Dictionary specifications

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

Version History

Version	Date	Modified By	Description of Change
V0.1	23/05/2011	M.Doronin	first draft
V0.2	03/06/2011	M.Doronin	corrections based on feedback
V11.12	21/12/2011	M.Doronin	update of autogenerated dictionaries

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CONTENTS

CHAPTER

ONE

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.

CHAPTER

TWO

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 AtomStates

Requesting information about atoms, including the states information.

2.2 Atoms

Requesting information about atoms, without their states.

2.3 Collisions

collisional process data

2.4 Functions

2.5 Methods

method information

2.6 MoleculeQuantumNumbers

Request the full molecule information, including states and quantum numbers.

2.7 MoleculeStates

request molecules, including their states but excluding the quantum numbers

2.8 Molecules

Request molecules, without information about their states.

2.9 NonRadiativeTransitions

non-radiative transitions data

2.10 Particles

request particle information only

2.11 Processes

data for all available processes

2.12 RadiativeCrossections

2.13 RadiativeTransitions

radiative transitions data

2.14 Solids

Restrict the search to databases containing information about solids.

2.15 Sources

source reference information

2.16 Species

only brief species information, without states

2.17 States

complete states information

CHAPTER

THREE

RESTRICTABLES

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 AtomMass

The atomic mass is the mass of an atom expressed in unified atomic mass unit u. It is defined as 1/12 of the rest mass of an unbound carbon-12 atom in its nuclear and electronic ground state. 1 u = 1.660538782(83)E-27 kg.

Units: u

Type: floating-point number

Constraints: >1

3.3 AtomMassNumber

Atomic mass number (A), also called mass number or nucleon number, is the total number of protons and neutrons (together known as nucleons) in an atomic nucleus. Because protons and neutrons both are baryons, the mass number A is identical with the baryon number B as of the nucleus as of the whole atom or ion. The mass number is different for each different isotope of a chemical element.

Type: integer number

Constraints: >0

3.4 AtomNuclearCharge

Atomic number or nuclear charge

Type: integer number

Constraints: >0

3.5 AtomNuclearSpin

The total angular momentum of a nucleus, usually represented as I. For electrons spin and orbital angular momentum are treated separately but particles in a nucleus generally behave as a single entity with intrinsic angular momentum I. Associated with each nuclear spin is a nuclear magnetic moment which produces magnetic interactions with its environment.

Type: floating-point number

Constraints:

3.6 AtomStateCoupling

Coupling scheme used to describe the state. Currently five coupling schemes are supported LS, jj, J1J2, jK and LK. For a detailed description of these and other schemes see, e.g., Atomic Spectroscopy at http://physics.nist.gov/Pubs/AtSpec/index.html

Type: string

Constraints:

3.7 AtomStateHyperfineMomentum

Type: floating-point number

Constraints:

3.8 AtomStateIonizationEnergy

Ionization energy in eV

Units: 1/cm

Type: floating-point number

Constraints: >0

3.9 AtomStateKappa

Relativistic correction.

Type: floating-point number

Constraints:

3.10 AtomStateLandeFactor

Lande factor

Type: floating-point number

Constraints:

3.11 AtomStateMagneticQuantumNumber

Magnetic quantum number of a state, can be integer or half-integer, positive and negative.

Type: floating-point number

Constraints:

3.12 AtomStateParity

State parity. Can have values: “even”, “odd” or “undefined”

Type: string

Constraints:

3.13 AtomStatePolarizability

State polarizability.

Type: floating-point number

Constraints:

3.14 AtomStateQuantumDefect

The quantum defect is a correction applied to the potential to account for the fact that the inner electrons do not entirely screen the corresponding charge of the nucleus. It is particularity important for atoms with single electron in the outer shell.

Type: floating-point number

Constraints:

3.15 AtomStateTotalAngMom

Type: integer number

Constraints:

3.16 AtomSymbol

Atomic name

Type: string

Constraints:

3.17 CollisionCode

Type: string

Constraints:

3.18 CollisionIAEACode

Type: string

Constraints:

3.19 EnvironmentSpeciesConcentration

Type: floating-point number

Constraints:

3.20 EnvironmentSpeciesMoleFraction

Type: floating-point number

Constraints:

3.21 EnvironmentSpeciesPartialPressure

Type: floating-point number

Constraints:

3.22 EnvironmentTemperature

Environment temperature

Units: K

Type: floating-point number

Constraints: >0

3.23 EnvironmentTotalNumberDensity

Units: 1/cm3

Type: floating-point number

Constraints:

3.24 EnvironmentTotalPressure

Environment total pressure

Units: Pa

Type: floating-point number

Constraints: >=0

3.25 FunctionID

Type: string

Constraints:

3.26 FunctionName

Type: string

Constraints:

3.27 Inchi

The IUPAC International Chemical Identifier (InChI) is a textual identifier for chemical substances, designed to provide a standard and human-readable way to encode atomic and molecular information and facilitate the search and exchange of such such information in databases and on the web.

Type: string

Constraints:

3.28 InchiKey

InChi key is hashed, fixed-length (currently 27 character) form of International Chemical Identifier (InChI) string describing a given atom/ion/isotope. InChIKeys consist of 14 characters resulting from a hash of the connectivity information of the InChI, followed by a hyphen, followed by 9 characters resulting from a hash of the remaining layers of the InChI, followed by a single character indication the version of InChI used, another hyphen, followed by single checksum character. More information about InChI and InChI Key can be found at http://www.iupac.org/inchi/

Type: string

Constraints:

3.29 IonCharge

Ionization stage with 0 for neutral

Type: integer number

Constraints: >=0

3.30 MethodCategory

Method category. Allowed values are: experiment, theory, ritz, recommended, evaluated, empirical, scalingLaw, semiempirical, compilation, derived

Type: string

Constraints:

3.31 MoleculeChemicalName

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

Type: string

Constraints:

3.32 MoleculeMolecularWeight

Units: u

Type: floating-point number

Constraints:

3.33 MoleculeNormalModeHarmonicFrequency

Units: MHz

Type: floating-point number

Constraints:

3.34 MoleculeProtonation

Type: string

Constraints:

3.35 MoleculeQNJ

Type: string

Constraints:

3.36 MoleculeQNK

Type: string

Constraints:

3.37 MoleculeQNKa

Type: string

Constraints:

3.38 MoleculeQNKc

Type: string

Constraints:

3.39 MoleculeQNv

Type: string

Constraints:

3.40 MoleculeQNv1

Type: string

Constraints:

3.41 MoleculeQNv2

Type: string

Constraints:

3.42 MoleculeQNv3

Type: string

Constraints:

3.43 MoleculeStateNuclearSpinIsomer

Nuclear spin isomer (symetry) of a molecular state.

Type: string

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

3.44 MoleculeStoichiometricFormula

Molecular stoichiometric formula

Type: string

Constraints:

3.45 NonRadTranEnergy

Type: floating-point number

Constraints:

3.46 NonRadTranProbability

Type: floating-point number

Constraints:

3.47 NonRadTranWidth

Type: floating-point number

Constraints:

3.48 NormalModeSymmetry

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

Type: string

Constraints:

3.49 ParticleName

Particle name, one of photon, electron, muon, positron, neutron, alpha, cosmic

Type: string

Constraints:

3.50 Pressure

Pressure as a Restrictable alone. Each node can decide itself how to interpret and treat this, if it makes sense to its data.

