The 'Case-By-Case' Schema for Molecular States in XSAMS - v0.2.1

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Introduction

The 'case-by-case' XML description of molecular states within XSAMS is designed to provide a straightforward and 'flat' data structure for representing the quantum numbers and symmetries that define a molecular state. As of version 0.2.1, 12 cases have been implemented, covering the needs of the HITRAN, CDMS, and BASECOL databases.
Each case is identified by a `prefix` and a `version`, and belongs to the namespace given (currently) by the URI `http://www.ucl.ac.uk/~ucapch0/XSAMS/cases/<prefix>/<version>`. At least for the time being, it is suggeested that validation is through Namespace Validation Dispatch Language (NVDL). This may be implemented by including the relevant processing instruction in the XSAMS XML instance document, after the XML declaration. For example, using the oxygen editor

```
<?xml version="1.0" encoding="UTF-8"?>
<?oxygen NVDLSchema="cbc.nvdl"?>
...
```

The NVDL Schema document, `cbc.nvdl` contains a set of rules which link the namespaces encountered in the XML document with the Schemata required to validate them. An sample NVDL document may be downloaded from `http://www.ucl.ac.uk/~ucapch0/XSAMS/`.

The Cases

The identified cases are described in the following section; some examples are given below. It should be noted that the rovibronic states of different electronic states of a molecule may be described using different cases. For example, the ground, $X^2\Pi$ electronic state of NO may be described within the `hunda` case whereas the excited, $A^2\Sigma^+$ electronic state would be better described using the `hundb` case. The electronic state is identified by its single-letter spectroscopic symbol (X, A, a, B, etc.)
There follows a list of the cases identified in version 0.2.1 of XSAMS with some examples:

1. Diatomic closed shell (`dcs`): CO, N_2, NO^+
2. Hund's case (a) diatomics (`hunda`): NO, OH [for low J]
3. Hund's case (b) diatomics (`hundb`): O_2, OH [for high J]
4. Closed-shell, linear triatomic molecules (`ltcs`): CO_2, HCN
5. Closed-shell, non-linear triatomic molecules (`nltcs`): H_2O
6. Closed-shell, symmetric top molecules (`stcs`): NH_3, CH_3Cl
7. Closed-shell, linear, polyatomic molecules (`lpcs`): C_2H_2
8. Closed-shell, asymmetric top molecules (`asymcs`): C_2H_4
9. Open-shell, asymmetric top molecules (`asymos`): CH_3O

10. Closed-shell, spherical top molecules (`sphcs`): CH_4, SF_6
11. Open-shell, spherical top molecules (`sphos`)
12. General case for arbitrary quantum numbers and symmetry (`gen`)

Examples

The element `<case:QNs>` should be placed within the XSAMS element `MolecularState` (although this cannot be enforced using NVDL). Some examples follow.

Example 1: a rovibrational state of CO

The $v = 0, J = 1$ state of the ground electronic state of CO has the following representation in the 'case-by-case' formulism:

```
<dcs:QNs>
   <dcs:ElecStateLabel>X</dcs:ElecStateLabel>
   <dcs:J>0</dcs:J>
   <dcs:v>1</dcs:v>
</dcs:QNs>
```

Example 2: a rovibrational state of NH_3

The $J = 22, K = 10$ rotational state of the $(1, 0^+, 0^0, 2^2)$ vibrational level of NH_3 could be represented by the following XML:

```
<stcs:QNs>
   <stcs:ElecStateLabel>X</stcs:ElecStateLabel>
   <stcs:J>20</stcs:J>
   <stcs:K>10</stcs:K>
   <stcs:vi mode="1">1</stcs:vi>
   <stcs:vi mode="2">0</stcs:vi>
   <stcs:vi mode="3">0</stcs:vi>
   <stcs:vi mode="4">2</stcs:vi>
   <stcs:li mode="3">0</stcs:li>
   <stcs:li mode="4">2</stcs:li>
   <stcs:vibInv>s</stcs:vibInv>
</stcs:QNs>
```

