BASECOL and VAMDC: A new way to access and manipulate molecular collisional data for interstellar applications

http://basecol.obspm.fr/

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Basecol Presentation

BASECOL is devoted to collisional ro-vibrational excitation of molecules by colliders such as atom, ion, molecule or electron.

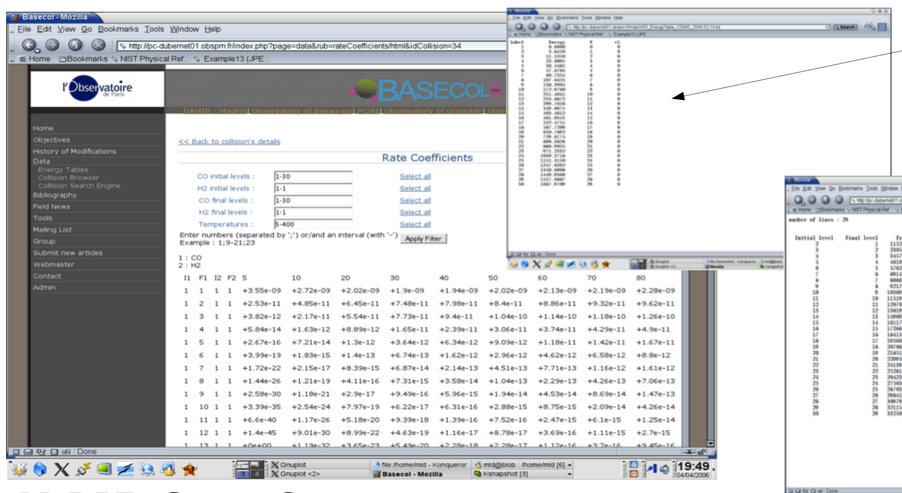
The database is composed of several parts:

- a status page with information about the needs for astrophysics, the current calculations and experiments being carried out, the possibility to contact the relevant groups.
- a bibliographic database (papers are read and associated to very precise keywords given back to the user in the query response)
- calculated collisional rates
- graphical visualization of collisional rates
- fitted and analytic functions of the collisional rates and the associated coefficients
- information on the methods used in the calculation of cross sections and rate coefficients (chain of errors)
- energy levels of the molecules (coming from spectroscopic databases or used in the theoretical calculations)

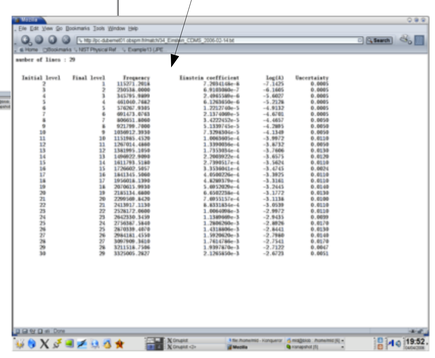
Use of BASECOL in non-LTE media

The usual difficulty met by astrophysical users is to combine collisional data from a database such as BASECOL with spectroscopic data coming from other native databases such as CDMS, JPL or any other databases.
Combination of data implies the possibility to match molecular states that are very often described differently in JPL, CDMS and BASECOL.

In order to overcome this problem BASECOL has imported spectroscopic data from JPL/CDMS, and for each molecule scientific work was done locally in order to transform CDMS/JPL molecular description into BASECOL internal description, and then a complete and coherent set of data including spectroscopic and collisional data were prepared for the users.
This required lengthy manipulation of data for each individual molecule, that will not be necessary any more within the VAMDC infrastructure.

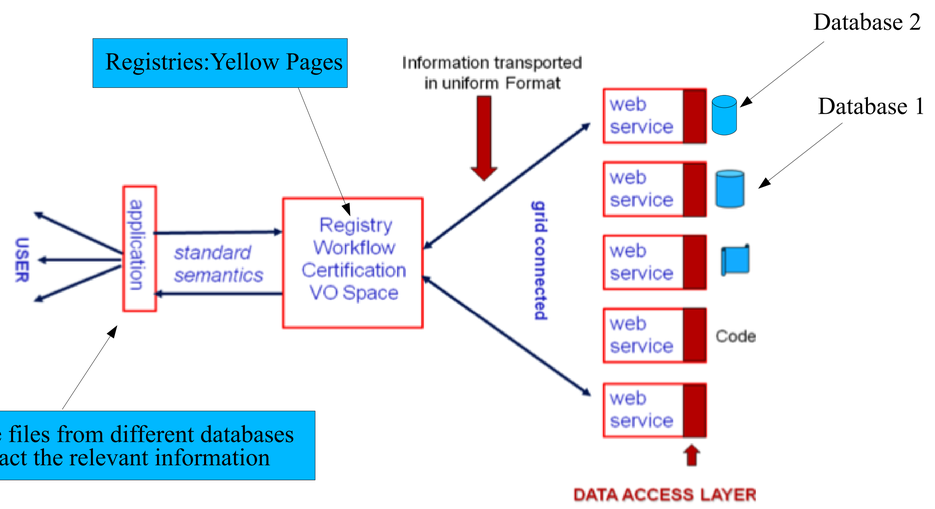


CMDS Spectroscopic Data
Locally processed by « hand »:
A script, validated by a scientist,
Transforms CDMS data
(for example Quantum Numbers)
into internal BASECOL format



