

Ro-Vibrational Collisional Excitation Database : BASECOL – <http://www.obspm.fr/basecol>

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Abstract

The BASECOL database is presented. The 2004 Version contains bibliographical and numerical data on collisional ro-vibrational excitation of molecules by H, He and H₂. It provides collisional rotational and ro-vibrational excitation rate coefficients for molecules of astrophysical interest, the molecular energy levels and a complete description of the chain of errors. It gives information on current calculations and is designed as a reference database to be used by both astrophysicists and physicists.

Keywords:

database, collision, molecules rotation vibration, excitation

1. Introduction

In view of the scientific preparation of the Heterodyne Instrument for the Far-Infrared on board the Herschel Space Observatory (HSO) [1] and of ALMA [2], particular needs have been pointed out for data on collisional ro-vibrational excitation of molecules by the abundant H, He and H₂ species present in interstellar environments.

These questions were addressed initially by the *Basemol* [3] group and a list of fundamental and urgent molecules was set.

This database, called **BASECOL** is devoted to collisional ro-vibrational excitation of molecules by colliders such as atom, ion, molecule or electron. An international working group of molecular physicists and astrophysicists involved in the calculations and use of ro-vibrational cross-sections is planned in order to ensure the continuity and the quality of the database.

2. Content

We are primarily focusing on collisional systems of interest for various interstellar cold molecular environment. 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 asso-

ciated 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)

The bibliographic database and the numerical database are linked together and are designed using a MySQL SGDB with a PHP interface. The Administration section is extremely flexible with the possibility of adding new capabilities.

Rate coefficients for the systems given in Table 1 are currently available via a restricted access. The data are fully documented and the quality of the data is assessed in detail. This is a major feature of this database.

All tables have output format in HTML or ASCII. The rate coefficients tables are linked to tables containing the correspondence between labelling of states and their

Table 1 List of molecules in 2004 version of BASECOL

$C_3H_2 + He$	$CH_3OH + He, H_2$	$CO + H, He, H_2$	$H_2O + He, H_2$
$CS + H_2$	$H_2 + H, He, H_2$	$HD + H, He, H_2$	$HCl + He$
$H_2CO + He$	$HDO + He$	$OCS, HCS^+ + He$	$SO, SiO + H_2$
$HCO^+ + H_2$	$SO_2 + He$	$HCN, HC_3N + He$	$SiC_2 + He$

quantum numbers and energy levels. They are also linked to tables containing the corresponding fitted coefficients as well as the fitted functions. A graphic interface allows to visualize calculated rate coefficients for any transition, to compare fitted and calculated rate coefficients and to compare different sets of calculations.

This database is intended to be useful to astrophysicists and is maintained by physicists. It also provides a link between astrophysicists and physicists interested in carrying on calculations or experiments. A mailing list is available and users are encouraged to register.

We are also addressing the issue of compatibility of the output of the database within the framework of the

Virtual Observatories [4], in relation both with WEB tools for spectral analysis and with other databases.

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References

- [1] <http://www.sron.nl/divisions/lea/hifi/>
- [2] <http://www.alma.nrao.edu/>
- [3] <http://www.lra.ens.fr/~pcmi/herschel-alma.html>
- [4] <http://www.ivoa.net>