International
Virtual
Observatory
Alliance

Atomic and Molecular Lines Data Model

Version 0.5

Draft Document 30 January 2006

This version:
ThisVersion-30Jan2006
Latest version:
http://www.ivoa.net/Documents/latest/LDM_v0.5
Previous versions:

Editors: Pedro Osuna, Matteo Guainazzi

Authors:
Marie-Lise Dubernet
Pedro Osuna
Matteo Guainazzi
Jesus Salgado
Evelyne Roueff

Status of This Document

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Abstract

This document presents a proposal for a Data Model to describe Atomic and Molecular Lines within the VO context in distributed repositories around the world.

The main objective of the model is to give access to the relevant information that will allow the identification and search of lines within VO environments.

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 acknowledgements section).

Acknowledgements

The authors wish to acknowledge all the people and institutes, atomic and molecular database experts and physicists who have collaborated through different discussions to the building up of the concepts described in this document.

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 this 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 **states** (it goes without saying that this concept has not to be intended as restricted to bound-bound transitions, but encompasses as well free-bound transitions, although it does not include free-free transitions, currently).

Each transition is defined through the pair of "**Levels**" between which it occurs. In turn the "Levels" are characterized by the attributes of the "**Species**" to which they belong, and 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 processes which modify the intrinsic properties of a "Line" (monochromaticity, 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 server 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 Line Data Model does not explicitly address non-electromagnetic transitions.

2 Data Model

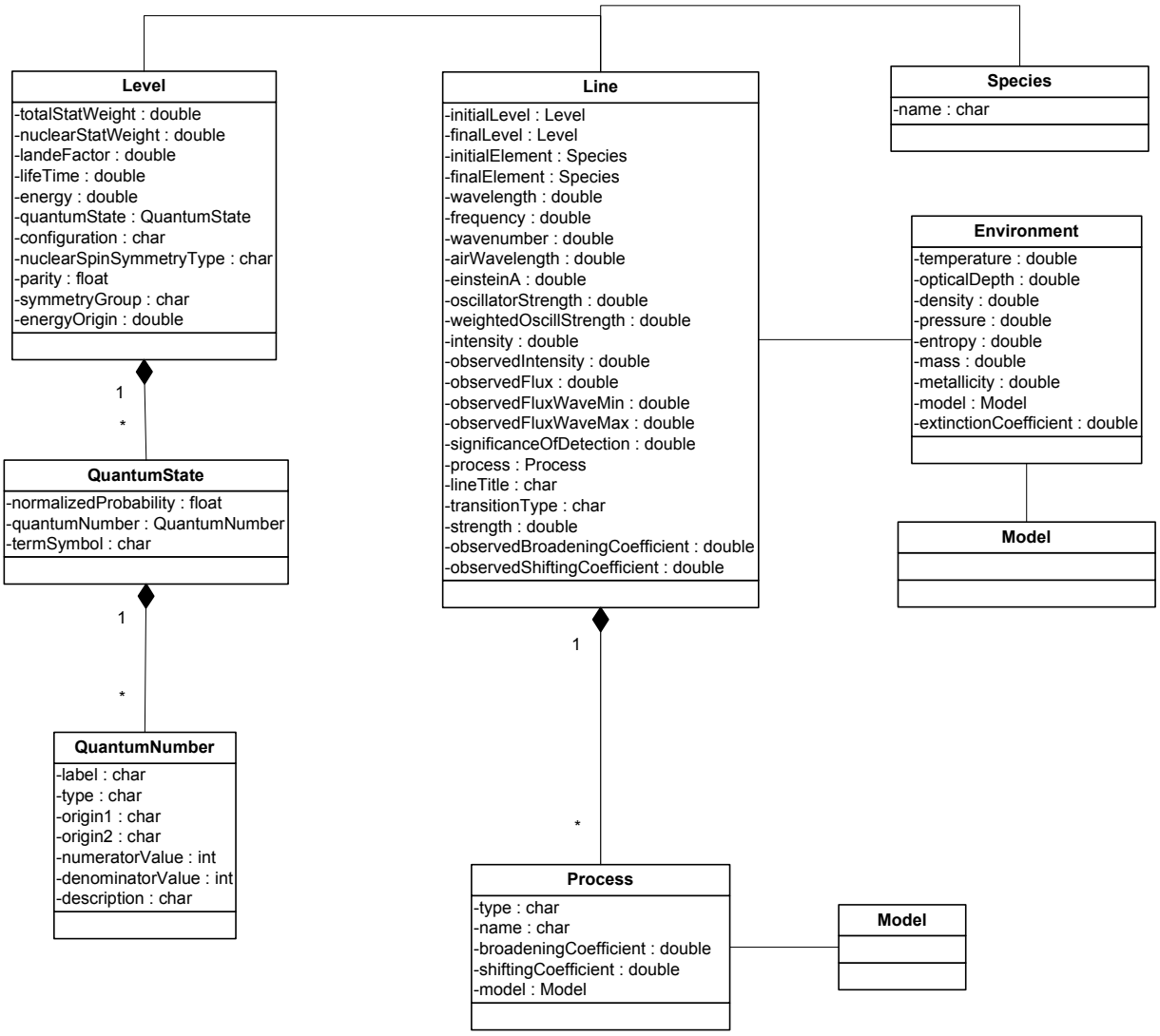
We have attempted to create a Data Model for Lines that would be useful to retrieve information from databases both of observed astronomical lines and atomic or molecular lines. There exist lots of line databases around the world, exposing different parameters. We have tried to cover the most relevant of those.

