FIRST ASTRONOMICAL DETECTION OF THE CUMULENE CARBON CHAIN MOLECULE H₂C₆ IN TMC-1

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ABSTRACT

The cumulene carbenes are important components of hydrocarbon chemistry in low-mass star-forming cores. Here we report the first astronomical detection of the long-chain cumulene carbene H₂C₆ in the interstellar cloud TMC-1, from observations of two of its rotational transitions: $J_{K_a} = 7_{1,7} \rightarrow 6_{1,6}$ at 18.8 GHz and $8_{1,8} \rightarrow 7_{1,7}$ at 21.5 GHz, using NASA’s Deep Space Network 70 m antenna at Goldstone, California. In addition we also observed the shorter cumulene carbene H₂C₄ at the same position. The fractional abundance of H₂C₆ relative to H₂ is about $4.7 \times 10^{-11}$ and that of H₂C₄ is about $1.1 \times 10^{-7}$. The abundance of H₂C₆ is in fairly good agreement with gas-phase chemical models for young molecular cloud cores, but the abundance of H₂C₄ is significantly larger than predicted.

Subject headings: interstellar: molecules — line: identification — molecular processes — radio lines — stars: formation

1. INTRODUCTION

The detection of new cumulene carbenes is important for determining the hydrocarbon chemistry in low-mass star-forming cores (cf. Bettens & Herbst 1996). The cumulene carbene chains are also of interest in astronomy for their possible role as carriers of the diffuse interstellar bands (McCarthy et al. 1997). Here we report the first astronomical detection of H₂C₆ (hexapentaenylidene) in the dark cloud TMC-1. The identification of this highly reactive isomer of triacetylene (HC₅H) was made possible by the recent laboratory detection of the rotational spectrum of both H₂C₅ and H₂C₆ (McCarthy et al. 1997) and by the high sensitivity of NASA’s Deep Space Network (DSN) antennas at centimeter wavelengths.

The shorter cumulene carbenes propadienylidene H₂C₃ (Cernicharo et al. 1991; Kawaguchi et al. 1991) and butatrienylidene H₂C₄ (Kawaguchi et al. 1991) were also observed at the same position as H₂C₆, allowing comparison with abundances predicted by chemical models. Both H₂C₅ and H₂C₆ have linear carbon backbones and C₂ symmetry and, because of the off-axis equivalent H-atoms, they both have ortho ($K = \pm 1$, odd) and para ($K = 0$, even) rotational ladders, between which both radiative and collisional transitions are forbidden. In cold molecular clouds we expect 3/4 of the population to be in the lowest lying ortho ($K = \pm 1$) ladders and emission from these to be slightly stronger than from the para ($K = 0$) ladder.

In addition to H₂C₆, several other complex molecules were observed in TMC-1, for the purpose of clarifying hydrocarbon chemistry in these star-forming cores. We find that the carbon-chain molecules vary in abundance among the three principal velocity components. The distribution of the cumulene carbenes is similar to those of other complex carbon compounds, such as the cyanopolyynes HC₅N and the carbon-chain radicals C₆H, but differs from that of the cyclopropenylidene ring, c-C₃H₂. The observed ratios of abundances in TMC-1 are compared with gas-phase chemical models.

2. OBSERVATIONS

The observations were made with NASA’s DSN 70 m antenna at Goldstone, California during 1996 October and November. In addition to H₂C₆, five other molecules (HC₅N, C₆H, H₂C₄, H₂C₅, and c-C₃H₂) were observed as part of an ongoing effort to study the carbon chemistry in TMC-1. The relevant transitions and line frequencies are listed in Table 1.

The observations were made with a broadband (17.5–26 GHz) cooled HEMT receiver with typical system temperatures of 50–65 K and the 2 million channel wide-band spectrometer analyzer (WBSA). The spectra were smoothed to resolutions in the range of 0.03 to 0.15 km s⁻¹ with a total spectral range of 20 to 40 MHz (cf. Langer et al. 1995). All observations, except that of the 18.4 GHz transition of H₂C₆, were made using position switching. In this mode the spectra were obtained by taking the difference between successive ON and OFF source integrations. To suppress baseline irregularities of instrumental and atmospheric origin, the right ascension of the OFF source position was also chosen to be 6 minutes in time to the west or east of the ON source position such that each ON-OFF pair had the same mean elevation. The presence of several stronger lines in the passband of the 21.5 GHz line of H₂C₅ and the 20.8 GHz line of H₂C₄ allowed us to check our calibration during each observing session. Following the detection of the 21.5 GHz line of H₂C₅, a frequency switching option was implemented for the DSN-WBSA system. We used this mode for the observations of the 18.8 GHz transition of H₂C₆ using an LO offset of 0.5 MHz between the signal and reference frequencies.

