# Dictionary specifications

**Document Information**


| | |
|---|---|
| **Editors:** | M. Doronin |
| **Authors:** | M. Doronin, C. Hill, T. Marquart |
| **Contributors:** | VAMDC WP6 working group |
| **Type of document:** | standards documentation |
| **Status:** | draft |
| **Distribution:** | public |
| **Work package:** | WP6 |
| **Version:** | 12.07 |
| **Date:** | 06/08/2011 |
| **Document code:** | |
| **Document URL:** | http://www.vamdc.org/documents/dictionary_v12.07.pdf |



**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 |
| V12.07 | 06/08/2012 | M.Doronin | update of autogenerated dictionaries |
| | | | |



**Acknowledgements**

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

# CONTENTS

CHAPTER

ONE

# CHANGELOG

The Restrictables, Requestables and Returnables continue to evolve to reflect the changes to the XML Schema (XSAMS) and the query language. Listed below are the additions and deletions for each category. Note that a renaming will be represented as deletion of the old and addition of the new keyword.

## 1.1 Changes between 11.12 and 12.07 releases:

### 1.1.1 Requestables

Added MoleculeBasisStates keyword, renamed RadiativeCrossections into RadiativeCrossSections

### 1.1.2 Restrictables

#### Deletions:

- NormalModeSymmetry
- Pressure (EnvironmentPressure should be used instead)
- Temperature (EnvironmentTemperature should be used instead)
- RadTransBandCentre
- RadTransBandWidth

Additions:

- SpeciesID
- VAMDCSpeciesID

### 1.1.3 Returnables

Returnables evolve a lot with each XSAMS and Python Node Software release, so no precise changelog is given.

## 1.2 Changes before 11.12 release:

### 1.2.1 Restrictables

#### Additions:

AtomStateTotalAngMom, Inchi, IonCharge, MethodCategory, MoleculeQNJ, MoleculeQNK, MoleculeQNKa, MoleculeQNKc, MoleculeQNv, MoleculeQNv1, MoleculeQNv2, MoleculeQNv3, MoleculeStateNuclearSpinI-

somer, ParticleName, RadTransBroadeningDoppler, RadTransBroadeningInstrument, RadTransBroadeningNatural, RadTransBroadeningPressure, StateEnergy, StateLifeTime, StateStatisticalWeight

#### Deletions:

AtomInchi, AtomInchiKey, AtomIonCharge, AtomStateEnergy, AtomStateID, AtomStateLifeTime, AtomStateStatisticalWeight, CollisionThreshold, MoleculeInchi, MoleculeInchiKey, MoleculeNormalModeIntensity, MoleculeStateCharacLifeTime, MoleculeStateCharacNuclearSpinSymmetry, MoleculeStateEnergy, MoleculeStateID

### 1.2.2 Requestables

#### Additions:

Functions, RadiativeCrossections

#### Deletions:

None

CHAPTER

TWO

# 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.

## 2.1 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.

## 2.2 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.

## 2.3 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.

## 2.4 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

THREE

# 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.

## 3.1 AtomStates

Requesting information about atoms, including the states information.

## 3.2 Atoms

Requesting information about atoms, without their states.

## 3.3 Collisions

collisional process data

## 3.4 Functions

## 3.5 Methods

method information

## 3.6 MoleculeBasisStates

The basis states for a set of molecular states expressed as a linear combination on some basis

## 3.7 MoleculeQuantumNumbers

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

## 3.8 MoleculeStates

request molecules, including their states but excluding the quantum numbers

## 3.9 Molecules

Request molecules, without information about their states.

## 3.10 NonRadiativeTransitions

non-radiative transitions data

## 3.11 Particles

request particle information only

## 3.12 Processes

data for all available processes

## 3.13 RadiativeCrossSections

Absorption (or emission?) cross sections as a function of wavelength or frequency-equivalent

## 3.14 RadiativeTransitions

radiative transitions data

## 3.15 Solids

Restrict the search to databases containing information about solids.

## 3.16 Sources

source reference information

## 3.17 Species

only brief species information, without states

## 3.18 States

complete states information

CHAPTER

FOUR

# 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.

## 4.1 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:**

## 4.2 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

## 4.3 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

## 4.4 AtomNuclearCharge

Atomic number or nuclear charge

**Type:** integer number

**Constraints:** >0

## 4.5 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:**

## 4.6 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:**

## 4.7 AtomStateHyperfineMomentum

**Type:** floating-point number

**Constraints:**

## 4.8 AtomStateIonizationEnergy

Ionization energy in eV

**Units:** 1/cm

**Type:** floating-point number

**Constraints:** >0

## 4.9 AtomStateKappa

Relativistic correction.

**Type:** floating-point number

**Constraints:**

## 4.10 AtomStateLandeFactor

Lande factor

**Type:** floating-point number

**Constraints:**

## 4.11 AtomStateMagneticQuantumNumber

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

**Type:** floating-point number

**Constraints:**

## 4.12 AtomStateParity

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

**Type:** string

**Constraints:**

## 4.13 AtomStatePolarizability

State polarizability.

**Type:** floating-point number

**Constraints:**

## 4.14 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:**

## 4.15 AtomStateTotalAngMom

**Type:** integer number

**Constraints:**

## 4.16 AtomSymbol

Atomic name

**Type:** string

**Constraints:**

## 4.17 CollisionCode

**Type:** string

**Constraints:**

## 4.18 CollisionIAEACode

**Type:** string

**Constraints:**

## 4.19 EnvironmentSpeciesConcentration

The concentration of a species contributing to an Environment

**Type:** floating-point number

**Constraints:**

## 4.20 EnvironmentSpeciesMoleFraction

The mole fraction of a species contributing to an Environment

**Type:** floating-point number

**Constraints:**

## 4.21 EnvironmentSpeciesPartialPressure

The partial pressure of a species contributing to an Environment

**Type:** floating-point number

**Constraints:**

## 4.22 EnvironmentTemperature

Environment temperature

**Units:** K

**Type:** floating-point number

**Constraints:** >0

## 4.23 EnvironmentTotalNumberDensity

The total number density of particles comprising an Environment

**Units:** 1/cm3

**Type:** floating-point number

**Constraints:**

## 4.24 EnvironmentTotalPressure

Environment total pressure

**Units:** Pa

**Type:** floating-point number

**Constraints:** >=0

## 4.25 FunctionID

A unique identifier for this function, of the form 'Fxxx'

**Type:** string

**Constraints:**

## 4.26 FunctionName

The name of this function

**Type:** string

**Constraints:**

## 4.27 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:**

## 4.28 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:**

## 4.29 IonCharge

Ionization stage with 0 for neutral

**Type:** integer number

**Constraints:** >=0

## 4.30 MethodCategory

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

**Type:** string

**Constraints:**

## 4.31 MoleculeChemicalName

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

**Type:** string

**Constraints:**

## 4.32 MoleculeMolecularWeight

**Units:** u

**Type:** floating-point number

**Constraints:**

## 4.33 MoleculeNormalModeHarmonicFrequency

The harmonic frequency of a normal mode.

**Units:** MHz

**Type:** floating-point number

**Constraints:**

## 4.34 MoleculeProtonation

**Type:** string

**Constraints:**

## 4.35 MoleculeQNJ

The molecular J quantum number for total angular momentum excluding nuclear spin

**Type:** floating-point number

**Constraints:**

## 4.36 MoleculeQNK

K is the quantum number associated with the projection of the total angular momentum excluding nuclear spin, J, onto the molecular symmetry axis.

**Type:** integer number

**Constraints:**

## 4.37 MoleculeQNKa

Ka is the rotational quantum label of an asymmetric top molecule, correlating to K in the prolate symmetric top limit.

**Type:** integer number

**Constraints:**

## 4.38 MoleculeQNKc

Kc is the rotational quantum label of an asymmetric top molecule, correlating to K in the oblate symmetric top limit.

**Type:** integer number

**Constraints:**

## 4.39 MoleculeQNv

For diatomic molecules, the vibrational quantum number, v

**Type:** integer number

**Constraints:**

## 4.40 MoleculeQNv1

The v1 vibrational quantum number.

**Type:** integer number

**Constraints:**

## 4.41 MoleculeQNv2

The v2 vibrational quantum number.

**Type:** integer number

**Constraints:**

## 4.42 MoleculeQNv3

The v3 vibrational quantum number.

**Type:** integer number

**Constraints:**

## 4.43 MoleculeStateNuclearSpinIsomer

Nuclear spin isomer (symmetry) of a molecular state. Can take values like 'ortho','para','A','E','meta', etc.

