Water formation by OH + H_2 on grain surfaces at 10 K: large isotope effects by quantum tunneling

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Water (H_2O) is the most abundant solid component in icy grain mantles in molecular clouds. It is widely accepted that grain-surface reactions play a pivotal role for H_2O formation in those environments. One of the representative pathways is the reaction of hydroxyl radicals (OH) with H_2 molecules;

$$OH + H_2 \rightarrow H_2O + H, \quad (1)$$

whose activation barrier is about 2100 K in the gas phase [1]. Due to the large barrier, it is unlikely that reaction (1) thermally occurs on the surface of interstellar grains at as low as 10 K; it should proceed through quantum tunneling. However, it remains unknown whether the tunneling surface reaction really occurs at such low temperatures.

In the present study, we performed laboratory experiments on the formation of H_2O through quantum tunneling reaction (1) under astrophysically relevant conditions.

When H_2 was codeposited onto a cold (10 K) substrate with OH, which was produced by dissociating H_2O in a microwave-induced plasma and cooled down to 100 K, the formation of H_2O was observed in the infrared absorption spectrum of the reaction products.

We next performed similar experiments by using D_2 instead of H_2 in order to measure isotope effects on the reaction. If OH react with D_2, HDO is formed by the following reaction:

$$OH + D_2 \rightarrow HDO + D. \quad (2)$$

We found that HDO was actually formed by the codeposition of D_2 with OH. However, the efficiency of reaction (2) was about 10% of that of reaction (1) under the same experimental conditions. The relative efficiency of reactions (1) and (2), as well as that of other reactions using OH and H_2 isotopologues (OD, HD, and D_2) was summarized in Figure 1 where the width of arrows represent the relative efficiency of each reaction. H-atom abstraction from H_2 or HD (thick arrows) was more effective than D-atom abstraction from HD or D_2 (thin arrows). The observed difference in the reaction efficiency can be explained with a difference in the effective mass of each reaction. Therefore, the strong mass-dependence of reactions clearly indicates that reaction (1) proceeds through quantum tunneling at 10 K.

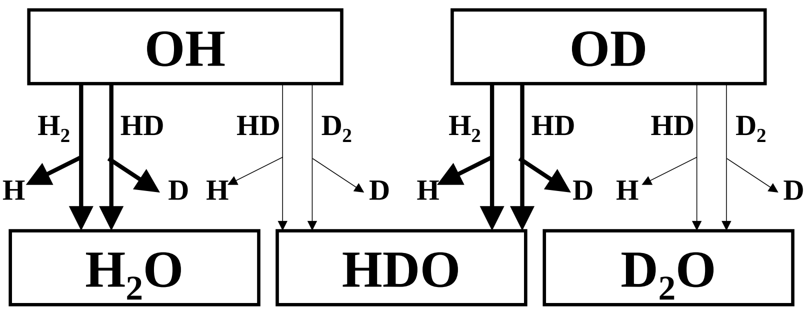

Figure 1: Schematic illustration of reaction efficiency; thick and thin arrows represent effective and less effective reactions, respectively. The relative efficiency is approximated as 1 to 0.1.

References

[1] R. Atkinson et al. 2004, Atmos. Chem. Phys. 4, 1461.