Dictionary specifications

Abstract: This document describes the list of global keywords used in VAMDC software.
Version History

<table>
<thead>
<tr>
<th>Version</th>
<th>Date</th>
<th>Modified By</th>
<th>Description of Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>V0.1</td>
<td>23/05/2011</td>
<td>M.Doronin</td>
<td>first draft</td>
</tr>
<tr>
<td>V0.2</td>
<td>03/06/2011</td>
<td>M.Doronin</td>
<td>corrections based on feedback</td>
</tr>
</tbody>
</table>

Disclaimer

The information in this document is subject to change without notice. Company or product names mentioned in this document may be trademarks or registered trademarks of their respective companies.

All rights reserved

The document is proprietary of the VAMDC consortium members. No copying or distributing, in any form or by any means, is allowed without the prior written agreement of the owner of the property rights.

This document reflects only the authors’ view. The European Community is not liable for any use that may be made of the information contained herein.

Acknowledgements

VAMDC is funded under the “Combination of Collaborative Projects and Coordination and Support Actions” Funding Scheme of The Seventh Framework Program. Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure. Grant Agreement number: 239108.
# CONTENTS

1 The VAMDC keywords
   1.1 Keywords origin ........................................... 1
   1.2 Keywords use ............................................. 1
   1.3 Use of Keywords for the Registry ............................. 1
   1.4 Units ...................................................... 2

2 Requestables .............................. 3
   2.1 Collisions ............................................... 3
   2.2 Methods ............................................... 3
   2.3 NonRadiativeTransitions ................................. 3
   2.4 Processes ............................................. 3
   2.5 RadiativeTransitions .................................. 3
   2.6 Sources ............................................... 3
   2.7 Species .................................................. 3
   2.8 States ................................................... 4

3 Restrictables .......................... 5
   3.1 AsOfDate ................................................. 5
   3.2 AtomInchi ................................................ 5
   3.3 AtomInchiKey ............................................ 5
   3.4 AtomIonCharge ........................................... 5
   3.5 AtomMass ................................................ 5
   3.6 AtomMassNumber ........................................ 6
   3.7 AtomNuclearCharge ...................................... 6
   3.8 AtomNuclearSpin ......................................... 6
   3.9 AtomStateCoupling ..................................... 6
   3.10 AtomStateEnergy ....................................... 6
   3.11 AtomStateHyperfineMomentum ............................ 6
   3.12 AtomStateID ............................................ 6
   3.13 AtomStateIonizationEnergy ............................. 7
   3.14 AtomStateKappa ........................................ 7
   3.15 AtomStateLandeFactor ................................ 7
   3.16 AtomStateLifeTime .................................... 7
   3.17 AtomStateMagneticQuantumNumber ......................... 7
   3.18 AtomStateMixingCoefficient ............................ 7
   3.19 AtomStateParity ....................................... 7
   3.20 AtomStatePolarizability ................................ 8
   3.21 AtomStateQuantumDefect ................................ 8
   3.22 AtomStateStatisticalWeight .............................. 8
   3.23 AtomSymbol ............................................. 8
   3.24 CollisionIAEACode ..................................... 8
   3.25 CollisionThreshold .................................... 8
   3.26 EnvironmentSpeciesConcentration ......................... 8
In VAMDC, different pieces of software need to communicate to each other. Apart from protocols and schema, a common vocabulary is needed. By this we mean a list of “global keywords” that should consist of reasonably short, human-readable keywords which uniquely define a certain type of information or data. In the following we describe how the keywords were created and how they are used in different parts of VAMDC software. The common gain in the various aspects is that the vocabulary allows to split the tasks that are common to all data sets from the database-specific information and routines. Thereby it becomes possible to implement software that can be re-used by multiple datasets, reducing the deployment on a new data set to implementing the parts that are truly specific for it.

1.1 Keywords origin

In order to compile a list of well-defined names for all kinds of information that VAMDC datasets can contain, we started from the XSAMS schema for atomic and molecular data, that is used as a main data model within the project.

Flattened and stripped, xsams-derived keywords took form like AtomStateLandeFactor, SourceAuthorName, MolecularSpeciesIonCharge.

The keywords representing desired branches of XSAMS like Species, Processes, RadiativeTransitions, Collisions were added, those would find use in future VSS2 query language.

1.2 Keywords use

The VAMDC keywords form three overlapping subsets:

- **Restrictables**, used in registries and in VSS query language, any client software and VAMDC user portal must use them to be able to request the data from VAMDC.

- **Returnables** that are currently used in registries and internally in the Django TAP-VAMDC service implementation, they define placeholders in XSAMS tree for user data output.

- **Requestables** that are due to be added to the VSS2 version of the query language. They would describe the branches of the XSAMS schema client wants to see in the output document produced by the service.

1.3 Use of Keywords for the Registry

The two aforementioned dictionaries RETURNABLES and RESTRICTABLES contain the most important information about each data set in the form of global keywords: what kind of data is contained in the database and which of these make sense to restrict in the query. By using only the keys in these key-value pairs we can compile this information in a format (XML-template) that the registry understands. Once this extension to the registry is specified, the portal will be able to decide from the information in the registry which databases might have a sensible answer to a particular query and only send it to these.
1.4 Units

In data model VAMDC does not enforce the use of a certain unit for a certain physical quantity. However, in order to make queries understood by all nodes, the keywords that are used as RESTRICTABLE have a default unit, which is the one used in the query. This means that each node must be aware and convert the query to its internal unit before executing the query. For returned data the node is free to use whatever applicable units from XSAMS UnitsType.
REQUESTABLES

Requestables, a future part of the VSS2 query language, defines a user-selectable branches of XSAMS schema for output. For example, client could request only species information, without any process data.

2.1 Collisions

collisional process data

2.2 Methods

method information

2.3 NonRadiativeTransitions

non-radiative transitions data

2.4 Processes

data for all available processes

2.5 RadiativeTransitions

radiative transitions data

2.6 Sources

source reference information

2.7 Species

only brief species information, without states
2.8 States

complete states information
The following keywords may be used as restrictables in TAP-VAMDC queries using VSS1 language, also they are added to registry for each new node.

Note that each node supports only a small subset of the keywords. The list of supported keywords may be retrieved through VOSI Capabilities service endpoint. See the TAP-VAMDC documentation for further details.

