THE ASTROPHYSICAL JOURNAL, 223:L105–L107, 1978 July 15

THE DETECTION OF HC_9N IN INTERSTELLAR SPACE

N. W. BROTEN, T. OKA, L. W. AVERY, AND J. M. MACLEOD
Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa
AND
H. W. KROTO
School of Molecular Sciences, University of Sussex, Brighton
Received 1978 March; accepted 1978 May 10

ABSTRACT

With a molecular weight of 123 amu, and 11 atoms, HC_9N (cyano-octatetra-yne) is the heaviest and largest molecule yet detected in interstellar space. The $J = 18 \rightarrow 17$ and $J = 25 \rightarrow 24$ transitions have been observed in Heiles's Cloud 2 by using a molecular constant obtained by extrapolation from the lighter cyanopolyyne molecules. The column density is estimated to be 3.2×10^{12} cm^{-2}, down by a factor of 4 from that of HC_9N in the same source.

Subject headings: interstellar: molecules — molecular processes

I. INTRODUCTION

The recent detections of the long linear molecules HC_5N and HC_7N in appreciable abundance in the dark dust cloud Heiles's Cloud 2 (MacLeod, Avery, and Broten 1978; Kroto *et al.* 1978) have prompted us to undertake a search for the next member of the series, cyano-octatetra-yne (H—C≡C—C≡C—C≡C—C≡C—C≡N). In contrast to the situation for HC_5N and HC_7N, where laboratory frequencies were available (Alexander, Kroto, and Walton 1976; Kirby, Kroto, and Walton 1978), HC_9N has not yet been made in the laboratory. In view of the very long integration times anticipated for the search, an accurate method of estimating the value of the molecular constant B_0 had to be developed. The procedure we used is described by Oka (1978) and involves extrapolation of the molecular constants which have been measured for the lighter molecules HCN, HC_9N, HC_5N, and HC_7N. Using our calculated B_0 for HC_9N, we predicted the frequency of the $J = 18 \rightarrow 17$ and $J = 25 \rightarrow 24$ transitions and subsequently detected both of these transitions in the molecular ridge in Heiles's Cloud 2. We believe this to be the first interstellar molecule detected on the basis of a calculated rotational constant with no previous spectroscopic study.

With a molecular weight of 123 amu, HC_9N now replaces HC_7N as the heaviest known interstellar molecule.

II. OBSERVATIONS AND DETERMINATION OF B_0

Our predicted value for B_0 was 290.523 MHz, yielding a predicted frequency for the $J = 18 \rightarrow 17$ transition of 10458.8 MHz. Observations at this frequency were carried out with the 46 m telescope of the Algonquin Radio Observatory[1] in 1977 June, August, October, and November. The system temperature was 120 K, the telescope beamwidth was 2'.7, and the beam efficiency was $\eta_B = 0.65$. A dual bank spectrometer was used in the total power mode, with frequency resolutions of 30 kHz and 10 kHz (0.86 km s^{-1} and 0.29 km s^{-1}). The observing techniques used are summarized by Avery *et al.* (1976).

Observations were made at only one position in Heiles's Cloud 2, near the peak of the HC_5N ridge. This position was α (1950) = $04^h38^m38^s.6$, δ(1950) = 25°35'00". The total on-source observing time was 25 hours, yielding a channel-to-channel rms noise of 3.1 mK (30 kHz filters) and 5.7 mK (10 kHz filters).

A spectral line of 20 mK antenna temperature was detected at a rest frequency of 10458.634 MHz, with an assumed radial velocity of 5.8 km s^{-1} (based on HC_5N and HC_7N velocities at this position). The observed line is shown in Figure 1*a*, and its parameters are listed in Table 1. We identified this line with the $J = 18 \rightarrow 17$ transition of HC_9N. Using a centrifugal distortion constant $D_0 = 1.01$ Hz, estimated from $D_0(HC_9N) = D_0(HC_7N) \times [B_0(HC_9N)/B_0(HC_7N)]^2$, we obtained a revised estimate for B_0:

$$B_{01} = 290.5183 \pm 0.0002 \text{ MHz},$$

where the bulk of the uncertainty arises from an uncertainty of ± 0.25 km s^{-1} in V_{LSR}.