**Type:** string

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

## 4.44 MoleculeStoichiometricFormula

Molecular stoichiometric formula

**Type:** string

**Constraints:**

## 4.45 NonRadTranEnergy

**Type:** floating-point number

**Constraints:**

## 4.46 NonRadTranProbability

**Type:** floating-point number

**Constraints:**

## 4.47 NonRadTranWidth

**Type:** floating-point number

**Constraints:**

## 4.48 ParticleName

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

**Type:** string

**Constraints:**

## 4.49 RadTransBroadeningDoppler

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

**Type:** string

**Constraints:**

## 4.50 RadTransBroadeningInstrument

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

**Type:** string

**Constraints:**

## 4.51 RadTransBroadeningNatural

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

**Type:** string

**Constraints:**

## 4.52 RadTransBroadeningPressure

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

**Type:** string

**Constraints:**

## 4.53 RadTransEffectiveLandeFactor

Effective Lande factor for a given transition

**Type:** floating-point number

**Constraints:**

## 4.54 RadTransEnergy

The energy of a radiative transition

**Type:** floating-point number

**Constraints:**

## 4.55 RadTransFrequency

Radiative transition frequency.

**Units:** MHz

**Type:** floating-point number

**Constraints:**

## 4.56 RadTransProbabilityA

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

**Units:** 1/s

**Type:** floating-point number

**Constraints:** >= 0

## 4.57 RadTransProbabilityIdealisedIntensity

**Type:** floating-point number

**Constraints:**

## 4.58 RadTransProbabilityLineStrength

Line profile-integrated absorption for transition between two energy levels. Line strength K = hν / 4π (n<sub>1</sub> B<sub>12</sub> - n<sub>2</sub> B<sub>21</sub>)

**Units:** 1/cm

**Type:** floating-point number

**Constraints:** >0

## 4.59 RadTransProbabilityLog10WeightedOscillatorStrength

**Type:** floating-point number

**Constraints:**

## 4.60 RadTransProbabilityOscillatorStrength

**Type:** floating-point number

**Constraints:**

## 4.61 RadTransProbabilityWeightedOscillatorStrength

**Type:** floating-point number

**Constraints:**

## 4.62 RadTransWavelength

Radiative transition vacuum wavelength

**Units:** A

**Type:** floating-point number

**Constraints:**

## 4.63 RadTransWavenumber

Radiative transition wavenumber.

**Type:** floating-point number

**Constraints:**

## 4.64 SourceCategory

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

**Type:** string

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

## 4.65 SourceYear

Publication Year

**Type:** integer number

**Constraints:** >0

## 4.66 SpeciesID

Node-specific species identifier, last measure to uniquely identify species if any other identifiers collide

**Type:** string

**Constraints:**

## 4.67 StateEnergy

Energy of the level

**Units:** 1/cm

**Type:** floating-point number

**Constraints:** >=0

## 4.68 StateLifeTime

Life time of an atomic state in s.

**Units:** s

**Type:** floating-point number

**Constraints:** >0

## 4.69 StateStatisticalWeight

**Type:** floating-point number

**Constraints:**

## 4.70 VAMDCSpeciesID

Internal VAMDC species identifier, inchikey plus suffix, used in case inchikeys collide for molecules.

**Type:** string

**Constraints:**

CHAPTER

FIVE

# 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.

## 5.1 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
- SomeKeywordAccuracy
- SomeKeywordAccuracyConfidence
- SomeKeywordAccuracyRelative
- SomeKeywordAccuracyType
- SomeKeywordEval
- SomeKeywordEvalMethod
- SomeKeywordEvalRecommended
- SomeKeywordEvalRef
- SomeKeywordEvalComment

## 5.2 The list of Returnables

### 5.2.1 CollisionTabulatedDataYAccuracyMethod

**Type:** string

**Constraints:**

### 5.2.2 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:**

### 5.2.3 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:**

### 5.2.4 AtomIonCharge

Ionization stage with 0 for neutral

**Type:** integer number

**Constraints:** >=0

### 5.2.5 AtomIsoelectronicSequence

**Type:** string

**Constraints:**

### 5.2.6 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

### 5.2.7 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

### 5.2.8 AtomNuclearCharge

Atomic number or nuclear charge

**Type:** integer number

**Constraints:** >0

### 5.2.9 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:**

### 5.2.10 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:**

### 5.2.11 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:**

### 5.2.12 AtomStateComponentMethod

**Type:** string

**Constraints:**

### 5.2.13 AtomStateComponentRef

**Type:** string

**Constraints:**

### 5.2.14 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:**

### 5.2.15 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:**

### 5.2.16 AtomStateCoreTermJ1J2

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

**Type:** integer number

**Constraints:**

### 5.2.17 AtomStateCoreTermJJ

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

**Type:** integer number

**Constraints:**

### 5.2.18 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:**

### 5.2.19 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:**

### 5.2.20 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:**

### 5.2.21 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

### 5.2.22 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:**

### 5.2.23 AtomStateCoreTermLKLSymbol

Core angular momentum symbol???

For example, "p".

**Type:** integer number

**Constraints:**

### 5.2.24 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

### 5.2.25 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

### 5.2.26 AtomStateCoreTermLSLSymbol

For example, "p".

**Type:** string

**Constraints:**

### 5.2.27 AtomStateCoreTermLSMultiplicity

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

**Type:** integer number

**Constraints:** >0

### 5.2.28 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

### 5.2.29 AtomStateCoreTermLSSeniority

Seniority for core electrons.

**Type:** integer number

**Constraints:** >=0

### 5.2.30 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:**

### 5.2.31 AtomStateCoreTotalAngMom

**Type:** integer number

**Constraints:**

### 5.2.32 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:**

### 5.2.33 AtomStateDescription

Good luck

**Type:** string

**Constraints:**

### 5.2.34 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:**

### 5.2.35 AtomStateEnergy

Energy of the level

**Units:** 1/cm

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:** >=0

### 5.2.36 AtomStateHyperfineConstantA

Hyperfine splitting due to magnetic dipole interaction

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.37 AtomStateHyperfineConstantB

Hyperfine splitting due to electric quadrupole interaction

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.38 AtomStateHyperfineMomentum

**Type:** floating-point number

**Constraints:**

### 5.2.39 AtomStateID

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

**Type:** string

**Constraints:**

### 5.2.40 AtomStateIonizationEnergy

Ionization energy in eV

**Units:** 1/cm

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:** >0

### 5.2.41 AtomStateKappa

Relativistic correction.

**Type:** floating-point number

**Constraints:**

### 5.2.42 AtomStateLandeFactor

Lande factor

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.43 AtomStateLifeTime

Life time of an atomic state in s.

**Units:** s

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:** >0

### 5.2.44 AtomStateMagneticQuantumNumber

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

**Type:** floating-point number

**Constraints:**

### 5.2.45 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:**

### 5.2.46 AtomStateMixingCoeffClass

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

**Type:** string

**Constraints:**

### 5.2.47 AtomStateParity

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

**Type:** string

**Constraints:**

### 5.2.48 AtomStatePolarizability

State polarizability.

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.49 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:**

### 5.2.50 AtomStateRef

The bibliographical references for a particular atomic state.

**Type:** string

**Constraints:**

### 5.2.51 AtomStateShellID

Atomic shell ID generated by a database.

**Type:** string

**Constraints:**

### 5.2.52 AtomStateShellKappa

Relativistic correction.

**Type:** floating-point number

**Constraints:**

### 5.2.53 AtomStateShellNumberOfElectrons

Number of electrons in a specific shell.

**Type:** integer number

**Constraints:** >0

### 5.2.54 AtomStateShellOrbitalAngMom

**Type:** integer number

**Constraints:**

### 5.2.55 AtomStateShellOrbitalAngMomSymbol

Shell angular momentum symbol?.

**Type:** string

**Constraints:**

### 5.2.56 AtomStateShellPairID

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

**Type:** string

**Constraints:**

### 5.2.57 AtomStateShellPairShell1ID

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

**Type:** string

**Constraints:**

### 5.2.58 AtomStateShellPairShell1Kappa

Relativistic correction for shell 1 in a pair.

**Type:** floating-point number

**Constraints:**

### 5.2.59 AtomStateShellPairShell1NumberOfElectrons

Number of electrons in shell 1 in a pair.

**Type:** integer number

**Constraints:** >0

### 5.2.60 AtomStateShellPairShell1OrbitalAngMom

Orbital angular momentum of shell 1 in a pair.

**Type:** integer number

**Constraints:** >=0

### 5.2.61 AtomStateShellPairShell1OrbitalAngmomSymbol

Orbital angular momentum symbol for shell 1 in a pair.

**Type:** string

**Constraints:**

### 5.2.62 AtomStateShellPairShell1Parity

Parity of shell 1 in a pair.

**Type:** string

**Constraints:**

### 5.2.63 AtomStateShellPairShell1QN

Principal quantum number of shell 1 in a pair.