We give in what follows a standard UML diagram describing a Line. It is followed by an XML Schema description.

Note on physical quantities: *all physical quantities represented by a number and associated accuracy in this document should contain a pointer to the relevant IVOA Quantity model as soon as it is available.*

Only the basic properties of the Quantity will be required: its value and its units. Including errors in the measurements should be an asset. As the Quantity data model and corresponding unit is not yet available, we delay its inclusion in this document, which shall be updated to include those as soon as possible.
Therefore, no quantities, units and errors are treated systematically in this document.
At this time, and while waiting to consolidate this point, data providers are encouraged to use S.I. units throughout the present model.

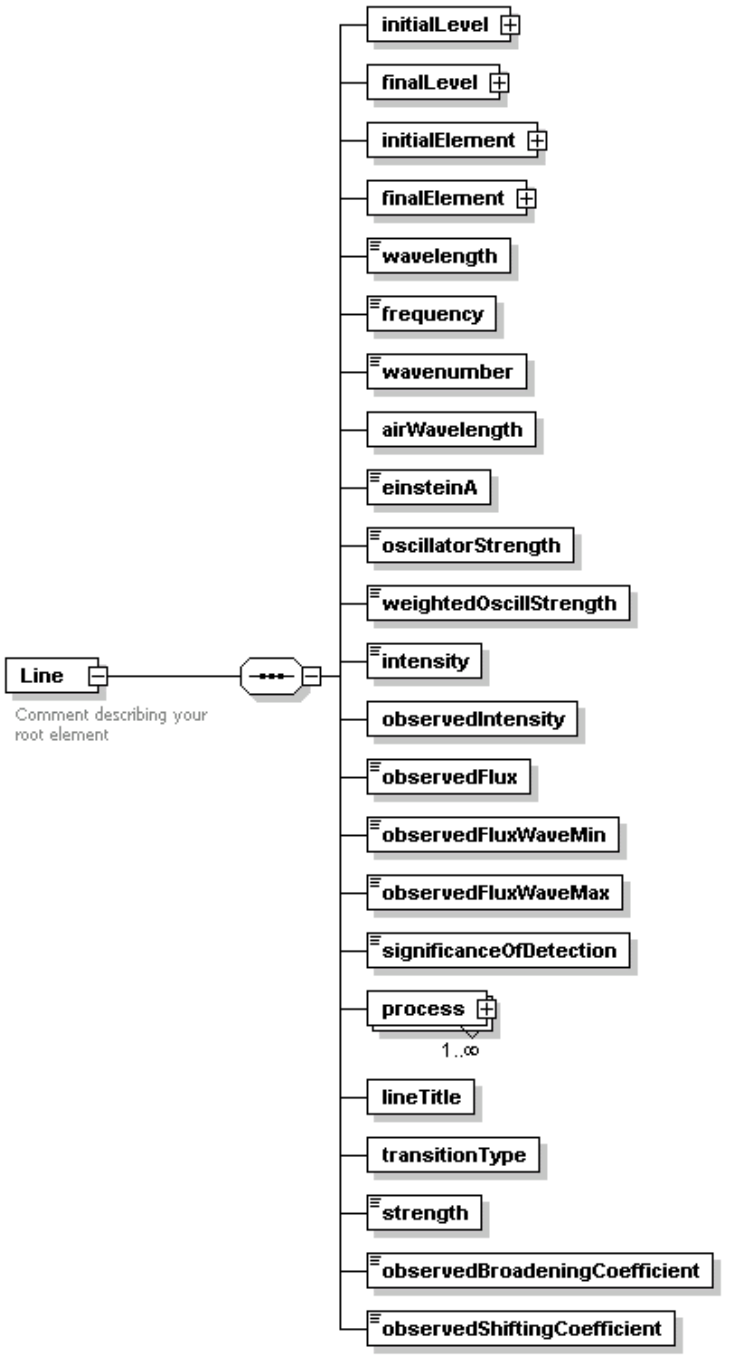
2.1 UML Data Model



2.2 Objects Description

2.2.1 Line

This class includes observables 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.



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2.2.1.1 Line.initialLevel

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

2.2.1.2 Line.finalLevel

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

2.2.1.3 Line.initialElement

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

2.2.1.4 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".

2.2.1.5 Line.wavelength

Wavelength in the vacuum of the transition originating the line.

2.2.1.6 Line.frequency

Frequency in the vacuum of the transition originating the line.

2.2.1.7 Line.wavenumber

Wavenumber in the vacuum of the transition originating the line.

2.2.1.8 Line.airWavelength

Wavelength in the air of the transition originating the line.

2.2.1.9 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".

2.2.1.10 Line.oscillatorStrength

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

$$A_{if} = [(8\pi^2 e^2 \nu^2)/(4\pi\varepsilon_0 m_e c^3)] (g_f/g_i) f_{fi} = [4\pi h \alpha \nu^2/ c^2 m_e](g_f/g_i) f_{fi}$$

where A_{if} is the Einstein A-coefficient for spontaneous emission between "initialLevel" and "finalLevel" - characterized by the energy difference $h\nu_{if}$, α ($= 2\pi e^2/hc\,4\pi\varepsilon_0$), 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. Units are MKSA with ε_0 expressed in $C^2.N^{-1}.m^{-2}$.