The detections reported here were made toward TMC-1 at a position [$\alpha(1950) = 4°38′41″$ and $\delta(1950) = 25°35′40″$] corresponding to the strongest HC₅N and H₂C₅ emission observed at $v_{LSR} = 5.8$ km s⁻¹ in our DSN 70 m high spectral

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resolution maps (Velusamy et al. 1997). The on source integration times for the H\textsubscript{2}C\textsubscript{6} lines were 23 and 18 hr for the 21.5 and 18.8 GHz transitions, respectively, and yielded a corresponding rms of 2.5 and 3.5 mK at spectral resolutions of 0.14 and 0.12 km s\textsuperscript{-1}.

### 3. RESULTS

In Figure 1 we show the spectra for the two transitions of H\textsubscript{2}C\textsubscript{4} and those of C\textsubscript{3}H and HC\textsubscript{5}N. The H\textsubscript{2}C\textsubscript{6} 21.5 GHz transition, HC\textsubscript{5}N, and C\textsubscript{3}H were observed simultaneously in the same passband. The spectrum of the 2\textsubscript{01} \rightarrow 1\textsubscript{00} transition of H\textsubscript{2}C\textsubscript{6} at 17.9 GHz in TMC-1 is shown in Figure 1b, along with the lines of H\textsubscript{2}C\textsubscript{6}, C\textsubscript{3}H, and c-C\textsubscript{3}H\textsubscript{2}. The H\textsubscript{2}C\textsubscript{4} and H\textsubscript{2}C\textsubscript{6} spectra peak at \~6 km s\textsuperscript{-1} with antenna temperatures \( T_a \) = 180 and 9 mK, respectively. Previous high spectral resolution studies of carbon-chain molecules in TMC-1, such as CCS and HC\textsubscript{5}N (Langer et al. 1995), revealed that there are three velocity components at 5.7, 5.9, and 6.1 km s\textsuperscript{-1} with very narrow linewidths \~0.15 to 0.20 km s\textsuperscript{-1}. Our detection of H\textsubscript{2}C\textsubscript{6} in TMC-1 supports the suggestion of a tentative assignment of a weak unblended and a blended 3 mm line in IRC +10216 (Guélin et al. 1997).

In Figure 1 it appears that the strongest H\textsubscript{2}C\textsubscript{4} and H\textsubscript{2}C\textsubscript{6} emission is at 5.9 km s\textsuperscript{-1}. The slight asymmetry in the line profiles is most likely due to a second, weaker (partially blended) component at 6.1 km s\textsuperscript{-1}, exactly what is seen in the velocity structure of C\textsubscript{5}H and probably that of C\textsubscript{6}H. There is no evidence in H\textsubscript{2}C\textsubscript{4} and H\textsubscript{2}C\textsubscript{6} for a component at 5.7 km s\textsuperscript{-1}. In contrast, c-C\textsubscript{3}H\textsubscript{2} and its linear isomer H\textsubscript{2}C\textsubscript{3} show strong emission at 5.7 and 5.9 km s\textsuperscript{-1} and only slightly less emission at 6.1 km s\textsuperscript{-1}. The presence of strong c-C\textsubscript{3}H\textsubscript{2} and H\textsubscript{2}C\textsubscript{3} emission

