Formation mechanism of 1- and 2-propanols in reaction CO and C_2H_5

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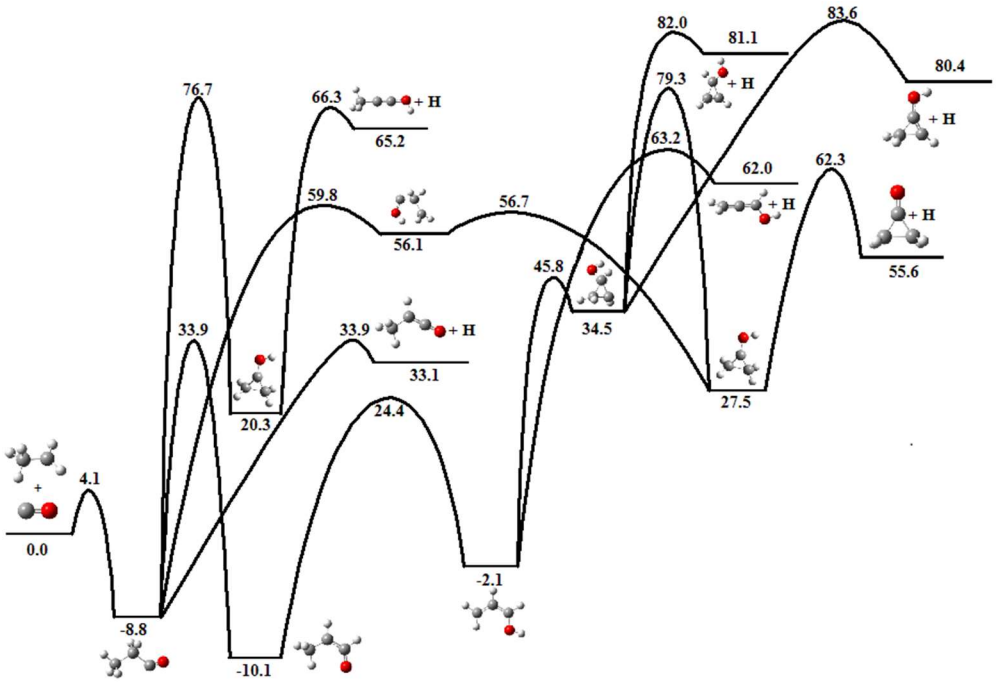
The synthesis of organics in molecular clouds and in star forming regions such as the Taurus Molecular Cloud (TMC-1) and Sagittarius B2, respectively, has been linked to the processing of low temperature (10 K) ice-coated nanoparticles (interstellar grains) by ionizing radiation such as the internal ultraviolet photon field and galactic cosmic rays (GCRs) in cold molecular clouds and in star forming regions. Interstellar grains represent carbonaceous and/or silicate-based nanoparticles coated with ice mantles a few hundred nanometers thick consisting of mixtures of at least water (H_2O), methanol (CH_3OH), carbon monoxide (CO), carbon dioxide (CO_2), methane (CH_4), formaldehyde (H_2CO), and ammonia (NH_3). The densest parts of these molecular clouds undergo gra-vitational collapse ultimately leading to star forming regions. In these environments, heating raises temperatures up to 300 K thus leading to a (partial) sublimation of the complex organic molecules into the gas phase, where they can be searched for and detected by radio telescopes with star forming regions resembling memory records of cold molecular clouds. Since the transition from a cold molecular cloud to star forming regions depends strongly on the molecular composition, it is imperative to unravel the basic processes of how key classes of organics are formed in those environments.

This study proposes a mechanism for the formation of 1- and 2-propanols through the reaction of carbon monoxide and ethane radical, which, in turn, may be present or formed from components of space ice. The energies and molecular parameters of the local minima and transition states involved in the reaction were computed at the B3LYP/6-311G(d,p) level of theory with a chemical accuracy of 0.01–0.02 Å for bond lengths as well as 1–2° for bond angles.



Potential energy surface (PES) for the ethyl reaction with carbon monooxide. This PES was calculated at the B3LYP/6-311G(d,p) level of theory.The relative energies are given in kCal/mol.