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.

2.2.1.11 Line.weightedOscillatorStrength

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

2.2.1.12 Line.intensity

The expected intensity of a line originating in the transition between "initialLevel" and "finalLevel" in an isolated undisturbed system (i.e., whenever no "Process" modifying the line profile and or intensity is taken into account). It can be expressed in absolute physical units or in relative units with respect to a reference line.

2.2.1.13 Line.observedIntensity

Peak intensity of an observed line. It can be expressed in absolute physical units or in relative units with respect to a reference line.

2.2.1.14 Line.observedFlux

Integrated intensity of the line profile over a given wavelength range

2.2.1.15 Line.observedFluxWaveMin

Minimum wavelength for observedFlux integration.

2.2.1.16 Line.observedFluxWaveMax

Maximum wavelength for observedFlux integration.

2.2.1.17 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).

2.2.1.18 Line.process

A string describing the process which produces the line in an astrophysical plasma, or modifying the intensity or the profile of a line. Lines for which "Process" does not apply are assumed to be strictly monochromatic, unblended and unresolved, i.e. mathematically described by a delta function.

2.2.1.19 Line.title

A small description title identifying the line.

2.2.1.20 Line.transitionType

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

$$\int \phi^*_f e^{i\vec{k}\vec{r}} l\nabla\phi_i d^3x$$

Possible values correspond to, e.g., "electric dipole", "magnetic dipole", "electric quadrupole" etc

2.2.1.21 Line.strength

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

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

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:

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

2.2.1.22 Line.observedBroadeningCoefficient

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

2.2.1.23 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).

2.2.2 Species

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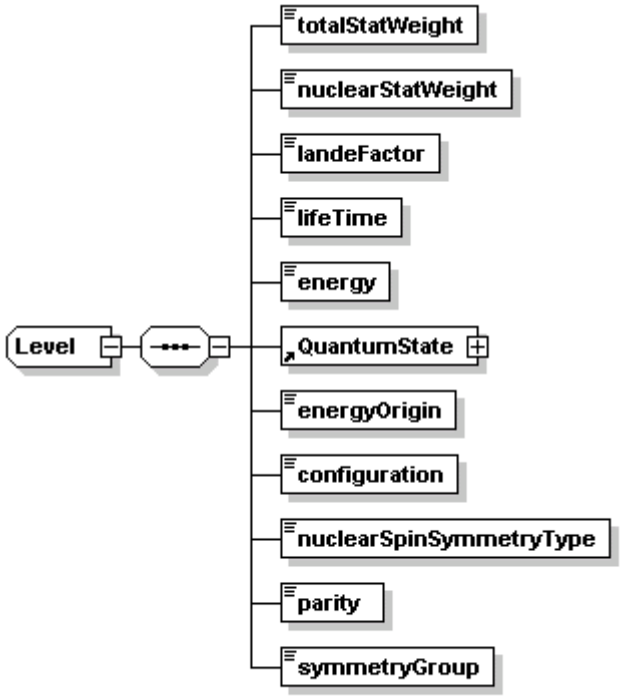
2.2.2.1 Species.name

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 I for standard chemical element names).

2.2.3 Level



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2.2.3.1 Level.totalStatWeight

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

2.2.3.2 Level.nuclearStatWeight

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

2.2.3.3 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:

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

where H is the magnetic field strength.

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 μ_j in the fine structure interaction:

$$\mu_j = g_j \mu_B J / \hbar$$

where μ_B is the Bohr magneton. In terms of pure quantum numbers:

$$g_j(J,L,S) \equiv 1 + [J(J+1) + S(S+1) + L(L+1)]/[2J(J+1)]$$

2.2.3.4 Level.lifeTime

Intrinsic lifetime of a level due to its radiative decay.

2.2.3.5 Level.energy

The binding energy of an electron belonging to the level.

2.2.3.6 Level.quantumState

Association to QuantumState. See below.

2.2.3.7 Level.nuclearSpinSymmetryType

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

2.2.3.8 Level.parity

Eigenvalue of the parity operator.

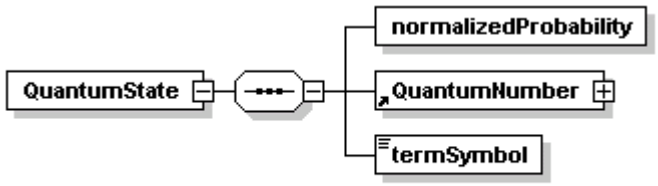
2.2.3.9 Level.configuration

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, 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 3*d*, ….. Closed shell configurations may be omitted from the enumeration.

2.2.3.10 Level.symmetryGroup

It is the Molecular Point Group. A description can be found in « Notations and Conventions in Molecular Spectroscopy: Part 2. Symmetry notation » (IUPAC Recommendations 1997), Pure & Appl. Chem., Vol. 69, no. 8, pp. 1641-1649, 1997.

2.2.4 QuantumState



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2.2.4.1 QuantumState.normalizedProbability

Element p_i of the "density matrix" $\rho \equiv \sum |\psi_i > p_i < \psi_i|$ which gives the

normalized probability to find the system in a given state.

2.2.4.2 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 section 2.2.5 below.