Using the above value of B_{01}, we calculated the expected laboratory frequency of the $J = 25 \rightarrow 24$ transition to be 14525.850 ± 0.012 MHz.

The 43 m radio telescope at the National Radio Astronomy Observatory,[2] Green Bank, West Virginia, was used to search for this transition in 1977 November. A dual channel parametric amplifier gave a system temperature of ~130 K. The beamwidth was ~2'.2 and the beam efficiency ~0.65. The 384-channel Mark II autocorrelation spectrometer was used in the parallel mode, with a total bandwidth of 1.25 MHz. This gave a

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

[2] Operated by Associated Universities, Inc., under contract with the National Science Foundation.

NRCC 16756

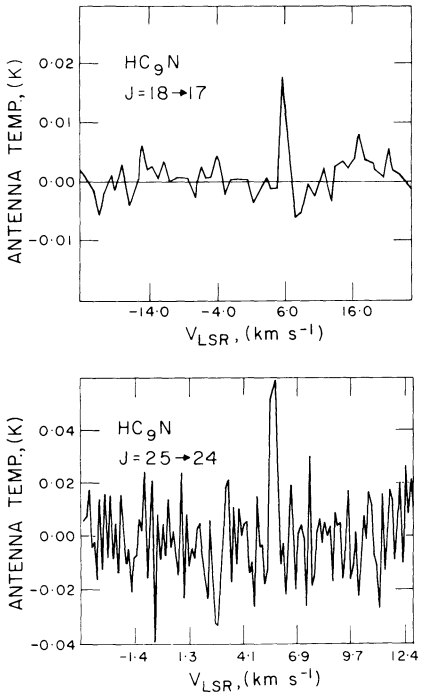

FIG. 1.—(*a*) Observed antenna temperature of the $J = 18 \rightarrow 17$ transition of HC_9N in Heiles's Cloud 2. The resolution is 30 kHz (0.86 km s^{-1}). (*b*) Observed antenna temperature of the $J = 25 \rightarrow 24$ transition of HC_9N in Heiles's Cloud 2. The channel separation is 6.5 kHz (0.13 km s^{-1}) and the effective resolution is 7.9 kHz (0.16 km s^{-1}).

channel separation of 6.5 kHz (0.13 km s^{-1}). Observations were made at $\alpha(1950) = 04^h38^m38^s6$, $\delta(1950) = 25°35'00''$, near the maximum HC_5N position in Cloud 2. The total observing time on source was 18 hours, and the rms noise on the final spectrum was 15 mK.

A spectral line was detected at a rest frequency of 14525.862 MHz. The observed line is shown in figure 1*b*, and its parameters are listed in Table 1.

Our measured rest frequency for this line agrees within 12 kHz with the predicted frequency of the $J = 25 \rightarrow 24$ transition of HC_9N, based on B_{01}. We thus consider that the observation of these two spectral lines constitutes the detection of HC_9N in interstellar space.

From our measurements of the $J = 25 \rightarrow 24$ transition, we can obtain a second revised estimate, B_{02}, for the molecular constant of 290.5185 MHz $\pm$0.0002.

Taking the mean of B_{01} and B_{02}, we obtain our best estimate for B_0 of 290.5184 $\pm$ 0.0002 MHz. We stress that the major uncertainty in this figure arises as a result of an uncertainty of $\pm$0.25 km s^{-1} in the radial velocity of the emitting gas. Even so, the accuracy to which we have determined B_0 for HC_9N by astronomical measurements is comparable with the accuracy to which Kirby *et al.* have determined B_0 for HC_7N by laboratory measurements (B_0 = 564.00074 $\pm$ 0.00016 MHz).