**Type:** integer number

**Constraints:** >0

### 5.2.64 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

### 5.2.65 AtomStateShellPairShell1TermJJ

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

**Type:** floating-point number

**Constraints:** >0

### 5.2.66 AtomStateShellPairShell1TermJKJ

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

**Type:** floating-point number

**Constraints:** >0

### 5.2.67 AtomStateShellPairShell1TermJKK

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

**Type:** floating-point number

**Constraints:** >0

### 5.2.68 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

### 5.2.69 AtomStateShellPairShell1TermLKK

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

**Type:** floating-point number

**Constraints:** >0

### 5.2.70 AtomStateShellPairShell1TermLKL

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

**Type:** integer number

**Constraints:** >=0

### 5.2.71 AtomStateShellPairShell1TermLKLSymbol

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

**Type:** string

**Constraints:**

### 5.2.72 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

### 5.2.73 AtomStateShellPairShell1TermLSL

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

**Type:** integer number

**Constraints:** >=0

### 5.2.74 AtomStateShellPairShell1TermLSLSymbol

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

**Type:** string

**Constraints:**

### 5.2.75 AtomStateShellPairShell1TermLSMultiplicity

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

**Type:** integer number

**Constraints:** >0

### 5.2.76 AtomStateShellPairShell1TermLSS

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

**Type:** floating-point number

**Constraints:** >=0

### 5.2.77 AtomStateShellPairShell1TermLSSeniority

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

**Type:** integer number

**Constraints:** >=0

### 5.2.78 AtomStateShellPairShell1TermLabel

Term label for shell 1.

**Type:** string

**Constraints:**

### 5.2.79 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

### 5.2.80 AtomStateShellPairShell2ID

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

**Type:** string

**Constraints:**

### 5.2.81 AtomStateShellPairShell2Kappa

Relativistic correction for shell 2 in a pair.

**Type:** floating-point number

**Constraints:**

### 5.2.82 AtomStateShellPairShell2NumberOfElectrons

Number of electrons in shell 2 in a pair.

**Type:** integer number

**Constraints:** >0

### 5.2.83 AtomStateShellPairShell2OrbitalAngMom

Orbital angular momentum of shell 2 in a pair.

**Type:** integer number

**Constraints:** >=0

### 5.2.84 AtomStateShellPairShell2OrbitalAngMomSymbol

Orbital angular momentum symbol for shell 2 in a pair.

**Type:** string

**Constraints:**

### 5.2.85 AtomStateShellPairShell2Parity

Parity of shell 2 in a pair.

**Type:** string

**Constraints:**

### 5.2.86 AtomStateShellPairShell2QN

Principal quantum number of shell 2 in a pair.

**Type:** integer number

**Constraints:** >0

### 5.2.87 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

### 5.2.88 AtomStateShellPairShell2TermJJ

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

**Type:** floating-point number

**Constraints:** >0

### 5.2.89 AtomStateShellPairShell2TermJKJ

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

**Type:** floating-point number

**Constraints:** >0

### 5.2.90 AtomStateShellPairShell2TermJKK

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

**Type:** floating-point number

**Constraints:** >0

### 5.2.91 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

### 5.2.92 AtomStateShellPairShell2TermLKK

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

**Type:** floating-point number

**Constraints:** >0

### 5.2.93 AtomStateShellPairShell2TermLKL

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

**Type:** integer number

**Constraints:** >=0

### 5.2.94 AtomStateShellPairShell2TermLKLSymbol

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

**Type:** integer number

**Constraints:**

### 5.2.95 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

### 5.2.96 AtomStateShellPairShell2TermLSL

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

**Type:** integer number

**Constraints:** >=0

### 5.2.97 AtomStateShellPairShell2TermLSLSymbol

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

**Type:** string

**Constraints:**

### 5.2.98 AtomStateShellPairShell2TermLSMultiplicity

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

**Type:** integer number

**Constraints:** >0

### 5.2.99 AtomStateShellPairShell2TermLSS

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

**Type:** floating-point number

**Constraints:** >=0

### 5.2.100 AtomStateShellPairShell2TermLSSeniority

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

**Type:** integer number

**Constraints:** >=0

### 5.2.101 AtomStateShellPairShell2TermLabel

Term label for shell 2.

**Type:** string

**Constraints:**

### 5.2.102 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

#### 5.2.103 AtomStateShellPairTermJ1J2

**Type:** integer number

**Constraints:**

#### 5.2.104 AtomStateShellPairTermJJ

**Type:** integer number

**Constraints:**

#### 5.2.105 AtomStateShellPairTermJKJ

**Type:** integer number

**Constraints:**

#### 5.2.106 AtomStateShellPairTermJKK

**Type:** integer number

**Constraints:**

#### 5.2.107 AtomStateShellPairTermJKS2

**Type:** integer number

**Constraints:**

#### 5.2.108 AtomStateShellPairTermLKK

**Type:** integer number

**Constraints:**

#### 5.2.109 AtomStateShellPairTermLKL

**Type:** integer number

**Constraints:**

#### 5.2.110 AtomStateShellPairTermLKLSymbol

**Type:** integer number

**Constraints:**

#### 5.2.111 AtomStateShellPairTermLKS2

**Type:** integer number

**Constraints:**

### 5.2.112 AtomStateShellPairTermLSL

**Type:** integer number

**Constraints:**

### 5.2.113 AtomStateShellPairTermLSLSymbol

**Type:** integer number

**Constraints:**

### 5.2.114 AtomStateShellPairTermLSMultiplicity

**Type:** integer number

**Constraints:**

### 5.2.115 AtomStateShellPairTermLSS

**Type:** integer number

**Constraints:**

### 5.2.116 AtomStateShellPairTermLSSeniority

**Type:** integer number

**Constraints:**

### 5.2.117 AtomStateShellPairTermLabel

**Type:** string

**Constraints:**

### 5.2.118 AtomStateShellParity

**Type:** integer number

**Constraints:**

### 5.2.119 AtomStateShellPrincipalQN

**Type:** integer number

**Constraints:**

### 5.2.120 AtomStateShellTermJ1J2

**Type:** integer number

**Constraints:**

#### 5.2.121 AtomStateShellTermJJ

**Type:** integer number

**Constraints:**

#### 5.2.122 AtomStateShellTermJKJ

**Type:** integer number

**Constraints:**

#### 5.2.123 AtomStateShellTermJKS

**Type:** integer number

**Constraints:**

#### 5.2.124 AtomStateShellTermK

**Type:** integer number

**Constraints:**

#### 5.2.125 AtomStateShellTermLKK

**Type:** integer number

**Constraints:**

#### 5.2.126 AtomStateShellTermLKL

**Type:** integer number

**Constraints:**

#### 5.2.127 AtomStateShellTermLKLSymbol

**Type:** string

**Constraints:**

#### 5.2.128 AtomStateShellTermLKS2

**Type:** integer number

**Constraints:**

#### 5.2.129 AtomStateShellTermLSL

**Type:** integer number

**Constraints:**

### 5.2.130 AtomStateShellTermLSLSymbol

**Type:** integer number

**Constraints:**

### 5.2.131 AtomStateShellTermLSMultiplicity

**Type:** integer number

**Constraints:**

### 5.2.132 AtomStateShellTermLabel

**Type:** integer number

**Constraints:**

### 5.2.133 AtomStateShellTermS

**Type:** integer number

**Constraints:**

### 5.2.134 AtomStateShellTermSeniority

**Type:** integer number

**Constraints:**

### 5.2.135 AtomStateShellTotalAngMom

**Type:** integer number

**Constraints:**

### 5.2.136 AtomStateStatisticalWeight

**Type:** floating-point number

**Constraints:**

### 5.2.137 AtomStateSuperShellNumberOfElectrons

**Type:** integer number

**Constraints:**

### 5.2.138 AtomStateSuperShellPrincipalQN

**Type:** integer number

**Constraints:**

### 5.2.139 AtomStateTermJ1J2

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

**Type:** integer number

**Constraints:**

### 5.2.140 AtomStateTermJJ

**Type:** integer number

**Constraints:**

### 5.2.141 AtomStateTermJKJ

**Type:** integer number

**Constraints:**

### 5.2.142 AtomStateTermJKK

**Type:** integer number

**Constraints:**

### 5.2.143 AtomStateTermJKS

**Type:** integer number

**Constraints:**

### 5.2.144 AtomStateTermLKK

**Type:** integer number

**Constraints:**

### 5.2.145 AtomStateTermLKL

**Type:** integer number

**Constraints:**

### 5.2.146 AtomStateTermLKLSymbol

**Type:** integer number

**Constraints:**

### 5.2.147 AtomStateTermLKS2

**Type:** integer number

**Constraints:**

### 5.2.148 AtomStateTermLSL

**Type:** integer number

**Constraints:**

### 5.2.149 AtomStateTermLSLSymbol

**Type:** string

**Constraints:**

### 5.2.150 AtomStateTermLSMultiplicity

**Type:** integer number

**Constraints:**

### 5.2.151 AtomStateTermLSS

**Type:** floating-point number

**Constraints:**

### 5.2.152 AtomStateTermLSSeniority

**Type:** integer number

**Constraints:**

### 5.2.153 AtomStateTermLabel

**Type:** string

**Constraints:**

### 5.2.154 AtomStateTotalAngMom

**Type:** integer number

**Constraints:**

### 5.2.155 AtomSymbol

Atomic name

**Type:** string

**Constraints:**

### 5.2.156 BasisState

A single basis state in the description of a molecular state as an expansion in some basis

