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THE DETECTION OF CYANOHEXATRIYNE, H(C ≡ C)$_3$CN, IN HEILES'S CLOUD 2

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ABSTRACT

The $J = 9 \rightarrow 8$ and $21 \rightarrow 20$ rotational transitions of the heavy linear molecule cyanohexatriyne, H(C ≡ C)$_3$CN, have been detected in Heiles's Cloud 2, a dark cloud at a distance of 115 pc in Taurus. This molecule, which contains eight heavy atoms and has a molecular weight of 99 amu, was synthesized specifically for the purpose of interstellar detection. Statistical-equilibrium calculations indicate a total column density of 2.7×10^{13} molecules cm^{-2}. This abundance is down by a factor of only 2 from that of H(C ≡ C)$_2$CN.

Subject heading: interstellar: molecules

I. INTRODUCTION

Hydrogen cyanide, HCN, and cyanoethyne (cyanoacetylene), HC ≡ CCN, are known to be quite abundant in interstellar clouds (Morris *et al.* 1976). To aid in the search for the next member of the series, the long linear molecule cyanobutadiyne (cyanodiacetylene), H(C ≡ C)$_2$CN, was synthesized in 1975 and its rotational spectrum studied by Alexander, Kroto, and Walton (1976).

Subsequently, cyanobutadiyne was discovered in Sgr B2 by Avery *et al.* (1976). An analysis of the observed lines in Sgr B2 indicated that the total column density of cyanobutadiyne is not much smaller than that of cyanoacetylene (Broten *et al.* 1976).

For molecules of similar atomic constitution and dipole moment, the geometric configuration which most favors detection is a linear one because of dilution arising from the many K components of nonlinear species. The cyanopolyynes, such as cyanoacetylene and cyanobutadiyne, fit this requirement.

The next member of the cyanopolyyne series, cyanohexatriyne, [H(C ≡ C)$_3$CN], has now been synthesized and studied specifically with a view to detecting this species in interstellar space. An analysis of the $J = 24 \leftarrow 23$ to $35 \leftarrow 34$ transitions observed in the laboratory yielded $B_0 = 564.00074 \pm 0.00016$ MHz and $D_0 = 0.00382 \pm 0.000087$ kHz (Kirby, Kroto, and Walton 1978). The nitrogen quadrupole hyperfine structure can be estimated assuming $eqQ = -4.12$ MHz as in cyanobutadiyne (Broten *et al.* 1976) and is given in Table 1 for the $J = 9 \rightarrow 8$ transition.

II. OBSERVATIONS

On the basis of the laboratory data, a search was made during 1977 March 26–30 for the $J = 9 \rightarrow 8$ transition of cyanohexatriyne (at 10152.002 MHz) by using the 46 m telescope of the Algonquin Radio Observatory.[1] At 10.15 GHz, the half-power beamwidth of the antenna is 2.′7 and the beam efficiency, η_B, is 0.65. An antenna temperature of 1 K corresponds to a flux density of approximately 4 Jy for a point source. The system noise temperature at the zenith is about 120 K. The spectrometer, which was used in the total-power mode, is a dual bank filter system that permitted simultaneous observations at spectral resolutions of 30 kHz (0.90 km s^{-1}) and 10 kHz (0.30 km s^{-1}). The observing procedure was essentially as described by Avery *et al.* (1976).

TABLE 1

PREDICTED $J = 9 \rightarrow 8$ FREQUENCIES AND INTENSITIES OF THE HYPERFINE COMPONENTS FOR CYANOHEXATRIYNE

$F' \rightarrow F''$	ω (MHz)	$\Delta\omega$ (MHz)	Relative Intensity
9→9	10150.538	−1.464	0.41
8→7	10151.990	−0.012	29.41
9→8	10152.002	0.000	32.92
10→9	10152.010	+0.008	36.84
8→9	10152.174	+0.172	0.001
8→8	10153.638	+1.636	0.41

NOTE.—Calculated with $B_0 = 564.00074$ MHz; $D_0 = 0.00382$ kHz; $eqQ = -4.12$ MHz.

