

Quantum dynamics study of rate constant for a reactive collision of astrophysical interest : the $D^+ + H_2$ reaction

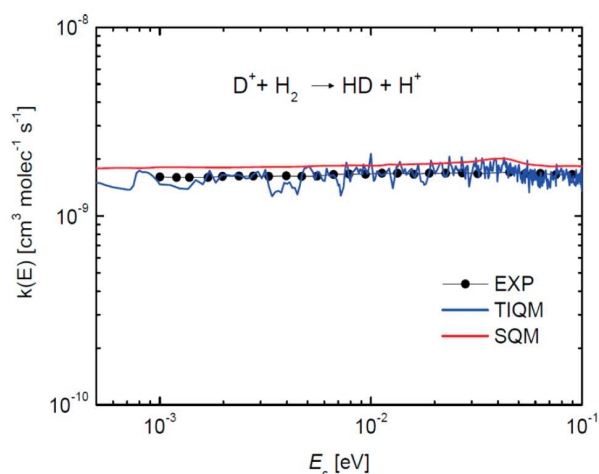
Y. Scribano¹, P. Honvault² et T. Gonzalez Lezana³

¹ Lab. Univers et Particules de Montpellier, UMR CNRS 5299, Univ. Montpellier II, 34095 Montpellier Cedex, France,

² Lab. Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS - Univ. Bourgogne, 21078 Dijon Cedex, France,

³ Instituto de Fisica Fundamental, CSIC, Serrano 123, 28006 Madrid, Spain.

For chemistry networks describing the reactions for the early universe [1] and especially for accurate models of the enrichment of deuterated molecules observed, we need to know in detail many state-to-state rate coefficients. For instance, Glover and Abel [2] modeled the chemistry of H_2 and HD primordial gas using a chemical network consisting of 115 reactions between 16 species. Today most of the rate coefficients of interesting reactions are still unknown or with a poor accuracy. For example, the uncertainty about the rate coefficient for the reaction directly affects model predictions for the HD abundance and thereby the cooling rate of the primordial gas. It is therefore of astrophysical importance to determine an accurate value of these rates, and helping to understand the cooling requires a complete set of the state-to-state rate coefficients as well as the total rate coefficient. In this talk, I will illustrate how first principles calculations can furnish us the way to determine accurately the rate constants for low temperature ($T < 100$ K). I will present the Time Independent Quantum Mechanical (TIQM) and Statistical Quantum Mechanical (SQM) results for the $D^+ + H_2$ reaction at low temperature using the accurate ab initio potential energy surface of Velilla *et al.* determined for H^+_3 [3]. The state to state cross sections at low collisional energies and rate coefficients at low temperature have been computed [4,5,6,7] and compared to the available experimental data [8].



Références :

- [1] Glover S.C. O., Savin. D. W., Mon. Not. R. Astron. Soc. 393, 911 (2009).
- [2] Glover S.C. O., Abel T, Mon. Not. R. Astron. Soc. 388, 1627 (2008).
- [3] Velilla L. et al., J. Chem. Phys., 129, 084307 (2008).
- [4] P. Honvault, Y. Scribano, J. Phys. Chem. A 117, 9778 (2013).
- [5] T. Gonzalez-Lezana, P. Honvault, Y. Scribano, J. Chem. Phys. 139, 054301 (2013).
- [6] P. Honvault, Y. Scribano, J. Phys. Chem. A 117, 13205 (2013).
- [7] T. Gonzalez-Lezana, Y. Scribano, P. Honvault, J. Phys. Chem. A in press (2014).
- [8] Gerlich D. and Schlemmer S., Planet. Space Sci. , 50, 1287 (2002).