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Virtual
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Simple Spectral Lines Data Model

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Status of This Document

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Abstract

This document represents a proposal for a Data Model to describe Spectral Line Transitions in the context of the Simple Line Access Protocol defined by the IVOA (c.f. Ref[] IVOA Simple Line Access protocol)

The main objective of the model is to integrate with and support the Simple Line Access Protocol, with which it forms a compact unit. This integration allows seamless access to Spectral Line Transitions available worldwide in the VO context.

This model does not deal with the complete description of Atomic and Molecular Physics, which scope is outside of this document.

In the astrophysical sense, a *line* is considered as the result of a *transition* between two *levels*. Under the basis of this assumption, a whole set of objects and attributes have been derived to define properly the necessary information to deal with lines appearing in astrophysical contexts.

The document has been written taking into account available information from many different Line data providers (see acknowledgments section).

Acknowledgments

Contents

1 Introduction

Atomic and molecular line databases are a fundamental component in our process of understanding the physical nature of astrophysical plasmas. Density, temperature, pressure, ionization state and mechanism, can be derived by comparing the properties (energy, profile, intensity) of emission and absorption lines observed in astronomical sources with atomic and molecular physics data.

The latter have been consolidated through experiments in Earth's laboratories, whose results populate a rich wealth of databases around the world. Accessing the information of these databases in the Virtual Observatory (VO) framework is a fundamental part of the VO mission.

This document aims at providing a simple framework, both for atomic and molecular line databases, as well as for databases of observed lines in all energy ranges, or for VO-tools, which can extract emission/absorption line information from observed spectra or narrow-band filter photometry.

The Model is organized around the concept of "**Line**", defined as the results of a **transition** between two **levels** (this concept applies to bound-bound and free-bound transitions, but not free-free transitions). In turn each "Level" is characterized by   one (or more) "**QuantumState**". The latter is characterized by a proper set of "**QuantumNumber**".

The object "**Species**" represents a placeholder for a whole new model to represent the atomic and molecular properties of matter. This will take form in a separate document. We reserve here one single attribute for the time being, the name of the species (including standard naming convention for ionised species), and shall be pointing to the future model whenever available.

Any process which modifies the intrinsic properties of a "Line" (monochromatic character, laboratory wavelength etc.) is described through the attributes of "**Process**", which allows as well to describe the nature of the process responsible for the line generation, whenever pertinent. The element "**Environment**" allows service providers to list physical properties of the line-emitting/absorbing plasma, derived from the properties of the line emission/absorption complex. Both "Process" and "Environment" contain hooks to VO "**Model**"s for theoretical physics (placeholders for future models).

The present Simple Spectral Line Data Model does not explicitly address non-electromagnetic transitions.

2 Data model

We have attempted to create a Simple Data Model for Spectral Lines that would be useful to retrieve information from databases both of observed astronomical lines and laboratory atomic or molecular lines.

We give in what follows a standard UML diagram describing a Line.
UML Data Model
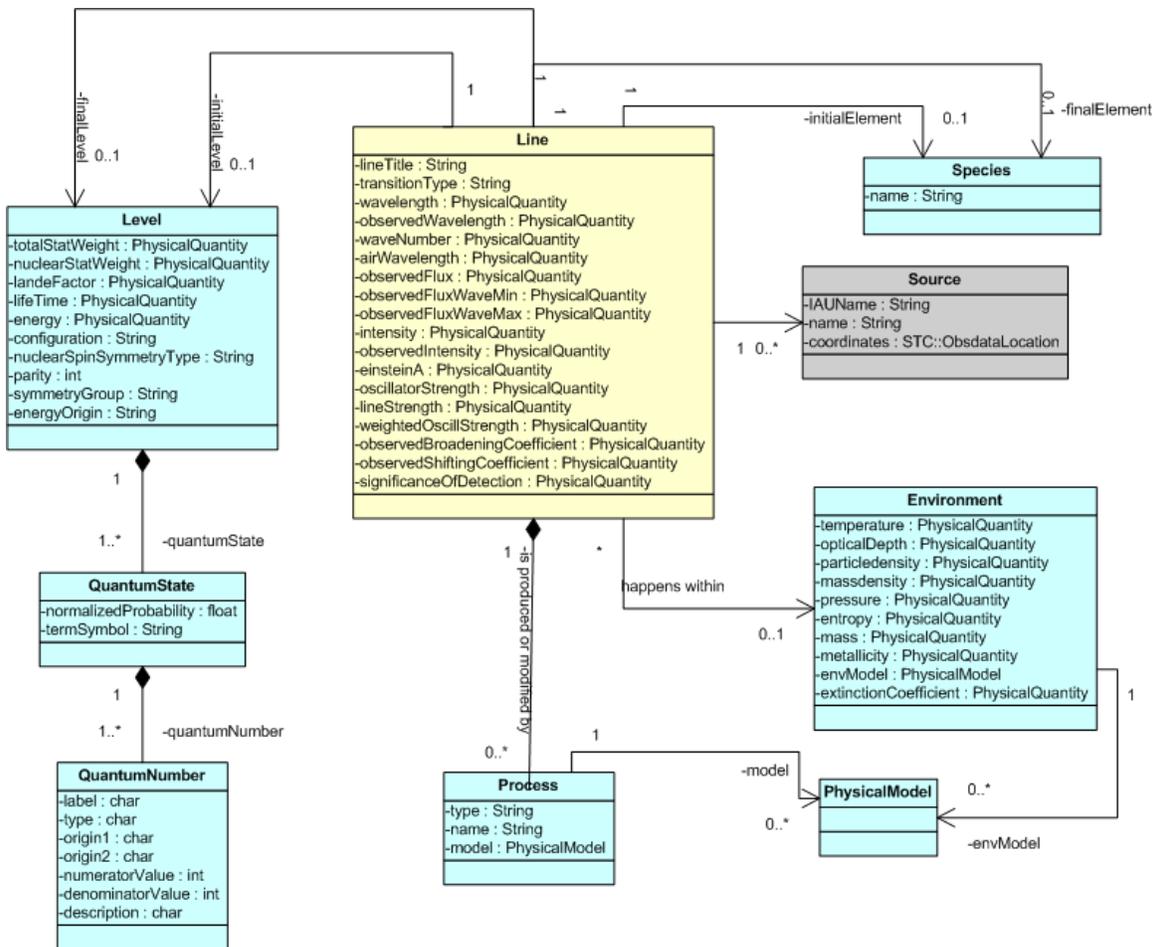
2.1 Objects Description

2.1.1 PhysicalQuantity

Class used to describe a physical measurement. This could be superseded by a general IVOA Quantity DM definition. It contains the basic information to understand a Quantity.

Although the definition of the physical quantity object is out of the scope of the present DM, here we attach a UML description of it as per DM working group discussion.
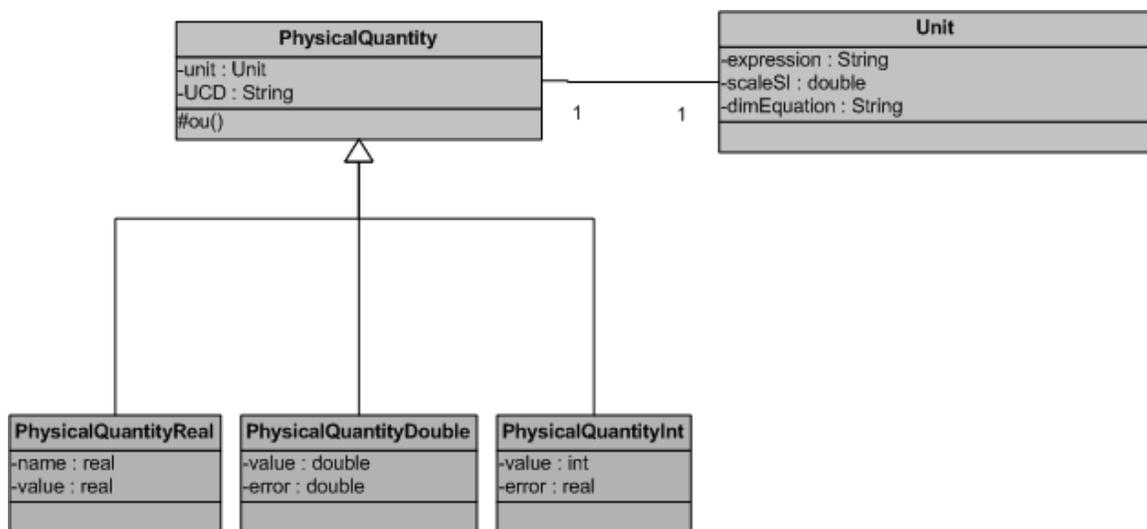
2.1.1.1 PhysicalQuantity.value
Value of the measure. General Number format.

2.1.1.2 PhysicalQuantity.error
General error of the measure. General Number format. Please note that this is the total error. A more formal description should be provided in a general IVOA Physical Quantity Data Model.

