Atomic and Molecular Uniform Content Descriptors
Working Draft
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Table des matières

Chapitre 1

Introduction

UCD are meant to be used within the context of Virtual Observatories. The first UCD's generation was created at the CDS in order to label concepts in tables' columns.

The present Atomic and Molecular UCD are not well defined, they are not complete, they don't follow any logical classification. In this document we address all these points and we provide a starting working sheet.

We divide the field in 5 main topics :
– identification of elements with **phys.at.element** and **phys.mol.element**
– identification of levels with **phys.at.level** and **phys.mol.level**
– radiative transitions between bound states with **phys.at.trans** and **phys.mol.trans**
– photon-matter interaction **phys.at.photo**, **phys.mol.photo** and matter-matter interaction **phys.at.coll**, **phys.mol.coll**
– some specific UCDs for various quantities

We separated Atomic Physics from Molecular Physics. Nevertheless many UCDs have identical meaning in both fields. The first draft should list all possible UCDs in both fields. The second draft will concatenate the information. We propose to state *phys.mol* or *phys.at* in order to indicate atomic or molecular physics. Then **.at** or **.mol** can be removed from common UCDs.

Chapitre 2

UCD for Atomic Physics

2.1 identification of elements : *phys.at.element*

phys.at.element : atomic element
  – **phys.at.name** : name of the element [Actinium, Lead, ...]
  – **phys.at.number** : atomic number [Z]
  – **phys.at.symbol** : [He, H ...]
  – **phys.at.ion** : ionisation stage [CII]
  – **phys.at.isotopic** : [^{9}Be, ^{10}Be]
  – **phys.at.weight** : atomic weight (shall we make a difference between weight and mass ?)
  – **phys.at.qn.I** : nuclear spin quantum number (see below for explanation of *phys.at.qn*)

2.2 identification of levels : *phys.at.level*

phys.at.level
    : atomic level
  – **phys.at.term** : atomic term
  – **phys.at.configuration** : atomic configuration
  – **phys.at.parity** : parity
  – **phys.at.sweight** : statistical weight
  – **phys.at.lande** : lande factor
  – **phys.at.lifetime** : lifetime
  – **phys.at.qn** : atomic quantum numbers
    – **.S** : electronic spin
    – **.L** : electronic L
    – **.J** : resulting from coupling of S and L
    – **.F** : resulting from coupling of J and I

  .final and **.initial** should be be added right at the end of words such as *phys.at.level.term* or *phys.at.level.configuration*, in order to specify initial and final states of a transition. This is done when initial and final states are given into individual columns. When initial and final states are given in the same column, one should use *phys.at.trans* and its derived words.
  – **.final** : final state
  – **.initial** : initial state

2.3 radiative transitions between bound states : *phys.at.trans*

phys.at.trans : atomic transition
    Some identification words of levels can be re-used here, such as :
  – **phys.at.term** : atomic term (initial state → final state)

- **phys.at.configuration** : atomic configuration (initial state → final state)
- **phys.at.parity** : parity (initial state → final state)
- **phys.at.sweight** : statistical weight (initial state → final state)

Other words can be added for radiative processes between bound states :
- **phys.at.wavelength** : wavelength of atomic transition in the air
- **phys.at.wavenumber** : energy of the transition in wavenumber
- **phys.at.prob** : Einstein A coefficient
- **phys.at.osc-strength** : oscillator strength f (when qualifying *phys.at.trans*).
- **phys.at.w-osc-strength** : weighted oscillator strength gf

2.4 photon-matter interaction (with at least one continuum state) and collisions

phys.at.photo : photon-matter interaction with at least one continuum state
phys.at.coll : collision involving electrons, atoms, ions and molecules

Various processes can be associated with these interactions and various observables can be measured, observed or calculated. We will indicate next to the definition whether this can be applied to *phys.at.photo* by (P), *phys.at.coll*(C) or both (PC).