Units: Pa

Type: floating-point number

Constraints: >=0

3.51 RadTransBandCentre

Type: floating-point number

Constraints:

3.52 RadTransBandWidth

Type: floating-point number

Constraints:

3.53 RadTransBroadeningDoppler

Only Restrictable (not NULL) to make a query where there is Broadening information.

Type: string

Constraints:

3.54 RadTransBroadeningInstrument

Only Restrictable (not NULL) to make a query where there is Broadening information.

Type: string

Constraints:

3.55 RadTransBroadeningNatural

Only Restrictable (not NULL) to make a query where there is Broadening information.

Type: string

Constraints:

3.56 RadTransBroadeningPressure

Only Restrictable (not NULL) to make a query where there is Broadening information.

Type: string

Constraints:

3.57 RadTransEffectiveLandeFactor

Effective Lande factor for a given transition

Type: floating-point number

Constraints:

3.58 RadTransEnergy

Type: floating-point number

Constraints:

3.59 RadTransFrequency

Type: floating-point number

Constraints:

3.60 RadTransProbabilityA

The Einstein coefficient for spontaneous radiative de-excitation (emission) A.

Units: 1/s

Type: floating-point number

Constraints: >= 0

3.61 RadTransProbabilityIdealisedIntensity

Type: floating-point number

Constraints:

3.62 RadTransProbabilityLineStrength

Line profile-integrated absorption for transition between two energy levels. Line strength K = hν / 4π (n₁ B₁₂ - n₂ B₂₁)

Units: 1/cm

Type: floating-point number

Constraints: >0

3.63 RadTransProbabilityLog10WeightedOscillatorStrength

Type: floating-point number

Constraints:

3.64 RadTransProbabilityOscillatorStrength

Type: floating-point number

Constraints:

3.65 RadTransProbabilityWeightedOscillatorStrength

Type: floating-point number

Constraints:

3.66 RadTransWavelength

Units: A

Type: floating-point number

Constraints:

3.67 RadTransWavenumber

Type: floating-point number

Constraints:

3.68 SourceCategory

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

Type: string

Constraints: Journal | Book | Proceedings | On-line

3.69 SourceYear

Publication Year

Type: integer number

Constraints: >0

3.70 StateEnergy

Energy of the level

Units: 1/cm

Type: floating-point number

Constraints: >=0

3.71 StateLifeTime

Life time of an atomic state in s.

Units: s

Type: floating-point number

Constraints: >0

3.72 StateStatisticalWeight

Type: floating-point number

Constraints:

3.73 Temperature

Temperature as a Restrictable alone. Each node can decide itself how to interpret and treat this, if it makes sense to its data.

Units: K

Type: floating-point number

Constraints: >0

CHAPTER

FOUR

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 possibilty 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

The IUPAC International Chemical Identifier (InChI) is a textual identifier for chemical substances, designed to provide a standard and human-readable way to encode atomic and molecular information and facilitate the search and exchange of such such information in databases and on the web.

Type: string

Constraints:

4.2.2 AtomInchiKey

InChi key is hashed, fixed-length (currently 27 character) form of International Chemical Identifier (InChI) string describing a given atom/ion/isotope. InChIKeys consist of 14 characters resulting from a hash of the connectivity information of the InChI, followed by a hyphen, followed by 9 characters resulting from a hash of the remaining layers of the InChI, followed by a single character indication the version of InChI used, another hyphen, followed by single checksum character. More information about InChI and InChI Key can be found at http://www.iupac.org/inchi/

Type: string

Constraints:

4.2.3 AtomIonCharge

Ionization stage with 0 for neutral

Type: integer number

Constraints: >=0

4.2.4 AtomMass

The atomic mass is the mass of an atom expressed in unified atomic mass unit u. It is defined as 1/12 of the rest mass of an unbound carbon-12 atom in its nuclear and electronic ground state. 1 u = 1.660538782(83)E-27 kg.

Units: u

Type: floating-point number

Has **DataType** suffixes support

Constraints: >1

4.2.5 AtomMassNumber

Atomic mass number (A), also called mass number or nucleon number, is the total number of protons and neutrons (together known as nucleons) in an atomic nucleus. Because protons and neutrons both are baryons, the mass number A is identical with the baryon number B as of the nucleus as of the whole atom or ion. The mass number is different for each different isotope of a chemical element.

Type: integer number

Constraints: >0

4.2.6 AtomNuclearCharge

Atomic number or nuclear charge

Type: integer number

Constraints: >0

4.2.7 AtomNuclearSpin

The total angular momentum of a nucleus, usually represented as l. For electrons spin and orbital angular momentum are treated separately but particles in a nucleus generally behave as a single entity with intrinsic angular momentum I. Associated with each nuclear spin is a nuclear magnetic moment which produces magnetic interactions with its environment.

Type: floating-point number

Constraints:

4.2.8 AtomSpeciesID

Reference key generated by the node software that connects processes and states to specific species. Each such key points at a single Species block in the XSAMS structure,

Type: string

Constraints:

4.2.9 AtomStateComponentComment

Sate description involves particular basis in which the wavefunction can be described by a number of components and corresponding quantum numbers. In this case a comment can be added to each component.

Type: string

Constraints:

4.2.10 AtomStateComponentMethod

Type: string

Constraints:

4.2.11 AtomStateComponentRef

Type: string

Constraints:

4.2.12 AtomStateCompositionComment

Atomic state is describe in particular framework resulting in specific presentation of the wavefunction. This comment is supposed to clarify the basis used for representing the specific state.

Type: string

Constraints:

4.2.13 AtomStateConfigurationLabel

String representing configuration in a condensed form. For instance, one may prefer to make use of a short configuration label 2s2.2p instead of providing details of shell populations etc.

Type: string

Constraints:

4.2.14 AtomStateCoreTermJ1J2

J1 or J2 quantum number for atomic core described in J1J2 coupling.

Type: integer number

Constraints:

4.2.15 AtomStateCoreTermJJ

j quantum number for the jj coupling view of an atomic core.

Type: integer number

Constraints:

4.2.16 AtomStateCoreTermJKJ

J quantum number for the JK coupling view of an atomic core. J can be integer or half-integer.

Type: floating-point number

Constraints:

4.2.17 AtomStateCoreTermJKK

K quantum number for the JK coupling view of an atomic core. K can be integer or half-integer.

Type: floating-point number

Constraints:

4.2.18 AtomStateCoreTermJKS2

S2 quantum number for the JK coupling view of an atomic core. S2 is the spin of the "external" term that couples with K to produce J. S2 is usually half-integer.

Type: floating-point number

Constraints:

4.2.19 AtomStateCoreTermLKK

K quantum number for the LK coupling view of an atomic core. K is the angular momentum of the "final" term is produced by the coupling of the total angular momentum L with the spin of the core S1. K is usually half-integer.

