REEVALUATION OF THE C_4H ABUNDANCE BASED ON THE REVISED DIPOLE MOMENT

TAKAHIRO OYAMA, *Department of Materials and Life Sciences, Sophia University, Tokyo, Japan*; YOSHIHIRO SUMIYOSHI, *Division of Pure and Applied Science, Faculty of Science and Technology, Gunma University, Maebashi, Japan*; MITSUNORI ARAKI, *Research Institute for Science and Technology, Tokyo University of Science, Noda, Japan*; SHURO TAKANO, *College of Engineering, Nihon University, Fukushima, Japan*; NOBUHIKO KUZE, *Department of Materials and Life Sciences, Sophia University, Tokyo, Japan*; KOICHI TSUKIYAMA, *Faculty of Science Division I, Tokyo University of Science, Shinjuku-ku, Tokyo, Japan*.

C_nH molecules are the simplest linear carbon chains in space. They are crucial for not only probes of young clouds but also benchmarks of calculations of chemical reaction network. However, their abundances occasionally show anomaly. For example, observed column densities of C_4H in various sources are one order of magnitude higher than theoretically estimated values. Herbst & Osamura suggested that these excesses of C_4H come from the theoretically determined dipole moment of C_4H.[a] The dipole moment in the electronic ground state of $^2\Sigma^+$ was calculated to be 0.87 D by the RCCSD(T)/aug-cc-pVDZ level of *ab initio* theory.[b] However, the mixing of wavefunctions between the ground state and the low-lying electronic excited state of $^2\Pi$ having the large dipole moment of 4.4 D occurs, giving a higher dipole moment to the ground state. By using a higher dipole moment, a smaller column density is derived via observed line intensities. In the present study, we re-calculated the dipole moment of C_4H by quantum chemical calculations including the mixing.[c] The calculations were carried out by the multi-reference configuration interaction level of *ab initio* theory using the cc-pVQZ basis set. The new dipole moment was derived to be 2.10 D, which is about 2.4 times larger than the value of 0.87 D used so far. Reported lines of C_4H were analyzed to revise column densities by using the new dipole moment. Revised values are about a factor of 6 smaller than those in the previous works. Using the revised column density of C_4H, abundances of the $C_{2n}H$ ($n = 1$–4) series show exponential smooth decreases with carbon-chain length in various sources.

[a]Herbst & Osamura, 2008, *ApJ*, **679**, 1670. [b]Woon, 1995, *Chem. Phys. Lett.* **244**, 45. [c]Oyama *et al.*, 2020, *ApJ*, **890**, 39.