3.1 AsOfDate

Return data excluding any additions or improvements that were made after the given date (YYYY-MM-DD). This allows for reproducing an earlier query. Note that probably not all nodes support this.

Type: string

Constraints:

3.2 AtomInchi

Type: string

Constraints:

3.3 AtomInchiKey

Type: string

Constraints:

3.4 AtomIonCharge

Ionization stage with 0 for neutral

Type: integer number

Constraints: >=0

3.5 AtomMass

Atomic mass in Daltons, which is the same as the unified mass units (1Da = 1u = 1.660 538 86 (28) e-27)

Units: u
3.6 AtomMassNumber

Units: u
Type: integer number
Constraints:

3.7 AtomNuclearCharge

Atomic number or nuclear charge
Type: integer number
Constraints: >0

3.8 AtomNuclearSpin

Type: floating-point number
Constraints:

3.9 AtomStateCoupling

Type: string
Constraints:

3.10 AtomStateEnergy

Energy of the level
Type: floating-point number
Constraints: >=0

3.11 AtomStateHyperfineMomentum

Type: floating-point number
Constraints:

3.12 AtomStateID

ID for an atomic state, e.g. for linking a process to the state
Type: string
Constraints:
3.13 AtomStateIonizationEnergy

Ionization energy in eV
Type: floating-point number
Constraints: >0

3.14 AtomStateKappa

Type: floating-point number
Constraints:

3.15 AtomStateLandeFactor

Lande factor
Type: floating-point number
Constraints:

3.16 AtomStateLifeTime

Life time of an atomic state in s.
Units: s
Type: floating-point number
Constraints: >0

3.17 AtomStateMagneticQuantumNumber

Type: floating-point number
Constraints:

3.18 AtomStateMixingCoefficient

Type: floating-point number
Constraints:

3.19 AtomStateParity

Type: string
Constraints:
3.20  AtomStatePolarizability

Type: floating-point number

Constraints:

3.21  AtomStateQuantumDefect

Type: floating-point number

Constraints:

3.22  AtomStateStatisticalWeight

Type: floating-point number

Constraints:

3.23  AtomSymbol

Atomic name

Type: string

Constraints:

3.24  CollisionIAEACode

Type: string

Constraints:

3.25  CollisionThreshold

Type: floating-point number

Constraints:

3.26  EnvironmentSpeciesConcentration

Type: floating-point number

Constraints:

3.27  EnvironmentSpeciesMoleFraction

Type: floating-point number

Constraints:
3.28 EnvironmentSpeciesPartialPressure

Type: floating-point number

Constraints:

3.29 EnvironmentTemperature

Environment temperature

Units: K

Type: floating-point number

Constraints: >0

3.30 EnvironmentTotalNumberDensity

Units: 1/cm3

Type: floating-point number

Constraints:

3.31 EnvironmentTotalPressure

Environment total pressure

Units: bar

Type: floating-point number

Constraints: >0

3.32 FunctionID

Type: string

Constraints:

3.33 FunctionName

Type: string

Constraints:

3.34 InchiKey

International Chemical Identifier (InChI) key (27-character or 14-character first part)

Type: string

Constraints:
3.35 MoleculeChemicalName

Conventional molecule name, e.g. CO2, NH3, Feh (may not be unique)
Type: string
Constraints:

3.36 MoleculeInchi

Type: string
Constraints:

3.37 MoleculeInchiKey

Type: string
Constraints:

3.38 MoleculeMolecularWeight

Type: floating-point number
Constraints:

3.39 MoleculeNormalModeHarmonicFrequency

Type: floating-point number
Constraints:

3.40 MoleculeNormalModeIntensity

Type: floating-point number
Constraints:

3.41 MoleculeStateCharacLifeTime

Molecular state lifetime in seconds
Units: s
Type: floating-point number
Constraints: >0
3.42 MoleculeStateCharacNuclearSpinSymmetry

Type: string
Constraints: (ortho|para|A|E|none)

3.43 MoleculeStateEnergy

Type: floating-point number
Constraints:

3.44 MoleculeStateID

Type: string
Constraints:

3.45 MoleculeStoichiometricFormula

Molecular stoichiometric formula
Type: string
Constraints:

3.46 NonRadTranEnergy

Type: floating-point number
Constraints:

3.47 NonRadTranProbability

Type: floating-point number
Constraints:

3.48 NonRadTranWidth

Type: floating-point number
Constraints:

3.49 NormalModeSymmetry

The character of the irreducible representation for this vibrational normal mode in the molecular point group
Type: string
Constraints:
3.50 RadTransBandCentre

Type: floating-point number
Constraints:

3.51 RadTransBandWidth

Type: floating-point number
Constraints:

3.52 RadTransEffectiveLandeFactor

Effective Lande factor for a given transition
Type: floating-point number
Constraints:

3.53 RadTransEnergy

Type: floating-point number
Constraints:

3.54 RadTransFrequency

Type: floating-point number
Constraints:

3.55 RadTransProbabilityA

Type: floating-point number
Constraints:

3.56 RadTransProbabilityIdealisedIntensity

Type: floating-point number
Constraints:

3.57 RadTransProbabilityLineStrength

Type: floating-point number
Constraints:
3.58  **RadTransProbabilityLog10WeightedOscillatorStrength**

Type: floating-point number

**Constraints:**

3.59  **RadTransProbabilityOscillatorStrength**

Type: floating-point number

**Constraints:**

3.60  **RadTransProbabilityWeightedOscillatorStrength**

Type: floating-point number

**Constraints:**

3.61  **RadTransWavelength**

Units: Å

Type: floating-point number

**Constraints:**

3.62  **RadTransWavenumber**

Type: floating-point number

**Constraints:**

3.63  **SourceCategory**

Type of publication, e.g. journal, book etc.

Type: string

**Constraints:** Journal | Book | Proceedings | On-line

3.64  **SourceYear**

Publication Year

Type: integer number

**Constraints:** >0
The following keywords are used as **Returnables** in Django implementation of TAP-VAMDC node software. **Returnables** is an internal concept of the Django implementation, defining the names of the placeholders in the schema, where data producer may put his data. There is no requirement for other implementations of VAMDC-TAP to include support for them. Some of the keywords suppose additional suffixes that allows them to be expanded into **DataType** xsams object. For further information see the Django TAP-VAMDC documentation.

