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OBSERVATIONS OF THE ¹³C ISOMERS OF CYANOACETYLENE: IMPLICATIONS FOR CARBON ISOTOPE STUDIES IN THE MILKY WAY

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ABSTRACT

Observations of the $J = 1 \rightarrow 0$ rotational transitions of HC₃N, H¹³CCCN, HC¹³CCN, and HCC¹³CN are used to search for fractionation among the three ¹³C isomers in the Galactic molecular cloud Sgr B2. Based on these high signal-to-noise observations (S/N \sim 10), we conclude that there is no evidence for fractionation in the three ¹³C isomers. Our observations are consistent with an earlier suggestion that the HC₃N $J = 1 \rightarrow 0$ transition is a weak maser in Sgr B2. In addition to Sgr B2, we have also observed the Galactic molecular clouds TMC-1 and Sgr A. We derive ${}^{12}C/{}^{13}C$ ratios of 11 ± 2 for Sgr B2 and $61{}^{+28}_{-16}$ for TMC-1. Subject headings: interstellar: abundances - interstellar: molecules - molecular processes

I. INTRODUCTION

Some of the most important input data for understanding the chemical evolution of our Galaxy arises from detailed studies of the distribution and abundance of the rare isotopes D, ¹³C, ¹⁵N, ¹⁷O, ¹⁸O, ²⁹Si, ³³S, and ³⁴S relative to their main isotopic forms in the interstellar medium. The most widely studied of these isotopes is ¹³C. Unfortunately, accurate measurements of the ¹²C/¹³C ratio have suffered from uncertainties due to possible chemical fractionation (e.g., HC₃N and CO) and optical depth effects (e.g., CO). We address the first of those problems here.

Initially, the $J = 1 \rightarrow 0$ rotational transitions of cyanoacetylene $(H^{12}C^{12}C^{12}C^{14}N)^5$ seemed to offer an ideal way for determining the ¹²C/¹³C isotope ratio. This transition was almost certain to be optically thin at the temperatures and densities typically found in molecular clouds, and there was no reason to suspect substantial isotopic fractionation. Further, the three ¹³C isomers of cyanoacetylene made it possible to check directly for isotopic fractionation. Unfortunately, Morris et al. (1976) found evidence that this transition was masing weakly in Sgr B2. To make matters worse, observations by Churchwell, Walmsley, and Winnewisser (1977, hereafter CWW) found that in the $J = 1 \rightarrow 0$ transition the line strength of one of the ¹³C isomers (H¹³CCCN) was twice as strong as the two remaining ¹³C isomers (HC¹³CCN and HCC¹³CN) in the molecular cloud Sgr B2. This result indicated the possibility of strong isotopic fractionation during the formation of HC₃N and cast doubt on the utility of HC₃N as a probe of the $^{12}C/^{13}C$ ratio.

Wannier and Linke (1978) addressed the question of fractionation in HC₃N by observing its $J = 9 \rightarrow 8$ transitions. They found no evidence for fractionation among the ¹³C isomers to a level of $\pm 5\%$. The interpretation of this result, in apparent conflict with CWW, was complicated by a number of

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 5 In the rest of the chemical formulae for cyanoacetylene in this paper, we will denote ^{12}C and ^{14}N by C and N, respectively.

factors. First of all, the higher-J transitions $(J \ge 3)$ are observed to have velocities of peak emission intensity slightly lower (55–60 km s⁻¹) than that of the $J = 1 \rightarrow 0$ and $J = 2 \rightarrow 1$ transitions (60–65 km s⁻¹). This velocity shift could arise from the fact that the higher-J transitions originate in a different part of the cloud complex. A second factor contributing to the velocity difference between the higher and lower J radiation is the possible weak masing of the $J = 1 \rightarrow 0$ transition. In this case, the line originates along the path of highest gain through the cloud rather than at the velocity of maximum thermal emission, which the higher-J transitions trace. Finally, the accurate determination of the isomer ratios is complicated by the fact that the lines of two of the ¹³C isomers are not cleanly separated for sources with line widths as large as those found in Sgr B2.

Because of the importance of these results to the study of the chemical evolution of ¹³C, and because of the improvements in receivers since the earlier work, we felt it appropriate to make new observations. In this paper, we present observations of the $J = 1 \rightarrow 0$ transitions of HC₃N and its three ¹³C isomers in the molecular clouds Sgr B2, TMC-1, and Sgr A, and report upper limits for many other molecular clouds. The observations are presented in § II. In § III we discuss Sgr B2, TMC-1, and Sgr A individually and address the question of fractionation among the ¹³C isomers of HC₃N in Sgr B2. In § IV we address the problem of the non-LTE hyperfine ratio observed in the $J = 1 \rightarrow 0$ transition of HC₃N in Sgr B2.