Observables :

- **.cross-section** : cross sections
- **.osc-strength** : oscillator strength
- **.rate-coeff** : rate coefficient
- **.coll-strength** : collisional strength
- **.line-broad-coeff** : line broadening coefficient
- **.line-shift-coeff** : line shifting coefficient
- **.branching-ratio** : branching ratio in processes

Processes :

- **phys.at(mol).ionization** : concerns ionization process (PC)
- **phys.at(mol).detachment** : concerns photo-detachment (P)
- **phys.at(mol).photon-scattering** (P)
  - **.raman**
  - **.thompson**
  - **.rayleigh**
  - **.two-photon**
- **phys.at(mol).depolarisation**
  - **.orientation**
  - **.alignment**
- **phys.at(mol).radiative-recombination**
- **phys.at.dielectronic-recombination**
- **phys.at(mol).radiative.charge-transfer**
- **phys.at(mol).charge-transfer**
- **phys.at(mol).stark**
- **phys.at.excitation**
  - **.electronic**
  - **.fine**
  - **.hyperfine**

Example

- **phys.at.ionization** : concerns ionization process (PC)
  - **.cross-section** : atomic ionization cross sections (PC)
  - **.osc-strength** : atomic ionization oscillator strength (PC)

2.5 misc

There is still some work to be done on properties of atoms (improve the description)

– *phys.at.moment* : moment
  – **.magnetic** : magnetic moment
  – **.electric** : electric moment
– *phys.at.polarisability* : polarisability
– *phys.at.ionization.energy* : ionization energy
– *phys.at.energy.incident* : incident energy of a particule in a process (photon, electron, heavy particule)
– *phys.at.perturbator* : identify the perturbator in a process

Chapitre 3

UCD for Molecular Physics

3.1 identification of elements : *phys.mol.element*

phys.mol.element
  : molecular element
  – **phys.mol.name** : name of the element [water, ...]
  – **phys.mol.symbol** : [H_2O, H_2 ...]
  – **phys.mol.ion** : ionisation stage [H_2O^+]
  – **phys.mol.isotopic** : [HDO, ...]
  – **phys.mol.diatomic** : diatomic molecule
  – **phys.mol.linear-polyatomic** : linear polyatomic
  – **phys.mol.symmetric** : symmetrical molecule
  – **phys.mol.spherical** : spherical molecule
  – **phys.mol.asymmetric** : asymmetric molecule
  The identification of the type of rotor is important for the identification of the quantum numbers.

3.2 identification of levels : *phys.mol.level*

phys.mol.level
  : molecular level
  – **phys.mol.state** : molecular electronic state (X, A, B, C, ..)
  – **phys.mol.configuration** : molecular electronic configuration
  – **phys.mol.parity** : parity
  – **phys.mol.sweight** : statistical weight
  – **phys.mol.lifetime** : lifetime
  – **phys.mol.qn** : molecular quantum numbers
    – **.N** : rotational (all molecules)
    – **.K** : projection of N (used for symmetrical molecules)
    – **.KC** : used for asymmetric molecules
    – **.KB** : used for asymmetric molecules
    – **.TAU** : used for asymmetric molecules
    – **.nu** : vibration (there are 3X-5 degrees of vibration for linear molecules and 3X-6 for non linear molecules, where X is the number of atoms)
    – **.l** : orbital momentum of vibration
    – **.S** : electronic spin
    – **.I** : nuclear spin
    – **.symmetry-type** : electronic orbital
    – **.J** : resulting from coupling of S and N
    – **.F** : resulting from coupling of J and I
  Molecules have electronic, rotational and vibrationnal degrees of freedom, that should be clearly indicated by :
  – **phys.mol.electronic** : concerns the electronic levels

    – **phys.mol.rotation** : concerns the rotational levels
    – **phys.mol.vibration** : concerns the vibrational levels

3.3 Photon-matter and collisional processes (see atomic section for common items)

– **phys.mol.dissociative-recombination**
– **phys.mol.chemical-reaction**
– **phys.mol.radiative-association**
– **phys.mol.excitation**
    – **.electronic**
    – **.rotation**
    – **.vibration**
    – **.ro-vibration**
    – **.ro-vibronic**

3.4 misc

– *phys.mol.dipole* : dipole moment
    – **.magnetic** : magnetic dipole moment
    – **.electric** : electric dipole moment
– *phys.mol.quadrupole* : quadrupole moment
    – **.magnetic** : magnetic quadrupole moment
    – **.electric** : electric quadrupole moment
– *phys.mol.polarisability* : polarisability
– *phys.mol.energy.incident* : incident energy of a particule in a process (photon, electron, heavy particule)
– *phys.mol.perturbator* : identify the perturbator in a process