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CCH $N=4-3$ emission from dense interstellar clouds

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Summary. We have searched for $N=4$–3 rotational line emission from the ethynyl radical CCH, at 349 GHz toward a number of galactic molecular clouds. We have detected emission from ten giant molecular clouds and have derived CCH column densities on the order of 10^{14}–10^{15} cm^{-2}. We find that CCH emission arises from dense gas, $n(H_2) \sim 10^4$–10^5 cm^{-3}, but not from very dense material, $n(H_2) > 10^6$ cm^{-3}, nor from hot gas such as the "hot core" region in Orion. We show that our observations are consistent with our knowledge of interstellar chemistry.

Key words: interstellar medium: molecules – interstellar medium: abundances.

1. Introduction

The ethynyl radical, CCH, was identified in interstellar clouds by Tucker et al. (1974) and several surveys have been performed in the $N=1-0$ rotational lines (Wootten et al., 1980; Huggins et al., 1984). These observations have shown that CCH is widespread in the Galaxy being detected in giant molecular clouds and dark dust clouds, as well as in absorption in spiral arm gas glouds (Nyman, 1984) and in the circumstellar envelopes of carbon-rich stars (Huggins et al., 1984). These low frequency observations indicate that emission from CCH is optically thin, in contrast with observations of the $N=3-2$ lines at 262 GHz by Ziurys et al. (1982) and Blake et al. (1986), which suggest that these lines are optically thick.

The $N=4-3$ transition of CCH at 349.4 GHz has been detected in Orion by Loren and Wootten (1986) and by White et al. (1986) who made a partial map of its distribution. In this paper we report the results of a search for $N=4-3$ emission toward several giant molecular clouds. Our observations and results are presented in the following section. Ethynyl is the simplest hydrocarbon containing more than one carbon atom. It is of interest chemically because it may be linked through its formation to the unobservable (at radio wavelengths) molecules methane, CH_4, and acetylene, C_2H_2, and, through its destruction, to the C_3- and C_4-hydrocarbons. Ethynyl has been identified as a key reactant in complex molecule formation in both interstellar clouds and carbon-rich circumstellar envelopes (e.g. Millar and Nejad, 1985. Nejad and Millar, 1987). We discuss the chemical implications of our observations in Sect. 3.

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2. Observational results

2.1. Observations

Our observations were carried out with the 3.8 m United Kingdom Infrared Telescope (UKIRT) on Mauna Kea, Hawaii during August 1985 using the Queen Mary College InSb heterodyne receiver (White et al., 1986). The system noise temperature was typically 300–400 K (single sideband equivalent), sky attenuation was checked frequently using standard chopper wheel calibration techniques and an rms pointing error of $<5''$ and a HPBW of $55''$ were obtained by star tracking and observations of Jupiter.

Our observed antenna temperatures have been converted to corrected radiation temperature, T_R^* (Kutner and Ulich, 1981) by dividing by $\eta_{fss}=0.88$ (White et al., 1986) which corrects for all atmospheric and telescope losses. In order to derive the true radiation temperature, T_R, we must divide T_R^* by η_c, the coupling efficiency, which takes into account the source size relative to the beam size. Figure 1 of White et al. (1986) gives η_c as a function of source size for the QMC/UKIRT system at 345 GHz. The partial map of CCH in Orion by White et al. gives a source size $\gtrsim 3'$, while sizes derived from CS observations (Linke and Goldsmith, 1980; Snell et al. 1984) of sources in which we have detected CCH, also are $\sim 3'$ (see Table 3 for details). For simplicity, we adopt a size of $3'$ for all sources in which we have detected CCH. This implies $\eta_c=0.9$, the value we have used in calculating column densities although we present the data in our tables and figures in terms of T_R^*.

