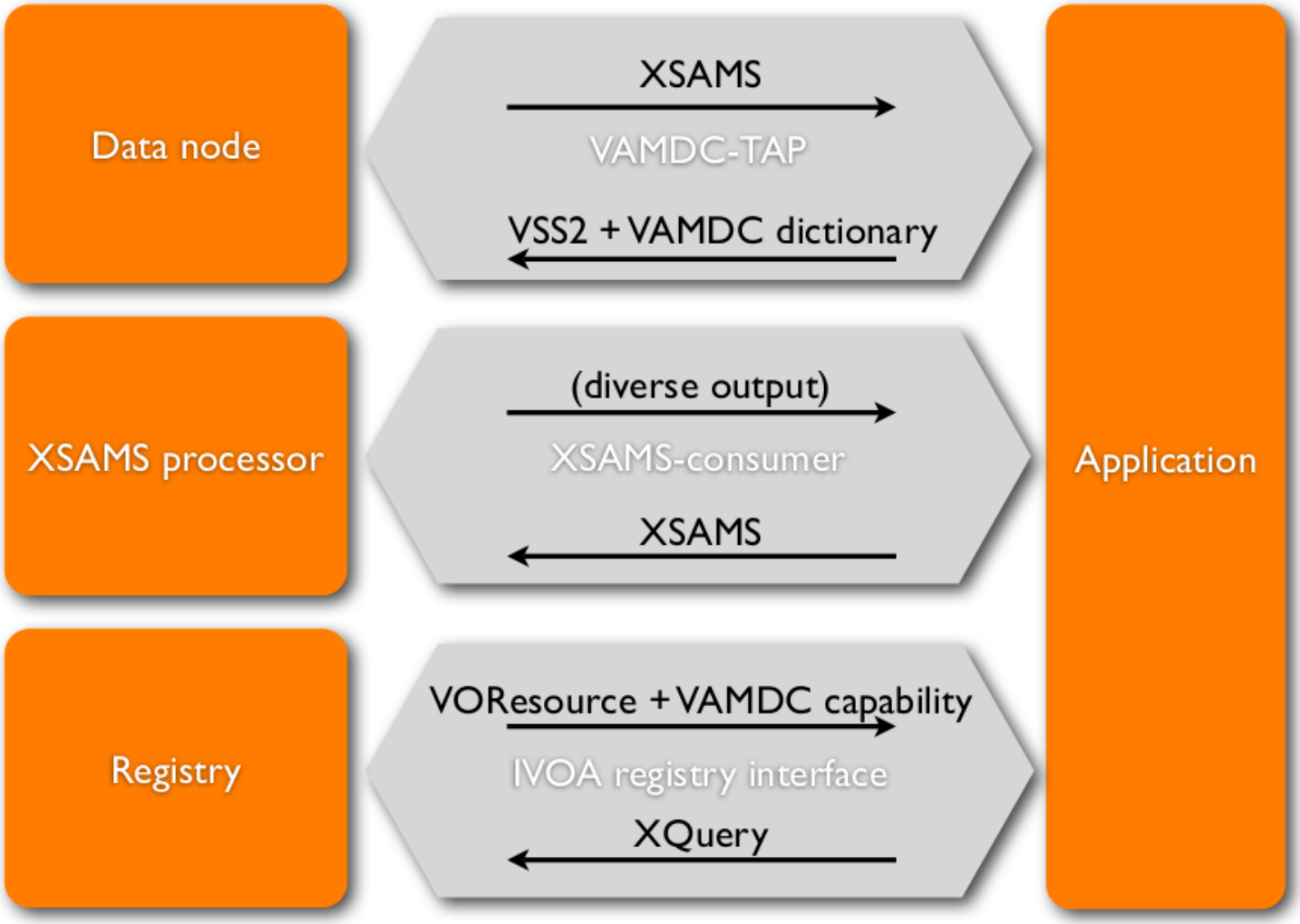
