

Access to Atomic and Molecular Data/Databases in the VO

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Abstract. 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. We report here on our current project concerning the access to Atomic and Molecular Physics Databases within the Virtual Observatories, addressing the organisation/access of data for specific astrophysical applications and the use of standards for interoperability. As an example we present the current status of a numerical and bibliographical database concerning collisional ro-vibrational excitation rate coefficients of molecules (<http://basecol.obs-besancon.fr>)

1. Presentation

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 (<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 can 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.
- The 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. We set up a discussion forum on the subject at (<https://maillist.obs-besancon.fr/wws/info/vo-physique>).

A follow up of the project can be found on

(<http://wwwusr.obspm.fr/~vo-phys/PAGE-VO/main.html>).

2. A case study: the scientific preparation of HIFI (HSO) and ALMA

In view of the scientific preparation of the HIFI instrument of the Herschel Space Observatory (HSO) (<http://www.sron.nl/divisions/lea/hifi/>) and of ALMA (<http://www.alma.nrao.edu/>), particular needs have been pointed out for:

- data on collisional ro-vibrational excitation of molecules
- data on millimeter and submillimeter spectral data.

These questions are addressed respectively by the

Basemol (<http://www.lra.ens.fr/~pcmi/herschel-alma.html>) and (*Astro-spec*) working groups.

2.1. The BASECOL database and related projects

In this framework, different groups have been set up to carry out calculations on collisional ro-vibrational excitation of molecules and to build a related bibliographic and numerical database.

This database, called **BASECOL** (<http://basecol.obs-besancon.fr>) is devoted to collisional ro-vibrational excitation of molecules by colliders such as atom, ion, molecule or electron. We have constituted a national working group of molecular physicists involved in the calculations of ro-vibrational cross-sections, in order to ensure the continuity and the quality of the database. We are currently enlarging the collaboration to the international molecular physicists community.

2.2. Current Status and future plans

We are primarily focusing on collisional systems of interest for various astrophysical media. The database is composed of several parts:

- a bibliographic database (papers are read and associated to very precise keywords),
- calculated collisional rates or cross-sections,
- information on the molecular data used in the cross section calculations, various informations on ro-vibrational excitation of molecules.

For systems of astrophysical interest, we will:

- provide full information on the chain of errors of the data and give some recommendations

- continue to update the content of the bibliographic database, as well as introducing new choices such as references on excitation of molecules colliding on a surface
- put on line all the calculated rate coefficients found in the literature and provide fits of these rate coefficients.

Access is currently available via a classical WEB interface with an interactive query page for the bibliographic database. An interactive access to the collisional rates and cross-sections is underway.

We are also addressing the issue of compatibility of the output of the database within the framework of the Virtual Observatories, in relation both with WEB tools for spectral analysis and with other databases such as the UMIST Database for Astrophysics (<http://www.rate99.co.uk/>) and the Cologne Database for Molecular Spectroscopy (<http://www.ph1.uni-koeln.de/vorhersagen/>).

We have created a discussion forum at (<https://maillist.obs-besancon.fr/wws/info/web-collision>).

The BASECOL database will be used both in the modelling of astrophysical objects (such as the model of Photo-Dissociation Regions (PDR) currently available at (<http://aristote.obspm.fr/MIS/>)) and in the interpretation of observed spectra (CASSIS) for HSO: analysis of observations for the search of new species and the determination of physical conditions.

2.3. Use of standards for interoperability

Definition of data: UCDs

We are currently addressing the semantic definition of the Atomic and Molecular Data, in collaboration with CDS, that is, by defining UCDs (<http://cdsweb.u-strasbg.fr/doc/UCD.htx>) related to atomic and molecular data. Both the BASECOL database (<http://basecol.obs-besancon.fr>) and the MOLAT database (<http://molat.obspm.fr>) of the Paris Observatory are going to be used to test the UCDs.

The work in progress is the following:

- go through the existing UCDs and simplify the structure (remove useless UCDs)
- Work out new UCDs, in particular for molecular physics
- As an example: atomic and molecular processes could appear in different levels: “AT” and “MOL”, instead of one level “AT”, as it is at present.

Representing Physics data in VOTable

VOTable (<http://cdsweb.u-strasbg.fr/doc/VOTable/>) is an XML standard which was especially designed to transfer astronomical data in tabular form. In molecular physics, the data that are often data cubes (or even “hypercubes”): for instance the effective collisional rate coefficients as a function of initial and final quantum numbers and temperatures. To be able to represent these data in VOTable, we need some kind of “projection” mechanism to place data cube “slices” into VOTable’<TABLE>s. Two solutions can be considered:

- put slices contiguously in one <TABLE> using repeated <FIELD>s; this solution has been used for some molecular data available in the CDS VizieR

catalogue service [see table 4 of catalogue VI/51 about collisional excitation rate of H₂CO from (Green 1994)];

- put one slice in one <TABLE>; then all <TABLE>s must have the same <FIELD>s.

In both cases, we need a further analyser next to the VOTable parser in order to join data of the same type belonging to either different <FIELD>s or to a given <FIELD>s in successive <TABLE>s.

To gather people interested in these matters and share experiences and questions, a Birds of a Feather session has been organised (Dubernet 2004).

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References

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