III. DISCUSSION

We have carried out statistical equilibrium calculations for HC_9N, making the following assumptions:

a) The HC_9N cloud is optically thin.

b) The HC_9N coexists spatially with HC_5N. We have not looked for HC_9N at any other position in Cloud 2, so we do not know that this is the case. However, we shall assume a molecular cloud size of 6'.0 × 1'.3 and include appropriate beam-dilution factors.

c) The dipole moment of HC_9N is 5.6 debye. This value is an extrapolation, based on the known dipole moments of HCN, HC_3N, and HC_5N.

d) The neutral hydrogen density is 4×10^4 cm^{-3} (Churchwell, Winnewisser, and Walmsley 1978).

e) The kinetic temperature is 11 K.

f) The line width (FWHP) is 0.4 km s^{-1}, independent of frequency.

g) There are hard collisions, with $\Delta J \leq 5$.

Details of the statistical equilibrium program are given in Avery *et al.* 1978. Using the above assumptions, and the observed integrated antenna temperature at 10.46 GHz, the total column density NL of HC_9N molecules at the position given earlier in Cloud 2 is 3.2×10^{12} cm^{-2}. This column density is down by a factor of ~4 from that of HC_7N in the same cloud.

The column densities of the cyanopolyynes HC_3N to HC_9N in Cloud 2 are listed in Table 2, based on 10GHz observations at ARO for HC_5N, HC_7N, and HC_9N, and 9 GHz Bonn observations of HC_3N (Churchwell *et al.*) For HC_5N, HC_7N, and HC_9N we have uniformly assumed the same parameters as listed in (*a*)–(*g*) above, except that for HC_5N, $\tau(4 \rightarrow 3) \approx 0.3$ has been taken into account in computing the column density of HC_5N. The results do not depend strongly on the assumed value of ΔJ.

It can be seen from Table 2 that each time two more carbon atoms are added to a cyanopolyyne, HC_nN, where n = 3, 5, 7, the abundance drops by a factor of ~4. It will be interesting to see whether this pattern of abundances holds true for other dust clouds containing these linear molecules. We have not yet attempted to detect HC_9N in any other sources.

TABLE 1

OBSERVED LINE PARAMETERS FOR HC_9N

Transition	T_A (K)	ΔV (km s^{-1})	$\int T_A \Delta V$ (K km s^{-1})	V_{LSR} (km s^{-1})
J=18→17 (ARO):				
0.86 km s^{-1} resolution....	0.019±0.003	0.86	0.020±0.003	5.8*
0.29 km s^{-1} resolution....	0.021±0.006	0.6±0.2	0.013±0.003	5.8*
J=25→24 (NRAO).....	0.073±0.012	0.35±0.08	0.027±0.008	5.8*

* Assumed.

TABLE 2

CYANOPOLYYNE COLUMN DENSITIES IN HEILES'S CLOUD 2

Molecule	Transition	ν(GHz)	$NL(10^{13}$ cm$^{-2})$
HC_3N.....	$J=1\rightarrow0$	9.098	$\gtrsim10$*
HC_5N.....	$J=4\rightarrow3$	10.651	5.0
HC_7N.....	$J=9\rightarrow8$	10.152	1.2
HC_9N.....	$J=18\rightarrow17$	10.459	0.32

* Estimate by Churchwell *et al.* (1978) based on measurements at their position (0,0), which they state is on the flank of the cloud; it is thus probably an underestimate.

IV. PREDICTIONS FOR $HC_{11}N$ AND $HC_{13}N$

The lines of HC_9N which we have detected are very weak, and it is of considerable interest to inquire whether it will be possible to detect heaver cyanopolyynes, using present-day systems. In figure 2, in addition to the curve of brightness temperature T_b versus frequency for HC_9N in Cloud 2, we have included several curves for other cyanopolyynes in Cloud 2 based on the same set of assumptions for T_K, $N(H_2)$, etc., given in § III. However, these curves are plotted for the same total column density of $NL = 1 \times 10^{13}$ cm^{-2} for all species, and must be scaled up or down to get the true brightness temperatures. Two effects can be noted:

i) The heavier the molecule, the lower the frequency at which its brightness temperature peaks.

ii) Even with the assumption of the same column density, the peak value of T_b decreases as the molecules become heavier.