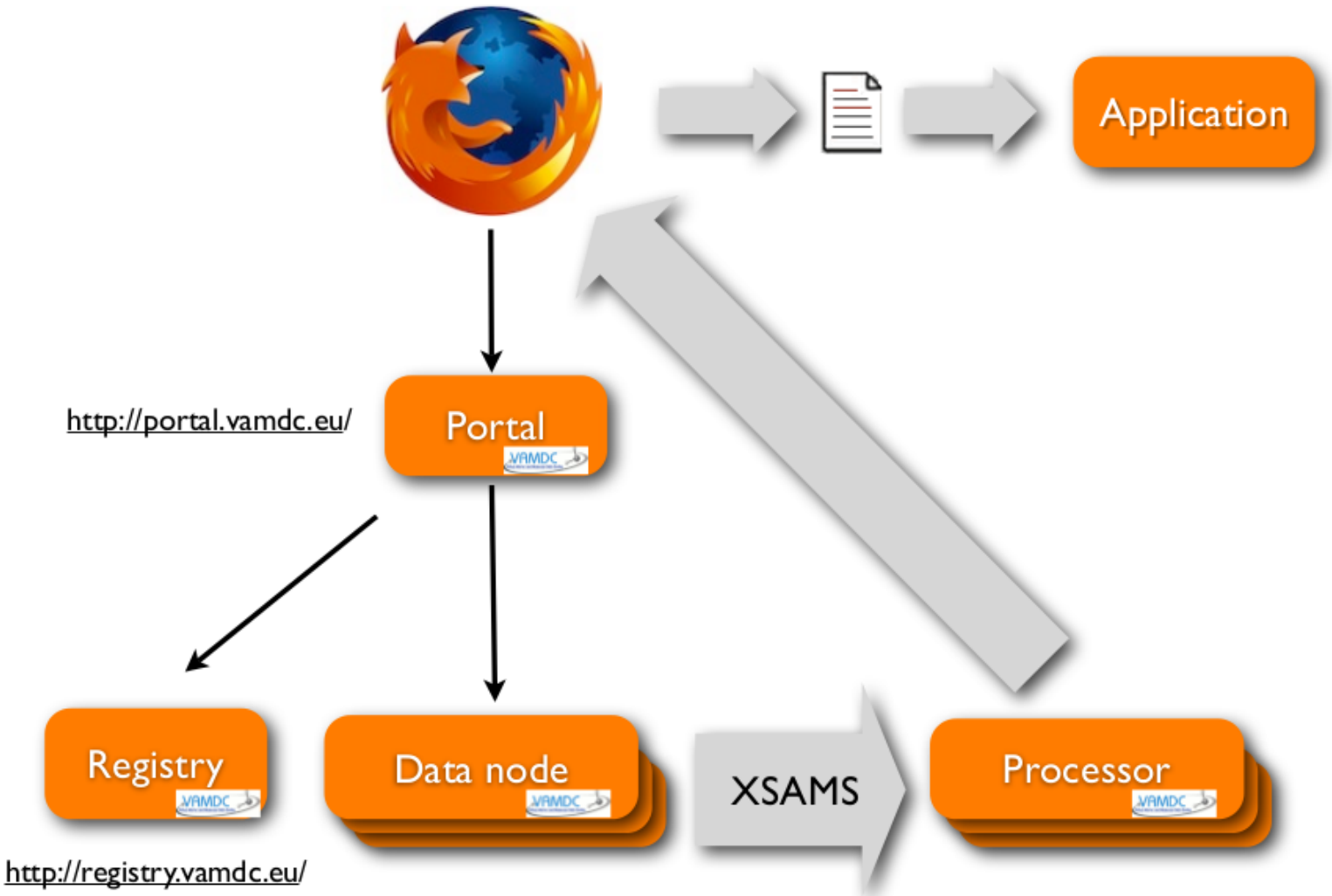
VAMDC consortium