Example 3: two states of different electronic states of MgH

This example shows two states of the MgH radical, using different cases for the $X^2\Sigma^+$ and $A^2\Pi$ electronic states:

```
<MolecularState stateID="S1-MgH-1">
  <Description>
    A state in the ground electronic state, X(2Sigma+), of MgH
  </Description>
  <MolecularStateCharacterisation>
    <StateEnergy energyOrigin="Zero-point from calculation based on N^2 Hamiltonian">
```

```
      <Value units="1/cm">0.</Value>
    </StateEnergy>
    <TotalStatisticalWeight>4</TotalStatisticalWeight>
  </MolecularStateCharacterisation>
  <hundb:QNs>
    <hundb:ElecStateLabel>X</hundb:ElecStateLabel>
    <hundb:J>0.5</hundb:J>
    <hundb:S>0.5</hundb:S>
    <hundb:N>0</hundb:N>
    <hundb:SpinComponentLabel>1</hundb:SpinComponentLabel>
    <hundb:Lambda>0</hundb:Lambda>
    <hundb:v>0</hundb:v>
    <hundb:parity>+</hundb:parity>
    <hundb:kronigParity>e</hundb:kronigParity>
  </hundb:QNs>
</MolecularState>
  ...
<MolecularState stateID="S1001-MgH-1">
  <Description>
    A state in the first excited electronic state, A(2Pi) of MgH
  </Description>
  <MolecularStateCharacterisation>
    <StateEnergy energyOrigin="Zero-point of electronic ground state">
      <Value units="1/cm">19278.13</Value>
    </StateEnergy>
    <TotalStatisticalWeight>4</TotalStatisticalWeight>
  </MolecularStateCharacterisation>
  <hunda:QNs>
    <hunda:ElecStateLabel>A</hunda:ElecStateLabel>
    <hunda:J>0.5</hunda:J>
    <hunda:S>0.5</hunda:S>
    <hunda:Omega>0.5</hunda:Omega>
    <hunda:Lambda>1</hunda:Lambda>
    <hunda:v>0</hunda:v>
    <hunda:parity>-</hunda:parity>
    <hunda:kronigParity>f</hunda:kronigParity>
  </hunda:QNs>
</MolecularState>
```

Diatomic closed-shell molecules: dcs

`ElecStateLabel`

Element

`<dcs:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state: X, A, a, B, etc..

Restrictions

- string.

J

Element

`<dcs:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer.

v

Element

`<dcs:v>`

Attributes

None.

Description

v is the vibrational quantum number.

Restrictions

- non-negative integer.

F_1

Element

`<dcs:F1>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$ to form the intermediate angular momentum.

Description

F_1 is the intermediate angular momentum quantum number associated with the coupling of the rotational angular momentum and nuclear spin of nucleus 1 where two such couplings are resolved: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$; F_1 is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.
- $|J - I_1| \leq F_1 \leq J + I_1$.

F

Element

`<dcs:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$ (or $\boldsymbol{F_1}$) to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I_1}$ if only one such coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_1} + \boldsymbol{I_2}$ if both couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<dcs:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`parity`

Element

`<dcs:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

`asSym`

Element

`<dcs:asSym>`

Attributes

None.

Description

`asSym` is (for diatomic molecules with a centre of inversion) 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 the identical nuclei ($\hat{P}_{12}$), according to whether they are bosons or fermions respectively.

Restrictions

- 's' or 'a'.

Hund's case (a) diatomics: hunda

`ElecStateLabel`

Element

`<hunda:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state: X, A, a, B, etc..

Restrictions

- string.

J

Element

`<hunda:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin: $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S} + \boldsymbol{R}$.

Restrictions

- non-negative integer or half-odd integer.

S

Element

`<hunda:S>`

Attributes

None.

Description

S is the quantum number associated with the total electronic spin angular momentum, $\boldsymbol{S}$.

Restrictions

- non-negative integer or half-odd integer.

$|\Sigma|$

Element

`<hunda:Sigma>`

Attributes

None.

Description

$|\Sigma|$ is the quantum number associated with the magnitude of the projection of $\boldsymbol{S}$ onto the molecular axis.

Restrictions

- non-negative integer or half-odd integer.
- $|\Sigma| = S, S-1, \cdots, \frac{1}{2}$ or 0.

Ω

Element

`<hunda:Omega>`

Attributes

None.

Description

Ω is the quantum number associated with the projection of the total angular momentum (excluding nuclear spin), $\boldsymbol{J}$, onto the molecular axis: $\Omega = |\Lambda + \Sigma|$ (or $\Omega = |\Lambda| + \Sigma$ if $S > |\Lambda| > 0$).

Restrictions

- non-negative integer or half-integer.
- $|\Omega| \leq J$.

$|\Lambda|$

Element

`<hunda:Lambda>`

Attributes

None.

Description

$|\Lambda|$ is the quantum number associated with the magnitude of the projection of the total electronic orbital angular momentum, $\boldsymbol{L}$, onto the molecular axis.

Restrictions

- non-negative integer.

v

Element

`<hunda:v>`

Attributes

None.

Description

v is the vibrational quantum number.

Restrictions

- non-negative integer.

F_1

Element

`<hunda:F1>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$ to form the intermediate angular momentum.

Description

F_1 is the intermediate angular momentum quantum number associated with the coupling of the rotational angular momentum and nuclear spin of nucleus 1 where two such couplings are resolved: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$; F_1 is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.
- $|J - I_1| \leq F_1 \leq J + I_1$.

