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Letter to the Editor

Detection of a new linear carbon chain radical: C_7H

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Abstract. Following our discovery of C_8H in IRC+10216 (Cernicharo & Guélin 1996), we report the detection in this circumstellar envelope of another linear carbon chain radical, C_7H. The microwave spectrum of C_7H has been recently observed in the laboratory (Travers et al. 1996a) and its rotational line frequencies are precisely known.

With this new detection, the family of acetylenic chain radicals (C_nH) observed in space is complete up to $n = 8$. The members with even numbers of carbon atoms are consistently more abundant than the odd number members; C_7H is found to be a factor of 4 less abundant than C_8H and a factor of 20 less abundant than C_5H.

Key words: stars: molecular data – stars: AGB – circumstellar matter – ISM: molecules – radio lines: stars

1. Introduction

The linear carbon chain radicals (C_nH, $n = 2, 8$) are of particular interest to interstellar chemistry. Unfamiliar on earth like nearly all carbon chains, they are thought to form in the gas phase by reactions of CCH, CC, C, or C^+ with hydrocarbons, especially acetylene (see e.g. Cherchneff & Glassgold 1993, Millar & Herbst 1994 –hereafter M&H, Thaddeus 1994). At the edges of circumstellar shells, they may also evaporate from grain mantles (Guélin et al. 1993). One way to discriminate between these processes is to measure the abundances of the longest possible chains. It has been proposed that long carbon chain molecules may lock up a substantial amount of interstellar carbon and give rise to some of the diffuse interstellar bands (Thaddeus 1994).

Recently, Cernicharo & Guélin (1996, hereafter C&G) discovered C_8H in the envelope of the evolved carbon star IRC+10216. C_8H, the second longest carbon chain molecule in space after HC_9N (Travers et al. 1996c), is a factor of 6–10 less abundant than C_6H, the next longest acetylenic radical. The large decrement may mean that the process leading to the formation of C_4H and C_6H becomes inefficient for much larger chains. This decrement is also large compared to those observed for the cyanopolyynes ($HC_5N/HC_7N/HC_9N \simeq 5/2.5/1$, Kawaguchi et al. 1995, hereafter KKIK) and, mostly, for C_3H and C_5H, two radicals with an odd number of C-atoms (C_3H/C_5H= 1.6/1). Since even and odd C-atom chains may be formed via different paths, it is important to measure the abundance of C_7H and to compare it to C_5H. C_7H, until now the only radical between CH and C_8H not detected in space, has just been observed in the laboratory and its microwave rotational frequencies are accurately determined (Travers et al. 1996a). On the basis of this data we have successfully searched for this molecule in IRC+10216.

2. Observations and results

The observations were carried out in May and July 1996 with the IRAM 30-m telescope, using two receivers with orthogonal polarizations. Both receivers were tuned to operate in a single sideband mode, with rejection of the upper sideband (USB) of more than 20 dB. The rejection was checked by searching for lines in the USB; we see no trace of such lines, except for the $J = 1 - 0$ line of $H^{13}CN$ (outside the limits of Fig. 1) and the $2 - 1$ line of ^{29}SiO, which appear as 70 mK and 6 mK features, respectively. The system noise temperature, corrected for ohmic and rear spillover losses and atmospheric emission, was 140 K for one receiver and 180 K for the other. The spectra, obtained in the standard wobbling mode with a reference field located $90''$ from the star, were flat and, except for a constant offset,

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required no baseline removal. The backend consisted of two banks of 1-MHz wide filters with sharp edges.

C_7H has a regular electronic ground state, with the $^2\Pi_{3/2}$ fine structure state (or $\Omega = 3/2$ ladder) 37 K above the $^2\Pi_{1/2}$ state (Travers et al. 1996a). Its Λ doubling constants are very small, yielding Λ doubling splittings much smaller than the Doppler linewidth (splittings $\simeq$ 2 MHz for the $J = 47.5 - 46.5$, $\Omega = 1/2$ transition and 0.2 MHz for the corresponding $\Omega = 3/2$ transition, vs Doppler width of 8.5 MHz).

Assuming a “cross-ladder” temperature similar to those of C_5H and C_6H ($T_{cross} \simeq T_k = 50 - 60$ K), we expect the population of the ground $^2\Pi_{1/2}$ state to be almost twice that of the $^2\Pi_{3/2}$ state and therefore the rotational lines in the $\Omega = 1/2$ ladder to be stronger. Moreover, since intensities of the lines in the lowest ladders of C_6H and C_8H are well described by rotational temperatures $T_{rot} = 35 - 50$ K, we expect the strongest C_7H lines observable with the IRAM 30-m telescope to lie at the lower end of the 3-mm band.

