Atomic and Molecular Databases for Astrophysics Needs, Usecases

Working Draft

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Chapter 1

Introduction

Numerical and bibliographical Databases in Atomic and Molecular Physics are essential for both the modelling of various astrophysical media and the interpretation of astrophysical spectra provided by ground or space-based telescopes. It is important to make atomic and molecular data widely available in interrelating databases with VO projects; this would allow:

- uniqueness of data used in astrophysical models
- automatic access to these data from web applications developed for spectrum analysis or modelling

Different steps have been identified in order to organise access to atomic and molecular data for astrophysical needs:

1. identify specific needs for specific applications
2. "validate" the relevant atomic and molecular data (precision, origin of the data: chain of errors)
3. get the data into a suitable scientific and technical format
4. semantic definition of the data

Point 1 was started with the organisation of a workshop (URL of limited use because it is in french, http://wwwusr.obspm.fr/ vo-phys/PAGE-VO/ATELIER/titre.html) where physicists and astrophysicists from various areas (solar physics, stars, planets, interstellar medium) met. The following conclusions could be drawn:

- data used in different models come from heterogeneous sources; they are either extracted from different databases (HITRAN, GEISA, VALD, CHIANTI, NIST, TOPbase, ...) or calculated by the user.
- data are not always reliable and the chain of errors is not known.

It is clear that a dedicated organisation of atomic and molecular data would be of the utmost interest.
The following chapters outline some talks given at the workshop (cited above). The texts have not been amended by the speakers.

Chapter 2

Stellar Physics

(B. Plez, plez@graal.univ-montp2.fr)

Wide range of needs for Stellar astrophysics

- Modelling of stellar interiors : Rosseland opacities on a wide range of physical conditions, monochromatic opacities (for e.g. radiative accelerations)
- Modelling of stellar atmospheres : monochromatic opacities, between about 100K and 10^5K, for atoms, molecules and grains
- Detailed modelling of spectra (abundances, etc..) : high spectral resolution, blending problems, hyperfine structure, isotopic shifts, etc
- Circumstellar medium : T $<$ 1000K, time dependent chemistry, photochemistry, grain-gas chemistry, etc...

Stellar interiors

- **Rosseland opacities** : Complete list of levels and transitions (including photoionisation) are needed, for a large number of atomic species (and all their ions) : *OP, OPAL, satisfactory*
- **Radiative accelerations** : same kind of data, but for an even larger number of elements (Li, etc..). Very accurate wavelengths are necessary (several elements have very close frequencies, .i.e. Li and Fe) : *OP is OK up to Ni - missing : Hg, rare earth (Eu, etc), Sc, Co, Sr, Y, Zr,* and they are observed in Hg-Mn, Am-Fm, stars.

Stellar Atmospheres: needs

- **Monochromatic Opacities** : Complete list of levels and transitions are needed, for a large number of atomic species and molecules (first few ions only). Temperature between a few 100K and 10^5K. Approximative wavelengths are OK. Important needs are more at the low temperature end (cool stars, brown dwarfs, giant planets)
- **LTE** : gf-values, excitation energies, wavelengths, collisional broadening parameters, etc..
- **non-LTE** : same data + collisional cross-sections
- **Important Molecules** (in bold those for which no satisfactory data exists, or not much work is being done : CH, CO, CN, **NH**, OH, TiO, $\mathbf{C_2}$, ZrO, VO, H_2O, HCN, $\mathbf{C_2H_2}$**,** $\mathbf{C_3}$, CH_4, ... electronic transitions, ro-vibrational transitions for very high v and J

Stellar Atmospheres : what is available

- Atomic lines :
  - VALD (www.astro.uu.se/ vald/). *not or very little update since 1999. Data quality included. Used for spectroscopic analysis.*
  - Kurucz (cfa-www.harvard.edu/amdata/ampdata/amdata.shtml) *large number of lines, uneven data quality*

- molecular lines:
  - HITRAN (cfa-www.harvard.edu.HITRAN). *incomplete, OK for low temperature (planets)*
  - Kurucz (cfa-www.harvard.edu/amdata/ampdata/amdata.shtml) : inequal content, but includes lists H_2O, TiO (Schwenke et al) of good quality
  - Scan (www.astro.ku.dk/ uffegj/) : Jørgensen, CH, CN, C_2, TiO and H_2O . *some problems with quality*
  - other lists for particular needs available from their authors

Chapter 3

Solar Physics

3.1 Atomic Physics (S. Sahal-Bréchot : sylvie.sahal-brechot@obspm.fr)

Type of studies

- Internal structure and radiative opacities
- Magnetism and dynamics of the solar atmosphere on various scales
- Solar instability : eruptions, coronal mass ejection
- Heating of the Solar corona and solar wind
- Spectroscopic and spectropolarimetric studies

Needs for what ?