2.1.1.3 PhysicalQuantity.unit
Unit in which the measure is expressed. Type, unit (see definition in next section). Both value and error should be expressed in the same units

2.1.2 Unit

Class used to describe a physical unit. This could be superseded by a general IVOA Unit DM definition. It contains the basic information to understand a Unit:

2.1.2.1 Unit.expression

String representation of the unit

2.1.2.2 Unit.scaleSI

Scaling reference of the unit described to the international system of units analogue, i.e., to the unit in the IS with the same dimensional equation

2.1.2.3 Unit.dimEquation

Dimensional equation representation of the unit. The format is a string with the dimensional equation, where M is mass, L is length, T is time, K is temperature and where the "^" has been sustracted.

```
 Examples:
1 Angstrom = 1.E-10 m
1.E-10 L

Unit.expression= Angstrom
Unit.scaleSI=1.E-10
Unit.dimEquation=L

1 erg/cm^2/s/Angstrom = 1.E7 Kg/m/s^3
1.E7 ML-1T-3

Unit.expression= erg/cm^2/s/Angstrom
Unit.scaleSI= 1.E7
Unit.dimEquation= ML-1T-3
```

See, e.g., IVOA SSAP for more examples

2.1.3 Line

This class includes observables, e.g. measured physical parameters, describing the line, as well as the main physical properties of the transition originating it.

Recombination and dissociations are expressed through atomic coefficients rather than through global properties.

2.1.3.1   Line.title

A small description title identifying the line. This is useful when identification is not secure or not yet established.

2.1.3.2   Line.initialLevel

A full description of the initial level of the transition, originating the line.

2.1.3.3   Line.finalLevel

A full description of the final level of the transition, originating the line

2.1.3.4   Line.initialElement

A full description of the initial state of the atom (including its ionization state) or molecule, where the line transition occurs.

2.1.3.5   Line.finalElement

A full description of the final state of the atom (including its ionization state) or molecule, where the line transition occurs. For bound-bound atomic transitions, it follows: "initialElement"="finalElement".

2.1.3.6   Line.wavelength

Wavelength in the vacuum of the transition originating the line.

2.1.3.7   Line.frequency

Frequency in the vacuum of the transition originating the line.

2.1.3.8   Line.wavenumber

Wavenumber in the vacuum of the transition originating the line.

2.1.3.9   Line.airWavelength

Wavelength in the air of the transition originating the line.

2.1.3.10   Line.einsteinA

Einstein A coefficient, defined as the probability per unit time s^{-1} for spontaneous emission in a bound-bound transition from "initialLevel" to "finalLevel".

2.1.3.11   Line.oscillatorStrength

If positive ("absorption oscillator strength"): the quantity f_{fi} defined by the relation:

$$A_{if} = \left(\frac{8\pi^2 e^2 v^2}{4\pi\varepsilon_0 m_e c^3} \right)\left(\frac{g_f}{g_i} \right) f_{fi} = \left(\frac{4\pi h \alpha v^2}{c^2 m_e} \right)\left(\frac{g_f}{g_i} \right) f_{fi}$$

where A_{if} is the Einstein A-coefficient for spontaneous emission between "initialLevel" and "finalLevel" - characterized by the energy difference $h v$-, $\alpha = \left(\frac{e^2}{\hbar c \, 4\pi\varepsilon_0} \right)$, m_e, c, and h are the usual symbols for the fine-structure constant, electron mass, speed of light and Planck constant, respectively; g_i is the statistical weight of the i-th level. The subscripts "i" and "f" refer to the "initialLevel" and "finalLevel", respectively. As usual throughout this document, units are S.I. with ε_0 expressed in $\frac{C^2}{Nm^2}$.

If negative ("emission oscillator strength") the quantity (f_{if}) is defined by:

$$-g_i f_{if} = g_f f_{fi} = gf$$

where gf is the weighted oscillator strength.

2.1.3.12   Line.weightedOscillatorStrength

The product between "oscillatorStrength" and the statistical weight g of the "initialLevel"

2.1.3.13   Line.intensity

This is a source dependent relative intensity, useful as a guideline for low density sources. These are values that are intended to represent the strengths of the lines of a spectrum as they would appear in emission. They may have been normalized. They can be expressed in absolute physical units or in relative units with respect to a reference line.

The difficulty of obtaining reliable relative intensities can be understood from the fact that in optically thin plasmas, the intensity of a spectral line is proportional to:

$$I_{ik} = N_k A_{ki} h \nu_{ik}$$

Where N_k is the number of atoms in the upper level k (population of the upper level), A_{ki} it the transition probability for transitions from upper level k to lower level i, and $h\nu_{ik}$ is the photon energy (or the energy difference between the upper level and lower level). Although both A_{ki} and ν_{ik} are well defined quantities for each line of a given atom, the population values N_k depend on plasma conditions in a given light source, and they are this different for different sources.

Taking into account this issue, the following points should be kept in mind when using relative intensities:

1. There is no common scale for relative intensities. The values from different databases or different publications use different scales. The relative intensities have meaning only within a given spectrum.
2. The relative intensities are most useful in comparing strengths of spectral lines that are not separated widely. This results from the fact that most relative intensities are not corrected for spectral sensitivity of the measuring instruments.

3. Relative intensities are source dependent (either laboratory or astrophysical detections)

2.1.3.14 Line.observedFlux
Integrated intensity of the line profile over a given wavelength range

2.1.3.15 Line.observedFluxWaveMin
Minimum wavelength for observedFlux integration.

2.1.3.16 Line.observedFluxWaveMax
Maximum wavelength for observedFlux integration.

2.1.3.17 Line.significanceOfDetection
The significance of line detection in an observed spectrum. It can be expressed in terms of signal-to-noise ratio, or detection probability (usually null hypothesis

probability that a given observed line is due to a statistical background fluctuation).

2.1.3.18   Line.transitionType

String indicating the first non zero term in the expansion of the operator $e^{i\vec{k}\vec{r}}$ in the atomic transition probability integral:

$$\int \phi^f e^{i\vec{k}\vec{r}} l \; \nabla\phi_i \quad d^3x$$

Possible values correspond to, e.g., "electric dipole", "magnetic dipole", "electric quadrupole", etc., or their corresponding common abbreviations E1, M1, E2, etc.

2.1.3.19   Line.strength

In theoretical works, the line strength S is widely used (Drake 1996):

$$S = S(i, k) = S(k, i) = |R_{ik}|^2 \quad where \quad R_{ik} = \langle \psi_k |P| \psi_i \rangle$$

Where ψ_i and ψ_k are the initial- and final-state wavefunction and R_{ik} is the transition matrix element of the appropriate multipole operator P. For example, the relationship between A, f, and S for electric dipole (E1 or allowed) transitions in S.I. units (A in s^{-1} , ν in s^{-1} , S in m^2 C^2, ε_0 in C^2.N^{-1}.m^{-2}, h in J.s) are:

$$A_{ik} = \left(\frac{4\pi h \alpha \nu^2}{c^2 m_e} \right) \left(\frac{g_k}{g_i} \right) f_{ki} = \left(\frac{16\pi^3 \nu^3}{3h\varepsilon_0 c^3 g_i} \right) S$$

2.1.3.20   Line.observedBroadeningCoefficient

Width of the line profile (expressed as Full Width Half Maximum) induced by a process of "type=Broadening".

2.1.3.21   Line.observedShiftingCoefficient

Shift of the transition laboratory wavelength(/frequency/wavenumber) induced by a process of "type=Energy shift". It is expressed by the difference between the peak intensity wavelength(frequency/wavenumber) in the observed profile and the laboratory wavelength(frequency/wavenumber).

2.1.4 Species

This class is a placeholder for a future model, providing a full description of the physical and chemical property of the chemical element of compound where the transition originating the line occurs

2.1.4.1 Species.name

Name of the chemical element or compound including ionisation status. Examples of valid names are: CIV for Carbon three times ionised, N2H+ for the Dyazenylium molecule, etc (see Appendix A for standard chemical element names).

2.1.5 Level

The scope of this class is to describe the quantum mechanics properties of each level, between which the transition originating the line occurs.

2.1.5.1 Level.totalStatWeight

Statistical weight associated to the level including all degeneracies, expressed as the total number of terms pertaining to a given level.

2.1.5.2 Level.nuclearStatWeight

The same as `Level.totalStatWeight` for nuclear spin states only

2.1.5.3 Level.landeFactor

A dimensionless factor *g* that accounts for the splitting of normal energy levels into uniformly spaced sublevels in the presence of a magnetic field. The level of energy E_0 is split into levels of energy:

$$E_0 + g\beta B(J) , E_0 + g\beta B(J-1) , \ldots, E_0 - g\beta B(J)$$

Where B is the magnetic field and β is a proportionality constant.

In the case of the L-S coupling (see [appendix C](#)), the Lande factor g_j is specified as the combination of atomic quantum numbers, which enters in the definition of the total magnetic moment m_j in the fine structure interaction:

$$m_j = \frac{g_j \mu_B J}{\hbar}$$

where μ_B is the Bohr magneton, defined as:

$$\mu_B = \frac{eh}{2\pi m_e}$$

Where
e is the elementary charge
h is the Planck constant
m_e is the electron rest mass

In terms of pure quantum numbers:

$$g_j(J, L, S) \equiv 1 + \frac{J(J+1) + S(S+1) + L(L+1)}{2J(J+1)}$$

2.1.5.4   Level.lifeTime
Intrinsic lifetime of a level due to its radiative decay.

2.1.5.5   Level.energy
The binding energy of an electron belonging to the level.

2.1.5.6   Level.energyOrigin
Human readable string indicating the nature of the energy origin. Examples: "Ionization energy limit", "Ground state energy" of an atom, "Dissociation limit" for a molecule, etc

2.1.5.7   Level.quantumState
A representation of the level quantum state through its set of quantum numbers

2.1.5.8 Level.nuclearSpinSymmetryType

A string indicating the type of nuclear spin symmetry. Possible values are:
"para", "ortho", "meta"

2.1.5.9 Level.parity

Eigenvalue of the parity operator. Values (+1,-1)

2.1.5.10 Level.configuration

For atomic levels, the standard specification of the quantum numbers **nPrincipal** (**n**) and **lElectronicOrbitalAngularMomentum (l)** for the orbital of each electron in the level; an exponent is used to indicate the numbers of electrons sharing a given **n** and **l**. For example, $1s^2, 2s^2, 2p^6, 5f$. The orbitals are conventionally listed according to increasing **n**, then by increasing **l**, that is, $1s$, $2s$, $2p$, $3s$, $3p$, $3d$, ... Closed shell configurations may be omitted from the enumeration.