The $^2\Sigma$ ground state of CCH shows fine structure, indicated by quantum number J, and hyperfine splitting, labelled by quantum number F. The $N=4-3$ rotational transition thus gives rise to 11 allowed transitions in the neighbourhood of 349.4 GHz (Ziurys et al., 1982). We observed at a central frequency of 349400.612 MHz (Sastry et al., 1981) with a spectral resolution of 1 MHz and a spectral bandwidth of 20–70 MHz, depending on the particular source. We thus detect a blend due to the $(N, J, F)=(4,7/2,4)-(3,5/2,3)$ and $(4,7/2,3)-(3,5/2,2)$ transitions which are separated by ~ 1.4 MHz (equivalent to a velocity separation of 1.2 km s^{-1}). This separation, barely resolvable by

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Table 1. CCH $N=4-3$ data

Source	R A (1980)	Dec (1950)	T_R^*	Δv (km s⁻¹)	v_{LSR} (km s⁻¹)
ρ Oph C	16 23 15	-24 19 30	< 0.65		
ρ Oph A	16 23 21	-24 16 49	< 0.15		
ρ Oph D	16 24 20	-24 22 42	< 0.44		
ρ Oph B	16 24 20	-24 20 49	< 0.22		
M17 SW	18 17 26	-16 14 54	1.16	5.5	20.0
M17 H_2	18 17 50	-16 09 45	< 0.58		
Serpens	18 27 24	01 12 40	< 0.15		
G34.3+0.1	18 50 46	01 10 46	< 0.44		
G35.2-0.75N	18 55 41	01 36 30	1.53	3.2	35.0
W51	19 21 27	14 24 30	1.3	8.7	57.0
S106	20 25 32	37 12 35	1.9	4.0	1.0
W75N	20 36 50	42 26 58	< 0.44		
DR21	20 37 14	42 09 12	1.16	4.0	-2.0
DR21 (OH)	20 37 14	42 12 08	0.95	3.5	-2.0
NGC 1333	03 25 26	31 06 18	< 0.58		
HH 7-11	03 25 58	31 05 46	< 0.58		
L 1551	04 28 40	18 01 45	< 0.44		
L 1641	05 32 24	-05 48 01	< 0.44		
NGC 1977	05 32 47	-04 58 11	1.45	2.5	11.2
OMC - 1[a]	05 32 47	-05 24 23	7.3	3.5	9.4
OMC - 2	05 33 00	-05 12 00	< 0.73		
OMC - 2(W)	05 33 00	-05 12 34	< 0.51		
OMC - 1(R)	05 32 51	-05 21 24	3.4	3.0	11.0
NGC 2024	05 39 12	-01 55 42	1.53	2.7	11.5
M78	05 43 35	-00 11 17	< 0.22		
Mon R2	06 05 20	-06 22 30	2.2	4.8	12.5
S255	06 10 01	18 00 00	< 0.87		

NOTE: [a] White et al. (1986)

our receiver, may account for some of the flat-topped and unusually broad line profiles we detected. For optically thin emission, this doublet carries about 42% of the total intensity in the $N=4-3$ transition, while the $(J,F)=(9/2,5)-(7/2,4)$ and $(9/2,4)-(7/2,3)$ doublet at 349.34 GHz should contain ~55% of the emission: we have chosen to observe the doublet at 349.4 Gz because this is observed to be the stronger of the two in Orion (White et al., 1986; Loren and Wootten, 1986).

2.2. Detections

Table 1 lists the sources in which we searched for the CCH $N=4-3$ line. This transition was detected in nine regions in addition to Orion-KL and the Orion 3′N, 1′E – the so-called "radical" – position. Table 1 gives values of peak T_R^* and, for sources in which CCH was detected, the lsr velocity (km s^{-1}) and the line width at half maximum, Δv (km s^{-1}). Figure 1 shows several of the observed line profiles.

2.3. Column densities

The (4,7/2,4) level of CCH lies 41.9 K above the ground state and requires densities in excess of 10^6 cm^{-3} in order to be thermalised. However, as we shall discuss in the following section, CCH is destroyed by chemical reactions in regions of very high density so that it is likely that the CCH we have detected is excited subthermally. This is true, for example, at the OMC-1(R) position – the "radical peak" – where observations of H_2CO by Evans et al. (1975) indicate $n(H_2)\sim10^5$ cm^{-3}. At Orion-KL, several distinct cloud components are apparent in the emission spectra of many molecules. However, neither our line parameters for the $N=4-3$ transition nor those for the $N=3-2$ transition (Ziurys et al., 1982; Blake et al., 1986) show emission from the high-density, $n(H_2)\sim10^7$ cm^{-3}, "hot core" region, but are consistent with the presence of CCH in the ambient ridge clouds, $n(H_2)\sim10^5$ cm^{-3}, a fact illustrated in the $N=4-3$ map presented by White et al. (1986).