F

Element

`<hunda:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$ (or $\boldsymbol{F_1}$) to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I_1}$ if only one such coupling is resolved; $\boldsymbol{F} = \boldsymbol{F_1} + \boldsymbol{I_2}$ if both couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<hunda:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`parity`

Element

`<hunda:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

`kronigParity`

Element

`<hunda:kronigParity>`

Attributes

None.

Description

`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. For integral J, the levels are called:

$$e \text{ if parity is } +(-1)^J,$$
$$f \text{ if parity is } -(-1)^J.$$

For half-odd integer J, the levels are called:

$$e \text{ if parity is } +(-1)^{J-\frac{1}{2}},$$
$$f \text{ if parity is } -(-1)^{J-\frac{1}{2}}.$$

.

Restrictions

- 'e' or 'f'.

`asSym`

Element

`<hunda:asSym>`

Attributes

None.

Description

`asSym` is (for diatomic molecules with a centre of inversion) 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 the identical nuclei ($\hat{P}_{12}$), according to whether they are bosons or fermions respectively.

Restrictions

- 's' or 'a'.

Hund's case (b) diatomics: hundb

`ElecStateLabel`

Element

`<hundb:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state: X, A, a, B, etc..

Restrictions

- string.

J

Element

`<hundb:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S} = \boldsymbol{L} + \boldsymbol{S} + \boldsymbol{R}$.

Restrictions

- non-negative integer or half-integer.
- $|N - S| \leq J \leq N + S$.

S

Element

`<hundb:S>`

Attributes

None.

Description

S is the quantum number associated with the total electronic spin angular momentum, $\boldsymbol{S}$.

Restrictions

- non-negative integer or half-odd integer.

N

Element

`<hundb:N>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.
- $N \geq |\Lambda|$.

SpinComponentLabel

Element

`<hundb:SpinComponentLabel>`

Attributes

None.

Description

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

Restrictions

- positive integer.

$|\Lambda|$

Element

`<hundb:Lambda>`

Attributes

None.

Description

$|\Lambda|$ is the quantum number associated with the magnitude of the projection of the total electronic orbital angular momentum, $\boldsymbol{L}$, onto the molecular axis.

Restrictions

- non-negative integer.

v

Element

`<hundb:v>`

Attributes

None.

Description

v is the vibrational quantum number.

Restrictions

- non-negative integer.

F_1

Element

`<hundb:F1>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$ to form the intermediate angular momentum.

Description

F_1 is the intermediate angular momentum quantum number associated with the coupling of the rotational angular momentum and nuclear spin of nucleus 1 where two such couplings are resolved: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$; F_1 is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.
- $|J - I_1| \leq F_1 \leq J + I_1$.

F

Element

`<hundb:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$ (or $\boldsymbol{F_1}$) to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I_1}$ if only one such coupling is resolved; $\boldsymbol{F} = \boldsymbol{F_1} + \boldsymbol{I_2}$ if both couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<hundb:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`parity`

Element

`<hundb:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

`kronigParity`

Element

`<hundb:kronigParity>`

Attributes

None.

Description

`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. For integral J, the levels are called:

$$e \text{ if parity is } +(-1)^J,$$
$$f \text{ if parity is } -(-1)^J.$$

For half-odd integer J, the levels are called:

$$e \text{ if parity is } +(-1)^{J-\frac{1}{2}},$$
$$f \text{ if parity is } -(-1)^{J-\frac{1}{2}}.$$

.

Restrictions

- 'e' or 'f'.

`asSym`

Element

`<hundb:asSym>`

Attributes

None.

Description

`asSym` is (for diatomic molecules with a centre of inversion) 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 the identical nuclei ($\hat{P}_{12}$), according to whether they are bosons or fermions respectively.

Restrictions

- 's' or 'a'.

Closed-shell, linear triatomic molecules: ltcs

Closed-shell, non-linear triatomics: nltcs

`ElecStateLabel`

Element

`<nltcs:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state: X, A, a, B, etc..

Restrictions

- string.

J

Element

`<nltcs:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer.

K_a

Element

`<nltcs:Ka>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.
- $K_a \leq J$.
- $K_a + K_c = J$ or $J + 1$.

K_c

Element

`<nltcs:Kc>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.
- $K_c \leq J$.
- $K_a + K_c = J$ or $J + 1$.

v_1

Element

`<nltcs:v1>`

Attributes

None.

Description

v_1 is the vibrational quantum number associated with the ν_1 normal mode.

Restrictions

- non-negative integer.

v_2

Element

`<nltcs:v2>`

Attributes

None.

