Exploring Nondiffusive Pathways to Acetaldehyde Formation in Interstellar Ices: Insights from Computational Studies

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The detection of acetaldehyde (CH_3CHO) in cold astrophysical environments, such as dark clouds and prestellar cores, challenges standard grain-surface chemistry models, which rely on radical diffusion. At temperatures of ∼10 K, radical mobility is extremely limited, making these pathways inefficient. To explain the presence of iCOMs in these cold cores, various chemical mechanisms have been proposed, including those based on nondiffusive pathways [1-6]. In this work, we present a computational investigation of a nondiffusive three-body (3-B) formation mechanism for CH_3CHO on interstellar water ices. The mechanism involves the hydrogenation of CO to form HCO in close proximity to a CH_3 radical, enabling immediate reaction without requiring diffusion. Using static quantum chemical calculations, we characterized the potential energy surface, including competing channels such as hydrogen abstraction. To assess the efficiency of the mechanism under realistic conditions, we performed *ab initio* molecular dynamics simulations at 10–25 K on a crystalline water-ice surface. Our results show that CH_3CHO can form via this nondiffusive pathway, though alternative products (CH_4 + CO or stable HCO) are also possible, leading to a distribution of outcomes. These findings highlight the importance of nondiffusive chemistry for explaining iCOM formation in cold interstellar environments.

References

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