

30 Years of Photodissociation Regions:

A symposium to honor David Hollenbach's lifetime in science
Asilomar, CA, USA - June 28th to July 3rd, 2015

INVITED TALK

Excitation coefficients for ions

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In order to retrieve actual molecular abundances from astrophysical observations of molecular spectral lines, knowledge of the rotational levels excitation schemes is essential. Actual excitation results of a trade-off between photon excitation and collisional excitation by the main constituents of the interstellar gas, electrons, molecular hydrogen, and, to a lesser extent, atomic hydrogen and helium. These rates are almost always obtained from theoretical investigations, by computing classical or quantum dynamics of the interaction of molecules with these colliders. However, recently, a series of experimental attempts are planned or are being tempted, to overcome this shortcoming.

Many types of molecules are observed and consequently, many collisions have been studied recently, like hydrides (Lanza et al. 2014), water and its isotopomers (Faure et al. 2012), organic molecules (Wiesenfeld and Faure 2013), atomic and molecular ions.

While for ISM cold or warm cloud, the main projectiles H_2 , the collisional effects in PDR are both due to electronic collisions (and molecular collisions (Wiesenfeld and Goldsmith 2014; Wiesenfeld and Masso 2014)). Computation of electronic collisional rates is performed mainly with the R-matrix theory (Tennyson 2010)

Scheme for computing inelastic rates goes into four steps:

1. Compute the interaction potential between the observed species and the projectile. The energy interaction is computed mainly by using *ab initio* quantum chemistry methods. The two molecules in interaction are taken as rigid. Usually a large number N of points are computed, each point being characterized by a set of intermolecular coordinates (one distance R , several angles Ω).
2. Fit the N points onto one single functional form $F(R, \Omega)$, suitable for the subsequent dynamics.
3. Perform the quantum dynamics for a series of collision energies E_k , resulting of inelastic cross sections $\sigma_{f \leftarrow i}(E_k)$.
4. Average the section $\sigma_{f \leftarrow i}(E_k)$ over the Maxwellian probability of kinetic energy at a given temperature T , to get the rate $k_{f \leftarrow i}(T)$

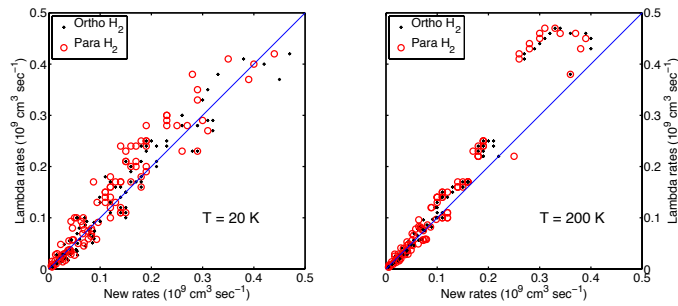


Figure 1: Comparison of deexcitation rates for HCO^+ in collision with H_2 . LAMBDA rates, Flower 1999. New rates, Wiesenfeld unpublished results.

This program has been applied with quite some success for several decades, and results are constantly updated with the improve of computer performance (see review papers like Roueff and Lique 2013; Dubernet et al. 2013).

The case of molecular ions bears special difficulties, because of both the long distance anisotropy of the interaction potential, and because of the large binding energy of the van der Waals complex between the molecular ion and H_2 . The same is true, but to a lesser extent for the interaction of atomic ions with molecular H_2 .

We shall present some very recent results concerning both the atomic species C[II] and the molecular species HCO^+ , both in collision with molecular hydrogen H_2 . It will be shown that remarkably, the actual excitation rates depend in a much weaker way on the details of the potential energy surface than their neutral counterparts. Collisional desexcitation rates are very large, because of the large, anisotropic charge-quadrupole and charge-induced dipole interactions, that decay slowly at large distances. An example of newly computed rates compared to the ones in the literature (LAMBDA database, <http://home.strw.leidenuniv.nl/moldata/>) appears in figure 1.

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