CYANODIACETYLENE (HC₃N) IN SAGITTARIUS B2

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Received 1978 April 12; accepted 1979 January 3

ABSTRACT

The \( J = 2 \rightarrow 1 \) and \( 3 \rightarrow 2 \) rotational transitions of cyanodiacylene have been observed in Sgr B2. Statistical equilibrium calculations have been carried out to construct a three-component model of the HC₃N cloud in Sgr B2 which is consistent with these observations, with our earlier observations of the \( J = 1 \rightarrow 0 \), \( 4 \rightarrow 3 \), and \( 8 \rightarrow 7 \) lines and with the data obtained by Guélin and Thaddeus for the \( J = 31 \rightarrow 30 \) to \( J = 37 \rightarrow 36 \) millimeter-wave transitions. The relative strength of the \( J = 1 \rightarrow 0 \) line requires the presence of an extensive, low-density envelope around the Sgr B2 molecular cloud which serves as a weak \( 1 \rightarrow 0 \) line maser. This envelope is characterized by an H₂ density of 100 cm⁻³ and a kinetic temperature of about 20 K. The maximum column density of HC₃N in Sgr B2 is found to be \( 1.6 \times 10^{14} \text{ cm}^{-2} \), equal to that of HC₅N.

Subject headings: interstellar; molecules — masers

I. INTRODUCTION

The heavy linear molecule cyanodiacylene, HC₃N (also referred to as cyanobutadiene), was discovered in Sgr B2 by Avery et al. (1976), who observed the \( J = 4 \rightarrow 3 \) rotational transition of the ground state at 10.651 GHz. Subsequently, the discovery was confirmed by detection of the \( J = 8 \rightarrow 7 \) and \( J = 1 \rightarrow 0 \) lines at 21.301 GHz and 2.663 GHz, respectively (Broten et al. 1976).

The small rotational constant of this molecule \( (B_0 = 1331.331 \text{ MHz}) \) results in a large number of lines at microwave frequencies. This fact, plus the simple spectrum associated with a linear molecule, makes cyanodiacylene useful for studying molecular excitation and for modeling physical conditions in the interstellar clouds where it can be detected.

In particular, Broten et al. (1976) found evidence that the \( J = 1 \rightarrow 0 \) line in Sgr B2 is enhanced relative to the \( J = 4 \rightarrow 3 \) and \( 8 \rightarrow 7 \) lines. They attributed this effect to an overpopulation in the \( J = 1 \) level relative to \( J = 0 \), resulting in weak maser amplification of the \( J = 1 \rightarrow 0 \) line. This population inversion arises in low-density regions where the collisional rates are small. It is caused by the strong dependence of the rate of downward radiative transitions upon \( J \). The variation with \( J \) of the radiative rates for the \( J \rightarrow J-1 \) transition is given by

\[
R_J \propto \frac{J^3}{2J+1} B_0^2 \mu^2,
\]

where \( \mu \) is the molecular dipole moment. Thus the downward rate from \( J = 2 \) is about 5 times greater than that from \( J = 1 \), resulting in an accumulation of population in \( J = 1 \) relative to the ground level if the rate of collisional excitations is approximately equal to the radiative rates. The downward rates become more equal as \( J \) increases, so the tendency for population inversion is strongest for the \( J = 1 \rightarrow 0 \) transition.

This effect was first investigated in detail by Goldsmith (1972), who showed that a negative excitation temperature for the \( J = 1 \rightarrow 0 \) line of CO can occur for a wide range of physical conditions. Morris et al. (1976, hereafter MTPZ) also discuss this phenomenon in connection with cyanacetylene, HC₅N.

Because there is observational evidence that the \( J = 1 \rightarrow 0 \) transition of cyanodiacylene is enhanced in Sgr B2, we have undertaken a statistical equilibrium study of this molecule to model the physical conditions implied by the observations. To determine the extent of the population inversions in the lowest levels of HC₃N, we have also observed in Sgr B2 the \( J = 2 \rightarrow 1 \) and \( 3 \rightarrow 2 \) lines at 5.325 GHz and 7.988 GHz. These new observational results are reported in the following section.

II. OBSERVATIONS

a) Detection of the \( J = 2 \rightarrow 1 \) Transition

The \( J = 2 \rightarrow 1 \) rotational transition of cyanodiacylene was detected in the direction of Sgr B2 (OH) \( (\alpha_{1950} = 17^h 44^m 11^s, \delta_{1950} = -28^\circ 22' 30'') \) with the 43 m telescope of NRAO. The observing period was 1976 July 11–18.