Nine sources were observed, but the line was detected only in Heiles's Cloud 2. The line was found at two positions separated by 6.′0, indicating that the H(C ≡ C)$_3$CN cloud is extended.

In order to confirm the identification, a search for the $J = 21 \rightarrow 20$ transition at 23687.890 MHz was undertaken on the 36.6 m radio telescope at Haystack Ob-

[1] The Algonquin Radio Observatory is operated by the National Research Council of Canada as a national radio astronomy facility.

TABLE 2

SUMMARY OF OBSERVATIONAL RESULTS IN CLOUD 2

TRANSITION	POSITION α(1950)	POSITION δ(1950)	ΔT_A* (K)	V_{LSR} (km s^{-1})	ΔV† (kms^{-1})
$J=9\rightarrow8$.....	$04^h38^m42^s0$	25°35′45″	0.08±0.01	5.85±0.15	1.0±0.3
	04 38 25.2	25 39 30	0.09±0.02	5.85±0.30	1.0±0.5
$J=21\rightarrow20$.....	04 38 42.0	25 35 45	0.206±0.023	5.93±0.02	0.35±0.05
	04 38 25.2	25 39 30	0.115±0.027	5.90±0.04	0.30±0.09
	04 38 11.8	25 42 30	0.133±0.024	5.83±0.04	0.53±0.11

* ΔT_A is antenna temperature of the line.

† ΔV is full width at half-maximum of unresolved three main hyperfine components.

servatory.[2] A maser radiometer was used in the observations, along with a 1024-channel autocorrelation spectrometer which gave a resolution of 4.88 kHz (0.062 km s^{-1}). The observations, which were made in total-power mode by using position switching, were carried out during 1977 July 15–17 and resulted in detection of the second line at three positions in Cloud 2. The observational results are summarized in Table 2.

Figures 1 and 2 show the spectra of the $J = 9 \rightarrow 8$ and $J = 21 \rightarrow 20$ lines obtained at $\alpha(1950) = 04^h38^m42^s0$, $\delta(1950) = 25°35'45''$, the position of the peak of the cyanobutadiyne distribution mapped by MacLeod, Avery, and Broten (1978). The observed $J = 9 \rightarrow 8$ line is consistent with the theoretical hyperfine structure (Table 1) for intrinsic line widths characteristic of Cloud 2 ($\sim$0.5 km s^{-1}). The three main hyperfine components of the $J = 21 \rightarrow 20$ line are separated by less than 5 kHz and are not resolved.

Table 3 contains our 3 σ upper limits and search coordinates for the sources in which cyanohexatriyne was not detected at 10.2 GHz.

III. DISCUSSION

To estimate the total column density of cyanohexatriyne, we have carried out statistical-equilibrium calculations incorporating the 50 lowest rotational levels of the ground vibrational state. We have assumed that the H(C ≡ C)$_3$CN cloud is optically thin and that it coexists spatially with H(C ≡ C)$_2$CN. On the basis of observations by Churchwell *et al.* 1978 of the $J = 9 \rightarrow 8$ line of H(C ≡ C)$_2$CN, we have approximated the H(C ≡ C)$_3$CN source distribution by a two-dimensional Gaussian with full widths at half-maximum of 1′.3 and 6′.0. The appropriate beam-dilution factors have been included in our calculations.

The dipole moment of H(C ≡ C)$_3$CN has not yet been determined, but we estimate it to be 5.0 debye. This estimate is based on the trend of the dipole moments of HCN, HC ≡ CCN, and H(C ≡ C)$_2$CN of 2.985 debye (Bhattacharya and Gordy 1960), 3.6 debye (Westenberg and Wilson 1950), and 4.33 debye (Alexander, Kroto, and Walton 1976).