2.2.4.3 QuantumState.termSymbol

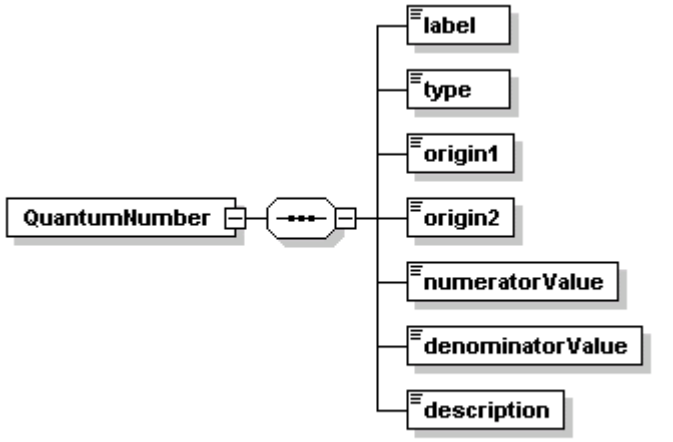
The term (symbol) to which this quantum state belongs, if applicable.

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 to write S, P, D, F, … for L=0,1,2,3,… and to write the numerical value for the multiplicity as a superscript at the left of the symbol for the L value. For instance, ^{5}P would describe a quintuplet term in which L=1 and S=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), Pure & Appl. Chem., Vol. 69, no. 8, pp. 1641-1649, 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.

2.2.5 QuantumNumber



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2.2.5.1 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

2.2.5.2 QuantumNumber.type

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

- **nPrincipal**
- **lElectronicOrbitalAngularMomentum**
- **sAngularMomentum**
- **jtotalAngularMomentum**
- **lMagneticQuantumNumber**
- **sMagneticQuantumNumber**
- **nuclearSpinI_I**
- **totalNuclearSpinI**
- **parity**
- **totalSpinMomentumS**
- **totalMagneticQuantumNumberS**
- **totalMolecularProjectionS**
- **totalElectronicOrbitalMomentumL**
- **totalMagneticQuantumNumberL**

- **totalMolecularProjectionL**
- **totalAngularMomentumJ**
- **totalMagneticQuantumNumberJ**
- **totalMolecularProjectionJ**
- **totalAngularMomentumF**
- **totalMagneticQuantumNumberF**
- **totalAngularMomentumJa**
- **rotationR**
- **molecularProjectionR**
- **asymmetricTau**
- **asymmetricKa**
- **asymmetricKc**
- **asymmetricKa**
- **vibrationNu_i**
- **vibrationLNu_i**
- **totalVibrationLNu**
- **vibronicAngularMomentumK**
- **vibronicAngularMomentumP**
- **vibrationSymmetry_i**
- **hinderedK1**
- **hinderedK2**

2.2.5.3 QuantumNumber.origin1

In the case of a QuantunNumber resulting from a coupling, the first originator of the coupling.

2.2.5.4 QuantumNumber.origin2

In the case of a QuantunNumber resulting from a coupling, the second originator of the coupling.

2.2.5.5 QuantumNumber.numeratorValue

The numerator of the quantum number value

2.2.5.6 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)

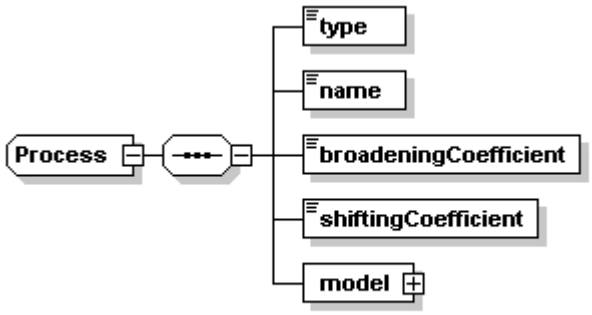
2.2.5.7 QuantumNumber.description

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

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

2.2.6 Process

The scope of this class is to spell out 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 models for each process.



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2.2.6.1 Process.type

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

2.2.6.2 Process.name

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

2.2.6.3 Process.broadeningCoefficient

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

2.2.6.4 Process.shiftingCoefficient

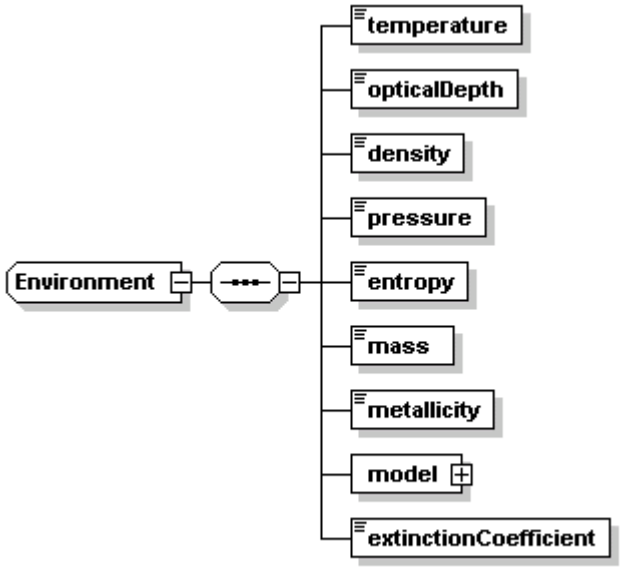
Shift of the transition laboratory wavelength(/frequency/wavenumber) of type=Energy shift". It is expressed by the difference between the peak intensity wavelength(/frequency/wavenumber) in the observed profile and the laboratory wavelength(/frequency/wavenumber).