Description

v_2 is the vibrational quantum number associated with the ν_2 normal mode.

Restrictions

- non-negative integer.

v_3

Element

`<nltcs:v3>`

Attributes

None.

Description

v_3 is the vibrational quantum number associated with the ν_3 normal mode.

Restrictions

- non-negative integer.

F_1

Element

`<nltcs:F1>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$ to form the intermediate angular momentum.

Description

F_1 is the intermediate angular momentum quantum number associated with the coupling of the rotational angular momentum and nuclear spin of nucleus 1 where two or more such couplings are resolved: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$; F_1 is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.
- $|J - I_1| \leq F_1 \leq J + I_1$.

F_2

Element

`<nltcs:F2>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{F_1}$ to form an intermediate angular momentum.

Description

F_2 is the intermediate angular momentum quantum number associated with the coupling of the rotational angular momentum and nuclear spin of nucleus 2 where three such couplings are resolved: $\boldsymbol{F_2} = \boldsymbol{F_1} + \boldsymbol{I_2}$; F_2 is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.
- $|F_1 - I_2| \leq F_2 \leq F_1 + I_2$.

F

Element

`<nltcs:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$, $\boldsymbol{F_1}$, or $\boldsymbol{F}$ to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I_1}$ if only one hyperfine coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_1} + \boldsymbol{I_2}$ if two couplings are resolved, or $\boldsymbol{F} = \boldsymbol{F_2} + \boldsymbol{I_3}$ if all three couplings are resolved.

Restrictions

- non-negative integer or half-integer.
- $|F_2 - I_3| \leq F \leq F_2 + I_3$.

r

Element

`<nltcs:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`parity`

Element

`<nltcs:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

asSym

Element

<nltcs:asSym>

Attributes

None.

Description

asSym is 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 the identical nuclei ($\hat{P}_{12}$), according to whether they are bosons or fermions respectively.

Restrictions

- 's' or 'a'.

Closed shell, symmetric-top molecules: stcs

`ElecStateLabel`

Element

`<stcs:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state.

Restrictions

- string.

J

Element

`<stcs:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer.

K

Element

`<stcs:K>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.
- $K \leq J$.

v_i

Element

`<stcs:vi>`

Attributes

`mode`: a positive integer, identifying the normal mode that this quantum number is associated with.

Description

v_i is the vibrational quantum number associated with the ν_i normal mode.

Restrictions

- non-negative integer.

l_i

Element

`<stcs:li>`

Attributes

`mode`: a positive integer, identifying the degenerate normal mode that this vibrational angular momentum quantum number is associated with.

Description

l_i is the vibrational angular momentum quantum number associated with the degenerate ν_i normal mode; positive and negative values distinguish l-type doubling components.

Restrictions

- non-negative integer.
- $|l_i| = v_i, v_i - 2, \cdots, 1$ or 0.

`vibInv`

Element

`<stcs:vibInv>`

Attributes

None.

Description

`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, NH_3).

Restrictions

- 's' or 'a'.

I

Element

`<stcs:I>`

Attributes

`nuclearSpinRef`: a label identifying the group of nuclear spins coupled to one another to form a total nuclear spin angular momentum.

Description

I is the quantum number associated with the total nuclear spin angular momentum: $\boldsymbol{I} = \boldsymbol{I_1} + \boldsymbol{I_2} + \cdots$ where nuclei $1, 2, \cdots$ have individual nuclear spin angular momenta $\boldsymbol{I_1}, \boldsymbol{I_2}, \cdots$.

Restrictions

- non-negative integer or half-integer.

F_j

Element

`<stcs:Fj>`

Attributes

- `nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_{j-1}}$ to form an intermediate angular momentum;
- j: an integer label identifying the order of the hyperfine coupling

.

Description

F_j is the intermediate angular momentum quantum number associated with the coupling of the nuclear spin angular momentum of nucleus j to the intermediate angular momentum: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$ or $\boldsymbol{F_j} = \boldsymbol{F_{j-1}} + \boldsymbol{I_j}$; $\boldsymbol{F_j}$ is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.

F

Element

`<stcs:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_j}$ to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J}+\boldsymbol{I_1}$ if only one such coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_{j-1}}+\boldsymbol{I_j}$ if two or more such couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<stcs:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`rotSym`

Element

`<stcs:rotSym>`

Attributes

None.

Description

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

Restrictions

- string.

`vibSym`

Element

`<stcs:vibSym>`

Attributes

None.

Description

`vibSym` is the symmetry species of the vibrational wavefunction, in some appropriate symmetry group.

Restrictions

- string.

`parity`

Element

`<stcs:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

Closed-shell, linear polyatomic molecules: lpcs

`ElecStateLabel`

Element

`<lpcs:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state.