We have searched for the three lowest ground state transitions of C_7H within the receiver band, the $J = 47.5 - 46.5, 48.5 - 47.5$ and $49.5 - 48.5$ transitions of the $\Omega = 1/2$ ladder, and in so doing we covered 2 transitions of the $\Omega = 3/2$ ladder. The observed spectra, are shown in Fig. 1 and the line parameters listed in Table 1. The integration time per spectrum (after addition of both polarization channels) is 11 – 15h and the resulting r.m.s. noise per 1 MHz channel is only 1.0–1.4 mK. Because the baselines are very flat, all features larger than 4 MHz and stronger than 2 mK are probably real.

Most lines observed in IRC+10216 with the 30-m telescope (see e.g., Fig. 1 of C&G) have sharp edges, a width of $\Delta v = 29.5$ km s^{-1}, and the cusped shape expected for optically thin lines arising in the outer expanding shell of this star. They are centred at exactly $V_{sys} = -26.4$ km s^{-1}, and are easy to identify even in crowded regions of the spectrum. One line in Fig. 1, with a rest frequency of 83035 MHz, appears narrower ($\sim$ 7 km s^{-1}); it is probably the $^3\Pi_0, v = 1, J = 2 - 1, f$ transition of vibrationally excited SiC (E/k = 1500 K), and probably arises in the inner envelope.

Besides the SiC line at 83035 MHz, 6 lines of Fig. 1 are readily identified. These are the two $N = 9 - 8$ spin-doublet components of $CCC^{13}CH$ (83048.4 and 83085.8 MHz), the two $N = 7 - 6$ spin-doublet components of MgNC in its first excited bending state ($v_2 = 1$), the $4_{14} - 3_{13}$ transition of $SiC^{13}C$ (86562.5 MHz) and the $J = 5 - 4$ transition of the rare $^{29}Si^{34}S$ isotopomer (86617.7 MHz). The frequencies of these 6 lines are precisely known from microwave laboratory measurements (Chen et al. 1995, Kagi et al. 1996, Cernicharo et al. 1991); their intensities are close to those expected from the corresponding lines of the main isotopomers or ground states. We note in this respect that the $v_2 = 1$ bending state of MgNC lies only 86 cm^{-1} above the ground state (Kagi et al. 1996) — i.e., low enough to be excited in the outer envelope, where MgNC is formed (Guélin et al. 1993). The best assigned C_7H lines have the standard 8.5 MHz (29.5 km s^{-1}) Doppler width. A seventh line, at 83131 MHz, is probably a blend of the $J = 5 - 4$, $K = 0, 1$ transitions of $^{13}CH_3CCH$: it has the correct frequency (83131 MHz) and is within a factor of 2 of the expected intensity (1 mK).