**Type:** string

**Constraints:**

### 5.2.157 BasisStateComment

A comment relating to this basis state

**Type:** string

**Constraints:**

### 5.2.158 BasisStateID

The ID for this basis state

**Type:** string

**Constraints:**

### 5.2.159 BasisStateMethod

Method relating to this basis state

**Type:** string

**Constraints:**

### 5.2.160 BasisStateRef

A source (reference) for this basis state

**Type:** string

**Constraints:**

### 5.2.161 CollisionCode

**Type:** string

**Constraints:**

### 5.2.162 CollisionComment

**Type:** string

**Constraints:**

### 5.2.163 CollisionDataSetComment

**Type:** string

**Constraints:**

### 5.2.164 CollisionDataSetDescription

**Type:** string

**Constraints:**

### 5.2.165 CollisionDataSetMethod

**Type:** string

**Constraints:**

### 5.2.166 CollisionDataSetRef

**Type:** string

**Constraints:**

### 5.2.167 CollisionFitDataAccuracy

**Type:** string

**Constraints:**

### 5.2.168 CollisionFitDataArgumentDescription

**Type:** string

**Constraints:**

### 5.2.169 CollisionFitDataArgumentLowerLimit

**Type:** string

**Constraints:**

### 5.2.170 CollisionFitDataArgumentName

**Type:** string

**Constraints:**

### 5.2.171 CollisionFitDataArgumentUnits

**Type:** string

**Constraints:**

### 5.2.172 CollisionFitDataArgumentUpperLimit

**Type:** string

**Constraints:**

### 5.2.173 CollisionFitDataComment

**Type:** string

**Constraints:**

### 5.2.174 CollisionFitDataFunction

**Type:** string

**Constraints:**

### 5.2.175 CollisionFitDataMethod

**Type:** string

**Constraints:**

### 5.2.176 CollisionFitDataParameter

**Type:** string

**Constraints:**

### 5.2.177 CollisionFitDataPhysicalUncertainty

**Type:** string

**Constraints:**

### 5.2.178 CollisionFitDataProductionDate

**Type:** string

**Constraints:**

### 5.2.179 CollisionFitDataRef

**Type:** string

**Constraints:**

### 5.2.180 CollisionGroup

Collision group label

**Type:** string

**Constraints:**

### 5.2.181 CollisionIAEACode

**Type:** string

**Constraints:**

### 5.2.182 CollisionID

Collision ID

**Type:** string

**Constraints:**

### 5.2.183 CollisionIntermediateSpecies

**Type:** string

**Constraints:**

### 5.2.184 CollisionIntermediateState

**Type:** string

**Constraints:**

### 5.2.185 CollisionMethod

**Type:** string

**Constraints:**

### 5.2.186 CollisionProductSpecies

**Type:** string

**Constraints:**

### 5.2.187 CollisionProductState

**Type:** string

**Constraints:**

### 5.2.188 CollisionReactantSpecies

**Type:** string

**Constraints:**

### 5.2.189 CollisionReactantState

**Type:** string

**Constraints:**

### 5.2.190 CollisionRef

**Type:** string

**Constraints:**

### 5.2.191 CollisionTabulatedData

**Type:** string

**Constraints:**

### 5.2.192 CollisionTabulatedDataComment

**Type:** string

**Constraints:**

### 5.2.193 CollisionTabulatedDataMethod

**Type:** string

**Constraints:**

### 5.2.194 CollisionTabulatedDataPhysicalUncertainty

**Type:** string

**Constraints:**

### 5.2.195 CollisionTabulatedDataProductionDate

**Type:** string

**Constraints:**

### 5.2.196 CollisionTabulatedDataRef

**Type:** string

**Constraints:**

### 5.2.197 CollisionTabulatedDataReferenceFrame

**Type:** string

**Constraints:**

### 5.2.198 CollisionTabulatedDataX

**Type:** floating-point number

**Constraints:**

### 5.2.199 CollisionTabulatedDataXAccuracy

**Type:** floating-point number

**Constraints:**

### 5.2.200 CollisionTabulatedDataXAccuracyComment

**Type:** string

**Constraints:**

### 5.2.201 CollisionTabulatedDataXAccuracyErrorFile

**Type:** string

**Constraints:**

### 5.2.202 CollisionTabulatedDataXAccuracyErrorList

**Type:** floating-point number

**Constraints:**

### 5.2.203 CollisionTabulatedDataXAccuracyErrorListN

**Type:** integer number

**Constraints:**

### 5.2.204 CollisionTabulatedDataXAccuracyErrorValue

**Type:** floating-point number

**Constraints:**

### 5.2.205 CollisionTabulatedDataXAccuracyMethodRef

**Type:** string

**Constraints:**

### 5.2.206 CollisionTabulatedDataXAccuracyRelative

**Type:** string

**Constraints:**

### 5.2.207 CollisionTabulatedDataXAccuracyType

**Type:** string

**Constraints:**

### 5.2.208 CollisionTabulatedDataXDataFile

**Type:** string

**Constraints:**

### 5.2.209 CollisionTabulatedDataXDataList

**Type:** floating-point number

**Constraints:**

### 5.2.210 CollisionTabulatedDataXDataListN

**Type:** integer number

**Constraints:**

### 5.2.211 CollisionTabulatedDataXDescription

**Type:** string

**Constraints:**

### 5.2.212 CollisionTabulatedDataXLinearSequenceIncrement

**Type:** floating-point number

**Constraints:**

### 5.2.213 CollisionTabulatedDataXLinearSequenceInitial

**Type:** floating-point number

**Constraints:**

### 5.2.214 CollisionTabulatedDataXLinearSequenceN

**Type:** integer number

**Constraints:**

### 5.2.215 CollisionTabulatedDataXParameter

**Type:** floating-point number

**Constraints:**

### 5.2.216 CollisionTabulatedDataXUnits

**Type:** string

**Constraints:**

### 5.2.217 CollisionTabulatedDataY

**Type:** floating-point number

**Constraints:**

### 5.2.218 CollisionTabulatedDataYAccuracy

**Type:** floating-point number

**Constraints:**

### 5.2.219 CollisionTabulatedDataYAccuracyComment

**Type:** string

**Constraints:**

### 5.2.220 CollisionTabulatedDataYAccuracyErrorFile

**Type:** string

**Constraints:**

### 5.2.221 CollisionTabulatedDataYAccuracyErrorList

**Type:** floating-point number

**Constraints:**

### 5.2.222 CollisionTabulatedDataYAccuracyErrorListN

**Type:** integer number

**Constraints:**

### 5.2.223 CollisionTabulatedDataYAccuracyErrorValue

**Type:** integer number

**Constraints:**

### 5.2.224 CollisionTabulatedDataYAccuracyMethodRef

**Type:** string

**Constraints:**

### 5.2.225 CollisionTabulatedDataYAccuracyRelative

**Type:** string

**Constraints:**

### 5.2.226 CollisionTabulatedDataYAccuracyType

**Type:** string

**Constraints:**

### 5.2.227 CollisionTabulatedDataYDataFile

**Type:** string

**Constraints:**

### 5.2.228 CollisionTabulatedDataYDataList

**Type:** floating-point number

**Constraints:**

### 5.2.229 CollisionTabulatedDataYDataListN

**Type:** integer number

**Constraints:**

### 5.2.230 CollisionTabulatedDataYDescription

**Type:** string

**Constraints:**

### 5.2.231 CollisionTabulatedDataYLinearSequenceIncrement

**Type:** floating-point number

**Constraints:**

### 5.2.232 CollisionTabulatedDataYLinearSequenceInitial

**Type:** floating-point number

**Constraints:**

### 5.2.233 CollisionTabulatedDataYLinearSequenceN

Number of elements in Linear Sequence

**Type:** integer number

**Constraints:**

### 5.2.234 CollisionTabulatedDataYParameter

**Type:** floating-point number

**Constraints:**

### 5.2.235 CollisionTabulatedDataYUnits

**Type:** string

**Constraints:**

### 5.2.236 CollisionThreshold

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.237 CollisionUserDefinition

**Type:** string

**Constraints:**

### 5.2.238 CrossSectionBandCentre

The centre wavenumber, wavelength, etc. of a feature in an tabulated cross section

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.239 CrossSectionBandModeComment

**Type:** string

**Constraints:**

### 5.2.240 CrossSectionBandModeDeltaV

List of dV values

**Type:** floating-point number

**Constraints:** >0

### 5.2.241 CrossSectionBandModeDeltaVID

ID of a normal mode when referenced in the assignment of a band in an assigned cross section

**Type:** string

**Constraints:**

### 5.2.242 CrossSectionBandModeMethod

**Type:** string

**Constraints:**

### 5.2.243 CrossSectionBandModeName

A string, optionally identifying a band in an assigned cross section, e.g. “asymmetric stretch”

**Type:** string

**Constraints:**

### 5.2.244 CrossSectionBandName

**Type:** string

**Constraints:**

### 5.2.245 CrossSectionBandWidth

The width of an assigned feature in a tabulated cross section (in units of wavenumber, wavelength, etc.)

