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

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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^{-1}, 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^{-1}. 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.

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References

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