

Photochemistry of six-membered hydrocarbons in solid parahydrogen

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Photochemical reactivities of cyclic hydrocarbons are interested in natural sciences, biological sciences, and astrochemistry, because the investigation of these ring molecules give us the useful information about the noble or unstable species formation and chemical reactions. In particular, since polycyclic aromatic hydrocarbons (PHAs) are one of the potential candidates for the carrier of diffuse interstellar bands (DIB) [1-3], it is important to understand the UV photochemical behavior of PHAs because interstellar molecules are constantly exposed to strong UV radiation. In this study, we investigate the photochemistry of six-membered hydrocarbons: benzene (Bz) [4], one of the simplest and most widely studied aromatic hydrocarbons, and 1,3-cyclohexadiene (1,3-CHD) [5] and 1,4-cyclohexadiene (1,4-CHD) [6], two double bonding at different position in ring, trapped in solid parahydrogen by a joint use of Fourier transform infrared spectroscopy and density functional theory (DFT) calculations, aiming to compare the photochemical stability, reactivity and photochemical products among three molecules. The mixture of hydrocarbons and parahydrogen were condensed on the cold substrate (4.2 K) cooled down by closed-cycle GM refrigerator. The sample was then irradiated by 193 nm photons of an ArF pulsed laser, and photoproducts were detected by FT-IR spectrometer. In order to confirm the spectral assignment of reactants and products, DFT calculations were also performed. In the IR spectra of 1,4-CHD in solid parahydrogen after ArF laser irradiation, we observed peaks of 1,3-CHD and Bz as photoproducts. Further irradiation using ArF, we observed the cyclohexadienyl radical, hexatriene derivatives, and small photofragment molecules. Comparing with the photochemical behavior of three six-membered hydrocarbons, the photochemical products and reactions mechanism of three molecules will be discussed.

References

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