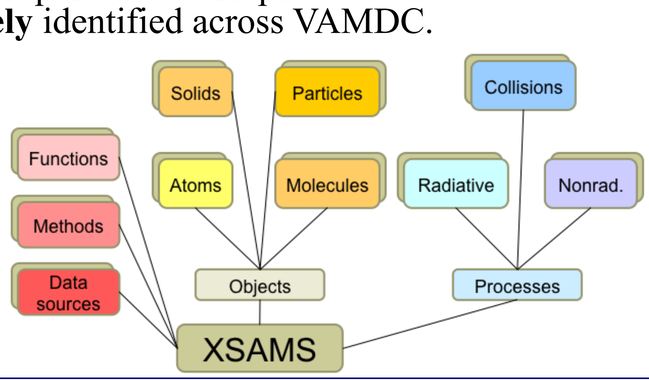
VAMDC Infrastructure

VAMDC infrastructure implies an output of databases into an unified format for description of data, the possibility of finding resources through registries using unified query language and finally integrating different sets of data from different databases.



VAMDC Outputs = XSAMS

The VAMDC's activities are based on the use of an XML schema XSAMS (XML Schema for Atomic & Molecular Spectroscopy) which has been developed under the auspices of the IAEA and aims to describe atomic, molecular and particle-surface interaction data in distributed databases around the world. XSAMS is currently being improved and extended within the VAMDC consortium. All Databases included in VAMDC provide an output in a XSAMS file where each data is **uniquely and uniformely** identified across VAMDC.

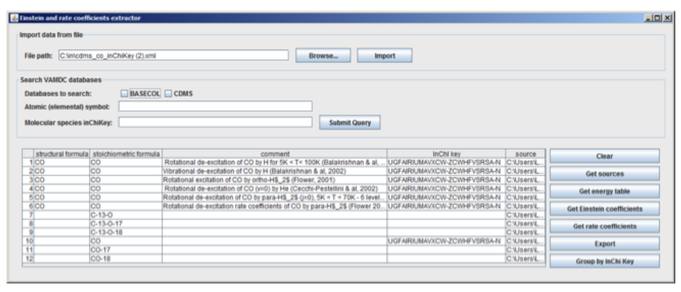


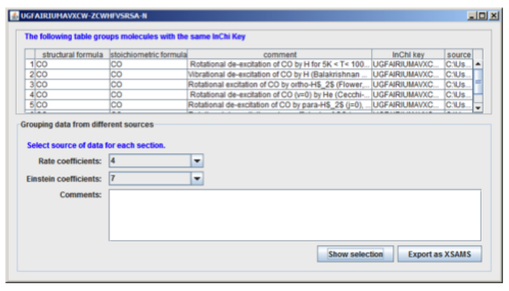
Client Tool to handle XSAMS files For spectroscopy and Collisions

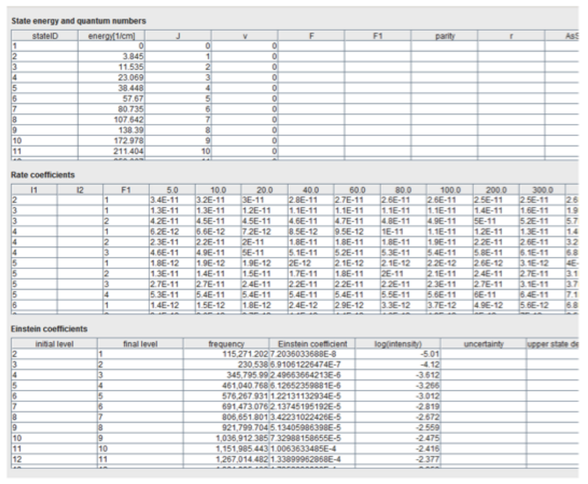
The aim of the client tool is to associate spectroscopic data provided by spectroscopic databases (CDMS, JPL, HITRAN, etc ..) with collisional data provided by collisional databases (BASECOL, ..) for a given molecule. This task is performed by the tool without knowledge of the physics underlying the XSAMS files. The tool knowns the XSAMS language and knows the rules of association of data.

Client Tool interrogates the registries to find spectroscopic and collisional information about a molecule. It retrieves different possible sets of data from different databases.

The user can associate sets of his own choice in order to create customized combination of spectroscopic and collisional data.







The client tool has combined set 7 of Spectroscopic data and set 5 of Collisional rate coefficients in order To create a single file.

This file can be output in the chosen format: XSAMS or ASCII.
The ASCII output can be Customized in a format compatible with input of astrophysical codes and then saved to local hard disk.

Advantage of such procedure:

** the user can choose the sets of data
** the user can use his own data and combine them with external databases

How to use your own data ?

VAMDC has created a set of **PUBLISHING TOOLS** that can be implemented on any database (Data Access Layer) or that takes your ASCII files and create a database compliant with XSAMS outputs and with VAMDC queries.

The **Client Tool** has the possibility to connect to your own Database entering your private URL, it has the possibility to upload a XSAMS file from your hard drive.

RELEASE OF STANDARDS AND SOFTWARE

All releases of standards and software will be made available on the VAMDC official website : http://www.vamdc.eu.

As VAMDC is in its R&D phase up to June 2012, releases will be made during that period WITHIN the VAMDC collaboration and FOR BETA TESTERS.

If you wish to become a BETA TESTER, please contact P.I. of VAMDC
marie-lise.dubernet@obspm.fr

After June 2012, releases will be fully public

Reference : Dubernet, M. L., et al, 2010, JQSRT, Volume 111, Issue 15, Pages 2151-2159

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