Systematic Determination of Complex Reaction Mechanisms in the Interstellar Medium

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Radical species in the interstellar medium (ISM) play a vital role in the formation of complex organic molecules (COMs). The primary radicals in the ISM, specifically H, OH, CO, HCO, CH_3O, CH_2 OH, CH_3, NH, and NH_2 can be formed through photodissociation of the molecules in ice mantles (e.g., H_2O, CH_4, H_2CO, CH_3OH, NH_3) or through surface reactions between atoms, radicals, and molecules.[1-3] Accumulation of primary radicals and molecules on the icy grain surfaces occurs at very low temperatures, generally at 10 K in dark clouds. Among the primary radicals, only H atoms may diffuse on the ice surfaces at 10 K. At relatively high temperatures, the so-called warming-up stage, other radical species and molecules may diffuse on the ice surfaces and react if they meet each other to form COMs. However, quantitative mechanistic details of the radical reactions on ices are difficult to characterize from experimental studies alone. Therefore, I aim to determine quantitative mechanistic details of the radical reactions on ices under interstellar conditions.[4-8] For this purpose, starting from the atoms, molecules, and primary radial species on ices, reaction mechanisms for the chemical evolution toward COMs will be systematically determined by using state-of-the-art quantum chemical methods.

References

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