

# Dynamical studies and product analysis of the reaction between $O(^1D)$ and $H_2/D_2$

Carolina M. A. Rio<sup>a</sup> and J. Brandão<sup>a</sup>

<sup>a</sup> Departamento de Química e Bioquímica, Faculdade de Ciências e Tecnologia, Universidade do Algarve, Campus de Gambelas, 8005-139 Faro, Portugal

The reaction  $O(^1D) + H_2 \rightarrow OH + H$  and its isotopic variants plays an important role in atmospheric chemistry and also is important in combustion chemistry. It has been taken as a prototype for insertion reactions. As a result, it has been subject of several experimental studies. Also theoretical studies of its dynamics have been carried out.

In absence of energy barrier, the long-range interactions [1] between reactants should play an important role on the dynamics of the reaction of  $O(^1D)$  with  $H_2$  that mainly occurs in the ground state potential energy surface for  $H_2O$  [2]. Quasiclassical and capture studies [3] on a new potential energy surface that carefully reproduces these interactions are in close agreement with the most recent estimates for the thermal rate constant, when the effects of the excited surfaces is taken into account.

In this work we study the dynamics of the  $O(^1D) + H_2/D_2$  reactions at fixed collision energies [4,5] using quasiclassical trajectories calculations on a double-valued potential energy surface for  $H_2O$  [2].

In order to compare with experiment we have calculated trajectories at fixed translational energies of 0.5, 1.0, 1.9, 3.0, and 5.0 kcal mol<sup>-1</sup>, for the  $O(^1D) + H_2$  reaction, while for  $O(^1D) + D_2$  reaction we have fixed it at 0.5, 1.0, 2.4, 5.0, and 5.3 kcal mol<sup>-1</sup>. In particular, we analyse the reactive cross section, the opacity function, and the differential cross sections. In this work we also study the isotopic effect (ratio  $H/D$ ,  $\Gamma_{H/D}$ ) and the energy distribution of the products for the  $O(^1D) + H_2/D_2$  reactions. The agreement found between our QCT results [3,4,5] and experiment reinforces the accuracy of the  $H_2O$  potential energy surface used.

This work was supported by the FCT under the POCTI/CTA/41252/2001 research project, co-financed by the European community fund, FEDER..

## References

- [1] João Brandão and Carolina M. A. Rio, *Chem. Phys. Lett.* (2003), 372(4), 866-872.
- [2] João Brandão and Carolina M. A. Rio, *J. Chem. Phys.* (2003), 119 (6), 3148-3159.
- [3] João Brandão and Carolina M. A. Rio, *Chem. Phys. Lett.* (2003), 377, 523-529.
- [4] Carolina M. A. Rio and João Brandão, "Isotopic effect of  $O(^1D) + H_2 / D_2 / DH$  reactions using a double-valued DMBE potential energy surface for  $H_2O$ " (to be published).
- [5] Carolina M. A. Rio and João Brandão, "Dynamical studies and product analysis on the  $O(^1D) + H_2 / D_2$  reactions" (to be published).