Another use case of returnables is the possibility to determine if it make sense to look for a certain piece of data in the output documents of the node. But even if the node declares that it has that kind of data in its output, there is no guarantee that it will be present in a response for a particular query.

### 4.1 Implicit Returnables

For the sake of not exploding the list below, keywords of a certain type are omitted. These are the ones that belong to a **DataType** in the XSAMS schema. A DataType has a value (the physical quantity itself) and can have units, comments, a method, references and an accuracy in different formats. Therefore, if a keyword *SomeKeyword* is marked as a DataType, the following words can also be used as Returnables, even though they are not listed below.

- SomeKeywordUnit
- SomeKeywordRef
- SomeKeywordComment
- SomeKeywordMethod
- SomeKeywordAccuracyCalibration
- SomeKeywordAccuracyQuality
- SomeKeywordAccuracySystematic
- SomeKeywordAccuracySystematicConfidence
- SomeKeywordAccuracySystematicRelative
- SomeKeywordAccuracyStatistical
- SomeKeywordAccuracyStatisticalConfidence
- SomeKeywordAccuracyStatisticalRelative
- SomeKeywordAccuracyStatLow
- SomeKeywordAccuracyStatLowConfidence
- SomeKeywordAccuracyStatLowRelative
- SomeKeywordAccuracyStatHigh
- SomeKeywordAccuracyStatHighConfidence
- SomeKeywordAccuracyStatHighRelative
4.2 The list of Returnables

4.2.1 AtomInchi

Type: string

Constraints:

4.2.2 AtomInchiKey

Type: string

Constraints:

4.2.3 AtomIonCharge

Ionization stage with 0 for neutral

Type: integer number

Constraints: >=0

4.2.4 AtomMass

Atomic mass in Daltons, which is the same as the unified mass units (1Da = 1u = 1.660 538 86 (28) e-27)

Units: u

Type: floating-point number

Has DataType suffixes support

Constraints: >1

4.2.5 AtomMassNumber

Units: u

Type: integer number

Constraints:

4.2.6 AtomNuclearCharge

Atomic number or nuclear charge

Type: integer number

Constraints: >0

4.2.7 AtomNuclearSpin

Type: floating-point number

Constraints:
4.2.8 AtomSpeciesID

Type: string
Constraints:

4.2.9 AtomStateComponentComments

Type: string
Constraints:

4.2.10 AtomStateComponentMethod

Type: string
Constraints:

4.2.11 AtomStateComponentRef

Type: string
Constraints:

4.2.12 AtomStateCompositionComments

Type: string
Constraints:

4.2.13 AtomStateConfigurationLabel

Type: string
Constraints:

4.2.14 AtomStateConfigurationLabel

Type: string
Constraints:

4.2.15 AtomStateCoreTermJ1J2

Type: integer number
Constraints:

4.2.16 AtomStateCoreTermJJ

Type: integer number
Constraints:
4.2.17 AtomStateCoreTermJKJ

Type: integer number

Constraints:

4.2.18 AtomStateCoreTermJKS

Type: integer number

Constraints:

4.2.19 AtomStateCoreTermK

Type: integer number

Constraints:

4.2.20 AtomStateCoreTermLKK

Type: integer number

Constraints:

4.2.21 AtomStateCoreTermLKL

Type: integer number

Constraints:

4.2.22 AtomStateCoreTermLKLsymbol

Type: integer number

Constraints:

4.2.23 AtomStateCoreTermLKS2

Type: integer number

Constraints:

4.2.24 AtomStateCoreTermLSL

Type: integer number

Constraints:

4.2.25 AtomStateCoreTermLSLSymbol

Type: string

Constraints:

4.2. The list of Returnables
4.2.26 AtomStateCoreTermLSMultiplicity

Type: integer number

Constraints:

4.2.27 AtomStateCoreTermLSSeniority

Type: integer number

Constraints:

4.2.28 AtomStateCoreTermLabel

Type: string

Constraints:

4.2.29 AtomStateCoreTermS

Type: integer number

Constraints:

4.2.30 AtomStateCoreTotalAngMom

Type: integer number

Constraints:

4.2.31 AtomStateCoupling

Type: string

Constraints:

4.2.32 AtomStateDescription

Good luck

Type: string

Constraints:

4.2.33 AtomStateElementCore

Type: string

Constraints:

4.2. The list of Returnables
4.2.34 AtomStateEnergy

Energy of the level
Type: floating-point number
Has DataTypes suffixes support
Constraints: >=0

4.2.35 AtomStateHyperfineConstantA

Hyperfine splitting due to magnetic dipole interaction
Type: floating-point number
Has DataTypes suffixes support
Constraints:

4.2.36 AtomStateHyperfineConstantB

Hyperfine splitting due to electric quadrupole interaction
Type: floating-point number
Has DataTypes suffixes support
Constraints:

4.2.37 AtomStateHyperfineMomentum

Type: floating-point number
Constraints:

4.2.38 AtomStateID

ID for an atomic state, e.g. for linking a process to the state
Type: string
Constraints:

4.2.39 AtomStateIonizationEnergy

Ionization energy in eV
Type: floating-point number
Has DataTypes suffixes support
Constraints: >0

4.2.40 AtomStateK

Type: string
Constraints:
4.2.41 AtomStateKappa
Type: floating-point number
Constraints:

4.2.42 AtomStateL
Type: string
Constraints:

4.2.43 AtomStateLandeFactor
Lande factor
Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.44 AtomStateLifeTime
Life time of an atomic state in s.
Units: s
Type: floating-point number
Has DataType suffixes support
Constraints: >0

4.2.45 AtomStateMagneticQuantumNumber
Type: floating-point number
Constraints:

4.2.46 AtomStateMixingCoeff
Type: string
Constraints:

4.2.47 AtomStateMixingCoeffClass
Type: string
Constraints:

4.2.48 AtomStateMixingCoeffClass
Type: string
Constraints:
4.2.49 AtomStateMixingCoefficient

Type: floating-point number

Constraints:

4.2.50 AtomStateParity

Type: string

Constraints:

4.2.51 AtomStatePolarizability

Type: floating-point number
Has DataType suffixes support

Constraints:

4.2.52 AtomStateQuantumDefect

Type: floating-point number
Has DataType suffixes support

Constraints:

4.2.53 AtomStateRef

Type: string

Constraints:

4.2.54 AtomStateS

Type: string

Constraints:

4.2.55 AtomStateS2

Type: string

Constraints:

4.2.56 AtomStateShellID

Type: string

Constraints:

4.2.57 AtomStateShellKappa

Type: floating-point number

Constraints:
4.2.58 AtomStateShellNumberOfElectrons
Type: integer number
Constraints:

4.2.59 AtomStateShellOrbitalAngMom
Type: integer number
Constraints:

4.2.60 AtomStateShellOrbitalAngMomSymbol
Type: string
Constraints:

4.2.61 AtomStateShellPairID
Type: string
Constraints:

4.2.62 AtomStateShellPairShell1ID
Type: string
Constraints:

4.2.63 AtomStateShellPairShell1Kappa
Type: floating-point number
Constraints:

4.2.64 AtomStateShellPairShell1NumberOfElectrons
Type: integer number
Constraints:

4.2.65 AtomStateShellPairShell1OrbitalAngMom
Type: integer number
Constraints:

4.2.66 AtomStateShellPairShell1OrbitalAngmomSymbol
Type: string
Constraints:
4.2.67 AtomStateShellPairShell1Parity
Type: string
Constraints:

4.2.68 AtomStateShellPairShell1QN
Type: integer number
Constraints:

4.2.69 AtomStateShellPairShell1TermJ1J2
Type: integer number
Constraints:

4.2.70 AtomStateShellPairShell1TermJJ
Type: integer number
Constraints:

4.2.71 AtomStateShellPairShell1TermJKJ
Type: integer number
Constraints:

4.2.72 AtomStateShellPairShell1TermJKS
Type: integer number
Constraints:

4.2.73 AtomStateShellPairShell1TermK
Type: integer number
Constraints:

4.2.74 AtomStateShellPairShell1TermLKK
Type: integer number
Constraints:

4.2.75 AtomStateShellPairShell1TermLKL
Type: integer number
Constraints:
4.2.76 AtomStateShellPairShell1TermLKLSymbol

Type: string
Constraints:

4.2.77 AtomStateShellPairShell1TermLKS2

Type: integer number
Constraints:

4.2.78 AtomStateShellPairShell1TermLSL

Type: integer number
Constraints:

4.2.79 AtomStateShellPairShell1TermLSLSymbol

Type: string
Constraints:

4.2.80 AtomStateShellPairShell1TermLSMultiplicity

Type: integer number
Constraints:

4.2.81 AtomStateShellPairShell1TermLSSeniority

Type: integer number
Constraints:

4.2.82 AtomStateShellPairShell1TermLabel

Type: string
Constraints:

4.2.83 AtomStateShellPairShell1TermS

Type: integer number
Constraints:

4.2.84 AtomStateShellPairShell1TotalAngMom

Type: integer number
Constraints:
4.2.85 AtomStateShellPairShell2ID
Type: string
Constraints:

4.2.86 AtomStateShellPairShell2Kappa
Type: floating-point number
Constraints:

4.2.87 AtomStateShellPairShell2NumberOfElectrons
Type: integer number
Constraints:

4.2.88 AtomStateShellPairShell2OrbitalAngMom
Type: integer number
Constraints:

4.2.89 AtomStateShellPairShell2OrbitalAngMomSymbol
Type: string
Constraints:

4.2.90 AtomStateShellPairShell2Parity
Type: string
Constraints:

4.2.91 AtomStateShellPairShell2QN
Type: integer number
Constraints:

4.2.92 AtomStateShellPairShell2TermJ1J2
Type: integer number
Constraints:

4.2.93 AtomStateShellPairShell2TermJJ
Type: integer number
Constraints:
4.2.94 **AtomStateShellPairShell2TermJKJ**

Type: integer number

Constraints:

4.2.95 **AtomStateShellPairShell2TermJKS**

Type: integer number

Constraints:

4.2.96 **AtomStateShellPairShell2TermJKS**

Type: integer number

Constraints:

4.2.97 **AtomStateShellPairShell2TermK**

Type: integer number

Constraints:

4.2.98 **AtomStateShellPairShell2TermLKK**

Type: integer number

Constraints:

4.2.99 **AtomStateShellPairShell2TermLKL**

Type: integer number

Constraints:

4.2.100 **AtomStateShellPairShell2TermLKL**

Type: integer number

Constraints:

4.2.101 **AtomStateShellPairShell2TermLKLSymbol**

Type: integer number

Constraints:

4.2.102 **AtomStateShellPairShell2TermLKS2**

Type: integer number

Constraints:
4.2.103 AtomStateShellPairShell2TermLSLSymbol

Type: integer number

Constraints:

4.2.104 AtomStateShellPairShell2TermLSMultiplicity

Type: integer number

Constraints:

4.2.105 AtomStateShellPairShell2TermLSSeniority

Type: integer number

Constraints:

4.2.106 AtomStateShellPairShell2TermLabel

Type: string

Constraints:

4.2.107 AtomStateShellPairShell2TermS

Type: integer number

Constraints:

4.2.108 AtomStateShellPairShell2TotalAngMom

Type: integer number

Constraints:

4.2.109 AtomStateShellPairTermJ1J2

Type: integer number

Constraints:

4.2.110 AtomStateShellPairTermJJ

Type: integer number

Constraints:

4.2.111 AtomStateShellPairTermJKJ

Type: integer number

Constraints:
4.2.112 AtomStateShellPairTermJKS
Type: integer number
Constraints:

4.2.113 AtomStateShellPairTermK
Type: integer number
Constraints:

4.2.114 AtomStateShellPairTermLKK
Type: integer number
Constraints:

4.2.115 AtomStateShellPairTermLKL
Type: integer number
Constraints:

4.2.116 AtomStateShellPairTermLKLSTSymbol
Type: integer number
Constraints:

4.2.117 AtomStateShellPairTermLKS2
Type: integer number
Constraints:

4.2.118 AtomStateShellPairTermLSL
Type: integer number
Constraints:

4.2.119 AtomStateShellPairTermLSLSTSymbol
Type: integer number
Constraints:

4.2.120 AtomStateShellPairTermLSMultiplicity
Type: integer number
Constraints:

4.2. The list of Returnables
4.2.121 AtomStateShellPairTermLSSeniority
Type: integer number
Constraints:

4.2.122 AtomStateShellPairTermLabel
Type: string
Constraints:

4.2.123 AtomStateShellPairTermS
Type: integer number
Constraints:

4.2.124 AtomStateShellParity
Type: integer number
Constraints:

4.2.125 AtomStateShellPrincipalQN
Type: integer number
Constraints:

4.2.126 AtomStateShellTermJ1J2
Type: integer number
Constraints:

4.2.127 AtomStateShellTermJJ
Type: integer number
Constraints:

4.2.128 AtomStateShellTermJKJ
Type: integer number
Constraints:

4.2.129 AtomStateShellTermJKS
Type: integer number
Constraints:
4.2.130 AtomStateShellTermK
Type: integer number
Constraints:

4.2.131 AtomStateShellTermLKK
Type: integer number
Constraints:

4.2.132 AtomStateShellTermLKL
Type: integer number
Constraints:

4.2.133 AtomStateShellTermLKLSymbol
Type: string
Constraints:

4.2.134 AtomStateShellTermLKS2
Type: integer number
Constraints:

4.2.135 AtomStateShellTermLSL
Type: integer number
Constraints:

4.2.136 AtomStateShellTermLSLSymbol
Type: integer number
Constraints:

4.2.137 AtomStateShellTermLSMultiplicity
Type: integer number
Constraints:

4.2.138 AtomStateShellTermLabel
Type: integer number
Constraints:
4.2.139 AtomStateShellTermS
Type: integer number
Constraints:

4.2.140 AtomStateShellTermSeniority
Type: integer number
Constraints:

4.2.141 AtomStateShellTotalAngMom
Type: integer number
Constraints:

4.2.142 AtomStateStatisticalWeight
Type: floating-point number
Constraints:

4.2.143 AtomStateSuperShellNumberOfElectrons
Type: integer number
Constraints:

4.2.144 AtomStateSuperShellPrincipalQN
Type: integer number
Constraints:

4.2.145 AtomStateTotalAngMom
Type: string
Constraints:

4.2.146 AtomSymbol
Atomic name
Type: string
Constraints:

4.2.147 CollisionComment
Type: string
Constraints:
4.2.148 CollisionDataSetComment

Type: string
Constraints:

4.2.149 CollisionDataSetDescription

Type: string
Constraints:

4.2.150 CollisionDataSetMethod

Type: string
Constraints:

4.2.151 CollisionDataSetRef

Type: string
Constraints:

4.2.152 CollisionFitDataAccuracy

Type: string
Constraints:

4.2.153 CollisionFitDataArgumentDescription

Type: string
Constraints:

4.2.154 CollisionFitDataArgumentLowerLimit

Type: string
Constraints:

4.2.155 CollisionFitDataArgumentName

Type: string
Constraints:

4.2.156 CollisionFitDataArgumentUnits

Type: string
Constraints:
4.2.157 CollisionFitDataArgumentUpperLimit

Type: string
Constraints:

4.2.158 CollisionFitDataComment

Type: string
Constraints:

4.2.159 CollisionFitDataFunction

Type: string
Constraints:

4.2.160 CollisionFitDataMethod

Type: string
Constraints:

4.2.161 CollisionFitDataParameter

Type: string
Constraints:

4.2.162 CollisionFitDataPhysicalUncertainty

Type: string
Constraints:

4.2.163 CollisionFitDataProductionDate

Type: string
Constraints:

4.2.164 CollisionFitDataRef

Type: string
Constraints:

4.2.165 CollisionIAEACode

Type: string
Constraints:
4.2.166 CollisionIntermediateSpecies
Type: string
Constraints:

4.2.167 CollisionIntermediateState
Type: string
Constraints:

4.2.168 CollisionMethod
Type: string
Constraints:

4.2.169 CollisionProductSpecies
Type: string
Constraints:

4.2.170 CollisionProductState
Type: string
Constraints:

4.2.171 CollisionRef
Type: string
Constraints:

4.2.172 CollisionSpecies
Type: string
Constraints:

4.2.173 CollisionState
Type: string
Constraints:

4.2.174 CollisionTabulatedDataComment
Type: string
Constraints:
4.2.175 CollisionTabulatedDataMethod
Type: string
Constraints:

4.2.176 CollisionTabulatedDataPhysicalUncertainty
Type: string
Constraints:

4.2.177 CollisionTabulatedDataProductionDate
Type: string
Constraints:

4.2.178 CollisionTabulatedDataRef
Type: string
Constraints:

4.2.179 CollisionTabulatedDataReferenceFrame
Type: string
Constraints:

4.2.180 CollisionTabulatedDataX
Type: floating-point number
Constraints:

4.2.181 CollisionTabulatedDataXDescription
Type: string
Constraints:

4.2.182 CollisionTabulatedDataXError
Type: floating-point number
Constraints:

4.2.183 CollisionTabulatedDataXN
Type: integer number
Constraints:
4.2.184 CollisionTabulatedDataXNegativeError

Type: string
Constraints:

4.2.185 CollisionTabulatedDataXParameter

Type: string
Constraints:

4.2.186 CollisionTabulatedDataXPositiveError

Type: floating-point number
Constraints:

4.2.187 CollisionTabulatedDataXUnits

Type: string
Constraints:

4.2.188 CollisionTabulatedDataY

Type: floating-point number
Constraints:

4.2.189 CollisionTabulatedDataYDescription

Type: string
Constraints:

4.2.190 CollisionTabulatedDataYError

Type: floating-point number
Constraints:

4.2.191 CollisionTabulatedDataYNegativeError

Type: floating-point number
Constraints:

4.2.192 CollisionTabulatedDataYPositiveError

Type: floating-point number
Constraints:
4.2.193 CollisionTabulatedDataYUnits

Type: string
Constraints:

4.2.194 CollisionThreshold

Type: floating-point number
HasDataType suffixes support
Constraints:

4.2.195 CollisionalTabulatedDataYN

Type: floating-point number
Constraints:

4.2.196 CrossSectionBandCentre

Type: floating-point number
HasDataType suffixes support
Constraints:

4.2.197 CrossSectionBandModeComment

Type: string
Constraints:

4.2.198 CrossSectionBandModeDeltaV

List of dV values
Type: floating-point number
Constraints: >0

4.2.199 CrossSectionBandModeDeltaVID

Type: string
Constraints:

4.2.200 CrossSectionBandModeMethod

Type: string
Constraints:
4.2.201 CrossSectionBandModeName

Type: string
Constraints:

4.2.202 CrossSectionBandName

Type: string
Constraints:

4.2.203 CrossSectionBandWidth

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.204 CrossSectionDescription

A string describing the cross section being given in a CrossSection element, e.g. ‘IR absorption cross section’
Type: string
Constraints:

4.2.205 CrossSectionEnvironment

Type: string
Constraints:

4.2.206 CrossSectionID

Type: string
Constraints:

4.2.207 CrossSectionSpecies

Type: string
Constraints:

4.2.208 CrossSectionState

Type: string
Constraints:
4.2.209 CrossSectionX

A list of whitespace-delimited values of the independent variable (e.g. wavelength) against which the cross section is given

Type: string

Constraints:

4.2.210 CrossSectionXDataFile

Datafile containing X data.