2.2.6.5 Process.model

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

2.2.7 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.



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2.2.7.1 Environment.temperature

The temperature in the line-producing plasma.

2.2.7.2 Environment.opticalDepth

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

2.2.7.3 Environment.density

The particle or mass density in the line-producing plasma.

2.2.7.4 Environment.pressure

The pressure in the line-producing plasma.

2.2.7.5 Environment.entropy

The entropy of the line-producing plasma.

2.2.7.6 Environment.mass

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

2.2.7.7 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.

2.2.7.8 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.

2.2.7.9 Model

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

2.3 XML Schema serialization

We give in what follows an xsd representation of the UML model presented above to help in the building of XML serialisations of the model. This xsd shall be available at the IVOA Dat Model pages (see references).

Note: this paragraph shall be modified before version 1.0 to point to the relevant place where the xsd should stay permanently.

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          totalMolecularProjectionS
          totalElectronicOrbitalMomentumL
          totalMagneticQuantumNumberL
          totalMolecularProjectionL totalAngularMomentumJ
          totalMagneticQuantumNumberJ
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          asymmetricKc asymmetricKa vibrationNu_i
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            type="xs:double" />
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            />
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          <xs:element name="metallicity" type="xs:double" />
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            type="xs:double" />
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      </xs:complexType>
    </xs:schema>
```

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 1.02"*** (IVOA Proposed Recommendation, 2005-07-12).

Items appearing in red are not currently in the Proposed UCD Recommendation and will be proposed for inclusion to the UCD board.

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
observedIntensity	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
symmetryGroup	phys.atmol.symmetrygroup

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

QuantumNumber	
label	meta.title
type	meta.title
origin1, origin2	meta.at.qn
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_2H^+) 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_2H^+ hyperfine structure components

J F_1 F → J'F'$_1$F'	**(MHz)**	**(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 *v* is the transition frequency – as derived assuming the same Local Standard Rest velocity for all observed spectral lines – and its relative uncertainty.

Estimates of the N_2H^+ optical depth, excitation temperature and intrinsic line width were made by fitting the hyperfine splitting complex. They yielded:

- τ_{tot} = 7.9±0.3
- T_{ext} = 4 .9±0.1 K
- Δv = 183±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) → (1,2) and (1,0) → (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 Quantity.error indicates the statistical uncertainty on a measured quantity.
Elements not belonging to the model described in this document are highlighted in blue.

