

## DETECTION OF THE HEAVY INTERSTELLAR MOLECULE CYANODIACETYLENE

L. W. AVERY, N. W. BROTON, J. M. MACLEOD, AND T. OKA

Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada

AND

H. W. KROTO

School of Molecular Sciences, University of Sussex, Brighton, England

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### ABSTRACT

The  $J = 4 \rightarrow 3$  rotational emission line of cyanodiacetylene  $\text{H}-\text{C}\equiv\text{C}-\text{C}\equiv\text{C}-\text{C}\equiv\text{N}$  has been detected in Sgr B2. If the molecules are assumed to be in thermal equilibrium at a temperature of 30 K, a column density of  $1.5 \times 10^{14} \text{ cm}^{-2}$  is obtained. This observation provides further evidence that heavy polyatomic molecules exist in abundance in Sgr B2.

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We have detected a new interstellar emission line in the molecular cloud Sgr B2 which we have attributed to the  $J = 4 \rightarrow 3$  rotational transition of cyanodiacetylene,  $\text{H}-\text{C}\equiv\text{C}-\text{C}\equiv\text{C}-\text{C}\equiv\text{N}$ . The frequency of the observed line agrees with the calculated value (10650.643 MHz) when a radial velocity for the molecular cloud of  $+62 \text{ km s}^{-1}$  is taken into account. This is a typical Doppler shift for most molecular lines found in Sgr B2. The identification will be confirmed if other transitions of this molecule can be detected, or if the hyperfine splitting can be resolved in a molecular cloud with small turbulence.

Cyanodiacetylene is a linear molecule with a large dipole moment. With a molecular weight of 75 amu, it is the heaviest molecule yet detected in interstellar space. The chain of 1 nitrogen and 5 carbon atoms contains more heavy atoms than any other molecule previously observed (cf. cyanoacetylene,  $\text{H}-\text{C}\equiv\text{C}-\text{C}\equiv\text{N}$  [Turner 1971] and vinyl cyanide,  $\text{CH}_2=\text{CH}-\text{C}\equiv\text{N}$  [Gardner and Winnewisser 1975a]). It is interesting to note that glycine, the simplest amino acid, has the same molecular weight. Unfortunately its microwave spectrum is unknown.

The microwave spectrum of cyanodiacetylene was observed in the laboratory recently by Alexander, Kroto and Walton (1975). The frequency of the  $J = 4 \rightarrow 3$  transition was calculated using their values of the rotational constant ( $B = 1331.3313 \pm 0.001 \text{ MHz}$ ) and the centrifugal distortion constant ( $D_J = 0.0257 \pm 0.002 \text{ kHz}$ ). The calculation is believed to have an accuracy of  $\pm 20 \text{ kHz}$ .

The lower rotational levels of cyanodiacetylene are shown in Figure 1. Because of its structural similarity, cyanoacetylene is also included. Cyanodiacetylene offers a large number of transitions at centimeter wavelengths because of its large moment of inertia.

The observations described here were made 1975 November 12-14 and 21-23 with the 46 m telescope of the Algonquin Radio Observatory.<sup>1</sup> At 10.7 GHz, the

<sup>1</sup>The Algonquin Radio Observatory is operated by the National Research Council of Canada as a national radio astronomy facility.

half-power beamwidth of the antenna is  $2'6$ , and the beam efficiency  $\eta_B$  is 0.65. An antenna temperature of 1 K corresponds to a flux density of approximately 4 Jy for a point source. The receiver is a cryogenically cooled parametric amplifier with a 3 dB bandwidth of 100 MHz. The system noise temperature at the zenith is about 120 K.

The ARO spectrometer, which was used in the total power mode, is a dual-bank filter system that permits simultaneous observations at two different spectral resolutions. Details of the spectrometer and the spectral processing procedure have been described by McLeish (1973).