The receiver, which was operated in the total power mode, was a dual-channel, cooled paramp, and the system temperature was typically 100 K when observing Sgr B2. Position switching was used with 10 minute source and reference scans for each spectrum. The reference scans were taken over the same range of hour angle as the corresponding source scans. Spectral information was obtained with the 384-channel autocorrelator in parallel configuration at a resolution of 52.4 kHz (2.95 km s⁻¹). At 5.3 GHz the antenna beamwidth was 5.4 and the beam efficiency, \( \eta_B \), was 0.65.

1 The National Radio Astronomy Observatory is operated by Associated Universities, Inc., under contract with the National Science Foundation.
The observed spectrum in the direction of Sgr B2 (OH). The positions and relative theoretical amplitudes (assuming thermal equilibrium) of the three strongest hyperfine components of the line are also shown. Table 1 contains a summary of the line parameters.

2) Detection of the $J = 3 \rightarrow 2$ Transition

The $J = 3 \rightarrow 2$ line was detected at Haystack Observatory, also in the direction of the Sgr B2 (OH) source, with the 37 m radio telescope. Observations were carried out from 1976 March 23 to 26. The receiver used was a cooled parang and the system temperature when observing Sgr B2 was typically 85 K. The spectrometer was a 100-channel autocorrelator with a frequency resolution of 166.7 kHz (6.24 km s$^{-1}$). Observations were made in the total power mode, using position switching at 5 minute intervals as described in § IIa. At 8.0 GHz the antenna beamwidth was 4\° and the beam efficiency was 0.55.

The $3 \rightarrow 2$ line is shown in Figure 1b and the observed parameters are listed in Table 1 along with other HC$_5$N data from Avery et al. (1976), Broten et al. (1976), and Guélin and Thaddeus (1978).

III. STATISTICAL EQUILIBRIUM CALCULATIONS

In our calculations of the statistical equilibrium of HC$_5$N, we have assumed that steady-state conditions prevail and have considered only the ground vibrational state. The linear structure of the molecule makes formulation of the equilibrium calculations particularly straightforward, although there are uncertainties in the various collisional cross sections. Because of the small value of $B_0$, a large number of levels must be included; we have considered between 50 and 90 levels, depending upon the assumed cloud temperature and degree of excitation of the molecule. Hyperfine splitting was neglected.

In evaluating the radiative rates, it is necessary to know the nature of the radiation field in the molecular cloud. We have assumed that all of the cyanodiacetylene ground-state transitions are optically thin. (The results of our calculations are consistent with this assumption.) Under such a condition, radiative trapping can be neglected and there are two principal sources of microwave radiation—the 2.8 K background and the galactic plane radiation, particularly that from the Sgr B2 continuum sources. The importance of the latter depends on the proximity of the H II regions to the molecular cloud. As this is not known, we have allowed the geometric dilution of the Sgr B2 continuum source to vary in the evaluation of the radiative rates. As discussed later, the best agreement with our observations was obtained with dilution factors small or zero, corresponding to the continuum sources subtending small solid angles as seen from the molecular cloud.

The collisional rates are dependent on total collisional cross sections and selection rules. Collisions with nonpolar H$_2$ molecules are primarily “hard” collisions which may result in level changes corresponding to large $\Delta J$, in contrast to collisions with...
polar molecules and charged particles which have selection rules \( \Delta J = 1 \) for dipole collisions or \( \Delta J = 2 \) for quadrupole collisions (Oka 1973).

Calculations have been carried out assuming only hard collisions. A total excitation cross section \( \sigma \) of \( 1.5 \times 10^{-14} \text{ cm}^2 \) was used. This value was obtained by scaling the total collisional cross section determined for HC\(_3\)N by Green and Chapman (1978) by a factor of 1.5 to allow for the greater length of HC\(_3\)N. For hard collisions, \( \sigma_{jJ} \), the excitation cross section from level \( J \) to level \( J'(J' > J) \) was taken to be

\[
\alpha_{J'} = \sigma Q g_J \exp \left( -E_J/kT \right) \quad \text{for} \quad J - J' \leq \Delta J_{\text{max}}
\]

and

\[
\alpha_{J'} = 0 \quad \text{for} \quad J - J' > \Delta J_{\text{max}}
\]