- radiative opacities and radiative accelerations (ETL, high T about 10000K, high density (log g = 4)
- energy levels and oscillator strength for ions (single and multicharged ions, such as FeIX to Fe XVII) **Top-Base : http://vizier.u-strasbg.fr/OP.htx**
- Line broadening by collisions with atomic hydrogen **VALD http://ams.astro.univie.ac.at/cgi-bin/vald/**

Needs for photosphere

- measurement of Stokes parameters with THEMIS on the solar disk (MTR mode) - Interpretation in terms of mapping of the magnetic field as a function of altitude $\vec{B}(x, y, z)$
- atomic (in particular Fe) lines, molecular lines in solar spots
- Needs : energy levels, oscillator strength, Lande Factor

Needs for photosphere et chromosphere

- measurement of Stokes parameters with THEMIS on the solar limb (multi-line mode) - " The second solar spectrum" : linear polarisation spectrum - needs for second solar spectrum :
  - atoms and ions (low ionization) - T = 5000K-7000K - - n_e about 10^{12} cm^{-3} - n_H about 10^{14} cm^{-3}-
  - Formation of polarized line in non-ETL
    * Energy levels with hyperfine structure **NIST**
    * Radiative excitation (oscillator strength) **NIST**
    * Excitation by electronic impact (cross-sections)
    * Depolarization by collisions with H (on going work at LERMA, data available)

Solar Instability : solar flares (chromospheric level)

- polarisation by electronic collision (1 to 40 eV) and by proton collision (1 to 100 keV)

- : data in LERMA (H : excitation of n=2 and 3 (done) for H_α, H : excitation of n= 4 (current) for H_β, Na : excitation of 3p)

- depolarisation by collisions with isotropic proton and electron (H : n=2, 3, 4 to be included)

Linear Polarisation of coronal lines on the solar limb, solar wind

- measurements of magnetic fields, velocity fields (bimaxwellian distribution of velocity : high anisotropy)

- 1rst measurement of polarisation with SUMER (O VI line 103.2 nm)

- 1rst detection of polarisation with CDS, XUV lines : He I 584, HeII 304, O IV 555+610, Mg IX 368, Mg X 610+625, Si XI 303

Corona heating

- Space-time analysis of thermodynamical quantities

- Intensity ratio of EUV and XUV lines on solar limb

- Energy levels, oscillator strength, cross section by electronic collision

Databases, see Weizman Institute : http://plasma-gate.weizmann.ac.il/DBfAPP.html

- CHIANTI http://wwwsolar.nrl.navy.mil/chianti.html for SOHO

- GAPHYOR with GENIE : energy levels, transition probabilities, cross sections http://gaphyor.lpgp.u-psud.fr/ and http://gap3.lpgp.u-psud.fr/GENIE/

- NIST Physical Reference Data Databases, Gaithersburg, MD (http://physics.nist.gov/PhysRefData/contents.html); Atomic Spectral Line broadening Bibliographic Database (http://physics.nist.gov/PhysRefData/Linebr/html/reffrm0.html)

- NIST Atomic spectroscopy Database (http://physics.nist.gov/cgi-bin/AtData/main_asd)

- Atomic and Molecular Databases for Astronomy (Harvard) (http://cfa-www.harvard.edu/amdata/ampdata/otherdb.html)

- Bibliographic Database on Atomic Transition Probabilities (http://physics.nist.gov/PhysRefData/Fvalbib/html/reffrm0.html)

- Electron-Impact Ionization Cross Section Database (http://physics.nist.gov/PhysRefData/Ionization/Xsection.html)

- VALD (http://www.astro.univie.ac.at/ vald/)

Chapter 4

Interstellar Medium

Interpretation of ISM spectra requires :

- step1: line frequencies of transitions in molecules (rotation, fine, hyperfine, vibration, ro-vibration) and for fine structure of some atoms, associated with identification of upper and lower levels (quantum numbers, energy levels, statistical weight, Einstein coefficients).
- step2 : for the same transitions, the collisional (de)-excitation rate coefficients are required (usually with H_2) for a range of temperature –¿ this is required to interpret spectra of non-LTE media
- step3 : prediction of synthetic spectra might require some initial guess on the abundances of molecules : these guesses might come from proper modelisation of the media including some chemistry (photo-processes and various reactive processes, etc...)