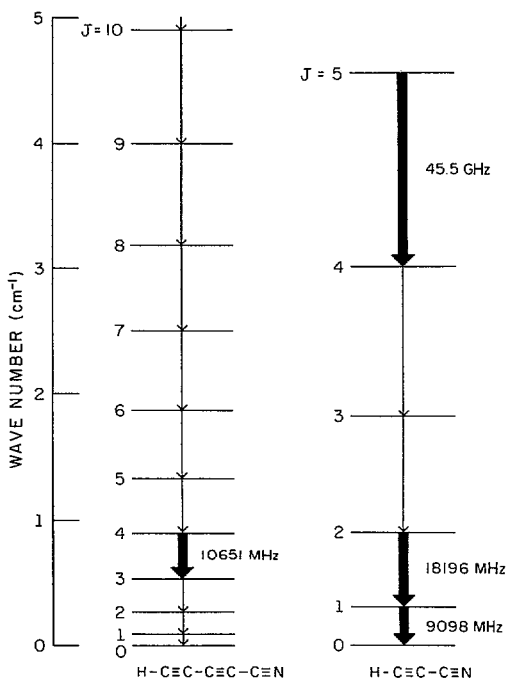


FIG. 1.—Lower rotational energy levels of cyanodiacetylene and cyanoacetylene. Transitions indicated by heavy arrows have been detected in interstellar clouds.

The difference between spectra for successive 10 minute periods on and off source were stored for further averaging. The off-source observations were taken at the same declination and hour angles as the on-source observations to remove systematic instrumental and background effects. The spectra were calibrated by observing W51 and DR 21.

We observed 2' north of the continuum peak of Sgr B2, and at the position of the Kleinmann-Low nebula in Orion. In each case positional accuracy was maintained by scanning the source to locate the continuum peak position and then offsetting by the required amount. The pointing was checked in this manner several times during each day's observations.

Figures 2 and 3 show the emission line we have attributed to cyanodiacetylene in Sgr B2, observed with resolutions of 100 kHz ( $2.8 \text{ km s}^{-1}$ ) and 30 kHz ( $0.8 \text{ km s}^{-1}$ ), respectively. The smooth line drawn through each spectrum is a simultaneous least-squares fit of Gaussian profiles and a composite baseline consisting of a straight line and a sine wave. The period of the sine wave is that of the ripple caused by multiple reflections between the prime-focus structure and the vertex of the main dish. Hyperfine splitting was calculated using the quadrupole coupling constant of cyanoacetylene ( $eqQ_N = -4.2 \text{ MHz}$  [Westenberg and Wilson 1950]). The three strong components with relative intensities of 0.24, 0.31 and 0.41, assuming thermal equilibrium, are shifted from the line center by  $-90 \text{ kHz}$  ( $F = 3 \rightarrow 2$ ),  $0 \text{ kHz}$  ( $F = 4 \rightarrow 3$ ), and  $+32 \text{ kHz}$  ( $F = 5 \rightarrow 4$ ), respectively. These components were not resolved in our observations. The components corresponding to  $F = 4 \rightarrow 4$ ,  $3 \rightarrow 3$ , and  $3 \rightarrow 4$  are weaker by a factor of about 50 and were not detected. The calculated frequencies and relative intensities of the six hyperfine components are shown in Figures 2 and 3.

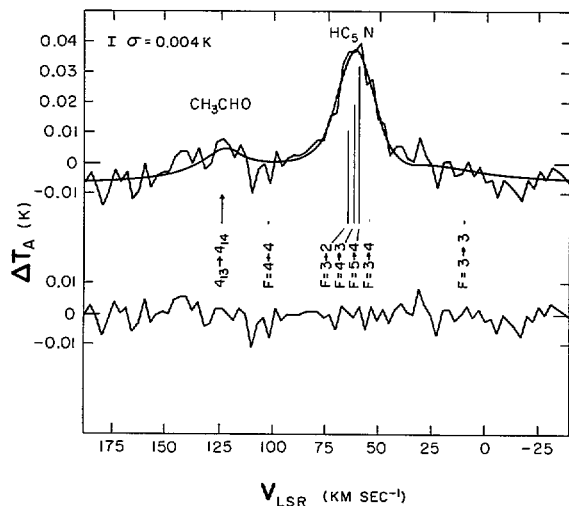


FIG. 2.—The emission line from Sgr B2 observed with 100 kHz resolution. The calculated frequencies and the relative intensities of the hyperfine lines of the  $J = 4 \rightarrow 3$  transition of cyanodiacetylene are indicated by vertical lines. Also shown is the expected frequency of the  $4_{13} \rightarrow 4_{14}$  line of acetaldehyde. The smooth line is a least-squares fit of Gaussian profiles and a composite baseline to the observed spectrum. The residuals are shown in the lower trace. The rms noise level is indicated by a vertical bar.