The equilibrium calculations were carried out by using several different collisional cross sections and combinations of dipole, quadrupole, and hard collisions. For an H_2 density of 3×10^3 cm^{-3}, the best agreement with our observations was achieved by using a kinetic temperature of 8 K and only hard collisions. The resulting total column density of cyanohexatriyne at the first position in Table 2 is 2.7×10^{13} cm^{-2}. MacLeod, Avery, and Broten (1978), using similar calculations and assumptions for H(C ≡ C)$_2$CN in Cloud 2, found a column density of 5.1×10^{13} cm^{-2}. For Sgr B2, our observations imply an upper limit to the cyanohexatriyne column density of 8×10^{13} cm^{-2}, assuming LTE and $T_{ex} = 30$ K.

Our statistical-equilibrium calculations do not show large departures from LTE for either H(C ≡ C)$_2$CN or H(C ≡ C)$_3$CN, and we conclude that LTE is a good approximation for these heavy molecules in Cloud 2. Under this approximation, if the brightness temperature of a transition from $J \rightarrow J - 1$ is ΔT_J and the full line width at half-maximum is ΔV_J (km s^{-1}), then ΔT_J is related to the molecular column density, N, through the equation

$$\Delta T_J \Delta V_J = \frac{8\pi^3}{3}\left(\frac{\ln 2}{\pi}\right)^{1/2} \times \frac{N_h(T_{ex} - T_{bg})\nu_J^2\mu^2}{k^2 T_{ex}^2 \exp\left[hB_0 J(J+1)/kT_{ex}\right]}. \quad (1)$$

In these expressions, T_{ex} is the excitation temperature of the line, T_{bg} the temperature of the microwave back-

TABLE 3

SUMMARY OF NEGATIVE RESULTS FOR THE $J = 9 \rightarrow 8$ TRANSITION

SOURCE	POSITION α(1950)	POSITION δ(1950)	RESOLUTION (kHz)	ΔT_A* (K)
Sgr B2.....	$17^h44^m11^s0$	−28°22′30″	100	<0.018
IRC 10216..	09 45 15.0	+13 30 40	100	<0.040
ρ Oph.....	16 23 30.0	−24 17 20	30	<0.056
DR 21.....	20 37 14.0	+42 09 00	30	<0.036
W Hya.....	13 46 12.0	−28 07 06	30	<0.032
Ori A†.....	05 32 50.8	−05 20 34	30	<0.047
OMC-2.....	05 33 00.0	−05 12 34	30	<0.028
NGC 2264..	06 38 28.4	+09 32 12	30	<0.075

* Values of ΔT_A are 3 σ upper limits.

† Position of maximum CN, N_2H^+, HCO^+ intensity (Turner and Thaddeus 1977).

[2] Radio astronomy at Haystack Observatory is supported by the National Science Foundation under grant AST75-14701.

ground, μ the molecular dipole moment, and ν_J the line frequency.

It is clear from equation (1) that, at similar frequencies, $\Delta T_J \Delta V_J$ for the cyanopolyynes is proportional to the total column density. It is independent of the molecular size as long as the exponential factor is not much larger than 1.

Table 4 shows the column densities of hydrogen cyanide and the cyanopolyynes in Sgr B2 and Cloud 2. The HC ≡ CCN abundance in Cloud 2 from Morris *et al.* (1976) may have to be increased by a factor of ~2 if the beam dilution for HC ≡ CCN is similar to that for the heavier molecules. The presence of cyanobutadiyne and cyanohexatriyne in nearly equal abundances in Cloud 2 may lead to a better understanding of heavy molecule formation in dark clouds. Unfortunately, ion-molecule models (Herbst and Klemperer

TABLE 4

COLUMN DENSITIES (cm^{-2}) OF HCN AND THE CYANOPOLYYNE COMPOUNDS

MOLECULE	SOURCE	
	Sgr B2	Cloud 2
HCN.....	3×10^{14}*	?
HC≡CCN.....	3×10^{14}†	$1\text{–}5\times10^{13}$†
H(C≡C)$_2$CN.....	2×10^{14}‡	5.1×10^{13}§
H(C≡C)$_3$CN.....	$<8\times10^{13}$‖	2.7×10^{13}‖

* Morris *et al.* 1973.
† Morris *et al.* 1976.
‡ Broten *et al.* 1976.
§ MacLeod *et al.* 1978.
‖ This paper.