The rotational excitation temperature, $T_{\rm rot}$, is unknown. Ziurys et al. (1982) estimated $T_{\rm rot}=9$ K in Orion, assuming optically thin $N=3-2$ emission. However, since this emission is likely to be optically thick, $T_{\rm rot}>9$ K; we present estimates for the column densities using values of $T_{\rm rot}$ in the range 10–50 K. In addition we shall assume that the $N=4-3$, $J=7/2-5/2$ blend which we observe is optically thin, although we know that this is not the case in Orion-KL. In this case, the column density in an upper level N is given by (Ziurys et al., 1982)

$$nL\,({\rm cm}^{-2})=\frac{3k\,(2N+1)\,T_R\,\Delta v}{8\pi^3\mu_D^2 N R_{hf}\,\nu},$$

where T_R is the peak radiation temperature, Δv is the line width at half-maximum, μ_D is the dipole moment, taken to be 0.8 D (Wilson and Green, 1977), $R_{hf}(=0.418)$ is the relative intensity of the hyperfine blend observed and the other symbols have their usual meaning. Using the integral expression for the partition function we find that the total column density is

$$N_T\,({\rm cm}^{-2})=2.13\;10^{11}\,T_{\rm rot}\,T_R\,\Delta v\,\exp(41.9/T_{\rm rot})$$

with Δv measured in km s^{-1}. Table 2 gives our estimates for N_T for those sources in which we detected emission. Typically $N_T\sim10^{14}$–10^{15} cm^{-2} in agreement with previous determinations (Tucker and Kutner, 1978; Wootten et al., 1980; Ziurys et al., 1982). In order to compare our results with those of theoretical models we need to know both the volume densities and column

