

Formation pathways of complex organic molecules: OH•projectile colliding with methanol ice mantle (CH₃OH)₁₀

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Abstract

In this article, we simulated the collisions of an OH• projectile impacting on a methanol cluster formed by ten units of methanol to mimic an ice mantle (CH₃OH)₁₀. The chemical processes occurring after the impact were studied through Born-Oppenheimer (ab-initio) molecular dynamics. We focus on collisions with initial kinetic impact energy of 10-22 eV, where the richest chemistry happens. We report the formation mechanisms of stable complex organic molecules (COMs) such as methoxymethanol CH₃OCH₂OH, formic acid HCOOH, formyl radical HCO, formaldehyde H₂CO and its elusive HCOH isomer. We show that CH₂(OH)₂, •CH₂OH or +CH₂OH are key intermediates to generate H₂CO and other COMs. We compare the outcomes using OH• with those using OH⁻ projectiles. These processes are likely relevant to the production of COMs in astrophysical environments. We discuss its formation mechanism and the astrophysical implications of these chemical pathways in star-forming regions.

Author keywords

Astrochemistry

Dust

Extinction

ISM: atoms

ISM: molecules

Molecular processes