

Molecular Dynamics Simulations of Interstellar Chemical Reactions

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While exploration missions such as Hayabusa2 and recent advances in the ALMA radio telescope have accelerated the discovery of complex organic molecules relevant to life in the interstellar medium, it is essential to recognize that these molecules are the final products of a sequence of chemical processes. Identifying the specific reactions responsible for their formation in interstellar space is particularly challenging, as direct observations and measurements provide only limited insight into the underlying pathways. To address this issue, theoretical reaction dynamics simulations play a crucial role in elucidating the elementary processes, including reaction efficiencies and branching fractions.

Through collision simulations, we have investigated the thermal rate coefficients and branching fractions of several elementary reactions [1–7], focusing particularly on ion–molecule interactions of H_3^+ with ethylene (C_2H_4) [1], isocyanic acid (HNCO) [6,7], and methanol (CH_3OH). In the interstellar medium, H_3^+ , widely regarded as a universal proton donor with strong proton affinity, plays a significant role in ion–molecule chemistry due to its high abundance. These reactions proceed efficiently in the absence of an entrance barrier and are primarily governed by strong attractive interactions such as charge–dipole and charge–induced dipole forces.

For the $\text{H}_3^+ + \text{HNCO}$ branching reaction [6], the temperature dependence of the rate coefficients obtained from our collision simulations departs from the predictions of classical capture theory, including those based on the modified Arrhenius and Su–Chesnavich equations. This deviation arises because the interaction between H_3^+ and HNCO comprises both attractive and repulsive components.

In addition, we carried out collision simulations for the $\text{H}_3^+ + \text{HNCO}$, $\text{H}_2\text{D}^+ + \text{HNCO}$, $\text{HD}_2^+ + \text{HNCO}$, and $\text{D}_3^+ + \text{HNCO}$ reactions to investigate the isotope effects [7]. In the $\text{H}_2\text{D}^+ + \text{HNCO}$ and $\text{HD}_2^+ + \text{HNCO}$ reactions, the abstraction of the lighter proton was preferred over that of the heavier deuteron at lower temperatures, owing to attractive interactions derived from the potential energy surface in these barrierless processes. These results suggest that, in barrierless reactions, the heavier deuteron—due to its greater mass and reduced mobility—is less likely to undergo efficient collisions with reactant molecules, thereby increasing the probability of proton abstraction relative to deuteron abstraction. This emphasizes the crucial influence of entrance channel dynamics in facilitating deuterium enrichment at low temperatures. The enrichment observed is attributed to a non-equilibrium isotope effect.

References

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