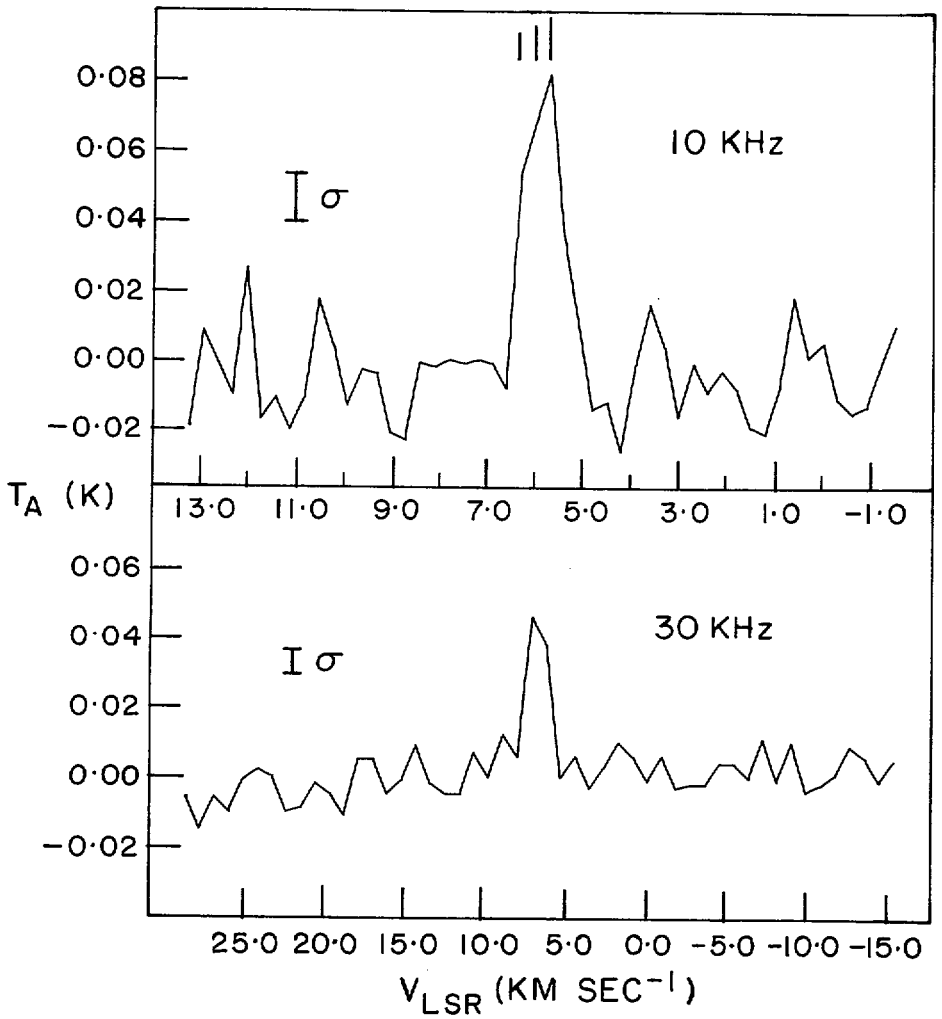

FIG. 1.—The $J = 9 \rightarrow 8$ line of H(C ≡ C)$_3$CN as observed at resolutions of 10 kHz and 30 kHz in Heiles's Cloud 2. The ordinate is antenna temperature. The positions and relative theoretical amplitudes of the three main hyperfine components are shown in the 10 kHz spectrum. In the 30 kHz spectrum the line appears weaker and broader than at 10 kHz because it was located midway between two spectrometer channels.