Restrictions

- string.

J

Element

`<lpcs:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer.

v_i

Element

`<lpcs:vi>`

Attributes

`mode`: a positive integer, identifying the normal mode that this quantum number is associated with.

Description

v_i is the vibrational quantum number associated with the ν_i normal mode.

Restrictions

- non-negative integer.

l_i

Element

`<lpcs:li>`

Attributes

`mode`: a positive integer, identifying the degenerate normal mode that this vibrational angular momentum quantum number is associated with.

Description

l_i is the vibrational angular momentum quantum number associated with the degenerate ν_i normal mode; positive and negative values distinguish l-type doubling components.

Restrictions

- non-negative integer.
- $|l_i| = v_i, v_i - 2, \cdots, 1$ or 0.

`vibInv`

Element

`<lpcs:vibInv>`

Attributes

None.

Description

`vibInv` is the parity of the vibrational wavefunction with respect to inversion through the molecular centre of mass in the molecular coordinate system..

Restrictions

- 'g' or 'u'.

`vibRefl`

Element

`<lpcs:vibRefl>`

Attributes

None.

Description

`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.

Restrictions

- '+' or '−'.

I

Element

`<lpcs:I>`

Attributes

`nuclearSpinRef`: a label, matching `/Q.+/` identifying the group of nuclear spins coupled to one another to form a total nuclear spin angular momentum.

Description

I is the quantum number associated with the total nuclear spin angular momentum: $\boldsymbol{I} = \boldsymbol{I_1} + \boldsymbol{I_2} + \cdots$ where nuclei $1, 2, \cdots$ have individual nuclear spin angular momenta $\boldsymbol{I_1}, \boldsymbol{I_2}, \cdots$.

Restrictions

- non-negative integer or half-integer.

F_j

Element

`<lpcs:Fj>`

Attributes

- `nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_{j-1}}$ to form an intermediate angular momentum;
- j: an integer label identifying the order of the hyperfine coupling

.

Description

F_j is the intermediate angular momentum quantum number associated with the coupling of the nuclear spin angular momentum of nucleus j to the intermediate angular momentum: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$ or $\boldsymbol{F_j} = \boldsymbol{F_{j-1}} + \boldsymbol{I_j}$; $\boldsymbol{F_j}$ is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.

F

Element

`<lpcs:F>`

Attributes

`nuclearSpinRef`: a label, matching `/Q.+/` identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_j}$ to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J}+\boldsymbol{I_1}$ if only one such coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_{j-1}}+\boldsymbol{I_j}$ if two or more such couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<lpcs:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`parity`

Element

`<lpcs:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

`kronigParity`

Element

`<lpcs:kronigParity>`

Attributes

None.

Description

`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. For integral J, the levels are called:

$$e \text{ if parity is } +(-1)^J,$$
$$f \text{ if parity is } -(-1)^J.$$

For half-odd integer J, the levels are called:

$$e \text{ if parity is } +(-1)^{J-\frac{1}{2}},$$
$$f \text{ if parity is } -(-1)^{J-\frac{1}{2}}.$$

.

Restrictions

- 'e' or 'f'.

asSym

Element

<lpcs:asSym>

Attributes

None.

Description

asSym is (for linear molecules with a centre of inversion) 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 the identical nuclei ($\hat{P}_{12}$), according to whether they are bosons or fermions respectively.

Restrictions

- 's' or 'a'.

Closed-shell, asymmetric top molecules: asymcs

`ElecStateLabel`

Element

`<asymcs:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state.

Restrictions

- string.

J

Element

`<asymcs:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer.

K_a

Element

`<asymcs:Ka>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.
- $K_a \leq J$.
- $K_a + K_c = J$ or $J + 1$.

K_c

Element

`<asymcs:Kc>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.
- $K_c \leq J$.
- $K_a + K_c = J$ or $J + 1$.

v_i

Element

`<asymcs:vi>`

Attributes

`mode`: a positive integer, identifying the normal mode that this quantum number is associated with.

Description

v_i is the vibrational quantum number associated with the ν_i normal mode.

Restrictions

- non-negative integer.

`vibInv`

Element

`<asymcs:vibInv>`

Attributes

None.

Description

`vibInv` is the parity of the vibrational wavefunction with respect to inversion through the molecular centre of mass in the molecular coordinate system..

Restrictions

- 's' or 'a'.

I

Element

`<asymcs:I>`

Attributes

`nuclearSpinRef`: a label identifying the group of nuclear spins coupled to one another to form a total nuclear spin angular momentum.

Description

I is the quantum number associated with the total nuclear spin angular momentum: $\boldsymbol{I} = \boldsymbol{I_1} + \boldsymbol{I_2} + \cdots$ where nuclei $1, 2, \cdots$ have individual nuclear spin angular momenta $\boldsymbol{I_1}, \boldsymbol{I_2}, \cdots$.