Type: floating-point number

Constraints: >0

4.2.20 AtomStateCoreTermLKL

L quantum number for the LK coupling view of an atomic core. L is the total angular momentum. L is integer.

Type: integer number

Constraints:

4.2.21 AtomStateCoreTermLKLSymbol

Core angular momentum symbol???

For example, “p”.

Type: integer number

Constraints:

4.2.22 AtomStateCoreTermLKS2

S2 quantum number for the LK coupling view of an atomic core. S2 is the spin of the “external” term. S2 is usually half-integer.

Type: floating-point number

Constraints: >0

4.2.23 AtomStateCoreTermLSL

L quantum number for the LS coupling view of an atomic core. L is the total orbital angular momentum of the core which couples to the total spin S to produce J. L is integer.

Type: integer number

Constraints: >=0

4.2.24 AtomStateCoreTermLSLSymbol

For example, “p”.

Type: string

Constraints:

4.2.25 AtomStateCoreTermLSMultiplicity

Multiplicity of the core. Multiplicity is 2*S+1, where S is the total spin of the core.

Type: integer number

Constraints: >0

4.2.26 AtomStateCoreTermLSS

S quantum number for the LS coupling view of an atomic core. S is the total spin which couples with the orbital angular momentum of the core L to produce J. S is integer or half-integer.

Type: floating-point number

Constraints: >=0

4.2.27 AtomStateCoreTermLSSeniority

Seniority for core electrons.

Type: integer number

Constraints: >=0

4.2.28 AtomStateCoreTermLabel

This string element is used to represent an atomic term in a condensed form, if necessary. For instance, one may prefer to make use of a term label 3P instead of separately indicating the term S and L values.

Type: string

Constraints:

4.2.29 AtomStateCoreTotalAngMom

Type: integer number

Constraints:

4.2.30 AtomStateCoupling

Coupling scheme used to describe the state. Currently five coupling schemes are supported LS, jj, J1J2, jK and LK. For a detailed description of these and other schemes see, e.g., Atomic Spectroscopy at http://physics.nist.gov/Pubs/AtSpec/index.html

Type: string

Constraints:

4.2.31 AtomStateDescription

Good luck

Type: string

Constraints:

4.2.32 AtomStateElementCore

Optional AtomicCore element (type AtomicCoreType), that is used to compactly represent the atomic core. For instance, one may prefer to use notation [Ne]3d to describe the excited configuration in a Na-like ion. In this case, it would be sufficient to only indicate the ElementCore element set to "Ne".

Type: string

Constraints:

4.2.33 AtomStateEnergy

Energy of the level

Units: 1/cm

Type: floating-point number

Has **DataType** suffixes support

Constraints: >=0

4.2.34 AtomStateHyperfineConstantA

Hyperfine splitting due to magnetic dipole interaction

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.35 AtomStateHyperfineConstantB

Hyperfine splitting due to electric quadrupole interaction

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.36 AtomStateHyperfineMomentum

Type: floating-point number

Constraints:

4.2.37 AtomStateID

ID for an atomic state, e.g. for linking a process to the state

Type: string

Constraints:

4.2.38 AtomStateIonizationEnergy

Ionization energy in eV

Units: 1/cm

Type: floating-point number

Has **DataType** suffixes support

Constraints: >0

4.2.39 AtomStateKappa

Relativistic correction.

Type: floating-point number

Constraints:

4.2.40 AtomStateLandeFactor

Lande factor

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.41 AtomStateLifeTime

Life time of an atomic state in s.

Units: s

Type: floating-point number

Has **DataType** suffixes support

Constraints: >0

4.2.42 AtomStateMagneticQuantumNumber

Magnetic quantum number of a state, can be integer or half-integer, positive and negative.

Type: floating-point number

Constraints:

4.2.43 AtomStateMixingCoeff

Mixing coefficient is the coefficient in the expansion of a wave function on a specific basis. It could be - squared (non-negative) or signed. The mandatory attribute mixingClass indicates the nature of the mixing coefficient and the specifics of the expansion.

Type: floating-point number

Constraints:

4.2.44 AtomStateMixingCoeffClass

Mandatory attribute of the mixing coefficient with one of the two values: “squared” or “signed”

Type: string

Constraints:

4.2.45 AtomStateParity

State parity. Can have values: “even”, “odd” or “undefined”

Type: string

Constraints:

4.2.46 AtomStatePolarizability

State polarizability.

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.47 AtomStateQuantumDefect

The quantum defect is a correction applied to the potential to account for the fact that the inner electrons do not entirely screen the corresponding charge of the nucleus. It is particularity important for atoms with single electron in the outer shell.

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.48 AtomStateRef

A string key that references specific atomic state..

Type: string

Constraints:

4.2.49 AtomStateShellID

Atomic shell ID generated by a database.

Type: string

Constraints:

4.2.50 AtomStateShellKappa

Relativistic correction.

Type: floating-point number

Constraints:

4.2.51 AtomStateShellNumberOfElectrons

Number of electrons in a specific shell.

Type: integer number

Constraints: >0

4.2.52 AtomStateShellOrbitalAngMom

Type: integer number

Constraints:

4.2.53 AtomStateShellOrbitalAngMomSymbol

Shell angular momentum symbol?.

Type: string

Constraints:

4.2.54 AtomStateShellPairID

ID for a pair of shells for mixed states assigned by a database.

Type: string

Constraints:

4.2.55 AtomStateShellPairShell1ID

ID for shell1 in a pair of shells assigned by a database.

Type: string

Constraints:

4.2.56 AtomStateShellPairShell1Kappa

Relativistic correction for shell 1 in a pair.

Type: floating-point number

Constraints:

4.2.57 AtomStateShellPairShell1NumberOfElectrons

Number of electrons in shell 1 in a pair.

Type: integer number

Constraints: >0

4.2.58 AtomStateShellPairShell1OrbitalAngMom

Orbital angular momentum of shell 1 in a pair.

Type: integer number

Constraints: >=0

4.2.59 AtomStateShellPairShell1OrbitalAngmomSymbol

Orbital angular momentum symbol for shell 1 in a pair.

Type: string

Constraints:

4.2.60 AtomStateShellPairShell1Parity

Parity of shell 1 in a pair.

Type: string

Constraints:

4.2.61 AtomStateShellPairShell1QN

Principal quantum number of shell 1 in a pair.

Type: integer number

Constraints: >0

4.2.62 AtomStateShellPairShell1TermJ1J2

J1 or J2 in J1J2 coupling for shell 1 in a pair. Can be integer of half-integer.

Type: floating-point number

Constraints: >0

4.2.63 AtomStateShellPairShell1TermJJ

j in jj coupling for shell 1 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.64 AtomStateShellPairShell1TermJKJ

j in jK coupling for shell 1 in pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.65 AtomStateShellPairShell1TermJKK

K in jK coupling for shell 1 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.66 AtomStateShellPairShell1TermJKS2

S2 (spin of external electrons) in jK coupling for shell 1 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.67 AtomStateShellPairShell1TermLKK

K in LK coupling for shell 1 in a pair. Could be integer or half-integer..

