

Hemiquantal treatment of low energy p+H₂ collisions

L. F. Errea^{*1}, Clara Illescas*, A. Macías*, L. Méndez*, B. Pons^{†2}, I. Rabadán*

^{*} Departamento de Química C-13, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain

[†] CELIA, Université de Bordeaux I – CNRS – CEA, 351 Cours de la Libération, 33405 Talence, France

Synopsis We present calculations of charge exchange and vibrational excitation cross sections in low energy p+H₂ collisions. These cross sections are obtained by means of an hemiquantal treatment which uses Diatomic In Molecules (DIM) diabatic wavefunctions of the H₃⁺ molecule. The hemiquantal approach allows to distinguish the nonreactive, dissociative and nuclear exchange contributions to the electronic reaction paths.

Collisions between protons and hydrogen molecules are the natural benchmark for the improvement and implementation of new theoretical approaches in ion-molecule collisions. Particularly interesting is the E ~ 1-100 eV impact energy range where nuclear exchange reactions compete with nonreactive nonadiabatic electron processes.

In order to explicitly describe reactive reaction paths, we have implemented a hemiquantal treatment of p+H₂ collisions. The hemiquantal approach is semiclassical [1]: it merges classical mechanics to describe the motion of the nuclei and a quantum representation of the electron dynamics. Concretely, the electron dynamics is described by the time-dependent Schrödinger equation which is solved by using a three-state DIM expansion. Simultaneously, the motion of both projectile and target nuclei is monitored under the influence of the common potential energy surface (PES) that is self-consistently built during the collision. Details on the theoretical approach will be given at the conference.

As an example of our results, we display in Fig. 1 the total electron capture cross section obtained for 2 < E < 500 eV. The contributions of nonreactive (NR), dissociative (D) and nuclear exchange (NE) paths to electron capture are included in the figure. The hemiquantal total cross section is in good agreement with measurements [2] at low E and reproduces the shape of previous vibronic calculations [3] at higher E.

For E < 100 eV, the total electron capture cross section presents a double-humped shape with maxima located at E ~ 6 eV and E ~ 30 eV. The first maximum corresponds to energies where NE paths are of great importance, while the second one is due to NR paths. In both energy regions, electron capture from H₂(v=0) occurs through a two-step mechanism involving intermediate H⁺+H₂(v) states; NR paths implies

quasiresonant v=3,4 states and NE paths involve even more excited vibrational states [4].

Besides vibrationally resolved cross sections, we will picture at the conference the nuclear and electron dynamics involved in the electron capture and vibrational excitation processes.

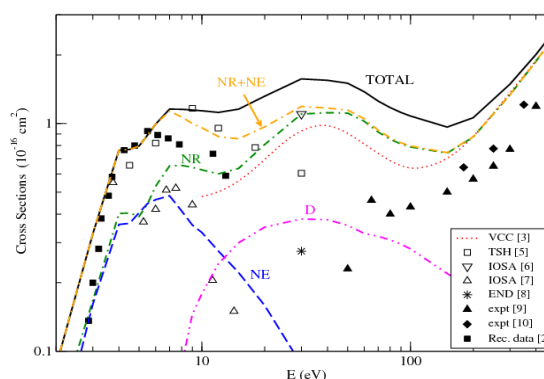


Figure 1. Single electron capture cross sections obtained by means of hemiquantal calculations for p+H₂ collisions. The contributions of nonreactive (NR), dissociative (D) and nuclear exchange (NE) processes to the total cross section are indicated. The results are compared to experimental data (filled symbols) and other calculations (open symbols) for total electron capture, as specified in the figure.

References

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¹ E-mail: lf.errea@uam.es

² E-mail: pons@celia.u-bordeaux1.fr