### TABLE 1

| Species | Transition | Frequency (MHz) | Reference |
|---------|------------|----------------|-----------|
| H\textsubscript{2}C\textsubscript{6} | \textsubscript{1}0,\textsubscript{1} \rightarrow \textsubscript{0},\textsubscript{0} | 21488.235 | McCarthy et al. |
| c-C\textsubscript{3}H\textsubscript{2} | \textsubscript{1}0,\textsubscript{0} \rightarrow \textsubscript{0},\textsubscript{0} | 18343.143 | Pickett et al. |
| H\textsubscript{2}C\textsubscript{4} | \textsubscript{2}0,\textsubscript{2} \rightarrow \textsubscript{1},\textsubscript{1} | 17863.810 | Travers et al. |
| C\textsubscript{5}H | \textsubscript{J}5/2 \rightarrow 9/2, \textsubscript{F} = 5 \rightarrow 4 | 21484.710 | Lovas |
| C\textsubscript{5}H | \textsubscript{J}7/2 \rightarrow 5/2, \textsubscript{F} = 4 \rightarrow 3 | 21485.262 | Lovas |
| C\textsubscript{6}H | \textsubscript{J}15/2 \rightarrow 13/2, \textsubscript{F} = 8 \rightarrow 7 | 21488.255 | McCarthy et al. |
| HC\textsubscript{9}N | \textsubscript{37} \rightarrow \textsubscript{36} | 21498.181 | Pickett et al. |

REFERENCES.—Lovas et al. 1992; Pickett, Poynter, & Cohen 1991; Travers et al. 1996; Lovas 1992; McCarthy et al. 1997.
at 5.7 km s\(^{-1}\) and the apparent absence of H\(_2\)C\(_6\) or H\(_2\)C\(_4\) emission at that velocity indicate that there is a significant chemical inhomogeneity in the hydrocarbon chemistry in TMC-1. Furthermore, the c-C\(_3\)H\(_2\) emission is much stronger than that of H\(_2\)C\(_3\) (\(T_d = 2.0\) K versus 0.12 K).

4. DISCUSSION

To estimate the abundances of H\(_2\)C\(_6\) and H\(_2\)C\(_4\) in TMC-1 we adopted a simple model in which we treat each rotational ladder as a separate linear rotor. The excitation of the ortho and para states can be treated separately, because the radiative and collisional transitions between them are negligible. For purposes of estimating abundances, the excitation of theortho ladder can be treated as two equivalent linear rotors. The energy levels of the \(K = \pm 1\) ladders are nearly equal and can be estimated within 1% by treating them as a linear rotor with \(B_0 = (B + C)/2\) (see McCarthy et al. 1997). Collisional rate coefficients for these species have not been calculated; we approximate their \(J\)-dependent values by using those derived for the linear chain molecule HCN (Green & Chapman 1978). We assume that the rotational population of H\(_2\)C\(_6\) has a normal ortho:para ratio of 3:1. Furthermore, reactive collisions with protonating ions can produce H\(_2\)C\(_6\)H\(^+\), which, upon decomposition to H\(_2\)C\(_6\) + H, will preserve the nuclear spins (Herbst 1977).

H\(_2\)C\(_6\) is highly polar, with a calculated dipole moment of 6.2 D (Maluendes & McLean 1992). The \(J = 8\) ortho levels lie \(-5\) K above the ortho ground state (\(J = 1\)) and these levels have an Einstein \(A\) coefficient of about \(2 \times 10^{-8}\) s\(^{-1}\). This yields a critical density \(n(H_2) \sim 5 \times 10^3\) cm\(^{-3}\), implying that the lower rotational levels are easily thermalized at the density in the cores of TMC-1. Figure 2 shows an excitation calculation for the \(K = -1\) ortho ladder of H\(_2\)C\(_6\) and the \(K = 0\) para ladder of H\(_2\)C\(_4\) (using a dipole moment of 4.5 D) for a range of fractional abundance gradients (in km s\(^{-1}\) pc\(^{-1}\)). For convenience, calculations were done with a large velocity gradient (LVG) code that is essentially equivalent to an LTE calculation for optically thin lines, as appropriate for the weak emission seen in H\(_2\)C\(_4\) and H\(_2\)C\(_6\). We assumed typical conditions found in the TMC-1 clumps: \(T_{\text{kin}} = 10\) K and \(n(H_2) = 10^6\) cm\(^{-3}\). The observed fractional abundances of H\(_2\)C\(_4\) and H\(_2\)C\(_6\), assuming \(\Delta V/\Delta L = 5\) km s\(^{-1}\) pc\(^{-1}\), are marked by filled triangles.