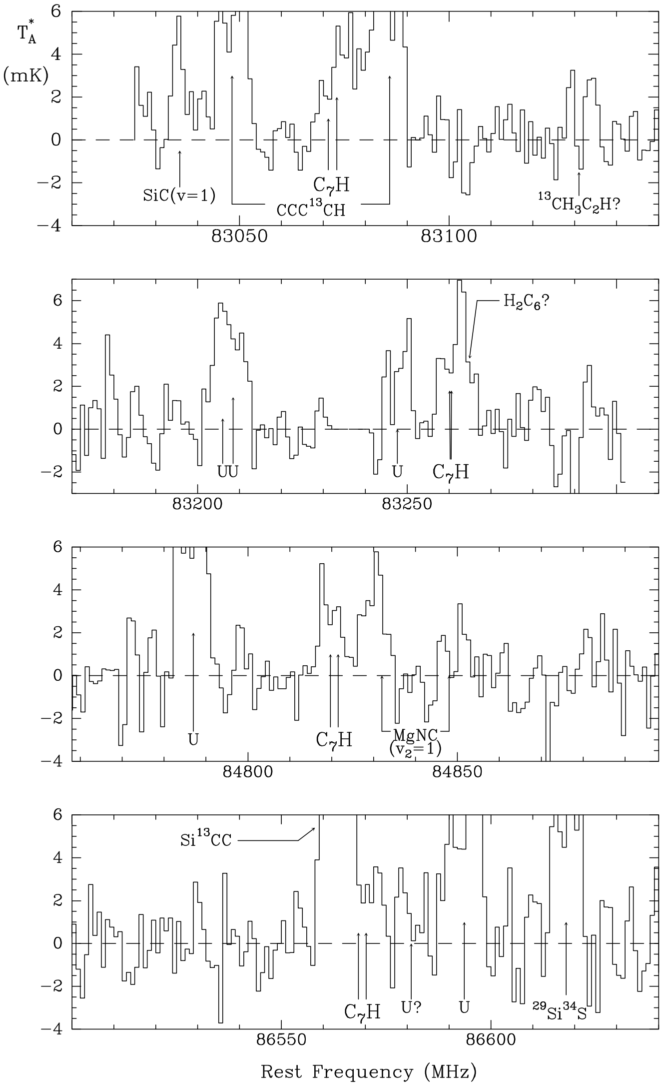

Fig. 1. Four 30-m telescope spectra covering 4 rotational transitions of C_7H (the Λ doublet components are indicated by vertical arrows). Two 8 MHz-wide intervals contaminated by strong lines from the upper sideband have been deleted. Unidentified lines are denoted ‘U’. Note the $N = 7 - 6$ doublet of vibrationally excited MgNC and the possible identification of H_2C_6 at 83264 MHz, on the right hand side of the C_7H line.

The positions of the C_7H $^2\Pi_{1/2}$ $J = 47.5 - 46.5, 48.5 - 47.5$ and $49.5 - 48.5$ Λ doublet components and of the $^2\Pi_{3/2}$ $J = 47.5 - 46.5$ components are indicated in Fig. 1 by vertical arrows. Each coincides with a weak line or line shoulder of intensity $\simeq$ 3 mK. The best line (84820 MHz) is well resolved from the nearby MgCN doublet and is 5σ in signal to noise. The other three lines (83073, 83261 and 86571 MHz) are blended on one side; their significance (derived from a fit of the confusion-free channels to a 8.5 MHz-wide rectangular line) is $4 - 5\sigma$. The fitted line rest frequencies agree to within the uncertainties with the C_7H transition frequencies (see Table 1).

There is little doubt that the lines at 83073, 83261, 84820 and 86571 MHz are real. Could they arise from species other than C_7H? We have searched for possible assignments of these lines in the standard catalogs of lines of astrophysical interest (e.g. Lovas 1984), as well as in our own line catalog. This latter (see Cernicharo et al. 1996) includes all the species and isotopomers observed in IRC+10216.

The only transitions within 6 MHz of our 4 lines are high J transitions of HC_9N and a transition of H_2C_6. In particular, the J = $146-145$ HC_9N line at 84820.6 MHz coincides with the 84820 MHz line, but its intensity is very probably too small to observe, because the abundance of HC_9N is low and the J = 146 level is too high in energy (E/k = 300 K vs T_{rot} = 23 K, according to KKIK).

HC_9N is 5 times less abundant than HC_7N in IRC+10216 and its $\lambda \geq 6$ mm lines are 5–7 times weaker than those of HC_7N (KKIK). At λ = 3 mm, the HC_9N/HC_7N intensity ratio drops abruptly; the J = 146 level of HC_9N, for example, lies 150 K above the J = 74 level of HC_7N yielding a Boltzmann factor $\exp((E_u - E'_u)/kT_{rot})$ = 700 for T_{rot} = 23 K. Since the $J = 74-73$ (83.46 GHz) and $J = 75-74$ (84.59 GHz) lines of HC_7N have intensities of $7-8$ mK and are only 2-3 times stronger than the 84820 MHz line, the contribution of HC_9N to that line is negligible. We note in this respect that the 4 to 78 GHz spectrum of HC_9N was recently measured in the laboratory by Travers et al. (1996b) and that the 3 mm transition frequencies are known to better than 40 kHz.

The rotational spectrum of the carbene H_2C_6 has also been recently measured in the laboratory by McCarthy et al. (1996b). The $31_{1,30} - 30_{1,29}$ transition has a frequency of 83264 MHz, too high to match the 83260 MHz line, but in good agreement with the blended $\simeq$ 3 mK line on its high frequency side. Another 3 mK line (outside the borders of Fig. 1) is detected at 83472 MHz, the frequency of the $31_{1,31} - 30_{1,30}$ transition of H_2C_6, lending further support to a possible detection of this molecule. Unfortunately, we have not covered other H_2C_6 transitions with a good enough sensitivity to confirm these tentative assignments.

