

# Reactivity of cationic pentane and its growth reaction

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In an interstellar chemistry, radical cations are ones of important species, because they are highly reactive. We have studied structures and ionization-induced reactions of monomers and clusters of radical cations in the gas phase by use of mass spectrometry, infrared spectroscopy, and theoretical calculations. Recently, we have investigated the reactivity of radical cations of alkanes. Through this, extremely high proton donor abilities of CH bonds of cationic alkanes have been elucidated, although neutral alkanes are typically aprotic.[1]

Figure 1 shows the structure of the di-hydrated cluster of cationic pentane. As seen in the figure, a proton of cationic pentane is transferred to the water moiety and is shared intermolecularly. No energy barrier in this proton transfer reaction is indicated by theoretical calculation. These results demonstrate the high proton donor ability of CH bonds in cationic pentane. The mechanism of its high proton donor ability is analyzed by infrared spectroscopy of cationic pentane monomer.[2]

Furthermore, we have determined the structure of cationic pentane dimer. Figure 2 shows the structure of cationic pentane dimer. The dimer cation are formed by the intermolecular semi-covalent bond type interaction between the hydrogen atoms. In the mass spectrum of the pentane dimer, the H<sub>2</sub>-loss fragment cation ( $m/z=142$ ) as well as the pentane dimer ( $m/z=144$ ) is observed. In this H<sub>2</sub>-loss fragment cation, the carbon atoms which lost the hydrogen atoms form the intermolecular hemibond. This hemibond formation would be a key for hydrocarbon growths.

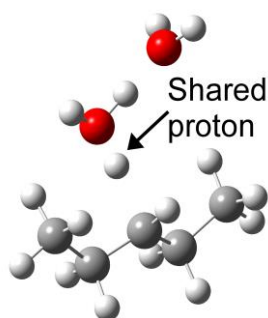


Figure 1: Structure of cationic pentane-(H<sub>2</sub>O)<sub>2</sub> cluster.

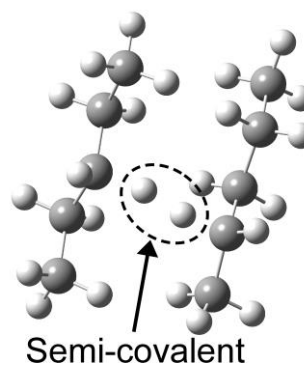


Figure 2: Structure of cationic pentane dimer.

## References

- [1] T. Endo, Y. Matsuda, A. Fujii, *J. Phys. Chem. Lett.* 8, 4716 (2017).
- [2] M. Xie, Y. Matsuda, and A. Fujii, *J. Phys. Chem. A.* 120, 6351 (2016).