I. Infrastructure
II. XSAMS format
III. XSAMS Processors

The core standards



Portal, nodes & processors



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XSAMS goals

- XSAMS stands for XML Schema for Atomic, Molecular and Solids (http://vamdc-standards.readthedocs.org/en/latest/dataModel/vamdcxsams/structure.html)

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

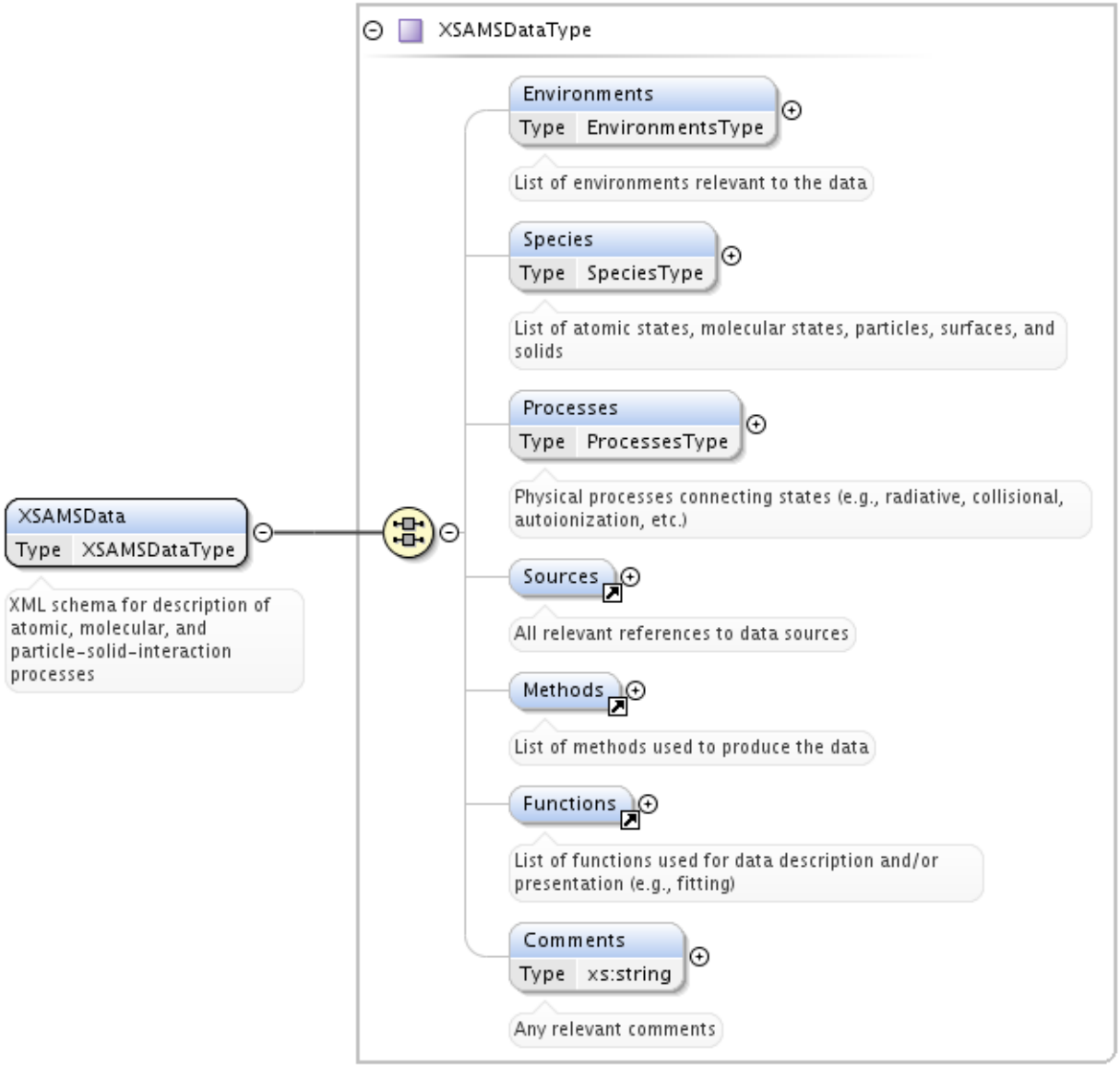
- Standard for exchange of atomic, molecular and particle-surface-interaction (AMPSI) data