Type: floating-point number

Constraints: >0

4.2.68 AtomStateShellPairShell1TermLKL

L in LK coupling for shell 1 in a pair. Could be integer or 0.

Type: integer number

Constraints: >=0

4.2.69 AtomStateShellPairShell1TermLKLSymbol

Orbital angular momentum symbol in LK coupling for shell 1 in a pair.

Type: string

Constraints:

4.2.70 AtomStateShellPairShell1TermLKS2

S2 (spin of external electrons) in jK coupling for shell 1 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.71 AtomStateShellPairShell1TermLSL

L in LS coupling for shell 1 in a pair. Could be integer or 0.

Type: integer number

Constraints: >=0

4.2.72 AtomStateShellPairShell1TermLSLSymbol

Orbital angular momentum symbol in LS coupling for shell 1 in a pair.

Type: string

Constraints:

4.2.73 AtomStateShellPairShell1TermLSMultiplicity

Multiplicity (2s+1) for shell 1 in a pair in LS coupling. Positive integer.

Type: integer number

Constraints: >0

4.2.74 AtomStateShellPairShell1TermLSS

Spin for shell 1 in a pair in LS coupling. Non-negative integer or half-integer.

Type: floating-point number

Constraints: >=0

4.2.75 AtomStateShellPairShell1TermLSSeniority

Seniority for shell 1 in a pair in LS coupling. Non-negative integer.

Type: integer number

Constraints: >=0

4.2.76 AtomStateShellPairShell1TermLabel

Term label for shell 1.

Type: string

Constraints:

4.2.77 AtomStateShellPairShell1TotalAngMom

Total angular momentum J for shell 1 in a pair. Could be non-negative integer or half-integer.

Type: floating-point number

Constraints: >=0

4.2.78 AtomStateShellPairShell2ID

ID for shell2 in a pair of shells assigned by a database.

Type: string

Constraints:

4.2.79 AtomStateShellPairShell2Kappa

Relativistic correction for shell 2 in a pair.

Type: floating-point number

Constraints:

4.2.80 AtomStateShellPairShell2NumberOfElectrons

Number of electrons in shell 2 in a pair.

Type: integer number

Constraints: >0

4.2.81 AtomStateShellPairShell2OrbitalAngMom

Orbital angular momentum of shell 2 in a pair.

Type: integer number

Constraints: >=0

4.2.82 AtomStateShellPairShell2OrbitalAngMomSymbol

Orbital angular momentum symbol for shell 2 in a pair.

Type: string

Constraints:

4.2.83 AtomStateShellPairShell2Parity

Parity of shell 2 in a pair.

Type: string

Constraints:

4.2.84 AtomStateShellPairShell2QN

Principal quantum number of shell 2 in a pair.

Type: integer number

Constraints: >0

4.2.85 AtomStateShellPairShell2TermJ1J2

J1 or J2 in J1J2 coupling for shell 2 in a pair. Can be integer of half-integer..

Type: floating-point number

Constraints: >0

4.2.86 AtomStateShellPairShell2TermJJ

j in jj coupling for shell 2 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.87 AtomStateShellPairShell2TermJKJ

j in jK coupling for shell 2 in a pair. Could be integer or half-integer..

Type: floating-point number

Constraints: >0

4.2.88 AtomStateShellPairShell2TermJKK

K in jK coupling for shell 2 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.89 AtomStateShellPairShell2TermJKS2

S2 (spin of external electrons) in jK coupling for shell 2 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.90 AtomStateShellPairShell2TermLKK

K in LK coupling for shell 2 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.91 AtomStateShellPairShell2TermLKL

L in LK coupling for shell 2 in a pair. Could be integer or 0.

Type: integer number

Constraints: >=0

4.2.92 AtomStateShellPairShell2TermLKLSymbol

Orbital angular momentum symbol in LK coupling for shell 2 in a pair.

Type: integer number

Constraints:

4.2.93 AtomStateShellPairShell2TermLKS2

S2 (spin of external electrons) in jK coupling for shell 2 in a pair. Could be integer or half-integer.

Type: floating-point number

Constraints: >0

4.2.94 AtomStateShellPairShell2TermLSL

L in LK coupling for shell 2 in a pair. Could be integer or 0.

Type: integer number

Constraints: >=0

4.2.95 AtomStateShellPairShell2TermLSLSymbol

Orbital angular momentum symbol in LS coupling for shell 2 in a pair.

Type: string

Constraints:

4.2.96 AtomStateShellPairShell2TermLSMultiplicity

Multiplicity (2s+1) for shell 2 in a pair in LS coupling. Positive integer.

Type: integer number

Constraints: >0

4.2.97 AtomStateShellPairShell2TermLSS

Spin for shell 2 in a pair in LS coupling. Non-negative integer or half-integer.

Type: floating-point number

Constraints: >=0

4.2.98 AtomStateShellPairShell2TermLSSeniority

Seniority for shell 2 in a pair in LS coupling. Non-negative integer.

Type: integer number

Constraints: >=0

4.2.99 AtomStateShellPairShell2TermLabel

Term label for shell 2.

Type: string

Constraints:

4.2.100 AtomStateShellPairShell2TotalAngMom

Total angular momentum J for shell 2 in a pair. Could be non-negative integer or half-integer.

Type: floating-point number

Constraints: >=0

4.2.101 AtomStateShellPairTermJ1J2

Type: integer number

Constraints:

4.2.102 AtomStateShellPairTermJJ

Type: integer number

Constraints:

4.2.103 AtomStateShellPairTermJKJ

Type: integer number

Constraints:

4.2.104 AtomStateShellPairTermJKK

Type: integer number

Constraints:

4.2.105 AtomStateShellPairTermJKS2

Type: integer number

Constraints:

4.2.106 AtomStateShellPairTermLKK

Type: integer number

Constraints:

4.2.107 AtomStateShellPairTermLKL

Type: integer number

Constraints:

4.2.108 AtomStateShellPairTermLKLSymbol

Type: integer number

Constraints:

4.2.109 AtomStateShellPairTermLKS2

Type: integer number

Constraints:

4.2.110 AtomStateShellPairTermLSL

Type: integer number

Constraints:

4.2.111 AtomStateShellPairTermLSLSymbol

Type: integer number

Constraints:

4.2.112 AtomStateShellPairTermLSMultiplicity

Type: integer number

Constraints:

4.2.113 AtomStateShellPairTermLSS

Type: integer number

Constraints:

4.2.114 AtomStateShellPairTermLSSeniority

Type: integer number

Constraints:

4.2.115 AtomStateShellPairTermLabel

Type: string

Constraints:

4.2.116 AtomStateShellParity

Type: integer number

Constraints:

4.2.117 AtomStateShellPrincipalQN

Type: integer number

Constraints:

4.2.118 AtomStateShellTermJ1J2

Type: integer number

Constraints:

4.2.119 AtomStateShellTermJJ

Type: integer number

Constraints:

4.2.120 AtomStateShellTermJKJ

Type: integer number

Constraints:

4.2.121 AtomStateShellTermJKS

Type: integer number

Constraints:

4.2.122 AtomStateShellTermK

Type: integer number

Constraints:

4.2.123 AtomStateShellTermLKK

Type: integer number

Constraints:

4.2.124 AtomStateShellTermLKL

Type: integer number

Constraints:

4.2.125 AtomStateShellTermLKLSymbol

Type: string

Constraints:

4.2.126 AtomStateShellTermLKS2

Type: integer number

Constraints:

4.2.127 AtomStateShellTermLSL

Type: integer number

Constraints:

4.2.128 AtomStateShellTermLSLSymbol

Type: integer number

Constraints:

4.2.129 AtomStateShellTermLSMultiplicity

Type: integer number

Constraints:

4.2.130 AtomStateShellTermLabel

Type: integer number

Constraints:

4.2.131 AtomStateShellTermS

Type: integer number

Constraints:

4.2.132 AtomStateShellTermSeniority

Type: integer number

Constraints:

4.2.133 AtomStateShellTotalAngMom

Type: integer number

Constraints:

4.2.134 AtomStateStatisticalWeight

Type: floating-point number

Constraints:

4.2.135 AtomStateSuperShellNumberOfElectrons

Type: integer number

Constraints:

4.2.136 AtomStateSuperShellPrincipalQN

Type: integer number

Constraints:

4.2.137 AtomStateTermJ1J2

J1 or J2 quantum number for atomic core described in J1J2 coupling.

Type: integer number

Constraints:

4.2.138 AtomStateTermJJ

Type: integer number

Constraints:

4.2.139 AtomStateTermJKJ

Type: integer number

Constraints:

4.2.140 AtomStateTermJKK

Type: integer number

Constraints:

4.2.141 AtomStateTermJKS

Type: integer number

Constraints:

4.2.142 AtomStateTermLKK

Type: integer number

Constraints:

4.2.143 AtomStateTermLKL

Type: integer number

Constraints:

4.2.144 AtomStateTermLKLSymbol

Type: integer number

Constraints:

4.2.145 AtomStateTermLKS2

Type: integer number

Constraints:

4.2.146 AtomStateTermLSL

Type: integer number

Constraints:

4.2.147 AtomStateTermLSLSymbol

Type: string

Constraints:

4.2.148 AtomStateTermLSMultiplicity

Type: integer number

Constraints:

4.2.149 AtomStateTermLSS

Type: floating-point number

Constraints:

4.2.150 AtomStateTermLSSeniority

Type: integer number

Constraints:

4.2.151 AtomStateTermLabel

Type: string

Constraints:

4.2.152 AtomStateTotalAngMom

Type: integer number

Constraints:

4.2.153 AtomSymbol

Atomic name

Type: string

Constraints:

4.2.154 CollisionCode

Type: string

Constraints:

4.2.155 CollisionComment

Type: string

Constraints:

4.2.156 CollisionDataSetComment

Type: string

Constraints:

4.2.157 CollisionDataSetDescription

Type: string

Constraints:

4.2.158 CollisionDataSetMethod

Type: string

Constraints:

4.2.159 CollisionDataSetRef

Type: string

Constraints:

4.2.160 CollisionFitDataAccuracy

Type: string

Constraints:

4.2.161 CollisionFitDataArgumentDescription

Type: string

Constraints:

4.2.162 CollisionFitDataArgumentLowerLimit

Type: string

Constraints:

4.2.163 CollisionFitDataArgumentName

Type: string

Constraints:

4.2.164 CollisionFitDataArgumentUnits

Type: string

Constraints:

4.2.165 CollisionFitDataArgumentUpperLimit

Type: string

Constraints:

4.2.166 CollisionFitDataComment

Type: string

Constraints:

4.2.167 CollisionFitDataFunction

Type: string

Constraints:

4.2.168 CollisionFitDataMethod

Type: string

Constraints:

4.2.169 CollisionFitDataParameter

Type: string

Constraints:

4.2.170 CollisionFitDataPhysicalUncertainty

Type: string

Constraints:

4.2.171 CollisionFitDataProductionDate

Type: string

Constraints:

4.2.172 CollisionFitDataRef

Type: string

Constraints:

4.2.173 CollisionIAEACode

Type: string

Constraints:

4.2.174 CollisionIntermediateSpecies

Type: string

Constraints:

4.2.175 CollisionIntermediateState

Type: string

Constraints:

4.2.176 CollisionMethod

Type: string

Constraints:

4.2.177 CollisionProductSpecies

Type: string

Constraints:

4.2.178 CollisionProductState

Type: string

Constraints:

4.2.179 CollisionReactantSpecies

Type: string

Constraints:

4.2.180 CollisionReactantState

Type: string

Constraints:

4.2.181 CollisionRef

Type: string

Constraints:

4.2.182 CollisionTabulatedDataComment

Type: string

Constraints:

4.2.183 CollisionTabulatedDataMethod

Type: string

Constraints:

4.2.184 CollisionTabulatedDataPhysicalUncertainty

Type: string

Constraints:

4.2.185 CollisionTabulatedDataProductionDate

Type: string

Constraints:

4.2.186 CollisionTabulatedDataRef

Type: string

Constraints:

4.2.187 CollisionTabulatedDataReferenceFrame

Type: string

Constraints:

4.2.188 CollisionTabulatedDataX

Type: floating-point number

Constraints:

4.2.189 CollisionTabulatedDataXDescription

Type: string

Constraints:

4.2.190 CollisionTabulatedDataXError

Type: floating-point number

Constraints:

4.2.191 CollisionTabulatedDataXN

Type: integer number

Constraints:

4.2.192 CollisionTabulatedDataXNegativeError

Type: string

Constraints:

4.2.193 CollisionTabulatedDataXParameter

Type: string

Constraints:

4.2.194 CollisionTabulatedDataXPositiveError

Type: floating-point number

Constraints:

4.2.195 CollisionTabulatedDataXUnits

Type: string

Constraints:

4.2.196 CollisionTabulatedDataY

Type: floating-point number

Constraints:

4.2.197 CollisionTabulatedDataYDescription

Type: string

Constraints:

4.2.198 CollisionTabulatedDataYError

Type: floating-point number

Constraints:

4.2.199 CollisionTabulatedDataYNegativeError

Type: floating-point number

Constraints:

4.2.200 CollisionTabulatedDataYPositiveError

Type: floating-point number

Constraints:

4.2.201 CollisionTabulatedDataYUnits

Type: string

Constraints:

4.2.202 CollisionThreshold

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.203 CollisionalTabulatedDataYN

Type: floating-point number

Constraints:

4.2.204 EnvironmentComment

Type: string

Constraints:

4.2.205 EnvironmentID

Type: string

Constraints:

4.2.206 EnvironmentRef

Type: string

Constraints:

4.2.207 EnvironmentSpecies

Type: string

Constraints:

4.2.208 EnvironmentSpeciesConcentration

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.209 EnvironmentSpeciesMoleFraction

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.210 EnvironmentSpeciesName

Type: string

Constraints:

4.2.211 EnvironmentSpeciesPartialPressure

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.212 EnvironmentSpeciesRef

Type: string

Constraints:

4.2.213 EnvironmentTemperature

Environment temperature

Units: K

Type: floating-point number

Has **DataType** suffixes support

Constraints: >0

4.2.214 EnvironmentTotalNumberDensity

Units: 1/cm3

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.215 EnvironmentTotalPressure

Environment total pressure

Units: Pa

Type: floating-point number

Has **DataType** suffixes support

Constraints: >=0

4.2.216 FunctionArgumentDescription

Type: string

Constraints:

4.2.217 FunctionArgumentLowerLimit

Type: floating-point number

Constraints:

4.2.218 FunctionArgumentName

Type: string

Constraints:

4.2.219 FunctionArgumentUnits

Type: string

Constraints:

4.2.220 FunctionArgumentUpperLimit

Type: floating-point number

Constraints:

4.2.221 FunctionComputerLanguage

Type: string

Constraints:

4.2.222 FunctionDescription

Type: string

Constraints:

4.2.223 FunctionExpression

Type: string

Constraints:

4.2.224 FunctionID

Type: string

Constraints:

4.2.225 FunctionName

Type: string

Constraints:

4.2.226 FunctionParameterDescription

Type: string

Constraints:

4.2.227 FunctionParameterName

Type: string

Constraints:

4.2.228 FunctionParameterUnits

Type: string

Constraints:

4.2.229 FunctionReferenceFrame

Type: string

Constraints:

4.2.230 FunctionSourceCodeURL

Type: string

Constraints:

4.2.231 FunctionSourceRef

Type: string

Constraints:

4.2.232 FunctionYDescription

Type: string

Constraints:

4.2.233 FunctionYLowerLimit

Type: floating-point number

Constraints:

4.2.234 FunctionYName

Type: string

Constraints:

4.2.235 FunctionYUnits

Type: string

Constraints:

4.2.236 FunctionYUpperLimit

Type: floating-point number

Constraints:

4.2.237 MethodCategory

Method category. Allowed values are: experiment, theory, ritz, recommended, evaluated, empirical, scalingLaw, semiempirical, compilation, derived

Type: string

Constraints:

4.2.238 MethodComment

Type: string

Constraints:

4.2.239 MethodRef

Type: string

Constraints:

4.2.240 MoleculeChemicalName

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

Type: string

Constraints:

4.2.241 MoleculeInchi

Type: string

Constraints:

4.2.242 MoleculeInchiKey

Type: string

Constraints:

4.2.243 MoleculeIonCharge

Molecule ion charge

Type: integer number

Constraints:

4.2.244 MoleculeMolecularWeight

Units: u

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.245 MoleculeNormalModeHarmonicFrequency

Units: MHz

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.246 MoleculeNormalModeIntensity

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.247 MoleculeNuclearSpins

Type: string

Constraints:

4.2.248 MoleculeNuclearSpinsAtomArray

Type: string

Constraints:

4.2.249 MoleculeNuclearSpinsBondArray

Type: string

Constraints:

4.2.250 MoleculeQNElecStateLabel

Type: string

Constraints:

4.2.251 MoleculeQNF

Type: string

Constraints:

4.2.252 MoleculeQNF1

Type: string

Constraints:

4.2.253 MoleculeQNF1nuclSpin

Type: string

Constraints:

4.2.254 MoleculeQNF2

Type: string

Constraints:

4.2.255 MoleculeQNF2nuclSpin

Type: string

Constraints:

4.2.256 MoleculeQNFj

Type: string

Constraints:

4.2.257 MoleculeQNFjj

Type: string

Constraints:

4.2.258 MoleculeQNFjnuclSpin

Type: string

Constraints:

4.2.259 MoleculeQNFnuclSpin

Type: string

Constraints:

4.2.260 MoleculeQNI

Type: string

Constraints:

4.2.261 MoleculeQNInuclSpin

Type: string

Constraints:

4.2.262 MoleculeQNJ

Type: string

Constraints:

4.2.263 MoleculeQNK

Type: string

Constraints:

4.2.264 MoleculeQNKa

Type: string

Constraints:

4.2.265 MoleculeQNKc

Type: string

Constraints:

4.2.266 MoleculeQNLambda

Type: string

Constraints:

4.2.267 MoleculeQNN

Type: string

Constraints:

4.2.268 MoleculeQNOmega

Type: string

Constraints:

4.2.269 MoleculeQNS

Type: string

Constraints:

4.2.270 MoleculeQNSigma

Type: string

Constraints:

4.2.271 MoleculeQNSpinComponentLabel

Type: string

Constraints:

4.2.272 MoleculeQNasSym

Type: string

Constraints:

4.2.273 MoleculeQNelecInv

Type: string

Constraints:

4.2.274 MoleculeQNelecRefl

Type: string

Constraints:

4.2.275 MoleculeQNkronigParity

Type: string

Constraints:

4.2.276 MoleculeQNl

Type: string

Constraints:

4.2.277 MoleculeQNl2

Type: string

Constraints:

4.2.278 MoleculeQNli

Type: string

Constraints:

4.2.279 MoleculeQNliMode

Type: string

Constraints:

4.2.280 MoleculeQNparity

Type: string

Constraints:

4.2.281 MoleculeQNr

Type: string

Constraints:

4.2.282 MoleculeQNrName

Type: string

Constraints:

4.2.283 MoleculeQNrotSym

Type: string

Constraints:

4.2.284 MoleculeQNrotSymGroup

Type: string

Constraints:

4.2.285 MoleculeQNv

Type: string

Constraints:

4.2.286 MoleculeQNv1

Type: string

Constraints:

4.2.287 MoleculeQNv2

Type: string

Constraints:

4.2.288 MoleculeQNv3

Type: string

Constraints:

4.2.289 MoleculeQNvi

Type: string

Constraints:

4.2.290 MoleculeQNviMode

Type: string

Constraints:

4.2.291 MoleculeQNvibInv

Type: string

Constraints:

4.2.292 MoleculeQNvibRefl

Type: string

Constraints:

4.2.293 MoleculeQNvibSym

Type: string

Constraints:

4.2.294 MoleculeQNvibSymGroup

Type: string

Constraints:

4.2.295 MoleculeQnCase

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

Type: string

Constraints:

4.2.296 MoleculeSpeciesID

Type: string

Constraints:

4.2.297 MoleculeStateEnergy

Units: 1/cm

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.298 MoleculeStateID

Type: string

Constraints:

4.2.299 MoleculeStateLifeTime

Molecular state lifetime in seconds

Units: s

Type: floating-point number

Has **DataType** suffixes support

Constraints: >0

4.2.300 MoleculeStateNuclearSpinIsomer

Nuclear spin isomer (symetry) of a molecular state.

Type: string

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

4.2.301 MoleculeStateNuclearStatisticalWeight

Nuclear statistical weight for a given molecular energy level

Type: integer number

Constraints: >0

4.2.302 MoleculeStateParameterMatrix

A space-separated list of values for the matrix. For an arbitrary matrix, it has nrows*ncols entries. For a diagonal matrix there are nrows=ncols entries. For a symmetric matrix there are nrows(nrows+1)/2 entries etc.

