



Dictionary specifications

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

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THE VAMDC KEYWORDS

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

RESTRICTABLES

The following keywords may be used as **restrictables** in TAP-VAMDC queries using VSSI 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 ($1\text{Da} = 1\text{u} = 1.660\,538\,86\,(28)\text{e-}27$)

Units: u

Type: floating-point number

Constraints: >1

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: (ortholparalAlElnone)

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: A

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

RETURNABLES

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 it's 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 ($1\text{Da} = 1\text{u} = 1.660\,538\,86\,(28)\text{e-}27$)

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:

4.2.26 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:

4.2.34 AtomStateEnergy

Energy of the level

Type: floating-point number

Has **DataType** suffixes support

Constraints: ≥ 0

4.2.35 AtomStateHyperfineConstantA

Hyperfine splitting due to magnetic dipole interaction

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.36 AtomStateHyperfineConstantB

Hyperfine splitting due to electric quadrupole interaction

Type: floating-point number

Has **DataType** 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 **DataType** 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 AtomStateShellPairTermLKLSymbol

Type: integer number

Constraints:

4.2.117 AtomStateShellPairTermLKS2

Type: integer number

Constraints:

4.2.118 AtomStateShellPairTermLSL

Type: integer number

Constraints:

4.2.119 AtomStateShellPairTermLSLSymbol

Type: integer number

Constraints:

4.2.120 AtomStateShellPairTermLSMultiplicity

Type: integer number

Constraints:

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

Has **DataType** suffixes support

Constraints:

4.2.195 CollisionalTabulatedDataYN

Type: floating-point number

Constraints:

4.2.196 CrossSectionBandCentre

Type: floating-point number

Has **DataType** 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 a_0 in the linear series $X_i = a_0 + a_1.i$ 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 a_0 in the linear series $X_i = a_0 + a_1.i$ 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 a_1 in the linear series $Y_i = a_0 + a_1.i$ 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 a_1 in the linear series $Y_i = a_0 + a_1.i$ 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:

4.2.231 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: >0

4.2.278 MoleculeStateCharacNuclearSpinSymmetry

Type: string

Constraints: (ortho|para|AlE|none)

4.2.279 MoleculeStateEnergy

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.280 MoleculeStateID

Type: string

Constraints:

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 NormalModeIntensity

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:

4.2.364 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.