Restrictions

- non-negative integer or half-integer.

F_j

Element

`<asymcs:Fj>`

Attributes

- `nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_{j-1}}$ to form an intermediate angular momentum;
- j: an integer label identifying the order of the hyperfine coupling

.

Description

F_j is the intermediate angular momentum quantum number associated with the coupling of the nuclear spin angular momentum of nucleus j to the intermediate angular momentum: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$ or $\boldsymbol{F_j} = \boldsymbol{F_{j-1}} + \boldsymbol{I_j}$; $\boldsymbol{F_j}$ is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.

F

Element

`<asymcs:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_j}$ to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J}+\boldsymbol{I_1}$ if only one such coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_{j-1}}+\boldsymbol{I_j}$ if two or more such couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<asymcs:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`rotSym`

Element

`<asymcs:rotSym>`

Attributes

None.

Description

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

Restrictions

- string.

`vibSym`

Element

`<asymcs:vibSym>`

Attributes

None.

Description

`vibSym` is the symmetry species of the vibrational wavefunction, in some appropriate symmetry group.

Restrictions

- string.

`parity`

Element

`<asymcs:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

Open-shell, asymmetric top molecules: asymos

`ElecStateLabel`

Element

`<asymos:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state.

Restrictions

- string.

J

Element

`<asymos:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer or half-odd integer.

S

Element

`<asymos:S>`

Attributes

None.

Description

S is the quantum number associated with the total electronic spin angular momentum, $\boldsymbol{S}$.

Restrictions

- non-negative integer or half-odd integer.

N

Element

`<asymos:N>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.

K_a

Element

`<asymos:Ka>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.
- $K_a \leq N$.
- $K_a + K_c = N$ or $N + 1$.

K_c

Element

`<asymos:Kc>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.
- $K_c \leq N$.
- $K_a + K_c = N$ or $N + 1$.

v_i

Element

`<asymos:vi>`

Attributes

`mode`: a positive integer, identifying the normal mode that this quantum number is associated with.

Description

v_i is the vibrational quantum number associated with the ν_i normal mode.

Restrictions

- non-negative integer.

`vibInv`

Element

`<asymos:vibInv>`

Attributes

None.

Description

`vibInv` is the parity of the vibrational wavefunction with respect to inversion through the molecular centre of mass in the molecular coordinate system..

Restrictions

- 's' or 'a'.

I

Element

`<asymos:I>`

Attributes

`nuclearSpinRef`: a label identifying the group of nuclear spins coupled to one another to form a total nuclear spin angular momentum.

Description

I is the quantum number associated with the total nuclear spin angular momentum: $\boldsymbol{I} = \boldsymbol{I_1} + \boldsymbol{I_2} + \cdots$ where nuclei $1, 2, \cdots$ have individual nuclear spin angular momenta $\boldsymbol{I_1}, \boldsymbol{I_2}, \cdots$.

Restrictions

- non-negative integer or half-integer.

F_j

Element

`<asymos:Fj>`

Attributes

- `nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_{j-1}}$ to form an intermediate angular momentum;
- j: an integer label identifying the order of the hyperfine coupling

.

Description

F_j is the intermediate angular momentum quantum number associated with the coupling of the nuclear spin angular momentum of nucleus j to the intermediate angular momentum: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$ or $\boldsymbol{F_j} = \boldsymbol{F_{j-1}} + \boldsymbol{I_j}$; $\boldsymbol{F_j}$ is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.

F

Element

`<asymos:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_j}$ to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J}+\boldsymbol{I_1}$ if only one such coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_{j-1}}+\boldsymbol{I_j}$ if two or more such couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<asymos:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`rotSym`

Element

`<asymos:rotSym>`

Attributes

None.

Description

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

Restrictions

- string.

`vibSym`

Element

`<asymos:vibSym>`

Attributes

None.

Description

`vibSym` is the symmetry species of the vibrational wavefunction, in some appropriate symmetry group.

Restrictions

- string.

`parity`

Element

`<asymos:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

Closed-shell, spherical-top molecules: sphcs

`ElecStateLabel`

Element

`<sphcs:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state.

Restrictions

- string.

J

Element

`<sphcs:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer.

v_i

Element

`<sphcs:vi>`

Attributes

`mode`: a positive integer, identifying the normal mode that this quantum number is associated with.

Description

v_i is the vibrational quantum number associated with the ν_i normal mode.

Restrictions

- non-negative integer.

l_i

Element

`<sphcs:li>`

Attributes

`mode`: a positive integer, identifying the degenerate normal mode that this vibrational angular momentum quantum number is associated with.