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.
In order to simplify, 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:= “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.origin1 := “J”`
- `Line.initialLevel.quantumState.origin2 := “I`$_1$`”`

- `Line.initialLevel.quantumState.quantumNumber. label:= “F“`
- `Line.initialLevel.quantumState.quantumNumber.type := “ totalAngularMomentumF “`
- `Line.initialLevel.quantumState.quantumNumber.description := “Resulting total angular momentum; coupling of I`$_2$` and F`$_1$`“`
- `Line.initialLevel.quantumState.quantumNumber.numeratorValue := 1`
- `Line.initialLevel.quantumState.quantumNumber.denominatorValue := 1`
- `Line.initialLevel.quantumState.origin1 := “F`$_1$`”`
- `Line.initialLevel.quantumState.origin2 := “I`$_2$`”`

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 spinsPure 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.origin1 := “J”
- Line.initialLevel.quantumState.origin2 := “I_1”

- 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.initialLevel.quantumState.origin1 := “J”
- Line.initialLevel.quantumState.origin2 := “I”

Line specific attributes:

- Line.wavelength:= $3.21755760 \times 10^{-6}$

Process specific attributes (two Process(es) present: EnergyShift and Broadening):

- Line.process.name:= “Local Standard Rest velocity“
- Line.process.type:= “Energy shift“
- Line.process.observedShiftingCoefficient:= 71074

- Line.process.type := „Broadening“
- Line.process.name := „Intrinsic line width“
- Line.observedBroadeningCoefficient := 183

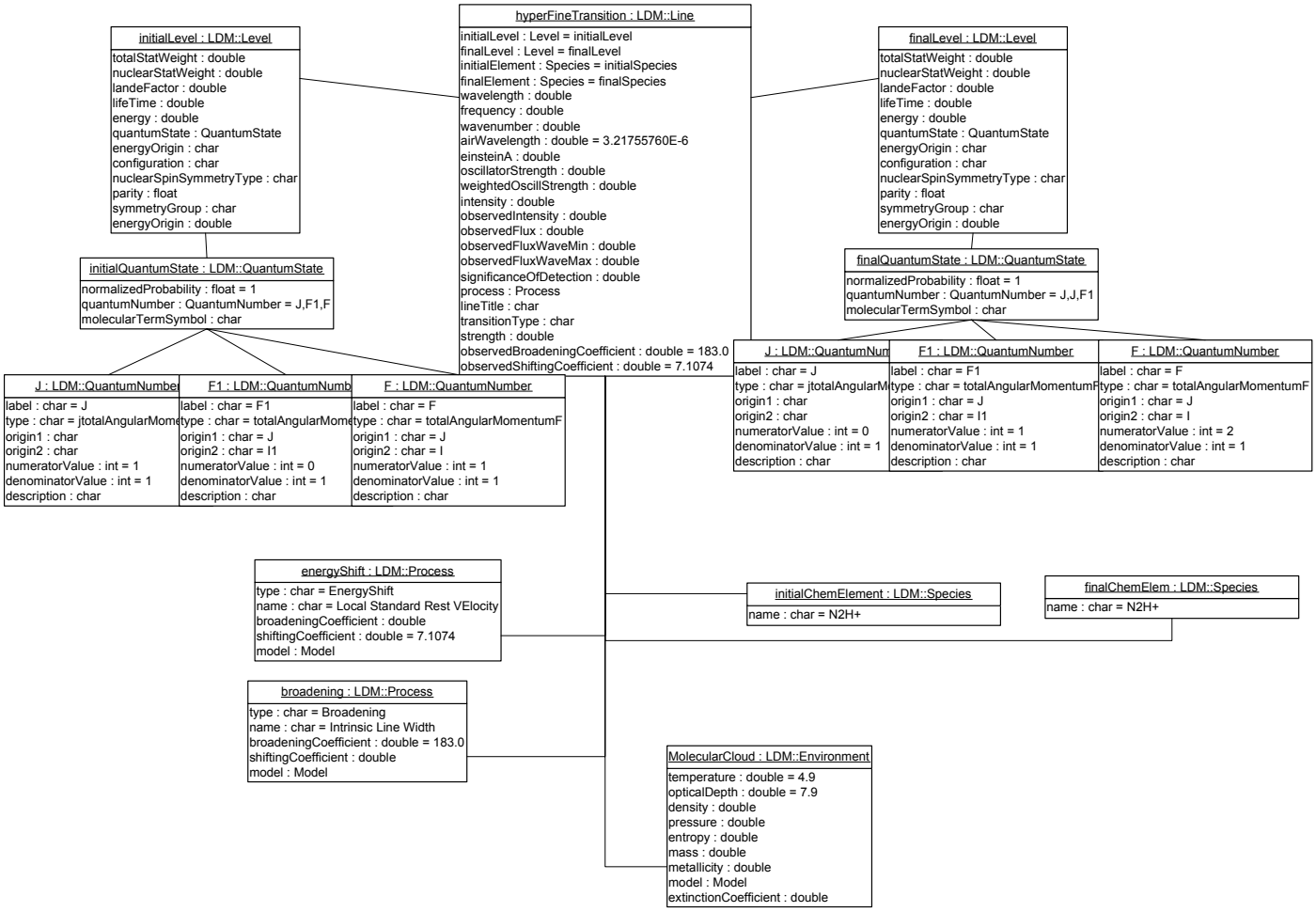
Environment specific attributes:

- `Line.Process.Model.ExcitationTemperature := 4.9`
- `Line.Process.Model.ExcitationTemperature.Error := 0.1`
- `Line.Process.Model.OpticalDepth := 7.9`
- `Line.Process.Model.OpticalDepthError := 0.3`

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

- `Line.species.name := “`N_2H^+`“`

4.1.2 UML instantiation diagram



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 ($kT \ll I$) – 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:= 3.1x10`$^{-9}$
- `Line.observedFlux := 4.3x10`$^{-4}$
- `Line.transitionType := „Radiative Recombination Continuum“`

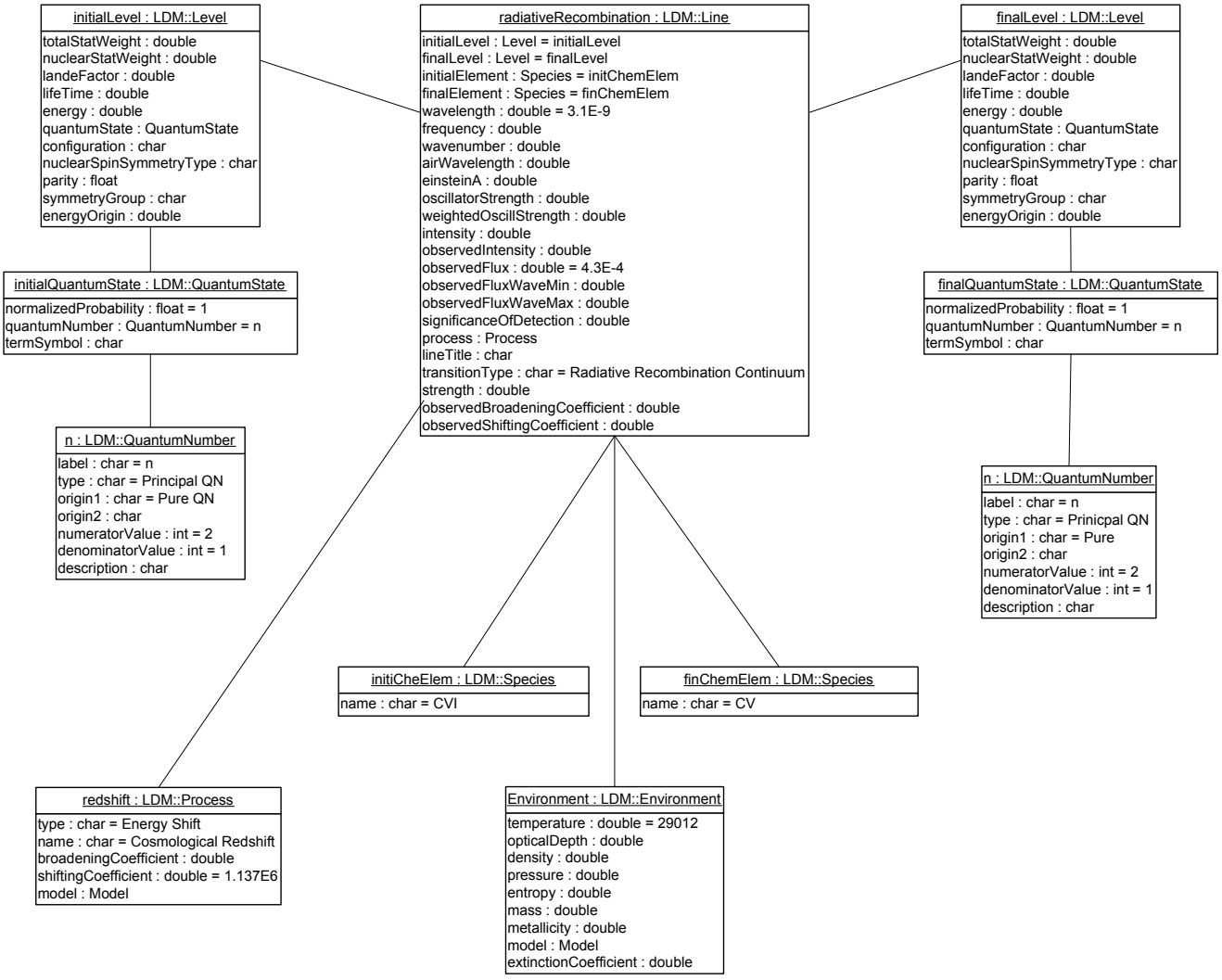
Process specific attributes

- `Line.Process.type := „Energy shift“`
- `Line.Process.name := „Cosmological redshift“`
- `Line.observedShiftingCoefficient := 1.137x10`^{6}

Environment:

- `Line.environment.Temperature := 1.9x10`^{5}

4.2.2 UML Instantiation diagram



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 $\boldsymbol{A}^2$, the component of $\boldsymbol{A}$ onto the internuclear axis $\boldsymbol{A}_z$, and the component of $\boldsymbol{A}$ on the laboratory quantization axis $\boldsymbol{A}_Z$. The basis function labels A, α and M_A correspond to eigenvalues of $\boldsymbol{A}^2$, $\boldsymbol{A}_z$, and $\boldsymbol{A}_Z$, 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 Quantum numbers for one electron systems

6.1.1 nPrincipal

principal quantum number n

6.1.2 lElectronicOrbitalAngularMomentum

orbital angular momentum of an electron $l = 0, 1, 2$ ....

$\hbar^2 l(l+1)$ is the eigenvalue of the $\boldsymbol{l}^2$ operator (called as well azimuthal quantum number).

6.1.3 sAngularMomentum

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

6.1.4 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 $\boldsymbol{j}^2$ operator, where $\mathbf{j} = \mathbf{l} + \mathbf{s}$.

6.1.5 lMagneticQuantumNumber