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.246 CrossSectionDescription

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

**Type:** string

**Constraints:**

### 5.2.247 CrossSectionEnvironment

Reference to an Environment ID describing the environment applicable to this cross section

**Type:** string

**Constraints:**

### 5.2.248 CrossSectionGroup

**Type:** string

**Constraints:**

### 5.2.249 CrossSectionID

ID label for this cross section data

**Type:** string

**Constraints:**

### 5.2.250 CrossSectionProcess

???

**Type:** string

**Constraints:**

### 5.2.251 CrossSectionSpecies

A reference to the ID of a species contributing to this cross section

**Type:** string

**Constraints:**

### 5.2.252 CrossSectionState

???

**Type:** string

**Constraints:**

### 5.2.253 CrossSectionX

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

**Type:** string

**Constraints:**

### 5.2.254 CrossSectionXDataFile

Datafile containing X data.

**Type:** string

**Constraints:**

### 5.2.255 CrossSectionXError

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

**Type:** floating-point number

**Constraints:**

### 5.2.256 CrossSectionXErrorList

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

**Type:** string

**Constraints:**

### 5.2.257 CrossSectionXLinearCount

The length of the linear series X_i = initial + increment * i giving the independent variable against which the cross section is given when this data series is an evenly-spaced series of values.

**Type:** integer number

**Constraints:**

### 5.2.258 CrossSectionXLinearIncrement

The increment step in the linear series X_i = initial + increment * 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:**

### 5.2.259 CrossSectionXLinearInitial

The initial value in the linear series X_i = initial + increment * 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:**

### 5.2.260 CrossSectionXName

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

**Type:** string

**Constraints:**

### 5.2.261 CrossSectionXUnit

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

**Type:** string

**Constraints:**

### 5.2.262 CrossSectionY

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

**Type:** string

**Constraints:**

### 5.2.263 CrossSectionYDataFile

Datafile containing Y data.

**Type:** string

**Constraints:**

### 5.2.264 CrossSectionYError

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

**Type:** floating-point number

**Constraints:**

### 5.2.265 CrossSectionYErrorList

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

**Type:** string

**Constraints:**

### 5.2.266 CrossSectionYLinearCount

The length of the linear series Y_i = initial + increment * i, giving the independent variable against which the cross section is given when this data series is an evenly-spaced series of values

**Type:** integer number

**Constraints:**

### 5.2.267 CrossSectionYLinearIncrement

The increment in the linear series Y_i = initial + increment * 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:**

### 5.2.268 CrossSectionYLinearInitial

The initial valie of the linear series Y_i = initial + increment * 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:**

### 5.2.269 CrossSectionYName

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

**Type:** string

**Constraints:**

### 5.2.270 CrossSectionYUnit

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

**Type:** string

**Constraints:**

### 5.2.271 EnvironmentComment

**Type:** string

**Constraints:**

### 5.2.272 EnvironmentID

An ID of the form “Exxx” identifying this Environment

**Type:** string

**Constraints:**

### 5.2.273 EnvironmentRef

A reference to the ID, of the form 'Exxx', identifying the environment referenced here

**Type:** string

**Constraints:**

### 5.2.274 EnvironmentSpecies

A species contributing to an Environment

**Type:** string

**Constraints:**

### 5.2.275 EnvironmentSpeciesConcentration

The concentration of a species contributing to an Environment

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.276 EnvironmentSpeciesMoleFraction

The mole fraction of a species contributing to an Environment

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.277 EnvironmentSpeciesName

The name of a species contributing to an Environment

**Type:** string

**Constraints:**

### 5.2.278 EnvironmentSpeciesPartialPressure

The partial pressure of a species contributing to an Environment

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.279 EnvironmentSpeciesRef

The reference to an ID of a species contributing to an Environment

**Type:** string

**Constraints:**

### 5.2.280 EnvironmentTemperature

Environment temperature

**Units:** K

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:** >0

### 5.2.281 EnvironmentTotalNumberDensity

The total number density of particles comprising an Environment

**Units:** 1/cm3

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.282 EnvironmentTotalPressure

Environment total pressure

**Units:** Pa

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:** >=0

### 5.2.283 FunctionArgumentDescription

Description of the function to an argument

**Type:** string

**Constraints:**

### 5.2.284 FunctionArgumentLowerLimit

The lower limit of validity for this argument to the fit or model function

**Type:** floating-point number

**Constraints:**

### 5.2.285 FunctionArgumentName

The name of this argument to the fit or model function

**Type:** string

**Constraints:**

### 5.2.286 FunctionArgumentUnits

The units of this argument to the fit or model function

**Type:** string

**Constraints:**

### 5.2.287 FunctionArgumentUpperLimit

The upper limit of validity for this argument to the fit or model function

**Type:** floating-point number

**Constraints:**

### 5.2.288 FunctionComputerLanguage

**Type:** string

**Constraints:**

### 5.2.289 FunctionDescription

A description of this function

**Type:** string

**Constraints:**

### 5.2.290 FunctionExpression

**Type:** string

**Constraints:**

### 5.2.291 FunctionID

A unique identifier for this function, of the form 'Fxxx'

**Type:** string

**Constraints:**

### 5.2.292 FunctionName

The name of this function

**Type:** string

**Constraints:**

### 5.2.293 FunctionParameterDescription

A description of this parameter to the fit or model function

**Type:** string

**Constraints:**

### 5.2.294 FunctionParameterName

A name of this parameter to the fit or model function

**Type:** string

**Constraints:**

### 5.2.295 FunctionParameterUnits

A units of this parameter to the fit or model function

**Type:** string

**Constraints:**

### 5.2.296 FunctionReferenceFrame

**Type:** string

**Constraints:**

### 5.2.297 FunctionSourceCodeURL

**Type:** string

**Constraints:**

### 5.2.298 FunctionSourceRef

**Type:** string

**Constraints:**

### 5.2.299 FunctionYDescription

**Type:** string

**Constraints:**

### 5.2.300 FunctionYLowerLimit

**Type:** floating-point number

**Constraints:**

### 5.2.301 FunctionYName

**Type:** string

**Constraints:**

### 5.2.302 FunctionYUnits

**Type:** string

**Constraints:**

### 5.2.303 FunctionYUpperLimit

**Type:** floating-point number

**Constraints:**

### 5.2.304 MethodCategory

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

**Type:** string

**Constraints:**

### 5.2.305 MethodComment

**Type:** string

**Constraints:**

### 5.2.306 MethodDescription

**Type:** string

**Constraints:**

### 5.2.307 MethodID

**Type:** string

**Constraints:**

### 5.2.308 MethodRef

**Type:** string

**Constraints:**

### 5.2.309 MoleculeBasisStates

The basis states for a set of molecular states expressed as a linear combination on some basis

**Type:** string

**Constraints:**

### 5.2.310 MoleculeBasisStatesComment

A Comment relating to this set of Basis states

**Type:** string

**Constraints:**

### 5.2.311 MoleculeBasisStatesMethod

A Method relating to this set of Basis states

**Type:** string

**Constraints:**

### 5.2.312 MoleculeBasisStatesRef

One or more source references relating to this set of Basis states

**Type:** string

**Constraints:**

### 5.2.313 MoleculeCASRegistryNumber

**Type:** string

**Constraints:**

### 5.2.314 MoleculeCNPIGroup

**Type:** string

**Constraints:**

### 5.2.315 MoleculeChemicalName

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

**Type:** string

**Constraints:**

### 5.2.316 MoleculeComment

**Type:** string

**Constraints:**

### 5.2.317 MoleculeIUPACName

**Type:** string

**Constraints:**

### 5.2.318 MoleculeInchi

**Type:** string

**Constraints:**

### 5.2.319 MoleculeInchiKey

**Type:** string

**Constraints:**

### 5.2.320 MoleculeIonCharge

Molecule ion charge

**Type:** integer number

**Constraints:**

### 5.2.321 MoleculeMolecularWeight

**Units:** u

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.322 MoleculeNormalModeDisplacementVectorComment

Comments concerning this normal mode's displacement vectors

**Type:** string

**Constraints:**

### 5.2.323 MoleculeNormalModeDisplacementVectorMethod

**Type:** string

**Constraints:**

### 5.2.324 MoleculeNormalModeDisplacementVectorRef

A reference to the atom in the molecule's structure to which this displacement vector applies

**Type:** string

**Constraints:**

### 5.2.325 MoleculeNormalModeDisplacementVectorX3

The x-component of this atom's displacement vector

**Type:** floating-point number

**Constraints:**

### 5.2.326 MoleculeNormalModeDisplacementVectorY3

The y-component of this atom's displacement vector

**Type:** floating-point number

**Constraints:**

### 5.2.327 MoleculeNormalModeDisplacementVectorZ3

The z-component of this atom's displacement vector

**Type:** floating-point number

**Constraints:**

### 5.2.328 MoleculeNormalModeElectronicState

A reference to the electronic state within which this normal mode applies

**Type:** string

**Constraints:**

### 5.2.329 MoleculeNormalModeHarmonicFrequency

The harmonic frequency of a normal mode.