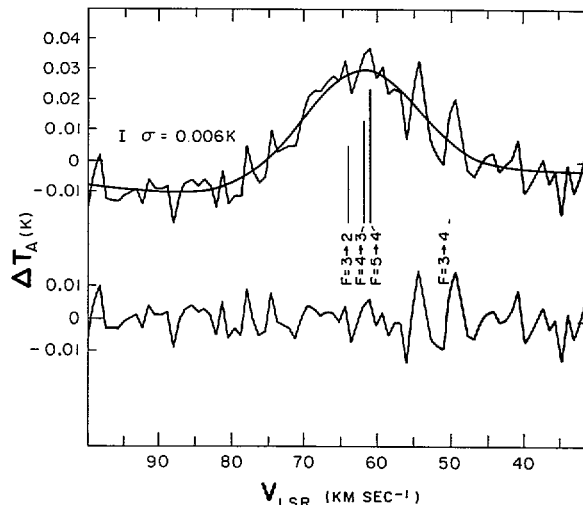


FIG. 3.—The emission line from Sgr B2 observed with 30 kHz resolution. See legend of Fig. 2 for details.

The expected position of the  $4_{13} \rightarrow 4_{14}$  transition of acetaldehyde ( $\text{CH}_3\text{CHO}$ ), based on a measured laboratory frequency of  $10648.428 \text{ MHz}$  (Bauder, Lovas, and Johnson 1974), is shown in Figure 2 by an arrow. There is an indication that this line is also present, but more observations are required before a detection can be claimed. For the present, we conclude that the antenna temperature of this line is less than  $0.01 \text{ K}$  in Sgr B2.

A summary of the results is given in Table 1. The cyanodiacetylene parameters for Sgr B2 are determined from the least-squares fit of a Gaussian profile to the spectral line. The average antenna temperature is  $0.037 \pm 0.002 \text{ K}$ . The velocity agrees well with that found for other molecules in this source, and the line width is similar to those found by McGee *et al.* (1973) for cyanoacetylene. The line parameters in Sgr B2 deduced from the 100 kHz and 30 kHz spectra are consistent allowing for experimental uncertainties. We did not detect the line in Orion. The values shown in the table are  $4\sigma$  upper limits.

Assuming that the cloud of cyanodiacetylene fills the beam, and that the excitation temperature is much greater than the background temperature, the weak line intensity implies that the cloud is optically thin. The first assumption is supported by the extent of the cyanoacetylene cloud (McGee *et al.* 1973). The excitation temperature for many other molecules in Sgr B2 lies in the range  $20\text{--}80 \text{ K}$  (cf. Cheung *et al.* 1969; Righini *et al.* 1975). The column density in the  $J = 4$  level can be written as (cf. Snyder 1972)

$$n_4 L = \frac{3ckT_{\text{ex}} f \Delta T dv}{8\pi^3 \nu_0^2 |\mu_{43}|^2 (T_{\text{ex}} - T_{\text{bg}})} \quad (1)$$

In this expression  $T_{\text{ex}}$  is the excitation temperature,  $T_{\text{bg}}$  the background temperature at the position of the cloud,  $\Delta T$  the brightness temperature of the spectral line, and  $\nu_0$  the center frequency of the line. The transition dipole matrix element  $|\mu_{J+1,J}|^2$  can be expressed as  $\mu^2(J+1)/(2J+3)$ , where the dipole moment  $\mu$  is 4.33 debyes for cyanodiacetylene.