Type: string

Constraints:

4.2.303 MoleculeStateParameterMatrixColRefs

This is a space-separated list of column names for the parameter matrix, as many as there are columns.

Type: string

Constraints:

4.2.304 MoleculeStateParameterMatrixForm

Molecular State parameter on matrix form; the matrix' form, such as "symmetric", "diagonal" etc.

Type: string

Constraints:

4.2.305 MoleculeStateParameterMatrixNcols

Molecular State parameters in matrix form; number of matrix columns

Type: integer number

Constraints:

4.2.306 MoleculeStateParameterMatrixNrows

Molecular state parameter data on matrix form, number of rows in matrix

Type: integer number

Constraints:

4.2.307 MoleculeStateParameterMatrixRowRefs

This is a space-separated list of row names for the parameter matrix, as many as there are rows.

Type: string

Constraints:

4.2.308 MoleculeStateParameterMatrixUnits

Molecular State parameters, units for data on matrix data form

Type: string

Constraints:

4.2.309 MoleculeStateParameterMatrixValues

Molecular State parameter on matrix form; type of matrix values: "real", "imaginary" or "complex".

Type: string

Constraints:

4.2.310 MoleculeStateParameterValueData

State parameter with a specific value

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.311 MoleculeStateParameterVectorDataUnits

Molecular State vector data units

Type: string

Constraints:

4.2.312 MoleculeStateParameterVectorRef

Molecular State parameter reference string giving context.

Type: string

Constraints:

4.2.313 MoleculeStateParameterVectorX3

Molecular State parameter vector coordinate X

Type: floating-point number

Constraints:

4.2.314 MoleculeStateParameterVectorY3

Molecular State parameter vector coordinate Y

Type: floating-point number

Constraints:

4.2.315 MoleculeStateParameterVectorZ3

Molecular State parameter vector coordinate Z

Type: floating-point number

Constraints:

4.2.316 MoleculeStateParameters

Additional parameters of molecular state

Type: string

Constraints:

4.2.317 MoleculeStateQuantumNumbers

Type: string

Constraints:

4.2.318 MoleculeStateTotalStatisticalWeight

Total statistical weight (degeneracy) for a given molecular energy level

Type: integer number

Constraints: >0

4.2.319 MoleculeStoichiometricFormula

Molecular stoichiometric formula

Type: string

Constraints:

4.2.320 MoleculeStructure

The molecular structure, as defined in CML

Type: string

Constraints:

4.2.321 NodeID

A unique string for each VAMDC node. For example used for xsams-internal referencing. This MUST be filled.

Type: string

Constraints:

4.2.322 NonRadTranComment

Type: string

Constraints:

4.2.323 NonRadTranEnergy

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.324 NonRadTranLowerState

Lower state of the transition

Type: string

Constraints:

4.2.325 NonRadTranMethod

Type: string

Constraints:

4.2.326 NonRadTranProbability

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.327 NonRadTranRef

Type: string

Constraints:

4.2.328 NonRadTranSpecies

Type: string

Constraints:

4.2.329 NonRadTranType

Type: string

Constraints:

4.2.330 NonRadTranUpperState

Upper state of the transition

Type: string

Constraints:

4.2.331 NonRadTranWidth

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.332 NormalModeHarmonicFrequency

The harmonic frequency of a normal mode

Units: 1/cm

Type: floating-point number

Has **DataType** suffixes support

Constraints: >0

4.2.333 NormalModeIntensity

Intensity of a normal mode

Units: km/mol

Type: floating-point number

Has **DataType** suffixes support

Constraints: >0

4.2.334 NormalModeSymmetry

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

Type: string

Constraints:

4.2.335 ParticleCharge

Type: string

Constraints:

4.2.336 ParticleComment

Type: string

Constraints:

4.2.337 ParticleMass

Type: string

Has **DataType** suffixes support

Constraints:

4.2.338 ParticleMethod

Type: string

Constraints:

4.2.339 ParticleName

Particle name, one of photon, electron, muon, positron, neutron, alpha, cosmic

Type: string

Constraints:

4.2.340 ParticlePolarization

Type: floating-point number

Constraints:

4.2.341 ParticleRef

Type: string

Constraints:

4.2.342 ParticleSpeciesID

Type: string

Constraints:

4.2.343 ParticleSpin

Type: floating-point number

Constraints:

4.2.344 RadTransBandCentre

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.345 RadTransBandWidth

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.346 RadTransBroadeningDopplerComment

Type: string

Constraints:

4.2.347 RadTransBroadeningDopplerEnvironment

Type: string

Constraints:

4.2.348 RadTransBroadeningDopplerLineshapeName

Type: string

Constraints:

4.2.349 RadTransBroadeningDopplerLineshapeParameter

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.350 RadTransBroadeningDopplerLineshapeParameterName

Type: string

Constraints:

4.2.351 RadTransBroadeningDopplerMethod

Type: string

Constraints:

4.2.352 RadTransBroadeningDopplerRef

Type: string

Constraints:

4.2.353 RadTransBroadeningInstrumentComment

Type: string

Constraints:

4.2.354 RadTransBroadeningInstrumentEnvironment

Type: string

Constraints:

4.2.355 RadTransBroadeningInstrumentLineshapeName

Type: string

Constraints:

4.2.356 RadTransBroadeningInstrumentLineshapeParameter

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.357 RadTransBroadeningInstrumentLineshapeParameterName

Type: string

Constraints:

4.2.358 RadTransBroadeningInstrumentMethod

Type: string

Constraints:

4.2.359 RadTransBroadeningInstrumentRef

Type: string

Constraints:

4.2.360 RadTransBroadeningNaturalComment

Type: string

Constraints:

4.2.361 RadTransBroadeningNaturalEnvironment

Type: string

Constraints:

4.2.362 RadTransBroadeningNaturalLineshapeName

Type: string

Constraints:

4.2.363 RadTransBroadeningNaturalLineshapeParameter

A broadening parameter for natural broadening.

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.364 RadTransBroadeningNaturalLineshapeParameterName

The name of natural broadening parameters.

Type: string

Constraints:

4.2.365 RadTransBroadeningNaturalMethod

Type: string

Constraints:

4.2.366 RadTransBroadeningNaturalRef

Type: string

Constraints:

4.2.367 RadTransBroadeningPressureComment

Type: string

Constraints:

4.2.368 RadTransBroadeningPressureEnvironment

Type: string

Constraints:

4.2.369 RadTransBroadeningPressureLineshapeName

Type: string

Constraints:

4.2.370 RadTransBroadeningPressureLineshapeParameter

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.371 RadTransBroadeningPressureLineshapeParameterName

Type: string

Constraints:

4.2.372 RadTransBroadeningPressureMethod

Type: string

Constraints:

4.2.373 RadTransBroadeningPressureRef

Type: string

Constraints:

4.2.374 RadTransComment

(String)

Type: string

Constraints:

4.2.375 RadTransCrossSectionBandCentre

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.376 RadTransCrossSectionBandModeComment

Type: string

Constraints:

4.2.377 RadTransCrossSectionBandModeDeltaV

List of dV values

Type: floating-point number

Constraints: >0

4.2.378 RadTransCrossSectionBandModeDeltaVID

Type: string

Constraints:

4.2.379 RadTransCrossSectionBandModeMethod

Type: string

Constraints:

4.2.380 RadTransCrossSectionBandModeName

Type: string

Constraints:

4.2.381 RadTransCrossSectionBandName

Type: string

Constraints:

4.2.382 RadTransCrossSectionBandWidth

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.383 RadTransCrossSectionDescription

A string describing the cross section being given in a CrossSection element, e.g. 'IR absorption cross section'

Type: string

Constraints:

4.2.384 RadTransCrossSectionEnvironment

Type: string

Constraints:

4.2.385 RadTransCrossSectionID

Type: string

Constraints:

4.2.386 RadTransCrossSectionSpecies

Type: string

Constraints:

4.2.387 RadTransCrossSectionState

Type: string

Constraints:

4.2.388 RadTransCrossSectionX

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

Type: string

Constraints:

4.2.389 RadTransCrossSectionXDataFile

Datafile containing X data.

