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## IR spectrum of ethylene cations isolated in solid Ar

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**[Introduction]** Unsaturated hydrocarbon cations are supposed to be abundant in the atmospheres of planets in the outer solar system and also have been found to dominate in hydrocarbon-bearing combustion process. The study of IR features of these species is important in understanding the fundamental of molecular structures; particularly the structure of these species is twisted relative to their neutral forms. Even ethylene cation, the simplest alkene cation, much remains to be learned about its ground-state properties. In previous work, Jacox and Thompson [1] reported the first direct IR observation of ethylene cation ( $C_2H_4^+$ ) produced by co-deposition of ethylene in a large excess of neon at 4.3 K with a beam of neon atoms that have been excited in a microwave discharge. Their work was summarized that the line, at  $1413.8\text{ cm}^{-1}$ , is assigned to the  $\nu_{12}$  ( $b_{1u}$ ) fundamental of  $C_2H_4^+$ . This peak agrees closely with the  $1411.7\text{ cm}^{-1}$  band recently assigned to this fundamental in gas-phase photoelectron spectroscopic studies. The absorption at  $3014.4\text{ cm}^{-1}$  attributed to  $\nu_{11}$  ( $b_{1u}$ ) of  $C_2H_4^+$ . One or more of the three weak absorptions between  $3141$  and  $3156\text{ cm}^{-1}$  may be contributed by  $\nu_9$  ( $b_{2u}$ ) of  $C_2H_4^+$ . The assignments of  $\nu_7$ ,  $\nu_{11}$ , and  $\nu_{12}$  fundamentals of  $C_2H_4^+$  have also been confirmed via deuterium-substituted experiments. Their work provided the detailed assignments of vibrational fundamentals of  $C_2H_4^+$ . However this molecular system is quite small, once the measurements toward to larger ones, the clear identification of spectral features between charged and neutral forms may be difficult. Hence, a new method to generate these species and characterize their spectral features is needed.

In our previous work, protonated aromatic hydrocarbons were generated by electron bombardment of aromatic hydrocarbons diluted in para- $H_2$  during matrix deposition. After irradiation of the matrix samples with 365 nm, trapped electrons were released and recombined with cationic species in the system. Thus, the IR features of cationic forms decreased in intensity and that of the neutral forms increased [2]. In the present work, gaseous Ar containing a small proportion of  $C_2H_4$  was bombarded with 300-eV electrons and then followed by condensation onto the cold target to form a matrix. The IR absorption spectra of the matrix sample were recorded to identify the products and the IR spectra of UV irradiation of the same matrix sample were subsequently recorded to identify the observed features of cations and neutrals.

**[Experiment]** A nickel-plated copper flat cooled to 10 K served as a cold substrate for matrix samples. The substrate was cooled with a ARS DE-204 closed-cycle helium refrigerator system and a turbomolecular pump provided the cryo-chamber vacuum, which was backed with a scroll pump, typically yielding a pressure of less than  $1 \times 10^{-8}$  Torr. The IR absorption spectra were recorded with a Fourier-transform infrared (FTIR) spectrometer (Bruker, Vertex 80) equipped with a KBr beamsplitter and a Hg-Cd-Te detector (cooled to 77 K), covering the spectral range of 500–4000  $\text{cm}^{-1}$ . Ethylene cations were produced by electron bombardment of a gaseous sample of Ar containing a small proportion of  $\text{C}_2\text{H}_4$  during deposition. An electron gun (Kimball Physics, Model EFG-7) was used to generate electron beams with energy of 300 eV and beam current of 200  $\mu\text{A}$  during the deposition period. A synchrotron radiation (BL-03 of NSRRC) was set emission at 350 nm (bandwidth: 1.5 nm) for further UV irradiation.

**[Result and Discussion]** A partial IR absorption spectrum of the sample  $\text{C}_2\text{H}_4/\text{Ar}$  (1/500) after deposition at 10 K shows intense IR lines at 948.2, 1440.1, and 2995.7  $\text{cm}^{-1}$  are respectively associated with the vibrational modes  $\nu_7$ ,  $\nu_{12}$ , and  $\nu_{11}$  of  $\text{C}_2\text{H}_4$ . Lines observed at 831.0 and 3112.0 (multiple lines)  $\text{cm}^{-1}$  with moderate intensities are assigned to  $\nu_{10}$  and  $\nu_9$ , respectively. Besides absorptions of the precursor, products generated via electron bombardment were also observed including  $\text{C}_2\text{H}_2$ ,  $\text{C}_2\text{H}_3$ ,  $\text{C}_3$ , and  $\text{C}_4\text{H}_2$ . Weak lines at 901.1, 1405.1, and 3028.9 (tentatively)  $\text{cm}^{-1}$  were observed and assigned to  $\text{C}_2\text{H}_4^+$ ; assignments were according to the report by Jacox and Thompson and the observed behaviors after irradiation of the matrix sample with UV light for 1 h.

### **[Reference]**

[1] Jacox, M. E.; Thompson, W. E. *J. Chem. Phys.* **2011**, 134, 064321.

[2] Bahou, M. ; Wu, Y.-J. ; Lee, Y-P. *Phys. Chem. Chem. Phys.* **2013**, 15, 1907.