Description

l_i is the vibrational angular momentum quantum number associated with the degenerate ν_i normal mode; positive and negative values distinguish l-type doubling components.

Restrictions

- non-negative integer.
- $|l_i| = v_i, v_i - 2, \cdots, 1$ or 0.

I

Element

`<sphcs:I>`

Attributes

`nuclearSpinRef`: a label identifying the group of nuclear spins coupled to one another to form a total nuclear spin angular momentum.

Description

I is the quantum number associated with the total nuclear spin angular momentum: $\boldsymbol{I} = \boldsymbol{I_1} + \boldsymbol{I_2} + \cdots$ where nuclei $1, 2, \cdots$ have individual nuclear spin angular momenta $\boldsymbol{I_1}, \boldsymbol{I_2}, \cdots$.

Restrictions

- non-negative integer or half-integer.

F_j

Element

`<sphcs:Fj>`

Attributes

- `nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_{j-1}}$ to form an intermediate angular momentum;
- j: an integer label identifying the order of the hyperfine coupling

.

Description

F_j is the intermediate angular momentum quantum number associated with the coupling of the nuclear spin angular momentum of nucleus j to the intermediate angular momentum: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$ or $\boldsymbol{F_j} = \boldsymbol{F_{j-1}} + \boldsymbol{I_j}$; $\boldsymbol{F_j}$ is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.

F

Element

`<sphcs:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_j}$ to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J}+\boldsymbol{I_1}$ if only one such coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_{j-1}}+\boldsymbol{I_j}$ if two or more such couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<sphcs:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`rotSym`

Element

`<sphcs:rotSym>`

Attributes

None.

Description

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

Restrictions

- string.

`vibSym`

Element

`<sphcs:vibSym>`

Attributes

None.

Description

`vibSym` is the symmetry species of the vibrational wavefunction, in some appropriate symmetry group.

Restrictions

- string.

`parity`

Element

`<sphcs:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

Open-shell, spherical-top molecules: sphos

`ElecStateLabel`

Element

`<sphos:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state.

Restrictions

- string.

J

Element

`<sphos:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer or half-odd integer.

S

Element

`<sphos:S>`

Attributes

None.

Description

S is the quantum number associated with the total electronic spin angular momentum, $\boldsymbol{S}$.

Restrictions

- non-negative integer or half-odd integer.

N

Element

`<sphos:N>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.

v_i

Element

`<sphos:vi>`

Attributes

`mode`: a positive integer, identifying the normal mode that this quantum number is associated with.

Description

v_i is the vibrational quantum number associated with the ν_i normal mode.

Restrictions

- non-negative integer.

l_i

Element

`<sphos:li>`

Attributes

`mode`: a positive integer, identifying the degenerate normal mode that this vibrational angular momentum quantum number is associated with.

Description

l_i is the vibrational angular momentum quantum number associated with the degenerate ν_i normal mode; positive and negative values distinguish l-type doubling components.

Restrictions

- non-negative integer.
- $|l_i| = v_i, v_i - 2, \cdots, 1$ or 0.

I

Element

`<sphos:I>`

Attributes

`nuclearSpinRef`: a label identifying the group of nuclear spins coupled to one another to form a total nuclear spin angular momentum.

Description

I is the quantum number associated with the total nuclear spin angular momentum: $\boldsymbol{I} = \boldsymbol{I_1} + \boldsymbol{I_2} + \cdots$ where nuclei $1, 2, \cdots$ have individual nuclear spin angular momenta $\boldsymbol{I_1}, \boldsymbol{I_2}, \cdots$.

Restrictions

- non-negative integer or half-integer.

F_j

Element

`<sphos:Fj>`

Attributes

- `nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_{j-1}}$ to form an intermediate angular momentum;
- j: an integer label identifying the order of the hyperfine coupling

.

Description

F_j is the intermediate angular momentum quantum number associated with the coupling of the nuclear spin angular momentum of nucleus j to the intermediate angular momentum: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$ or $\boldsymbol{F_j} = \boldsymbol{F_{j-1}} + \boldsymbol{I_j}$; $\boldsymbol{F_j}$ is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.

F

Element

`<sphos:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin being coupled to $\boldsymbol{J}$ or $\boldsymbol{F_j}$ to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J}+\boldsymbol{I_1}$ if only one such coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_{j-1}}+\boldsymbol{I_j}$ if two or more such couplings are resolved.

Restrictions

- non-negative integer or half-integer.

r

Element

`<sphos:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`rotSym`

Element

`<sphos:rotSym>`

Attributes

None.

Description

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

Restrictions

- string.

`vibSym`

Element

`<sphos:vibSym>`

Attributes

None.