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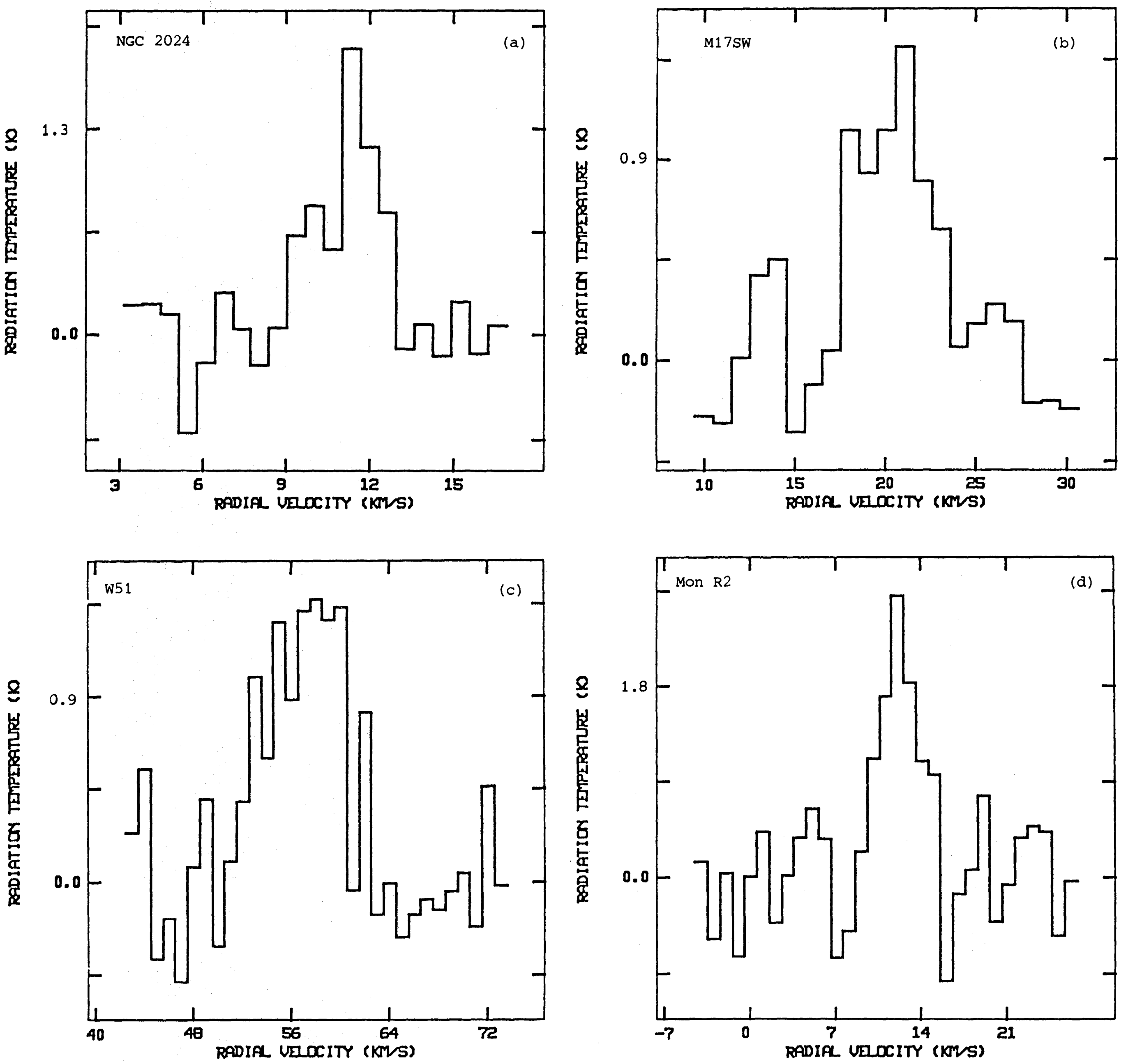

Fig. 1a–d. CCH $N=4-3$ lines observed toward **a** NGC 2024, **b** M17SW, **c** W51, and **d** Mon R2

densities of molecular hydrogen in our clouds. Table 3 lists these quantities although we note that the errors in both $n(H_2)$ and $N(H_2)$ are large and preclude a strict comparison between observations and theory. Nonetheless they should give fractional abundances of CCH correct to an order of magnitude. Typically $n(H_2) \sim 10^5$–$10^6\,\mathrm{cm}^{-3}$ and $N(H_2) \sim (2-10) \times 10^{23}\,\mathrm{cm}^{-2}$, leading to a fractional abundance of CCH, $x(\mathrm{CCH}) \sim 10^{-9}$–$10^{-10}$ if $T_{\mathrm{rot}} \gtrsim 20\,\mathrm{K}$.

3. Discussion

Our observations show that CCH is common in dense molecular clouds but not in extremely dense cores, $n > 10^6\,\mathrm{cm}^{-3}$, within these clouds nor in "hot core" regions such as in Orion. In this section we shall show that our results are reasonably consistent with current chemical models of interstellar clouds.

In dense interstellar clouds, the CCH radical is formed in the dissociative recombination of $C_2H_2^+$ and $C_2H_3^+$,

$$C_2H_2^+ + e \rightarrow \mathrm{CCH} + \mathrm{H} \tag{1a}$$

$$\rightarrow \mathrm{CH} + \mathrm{CH}, \tag{1b}$$

$$C_2H_3^+ + e \rightarrow \mathrm{CCH} + H_2 \tag{2a}$$

$$\rightarrow C_2H_2 + \mathrm{H}. \tag{2b}$$

It is destroyed in reactions with oxygen atoms

$$\mathrm{CCH} + \mathrm{O} \rightarrow \mathrm{CO} + \mathrm{CH} \tag{3}$$

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Table 2. Column density estimates for CCH[a]