Here \( \Delta J_{\text{max}} \) is the greatest amount by which \( J \) was allowed to change, \( g_J = (2J + 1) \) is the statistical weight of level \( J' \), \( E_J \) is the rotational energy of the level, \( \sigma \) is the total cross section of \( 1.5 \times 10^{-14} \text{ cm}^2 \), \( T \) is the kinetic temperature, and \( Q \) is the normalization factor

\[
Q = \left[ \sum_{J' > J}^{J + \Delta J_{\text{max}}} g_{J'} \exp \left( -E_{J'}/kT \right) \right]^{-1},
\]

where \( \zeta = J - \Delta J_{\text{max}} \) for \( J \geq \Delta J_{\text{max}} \) and \( \zeta = 0 \) for \( J < \Delta J_{\text{max}} \). The above choice of \( \alpha_{J'} \) corresponds to the most simple collision model of Van Vleck and Weisskopf (1945) except for the truncation at \( \Delta J_{\text{max}} \). The cross sections for the inverse processes were calculated from the principle of detailed balancing, so that

\[
\frac{\alpha_J}{\alpha_{J'}} = \frac{g_J}{g_{J'}} \exp \left( (E_J - E_{J'})/kT \right).
\]

The rate for the collision-induced transition \( J' \leftrightarrow J \) is then found to be

\[
C_{J'J} = \sigma_{J'J} \nu n,
\]

where \( \nu \) and \( n \) are the average thermal velocity and number density of the colliding species.

The radiative rates are given by

\[
R_{J-1,J-1} = B_{J,J-1} U(\nu_{J,J-1}) + A_{J-1,J-1}
\]

and

\[
R_{J,J-1} = B_{J,J-1} U(\nu_{J,J-1}),
\]

where the Einstein coefficients of absorption \( B_{J,J-1} \), induced emission \( B_{J,J-1} \), and spontaneous emission \( A_{J-1,J} \) are

\[
B_{J,J-1} = \frac{8\pi \alpha^2}{3h^2} \left( \frac{J}{2J-1} \right),
\]

\[
B_{J,J-1} = \frac{2J-1}{2J+1} B_{J,J-1},
\]

and

\[
A_{J-1,J} = \frac{8\pi \alpha^3}{3h} B_{J,J-1}.
\]

The energy density of radiation at \( \nu \) is given as

\[
U(\nu) = \frac{8\pi \alpha^3}{3h} \frac{1}{\exp(\hbar \nu/kT) - 1} \approx \frac{8\pi \alpha^3 kT}{c^3}.
\]

Once the appropriate rate coefficients are computed, the steady-state relative population of each molecular level may be found by solving the system simultaneous
standard equations of statistical equilibrium (for $J = 0, 1, \ldots, N - 1$)

$$-n(J) \sum_{J'}^{N-1} (R_{J'J} + C_{J'J}) + \sum_{J'}^{N-1} n(J') (R_{J'J} + C_{J'J}) = 0.$$  \hspace{1cm} (9)

In these equations $N$ is the number of molecular levels used in the calculations, and $n(J)$ the relative population of the $J$th level. Once the $n(J)$ values are known, $T_{ex}(J \rightarrow J - 1)$ is computed from the relation

$$T_{ex}(J \rightarrow J - 1) = \frac{h \nu_{J,J-1}}{k} \ln \left( \frac{g_J n(J) n(J - 1)}{g_{J-1} n(J - 1)} \right)^{-1}.$$  \hspace{1cm} (10)

The resultant $T_{ex}$ values may then be incorporated into the radiative-transfer equation to calculate spectral line brightness temperatures and antenna temperatures.

IV. SOURCE GEOMETRY

Transformation of excitation temperatures into beam-averaged brightness temperatures or antenna temperatures via the transfer equation is dependent upon the geometric configurations of both the molecular cloud and the background continuum source. It is therefore necessary for computational purposes to model the background brightness temperature distribution as well as the configuration and physical conditions in the molecular cloud.

The galactic center region, including the Sgr B2 continuum source, has been studied by a number of observers at various frequencies—e.g., Broten et al. (1965), Martin and Downes (1972), and Kapitzky and Dent (1974). Using the Cambridge One-Mile (1.67 km) Telescope with a beamwidth of 6° at 5 GHz, Martin and Downes (1972) found evidence of a number of discrete, bright condensations of angular size $\leq 10°$ in the Sgr B2 complex.