II. OBSERVATIONS

Cyanoacetylene is a linear polyatomic molecule without internal rotation. The rotational transitions are hyperfine-split as a result of the interaction of the electric quadrupole moment of the N nucleus (spin = 1) with the electronic charge distribution of the molecule. This hyperfine splitting is astrophysically important for $J \leq 3$. There is no net electronic angular momentum in cyanoacetylene, but there is still magnetic hyperfine splitting arising from the interaction of the magnetic dipole moment of the H nucleus with the small magnetic fields produced by molecular rotation $(I \cdot J \text{ interactions})$. This magnetic hyperfine splitting is usually $\sim 5 \text{ kHz} (0.2 \text{ km s}^{-1})$, much smaller than the Doppler line widths found in most interstellar clouds.

Observations of the $J = 1 \rightarrow 0$ transitions of HC₃N and its three ¹³C isomers were made on 1986 October 9-14 with the

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TABLE 1 OBSERVED ERFOLIENCIES

OBSERVED I REQUERCIES			
Molecule	$F \rightarrow F'$	Observed Frequency ^a (MHz)	
HC ₁ N	$1 \rightarrow 1$	9097.0346	
3	$2 \rightarrow 1$	9098.3321	
	$0 \rightarrow 1$	9100.2727	
H ¹³ CCCN	$1 \rightarrow 1$	8815.824	
	$2 \rightarrow 1$	8817.115	
	$0 \rightarrow 1$	8819.065	
HC ¹³ CCN	$1 \rightarrow 1$	9058.498	
	$2 \rightarrow 1$	9059.739	
	$0 \rightarrow 1$	9061.700	
HCC ¹³ CN	$1 \rightarrow 1$	9059.412	
	$2 \rightarrow 1$	9060.624	
	$0 \rightarrow 1$	9062.555	

^a HC₃N frequencies from de Zafra 1971. Isotopic frequencies from Churchwell, Walmsley, and Winnewisser 1977.

43 m telescope of the National Radio Astronomy Observatory.⁶ The frequencies observed are listed in Table 1. The positions, center velocities, and channel widths used for each source are listed in Table 2. In the frequency range observed (8.8-9.1 GHz), the beam efficiency was measured to be 0.84 and the beam size (HPBW) ranged between 3'2 at 9100.27 MHz and 3'.3 at 8815.82 MHz. The flux density scale was calibrated by continuum observations of NGC 7027 and Virgo A, which were assumed to have flux densities of 6.2 and 43.2 Jy, respectively. A single-channel Ku band maser upconverter receiver was used with a linearly polarized feed (p.a. = $202^{\circ}5$). The system temperature was typically 65-75 K throughout the observing run, somewhat higher than usual because of bad weather. The relative gains in each autocorrelator receiver quadrant were calibrated by taking continuum scans of the above calibration sources. The autocorrelator was split into four receivers so that we could observe the various isomers

⁶ The National Radio Astronomy Observatory is operated by Associated Universities, Inc., under contract with the National Science Foundation.

simultaneously. Our bandpass calibration procedure eliminated potential errors in comparing the relative strengths of the three ¹³C isomers. The fluctuation across the receiver bandpass was typically $\lesssim 15\%$ throughout the observing run.

The spectra reported here were taken by employing receiver bandwidths from 1.25 to 40 MHz to sample the \sim 200 MHz of total bandwidth available from the maser upconverter receiver. This provided us with a range of velocity resolutions from 0.2 to 2.6 km s⁻¹. The ¹²C transition of HC₃N was observed simultaneously with its three ¹³C isomers. This minimizes the influence of atmospheric effects which can cause errors when the two isotopic forms of the molecule are compared. The bulk of the Sgr B2 integration time on the H¹³CCCN isomer was obtained by Bania, Rood, and Wilson (1987) in one of the test bands used for their ³He⁺ observations. The spectra were taken employing the total power observing mode following the basic procedure outlined in Bania, Rood, and Wilson.

