Formation of formaldehyde through methanol-ice-mantle (CH3OH)10bombardment by OH+catión

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Abstract

Context. Formaldehyde H2CO was the first organic polyatomic molecule discovered in the interstellar medium to have been detected in a variety of sources. However, pathways to synthesize this molecule under interstellar conditions have yet to be discussed. Aims. We carried out a systematic study to analyze the chemical processes that can explain the H2CO formation mechanism toward a decamer of methanol (CH3OH)10 as target material to mimic an ice mantle bombarded by an OH+ cation. Methods. We performed Born-Oppenheimer (ab initio) molecular dynamics simulations to obtain the formation mechanisms of complex organic molecules (COMs) such as formaldehyde H2CO and its HCOH isomer. Results. We found that CH2OH+ and CH2(OH)2 are the main precursors to form H2CO and HCOH. We discuss its formation mechanisms and the astrophysical implications in star-forming regions. These processes are likely relevant to the production of COMs. © ESO 2021.

Author keywords

Astrochemistry; ISM: molecules; Molecular processes