We have used two Gaussian components to model the source structure found by Martin and Downes. Component A has an angular size of 4' (fullwidth at half-maximum) and produces a flux density of 45 Jy at 5 GHz. This represents the contribution of the extended component and all of the seven discrete sources except number 4 in the Martin-Downes model. Component B, which is superposed on the center of A, has an angular width of 12° and represents the strongest discrete source (number 4) in their model. It yields a flux density of 8 Jy at 5 GHz. These two Gaussian sources in our model are situated on a plateau which is of large angular size relative to the beamwidths of our telescopes and which has a brightness temperature of 2.0 K at 5 GHz. This third component represents the broad, diffuse galactic center emission (see, e.g., Broten et al. 1965) not detected in the Cambridge aperture synthesis observations.

This three-component model, with appropriate scaling of flux densities with frequency, accounts very well for our continuum observations of Sgr B2 at all the observed line frequencies, and, together with the 2.8 K microwave background, is taken to represent the continuum radiation in the direction of Sgr B2.

The HC$_3$N molecular cloud is assumed to be in front of and centered on the line of sight to the continuum source. For reasons to be discussed later, we have adopted a three-component model for the molecular cloud. For ease of calculation, the components were taken to be concentric cylinders of different radii oriented with their axes on the line of sight to the center of the continuum source. Each cylinder's length was taken equal to its diameter, and physical conditions were assumed constant within each component.

The resulting overall configuration of the model is shown schematically in Figure 2 with the three molecular cloud components labeled as regions I, II, and III in order of increasing size.

V. COMPUTATION OF LINE BRIGHTNESS TEMPERATURES

The transfer equation relating brightness temperature $T_B$ along a ray and $T_{ex}$ for an optically thin line
can be written
\[ \int T_g dv = T_{\text{ex}}(1 - T_e/T_{\text{ex}}) \int \tau dv. \]  
(11)

Here \( T_e \) is the brightness temperature of the background continuum source, \( \tau \) is optical thickness, \( v \) is velocity, and \( T_{\text{ex}} \) is assumed constant. For the transition \( J \rightarrow J - 1 \), the opacity integrated over all velocities is given by
\[ \int \tau dv = N_I A_{J,J-1} c^3 [\exp(hv_0/kT_{\text{ex}}) - 1]/8\pi v_0^3, \]  
(12)

where \( N_I \) is the column density of molecules in the upper level of the transition, \( A_{J,J-1} \) the Einstein rate for spontaneous radiative de-excitation, and \( v_0 \) the line frequency.

The beam-averaged brightness temperature of a source, \( T_B \), is related to \( T_B \) of equation (11) by
\[ T_B = \int T_B P d\Omega / \int P d\Omega, \]  
(13)

where \( P \) is the normalized antenna power pattern and the integrals are taken over 4sr.

Substitution of equation (12) into (11) leads to an expression for the beam-averaged brightness temperature (defined by eq. [13]) integrated over the line \( J \rightarrow J - 1 \) as follows:
\[ \int T_g dv = \left\{ A_{J,J-1} c^3 T_{\text{ex}} \left[ \exp(hv_0/kT_{\text{ex}}) - 1 \right] \right\} \int P N_I (1 - T_e/T_{\text{ex}}) d\Omega / 8\pi v_0^3 \int P d\Omega. \]  
(14)

Theoretical antenna temperatures may then be computed from \( T_B \), using the well-known relation
\[ T_A = \tau_B T_B. \]  
(15)

Evaluation of the integrals over angle in equation (14) is straightforward, although lengthy, for the geometry of our source model. If we assume that the telescope beams are Gaussian and neglect the curvature of the plane of the sky, the angle integrals can be transformed into integrals over polar coordinates and easily evaluated over the circular cross-sectional areas of regions I, II, and III of the molecular cloud model.

The final analytic form for
\[ \int T_g dv \]

involves many terms because of the geometric complexity of our model and so is not presented here.

VI. THE SAGITTARIUS B2 MOLECULAR CLOUD MODEL

A two-component model for Sgr B2 has been devised by MTPZ on the basis of observations of nine lines of cyanoacetylene. Their model consists of a relatively dense core \([n(H_2) \approx 10^6 \text{ cm}^{-3}\) and less dense halo \([n(H_2) \approx 10^4 \text{ cm}^{-3}\)] of angular diameters 2' and 5', respectively. The fit to their data was not particularly sensitive to the assumed kinetic temperature. They found \( T_K(\text{core}) = 20\text{–}50 \text{ K} \) and \( T_K(\text{halo}) = 20\text{–}80 \text{ K} \). The abundance of HC₃N relative to that of H₂ was about 100 times greater in the halo than in the core.