Type: string

Constraints:

4.2.211 CrossSectionXError

An error (accuracy) applying to each and every data point in the Cross section independent variable data series

Type: floating-point number

Constraints:

4.2.212 CrossSectionXErrorList

A list of errors (accuracy values), separated by whitespace, one for each of the data points listed in the cross section independent variable data series (e.g. wavenumber)

Type: string

Constraints:

4.2.213 CrossSectionXLinearA0

The coefficient a0 in the linear series \( X_i = a0 + a1.i \) giving the independent variable against which the cross section is given when this data series is an evenly-spaced series of values.

Type: floating-point number

Constraints:

4.2.214 CrossSectionXLinearA0

The coefficient a0 in the linear series \( X_i = a0 + a1.i \) giving the independent variable against which the cross section is given

Type: floating-point number

Constraints:

4.2.215 CrossSectionXName

The name of the independent variable against which the cross section is measured (e.g. wavenumber)

Type: string

Constraints:
4.2.216 CrossSectionXUnit

The units of the independent variable against which the cross section is measured (e.g. 1/cm)

Type: string

Constraints:

4.2.217 CrossSectionY

A whitespace-delimited list of data points comprising the cross section

Type: string

Constraints:

4.2.218 CrossSectionYDataFile

Datafile containing Y data.

Type: string

Constraints:

4.2.219 CrossSectionYError

A single error (accuracy) value applying to each and every data point of the cross section

Type: floating-point number

Constraints:

4.2.220 CrossSectionYErrorList

A white-space delimited list of error (accuracy) values for each data point given for the cross section

Type: string

Constraints:

4.2.221 CrossSectionYLinearA1

The coefficient a1 in the linear series \( Y_i = a0 + a1.i \) giving the independent variable against which the cross section is given when this data series is an evenly-spaced series of values

Type: floating-point number

Constraints:

4.2.222 CrossSectionYLinearA1

The coefficient a1 in the linear series \( Y_i = a0 + a1.i \) giving the independent variable against which the cross section is given

Type: floating-point number

Constraints:
4.2.223 CrossSectionYName

Name of the Cross Section parameter given (e.g. ‘sigma’)
Type: string
Constraints:

4.2.224 CrossSectionYUnit

Units of the cross section (e.g. ‘Mb’, ‘arbitrary’, ‘km/mol’)
Type: string
Constraints:

4.2.225 EnvironmentComment

Type: string
Constraints:

4.2.226 EnvironmentID

Type: string
Constraints:

4.2.227 EnvironmentRef

Type: string
Constraints:

4.2.228 EnvironmentSpecies

Type: string
Constraints:

4.2.229 EnvironmentSpeciesConcentration

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.230 EnvironmentSpeciesMoleFraction

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2. The list of Returnables
4.2.231 EnvironmentSpeciesName
Type: string
Constraints:

4.2.232 EnvironmentSpeciesPartialPressure
Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.233 EnvironmentSpeciesRef
Type: string
Constraints:

4.2.234 EnvironmentTemperature
Environment temperature
Units: K
Type: floating-point number
Has DataType suffixes support
Constraints: >0

4.2.235 EnvironmentTotalNumberDensity
Units: 1/cm3
Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.236 EnvironmentTotalPressure
Environment total pressure
Units: bar
Type: floating-point number
Has DataType suffixes support
Constraints: >0

4.2.237 FunctionArgumentDescription
Type: string
Constraints:
4.2.238 FunctionArgumentLowerLimit

Type: floating-point number

Constraints:

4.2.239 FunctionArgumentName

Type: string

Constraints:

4.2.240 FunctionArgumentUnits

Type: string

Constraints:

4.2.241 FunctionArgumentUpperLimit

Type: floating-point number

Constraints:

4.2.242 FunctionComputerLanguage

Type: string

Constraints:

4.2.243 FunctionDescription

Type: string

Constraints:

4.2.244 FunctionExpression

Type: string

Constraints:

4.2.245 FunctionID

Type: string

Constraints:

4.2.246 FunctionName

Type: string

Constraints:
4.2.247 FunctionParameterDescription
Type: string
Constraints:

4.2.248 FunctionParameterName
Type: string
 Constraints:

4.2.249 FunctionParameterUnits
Type: string
Constraints:

4.2.250 FunctionReferenceFrame
Type: string
Constraints:

4.2.251 FunctionSourceCodeURL
Type: string
Constraints:

4.2.252 FunctionSourceRef
Type: string
Constraints:

4.2.253 FunctionYDescription
Type: string
Constraints:

4.2.254 FunctionYLowerLimit
Type: floating-point number
Constraints:

4.2.255 FunctionYName
Type: string
Constraints:
4.2.256 FunctionYUnits
Type: string
Constraints:

4.2.257 FunctionYUpperLimit
Type: floating-point number
Constraints:

4.2.258 MethodComment
Type: string
Constraints:

4.2.259 MethodRef
Type: string
Constraints:

4.2.260 MoleculeChemicalName
Conventional molecule name, e.g. CO2, NH3, FeH (may not be unique)
Type: string
Constraints:

4.2.261 MoleculeID
Type: string
Constraints:

4.2.262 MoleculeInchi
Type: string
Constraints:

4.2.263 MoleculeInchiKey
Type: string
Constraints:

4.2.264 MoleculeMolecularWeight
Type: floating-point number
Has DataType suffixes support
Constraints:
4.2.265 MoleculeNormalModeHarmonicFrequency

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.266 MoleculeNormalModeIntensity

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.267 MoleculeNuclearSpins

Type: string
Constraints:

4.2.268 MoleculeNuclearSpinsAtomArray

Type: string
Constraints:

4.2.269 MoleculeNuclearSpinsBondArray

Type: string
Constraints:

4.2.270 MoleculeQn

Type: floating-point number
Constraints:

4.2.271 MoleculeQnAttribute

Molecular quantum number attribute(s)
Type: string
Constraints:

4.2.272 MoleculeQnCase

Case name for the case-by-case molecular state description
Type: string
Constraints:
4.2.273 **MoleculeQnComment**

Additional comments for molecular quantum numbers

*Type:* string

*Constraints:*

4.2.274 **MoleculeQnLabel**

Case label for the case-by-case molecular state description

*Type:* string

*Constraints:*

4.2.275 **MoleculeQnStateID**

*Type:* string

*Constraints:*

4.2.276 **MoleculeSpeciesID**

*Type:* string

*Constraints:*

4.2.277 **MoleculeStateCharacLifeTime**

Molecular state lifetime in seconds

*Units:* s

*Type:* floating-point number

Has *DataType* suffixes support

*Constraints:* 

4.2.278 **MoleculeStateCharacNuclearSpinSymmetry**

*Type:* string

*Constraints:* (ortho|para|A|E|none)

4.2.279 **MoleculeStateEnergy**

*Type:* floating-point number

Has *DataType* suffixes support

*Constraints:*

4.2.280 **MoleculeStateID**

*Type:* string

*Constraints:*

### 4.2. The list of Returnables
4.2.281 MoleculeStateQuantumNumbers
Type: string
Constraints:

4.2.282 MoleculeStoichiometricFormula
Molecular stoichiometric formula
Type: string
Constraints:

4.2.283 NodeID
A unique string for each VAMDC node. For example used for xsams-internal referencing. This MUST be filled.
Type: string
Constraints:

4.2.284 NonRadTranComment
Type: string
Constraints:

4.2.285 NonRadTranEnergy
Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.286 NonRadTranFinalState
Final state of the transition
Type: string
Constraints:

4.2.287 NonRadTranInitialState
Initial state of the transition
Type: string
Constraints:

4.2.288 NonRadTranMethod
Type: string
Constraints:
4.2.289 NonRadTranProbability

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.290 NonRadTranRef

Type: string
Constraints:

4.2.291 NonRadTranSpecies

Type: string
Constraints:

4.2.292 NonRadTranType

Type: string
Constraints:

4.2.293 NonRadTranWidth

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.294 NormalModeHarmonicFrequency

The harmonic frequency of a normal mode
Units: 1/cm
Type: floating-point number
Has DataType suffixes support
Constraints: >0

4.2.295 NormalModelIntensity

Intensity of a normal mode
Units: km/mol
Type: floating-point number
Has DataType suffixes support
Constraints: >0
4.2.296 NormalModeSymmetry

The character of the irreducible representation for this vibrational normal mode in the molecular point group

Type: string
Constraints:

4.2.297 RadTransBandCentre

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.298 RadTransBandWidth

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.299 RadTransBroadeningDopplerComment

Type: string
Constraints:

4.2.300 RadTransBroadeningDopplerEnvironment

Type: string
Constraints:

4.2.301 RadTransBroadeningDopplerLineshapeName

Type: string
Constraints:

4.2.302 RadTransBroadeningDopplerLineshapeParameter

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.303 RadTransBroadeningDopplerLineshapeParameterName

Type: string
Constraints:
4.2.304 RadTransBroadeningDopplerMethod
Type: string
Constraints:

4.2.305 RadTransBroadeningDopplerRef
Type: string
Constraints:

4.2.306 RadTransBroadeningInstrumentComment
Type: string
Constraints:

4.2.307 RadTransBroadeningInstrumentEnvironment
Type: string
Constraints:

4.2.308 RadTransBroadeningInstrumentLineshapeName
Type: string
Constraints:

4.2.309 RadTransBroadeningInstrumentLineshapeParameter
Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.310 RadTransBroadeningInstrumentLineshapeParameterName
Type: string
Constraints:

4.2.311 RadTransBroadeningInstrumentMethod
Type: string
Constraints:

4.2.312 RadTransBroadeningInstrumentRef
Type: string
Constraints:
4.2.313 RadTransBroadeningNaturalComment
Type: string
Constraints:

4.2.314 RadTransBroadeningNaturalEnvironment
Type: string
Constraints:

4.2.315 RadTransBroadeningNaturalLineshapeName
Type: string
Constraints:

4.2.316 RadTransBroadeningNaturalLineshapeParameter
A broadening parameter for natural broadening.
Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.317 RadTransBroadeningNaturalLineshapeParameterName
The name of natural broadening parameters.
Type: string
Constraints:

4.2.318 RadTransBroadeningNaturalMethod
Type: string
Constraints:

4.2.319 RadTransBroadeningNaturalRef
Type: string
Constraints:

4.2.320 RadTransBroadeningPressureComment
Type: string
Constraints:
4.2.321 RadTransBroadeningPressureEnvironment

Type: string
Constraints:

4.2.322 RadTransBroadeningPressureLineshapeName

Type: string
Constraints:

4.2.323 RadTransBroadeningPressureLineshapeParameter

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.324 RadTransBroadeningPressureLineshapeParameterName

Type: string
Constraints:

4.2.325 RadTransBroadeningPressureMethod

Type: string
Constraints:

4.2.326 RadTransBroadeningPressureRef

Type: string
Constraints:

4.2.327 RadTransComments

(String)
Type: string
Constraints:

4.2.328 RadTransEffectiveLandeFactor

Effective Lande factor for a given transition
Type: floating-point number
Has DataType suffixes support
Constraints:
4.2.329 RadTransEnergy

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.330 RadTransFinalStateRef

Type: string
Constraints:

4.2.331 RadTransFrequency

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.332 RadTransInitialStateRef

Type: string
Constraints:

4.2.333 RadTransProbabilityA

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.334 RadTransProbabilityIdealisedIntensity

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.335 RadTransProbabilityLineStrength

Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.336 RadTransProbabilityLog10WeightedOscillatorStrength

Type: floating-point number
Has DataType suffixes support
Constraints:
4.2.337 RadTransProbabilityMultipole
Type: string
Constraints:

4.2.338 RadTransProbabilityOscillatorStrength
Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.339 RadTransProbabilityWeightedOscillatorStrength
Type: floating-point number
Has DataType suffixes support
Constraints:

4.2.340 RadTransRefs
Type: string
Constraints:

4.2.341 RadTransShiftingComment
Type: string
Constraints:

4.2.342 RadTransShiftingEnv
Type: string
Constraints:

4.2.343 RadTransShiftingMethod
Type: string
Constraints:

4.2.344 RadTransShiftingParamAccCalib
Type: string
Constraints:

4.2.345 RadTransShiftingParamAccComment
Type: string
Constraints:
4.2.346 RadTransShiftingParamAccMethod
Type: string
Constraints:

4.2.347 RadTransShiftingParamAccQuality
Type: integer number
Constraints: >=0

4.2.348 RadTransShiftingParamAccRef
Type: string
Constraints:

4.2.349 RadTransShiftingParamAccStatHigh
Type: floating-point number
Constraints:

4.2.350 RadTransShiftingParamAccStatHighConfidence
Type: floating-point number
Constraints:

4.2.351 RadTransShiftingParamAccStatHighRelative
Type: string
Constraints:

4.2.352 RadTransShiftingParamAccStatLow
Type: floating-point number
Constraints:

4.2.353 RadTransShiftingParamAccStatLowConfidence
Type: floating-point number
Constraints:

4.2.354 RadTransShiftingParamAccStatLowRelative
Type: string
Constraints:
4.2.355  RadTransShiftingParamAccStatisticalConfidence
Type: floating-point number
Constraints:

4.2.356  RadTransShiftingParamAccStatisticalRelative
Type: string
Constraints:

4.2.357  RadTransShiftingParamAccSystematicConfidence
Type: floating-point number
Constraints:

4.2.358  RadTransShiftingParamAccSystematicRelative
Type: string
Constraints:

4.2.359  RadTransShiftingParamComment
Type: string
Constraints:

4.2.360  RadTransShiftingParamFitArgumentDescription
Type: string
Constraints:

4.2.361  RadTransShiftingParamFitArgumentLowerLimit
Type: floating-point number
Constraints:

4.2.362  RadTransShiftingParamFitArgumentName
List of argument names
Type: string
Constraints:

4.2.363  RadTransShiftingParamFitArgumentUnits
Type: string
Constraints:

4.2. The list of Returnables

57
4.2.364 RadTransShiftingParamFitArgumentUpperLimit
Type: floating-point number
Constraints:

4.2.365 RadTransShiftingParamFitFunction
Type: string
Constraints:

4.2.366 RadTransShiftingParamFitParameter
Type: string
Has DataType suffixes support
Constraints:

4.2.367 RadTransShiftingParamFitParameterName
Type: string
Constraints:

4.2.368 RadTransShiftingParamMethod
Type: string
Constraints:

4.2.369 RadTransShiftingParamName
Type: string
Constraints:

4.2.370 RadTransShiftingParamRef
Type: string
Constraints:

4.2.371 RadTransShiftingParamValue
Shifting parameter value
Type: floating-point number
Constraints:

4.2.372 RadTransShiftingParamValue
Type: floating-point number
Constraints:
4.2.373 RadTransShiftingParamValueUnits

Type: string

Constraints:

4.2.374 RadTransShiftingParamValueUnits

Type: string

Constraints:

4.2.375 RadTransShiftingParamValueUnits

Type: string

Constraints:

4.2.376 RadTransShiftingRef

Type: string

Constraints:

4.2.377 RadTransSpeciesRef

Type: string

Constraints:

4.2.378 RadTransWavelength

Units: A

Type: floating-point number

Has DataType suffixes support

Constraints:

4.2.379 RadTransWavenumber

Type: floating-point number

Has DataType suffixes support

Constraints:

4.2.380 SourceAuthorName

Name of one of the authors

Type: string

Constraints:
4.2.381 SourceCategory
Type of publication, e.g., journal, book etc.
Type: string
Constraints: Journal | Book | Proceedings | On-line

4.2.382 SourceID
Type: string
Constraints:

4.2.383 SourceName
E.g. JQSRT
Type: string
Constraints:

4.2.384 SourcePageBegin
Starting page number
Type: integer number
Constraints: >=0

4.2.385 SourcePageEnd
Type: string
Constraints:

4.2.386 SourceTitle
Full title of the paper
Type: string
Constraints:

4.2.387 SourceURI
Webb link to the publication
Type: string
Constraints:

4.2.388 SourceVolume
Volumen number
Type: integer number
Constraints: >0
4.2.389 SourceYear

Publication Year

**Type:** integer number

**Constraints:** >0
CUSTOM HTTP HEADERS OF TAP-VAMDC

“TAP-VAMDC” is the working title for the emerging data-access services that return data in XSAMS format. To provide the easily-accessible statistics of the response document, several custom HTTP headers were defined. They are reported for both HTTP HEAD and HTTP GET queries to the TAP-VAMDC sync endpoint.

5.1 Statistics

The following headers represent document statistics, all should be integer numbers.

- **VAMDC-COUNT-SPECIES** Total count of the atomic **Ion** and **Molecule** records with distinct SpecieID attribute.
- **VAMDC-COUNT-ATOMS** Count of the atomic **Ion** records with distinct SpecieID attribute.
- **VAMDC-COUNT-MOLECULES** Count of the **Molecule** records with distinct SpecieID attribute.
- **VAMDC-COUNT-SOURCES** Count of distinct **Source** records
- **VAMDC-COUNT-STATES** Count of distinct **State** records, both **AtomicState** and **MolecularState** combined
- **VAMDC-COUNT-COLLISIONS** Count of the **CollisionalTransition** elements of the **Processes** branch of XSAMS.
- **VAMDC-COUNT-RADIATIVE** Count of the **RadiativeTransition** elements of the **Processes** branch of XSAMS.
- **VAMDC-COUNT-NONRADIATIVE** Count of the **NonRadiativeTransition** elements of the **Processes** branch of XSAMS.

With a reasonable database layout the nodes should easily be able to gather these numbers by running COUNT queries on their corresponding tables.

5.2 Volume limitation

A TAP-XSAMS service can limit the amount of data it returns via the synchronous interface, for example to prevent the fetching of the whole database or for performance reasons. The service may then fill the HTTP-header of the response with the field **VAMDC-TRUNCATED** that indicates the percentage

**VAMDC-TRUNCATED**: 2.9 %
5.3 Document size estimate

VAMDC-APPROX-SIZE HTTP header is intended to provide the estimation of the size of the response document. It should return an integer value, representing estimate uncompressed document size in megabytes.