**Units:** MHz

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.330 MoleculeNormalModeID

The ID of this normal mode

**Type:** string

**Constraints:**

### 5.2.331 MoleculeNormalModeIntensity

Normal mode intensity

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.332 MoleculeNormalModeMethod

**Type:** string

**Constraints:**

### 5.2.333 MoleculeNormalModePointGroupSymmetry

The symmetry species of this normal mode within the point group of the molecule in the specified electronic state

**Type:** string

**Constraints:**

### 5.2.334 MoleculeNormalModeRef

**Type:** string

**Constraints:**

### 5.2.335 MoleculeOrdinaryStructuralFormula

The ordinary structural formula, as it is usually written, for the molecule

**Type:** string

**Constraints:**

### 5.2.336 MoleculeQNElecStateLabel

A label identifying the molecule's electronic state, e.g. 'X', 'A', 'b'

**Type:** string

**Constraints:**

### 5.2.337 MoleculeQNF

The molecular state quantum number for total angular momentum including nuclear spin

**Type:** floating-point number

**Constraints:**

### 5.2.338 MoleculeQNF1

The molecular state quantum number for angular momentum including hyperfine coupling with one nuclear spin, F1 = J + I1

**Type:** floating-point number

**Constraints:**

### 5.2.339 MoleculeQNF1nuclSpin

Identifier for the nucleus coupling its spin to give F1: F1 = J + I1

**Type:** string

**Constraints:**

### 5.2.340 MoleculeQNF2

The molecular state quantum number for angular momentum including hyperfine coupling with the second of two nuclear spins: F2 = F1 + I2

**Type:** floating-point number

**Constraints:**

### 5.2.341 MoleculeQNF2nuclSpin

Identifier for the second nucleus coupling its spin to give F2: F2 = F1 + I2

**Type:** string

**Constraints:**

### 5.2.342 MoleculeQNFj

The Fj quantum number, for some intermediate nuclear spin coupling: Fj = Fj-1 + Ij (j>1), or Fj = J + Ij (j=1)

**Type:** floating-point number

**Constraints:**

### 5.2.343 MoleculeQNFjj

The integer j, identifying the order of this nuclear spin coupling where several nuclear spins couple: Fj = Fj-1 + Ij (j>1)

**Type:** integer number

**Constraints:**

### 5.2.344 MoleculeQNFjnuclSpin

ID of the nuclear spin coupling to give quantum number Fj

**Type:** string

**Constraints:**

### 5.2.345 MoleculeQNFnuclSpin

ID of the nuclear spin coupling to give quantum number F, the total angular momentum (including nuclear spin).

**Type:** string

**Constraints:**

### 5.2.346 MoleculeQNI

The total nuclear spin quantum number for a coupled set of identical nuclear spins, I = I1 + I2 + ...

**Type:** floating-point number

**Constraints:**

### 5.2.347 MoleculeQNInuclSpin

**Type:** string

**Constraints:**

### 5.2.348 MoleculeQNJ

The molecular J quantum number for total angular momentum excluding nuclear spin

**Type:** floating-point number

**Constraints:**

### 5.2.349 MoleculeQNK

K is the quantum number associated with the projection of the total angular momentum excluding nuclear spin, J, onto the molecular symmetry axis.

**Type:** integer number

**Constraints:**

### 5.2.350 MoleculeQNKa

Ka is the rotational quantum label of an asymmetric top molecule, correlating to K in the prolate symmetric top limit.

**Type:** integer number

**Constraints:**

### 5.2.351 MoleculeQNKc

Kc is the rotational quantum label of an asymmetric top molecule, correlating to K in the oblate symmetric top limit.

**Type:** integer number

**Constraints:**

### 5.2.352 MoleculeQNLambda

Lambda is the quantum number associated with the magnitude of the projection of the total electronic orbital angular momentum, L, onto the molecular axis.

**Type:** integer number

**Constraints:**

### 5.2.353 MoleculeQNN

N is the quantum number associated with the total angular momentum excluding electronic and nuclear spin, N: J = N + S.

**Type:** integer number

**Constraints:**

### 5.2.354 MoleculeQNOmega

Omega is the quantum number associated with the projection of the total angular momentum (excluding nuclear spin), J, onto the molecular axis.

**Type:** floating-point number

**Constraints:**

### 5.2.355 MoleculeQNS

S is the quantum number associated with the total electronic spin angular momentum.

**Type:** floating-point number

**Constraints:**

### 5.2.356 MoleculeQNSigma

Sigma is the quantum number associated with the magnitude of the projection of S onto the molecular axis.

**Type:** floating-point number

**Constraints:**

### 5.2.357 MoleculeQNSpinComponentLabel

SpinComponentLabel is the positive integer identifying the spin-component label, Fx, where x=1,2,3,... in order of increasing energy for a given value of J - see Herzberg, Spectra of Diatomic Molecules, Van Nostrand, Princeton, N.J., 1950.

**Type:** string

**Constraints:**

### 5.2.358 MoleculeQNasSym

a/s-symmetry: the symmetry of the rovibronic wavefunction, ‘a’ or ‘s’ such that the total wavefunction including nuclear spin is symmetric or antisymmetric with respect to permutation of identical nuclei

**Type:** string

**Constraints:**

### 5.2.359 MoleculeQNelecInv

elecInv is the parity of the electronic wavefunction with respect to inversion through the molecular centre of mass in the molecular coordinate system (‘g’ or ‘u’)

**Type:** string

**Constraints:**

### 5.2.360 MoleculeQNelecRefl

The parity of the electronic wavefunction with respect to reflection in a plane containing the molecular symmetry axis in the molecular coordinate system (equivalent to inversion through the molecular centre of mass in the laboratory coordinate system), '+' or '-'

**Type:** string

**Constraints:**

### 5.2.361 MoleculeQNelecSym

**Type:** string

**Constraints:**

### 5.2.362 MoleculeQNelecSymGroup

**Type:** string

**Constraints:**

### 5.2.363 MoleculeQNkronigParity

kronigParity is the 'rotationless' parity: the parity of the total molecular wavefunction excluding nuclear spin and rotation with respect to inversion through the molecular centre of mass of all particles' coordinates in the laboratory coordinate system, 'e' or 'f'

**Type:** string

**Constraints:**

### 5.2.364 MoleculeQNl

The vibrational angular momentum quantum number, l

**Type:** integer number

**Constraints:**

### 5.2.365 MoleculeQNl2

For linear triatomic molecules, the vibrational angular momentum quantum number associated with the nu2 bending vibration: l2 = v2, v2-2, ..., 1 or 0

**Type:** integer number

**Constraints:**

### 5.2.366 MoleculeQNli

The vibrational angular momentum quantum number, l_i, associated with a degenerate vibrational mode, nu_i: li = vi, vi-2, ..., 1 or 0

**Type:** integer number

**Constraints:**

### 5.2.367 MoleculeQNliMode

An integer identifying the degenerate vibrational mode to which the li quantum number belongs

**Type:** integer number

**Constraints:**

### 5.2.368 MoleculeQNparity

Total parity: the parity of the total molecular wavefunction (excluding nuclear spin) with respect to inversion through the molecular centre of mass of all particles' coordinates in the laboratory coordinate system, the E* operation, '+' or '-'

**Type:** string

**Constraints:**

### 5.2.369 MoleculeQNr

r is a named, positive integer label identifying the state if no other good quantum numbers or symmetries are known.

**Type:** integer number

**Constraints:**

### 5.2.370 MoleculeQNrName

A name, identifying the ranking label, r

**Type:** string

**Constraints:**

### 5.2.371 MoleculeQNrotSym

rotSym is the symmetry species of the rotational wavefunction, in some appropriate symmetry group.

**Type:** string

**Constraints:**

### 5.2.372 MoleculeQNrotSymGroup

The symmetry group used in giving the rotational symmetry species label

**Type:** string

**Constraints:**

### 5.2.373 MoleculeQNrovibSym

**Type:** string

**Constraints:**

### 5.2.374 MoleculeQNrovibSymGroup

**Type:** string

**Constraints:**

### 5.2.375 MoleculeQNv

For diatomic molecules, the vibrational quantum number, v

**Type:** integer number

**Constraints:**

### 5.2.376 MoleculeQNv1

The v1 vibrational quantum number.

**Type:** integer number

**Constraints:**

### 5.2.377 MoleculeQNv2

The v2 vibrational quantum number.

**Type:** integer number

**Constraints:**

### 5.2.378 MoleculeQNv3

The v3 vibrational quantum number.

**Type:** integer number

**Constraints:**

### 5.2.379 MoleculeQNvi

The vi vibrational quantum number for the ith normal mode

**Type:** integer number

**Constraints:**

### 5.2.380 MoleculeQNviMode

An integer identifying the vibrational normal mode for the vi quantum number

**Type:** integer number

**Constraints:**

### 5.2.381 MoleculeQNvibInv

vibInv is the parity of the vibrational wavefunction with respect to inversion through the molecular centre of mass in the molecular coordinate system. Only really necessary for molecules with a low barrier to such an inversion (for example, NH3), 's' or 'a'.