Scoville, Solomon, and Penzias (1975, hereafter SSP) have also studied the Sgr B2 molecular cloud using transitions of CO, ¹²CO, CS, and H₂CO. They concluded that the cloud consists of a dense core about 6 pc (2') in diameter lying within an extended envelope of diameter 45 pc (15'). In their model the average H₂ density is \( 5 \times 10^3 \text{ cm}^{-3} \) in the core and \( 5 \times 10^3 \text{ cm}^{-3} \) in the extended source. The average kinetic temperature was estimated to be 20 K.

In our initial modeling of the cyanodiacylentene data, it became apparent that a three-component model would be necessary to account for our observations and still satisfy the observations of MTPZ and SSP. As discussed earlier, one of the observational facts that must be accounted for is the enhancement of the \( J = 1 \rightarrow 0 \) line of HC₃N. This may be achieved through a population inversion of the \( J = 1 \) level which results in amplification of the background continuum. For HC₃N we found that \( n(H_2) \) could not exceed \( 4 \times 10^3 \text{ cm}^{-3} \) if \( T_{\text{ex}}(1 \rightarrow 0) \) is to be negative; otherwise collisional processes destroy the inversion. It is therefore necessary to postulate the existence of a third, low-density region of the cloud in addition to the two components with \( N(H_2) > 10^4 \text{ cm}^{-3} \) found by SSP and MTPZ.

Table 2 summarizes our model of the HC₃N molecular cloud in Sgr B2. Because our HC₃N lines arise in the intermediate- and low-density regions II and III, we are not able to say anything about the dense inner core of the cloud from our observations. Thus the size of region I and its values of \( T_K \) and \( n(H_2) \) are taken from the core model of MTPZ. The column density for region I was computed so as to make the model consistent with the millimeter data of Guélin and Thaddeus (1978). In general, the model calculations of temperature and H₂ density are not strongly dependent upon the physical dimensions of the different regions. Our observations do not allow us to determine uniquely the sizes of the three regions. Rather, the calculations are sensitive to the total HC₃N column density in the telescope beam, which is the product of the molecular number density and the physical path length. Accordingly, we have chosen, for compatibility with the MPTZ model, the diameter of region II to be 5' and have arbitrarily taken the diameter of region III to be 10'.
TABLE 2
THE THREE-COMPONENT MODEL FOR THE SAGITTARIUS B2 MOLECULAR CLOUD

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Region I</th>
<th>Region II</th>
<th>Region III</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parsecs</td>
<td>7</td>
<td>15</td>
<td>30</td>
</tr>
<tr>
<td>$T_x$ K*</td>
<td>2.4</td>
<td>5</td>
<td>10</td>
</tr>
<tr>
<td>$\log n(H_2)$ cm$^{-3}$*</td>
<td>&gt; 25</td>
<td>25-35</td>
<td>10-35</td>
</tr>
<tr>
<td>$\log n(HC_3N)/n(H_2)$*</td>
<td>&gt; 5.3</td>
<td>3.5 ± 0.3</td>
<td>1.9 ± 0.3</td>
</tr>
<tr>
<td>$\log n(HC_3N)$ (cm$^{-3}$)</td>
<td>1.5 $\times$ 10$^{13}$</td>
<td>1.6 $\times$ 10$^{14}$</td>
<td>1.1 $\times$ 10$^{13}$</td>
</tr>
<tr>
<td>$\log n(H_2)$</td>
<td>(6.0)</td>
<td>(3.5)</td>
<td>(2.0)</td>
</tr>
<tr>
<td>$\log n(H_2)/n(HC_3N)$</td>
<td>&lt; -11.5</td>
<td>-9.0 ± 0.1</td>
<td>-8.8 ± 0.3</td>
</tr>
<tr>
<td>$\log n(HC_3N)$</td>
<td>(-12.2)</td>
<td>(-9.0)</td>
<td>(-8.9)</td>
</tr>
<tr>
<td>Total $H_2$ mass ($M_\odot$)</td>
<td>$1 \times 10^7$</td>
<td>$4 \times 10^5$</td>
<td>$9 \times 10^4$</td>
</tr>
<tr>
<td>Mass of HC$<em>3$N ($M</em>\odot$)</td>
<td>$5 \times 10^{-4}$</td>
<td>$3 \times 10^{-2}$</td>
<td>$8 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