If we assume that the abundance factor of ~4 continues to $HC_{11}N$, we can estimate the expected brightness temperature of the $J = 31 \rightarrow 30$ transition at 10.48 GHz to be ~39 mK in Heiles's Cloud 2. Such a line would give an antenna temperature of 10 mK in the 10 kHz filter bank of the Algonquin 46 m telescope, after allowing for beam dilution and beam efficiency. Detection of such a weak, narrow spectral line would be extremely difficult with present-day equipment.

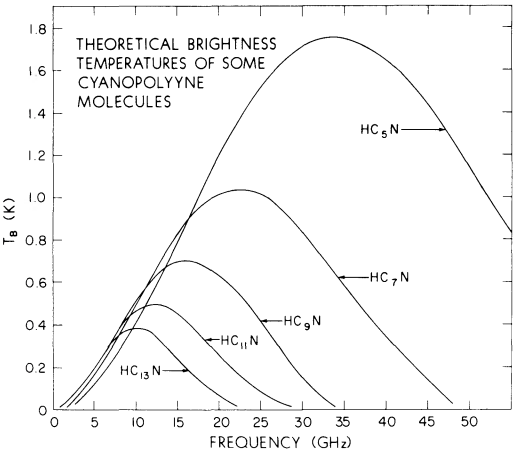

FIG. 2.—Brightness temperature versus frequency for several cyanopolyyne molecules, based on statistical equilibrium calculations using assumptions (*a*) to (*g*) listed in § III for HC_9N. For the heavier cyanopolyynes ($n > 5$), the dipole moment μ_{n+2} of $HC_{n+2}N$ was taken to be $\mu_n + 0.6$ debye, where μ_n is the dipole moment of HC_nN. For each cyanopolyyne, the same total column density $NL = 1 \times 10^{13}$ cm^{-2} has been used.

V. IMPLICATIONS FOR THE DIFFUSE INTERSTELLAR BANDS

Douglas (1977) has suggested that long chain carbon molecules C_n, where n may lie in the range 5–15, are the absorbing species which give rise to the well-known diffuse interstellar bands of optical astronomy. The presence of HC_5N, HC_7N, and now HC_9N in the interstellar medium suggests that long chain polyynes, which have no dipole moment and thus cannot be observed, are also very likely to be present. Douglas suggests that the shortest of the chains (C_2, C_3, C_4) are photodissociated in these regions, but chains beyond a certain length can lose the energy absorbed in the form of radiation by an internal conversion process, and thus are not readily photodissociated. This increase in stability of longer C_n molecules may reduce or arrest the decrease in abundance with chain length which has been observed up to HC_9N and may make possible the detection of some additional cyanopolyynes.

We thank the staff of the National Radio Astronomy Observatory for their kind hospitality and assistance during the Green Bank Observations. We appreciate the assistance of L. A. Higgs and A. Woodsworth during the computer reduction of the NRAO data. At Algonquin, special assistance in acquiring the astronomical data was capably provided by Paul Smith, Walter Turner, Rainer Glaeser, and Neil Armitage.

REFERENCES

Alexander, A. J., Kroto, H. W., and Walton, D. R. M. 1976, *J. Molec. Spectrosc.*, **62**, 175.
Avery, L. W., Broten, N.W., MacLeod, J. M., Oka, T., and Kroto, H. W. 1976, *Ap. J. (Letters)*, **205**, L173.
Avery, L. W., Oka, T., Broten, N. W., and MacLeod, J. M. 1978, in preparation.
Churchwell, E., Winnewisser, G., and Walmsley, C. M. 1978, *Astr. Ap.*, in press.
Douglas, A. E. 1977, *Nature*, **269**, 130.
Kirby, C., Kroto, H. W., and Walton, D. R. M. 1978, in preparation.
Kroto, H. W., Kirby, C., Walton, D. R. M., Avery, L. W., Broten, N. W., MacLeod, J. M., and Oka, T. 1978, *Ap. J. (Letters)*, **219**, L133.
MacLeod, J. M., Avery, L. W., and Broten, N. W. 1978, in preparation.
Oka, T. 1978, *J. Molec. Spectrosc.*, in press.

L. W. AVERY, N. W. BROTEN, J. M. MACLEOD, and T. OKA: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Canada

H. W. KROTO: School of Molecular Sciences, University of Sussex, Brighton, England