TABLE 1  
SUMMARY OF OBSERVATIONAL RESULTS

Source	Molecule	Resolution (kHz)	$\Delta T_A^*$ (K)	$V_{LSR}$ (km s <sup>-1</sup> )	$\Delta V^\dagger$ (km s <sup>-1</sup> )	Integration Time <sup>‡</sup> (minutes)
Sgr B2.....	HC <sub>5</sub> N	100	0.036 ± .002	62.6 ± 0.6	19.4 ± 1.5	470
		30	0.039 ± .005	61.6 ± 0.6	19.0 ± 2.2	470
Orion KL.....	CH <sub>3</sub> CHO	100	<0.015	...	...	470
	HC <sub>5</sub> N	30	<0.025	...	...	410

\*  $\Delta T_A$  is the antenna temperature of the line.

†  $\Delta V$  is the full line width at half-maximum.

‡ Time spent on source.

To evaluate expression (1) we take the line antenna temperature,  $\Delta T_A$ , and full width at half-maximum,  $\Delta\nu$ , to be 0.037 K and 0.688 MHz, respectively. Assuming a Gaussian line shape, the integral in equation (1) is expressed as  $1.064 \Delta\nu \Delta T$ , where  $\Delta T$  is  $\Delta T_A / \eta_B$ . At a position 2' north of the Sgr B2 continuum peak the measured antenna temperature was 1.8 K, corresponding to a brightness temperature of 2.8 K. The 2.7 K cosmic background must be added to obtain 5.5 K for  $T_{bg}$ . This is an upper limit since some of the emission may originate in front of the molecular cloud. The value of  $T_{ex}$  is not known; but as long as  $T_{ex} \gg T_{bg}$ , the column density of the  $J = 4$  level does not depend strongly on  $T_{ex}$ . The column density of cyanodiacetylene in the  $J = 4$  rotational level is calculated to be  $2.7 \times 10^{12}$  cm<sup>-2</sup> for  $T_{ex} = 30$  K and  $2.5 \times 10^{12}$  cm<sup>-2</sup> for  $T_{ex} = 50$  K. If we assume thermal equilibrium at temperature  $T$ , the total column density is given by

$$NL = n_J L \frac{kT}{hB} \frac{1}{2J+1} \exp\left[\frac{hBJ(J+1)}{kT}\right]. \quad (2)$$

For cyanodiacetylene this yields values of  $1.5 \times 10^{14}$  cm<sup>-2</sup> if  $T = 30$  K and  $2.2 \times 10^{14}$  cm<sup>-2</sup> if  $T = 50$  K.

It is interesting to compare the above abundance with that of cyanoacetylene in Sgr B2. The column density of cyanoacetylene has been discussed by many authors; the estimates differ by two orders of magnitude depending on the line observed. From observations of the  $J = 1 \rightarrow 0$  line in Sgr B2, Turner (1971) obtained

a column density of  $2.1 \times 10^{16}$  cm<sup>-2</sup> which is similar to a revised value obtained by McGee *et al.* (1973) (see Gardner and Winnewisser 1975*b*). However, from the observations of four transitions,  $J = 8 \rightarrow 7$  to  $11 \rightarrow 10$ , in the millimeter region, Morris *et al.* (1973) obtained  $3 \times 10^{14}$  cm<sup>-2</sup> in Sgr B2. The observation by Dickinson (1972) of the  $J = 2 \rightarrow 1$  transition also indicated a much smaller abundance than that found by Turner (1971). An inversion of the  $J = 1 \rightarrow 0$  transition of cyanoacetylene has been suggested (Morris *et al.* 1973; Gardner and Winnewisser 1975*b*) to explain this inconsistency.

The column density of cyanodiacetylene obtained from our measurements is close to that of cyanoacetylene obtained from high- $J$  transitions and, based on discussions by Morris *et al.* (1973), is about 5 times higher than that of HCN in Sgr B2. These relative abundances are surprising and will provide a test for current theories of molecular formation.

If the abundance of cyanodiacetylene is real and not due to some nonequilibrium condition, then this observation suggests that many types of heavy molecules may exist in Sgr B2. The difficulty of observing them may be due not to their low abundance but to the fact that the heavier molecules are distributed over more rotational levels.

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*Note added in proof.* We have subsequently confirmed the identification of HC<sub>5</sub>N by detection of the  $J = 8-7$  line in Sgr B2 at 21,301.247 MHz.