![Diagram](image-url)

**Fig. 2.** The antenna temperatures for the ortho levels of H\(_2\)C\(_6\) (solid lines) and para levels of H\(_2\)C\(_4\) (dashed lines) calculated using a LVG excitation model and approximating the energy levels with a simple linear rotor (see text) as a function of \(J\). The parameters are \(T_{\text{kin}} = 10\) K, \(n(H_2) = 10^6\) cm\(^{-3}\), and \(\Delta V/\Delta L = 1\) km s\(^{-1}\) pc\(^{-1}\). Curves for three fractional abundances (in units of km s\(^{-1}\) pc\(^{-1}\)) are shown for each molecule. The observed \(T_A\) for H\(_2\)C\(_6\) (filled triangle) and H\(_2\)C\(_4\) (filled circles) are marked in the figures along with their 1 \(\sigma\) error bars. Total fractional abundances need to include a factor for the ortho and para fractions, the velocity gradient, and antenna efficiency (see text).

![Diagram](image-url)

**Fig. 3.** Fractional abundances of five carbon chains, C\(_3\)H, C\(_4\)H\(_2\), H\(_2\)C\(_3\)H, H\(_2\)C\(_4\), and H\(_2\)C\(_5\)N as a function of number of carbons \(C_n\). These are taken from the early time solutions for the gas-phase chemical model of Millar et al. (1997) for a cold cloud core with \(T_{\text{kin}} = 10\) K and \(n(H_2) = 10^6\) cm\(^{-3}\). The observed fractional abundances of H\(_2\)C\(_4\) and H\(_2\)C\(_6\), assuming \(\Delta V/\Delta L = 5\) km s\(^{-1}\) pc\(^{-1}\), are marked by filled triangles.
hydrocarbon production up to 8 or 9 carbons, but does not include the carbon insertion reactions.

In Figure 3 we plot these model abundances for the carbon chains $C_2nH$, $C_{2n+1}H$, $H_2C_{2n}$, $H_2C_{2n+1}$, and $HC_{2n+1}N$, as well as a point for $c$-$C_3H_2$ for the physical conditions relevant to this core of TMC-1. Figure 3 uses the early-time results of Millar et al. (1997), as only this evolutionary stage has enough neutral carbon to produce a successful complex carbon chemistry with large hydrocarbon abundances. The late-times, or steady state, solutions have too little carbon and complex carbon species to explain the observations. This result is not surprising, as other tracers, such as CCS, confirm the ages of these dense core components to be $\leq$ a few $\times 10^5$ years (Kuiper, Langer, & Velusamy 1996; Velusamy et al. 1997). Note that the $C_nH$ radicals are predicted to be more abundant than the corresponding $H_2C_n$ cumulene carbenes, as observed. However, the Millar et al. (1997) model also predicts that $H_2C_6$ is more abundant than $H_2C_4$, which is exactly the opposite of what is observed. The measured $H_2C_4$ abundance agrees within a factor of 2 with their model calculations, while the predicted $H_2C_4$ fractional abundance is too low by a factor $\approx 25$. On the other hand, the observed $H_2C_4/H_2C_6$ ratio is consistent with the slope of the abundance versus chain length in the $C_nH$ radicals. However, some caution is in order regarding absolute abundances, because this model does not distinguish between different isomers such as triacetylene ($HC_6H$) and $H_2C_6$.

Bettens et al. (1995) explored the effects of various assumptions about the neutral-neutral reactions on the production of complex carbon molecules in interstellar clouds. Bettens & Herbst (1996) recommend using two of their chemical models which best explain the polyatomic species: the new standard model (NSM) and model 4 (M4). NSM is a modified version of the standard ion-molecule chemical scheme; in M4, rapid neutral-neutral reactions play a critical role. A key feature of M4 is that the reactions $O + C_n \rightarrow C_{n-1} + CO$ are assumed negligible for $n > 2$. Model M4 of Bettens et al. (1995) provides the best agreement with our $H_2C_4$ observations, but the calculated abundance is still too high by a factor of 5. The models appear to be sensitive to assumptions about the neutral-neutral reaction rate coefficients at low temperature. $H_2C_6$ and $H_2C_4$ are important diagnostics for discrimination among models of hydrocarbon chemistry in dense cores; however, more laboratory measurements and astronomical observations are needed to resolve the hydrocarbon chemistry in dense cores.

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