Source	T_{rot} (K) 10	20	50
M17 SW	10.0	2.4	1.8
G35.2-0.75N	7.6	1.9	1.3
W51	17.7	4.3	3.1
S106	11.9	2.9	2.1
DR21	7.2	1.8	1.2
DR21 (OH)	5.2	1.3	0.91
NGC 1977	5.7	1.4	0.99
OMC - 1[b]	39.9	9.8	7.0
OMC - 1 (R)	15.9	3.9	2.8
NGC 2024	6.4	1.6	1.1
Mon R2	16.6	4.1	2.9

NOTES: (a) Column densities are given in units of 10^{14} cm^{-2} and are calculated using T_R^* and Δv from Table 1 and the coupling efficiency η_c = 0.9 (see text). (b) Data for this position taken from White et al. (1986).

Table 3. Molecular hydrogen column densities, volume densities and source sizes for the regions in which we detected CCH emission

Source	$N(H_2)cm^{-2}$	$n(H_2)cm^{-3}$	Size (arcmin)	Ref.
M17 SW	4(23)[a]	6(4)	3 x 3	1
G35.2-0.75N	1.5(23)	6(5)	2 x 1	2,3
W51	2(24)	1(5)	4 x 3	1
S106	~ 6(23)		4 x 4	4[b]
DR21	3.9(23)	1.6(5)	>3 x 3	5
DR21 (OH)	6.0(23)	2.7(5)	>3 x 3	5
NGC 1977		3(4)-1(6)		6
OMC - 1	1(24)	1(5)	extended	7
OMC - 1(R)	3(23)	1(4)	extended	8
NGC 2024	3(23)[c]	1.6(6)	6 x 1	9
Mon R2	2.5(23)	2(5)	2.5 x 2.5	1

a a(b) = a x 10^b
b Using $N(NH_3)$ from ref 4 and assuming $x(NH_3) = 10^{-8}$
c Using N(CS) from ref 9 and assuming $x(CS) = 5 \times 10^{-10}$

References:- (1) Linke and Goldsmith 1980, (2) Dent et al. 1985a, (3) Dent et al. 1985b, (4) Little et al. 1979, (5) Richardson et al. 1986, (6) Kutner et al. 1985, (7) Evans et al. 1975, (8) Blake et al. 1987, (9) Evans et al. 1987

and in ion-molecule reactions with ions such as He^+, C^+ and so on, that with C^+

$$C^+ + CCH \rightarrow C_3^+ + H \tag{4}$$

being most important. The $C_2H_2^+$ and $C_2H_3^+$ ions are formed in reactions of C^+ with methane, CH_4,

$$C^+ + CH_4 \rightarrow C_2H_2^+ + H_2 \tag{5a}$$

$$\rightarrow C_2H_3^+ + H\,. \tag{5b}$$

$C_2H_2^+$ has a slow radiative association with H_2 ($k \sim 10^{-13}\,cm^3\,s^{-1}$ at 30–50 K, Herbst and Leung, 1986), while $C_2H_3^+$ is unreactive with H_2. As a result, reactions (1) and (2) are the dominant loss mechanisms for $C_2H_2^+$ and $C_2H_3^+$, and we can write the fractional abundance of CCH as

$$x(CCH) = \frac{0.5\,k_5\,x(C^+)\,x(CH_4)}{k_3\,x(0) + k_4\,x(C^+)}\,,$$

where $k_5 = k_{5a} + k_{5b}$, and we have assumed a branching ratio of 0.5 for each of reactions (1a) and (2a). We have neglected all ion-molecule loss routes for CCH other than that involving C^+. The rate coefficients k_4 and k_5 are known fairly accurately but the correct value for k_3 is unknown. Prasad and Huntress (1980) assumed an activation energy, $E_A \sim 250$ K for reaction (3) but Millar and Freeman (1984) found that such a large value implied an abundance of CCH much larger than observed in cold, dense clouds such as TMC-1, while $E_A = 0$ K gave too little CCH (see also Herbst and Leung, 1986). In the calculations presented here, we use $E_A = 40$ K and 90 K, the former value being that which gives reasonable agreement between theory and observation in TMC-1 (Millar and Nejad, 1985).