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

6.1.6 sMagneticQuantumNumber

spin magnetic quantum number, $m_s = +/- ½$ where $\hbar\, m_s$ is the eigenvalue of the $\boldsymbol{s}_z$ operator.

Other quantum numbers:

6.1.7 nuclearSpinI_i

nuclear spin of nucleus *i*

6.1.8 totalNuclearSpinI

nuclear spin of one nucleus.

6.1.9 parity

eigenvalue of the parity operator applied to the total wavefunction

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

6.2.1 totalSpinMomentumS

for n-electron system, it is the total spin quantum number S, S can be integral or half-integral. $S(S+1)\hbar^2$ is the eigenvalue of the $\boldsymbol{S}^2$ operator, where $\boldsymbol{S} = \sum_i^n \boldsymbol{s}_i$.

6.2.2 totalMagneticQuantumNumberS

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

6.2.3 totalMolecularProjectionS

projection of the total spin, Σ= -S, -S+1, ..., S-1, S, where $\hbar \Sigma$ is the eigenvalue of the $\boldsymbol{S}_z$ operator.

6.2.4 totalElectronicOrbitalMomentumL

for n-electron system, it is the total orbital angular momentum L, L is integral. $L(L+1)\hbar^2$ is the eigenvalue of the $\boldsymbol{L}^2$ operator, where $L = \sum_i^n \boldsymbol{l}_i$.

6.2.5 totalMagneticQuantumNumberL

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

6.2.6 totalMolecularProjectionL

absolute value of the projection of the total orbital momentum onto the intermolecular axis, Λ=0,...,L-1,L, where +/- $\hbar \Lambda$ is the eigenvalue of the $\boldsymbol{L}_z$ operator.

6.2.7 totalAngularMomentumJ

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

$$\boldsymbol{J} = \sum_i^n \boldsymbol{l}_i + \boldsymbol{s}_i$$

and for molecules:

$$\boldsymbol{J} = \sum_i^n \boldsymbol{s}_i + \boldsymbol{R} = \boldsymbol{S} + \boldsymbol{R}$$

6.2.8 totalMagneticQuantumNumberJ

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

6.2.9 totalMolecularProjectionJ

absolute value of the projection of the total angular momentum J onto the intermolecular axis, noted $\Omega = 0,..., J-1, J$, where $+/- \hbar \Omega$ is the eigenvalue of the $\boldsymbol{J_z}$ operator.

$$\Omega = \Sigma + \Lambda$$

6.2.10 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 $\boldsymbol{F^2}$ operator, where for atoms:

$$\boldsymbol{F} = \sum_i^n (\boldsymbol{l_i} + \boldsymbol{s_i}) + \boldsymbol{l} = \boldsymbol{J} + \boldsymbol{I}$$

and for molecules with m nuclear spins:

$$\boldsymbol{F} = \sum_i^n \boldsymbol{s_i} + \sum_i^m \boldsymbol{I_m} + + \boldsymbol{R} = \boldsymbol{S} + \boldsymbol{R} + \boldsymbol{I}$$

6.2.11 totalMagneticQuantumNumberF

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

6.2.12 totalAngularMomentumJa

is the total angular momentum J_a exclusive of nuclear and electronic spin, J_a is integral. $J_a(J_a+1)\hbar^2$ is the eigenvalue of the $\boldsymbol{J_a}^2$ operator, where $\boldsymbol{J_a} = \mathbf{L} + \mathbf{R}$. (case de Hund (c, d) for diatomic molecule).

6.3 Pure rotational quantum numbers

6.3.1 rotationR

rotational quantum number $R=0, 1, ...$ for the rotation of the nuclear framework. $R(R+1)\hbar^2$ is the eigenvalue of the $\boldsymbol{R}^2$ operator.

6.3.2 molecularProjectionR

for a symmetric top molecule it is the component of ***R*** along the molecular quantized axis, usually noted K. $\hbar K$ is the eigenvalue of the J_z operator, with values $K = -R, -R+1, ..., R-1, R$.

6.3.3 asymmetricTau