For molecular states, similar enumerations takes place involving appropriate representations.

2.1.6 QuantumState

2.1.6.1 QuantumState.mixingCoefficient

A positive or negative number (double) giving the squared or the signed linear coefficient corresponding to the associated component in the expansion of the eigenstate (QuantumState in the DM). It varies from 0 to 1 (or -1 to 1)

2.1.6.2 QuantumState.quantumNumber

In order to allow for a simple mechanism for quantum numbers coupling, the QuantumNumber object is reduced to the minimum set of needed attributes to identify a quantum number. Coupling is then implemented by specifying combinations of the different quantum numbers.

See Appendix C.

2.1.6.3 QuantumState.termSymbol

The term (symbol) to which this quantum state belongs, if applicable.

For example, in the case of Spin-Orbit atomic interaction, a term describes a set of (2S+1)(2L+1) states belonging to a definite configuration and to a definite L and S. The notation for a term is for the LS coupling is, at follows:

$$^{2S+1}L_J$$

where

- *S* is the total spin quantum number. $2S+1$ is the **spin multiplicity**: the maximum number of different possible states of *J* for a given (*L*,*S*) combination.
- *L* is the total orbital quantum number in spectroscopic notation. The symbols for L = 0,1,2,3,4,5 are S,P,D,F,G,H respectively.
- *J* is the total angular momentum quantum number, where
  $$|L-S| \leq J \leq L+S$$

For instance, $^3P_1$ would describe a term in which L=1, S=1 and J=1. If J is not present, this term symbol represents the 3 different possible levels (J=0,1,2)

See appendix C for more examples of different couplings.

For molecular quantum states, it is a shorthand expression of the group irreductible representation and angular momenta that characterize the state of a molecule, i.e its electronic quantum state. A complete description of the molecularTermSymbol can be found in « Notations and Conventions in Molecular Spectroscopy: Part 2. Symmetry notation » (IUPAC Recommendations 1997), C.J.H. Schutte et at, Pure & Appl. Chem., Vol. 69, no. 8, pp. 1633-1639, 1997. The molecular term symbol contains the irreductible representation for the molecular point groups with right subscripts and superscripts, and a left superscript indicating the electron spin multiciplicity, Additionaly it starts with an symbol ~X (i.e., ~ on X) (ground state), Ã, ~B (i.e. ~ on B), ... indicating excited states of the same multiplicity than the ground state X or ã, ~b (~ on b), ... for excited states of different   multiplicity.

2.1.7 QuantumNumber

  The scope of this class is to describe the set of quantum numbers describing each level.

2.1.7.1   QuantumNumber.label
The name of the quantum number. It is a string like "F", "J", "I1", etc., or whatever human readable string that identifies the quantum number

2.1.7.2　　　　　　　　QuantumNumber.type

A string describing the quantum number. Recommended values are (see Appendix B for a description):

```
totalNuclearSpinI
totalMagneticQuantumNumberI
totalMolecularProjectionI
nuclearSpin
parity
serialQuantumNumber
nPrincipal
lElectronicOrbitalAngularMomentum
sAngularMomentum
jTotalAngularMomentum
fTotalAngularMomentum
lMagneticQuantumNumber
sMagneticQuantumNumber
jMagneticQuantumNumber
fMagneticQuantumNumber
asymmetricTAU
asymmetricKA
asymmetricKC
totalSpinMomentumS
totalMagneticQuantumNumberS
totalMolecularProjectionS
totalElectronicOrbitalMomentumL
totalMagneticQuantumNumberL
totalMolecularProjectionL
totalAngularMomentumN
totalMagneticQuantumNumberN
totalMolecularProjectionN
totalAngularMomentumJ
totalMagneticQuantumNumberJ
totalMolecularProjectionJ
intermediateAngularMomentumF
totalAngularMomentumF
totalMagneticQuantumNumberF
vibrationNu
vibrationLNu
totalVibrationL
vibronicAngularMomentumK
vibronicAngularMomentumP
hinderedK1
hinderedK2
```

2.1.7.3　　　　　　　　QuantumNumber.numeratorValue

The numerator of the quantum number value

2.1.7.4　　　　　　　　QuantumNumber.denominatorValue

The denominator of the quantum number value. If not explicitly specified, it is defaulted to "1" (meaning that the corresponding quantum number value is a multiple integer)

2.1.7.5　　　　　　　　QuantumNumber.description

A human readable string, describing the nature of the quantum number. Standard descriptions are given at the Appendix B for those quantum numbers

whose names are given above.   For a quantum number not appearing above, the descritpion shall be given here.

2.1.8 Process

The scope of this class is to describe the physical process responsible for the generation of the line, or for the modification of its physical properties with respect to those measured in the laboratory. The complete description of the process is relegated to specific placeholder called "model" which will describe specific physical models for each process.

2.1.8.1   Process.type

String identifying the type of process. Possible values are: "Matter-radiation interaction", "Matter-matter interaction", "Energy shift", "Broadening".

2.1.8.2   Process.name

String describing the process: Example values (corresponding to the values of "type" listed above) are: "Photoionization", "Collisional excitation", "Gravitational redshift", "Natural broadening".

2.1.8.3   Process.model

A theoretical model by which a specific process might be described.

2.1.9 Environment

The scope of this class is describing the physical properties of the ambient gas, plasma, dust or stellar atmosphere where the line is generated.

2.1.9.1   Environment.temperature

The temperature in the line-producing plasma.

2.1.9.2   Environment.opticalDepth

The optical depth in the line-producing plasma for the transition described by "initialLevel" and "finalLevel".

2.1.9.3　　　　　　　　Environment.particledensity

The particle density in the line-producing plasma.

2.1.9.4　　　　　　　　Environment.massdensity

The mass density in the line-producing plasma.

2.1.9.5　　　　　　　　Environment.pressure

The pressure in the line-producing plasma.

2.1.9.6　　　　　　　　Environment.entropy

The entropy of the line-producing plasma.

2.1.9.7　　　　　　　　Environment.mass

The total mass of the line-producing gas/dust cloud or star.

2.1.9.8　　　　　　　　Environment.metallicity

As customary in astronomy, the metallicity of an element is expressed as the logarithmic ratio between the element and the Hydrogen abundance, normalized to the solar value. If the metallicity of a celestial object or plasma is expressed through a single number, this refers to the iron abundance.

2.1.9.9　　　　　　　　Environment.extinctionCoefficient

A quantitative observable k, which expresses the suppression of the emission line intensity due to the presence of optically thick matter along the line-of-sight. It is a measure of the intervening gas density through one of the following equations:

$$k = n\sigma = \kappa\rho$$

where n is the particle density, σ is the integrated cross section, κ is the integrated opacity and ρ the matter density.

2.1.9.10　　　　　　　　Model

Placeholder for future detailed theoretical models of the environment plasma where the line appears.

2.1.10 Source

This class gives a basic characterization of the celestial source, where an astronomical line has been observed

2.1.10.1 Source.IAUname

The IAUname of the source

2.1.10.2 Source.name

An alternative or conventional name of the source

2.1.10.3 Source.coordinates

Coordinates of the source. Link to IVOA Space Time Coordinates data model

3 UCDs

The following is a list of the UCDs that should accompany any of the object attributes in their different serializations.

They are based in *"The UCD1+ controlled vocabulary Version 1.23"* (IVOA Recommendation, 2 Apr 2007).

There is one table per each of the objects in the Data Model. The left column indicates the object attribute, and the right column the UCD. Items appearing in *(bold)* correspond to other objects in the model.

Line	
initialLevel	*(Level)*
finalLevel	*(Level)*
initialElement	*(ChemicalElement)*
finalElement	*(ChemicalElement)*
wavelength	em.wl
wavenumber	em.wn
frequency	em.freq
airWavelength	em.wl
einsteinA	phys.at.transProb
oscillatorStrength	phys.at.oscStrength
weightedOscillStrength	phys.at.WOscStrength
intensity	spect.line.intensity
observedFlux	phot.flux

observedFluxWaveMin	em.wl
observedFluxWaveMax	em.wl
significanceOfDetection	stat.snr
process	*(Process)*
lineTitle	meta.title
transitionType	meta.title
strength	spect.line.strength
observedBroadeningCoefficient	spect.line.broad
observedShiftingCoefficient	phys.atmol.lineShift

Species	
name	meta.title

Level	
type	meta.title
totalStatWeight	phys.atmol.sweight
nuclearStatWeight	phys.atmol.nucweigth
lifeTime	phys.atmol.lifetime
energy	phys.energy
quantumState	*(QuantumState)*
energyOrigin	phys.energy
landeFactor	phys.at.lande
nuclearSpinSymmetryType	phys.atmol.symmetrytype
parity	phys.atmol.parity
energyOrigin	phys.energy
configuration	phys.atmol.configuration

QuantumState	
normalizedProbability	stat.normalProb
quantumNumber	phys.atmol.qn
termSymbol	phys.atmol.termSymbol

QuantumNumber	
label	meta.title
type	meta.title
numeratorValue	meta.number
denominatorValue	meta.number
description	meta.note

Process	
model	*(Model)*
name	meta.title

Environment	
temperature	phys.temperature
opticalDepth	phys.absorption.opticalDepth
density	phys.density
pressure	phys.pressure
extinctionCoefficient	phys.absorption
entropy	phys.entropy
mass	phys.mass
metallicity	phys.abund.Z
model	*(Model)*

4 Working examples

4.1 *The Hyperfine Structure of N2H$^+$*

This example refers to the measurement of the hyperfine structure of the J=1→0 transition in diazenlyium (N$_2$H$^+$) at 93 Ghz (Caselli et al. 1995) toward the cold (kinetic temperature T$_K$~10 K) dense core of the interstellar cloud L1512. Due to the closed-shell $^1\Sigma$ configuration of this molecule, the dominant hyperfine interactions are those between the molecular electric field gradient and the electric quadrupole moments of the two nitrogen nuclei. Together they produce a splitting of the J=1→0 in seven components. The astronomical measurements are much more accurate than those obtainable on the Earth, due to the excellent spectral resolution (~0.18 km s^{-1} FWHM), which correspond to the thermal width at ~20K, much a lower temperature than achievable in the laboratory.