The four lines designated C_7H in Fig. 1 have no plausible alternate assignment. Could they be unrelated unidentified (U) lines? There are only 6 or 7 U lines with intensities $\geq$ 2 mK visible in this figure, which corresponds to one U-line per 80 MHz. A similar U-line density is found over the 82–86 MHz band in the new spectral survey. The chances that 4 U-lines agree within 1–2 MHz with C_7H are thus very small, so we conclude that we have detected C_7H.

As noted above, the $J = 47.5 - 46.5$ (83260.3 MHz) and $48.5 - 47.5$ (85013.0 MHz) transitions of the $^2\Pi_{3/2}$ state lie 37 K above the corresponding $^2\Pi_{1/2}$ state transitions. They give thus rise to lines $\exp(37/T_{cross})$ times weaker. The 83260.3 MHz line in Fig. 1 has about the same strength as the 83070 MHz ground state line which, taking into account the uncertainties on the line intensities, yields $T_{cross} > 40$ K. On the other hand, we have only marginally detected the 85013 MHz line, which appears as a weak (1.5 mK or 2σ) feature. This yields $T_{cross} < 60$ K.

3. The abundance of C_7H

The dipole moment of C_7H has been estimated by Pauzat et al. (1991) from SCF calculations ($\mu_\circ$ = 5.09 D) and, more recently, by Woon (1995) from high level coupled-cluster theory calculations with a large correlation consistent basis set ($\mu_\circ$ = 5.95 D). Because the SCF calculations are likely to underestimate $\mu_\circ$ by $\simeq$ 20% (Y. Ellinger *priv. comm.*), we adopt $\mu_\circ$ = 5.95 D in the following.

Table 1. Table 1: Observed Line Parameters

Frequency (MHz)	Transition $\Omega, J \rightarrow J'$	Obs-calc† (MHz)	E_u/k (K)	$\int T_a^* dv$ (K.kms^{-1})
83072.9‡ (15)	1/2, 47.5–46.5	1.0	92.7	0.06(2)
83261.0‡ (8)	3/2, 47.5–46.5	0.6	129.7	0.08(2)
84819.5 (10)	1/2, 48.5–47.5	-1.1	96.6	0.08(2)
85013 (2)	3/2, 48.5–47.5	2.5	133.7	0.03(2)
86571.5‡ (10)	1/2, 49.5–48.5	1.3	100.7	0.07(2)

† Calculated from laboratory measured constants (Travers et al. 1996a).
‡ Blended lines: the rest frequencies and integrated intensities are derived from a double-line fit, assuming lines with cusped shapes and width Δv = 29.5 km s^{-1}. The r.m.s. uncertainties (in parentheses) are in units of the last digit.

In order to estimate the C_7H column density, we need to know the rotational level population. Contrary to CO and HCN, which are observed throughout the CS envelope, the carbon chain radicals seem confined to a relatively thin shell of radius $R \simeq 15''$, temperature $T_k \simeq$ 50 K and density $n_{H_2} \simeq 10^{3-4}$ (Guélin et al. 1993). The line intensities of the long chain molecules are well described from λ = 1 cm to λ = 2 mm by $T_{rot} = 25-50$ K. For simplicity, we assume that the fractionnal abundance of C_7H, relative to H_2, is constant within a spherical shell of inner radius $12''$ and outer radius $18''$ and zero elsewhere and that the rotational level population within a fine structure state follows a Boltmann distribution with T_{rot} = 35 K. The integrated intensities of Table 1 then yield an average column density along the line of sight (twice the column density along a radius) of 1.4 10^{12} cm^{-2} for the $\Omega = 1/2$ state and, for T_{cross} = 50 K, a total column density of 2 10^{12} cm^{-2}.

Fig. 2 shows how the C_7H column density compares with those observed for the other carbon chain radicals. The latter were calculated from the 70–250 GHz data of Cernicharo et al. (1987, 1996) and the 28–50 GHz data of KKIK. A single value of T_{rot} was fitted for each species and we assumed the same spatial distribution as for C_8H. We used the dipole moments of Woon (1995), which, for C_5H and C_6H are significantly larger than those adopted by Cernicharo et al. (1987) and KKIK.

