

Formation of Complex Organic Molecules on Interstellar Grain Surfaces. Insights from Periodic Quantum Chemical Simulations

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About 200 molecular species were detected in the ISM. Some of them are complex organic molecules (COMs), molecules with more than 6 atoms containing one or multiple C atoms. Some COMs can reach a certain degree of complexity and can have a prebiotic relevance. Knowing whether COMs contributed or not to the chemical evolution needed for the emergence of life is one of the open questions in the origin of life studies. Two classes of models are invoked to explain the interstellar synthesis of COMs. One advocates formation of COMs on the grain surfaces [1, 2], in which dissociation of frozen hydrogenated species gives radicals, which in turn recombine to form COMs. The other postulates that they form via gas-phase reactions [3, 4], in which the frozen hydrogenated species desorb into the gas phase and react with other gaseous species to form COMs through a series of gas-phase processes. The problem in knowing which of the two models is correct and in which conditions each model is applicable mostly comes from a dramatic lack of experimental and theoretical data of gas-phase and on-surface reactions. This communication focuses on the formation of several COMs by recombination of their precursor radicals (e.g., $\text{CH}_3 + \text{HCO} \rightarrow \text{CH}_3\text{CHO}$; $\text{CH}_2\text{OH} + \text{HCO} \rightarrow \text{HOCH}_2\text{CHO}$, and others) on grain surfaces by means of quantum chemical simulations. Surfaces are based on a periodic approach of a slab model consisting of H_2O mixed with CO (Figure 1). Results indicate that, in addition to radical recombination, other processes are competitive reactive channels. The occurrence of these processes depends on several factors such as the nature of the radical recombination, the proximity of the reactants or the capability of the radicals to transfer their H atoms [5].

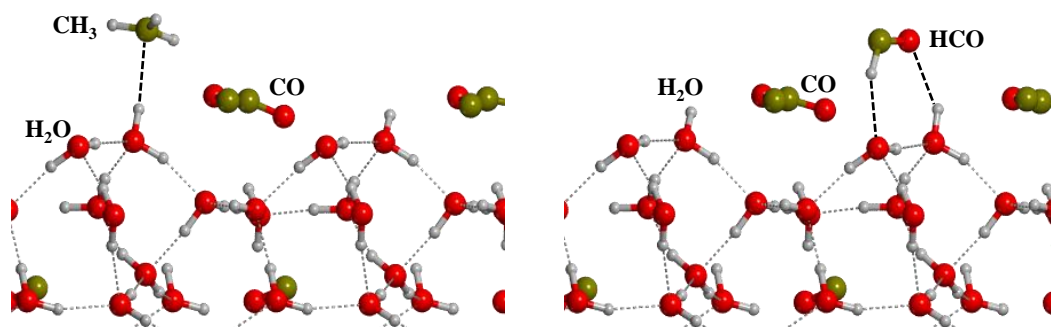


Figure 1: Surface slab model employed to simulate the recombination of radical species on surfaces. In this case the CH_3 and HCO radicals are adsorbed on the surface model.

References

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