Table 1 – Observed   properties of the N$_2$H$^+$ hyperfine structure components

J F$_1$ F → J'F'$_1$F'	ν (MHz)	$\sigma_\nu \, \Delta\nu$ (MHz)
1 0 1 → 0 1 2	93176.2650	0.0011
1 2 1 → 0 1 1	93173.9666	0.0012
1 2 3 → 0 1 2	93173.7767	0.0012
1 2 2 → 0 1 1	93173.4796	0.0012
1 1 1→ 0 1 0	93172.0533	0.0012
1 1 2 → 0 1 2	93171.9168	0.0012
1 1 0 → 0 1 1	93171.6210	0.0013

where ν is the transition frequency – as derived assuming the same Local Standard Rest velocity for all observed spectral lines – and $\sigma_\nu \, \Delta\nu$ its relative uncertainty.

 Estimates of the N$_2$H$^+$ optical depth, excitation temperature and intrinsic line width were made by fitting the hyperfine splitting complex. They yielded:

- $\tau_{tot} = 7.9 \pm 0.3$
- $T_{ext} = 4.9 \pm 0.1$

- $\Delta v = 183 \pm 1$ m s^{-1}

However, the same paper reports evidence for deviations from a single temperature excitation   in the following transitions: $(F_1, F) = (1,2) \rightarrow (1,2)$ and $(1,0) \rightarrow (1,1)$

We show below an example of instantiation of the current Line Data Model for one of the components of the N_2H^+ hyperfine transition (*e.g.* the transition in the first row of *Tab.1*).
In what follows, SI units are assumed whenever pertinent and PhysicalQuantity.error indicates the statistical uncertainty on a measured quantity.

4.1.1 The values in the model

In what follows we give the values attached to each of the model items pertinent for the case. For sake of simplicity, we report here the transition in the first row of Table 1 only. Likewise, the class attributes have been given values in pseudo-code way.

Initial Level (one QuantumState defined by three QuantumNumber(s)):

- `Line.initialLevel.quantumState.quantumNumber.label := "J"`
- `Line.initialLevel.quantumState.quantumNumber.type :=`
  `"totalAngularMomentumJ"`
- `Line.initialLevel.quantumState.quantumNumber.description := "Pure`
  `quantum number"`
- `Line.initialLevel.quantumState.quantumNumber.numeratorValue := 1`
- `Line.initialLevel.quantumState.quantumNumber.denominatorValue :=1`

- `Line.initialLevel.quantumState.quantumNumber. label:= "F₁"`
- `Line.initialLevel.quantumState.quantumNumber.type :=`
  `"totalAngularMomentumF"`
- `Line.initialLevel.quantumState.quantumNumber.description:=`
  `"Resulting angular momentum including nuclear spin for one`
  `nucleus; coupling of J and I₁"`
- `Line.initialLevel.quantumState.quantumNumber.numeratorValue := 0`

- `Line.initialLevel.quantumState.quantumNumber. label:= "F"`
- `Line.initialLevel.quantumState.quantumNumber.type :=`
  `"totalAngularMomentumF"`
- `Line.initialLevel.quantumState.quantumNumber.description :=`
  `"Resulting total angular momentum; coupling of I₂ and F₁"`
- `Line.initialLevel.quantumState.quantumNumber.numeratorValue := 1`
- `Line.initialLevel.quantumState.quantumNumber.denominatorValue :=1`

Final Level (one QuantumState defined by three QuantumNumber(s)):

- `Line.finalLevel.quantumState.quantumNumber. label:= "J"`
- `Line.finalLevel.quantumState.quantumNumber.type :=`
    `"jtotalAngularMomentum"`
- `Line.finalLevel.quantumState.quantumNumber.description := "Total`
    `angular momentum excluding nuclear spins. Pure quantum number"`
- `Line.finalLevel.quantumState.quantumNumber.numeratorValue := 1`
- `Line.initialLevel.quantumState.quantumNumber.denominatorValue :=1`

- `Line.initialLevel.quantumState.quantumNumber. label:= "F`$_1$`"`
- `Line.initialLevel.quantumState.quantumNumber.type :=`
    `"totalAngularMomentumF"`
- `Line.initialLevel.quantumState.quantumNumber.description:=`
    `"Resulting angular momentum including nuclear spin for one`
    `nucleus; coupling of J and I`$_1$`"`
- `Line.initialLevel.quantumState.quantumNumber.numeratorValue := 0`

- `Line.initialLevel.quantumState.quantumNumber. label:= "F"`
- `Line.initialLevel.quantumState.quantumNumber.type :=`
    `"totalAngularMomentumF"`
- `Line.initialLevel.quantumState.quantumNumber.description :=`
    `"Resulting total angular momentum; coupling of I and J"`
- `Line.initialLevel.quantumState.quantumNumber.numeratorValue := 2`
- `Line.initialLevel.quantumState.quantumNumber.denominatorValue :=`
    `1`

Line specific attributes:
- `Line.airWavelength.value:= 3.21755760x10`$^{-3}$
- `Line.airWavelength.unit.expression:= "m"`
- `Line.airWavelength.Unit.scaleSI:= 1`
- `Line.airWavelength.Unit.dimEquation:= "L"`

Process specific attributes (Broadening):

- `Line.process.type := "Broadening"`
- `Line.process.name := "Intrinsic line width"`
- `Line.observedBroadeningCoefficient.value := 183`
- `Line.observedBroadeningCoefficient.unit.expression := "m/s"`
- `Line.observedBroadeningCoefficient.Unit.scaleSI := 1`

- `Line.observedBroadeningCoefficient.Unit.dimEquation := "LT-1"`

Environment specific attributes:

- `Line.process.model.excitationTemperature.value := 4.9`
- `Line.process.model.excitationTemperature.error := 0.1`
- `Line.process.model.excitationTemperature.unit.expression := "K"`
- `Line.process.model.excitationTemperature.Unit.scaleSI := 1`
- `Line.process.model.excitationTemperature.Unit.dimEquation := "K"`
- `Line.process.model.opticalDepth.value := 7.9`
- `Line.process.model.opticalDepth.unit.expression := ""`
- `Line.process.model.opticalDepth.Unit.scaleSI := 1`
- `Line.process.model.opticalDepth.Unit.dimEquation := ""`
- `Line.process.model.opticalDepth.error := 0.3`

Initial and final (identical) **Specie(s)**:

- `Line.initialElement.name := "N_2H^+"`
- `Line.finalElement.name := "N_2H^+"`

Source specific attributes**:**

- `Line.source.name := "L1512"`

4.1.2 JSON representation

```
{
    "Line": {

        "source": {
            "name": "L1512"
        }

        "initialElement": {
            "name": "N2H+"
        }

        "finalElement": {
            "name": "N2H+"
        }
```

```
"initialLevel": {
        "quantumNumber": {
                "label": "J"
                "type": "totalAngularMomentumJ"
                "description": "Pure quantum number"
                "numeratorValue": "1"
                "denominatorValue": "1"
        }
        "quantumNumber": {
                "label": "F1"
                "type": "totalAngularMomentumF"
                "description": "Resulting angular momentum including
nuclear spin for one nucleus; coupling of J and I1"
                "numeratorValue": "0"
        }
        "quantumNumber": {
                "label": "F"
                "type": "totalAngularMomentumF"
                "description": 'Resulting total angular momentum;
coupling of I2 and F1"
                "numeratorValue": "1"
                "denominatorValue": "1"
        }
}

"finalLevel": {
        "quantumNumber": {
                "label": "J"
                "type": "jtotalAngularMomentum"
                "description":    "Total angular momentum excluding
nuclear spins. Pure quantum number"
                "numeratorValue": "1"
                "denominatorValue": "1"
        }
        "quantumNumber": {
                "label": "F1"
                "type": "totalAngularMomentumF"
                "description": "Resulting angular momentum including
nuclear spin for one nucleus; coupling of J and I1"
                "numeratorValue": "0"
        }
        "quantumNumber": {
                "label": "F"
                "type": "totalAngularMomentumF"
```

                              "description": "Resulting total angular momentum;
coupling of I and J"

                              "numeratorValue": "2"
                              "denominatorValue": "1"
                    }
          }

          "airWavelength": {
                    "value":   "3.21755760x10-3"
                    "unit": {
                              "expression": "m"
                              "scaleSI": "1"
                              "dimEquation": "L"
                    }
          }
          "process": {
                    "type": "Broadening"
                    "name": "Intrinsic line width"