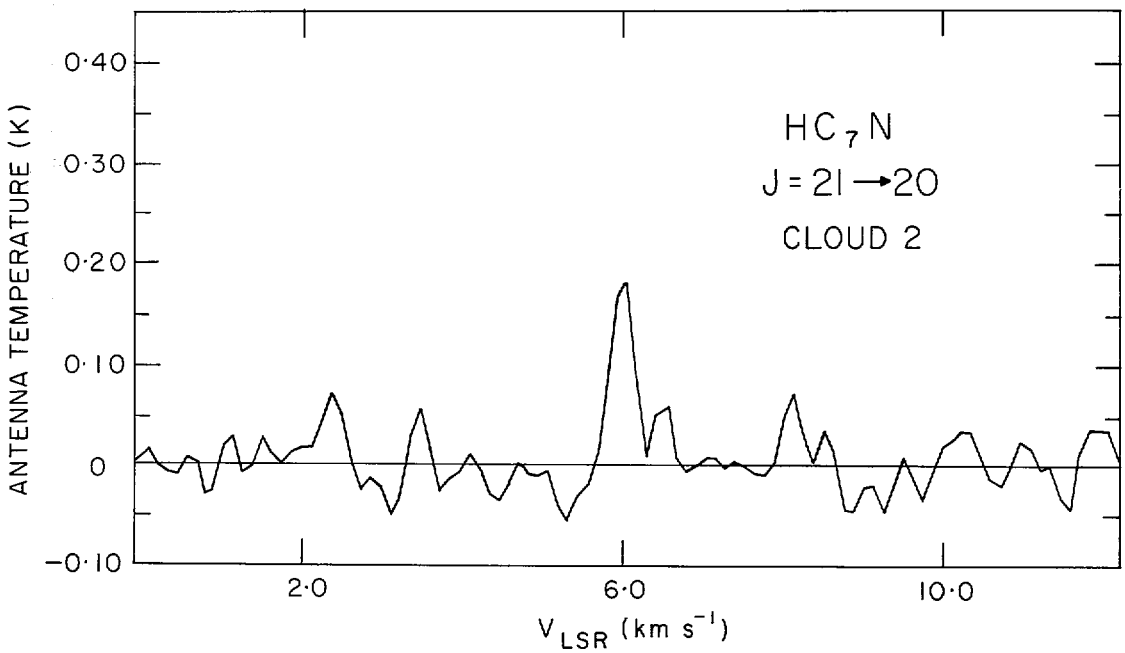

FIG. 2.—The $J = 21 \rightarrow 20$ line of $H(C \equiv C)_3CN$ in Cloud 2, filtered to a resolution of 19.5 kHz (0.25 km s^{-1})

1973; Watson 1973; Black and Dalgarno 1973) have not yet been developed for molecules with more than five atoms. Grain surface reactions (Allen and Robinson 1977; Iguchi 1975) have been developed for molecules with up to 11 atoms, but these molecules contained a maximum of four heavy atoms.

Allen and Robinson (1977) have estimated the theoretical abundance ratio $H(C \equiv C)_2CN/HC \equiv CCN$ by equating it with their $H(C \equiv C)_2/C \equiv CH$ ratio. For Sgr B2 this ratio is $\sim 3 \times 10^{-2}$, and $\sim 5 \times 10^{-4}$ for dark clouds of 10^6 yr age. Although their present model accounts very well for the $HC \equiv CCN$ abundance observed in Cloud 2 (Morris *et al.* 1976), it is quantitatively inadequate for $H(C \equiv C)_2CN$.

It is worth noting that Anders, Hayatsu, and Studier (1974) have experimentally studied catalytic surface reactions as a means of producing interstellar and meteoritic molecules. They found that a large variety of complex molecules could be produced in this manner, with a predominance of straight chain hydrocarbons over branched chains.

We believe that cyanohexatriyne with its eight heavy atoms makes more stringent demands upon theories of molecular formation than any other molecule yet detected. Other known interstellar molecules [e.g., ethanol, CH_3CH_2OH, and dimethyl ether, $(CH_3)_2O$] have the same total number of atoms but only three heavy atoms. The relatively high abundance of hydrogen makes these molecules easier to form through a series of reactions than $H(C \equiv C)_3CN$. If cyanohexatriyne were produced by successive encounters between simple carbon hydride compounds, then many reactions would be needed. It is not clear that there is sufficient time in sources such as Cloud 2 for these reactions to produce a detectable amount of $H(C \equiv C)_3CN$.

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