Description

`vibSym` is the symmetry species of the vibrational wavefunction, in some appropriate symmetry group.

Restrictions

- string.

`parity`

Element

`<sphos:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

Open-shell,linear triatomic molecules: ltos

`ElecStateLabel`

Element

`<ltos:ElecStateLabel>`

Attributes

None.

Description

`ElecStateLabel` is a label identifying the electronic state: X, A, a, B, etc..

Restrictions

- string.

J

Element

`<ltos:J>`

Attributes

None.

Description

J is the quantum number associated with the total angular momentum excluding nuclear spin, $\boldsymbol{J}$.

Restrictions

- non-negative integer.

S

Element

`<ltos:S>`

Attributes

None.

Description

S is the quantum number associated with the total electronic spin angular momentum, $\boldsymbol{S}$.

Restrictions

- non-negative integer or half-odd integer.

N

Element

`<ltos:N>`

Attributes

None.

Description

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

Restrictions

- non-negative integer.

v_1

Element

`<ltos:v1>`

Attributes

None.

Description

v_1 is the vibrational quantum number associated with the ν_1 normal mode.

Restrictions

- non-negative integer.

v_2

Element

`<ltos:v2>`

Attributes

None.

Description

v_2 is the vibrational quantum number associated with the doubly-degenerate ν_2 normal mode.

Restrictions

- non-negative integer.

l_2

Element

`<ltos:l2>`

Attributes

None.

Description

l_2 is the vibrational angular momentum quantum number associated with the degenerate bending vibration, ν_2; positive and negative values distinguish l-type doubling components.

Restrictions

- integer.
- $|l_2| = v_2, v_2 - 2, \cdots, 1$ or 0.

v_3

Element

`<ltos:v3>`

Attributes

None.

Description

v_3 is the vibrational quantum number associated with the ν_3 normal mode.

Restrictions

- non-negative integer.

F_1

Element

`<ltos:F1>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$ to form the intermediate angular momentum.

Description

F_1 is the intermediate angular momentum quantum number associated with the coupling of the rotational angular momentum and nuclear spin of nucleus 1 where two or more such couplings are resolved: $\boldsymbol{F_1} = \boldsymbol{J} + \boldsymbol{I_1}$; F_1 is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.
- $|J - I_1| \leq F_1 \leq J + I_1$.

F_2

Element

`<ltos:F2>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{F_1}$ to form an intermediate angular momentum.

Description

F_2 is the intermediate angular momentum quantum number associated with the coupling of the rotational angular momentum and nuclear spin of nucleus 2 where three such couplings are resolved: $\boldsymbol{F_2} = \boldsymbol{F_1} + \boldsymbol{I_2}$; F_2 is often not a good quantum number.

Restrictions

- non-negative integer or half-integer.
- $|F_1 - I_2| \leq F_2 \leq F_1 + I_2$.

F

Element

`<ltos:F>`

Attributes

`nuclearSpinRef`: a label identifying the nuclear spin coupled to $\boldsymbol{J}$, $\boldsymbol{F_1}$, or $\boldsymbol{F}$ to form the total angular momentum.

Description

F is the quantum number associated with the total angular momentum including nuclear spin: $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I_1}$ if only one hyperfine coupling is resolved, $\boldsymbol{F} = \boldsymbol{F_1} + \boldsymbol{I_2}$ if two couplings are resolved, or $\boldsymbol{F} = \boldsymbol{F_2} + \boldsymbol{I_3}$ if all three couplings are resolved.

Restrictions

- non-negative integer or half-integer.
- $|F_2 - I_3| \leq F \leq F_2 + I_3$.

r

Element

`<ltos:r>`

Attributes

`name`: a string identifying this ranking index.

Description

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

Restrictions

- positive integer.

`parity`

Element

`<ltos:parity>`

Attributes

None.

Description

`parity` is the 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 $\hat{E}^*$ operation.

Restrictions

- '+' or '−'.

`kronigParity`

Element

`<ltos:kronigParity>`

Attributes

None.

Description

`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. For integral J, the levels are called:

$$e \text{ if parity is } +(-1)^J,$$
$$f \text{ if parity is } -(-1)^J.$$

For half-odd integer J, the levels are called:

$$e \text{ if parity is } +(-1)^{J-\frac{1}{2}},$$
$$f \text{ if parity is } -(-1)^{J-\frac{1}{2}}.$$

.

Restrictions

- 'e' or 'f'.

`asSym`

Element

`<ltos:asSym>`

Attributes

None.

Description

`asSym` is (for linear molecules with a centre of inversion) 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 the identical nuclei ($\hat{P}_{12}$), according to whether they are bosons or fermions respectively.

Restrictions

- 's' or 'a'.