                    "model": {
                              "excitationTemperature": {
                                        "value": "4.9"
                                        "error": "0.1"
                                        "unit": {
                                                  "expression": "K"
                                                  "scaleSI": "1"
                                                  "dimEquation": "K"
                                        }
                              }
                              "opticalDepth": {
                                        "value": "7.9"
                                        "error": "0.3"
                                        "unit": {
                                                  "expression": ""
                                                  "scaleSI": "1"
                                                  "dimEquation": ""
                                        }
                              }
                    }
          }

          "observedBroadeningCoefficient": {
                    "value": "183"
                    "unit" : {
                              "expression": "m/s"

```json
                        "scaleSI": "1"
                        "dimEquation": "LT-1"
                }
            }
        }
    }
```

4.1.3 UML instantiation diagram
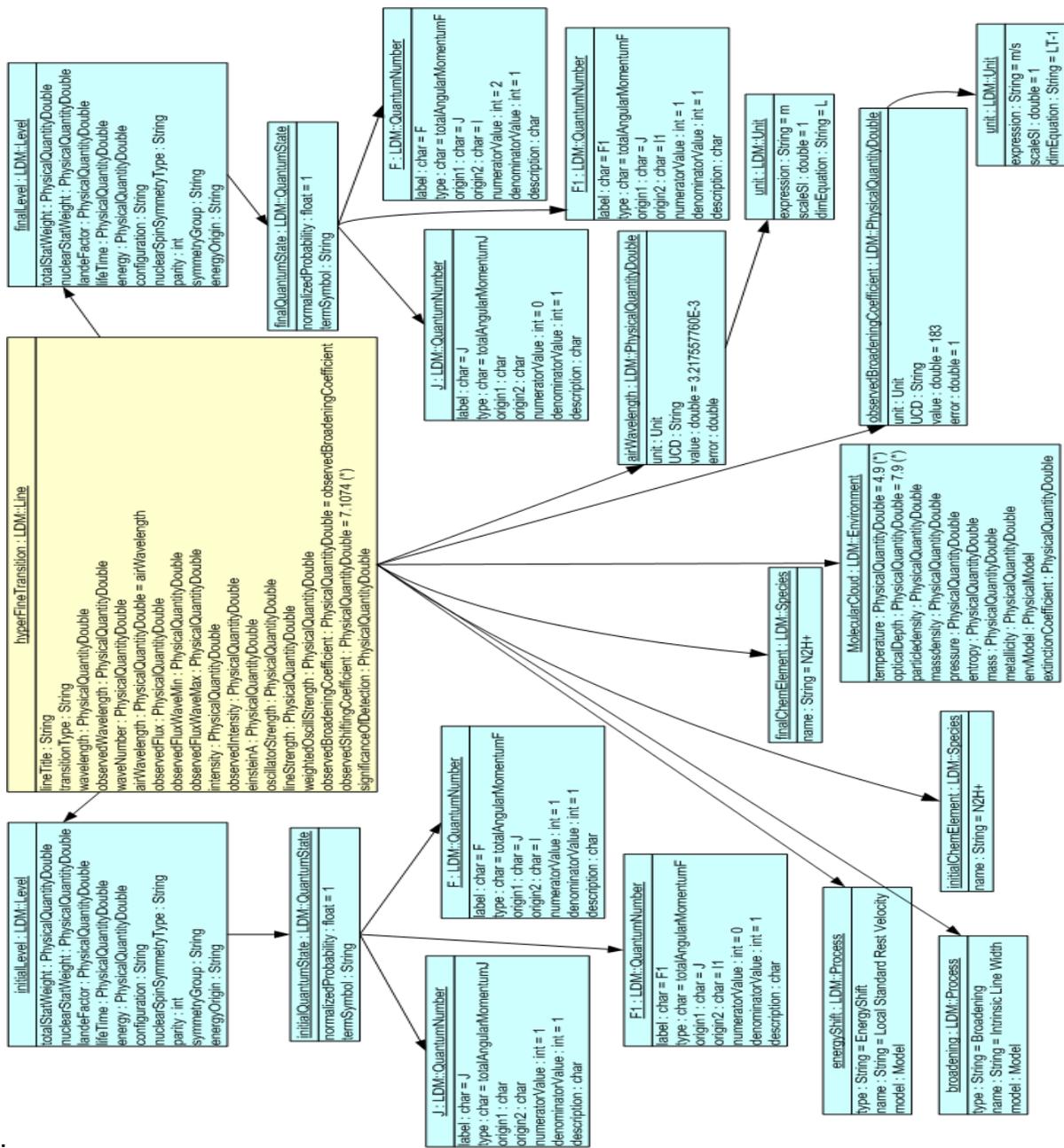
Please note that some physical quantities (marked with an asterisk) have not been fully instanced to simplify the graphics.

4.2 Radiative Recombination Continua: a diagnostic tool for X-Ray spectra of AGN

The advent of a new generation of large X-ray observatories is allowing us to obtain spectra of unprecedented quality and resolution on a sizeable number of Active Galactic Nuclei (AGN). This has revived the need for diagnostic tools, which can properly characterize the properties of astrophysical plasmas encompassing   the nuclear region, where the gas energy budget is most likely dominated by the high-energy AGN output.

  Among these spectra diagnostics, Radiative Recombination Continua (RRC) play a key role, as they unambiguously identify photoionized plasmas, and provide unique information on their physical properties. The first quantitative studies which recognized the importance of RRC in X-ray spectra date back to the early '90, using *Einstein* (Liedahl et al. 1991; Kahn & Liedahl 1991) and ASCA (Angelini et al. 1995) observations. The pioneer application of the RRC diagnostic to AGN is due to Kinkhabwala et al. (2002; K02), who analysed a long XMM-Newton/RGS observation of the nearby Seyfert 2 galaxy NGC1068 (z=0.003793, corresponding to a recession velocity of 1137 km s^{-1}). We will refer to the results reported in their paper hereafter.

  K02 report the detection of RRC from 6 different ionic species. Their observational properties are shown in Tab.3. The RRC temperature kT_e is

Tab.3 – Properties of the RRC features in the XMM-Newton/RGS spectrum of NGC1068

Ion	kT_e (eV)	Flux $(10^{-4}$ ph cm^{-2} s$^{-1})$	I (eV)
CV	2.5±0.5	4.3±0.4	392.1
CVI	4.0±1.0	2.8±0.3	490.0
NVI	3.5±2.0	2.1±0.2	552.1
NVII	5.0±3.0	1.1±0.1	667.1
OVII	4.0±1.3	2.4±0.2	739.3
OVIII	7.0±3.5	1.2±0.1	871.4

derived from the RRC profile fit, as the width of the RRC profile $\Delta E \approx kT_e$. The average RRC photon energy is $E \approx I + kT_e$, where I is the ionization potential of the

recombined state. If the plasma is highly over ionized (kT«I) – as expected in X-ray photoionized nebulae (Kallman & McCray 1982) – then $\Delta E/E \approx kT_e/I$. Therefore, the specification of kT_e (extracted from Tab.2 in K02) and I (extracted from table of photo ionization potentials) is enough to know the energy of the feature.

4.2.1 The values in the model

Initial Level description:
- `Line.initialLevel.quantumState.quantumNumber.label:= "n"`
- `Line.initialLevel.quantumState.quantumNumber.type:= "nPrincipal"`
- `Line.initialLevel.quantumState.quantumNumber.numeratorValue:=1`
- `Line.initialLevel.quantumState.quantumNumber.denominatorValue:=1`

Final Level:
- `Line.finalLevel.quantumState.quantumNumber.label:= "n"`
- `Line.finalLevel.quantumState.quantumNumber.type:= "nPrincipal"`
- `Line.finalLevel.quantumState.quantumNumber.numeratorValue:= 1`
- `Line.finalLevel.quantumState.quantumNumber.denominatorValue:= 1`

Initial Element:
- `Line.initialElement.species.name := "CVI"`

Final Element:
- `Line.finalElement.species.name := "CV"`

(Observed) **Line** specific attributes

- `Line.wavelength.value := 394.6`
- `Line.wavelength.unit.expression := "eV"`
- `Line.wavelength.Unit.scaleSI := 1.6E-19`
- `Line.wavelength.Unit.dimEquation := "ML2T-2"`

- `Line.observedFlux.value := 2.8E-4`
- `Line.observedFlux.error := 0.3E-4`
- `Line.observedFlux.unit.expression := "photons*cm-2*s-1"`
- `Line.observedFlux.unit.scaleSI = 1.E4`
- `Line.observedFlux.unit.dimEquation := "L-2T-1"`

- `Line.transitionType := "Radiative Recombination Continuum"`

Process specific attributes
- `Line.Process.type := "Energy shift"`
- `Line.Process.name := "Cosmological redshift"`

- `Line.observedShiftingCoefficient.value := 1137`
- `Line.observedShiftingCoefficient.unit.expression := "km/s"`
- `Line.observedShiftingCoefficient.unit.scaleSI := 1.E3`
- `Line.observedShiftingCoefficient.unit.dimEquation := "MT-1"`

Environment specific attributes:

- `Line.environment.temperature.value := 1.9E5`
- `Line.environment.temperature.unit.expression := "K"`
- `Line.environment.temperature.unit.scaleSI := 1`
- `Line.environment.temperature.unit.dimEquation := "K"`

