A classical trajectory approach for three body recombination reactions

Miguel Lara-Moreno[1*], Thierry Stoecklin[1] and Philippe. Halvick[1]

[1] *ISM, UMR5255 du CNRS, Institut des Sciences Moleculaires, 351 cours de la Liberation, 33405, Talence Cedex – France ;*

* E-mail : miguel-del-jesus.lara-moreno@u-bordeaux.fr

ABSTRACT

A recent method for classical trajectory calculations of three-body collision [1,2] will be revised and applied to the study of three body recombination (TBR) reaction $Cl^- + p\text{-}H_2 + p\text{-}H_2 = p\text{-}H_2Cl^- + p\text{-}H_2$. In this method the dynamics of the three-body system is obtained by recasting the 6 degrees of freedom of the system as a two-body collision in a 6D-dimensional space, as shown in Figure 1. A redefinition of the 6D hyper-spherical coordinates was done in order to gain more physical insight on the initial conditions and the kinematics. The TBR reaction rates for the formation of the $p\text{-}H_2Cl^-$ complex are computed in the temperature range 10 - 30 K and compared to recent experimental measurement.

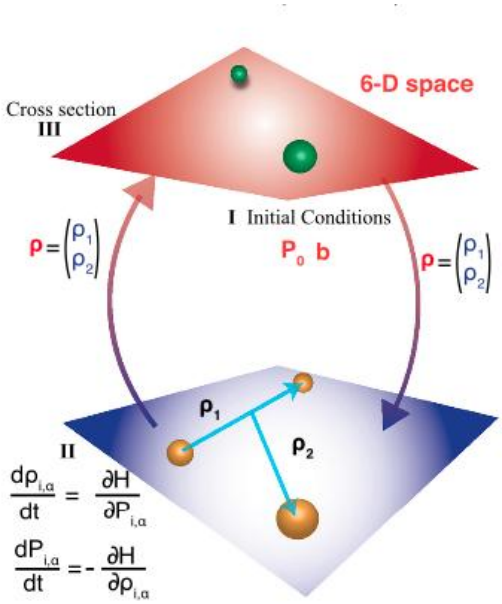

Figure 1 : Schematic representation of the method used for treating the three-body collision. [Taken from Ref. 2]

References

[1] J. Pérez-Ríos, Steve Ragole, Jia Wang, and Chris H. Greene, *J. Chem. Phys.* 140, 044307 (2014)

[2] Chris H. Greene, P. Giannakeas, and J. Pérez-Ríos, *Rev. Mod. Phys*, 89, (2017).