* The values in parentheses yielded theoretical values of brightness temperatures closest to the observed values. See Table 1 for comparison with observations.

over large ranges. Thus the ranges shown in Table 2 for temperature and $H_2$ density are based on estimates of the degree to which changing the values of one of these parameters in one of the regions, while holding all others constant, alters the strengths of the spectral lines which originate in that region. They do not represent rigorously determined limits for the different parameters.

The values in Table 2 were obtained assuming only hard collisions, $\Delta J_{\text{max}} = 20$, and neglecting the effects of the Sgr B2 continuum source (but not the 2.8 K background) on the radiative coefficients. Some calculations were made using smaller values of $\Delta J_{\text{max}}$ and nonzero geometric dilution factors for the continuum sources in Sgr B2. Both these changes act to decrease the degree of inversion of the $1 \rightarrow 0$ line, and make it more difficult to achieve the desired amplification. For example, taking dilution factors for the radiation from the continuum plateau and component A of the continuum model to be 0.5 and 0.3, respectively, results in equal amplitudes for the $1 \rightarrow 0$ and $2 \rightarrow 1$ lines.

Table 1 contains a comparison of observed line brightness temperatures for HC$_3$N and those predicted using the values in parentheses from Table 2.

VII. DISCUSSION AND CONCLUSIONS

We have devised a model of the Sgr B2 molecular cloud and continuum sources which accounts well for the HC$_3$N line observations and is basically consistent with the HC$_3$N model of MTPZ. The important new feature of our model is the presence of an extensive, very low-density molecular cloud surrounding the core and halo of the MTPZ model. This outermost region is taken to be 30 pc (10') in diameter and is characterized by an $H_2$ density of $\sim 100$ cm$^{-3}$ and $T_x \sim 20$ K.

Such a low density is characteristic of a diffuse cloud and is rather surprising in connection with Sgr B2, but, within the assumptions of our modeling, seems to be an inescapable consequence of the statistical equi-librium calculations. As discussed earlier, attempts to increase $n(H_2)$ above $4 \times 10^3$ cm$^{-3}$ destroy the $J = 1 \rightarrow 0$ line inversion.

For a particular molecule, the requirement for such inversion is that collisional and radiative rates for the levels involved be about equal. Because the radiative rates for HC$_3$N are much less than those for HC$_3$N, due to the much smaller rotational constant, the inversion of the $J = 1 \rightarrow 0$ line occurs at significantly lower $H_2$ densities for HC$_3$N. This explains why the presence of region III was not revealed by the HC$_3$N observations. Of course, the three-component model presented here can be, at best, only an approximation to reality and should be interpreted as representing a continuous density gradient in the cloud.

In our model, region III is the principal contributor to the observed brightness temperature of the $J = 1 \rightarrow 0$ and $2 \rightarrow 1$ lines. In fact, the first three lines are characterized by negative values of $T_x$ in this region. The $1 \rightarrow 0$ line is strongly inverted and the $2 \rightarrow 1$ line less so, but both lines amplify the continuum background in this part of the model. It is worth noting that, as shown in Table 1, the observed relatively narrow widths of the $1 \rightarrow 0$ line (11.6 km s$^{-1}$) and, to a lesser extent, the $2 \rightarrow 1$ line (16.2 km s$^{-1}$), are consistent with their origin in a different part of the molecular cloud than the higher $J$ lines. The $3 \rightarrow 2$ line originates equally in regions II and III; the $4 \rightarrow 3$ and $8 \rightarrow 7$ lines arise primarily in region II. The millimeter wavelength lines ($J = 31 \rightarrow 30$ to 37 36) observed by Guelin and Thaddeus (1978) originate entirely in the inner two regions.