Source specific attributes**:**

- `Line.source.name := "NGC1068"`

4.2.2 JSON representation

```
{
      "Line": {
            "transitionType":   "Radiative Recombination Continuum"
            "wavelength": {
                  "value":   "394.6"
                  "unit": {
                              "expression": eV"
                              "scaleSI": "1.6E-19"
                              "dimEquation": "ML2T-2"
                  }
            }
            "observedFlux": {
                  "value":   "2.8E-4"
                  "error": "0.3E-4"
                  "unit": {
                              "expression": photons*cm-2*s-1"
                              "scaleSI": "1.E4"
                              "dimEquation": "L-2T-1"
                  }
            }
            "source": {
                  "name": "NGC1068"
            }
            "initialElement": {
                  "name": "CVI"
            }
            "finalElement": {
```

```
                    "name": "CV"
            }
            "initialLevel": {
                    "quantumNumber": {
                            "label": "n"
                            "type": "nPrincipal"
                            "numeratorValue": "1"
                            "denominatorValue": "1"
                    }
            }
            "finalLevel": {
                    "quantumNumber": {
                            "label": "n"
                            "type": "nPrincipal"
                            "numeratorValue": "1"
                            "denominatorValue": "1"
                    }
            }
            "process": {
                    "type": "Energy shift"
                    "name": "Cosmological redshift"
            }
            "observedShiftingCoefficient": {
                    "value": "1137"
                    "unit" : {
                            "expression": "km/s"
                            "scaleSI": "1.E3"
                            "dimEquation": "MT-1"
                    }
            }
            "environment": {
                    "temperature": {
                            "value": "1.9E5"
                            "unit": {
                                    "expression": "K"
                                    "scaleSI": "1"
                                    "dimEquation": "K"
                            }
                    }
            }
        }
}
```

4.2.3 UML Instantiation diagram

initialLevel : LDM::Level
totalStatWeight : PhysicalQuantityDouble
nuclearStatWeight : PhysicalQuantityDouble
landeFactor : PhysicalQuantityDouble
lifeTime : PhysicalQuantityDouble
energy : PhysicalQuantityDouble
configuration : String
nuclearSpinSymmetryType : String
parity : int
symmetryGroup : String
energyOrigin : String

radiativeRecombination : LDM::Line
lineTitle : String
transitionType : String = Radiative Recombination Continuum
wavelength : PhysicalQuantityDouble = wavelength
observedWavelength : PhysicalQuantityDouble
waveNumber : PhysicalQuantityDouble
airWavelength : PhysicalQuantityDouble
observedFlux : PhysicalQuantityDouble = observedFlux
observedFluxWaveMin : PhysicalQuantityDouble
observedFluxWaveMax : PhysicalQuantityDouble
intensity : PhysicalQuantityDouble
observedIntensity : PhysicalQuantityDouble
einsteinA : PhysicalQuantityDouble
oscillatorStrength : PhysicalQuantityDouble
lineStrength : PhysicalQuantityDouble
weightedOscillStrength : PhysicalQuantityDouble
observedBroadeningCoefficient : PhysicalQuantityDouble
observedShiftingCoefficient : PhysicalQuantityDouble = observedShiftingCoefficient
significanceOfDetection : PhysicalQuantityDouble

finalLevel : LDM::Level
totalStatWeight : PhysicalQuantityDouble
nuclearStatWeight : PhysicalQuantityDouble
landeFactor : PhysicalQuantityDouble
lifeTime : PhysicalQuantityDouble
energy : PhysicalQuantityDouble
configuration : String
nuclearSpinSymmetryType : String
parity : int
symmetryGroup : String
energyOrigin : String

initialQuantumState : LDM::QuantumState
normalizedProbability : float = 1
termSymbol : String

finalQuantumState : LDM::QuantumState
normalizedProbability : float = 1
termSymbol : String

n : LDM::QuantumNumber
label : char = n
type : char = Principal QN
origin1 : char = Pure QN
origin2 : char
numeratorValue : int = 1
denominatorValue : int = 1
description : char

initiCheElem : LDM::Species
name : String = CVI

finChemElem : LDM::Species
name : String = CV

n : LDM::QuantumNumber
label : char
type : char = Principal QN
origin1 : char = Pure
origin2 : char = n
numeratorValue : int = 1
denominatorValue : int = 1
description : char

environment : LDM::Environment
temperature : PhysicalQuantityDouble = temperature
opticalDepth : PhysicalQuantityDouble
particledensity : PhysicalQuantityDouble
massdensity : PhysicalQuantityDouble
pressure : PhysicalQuantityDouble
entropy : PhysicalQuantityDouble
mass : PhysicalQuantityDouble
metallicity : PhysicalQuantityDouble
envModel : PhysicalModel
extinctionCoefficient : PhysicalQuantityDouble

wavelength : LDM::PhysicalQuantityDouble
unit : Unit
UCD : String
value : double = 349.6
error : double = 0.5

redshift : LDM::Process
type : String = Energy Shift
name : String = Cosmological Redshift
model : Model

unit : LDM::Unit
expression : String
scaleSI : double
dimEquation : String

temperature : LDM::PhysicalQuantityDouble
unit : Unit
UCD : String
value : double = 29012
error : double

observedFlux : LDM::PhysicalQuantityDouble
unit : Unit
UCD : String
value : double = 4.3E-4
error : double = 0.3E-4

unit : LDM::Unit
expression : String
scaleSI : double
dimEquation : String

unit : LDM::Unit
expression : String
scaleSI : double
dimEquation : String

observedShiftingCoefficient : LDM::PhysicalQuantityDouble
unit : Unit
UCD : String
value : double = 1137
error : double

unit : LDM::Unit
expression : String
scaleSI : double
dimEquation : String

4.3 References

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5 Appendix A: List of Atomic Elements

List of Elements extracted from the **IUPAC Commission on Atomic Weights and Isotopic Abundances**. **(http://www.chem.qmul.ac.uk/iupac/)**

List of Elements in Atomic Number Order.

At No	Symbol	Name	Notes
1	H	Hydrogen	1, 2, 3
2	He	Helium	1, 2
3	Li	Lithium	1, 2, 3, 4
4	Be	Beryllium	
5	B	Boron	1, 2, 3
6	C	Carbon	1, 2
7	N	Nitrogen	1, 2
8	O	Oxygen	1, 2
9	F	Fluorine	
10	Ne	Neon	1, 3
11	Na	Sodium	
12	Mg	Magnesium	
13	Al	Aluminium	
14	Si	Silicon	2
15	P	Phosphorus	
16	S	Sulfur	1, 2
17	Cl	Chlorine	3
18	Ar	Argon	1, 2
19	K	Potassium	1
20	Ca	Calcium	1
21	Sc	Scandium	
22	Ti	Titanium	
23	V	Vanadium	
24	Cr	Chromium	
25	Mn	Manganese	
26	Fe	Iron	
27	Co	Cobalt	
28	Ni	Nickel	
29	Cu	Copper	2
30	Zn	Zinc	
31	Ga	Gallium	
32	Ge	Germanium	
33	As	Arsenic	
34	Se	Selenium	
35	Br	Bromine	

36	Kr	Krypton	1, 3
37	Rb	Rubidium	1
38	Sr	Strontium	1, 2
39	Y	Yttrium	
40	Zr	Zirconium	1
41	Nb	Niobium	
42	Mo	Molybdenum	1
43	Tc	Technetium	5
44	Ru	Ruthenium	1
45	Rh	Rhodium	
46	Pd	Palladium	1
47	Ag	Silver	1
48	Cd	Cadmium	1
49	In	Indium	
50	Sn	Tin	1
51	Sb	Antimony	1
52	Te	Tellurium	1
53	I	Iodine	
54	Xe	Xenon	1, 3
55	Cs	Caesium	
56	Ba	Barium	
57	La	Lanthanum	1
58	Ce	Cerium	1
59	Pr	Praseodymium	
60	Nd	Neodymium	1
61	Pm	Promethium	5
62	Sm	Samarium	1
63	Eu	Europium	1
64	Gd	Gadolinium	1
65	Tb	Terbium	
66	Dy	Dysprosium	1
67	Ho	Holmium	
68	Er	Erbium	1
69	Tm	Thulium	
70	Yb	Ytterbium	1
71	Lu	Lutetium	1
72	Hf	Hafnium	
73	Ta	Tantalum	
74	W	Tungsten	
75	Re	Rhenium	
76	Os	Osmium	1
77	Ir	Iridium	
78	Pt	Platinum	
79	Au	Gold	
80	Hg	Mercury	

81	Tl	Thallium	
82	Pb	Lead	1, 2
83	Bi	Bismuth	
84	Po	Polonium	5
85	At	Astatine	5
86	Rn	Radon	5
87	Fr	Francium	5
88	Ra	Radium	5
89	Ac	Actinium	5
90	Th	Thorium	1, 5
91	Pa	Protactinium	5
92	U	Uranium	1, 3, 5
93	Np	Neptunium	5
94	Pu	Plutonium	5
95	Am	Americium	5
96	Cm	Curium	5
97	Bk	Berkelium	5
98	Cf	Californium	5
99	Es	Einsteinium	5
100	Fm	Fermium	5
101	Md	Mendelevium	5
102	No	Nobelium	5
103	Lr	Lawrencium	5
104	Rf	Rutherfordium	5, 6
105	Db	Dubnium	5, 6
106	Sg	Seaborgium	5, 6
107	Bh	Bohrium	5, 6
108	Hs	Hassium	5, 6
109	Mt	Meitnerium	5, 6
110	Ds	Darmstadtium	5, 6
111	Rg	Roentgenium	5, 6
112	Uub	Ununbium	5, 6
114	Uuq	Ununquadium	5, 6
116	Uuh	Ununhexium	see Note above
118	Uuo	Ununoctium	see Note above

1. Geological specimens are known in which the element has an isotopic composition outside the limits for normal material. The difference between the atomic weight of the element in such specimens and that given in the Table may exceed the stated uncertainty.