**Type:** string

**Constraints:**

### 5.2.382 MoleculeQNvibRefl

vibRefl is the parity of the vibrational wavefunction with respect to reflection in a plane containing the molecular symmetry axis in the molecular coordinate system, '+' or '-'.

**Type:** string

**Constraints:**

### 5.2.383 MoleculeQNvibSym

Vibrational wavefunction symmetry species

**Type:** string

**Constraints:**

### 5.2.384 MoleculeQNvibSymGroup

The symmetry group used to specify the vibrational wavefunction symmetry species

**Type:** string

**Constraints:**

### 5.2.385 MoleculeQnCase

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

**Type:** string

**Constraints:**

### 5.2.386 MoleculeSpeciesID

ID for the molecular species

**Type:** string

**Constraints:**

### 5.2.387 MoleculeStableMolecularProperties

Molecular properties such as molecular weight

**Type:** string

**Constraints:**

### 5.2.388 MoleculeStateDescription

A text description of this molecular state

**Type:** string

**Constraints:**

### 5.2.389 MoleculeStateEnergy

The energy of a molecular state

**Units:** 1/cm

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.390 MoleculeStateEnergyOrigin

A string identifying where the origin is taken for the energy of this molecular state

**Type:** string

**Constraints:**

### 5.2.391 MoleculeStateExpansionCoeff

**Type:** floating-point number

**Constraints:**

### 5.2.392 MoleculeStateExpansionCoeffStateRef

**Type:** string

**Constraints:**

### 5.2.393 MoleculeStateExpansionComments

**Type:** string

**Constraints:**

### 5.2.394 MoleculeStateExpansionMethodRef

**Type:** string

**Constraints:**

### 5.2.395 MoleculeStateExpansionSourceRef

One or more source references - these entries should match the sourceID attributes of the Sources.

**Type:** string

**Constraints:**

### 5.2.396 MoleculeStateFullyAssigned

A boolean value, asserting that the state is fully assigned (true) or not (false)

**Type:** string

**Constraints:**

### 5.2.397 MoleculeStateID

A string, of the form 'Sxxx' identifying this molecular state

**Type:** string

**Constraints:**

### 5.2.398 MoleculeStateLifeTime

Molecular state lifetime in seconds

**Units:** s

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:** >0

### 5.2.399 MoleculeStateMixingCoefficient

**Type:** string

**Constraints:**

### 5.2.400 MoleculeStateNuclearSpinIsomer

Nuclear spin isomer (symmetry) of a molecular state. Can take values like 'ortho','para','A','E','meta', etc.

**Type:** string

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

### 5.2.401 MoleculeStateNuclearStatisticalWeight

Nuclear statistical weight for a given molecular energy level

**Type:** integer number

**Constraints:** >0

### 5.2.402 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:**

### 5.2.403 MoleculeStateParameterMatrixColRefs

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

**Type:** string

**Constraints:**

### 5.2.404 MoleculeStateParameterMatrixForm

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

**Type:** string

**Constraints:**

### 5.2.405 MoleculeStateParameterMatrixNcols

Molecular State parameters in matrix form; number of matrix columns

**Type:** integer number

**Constraints:**

### 5.2.406 MoleculeStateParameterMatrixNrows

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

**Type:** integer number

**Constraints:**

### 5.2.407 MoleculeStateParameterMatrixRowRefs

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

**Type:** string

**Constraints:**

### 5.2.408 MoleculeStateParameterMatrixUnits

Molecular State parameters, units for data on matrix data form

**Type:** string

**Constraints:**

### 5.2.409 MoleculeStateParameterMatrixValues

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

**Type:** string

**Constraints:**

### 5.2.410 MoleculeStateParameterValueData

State parameter with a specific value

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.411 MoleculeStateParameterVectorDataUnits

Molecular State vector data units

**Type:** string

**Constraints:**

### 5.2.412 MoleculeStateParameterVectorRef

Molecular State parameter reference string giving context.

**Type:** string

**Constraints:**

### 5.2.413 MoleculeStateParameterVectorX3

Molecular State parameter vector coordinate X

**Type:** floating-point number

**Constraints:**

### 5.2.414 MoleculeStateParameterVectorY3

Molecular State parameter vector coordinate Y

**Type:** floating-point number

**Constraints:**

### 5.2.415 MoleculeStateParameterVectorZ3

Molecular State parameter vector coordinate Z

**Type:** floating-point number

**Constraints:**

### 5.2.416 MoleculeStateParameters

Additional parameters of molecular state

**Type:** string

**Constraints:**

### 5.2.417 MoleculeStateParity

**Type:** string

**Constraints:**

### 5.2.418 MoleculeStateQuantumNumbers

**Type:** string

**Constraints:**

### 5.2.419 MoleculeStateTotalStatisticalWeight

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

**Type:** integer number

**Constraints:** >0

### 5.2.420 MoleculeStoichiometricFormula

Molecular stoichiometric formula

**Type:** string

**Constraints:**

### 5.2.421 MoleculeStructure

The molecular structure, as defined in CML

**Type:** string

**Constraints:**

### 5.2.422 MoleculeURLFigure

**Type:** string

**Constraints:**

### 5.2.423 NodeID

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

**Type:** string

**Constraints:**

### 5.2.424 NonRadTranComment

**Type:** string

**Constraints:**

### 5.2.425 NonRadTranEnergy

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.426 NonRadTranGroup

non-radiative transition group label

**Type:** string

**Constraints:**

### 5.2.427 NonRadTranID

non-radiative transition ID

**Type:** string

**Constraints:**

### 5.2.428 NonRadTranLowerState

Lower state of the transition

**Type:** string

**Constraints:**

### 5.2.429 NonRadTranMethod

**Type:** string

**Constraints:**

### 5.2.430 NonRadTranProbability

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.431 NonRadTranProcess

**Type:** string

**Constraints:**

### 5.2.432 NonRadTranRef

**Type:** string

**Constraints:**

### 5.2.433 NonRadTranSpecies

**Type:** string

**Constraints:**

### 5.2.434 NonRadTranType

**Type:** string

**Constraints:**

### 5.2.435 NonRadTranUpperState

Upper state of the transition

**Type:** string

**Constraints:**

### 5.2.436 NonRadTranWidth

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.437 ParticleCharge

**Type:** string

**Constraints:**

### 5.2.438 ParticleComment

**Type:** string

**Constraints:**

### 5.2.439 ParticleMass

**Type:** string

Has **DataType** suffixes support

**Constraints:**

### 5.2.440 ParticleMethod

**Type:** string

**Constraints:**

### 5.2.441 ParticleName

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

**Type:** string

**Constraints:**

### 5.2.442 ParticlePolarization

**Type:** floating-point number

**Constraints:**

### 5.2.443 ParticleRef

**Type:** string

**Constraints:**

### 5.2.444 ParticleSpeciesID

**Type:** string

**Constraints:**

### 5.2.445 ParticleSpin

**Type:** floating-point number

**Constraints:**

### 5.2.446 RadTransBroadeningDopplerComment

Comments relating to this Doppler broadening process

**Type:** string

**Constraints:**

### 5.2.447 RadTransBroadeningDopplerEnvironment

A reference to an Environment ID, describing the environment (in particular, temperature) for this Doppler broadening process

**Type:** string

**Constraints:**

### 5.2.448 RadTransBroadeningDopplerLineshapeName

The name of the lineshape resulting from this Doppler broadening process ('gaussian', most likely).

**Type:** string

**Constraints:**

### 5.2.449 RadTransBroadeningDopplerLineshapeParameter

A parameter to the Doppler lineshape

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.450 RadTransBroadeningDopplerLineshapeParameterName

The name of a parameter for the Doppler lineshape.

**Type:** string

**Constraints:**

### 5.2.451 RadTransBroadeningDopplerMethod

A reference to the method by which this Doppler broadening process is determined.

**Type:** string

**Constraints:**

### 5.2.452 RadTransBroadeningDopplerRef

A source reference for Doppler broadening process.

**Type:** string

**Constraints:**

### 5.2.453 RadTransBroadeningInstrumentComment

Comments relating to instrumental line broadening

**Type:** string

**Constraints:**

### 5.2.454 RadTransBroadeningInstrumentEnvironment

The ID of an Environment element, describing the environment of the intstrumental broadening process

**Type:** string

**Constraints:**

### 5.2.455 RadTransBroadeningInstrumentLineshapeName

Instrument broadening lineshape name

**Type:** string

**Constraints:**

### 5.2.456 RadTransBroadeningInstrumentLineshapeParameter

An instrument broadening lineshape parameter

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.457 RadTransBroadeningInstrumentLineshapeParameterName

The name of a parameter used in the description of an instrument-broadening lineshape.

**Type:** string

**Constraints:**

### 5.2.458 RadTransBroadeningInstrumentMethod

A reference to the Method by which the instrument-broadening process is determined.

