Formation of acetaldehyde on mixed-ice grain surfaces

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Interstellar complex organic molecules (iCOMs) are defined as compounds with ≥6 atoms, in which at least one is carbon. [1] Since their discovery in star-forming regions, they have been gaining increasing interest, as they can be considered the precursors of more complex molecules, which can have biological relevance. [2] However, understanding how iCOMs are formed is still a matter of debate, as it is supposed that both gas-phase and on-grain chemistry are needed for their synthesis. [3], [4] Acetaldehyde is one of the most detected species, therefore its formation routes are of paramount interest in astrochemical models. [5]

In the gas phase, CH_3CHO appears to be efficiently synthesized from ethanol and from ethyl radical. [5], [6] On the surface, radical-radical recombinations are preferred, for being barrierless, even though the orientation of the fragments has a crucial role and side reactions like H-abstraction may take place. [7], [8] We investigated a new reaction pathway for the formation of acetaldehyde, namely $CH_3 + CO_{(ice)}$, where the CO is a component of the ice surface. Our H_2O:CO amorphous model contains 25% of carbon monoxide and was chosen to avoid H-abstraction reactions. We found that the reaction, in the case to follow a Langmuir-Hinshelwood mechanism, exhibits a high energy barrier to be surmountable in interstellar conditions, but when adopting a Eley-Rideal mechanism it is barrierless. Subsequent hydrogenation step is found to be barrierless depending on the orientation of the two radicals. Thus, we suggest this pathway to form acetaldehyde to be likely when a CH_3 radical coming from the gas phase lands on a CO-rich region in icy surfaces.

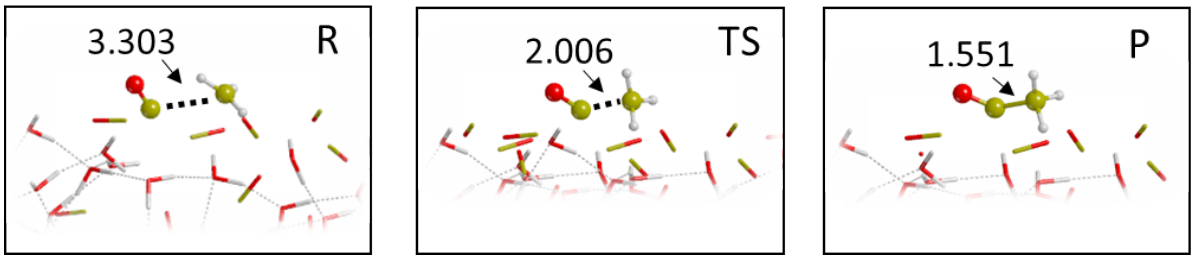

Figure 1: Reactant (R), transition state (TS), and product (P) of the reaction of CH_3 with a CO molecule of the (001) surface cut from our H_2O:CO amorphous ice model. Fragments involved in the reaction are represented as balls and sticks. Colour code: gray, H; brown, C; red, O. Distances are in Å.

References

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