Analysis of the column densities of C_4H using the revised dipole moment

T. Oyama,[1] H. Ozaki,[2] M. Araki,[1] Y. Sumiyoshi,[2] S. Takano,[3] A. Ohsugi,[1]
A. Ubagai,[1] Y. Minami,[1] N. Kuze[4] and K. Tsukiyama[1]

[1]*Department of Chemistry, Tokyo University of Science, Japan*
[2]*Division of Pure and Applied Science, Graduate School of Science and Technology, Gunma University, Japan*
[3]*Department of Physics, College of Engineering, Nihon University, Japan*
[4]*Department of Materials and Life Sciences, Sophia University, Japan*

A series of C_nH molecules are the simplest linear carbon chains. They are crucial for not only traces of young clouds but also benchmarks of chemical reaction network calculations. 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 *et al*. suggested that these excesses of C_4H come from the theoretically determined dipole moment of C_4H [1]. Based on the simple theory, the $^2\Sigma^+$ ground state of this molecule has the small dipole moment of 0.87 D [2]. However, the mixing of wavefunctions between the ground state and the low-lying $^2\Pi$ excited state 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. The calculations were carried out by the multi-reference configuration interaction (MRCI) level of *ab initio* theory using the aug-cc-pVQZ basis set. The new dipole moment was derived to be 2.366 D, which is three times higher 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 column densities are one order of magnitude lower than those in the previous works, as listed in Table 1. The column densities of C_nH molecules in IRC+10216 are described in Figure 1. Using the revised column density of C_4H, abundances of the C_nH series show a linearity. Trends of the other sources listed in Table 1 are also similar. These trends might be results of sequential formation of C_nH molecules in the sources.

Table 1: The column densities of C_4H.

	Previous work		Re-analysis	
Objects	N / cm^{-2}	T / K	N / cm^{-2}	T / K
L483[a]	6.9E+13	10	1.4(2)E+13	7.9(8)
TMC-1 CP[b]	2.9E+14	6.7	4.2E+13	6.7
Barnard 1[a]	2.5E+14	5	3.4E+13	5
L134N[a]	6.1E+13	5	8.3E+12	5
Horsehead[a]	3.0E+13	15	4.1E+12	15
Orion Bar[a]	2.5E+13	15	3.2E+12	15
L1527[c]	1.0E+14	14.3	2.37(8)E+13	14.5(9)
Lupus-1A[d]	5.0E+14	7.3	6.7E+13	7.3
IRC+10216[e]	3.0E+15	35	4.1E+14	35

[a] Ref. 3. [b] Ref. 4. [c] Ref. 5. [d] Ref. 6. [e] Ref. 7.

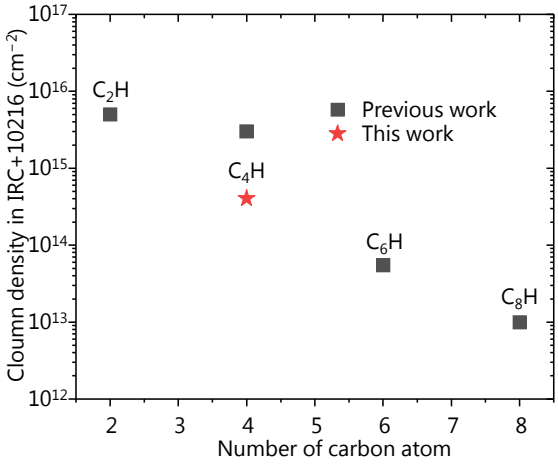

Figure 1: The column densities of C_nH molecules in IRC+10216.

References

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