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

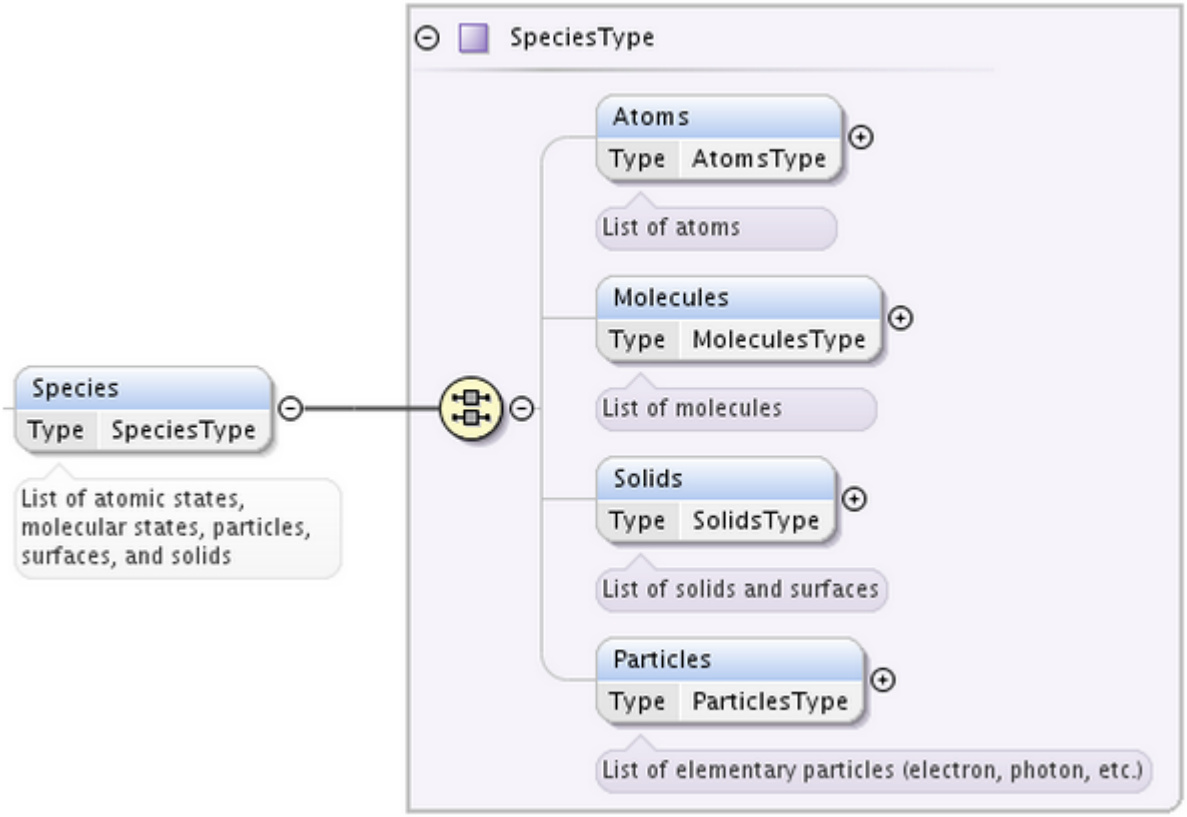
- Correctness or applicability of the data is left to the producer responsibility