2. Range in isotopic composition of normal terrestrial material prevents a more precise value being given; the tabulated value should be applicable to any normal material.

3. Modified isotopic compositions may be found in commercially available material because it has been subject to an undisclosed or inadvertant isotopic fractionation. Substantial deviations in atomic weight of the element from that given in the Table can occur.

4. Commercially available Li materials have atomic weights that range between 6.939 and 6.996; if a more accurate value is required, it must be determined for the specific material [range quoted for 1995 table 6.94 and 6.99].

5. Element has no stable nuclides. The value enclosed in brackets, e.g. [209], indicates the mass number of the longest-lived isotope of the element. However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

The names and symbols for elements 112-118 are under review. The temporary system recommended by J Chatt, *Pure Appl. Chem.*, **51**, 381-384 (1979) is used above. The names of elements 101-109 were agreed in 1997 (See *Pure Appl. Chem., 1997, 69, 2471-2473*),for element 110 in 2003 (see *Pure Appl. Chem., 2003, 75, 1613-1615*) and for element 111 in 2004 (see *Pure Appl. Chem., 2004, 76, 2101-2103*).

6   Appendix B: List of quantum numbers

The list contains the most usual quantum numbers in atomic and molecular spectroscopy. The list is not exhaustive and is opened to new entries.

Note for molecules: Angular momemtum basis functions, $|A \alpha M_A >$, can be simultaneous eigenfunctions of three types of operators : the magnitude A^2, the component of A onto the internuclear axis A_z, and the component of A on the laboratory quantization axis A_Z. The basis function labels A, α and M_A correspond to eigenvalues of A^2, A_z, and A_Z, respectively $\hbar^2 A(A+1)$, $\hbar \alpha$ and $\hbar M_A$.

Note for intermediate coupling: Intermediate coupling occurs in both atomic and molecular physics. The document below gives some explanations about intermediate coupling in atomic physics, these explanations can be transposed to molecular physics (as for intermediate coupling between different Hund's cases). As described below, levels can be labelled by the least objectionable coupling case, by linear combinaison of pure coupling basis functions (the linear coefficients can be determined in a theoretical approach: *this is planned for in the*

data model), or simply by a sort of serial number (see **serialQuantumNumber** below)

6.1 Various Quantum numbers

6.1.1 totalNuclearSpinI

total nuclear spin of one atom or a molecule, I

6.1.2 totalMagneticQuantumNumberI

total magnetic quantum number, $M_I = -I, -I+1, ..., I-1, I$ where $\hbar M_I$ is the eigenvalue of the $\hat{I}_z$ operator

6.1.3 totalMolecularProjectionI

total nuclear spin projection quantum number Ω_I, $\Omega_I = -I, -I+1, ..., I-1, I$ where $\hbar \Omega_I$ is the eigenvalue of the $\hat{I}_z$ operator

6.1.4 nuclearSpin

nuclear spin of individual nucleus i which composes a molecule, noted; I_i

6.1.5 parity

eigenvalue of the parity operator applied to the total wavefunction. It takes the value "0" for even parity and "1" for odd parity

6.1.6 serialQuantumNumber

A serial quantum number that labels states to which no good or nearly good quantum numbers can be assigned to.

6.2 Quantum numbers for hydrogenoids

6.2.1 nPrincipal

principal quantum number n

6.2.2 lElectronicOrbitalAngularMomentum

orbital angular momentum of an electron $l = 0,1,2,...$ where $\hbar^2(l+1)$ is the eigenvalue of the $\hat{l}^2$ operator (called as well azimuthal quantum number).

6.2.3 sAngularMomentum

spin angular momentum of an electron, $s = \dfrac{1}{2}$ only where $\hbar^2 s(s+1)$ is the eigenvalue of the $\hat{s}^2$ operator)

6.2.4 jTotalAngularMomentum

total angular momentum of one electron j, $j = l-1/2(l>0)$ and $j = l+1/2$. $\hbar^2 j(j+1)$ is the eigenvalue of the $\hat{j}^2$ operator, where $\hat{j} = \hat{l} + \hat{s}$

6.2.5 fTotalAngularMomentum

total angular momentum f, including nuclear spin I. $\hbar^2 f(f+1)$ is the eigenvalue of the $\hat{f}^2$ operator, where $\hat{f} = \hat{j} + \hat{I}$

6.2.6 lMagneticQuantumNumber

orbital magnetic quantum number, $m_l = -l,-l+1,...,l-1,l$ where $\hbar m_l$ is the eigenvalue of the $\hat{l}_z$ operator

6.2.7 sMagneticQuantumNumber

spin magnetic quantum number, $m_s = \pm 1/2$ where $\hbar m_s$ is the eigenvalue of the $\hat{s}_z$ operator

6.2.8 jMagneticQuantumNumber

orbital magnetic quantum number, $m_j = -j,-j+1,..., j-1, j$ where $\hbar m_j$ is the eigenvalue of the $\hat{j}_z$ operator

6.2.9 fMagneticQuantumNumber

orbital magnetic quantum number, $m_f = -f, -f+1, ..., f-1, f$ where $\hbar m_f$ is the eigenvalue of the $\hat{f}_z$ operator

6.3 Pure rotational quantum numbers

6.3.1 asymmetricTAU

Index τ labelling asymmetric rotational energy levels for a given rotational quantum number N.

Note: The solution of the Schrödinger equation for an asymmetric-top molecule gives for each value of N, (2N+1) eigenfunctions with its own energy. It is customary to keep track of them by adding the subscript τ to the N value (N_τ). This index τ goes from -N for the lowest energy of the set to +N for the highest energy, and is equal to $(K_a - K_c)$.

6.3.2 asymmetricKA

For a given N, energy levels may be specified by K_a K_c (or K_{-1} K_1, or K_- K_+ are alternative notations), where K_a is the K quantum number for the limiting prolate (B=C) and K_c for the limiting oblate (B=A). In the notation (K_{-1} K_1) the subscripts "1" and "-1" correspond to values of the asymmetry parameter $\kappa = \dfrac{2B - A - C}{A - C}$

where A, B, C are rotational constants of the asymmetric molecule (by definition A>B>C)

6.3.3 asymmetricKc

see **asymmetricKA**

6.4 Quantum numbers for n electron systems (atoms and molecules)

6.4.1 totalSpinMomentumS

it is the total spin quantum number S, S can be integral or half-integral.
$\hbar^2 S(S+1)$ is the eigenvalue of the $\hat{S}^2$ operator, where $\hat{S} = \Sigma_{i=1}^{N} \hat{s}_i$

6.4.2 totalMagneticQuantumNumberS

total spin magnetic quantum number, $M_S = -S, -S+1, ..., S-1, S$ where $\hbar M_S$ is the eigenvalue of the $\hat{S}^2$ operator.

6.4.3 totalMolecularProjectionS

total spin projection quantum number Σ, $\Sigma = -S, -S+1, ..., S-1, S$, where $\hbar \Sigma$ is the eigenvalue of the $\hat{S}^2$ operator.

6.4.4 totalElectronicOrbitalMomentumL

it is the total orbital angular momentum L, L is integral. $\hbar^2 L(L+1)$ is the eigenvalue of the $\hat{L}^2$ operator, where $\hat{L} = \Sigma_{i=1}^{n} \hat{l}_i$

6.4.5 totalMagneticQuantumNumberL

total orbital magnetic quantum number, $M_L = -L, -L+1, ..., L-1, L$, where $\hbar M_L$ is the eigenvalue of the $\hat{L}_Z$ operator.

6.4.6 totalMolecularProjectionL

total orbital projection quantum number, $\Lambda = 0, 1, ..., L-1, L$ where $\hbar \Lambda$ is the absolute value of the eigenvalue of the $\hat{L}_Z$ operator (Hund's cases (a) and (b) in the case of a diatomic)

6.4.7 totalAngularMomentumN

is the total angular momentum N exclusive of nuclear and electronic spin, N is integral. For a molecule in a close-shell state **totalAngularMomemtumN** is the pure rotational angular momentum.

6.4.8 totalMagneticQuantumNumberN

total orbital magnetic quantum number, $M_N = -N, -N+1, ..., N-1, N$ where $\hbar M_N$ is the eigenvalue of the $\hat{N}_Z$ operator

6.4.9 totalMolecularProjectionN

absolute value of the component of the angular momentum N along the axis of a symmetric (or quasi-symmetric) rotor, usually noted K. $\pm \hbar K$ is the eigenvalue of the $\hat{N}_z$ operator, with values $K = 0,..., N-1, N$

For open shell diatomic molecules, it corresponds to "totalMolecularProjectionL" (Λ), so we advise to preferentially use "totalMolecularProjectionL"

Note: The symbol K is also used in spectroscopy to describe the component of the vibronic angular momentum (excluding spin) along the axis for linear polyatomic molecules. In this model, we prefer to uniquely identify this specific case by a different type of Quantum Number: "vibronicAngularMomentumK", defined thereafter.

6.4.10   totalAngularMomentumJ

is the total angular momentum J exclusive of nuclear spin, J can be integral or half-integral.

For atoms:

$$\hat{J} = \Sigma_{i=1}^{n}(\hat{l}_i + \hat{s}_i)$$

For molecules:

$$\hat{J} = \hat{N} + \Sigma_{i=1}^{n}\hat{s}_i = \hat{N} + \hat{S}$$

6.4.11   totalMagneticQuantumNumberJ

total magnetic quantum number, $M_J = -J, -J+1, ..., J-1, J$ where $\hbar M_J$ is the eigenvalue of the $\hat{J}_z$ operator.