The C_nH radicals with odd n appear consistently less abundant than the radicals with even n, and the convergence of the 'odd' and 'even' curves, observed between n = 3 and n = 6, does not continue at larger n. The 'even' and 'odd' curves show both a flat section (the first two species have similar abundances), followed by a fairly steep slope with a decrease by

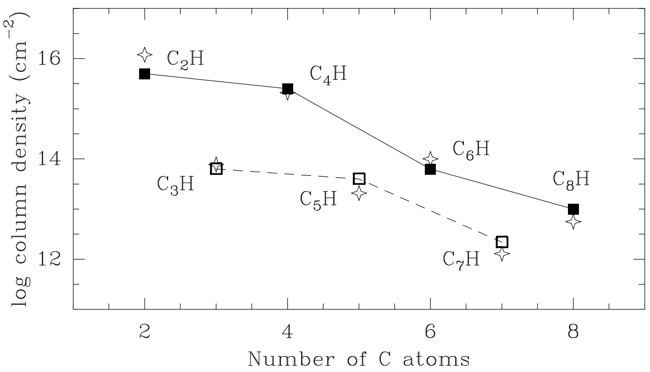

Fig. 2. Observed (squares) and predicted (stars) column densities of the carbon chain radicals C_nH in IRC+10216. The observed column densities have been calculated in the case of a spherical shell source of inner radius 12″ and outer radius 18″ (see text). The predicted column densities are from M&H.

a factor of 10–20 for each additional CC group. The near constant slope suggests that the long chains are formed sequentially (C_6H from C_4H and C_7H from C_5H) by similar-type reactions; the relatively low abundances of the first two species, C_2H and C_3H, suggest, on the other hand, a distinct formation mechanism (which, for C_2H might be photodissociation). This behaviour is fairly similar to that predicted by neutral-neutral reaction models: we have plotted on Fig. 2 the abundances calculated by M&H in the case of a medium-high acetylene abundance ($2.5\,10^{-5}$). The agreement is obviously good. It should not, however, be considered as conclusive, because it depends largely on the values adopted for the acetylene abundance and the UV radiation intensity, two parameters which largely control the positions and slope of the curves. The model, moreover, predicts that C_2H, C_3H and C_4H peak at different distances from the star, contrary to observation (Guélin et al. 1993).

The Millar & Herbst model can be used, in principle, to estimate the abundance of the next carbon chain radical, C_9H, to see if it is possible to detect it. M&H quote $C_9H/C_7H \simeq 1$, but the large C_9H abundance mostly results from a truncation of their reaction network for $n > 9$ in which most destruction channels of C_9H are ignored. More probably, $C_9H/C_7H \simeq C_7H/C_5H$, in which case C_9H will be very difficult to detect in IRC+10216, despite a predicted large dipole moment and known rest frequencies (McCarthy et al. 1996a).

4. Summary and prospects

We have detected in IRC+10216 3 rotational lines from the lower ($^2\Pi_{1/2}$) fine structure state of C_7H and one from the upper ($^2\Pi_{3/2}$) fine structure state. The lines have frequencies between 83 and 87 GHz and quantum numbers J_u between 47.5 and 49.5.

The C_7H column density, calculated for a rotation temperature of 35 K, is $\simeq 2\,10^{12}$ cm^{-2}. It is about 20 times smaller than the column density of C_5H and 4 times smaller than that of C_8H. The sharp abundance decrements observed between C_5H and C_7H, on the one hand, and between C_6H and C_8H, on the other hand, reduce the liklihood that a large fraction of the carbon in IRC+10216 is locked into long carbon chains. The situation could however be different in dense dark clouds like TMC1 or in the diffuse interstellar gas.

Observation of other lines with very different J numbers would be needed to determine directly the rotation temperature of C_7H and to better constrain the abundance of this radical. This, however, may turn out to be difficult. The line intensities observed with the 30-m telescope (HPBW= 28″, beam efficiency B_{eff} = 0.75) are 2–3 mK, close to the detection limit for 8 MHz-wide lines with this instrument. Lines with much higher J are probably too weak to detect. The line strength, which increases at lower frequencies, probably peaks at about 50 GHz, i.e., at the upper end of the NRO 7-mm receiver tuning band. The two-fold higher expected line intensity suggests that detection of the 50 GHz lines may be possible. A search for C_7H should also be made in the dark cloud TMC1, because the formation mechanisms of carbon chain radicals may be quite different in TMC1 and IRC+10216.

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