We have carried out a time-dependent chemical kinetic calculation using the dense cloud model described by Millar et al. (1987) for a gas temperature of 30 K and $n(H_2) = 10^4$–$10^7\,cm^{-3}$.

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Table 4. Theoretical steady state fractional abundances for dense interstellar clouds with $T = 30$ K

$n(H_2)cm^{-3}$	$x(C^+)$	$x(O)$	$x(CH_4)$	$x(CCH)$ E_A=40K	90K
1.0(4)[a]	9.2(-10)	3.5(-5)	7.9(-8)	9.2(-11)	4.6(-10)
1.0(5)	9.3(-11)	3.5(-5)	1.0(-7)	1.2(-11)	6.1(-11)
1.0(6)	9.4(-12)	3.5(-5)	1.2(-7)	1.4(-12)	7.2(-12)
1.0(7)	9.7(-13)	3.5(-5)	1.7(-7)	1.7(-13)	8.7(-13)

[a] $a(b) = a \times 10^b$

Our detailed results show that $k_3 x(O) > k_4 x(C^+)$ so that an approximate equation for $x(CCH)$ is

$$x(CCH) = 0.5 k_5 x(C^+)\, x(CH_4)/k_3 x(O).$$

For either value of E_A, this expression gives values of $x(CCH)$ at steady-state less than a factor of two lower than those obtained from the detailed calculations for $n(H_2) \geqq 10^4\,cm^{-3}$ and thus can be used to study the density and temperature dependence of $x(CCH)$.

Table 4 contains some results, specifically the fractional abundances of C^+, O, CH_4, and CCH at steady-state ($t > 10^7$ yr), from the full time-dependent calculation for $E_A = 40$ K and $E_A = 90$ K. The abundances of C^+, O, and CH_4 are independent of the choice of E_A. It is clear that the decrease in $x(CCH)$ as $n(H_2)$ increases is due essentially to the decrease in $x(C^+)$. The C^+ ion is produced in the reaction

$$He^+ + CO \rightarrow C^+ + O + He \quad (6)$$

where the He^+ is produced by cosmic-ray ionisation of helium, which Millar and Nejad (1985) have shown gives rise to an inverse dependence of $x(He^+)$, and hence $x(C^+)$, on density. Thus, the non-detection of CCH in regions of very high density, $n(H_2) \gtrsim 10^6\,cm^{-3}$, is due to (i) the low fractional abundance of C^+ and (ii) destruction by O atoms, a significant population of which remains in the gas phase at high density. Likewise the non-detection of CCH is 'hot core' regions may be due to very efficient destruction by O atoms since the high kinetic temperatures of such sources ensure that the activation energy in reaction (3) is overcome. However detailed chemical models of the Orion Hot Core by Brown et al. (1988) argue for a different explanation. They argue that the non-detection of CCH (and other radicals) is due to the accretion and subsequent hydrogenation of CCH (to C_2H_2) on the surface of interstellar dust grains in a cold clump of gas which eventually evolves into the hot core.

Finally, we note that the fractional abundances observed are in general agreement with the calculated steady-state values for $n \gtrsim 10^5\,cm^{-3}$ if $E_A \sim 90$ K. This is contrary to the conclusion of Prasad and Huntress (1980) and is due to the more accurate rate coefficients and more detailed and extensive hydrocarbon chemistry used in the present model.

4. Conclusions

We have detected $N = 4-3$ rotational line emission from the radial CCH toward a number of galactic molecular clouds. Our observed fractional abundances are consistent with a theoretical model in which the CCH arises in gas with a density $\sim 10^5\,cm^{-3}$ but not in denser gas, $n(H_2) \gtrsim 10^6\,cm^{-3}$, implying that, as observed, the CCH is excited sub-thermally. The CCH abundance is consistent with a formation mechanism involving C^+, whose fractional abundance decreases as the density increases, and destruction by oxygen atoms, whose fractional abundance is independent of density. The observed column densities and derived fractional abundances of CCH are in reasonable agreement with current models of interstellar chemistry and suggest that time-dependent effects such as those invoked by Prasad and Huntress (1980) are not required.

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