- Current version is 12.07

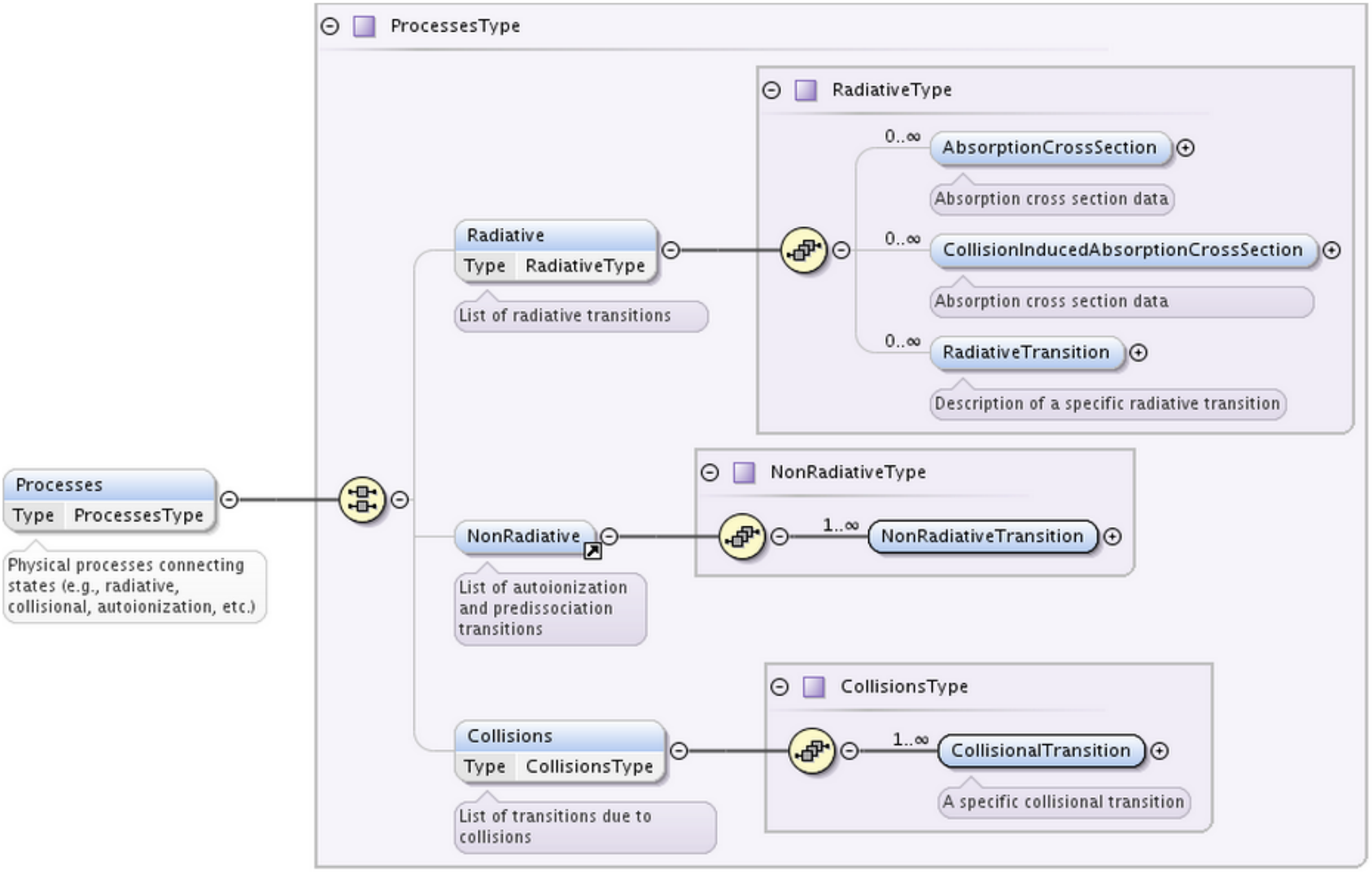
XSAMS structure : root element



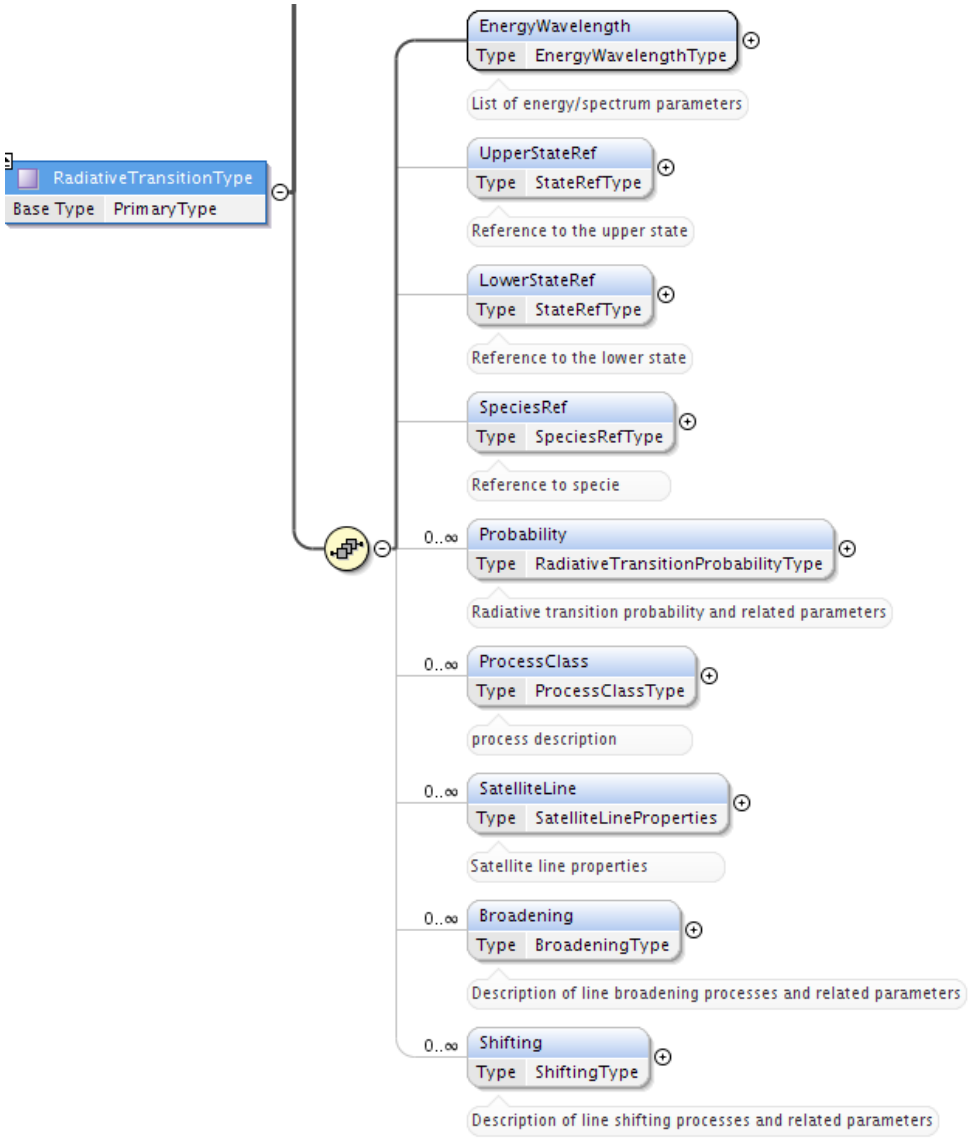
XSAMS structure : species element



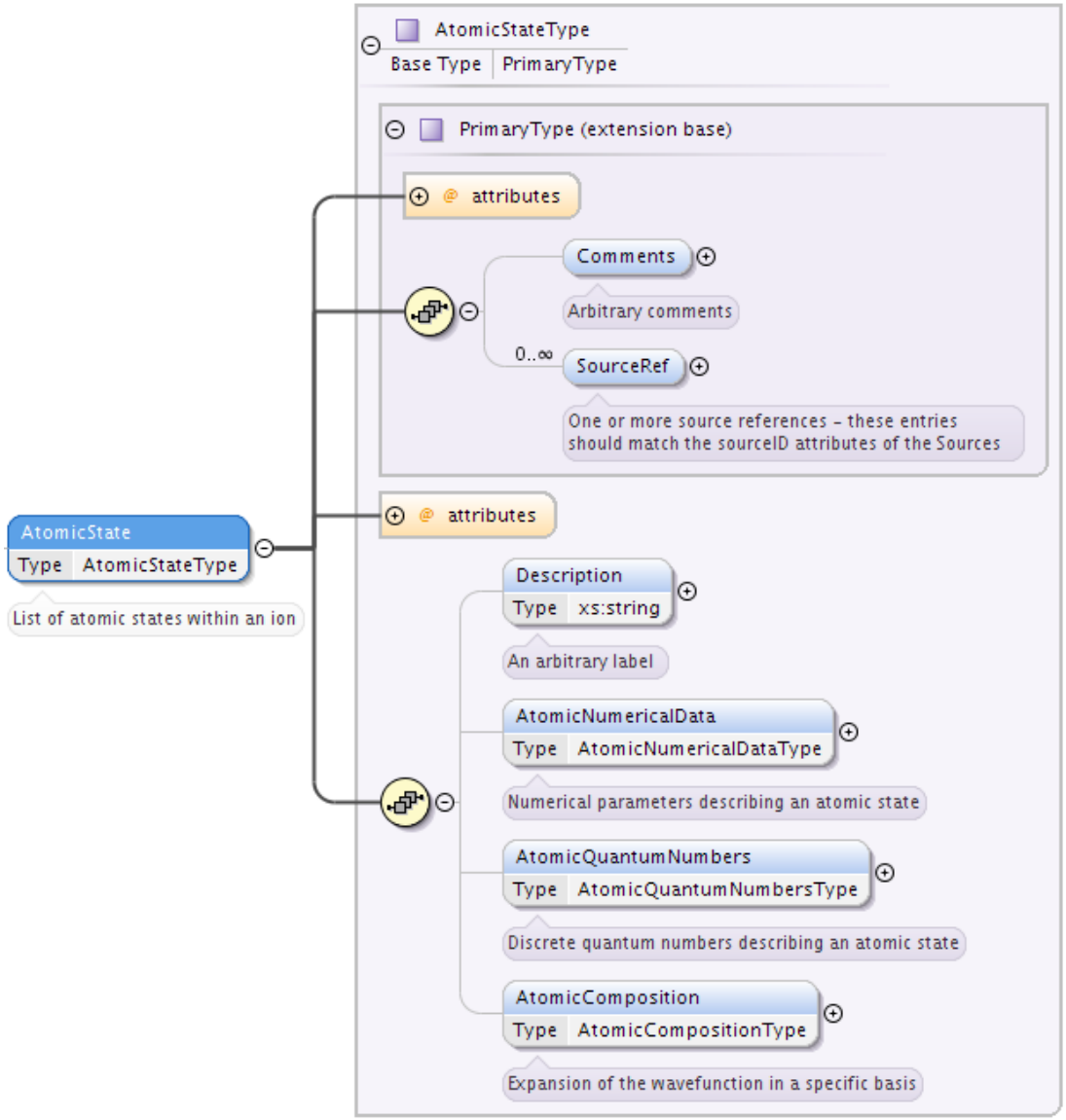
XSAMS structure : processes element



Radiative transition



Atomic State



Radiative transition

```
<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

Species identification

- It is done thanks to InChIKey
- 27 characters string, SHA-256 hash of InchI description of the species
- IUPAC International Chemical Identifier, standard way to encode molecular information
- We have a species database to do the mapping between InChIKeys and molecule names
- The DB contains link between isotopes of a species
- Example on the portal (not used for atoms)

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XSAMS Processors

- They are 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

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

- As they are registered in the VAMDC registry, they must provide VOS capabilities functionnality

- They provide a simple web interface to upload XSAMS files and or be calle 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 documer then stays available on the server with this id

Current Processors

