Laboratory Spectroscopy of 1,2,3-butatriene cation $H_2CCCCH_2^+$ as a Candidate for a Diffuse Interstellar Band Carrier

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The diffuse interstellar bands (DIBs) were first discovered in the optical absorption spectra on stars in about 1920. Carbon chain molecules were suggested as candidates for DIB carriers in 1977 by Douglas [1]. Although large number of carbon chain molecules have been tested based on this suggestion, DIBs have not been identified yet. In this study, an emission spectrometer with hollow-cathode glow discharge and extended negative glow discharge systems produced a spectrum including the 4905 Å band from 2-butyne $H_3C{-}C{\equiv}C{-}CH_3$ as the precursor. Photoelectron spectroscopy of H_2CCCCH_2 [2] indicated that the simple carbon chain molecule $H_2CCCCH_2^+$ (1,2,3-butatriene cation) produces a $^2B_{3u}$–X^2B_{2g} electronic transition at 4905 Å. However, the 4905 Å band does not match the reported DIBs. If the assignment of the 4905 Å band to $H_2CCCCH_2^+$ is true, it becomes doubtful as to whether carbon chain molecules are carriers of DIBs.

We confirmed the assignment of the band by using chemical and physical investigations [3]. The chemical behavior of the band was tested using several kinds of precursors in the discharge. Physical investigation by electrode switching indicated that the origin of the 4905 Å band has a positive charge. The accompanying bands at around 4905 Å were analyzed by the double-minimum torsional potential mode as shown in Figure 1. All of the investigations and the analysis gave the consistent results with the assignment. Therefore the observed 4905 Å band was surely assigned to $H_2CCCCH_2^+$. This cation does not correspond to the currently-known DIBs, even though this is one of the basic unsaturated carbon chain molecules. A question about carbon chain molecules as carriers of DIBs may be raised.

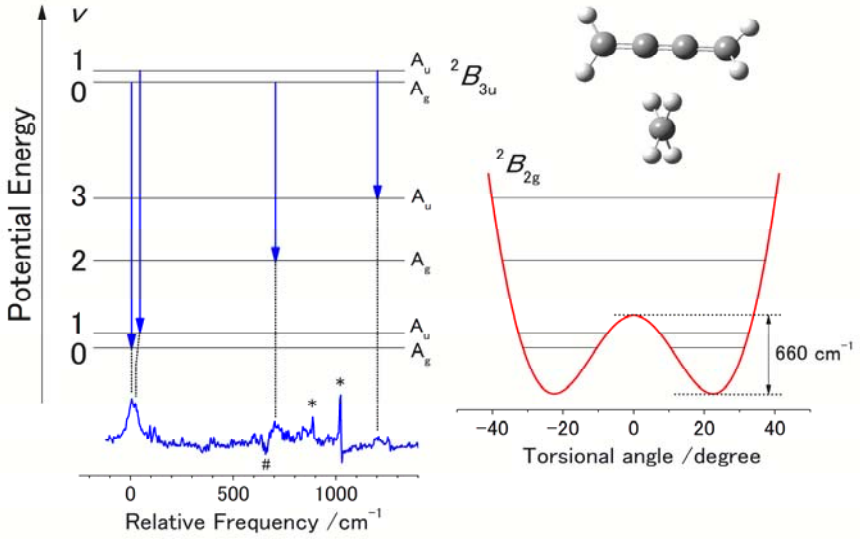

Figure 1: The observed vibronic bands of the $^2B_{3u}$–X^2B_{2g} electronic transition of $H_2CCCCH_2^+$ (left). The vibrational structure and the obtained double-minimum torsional potential (right).

References

[1] A.E. Douglas, 1977, Nat 269, 130.
[2] F. Brogli, *et al*., 1974, Chem. Phys. 4, 107.
[3] M. Araki, S. Uchida, Y. Matsushita, & K. Tsukiyama, 2014, Journal of Molecular Spectroscopy 297, 51.