Radical binding and radical reactions on interstellar ices: a combined experimental and quantum chemical study

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Abstract

The building blocks of molecules, which lead to the origin of life in the Universe, can be formed on cosmic ice dust grains in the interstellar medium (ISM).[1] For a quantitative understanding of the chemical evolution towards complex molecules (COMs), it is essential to know the behaviour of relatively small radical species on ice grains at low temperatures (e.g., 10 K).[2] However, elementary radical processes, such as radical adsorption, diffusion, and chemical reactions when encountering each other are still unknown, and treated as a "black box" in the astrochemical models in determining the chemical evolution in the universe. To overcome this limitation, we use a multidisciplinary approach, where we connect quantum chemistry and low-temperature sciences to study the radical processes on ices.

The binding energies of the radicals on ices determine their desorption probability and influence their surface mobility, both of which are critical in determining their reactivity. The computed binding energy of the radical is sensitive to the dangling hydrogen or dangling oxygen at the binding site. As a result, a range of binding energies was observed for the radical species.[3-7] We have also studied the radical reactions on ices; OCS + H,[4] PH_3 + D,[5] CH_3SH + H, and CH_3OH + OH. Computed reaction paths of the radical reactions on ices explained the experimentally observed products, where quantum tunnelling plays a key role in achieving the reactions at low temperatures. Our combined quantum chemical and experimental studies give important mechanistic insights into the COMs formation in the ISM.

References

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