A new path for H_2 formation supposed to occur in the CO rich ice-mantle

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Low temperature surface or solid-phase radical reaction on interstellar dusts has been paid much attention for the understanding of chemical evolution of molecules in dark clouds. Several stationary points for reactions of CO with H atom yielding HCO and HOC were examined at the level of MR-SDCI/cc-pVTZ (Fig.1). Throughout the following exothermal reactions (1), (2), and (3), ice-mantle serves as the reaction-heat absorber in making the reaction facilitate.

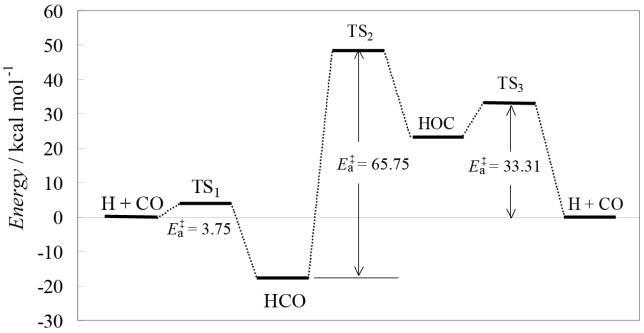

Fig. 1 Energy profile for the reactions between H and CO.

First, the reaction,

$$H + CO \rightarrow HCO, \qquad (1)$$

has a reaction barrier of ca. 3.75 kcal/mol. At the typical temperature of 15 K in the molecular cloud, the barrier in the reaction is too high, so that only tunneling reaction would be feasible between the reactants adsorbed on neighboring sites (Langmuir-Hinshelwood mechanism). Tunneling probability is calculated to be as small as 1.7×10^{-10}, but hydrogen atom trapped in a potential well on the ice-surface will repeat the collision with CO through *ca* 10^{13} oscillations/sec, resulting in the completion of tunneling in 3.2 msec.

The succeeding reaction with H atom, which approaches from (A) side in Fig. 2, results in hydrogen abstraction from HCO yielding H_2 and CO molecules,

$$H + HCO \rightarrow H_2 + CO \qquad (2),$$

as shown by successive red-arrow marks. Alternatively, the approach from (B) side results in formaldehyde formation.

$$H + HCO \rightarrow H_2CO. \qquad (3)$$

Both reactions (2) and (3) are calculated to be a down-hill reaction without activation energy barrier.

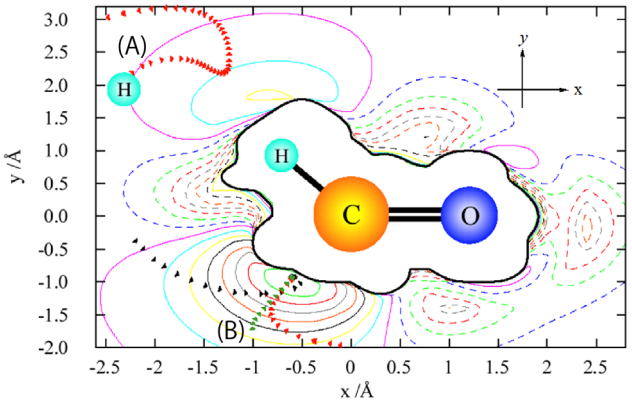

Fig. 2 2D potential energy surface around HCO.

Accordingly, combination of reactions (1) and (2) will make a H_2 production cycle. Here, CO behaves just like the catalyst in the cycle. This is another new reaction path for the H_2 production from H atoms in space through neutral reaction (*cf.* [1]).

[1] J. Takahashi, K. Masuda, and M. Nagaoka, ApJ, **520**,724 (1999).