6.4.12   totalMolecularProjectionJ

absolute value of the component of the angular momentum J along the molecular axis, noted $\Omega = 0, ..., J-1, J$ where $\pm \hbar \Omega$ is the eigenvalue of the $\hat{J}_z$ operator.

For linear molecules with no nuclear spin (or no nuclear spin coupled to the molecular axis), it is the absolute value of the component of the total electronic angular momentum $\hat{L} + \hat{S}$ on the molecular axis (Hund's cases (a) and (c)).

When Λ and Σ are defined (Hund's case (a)): $\Omega = \left| \Lambda \pm \Sigma \right|$

For linear molecules with a nuclear spin coupled to the molecular axis, it includes as well the component Ω_I of the nuclear spin on the molecular axis.

6.4.13   intermediateAngularMomemtunF

is associated to the intermediate quantum number F_i where $\hat{F}_i = \hat{I}$ (or $\hat{I}_j$) + any other vector

6.4.14   totalAngularMomentumF

is the total angular momentum F including nuclear spin, F can be integral or half-integral. $F(F+1)\hbar^2$ is the eigenvalue of the $\hat{F}^2$ operator, where for atoms:

$$\hat{F} = \Sigma_{i=1}^{n}(\hat{l}_i + \hat{s}_i) + \hat{I} = \hat{J} + \hat{I}$$

and for molecules with *m* nuclear spins:
$$\hat{F} = \hat{J} + \Sigma_{i=1}^{n}\hat{I}_i = \hat{J} + \hat{I}$$

6.4.15   totalMagneticQuantumNumberF

total magnetic quantum number, $M_F = -F, -F+1, ..., F-1, F$ where $\hbar M_F$ is the eigenvalue of the $\hat{F}_Z$ operator

6.5 *Vibrational and (ro-)vibronic quantum numbers*

6.5.1 vibrationNu

vibrational modes v_i (following Mulliken conventions). By default the vibrational mode is a normal mode. If the vibrational mode is fairly localised, the bond description will be included in the attribute "description" of "QuantumNumber"

6.5.2 vibrationLNu

angular momentum associated to degenerate vibrations, $l_i = v_i, v_i - 2, v_i - 4, ..., 1$ or 0

6.5.3 totalVibrationL

total vibrational angular momentum is the sum of all angular momenta $\pm l_i$ associated to degenerate vibrations: $l_v = \left| \Sigma_i (\pm l_i) \right|$

6.5.4 vibronicAngularMomentumK

is the sum of the total vibrational angular momentum l_v and of the electronic orbital momentum about the internuclear axis $\Lambda : K = \left| \pm l_v \pm \Omega \right|$

here K (l_v and Λ) are unsigned quantities. This is used for linear polyatomic molecules. (see p.25 Volume III pf Herzberg, and REC. (recommendation) 17 of Muliken, 1955)

6.5.5 vibronicAngularMomentumP

is the sum of the total vibrational angular momentum l_v and of the total electronic orbital momentum about the internuclear axis $\Omega : P = \left| \pm l_v \pm \Omega \right|$

here P (l_v and Ω) are unsigned quantities. This is used for linear polyatomic molecules. (see p.26 Volume III pf Herzberg, and REC. 18 of Muliken, 1955)

6.5.6 rovibronicAngularMomentumP

total resultant axial angular momentum quantum number including electron spin: $P = \left| K + \Sigma \right|$. (REC. 26 of Mulliken, 1955)

6.5.7 hinderedK1, hinderedK2

for internal free rotation of 2 parts of a molecule, (see p.492, Volume II of Herzberg), 2 additional projection quantum numbers are necessary: k_1 and k_2, such that total rotational energy is given by:

$$F(N,K,k_1,k_2) = BN(N+1)BK^2 + A_1 k_1^2 + A_2 k_2^2$$

Where N is **totalAngularMomentumN** and K is **totalMolecularProjectionN** (see p.492, Volume II of Herzberg (1964))

7 APPENDIX C:Description of couplings for atomic Physics

7.1 LS coupling

Usually the strongest interactions among the electrons of an atom are their mutual Coulomb repulsions. These repulsions affect only the orbital angular momenta, and not the spins. It is thus most appropriate to first couple together all the orbital angular momenta to give eigenfunctions
of L^2 and L_z, with L the total orbital angular momentum of the atom. Similarly all spins are coupled together to give the eigenfunctions of S^2 and S_z, with S the total spin angular momentum; then L and S are coupled together to give eigenfunctions of J^2 and J_z, where $J=L+S.$

When the coupling conditions within an atom correspond closely to pure LS-coupling conditions, then the quantum states of an atom can be accurately described in terms of LS-coupling quantum numbers:

Giving values of L and S specifies a term, or more precisely a ``LS term", because on may also refer to ``terms" of a different sort when discussing other coupling schemes (In order to completely specify a term it is necessary to give not only values of L and S, but also values of all lower-order quantum numbers, such as $n_i l_i$.

- Giving values of L, S, J specifies a level
- Giving values of L, S, J, M_J specifies a state
- The value of (2S+1) is called the multiplicity of the term

For LS-coupled functions, the notation introduced by Russel and Saunders is universally used : $^{2S+1}L_J$, where numerical values are to be substituted for (2S+1) and J, and the appropriate letter symbol is used for L (S, P, ..); except when discussing the Stark or Zeeman effect, there is usually no need to specify the value of M_J .

7.2 jj coupling

With increasing Z, the spin-orbit interactions become increasingly more important; in the limit in which these interactions become much stronger than the Coulom terms, the coupling conditions approach pure jj coupling.

In the jj-coupling scheme, basis functions are formed by first coupling the spin of each electron to its own orbital angular momentum, and then coupling together the various resultants j_i in some arbitrary order to obtain the total angular momentum J.

For two-electron configurations, the coupling scheme may be described by the condensed notation $[(l_1 s_1)j_1 , (l_2, s_2)j_2]JM_J$ with the usual jj-notation for energy levels $(j_1, j_2)_J$ [analogous to the Russel Saunders notation $^{2S+1}L_J$].

7.3 jK coupling

For configurations containing only two electron outside of closed shells, the common limiting type of pair coupling (energy levels tend to appear in pairs), jK coupling, occurs when the strongest interaction is the spin-orbit interaction of the more tightly bound electron, and the next strongest interaction is the spin-independent (direct) portion of the Coulomb interaction between the 2 electrons. The corresponding angular-momemtum coupling scheme is $l_1 + s_1 = j_1$, $j_1 + l_2 = K$, $K + s_2 = J$, or notation $\{[(l_1 s_1)j_1 , l_2]K,s_2\}JM$ with the standard energy level notation $j_1[K]_J$.

7.4 LK coupling

The other limiting form of pair coupling is called LK (or Ls) coupling. In two-electron configurations, it corresponds to the case in which the direct Coulomb interaction is greater then the spin-orbit interaction of either electron, and the spin-orbit interaction of the inner electron is next most important. The coupling scheme is $l_1 + l_2 = L$, $L + s_1 = K$, $K + s_2 = J$, or notation $\{[(l_1 l_2)L, s_1]K,s_2\}JM$ with the standard energy level notation $L[K]_J$.

7.5 Intermediate coupling

Frequently the coupling conditions do not lie particularly close even to one of these four cases; such situation is referred to as intermediate coupling. The energy levels can only be labelled in terms of the least objectionable of the four pure-coupling schemes (with the understanding that these labels may give a poor description of the true angular-momentum properties of the corresponding quantum states). In many cases, however, the coupling conditions are so hopelessly far from any pure-coupling scheme that it is meaningless to do anything more than label the energy levels and quantum states by means of serial numbers or some similar arbitrary device, or to list the values of the largest few eigenvector components (or the squares thereof) in the expansion of the total wavefunction.

   "The wavefunctions of levels are often expressed as eigenvectors that are linear combinations of basis states in one of the standard coupling schemes. Thus, the wave function $\Psi(\alpha J)$ for a level labeled αJ might be expressed in terms of normalized LS coupling basis states $\Phi(\gamma SLJ)$: $\Psi(\alpha J)=\sum_{\gamma SL} c(\gamma SLJ)\Phi(SLJ)$ The $c(\gamma SLJ)$ are expansion coefficients , and $\sum_{\gamma SL} |c(SLJ|^2 = 1$ (Martin & Wiese)

The expansion coefficients are called "mixingCoefficient" in this document.

The squared expansion coefficients for the various γSL terms in the composition of the αJ level are conveniently expressed as percentages, whose sum is 100%. The notation for RS basis states has been used only for concreteness; the eigenvectors may be expressed in any coupling scheme, and the coupling schemes may be different for different configurations included in a single calculation (with configuration interaction). « Intermediate coupling » conditions for a configuration are such that calculations in both LS and jj coupling yield some eigenvectors representing significant mixtures of basis states.
The largest percentage in the composition of a level is called the *purity* of the level in that coupling scheme. The coupling scheme (or combination of coupling schemes if more than one configuration is involved) that results in the largest average purity for all the levels in a calculation is usually best for naming the levels. With regard to any particular calculation, one does well to remember that, as with other calculated quantities, the resulting eigenvectors depend on a specific theoretical model and are subject to the inaccuracies of whatever approximations the model involves.
Theoretical calculations of experimental energy level structures have yielded many eigenvectors having significantly less than 50% purity in any coupling scheme. Since many of the corresponding levels have nevertheless been assigned names by spectroscopists, some caution is advisable in the acceptance of level designations found in the literature. »