- Bibtex : extract references informations from a XSAMS document and returns them in 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

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

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

Transformation result example

Menu

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

Sources

Id	Title	Origin	Authors	Year	Link
BTopbase-19	Atomic data for opacity calculations. VII - Energy levels, f values and photoionisation cross sections for He-like ions	journal : Journal of Physics B Atomic Molecular Physics (Vol : 20 , Page Begin : 6457 , Page End : 6476)	Fernley, J. A.; Seaton, M. J.; Taylor, K. T.;	1987	http://cdsads.u-strasbg.fr/abs/1987JPhB...20.6457F
BTopbase-26		journal : unpublished	Seaton, M. J.;	1995	http://xsams-processors.obspm.fr/applyXSL/atomicxsams2html/result/1021

Results from Topbase VAMDC node

Unselect all	Spec Ion	Wavelength(A)	A	Weighted Oscillator Strength	Lower state source	Lower energy(Ry)	Lower ionization(Ry)	Lower lifetime	Lower statistical weight	Lower parity	Lower mixing coeff	Lower configuration	Lower term label	Lower coupling	Upper state source	Upper energy(Ry)	Upper ionization(Ry)	Upper lifetime	Upper statistical weight	Upper parity	Upper mixing coeff	Upper configuration	Upper term label	Upper coupling
