The Behavior of Carbon Atoms on the Surface of Amorphous Solid Water

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Significant advances in observational astronomy, such as the James Webb Space Telescope, have revealed the chemical diversity of interstellar media. In dense, cold regions of interstellar media, so-called molecular clouds, cosmic dust is typically covered with ice, where amorphous solid water (ASW) is the major component. The chemistry on the surface of icy dust grains is known to play an important role in the formation of molecular species. Chemical reactions involving carbon (C) atoms are essential in the formation of complex organic molecules (COMs); in astrochemistry, all molecules with six or more atoms, of which at least one of them is a C atom, are called COMs.

Recently, C atom reactions with light species (e.g., H atoms, H₂O, CO, and NH₃) in lowtemperature ice have been extensively studied and the COMs formation has been reported. These experiments were performed by co-depositing C atoms and other species onto a substrate. However, these simulation experiments may not fully reflect the chemistry occurring in molecular clouds, where atoms and molecules are slowly deposited from gas phase onto icy grains. In other words, adsorbates remain on the surface of icy grains for a long time before encountering other species, in contrast to co-deposition experiments where rapid deposition rate facilitates immediate reaction. To extrapolate laboratory experiments to realistic environments, it is necessary to determine each elementary physicochemical process, such as adsorption, surface diffusion, and reaction. By developing an *in situ* C-atom detection method, we revealed the adsorption scheme for C atoms on ice (physisorbed and chemisorbed states) and determined the activation energy for C atom diffusion on the surface of ice.¹ The reactivity of adsorbed C atoms with nonenergetic H atoms was also investigated to understand the role of adsorption states in the formation of methane via the C + 4H \rightarrow CH₄ reaction.²

The C atoms adsorbed on ASW were classified into three types; (i) C atoms that readily react with H₂O to produce formaldehyde, (ii) those remain physisorbed for a prolonged period, and (iii) physisorbed C atoms that transform into the chemisorbed state. For type (ii) C atoms, the activation energy for surface diffusion was determined to be 88 meV, indicating that diffusive C-atom reactions are activated at approximately 22 K on interstellar ice. The reactivity of C atoms with H atoms was investigated to elucidate the CH₄ formation mechanisms. We found that only physisorbed C atoms yielded CH₄. Based on these experimental findings, we draw a plausible scenario for the fate of C atoms accreting interstellar icy grains.

¹ Tsuge, M. et al. Surface Diffusion of Carbon Atoms as a Driver of Interstellar Organic Chemistry. *Nat. Astron.* **2023**, 7, 1351.

² Tsuge, M. et al. Methane Formation Efficiency on Icy Grains: Role of Adsorption States. Submitted.