Index τ labelling asymmetric rotational energy levels for a given rotational quantum number R. Note: The solution of the Schrödinger equation for an asymmetric-top molecule gives for each value of R, (2R+1) eigenfunctions with its own energy. It is customary to keep track of them by adding the subscript τ to the R_τ value. This index τ goes from -R for the lowest energy of the set to +R for the highest energy, and is equal to $(k_a - k_c)$.

6.3.4 asymmetricKa

For a given R 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 and k_c for the limiting oblate. In the notation (k_{-1} k_1) the subscripts “1” and “-1” correspond to values of the asymmetry parameter $\kappa = (2B-A-C)(A-C)$, where A, B, C are rotational constants of the asymmetric molecule.

6.3.5 asymmetricKc

see **asymmetricKa**

6.4 Vibrational and vibronic quantum numbers

6.4.1 vibrationNu_i

vibrational quantum number v_i (following Mulliken conventions)

6.4.2 vibrationLNu_i

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

6.4.3 totalVibrationLNu

total vibrational angular momentum is the sum of all angular momenta +/- l_i associated to degeneratevibrations: $l_v = | \Sigma_i\_i +/- l_i |$

6.4.4 vibronicAngularMomentumK

is the sum of the total vibrational angular momentum l_{nu} and of the electronic orbital momentum about the internuclear axis Λ : $K = / +/- l_v \ +/- \Lambda /$; here K (l_v and Λ) are unsigned quantities

6.4.5 vibronicAngularMomentumP

is the sum of the total vibrational angular momentum l_{nu} and of the total electronic orbital momemtum about the internuclear axis Ω : $K = / +/- l_v \ +/- \Omega /$; here K (l_v and Ω) are unsigned quantities

6.4.6 vibrationSymmetry_i

symmetry of individual vibrational modes v_i

6.4.7 hinderedK1, hinderedK2

for internal free rotation of 2 parts of a molecule, 2 additional projection quantum numbers are necessary: k_1 and k_2, such that the total rotationnal energy is given by: $F(R,K,k_1,k_2) = BR(R+1) - BK^2 + A_1k_1^2 + A_2k_2^2$ where R is **rotationR** and K is **molecularProjectionR**

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 $\boldsymbol{L^2}$ and $\boldsymbol{L_Z}$, with $\boldsymbol{L}$ the total orbital angular momentum of the atom. Similarly all spins are coupled together to give the eigenfunctions of $\boldsymbol{S^2}$ and $\boldsymbol{S_Z}$, with $\boldsymbol{S}$ the total spin angular momentum; then $\boldsymbol{L}$ and $\boldsymbol{S}$ are coupled together to give eigenfunctions of $\boldsymbol{J^2}$ and $\boldsymbol{J_Z}$, where $\boldsymbol{J=L+S.}$

When the coupling conditions within an atom correspond closely to pure LS-coupling conditions, then the quantum states of an atom can be accuratly 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 $\boldsymbol{j_i}$ 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 $\mathbf{l_1 + s_1 = j_1}$, $\mathbf{j_1 + l_2 = K}$, $\mathbf{K + s_2 = J}$, 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 $\boldsymbol{l_1 + l_2 = L,\ \ L + s_1 = K,\ K + s_2 = J}$, 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 $\sum_{\gamma SL} |c(\gamma SLJ|^2 = 1$ (Martin & Wiese)

The expansion coefficients are called "normalizedProbability" 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 caclculations 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 combinaison 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 signigicantly less than 50% purity in any coupling scheme. Since many of the corresponding levels have nevertheless been assigned names by spectroscopists, some caution is adviable in the acceptance of level designations found in the literature. »