**Type:** string

**Constraints:**

### 5.2.459 RadTransBroadeningInstrumentRef

A Source reference for the instrument-broadening process.

**Type:** string

**Constraints:**

### 5.2.460 RadTransBroadeningNaturalComment

Comments relating to this natural (radiative) broadening process

**Type:** string

**Constraints:**

### 5.2.461 RadTransBroadeningNaturalEnvironment

The ID of an Environment element, describing the environment of this natural broadening process

**Type:** string

**Constraints:**

### 5.2.462 RadTransBroadeningNaturalLineshapeName

The name of the line shape used to describe this natural line broadening

**Type:** string

**Constraints:**

### 5.2.463 RadTransBroadeningNaturalLineshapeParameter

A broadening parameter for natural broadening.

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.464 RadTransBroadeningNaturalLineshapeParameterName

The name of natural broadening parameters.

**Type:** string

**Constraints:**

### 5.2.465 RadTransBroadeningNaturalMethod

A reference to the Method by which this natural broadening line shape was determined

**Type:** string

**Constraints:**

### 5.2.466 RadTransBroadeningNaturalRef

A Source reference for this natural broadening line shape

**Type:** string

**Constraints:**

### 5.2.467 RadTransBroadeningPressureComment

Comments relating to this pressure broadening process

**Type:** string

**Constraints:**

### 5.2.468 RadTransBroadeningPressureEnvironment

A reference to the Environment element describing the environment (temperature, pressure, composition) of this pressure broadening process

**Type:** string

**Constraints:**

### 5.2.469 RadTransBroadeningPressureLineshapeName

The name of the line shape used to describe the line broadening by pressure-broadening.

**Type:** string

**Constraints:**

### 5.2.470 RadTransBroadeningPressureLineshapeParameter

A parameter to the pressure-broadened line shape.

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.471 RadTransBroadeningPressureLineshapeParameterName

The name of this parameter to the pressure-broadened line shape.

**Type:** string

**Constraints:**

### 5.2.472 RadTransBroadeningPressureMethod

A reference to the Method by which this pressure-broadened line shape was determined.

**Type:** string

**Constraints:**

### 5.2.473 RadTransBroadeningPressureRef

A Source reference for this pressure-broadened line shape.

**Type:** string

**Constraints:**

### 5.2.474 RadTransComment

(String)

**Type:** string

**Constraints:**

### 5.2.475 RadTransEffectiveLandeFactor

Effective Lande factor for a given transition

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.476 RadTransEnergy

The energy of a radiative transition

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.477 RadTransFrequency

Radiative transition frequency.

**Units:** MHz

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.478 RadTransGroup

Radiative transition group label

**Type:** string

**Constraints:**

### 5.2.479 RadTransID

Transition ID

**Type:** string

**Constraints:**

### 5.2.480 RadTransLowerStateRef

Reference to the lower State of this radiative transition.

**Type:** string

**Constraints:**

### 5.2.481 RadTransProbabilityA

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

**Units:** 1/s

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:** >= 0

### 5.2.482 RadTransProbabilityIdealisedIntensity

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.483 RadTransProbabilityKind

**Type:** string

**Constraints:**

### 5.2.484 RadTransProbabilityLineStrength

Line profile-integrated absorption for transition between two energy levels. Line strength K = hν / 4π (n<sub>1</sub> B<sub>12</sub> - n<sub>2</sub> B<sub>21</sub>)

**Units:** 1/cm

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:** >0

### 5.2.485 RadTransProbabilityLog10WeightedOscillatorStrength

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.486 RadTransProbabilityOscillatorStrength

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.487 RadTransProbabilityWeightedOscillatorStrength

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.488 RadTransProcess

Transition process, deexcitation or excitation

**Type:** string

**Constraints:**

### 5.2.489 RadTransRefs

**Type:** string

**Constraints:**

### 5.2.490 RadTransShifting

The pressure-shifting process for a radiative transition.

**Type:** string

**Constraints:**

### 5.2.491 RadTransShiftingComment

Comments relating to this pressure-shifting process.

**Type:** string

**Constraints:**

### 5.2.492 RadTransShiftingEnv

A reference to an Environment element giving the environment (pressure, temperature, composition) in which this pressure-shifting process occurs.

**Type:** string

**Constraints:**

### 5.2.493 RadTransShiftingMethod

Reference to the Method by which this pressure-shifting process was determined.

**Type:** string

**Constraints:**

### 5.2.494 RadTransShiftingName

**Type:** string

**Constraints:**

### 5.2.495 RadTransShiftingParam

Shifting parameter value

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.496 RadTransShiftingParamFitArgumentDescription

**Type:** string

**Constraints:**

### 5.2.497 RadTransShiftingParamFitArgumentLowerLimit

**Type:** floating-point number

**Constraints:**

### 5.2.498 RadTransShiftingParamFitArgumentName

List of argument names

**Type:** string

**Constraints:**

### 5.2.499 RadTransShiftingParamFitArgumentUnits

**Type:** string

**Constraints:**

### 5.2.500 RadTransShiftingParamFitArgumentUpperLimit

**Type:** floating-point number

**Constraints:**

### 5.2.501 RadTransShiftingParamFitFunction

**Type:** string

**Constraints:**

### 5.2.502 RadTransShiftingParamFitParameter

**Type:** string

Has **DataType** suffixes support

**Constraints:**

### 5.2.503 RadTransShiftingParamFitParameterName

**Type:** string

**Constraints:**

### 5.2.504 RadTransShiftingParamName

**Type:** string

**Constraints:**

### 5.2.505 RadTransShiftingRef

Reference to a Source for this pressure-shifting process.

**Type:** string

**Constraints:**

### 5.2.506 RadTransSpeciesRef

**Type:** string

**Constraints:**

### 5.2.507 RadTransTransitionType

A string, 'excitation' or 'deexcitation', determining whether a radiative transition is given in absorption or emission respectively

**Type:** string

**Constraints:**

### 5.2.508 RadTransUpperStateRef

The upper state for the transition

**Type:** string

**Constraints:**

### 5.2.509 RadTransWavelength

Radiative transition vacuum wavelength

**Units:** A

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.510 RadTransWavenumber

Radiative transition wavenumber.

**Type:** floating-point number

Has **DataType** suffixes support

**Constraints:**

### 5.2.511 SolidComment

**Type:** string

**Constraints:**

### 5.2.512 SolidLayerComment

**Type:** string

**Constraints:**

### 5.2.513 SolidLayerComponentComment

**Type:** string

**Constraints:**

### 5.2.514 SolidLayerComponentElementSymbol

**Type:** string

**Constraints:**

### 5.2.515 SolidLayerComponentMethod

**Type:** string

**Constraints:**

### 5.2.516 SolidLayerComponentNuclearCharge

**Type:** string

**Constraints:**

### 5.2.517 SolidLayerComponentPercentage

**Type:** floating-point number

**Constraints:**

### 5.2.518 SolidLayerComponentRef

**Type:** string

**Constraints:**

### 5.2.519 SolidLayerComponentStochiometricValue

**Type:** floating-point number

**Constraints:**

### 5.2.520 SolidLayerName

**Type:** string

**Constraints:**

### 5.2.521 SolidLayerTemperature

**Type:** string

Has **DataType** suffixes support

**Constraints:**

### 5.2.522 SolidLayerThickness

**Type:** string

Has **DataType** suffixes support

**Constraints:**

### 5.2.523 SolidLayerTopology

**Type:** string

**Constraints:**

### 5.2.524 SolidMethod

**Type:** string

**Constraints:**

### 5.2.525 SolidRef

**Type:** string

**Constraints:**

### 5.2.526 SolidSpeciesID

**Type:** string

**Constraints:**

### 5.2.527 SourceArticleNumber

**Type:** string

**Constraints:**

### 5.2.528 SourceAuthorName

Name of one of the authors

**Type:** string

**Constraints:**

### 5.2.529 SourceCategory

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

**Type:** string

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

#### 5.2.530 SourceComments

Comments and notes connected with a Source (reference)

**Type:** string

**Constraints:**

#### 5.2.531 SourceDOI

**Type:** string

**Constraints:**

#### 5.2.532 SourceID

**Type:** string

**Constraints:**

#### 5.2.533 SourceName

E.g. JQSRT

**Type:** string

**Constraints:**

#### 5.2.534 SourcePageBegin

Starting page number

**Type:** integer number

**Constraints:** >=0

#### 5.2.535 SourcePageEnd

**Type:** string

**Constraints:**

#### 5.2.536 SourceTitle

Full title of the paper

**Type:** string

**Constraints:**

#### 5.2.537 SourceURI

Webb link to the publication

**Type:** string

**Constraints:**

### 5.2.538 SourceVolume

Volumen number

**Type:** integer number

**Constraints:** >0

### 5.2.539 SourceYear

Publication Year

**Type:** integer number

**Constraints:** >0

CHAPTER

SIX

# 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.

## 6.1 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.

## 6.2 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 %

## 6.3 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.