It might be thought surprising that, in spite of the large path length through the low-density region III, the observed width of the $J = 1 \rightarrow 0$ line of HC$_3$N ($\sim 11.6$ km s$^{-1}$) is considerably less than the $\sim 50$ km s$^{-1}$ width of the $J = 1 \rightarrow 0$ line of CO from Sgr B2 (SSP) which also originates in an extensive region. However, two important points should be considered. a) The $J = 1 \rightarrow 0$ CO line has a large optical depth in Sgr B2, whereas HC$_3$N is believed to be optically thin. A better comparison can be made with C$^{18}$O, for
which the $J = 1 \rightarrow 0$ line is probably optically thin (SSP). This line has a width of $\sim 25 \text{ km s}^{-1}$, more comparable with the HC$_3$N line.

b) About two-thirds of the intensity of the $J = 1 \rightarrow 0$ line of HC$_3$N, as observed with the 8/2 beam of the Parkes 210 foot (64 m) telescope, arises from amplification of component A of our continuum model, and the remainder of the line arises chiefly from amplification of the continuum plateau. Component A has an angular width of $4'$, so the width of the observed $J = 1 \rightarrow 0$ line will depend on the radial velocity dispersion in region III along a $4'$ diameter cylinder outside of region II. The higher $J$ lines, on the other hand, originate in regions I and II, so their widths reflect the velocity dispersion in these much denser parts of the cloud. Our observations thus imply that velocity dispersion in the low-density envelope is less than that in the inner components of the model.

One of the interesting results of our study is that in the densest region the ratio of $n$(HC$_3$N) to $n$(H$_2$) is three orders of magnitude less than it is in region II and III. MTPZ found that HC$_3$N was also depleted relative to H$_2$ in the core of their model.

The column density of HC$_3$N in Sgr B2 was computed by Broten et al. (1976), under the assumption of thermodynamic equilibrium, to be $1.6 \times 10^{14} \text{ cm}^{-2}$ on the basis of the $J = 4 \rightarrow 3$ and $8 \rightarrow 7$ lines. The column density in our model is greatest in region II and also equals $1.6 \times 10^{14} \text{ cm}^{-2}$ in agreement with the LTE results. This is equal to the column density for HC$_3$N in the same source (MTPZ), which suggests that, in region II, either both molecules are made with comparable efficiency, or else, assuming both are synthesized from lighter molecules, that HC$_3$N has a longer lifetime than HC$_5$N. However, comparison with the MTPZ model indicates that in region I the ratio $N$(HC$_3$N)/$N$(H$_2$) is an order of magnitude less than the ratio $N$(HC$_5$N)/$N$(H$_2$). It would appear that the relative depletion of HC$_3$N with respect to HC$_5$N in this region is related to the large density of H$_2$.

The model can be used to predict the frequency range over which the cyanodiacetylene lines in Sgr B2 should be strongest. For $4 < J_{\text{upper}} < 29$, region II is the dominant contributor to $T_B$ (assuming telescope apertures of 150 feet [46 m] up to $J = 8 \rightarrow 7$, and 36 feet [11 m] for the higher $J$ lines). Beyond $J = 29$, the contribution from region I becomes predominant. If we assume the 36 foot telescope of NRAO were used for observing, the beam-averaged brightness temperature for the HC$_3$N lines maximizes at 0.60 K for $14 < J_{\text{upper}} < 18$; i.e., for frequencies between 37 and 48 GHz. The predicted value of $T_B$ for the $J = 45 \rightarrow 44$ line ($\sim 120$ GHz), which originates entirely in region I, is 0.02 K.

In conclusion, it is important to note that an infrared radiation field has not been incorporated into the equilibrium calculations for this study. The inclusion of excited vibrational levels would complicate the calculations considerably and also would require more complete knowledge of the molecule than is now available. The importance of this omission is difficult to assess. The lowest-lying excited vibrational level of HC$_3$N is estimated to lie about 80 cm$^{-1}$ above the ground state. Harvey, Campbell, and Hoffmann (1977), from observations in the far-infrared, have deduced that the infrared brightness temperature of Sgr B2 is about 40 K. The possibility exists that the rotational excitation of HC$_3$N in the ground vibrational state is controlled by infrared excitation to higher vibrational levels followed by radiative decay. It is not clear whether this process could produce the observed inversion of the $1 \rightarrow 0$ line without the necessity of the low H$_2$ densities required if collisional and microwave processes dominate the excitation. Such a possibility should be studied when the necessary molecular data become available.

We appreciate the hospitality extended us by Haystack Observatory and NRAO and would like to thank the staffs of both facilities for their assistance in making the observations reported here. We also thank Dr. M. Guélin and Dr. P. Thaddeus for making their data available to us in advance of publication.

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