# Formation of complex organic molecules in ice mantles: An ab initio molecular dynamics study

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We present a detailed simulation of a dust grain covered by a decamer of (CH3OH)10-ice-mantle, bombarded by an OH- closed-shell molecule with kinetic energies from 10-22 eV. The chemical pathways are studied through Born-Oppenheimer (ab initio) molecular dynamics. The simulations show that methanol ice-mantles can be a key generator of complex organic molecules (COMs). We report the formation of COMs such as methylene glycol (CH2(OH)2) and the OCH2OH radical, which have not been detected yet in the interstellar medium (ISM). We discuss the chemical formation of new species through the reaction of CH3OH with the hydroxyl projectile. The dependence of the outcome on the kinetic energy of the projectile and the implications for the observation and detection of these molecules might explain why the methoxy radical (CH3·) has been observed in a wider range of astrophysical environments than the hydroxymethyl (CH2·) isomer. Because of the projectile kinetic energies required for these reactions to occur, we suggest that these processes are likely relevant in the production of COMs in photodissociation and shock regions produced by high-velocity jets and outflows from young stellar objects. 

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