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Hydrogenation and deuteration of solid aromatic hydrocarbon by quantum tunneling

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Surface tunneling reactions on interstellar dust (e.g., CO + H or D) are crucial to explain the abundances of organic molecules like methanol and their deuterated isotopologues observed in cold dense interstellar regions ($\leq$ 100 K), such as molecular clouds, where thermally activated reactions rarely occur at low temperatures. Aromatic and aliphatic hydrocarbons are two of the main components of interstellar and circumstellar dust, and benzene (C_6H_6) must be a precursor of interstellar polycyclic aromatic hydrocarbons (PAHs) and hydrogenated amorphous carbon grains. The present study investigates the following hydrogenation/deuteration reactions of amorphous solid C_6H_6 over a wide temperature range (10-50 K).

C_6H_6 + H(D) $\rightarrow$ C_6H_7(C_6H_6D) E_a = 18.2 kJ mol^{-1}, [R1]
C_6H_7 + H(D) $\rightarrow$ C_6H_8($C_6H_6D_2$), [R2]
C_6H_8 + H(D) $\rightarrow$ C_6H_9($C_6H_6D_3$) E_a = 6.3 kJ mol^{-1}, [R3]
C_6H_9 + H(D) $\rightarrow$ C_6H_{10}($C_6H_6D_4$), [R4]
C_6H_{10} + H(D) $\rightarrow$ C_6H_{11}($C_6H_6D_5$) E_a = 10.5 kJ mol^{-1}, [R5]
C_6H_{11} + H(D) $\rightarrow$ C_6H_{12}($C_6H_6D_6$). [R6]

E_a is the activation barrier for H-atom addition in the gas phase. The radical recombination reactions R2, R4, and R6 are barrierless on the surface. We experimentally demonstrate that cold H and D atoms can efficiently add to solid benzene by tunneling at temperatures as low as 10-50 K. The present study is the first report on a nonenergetic deuteration process of aromatic hydrocarbons at low temperatures. In comparison to C_6H_6, PAHs tend to have lower activation barriers to H or D addition owing to the higher flexibility. Therefore, we suggest that interstellar aromatic hydrocarbons including PAHs and C_6H_6 can be hydrogenated or deuterated by the tunneling of H or D atoms at low temperatures. The deuteration of interstellar aromatic hydrocarbons is of particular important, because these molecules represent a major carrier of deuterium enrichment observed in carbonaceous meteorites and interplanetary dust particles. As the gaseous atomic D/H ratio in molecular clouds can be also strongly enhanced for elemental ratios of 1.5×10^{-5} to 10^{-2}-10^{-1}, our results suggest that tunneling might represent a major deuteration mechanism for interstellar aromatic hydrocarbons, because surface tunneling is especially facilitated in the cold dense interstellar environments.

Keywords: Aromatic hydrocarbons, hydrogenation, deuterium enrichment, quantum tunneling, molecular clouds