☑	He 2	303.797315958	20043477020.3	0.832	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.0	1.0	0.0	6	odd	1.0	2p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	256.328953298	5346620510.16	0.158	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.555556	0.444444	0.0	6	odd	1.0	3p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	243.037852766	2183221280.01	0.058	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.75	0.25	0.0	6	odd	1.0	4p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	237.341653092	1101219463.61	0.0279	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.84	0.16	0.0	6	odd	1.0	5p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	234.357922757	631513908.254	0.0156	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.888889	0.111111	0.0	6	odd	1.0	6p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	232.59481688	395770867.642	0.00963	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.9183674	0.0816326	0.0	6	odd	1.0	7p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	231.464621682	264355160.481	0.00637	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.9375	0.0625	0.0	6	odd	1.0	8p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	230.696085868	185072066.972	0.00443	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.9506173	0.0493827	0.0	6	odd	1.0	9p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	230.149481786	134741888.818	0.00321	BTopbase-26	0.0	4.0	0.0	2	even	1.0	1s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.96	0.04	0.0	6	odd	1.0	10p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	1640.50419377	718757126.967	0.87	BTopbase-26	3.0	1.0	0.0	2	even	1.0	2s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.555556	0.444444	0.0	6	odd	1.0	3p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	1215.18926383	310167988.746	0.206	BTopbase-26	3.0	1.0	0.0	2	even	1.0	2s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.75	0.25	0.0	6	odd	1.0	4p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	1084.99041413	158462958.42	0.0839	BTopbase-26	3.0	1.0	0.0	2	even	1.0	2s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.84	0.16	0.0	6	odd	1.0	5p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	1025.31581319	91577795.9217	0.0433	BTopbase-26	3.0	1.0	0.0	2	even	1.0	2s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.888889	0.111111	0.0	6	odd	1.0	6p	2Podd	L=1 S=0.5 Multiplicity=2
☑	He 2	992.404508123	57567891.7302	0.0255	BTopbase-26	3.0	1.0	0.0	2	even	1.0	2s	2Seven	L=0 S=0.5 Multiplicity=2	BTopbase-26	3.9183674	0.0816326	0.0	6	odd	1.0	7p	2Podd	L=1 S=0.5 Multiplicity=2