Type: string

Constraints:

4.2.390 RadTransCrossSectionXError

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

Type: floating-point number

Constraints:

4.2.391 RadTransCrossSectionXErrorList

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:

4.2.392 RadTransCrossSectionXLinearA0

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:

4.2.393 RadTransCrossSectionXName

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

Type: string

Constraints:

4.2.394 RadTransCrossSectionXUnit

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

Type: string

Constraints:

4.2.395 RadTransCrossSectionY

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

Type: string

Constraints:

4.2.396 RadTransCrossSectionYDataFile

Datafile containing Y data.

Type: string

Constraints:

4.2.397 RadTransCrossSectionYError

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

Type: floating-point number

Constraints:

4.2.398 RadTransCrossSectionYErrorList

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

Type: string

Constraints:

4.2.399 RadTransCrossSectionYLinearA1

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:

4.2.400 RadTransCrossSectionYName

Name of the Cross Section parameter given (e.g. 'sigma')

Type: string

Constraints:

4.2.401 RadTransCrossSectionYUnit

Units of the cross section (e.g. 'Mb', 'arbitrary', 'km/mol')

Type: string

Constraints:

4.2.402 RadTransEffectiveLandeFactor

Effective Lande factor for a given transition

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.403 RadTransEnergy

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.404 RadTransFrequency

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.405 RadTransLowerStateRef

Type: string

Constraints:

4.2.406 RadTransProbabilityA

The Einstein coefficient for spontaneous radiative de-excitation (emission) A.

Units: 1/s

Type: floating-point number

Has **DataType** suffixes support

Constraints: >= 0

4.2.407 RadTransProbabilityIdealisedIntensity

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.408 RadTransProbabilityLineStrength

Line profile-integrated absorption for transition between two energy levels. Line strength K = hν / 4π (n₁ B₁₂ - n₂ B₂₁)

Units: 1/cm

Type: floating-point number

Has **DataType** suffixes support

Constraints: >0

4.2.409 RadTransProbabilityLog10WeightedOscillatorStrength

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.410 RadTransProbabilityMultipole

Type: string

Constraints:

4.2.411 RadTransProbabilityOscillatorStrength

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.412 RadTransProbabilityWeightedOscillatorStrength

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.413 RadTransRefs

Type: string

Constraints:

4.2.414 RadTransShifting

Type: string

Constraints:

4.2.415 RadTransShiftingComment

Type: string

Constraints:

4.2.416 RadTransShiftingEnv

Type: string

Constraints:

4.2.417 RadTransShiftingMethod

Type: string

Constraints:

4.2.418 RadTransShiftingName

Type: string

Constraints:

4.2.419 RadTransShiftingParam

Shifting parameter value

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.420 RadTransShiftingParamFitArgumentDescription

Type: string

Constraints:

4.2.421 RadTransShiftingParamFitArgumentLowerLimit

Type: floating-point number

Constraints:

4.2.422 RadTransShiftingParamFitArgumentName

List of argument names

Type: string

Constraints:

4.2.423 RadTransShiftingParamFitArgumentUnits

Type: string

Constraints:

4.2.424 RadTransShiftingParamFitArgumentUpperLimit

Type: floating-point number

Constraints:

4.2.425 RadTransShiftingParamFitFunction

Type: string

Constraints:

4.2.426 RadTransShiftingParamFitParameter

Type: string

Has **DataType** suffixes support

Constraints:

4.2.427 RadTransShiftingParamFitParameterName

Type: string

Constraints:

4.2.428 RadTransShiftingParamName

Type: string

Constraints:

4.2.429 RadTransShiftingRef

Type: string

Constraints:

4.2.430 RadTransSpeciesRef

Type: string

Constraints:

4.2.431 RadTransUpperStateRef

The upper state for the transition

Type: string

Constraints:

4.2.432 RadTransWavelength

Units: A

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.433 RadTransWavenumber

Type: floating-point number

Has **DataType** suffixes support

Constraints:

4.2.434 SolidComment

Type: string

Constraints:

4.2.435 SolidLayerComment

Type: string

Constraints:

4.2.436 SolidLayerComponentComment

Type: string

Constraints:

4.2.437 SolidLayerComponentElementSymbol

Type: string

Constraints:

4.2.438 SolidLayerComponentMethod

Type: string

Constraints:

4.2.439 SolidLayerComponentNuclearCharge

Type: string

Constraints:

4.2.440 SolidLayerComponentPercentage

Type: floating-point number

Constraints:

4.2.441 SolidLayerComponentRef

Type: string

Constraints:

4.2.442 SolidLayerComponentStochiometricValue

Type: floating-point number

Constraints:

4.2.443 SolidLayerName

Type: string

Constraints:

4.2.444 SolidLayerTemperature

Type: string

Has **DataType** suffixes support

Constraints:

4.2.445 SolidLayerThickness

Type: string

Has **DataType** suffixes support

Constraints:

4.2.446 SolidLayerTopology

Type: string

Constraints:

4.2.447 SolidMethod

Type: string

Constraints:

4.2.448 SolidRef

Type: string

Constraints:

4.2.449 SolidSpeciesID

Type: string

Constraints:

4.2.450 SourceAuthorName

Name of one of the authors

Type: string

Constraints:

4.2.451 SourceCategory

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

Type: string

Constraints: Journal | Book | Proceedings | On-line

4.2.452 SourceComments

Comments and notes connected with a Source (reference)

Type: string

Constraints:

4.2.453 SourceDOI

Type: string

Constraints:

4.2.454 SourceID

Type: string

Constraints:

4.2.455 SourceName

E.g. JQSRT

Type: string

Constraints:

4.2.456 SourcePageBegin

Starting page number

Type: integer number

Constraints: >=0

4.2.457 SourcePageEnd

Type: string

Constraints:

4.2.458 SourceTitle

Full title of the paper

Type: string

Constraints:

4.2.459 SourceURI

Webb link to the publication

Type: string

Constraints:

4.2.460 SourceVolume

Volumen number

Type: integer number

Constraints: >0

4.2.461 SourceYear

Publication Year

Type: integer number

Constraints: >0

CHAPTER

FIVE

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.