Isotopic effect in the O(^1D) + DH reaction and H + OD ⇆ OH + D equilibrium.

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In this work a recent double-valued potential energy surface for water molecule [1] is used in order to study the isotopic effect in O(^1D) + DH reaction, by using quasiclassical trajectory calculations (QCT).

This reaction and the respective isotopic effect has been the subject of several theoretical [2,3,4] and experimental [5,6,7] studies; these two types of results are not coincident, being the theoretical results strongly dependent on the potential energy surface (PES) used. In the literature we have found a large range of experimental values for the ratio OD/OH, $\Gamma_{OD/OH}$ or $\Gamma_{H/D}$: 1.13 ± 0.08 [8] - 1.9 [9] and, in an experimental recent work, Jensen and collaborators [10] refer to a value next to two. Besides, Hsu and collaborators [6] have presented an experimental results at 2.05 kcal mol^{-1} collision energy. In another work [7] these authors present the angular distributions of the products for the reaction of O(^1D) with DH at 3.7 and 4.55 kcal mol^{-1}, and also show the contribution of the abstraction and insertion mechanisms.

Here we compare our results with those already published. Possible contributions of the excited surfaces are also taken into account. At 2.05, 3.7, and 4.55 kcal mol^{-1} collision energies we have studied the cross section, the life time for the complex formed, the opacity function, the energy distribution of the products, the isotopic effect OD/OH and the angular distribution of the products. We also discuss the contribution of the insertion and abstraction mechanisms. In order to corroborate experimental results, we have also studied the H + OD ⇆ OH + D equilibrium.

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