Dictionary specifications

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

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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 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
The following keywords may be used as restrictables in TAP-V AMDC 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. $1 \text{ u} = 1.660538782(83)\times10^{-27} \text{ kg}$.

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
3.5 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:** >0

3.6 AtomStateCoupling

Coupling scheme used to describe the state. Currently five coupling schemes are supported LS, \( jj \), \( J_1J_2 \), \( jK \) 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:**

3.5. AtomNuclearSpin
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 particularly 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 \( K = \frac{h \nu}{4\pi} \left( n_{1} B_{12} - n_{2} B_{21} \right) \)

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: Å
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
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

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 $I$. 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:

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

State 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. The list of Returnables
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: \( \geq 0 \)

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: \( \text{1/cm} \)

Type: floating-point number

Has DataTypes suffixes support
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 particularly 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

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4.2. The list of Returnables
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. The list of Returnables
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. The list of Returnables
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. The list of Returnables
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. The list of Returnables
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  MoleculeQNI
Type: string
Constraints:

4.2.277  MoleculeQNI2
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: \(1/\text{cm}\)
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 (symmetry) 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
HasDataType 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 DataTypes 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 DataTypes suffixes support
Constraints:

4.2.332 NormalModeHarmonicFrequency

The harmonic frequency of a normal mode
Units: 1/cm
Type: floating-point number
Has DataTypes 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. The list of Returnables 60
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. The list of Returnables
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 $a_0$ 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:

4.2.393 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 $a_1$ in the linear series $Y_i = a_0 + a_1i$ 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. The list of Returnables
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 $K = \frac{h\nu}{4\pi}(n_{1}B_{12} - n_{2}B_{21})$
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. The list of Returnables
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 Data Type 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: Å
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 DataTypes suffixes support
Constraints:

4.2.445 SolidLayerThickness

Type: string
Has DataTypes suffixes support
Constraints:

4.2. The list of Returnables
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

4.2. The list of Returnables
“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.