III. RESULTS

a) Sgr B2

We measured the intensities of the $J = 1 \rightarrow 0$ transitions of HC₃N and its ¹³C isomers. Because of the large velocity dispersion in this molecular cloud, the lines from two of the isomers, HC¹³CCN and HCC¹³CN, are blended. We present in Table 3 the measured line parameters as determined from Gaussian fits to the various spectral features, and we show the spectra and Gaussian fits in Figure 1. For HC₃N two velocity components are visible, one at 63 km s^{-1} and another at 80 km s^{-1} . Note that the 63 km s^{-1} feature has a distinctly non-Gaussian shape. It has been suggested that this non-Gaussian shape could be due to contributions from four separate velocity components (McGee, Newton, and Butler 1975) or might be the result of a weak maser (Morris et al. 1976). We discuss this problem in § IV below.

With 34 hr of integration time, our spectra for H¹³CCCN are far better than any obtained before. As with HC₃N, there are velocity components at 63 and 80 km s⁻¹. The blended HC¹³CCN and HCC¹³CN lines are shown both using the same velocity scale as for H¹³CCCN and with a larger velocity

	TABLE	2
OBSERVED	SOURCE	PARAMETERS

Source	α(1950)	δ(1950)	Center Velocity (km s ⁻¹)	Channel Width (km s ⁻¹)
ГМС-2	04 ^h 29 ^m 43 ^s 0	+24°18′54″	+ 6.1	0.7
ГМС-1	04 38 38.5	+25 36 26	+ 5.6	0.2
1544	05 01 14.0	+250700	+ 7.0	0.7
Orion-KL	05 32 47.0	-05 24 20	+8.3	0.7
Virgo A ^a	12 28 17.6	+124002		
[183 4N	15 51 32.7	$-02\ 39\ 31$	+ 2.4	0.2
o Oph B	16 24 10.0	-24 22 42	+ 3.6	0.2
Sor A	17 42 36.2	-28 57 52	+48.8	1.3
Sor B2	17 44 10.7	$-28\ 22\ 17$	+65.2	1.3, ^b 2.6 ^c
W31C	18 06 25.0	-20 19 48	+0.0	0.6
W33	18 11 19.5	-17 56 40	+ 33.5	0.6
778	19 24 26.4	+23 3000	+9.9	0.6
B335	19 34 36.0	+072730	+8.4	0.6
DR 21 (OH)	20 37 14.0	+421200	-4.0	0.6
NGC 7027ª	21 05 09.4	+420203		
N7538 (OH)	23 11 37.0	+61 11 59	-62.0	0.6
\$162	23 18 28.1	+60 55 11	-45.0	0.6

^a Continuum calibration source.

^b For HC₃N.
 ^c For H¹³CCCN, HC¹³CCN, and HCC¹³CN.

1988ApJ...334..182M

184

TABLE 3 SAGITTADHIS R2 MEASURED LINE PARAMETERS

SHOTTING DE MENSORED EINE I ARAMETERS					
Isomer	$F \rightarrow F'$	V _{LSR} ^a (km s ⁻¹)	FWHM ^a (km s ⁻¹)	T _A (mK)	I _{REL} ^b
HC ₃ N	$0 \rightarrow 1$	63.10	18.10	96 + 9	0.4
0	$0 \rightarrow 1$	80.55	17.45	11 + 10	
	$2 \rightarrow 1$	63.10	18.10	$1150 + 9^{\circ}$	5.0
	$2 \rightarrow 1$	63.10	14.61	$1219 + 22^{d}$	
	$2 \rightarrow 1$	80.55	17.45	157 + 9	5.0
	$1 \rightarrow 1$	63.10	18.10	441 ± 9	1.9
	$1 \rightarrow 1$	80.55	17.45	56 ± 9	1.8
H ¹³ CCCN	$0 \rightarrow 1$	60.00	18.10	9 ± 1	1.2
	$2 \rightarrow 1$	60.00	18.10	39 ± 1	5.0
	$2 \rightarrow 1$	78.45	17.45	7 ± 1	
	$1 \rightarrow 1$	60.00	18.10	22 ± 1	2.8
HC ¹³ CCN	$0 \rightarrow 1$		-11.		
	$2 \rightarrow 1$	60.31	18.10	46 + 2	50
	$1 \rightarrow 1$	60.31	18.10	$\frac{10}{27 \pm 2}$	2.9
HCC ¹³ CN	$0 \rightarrow 1$				
	$2 \rightarrow 1$	60.31	18 10	43 + 2	50
	$1 \rightarrow 1$	60.31	18.10	$\frac{40 \pm 2}{29 \pm 2}$	3.4

^a Standard error assumed to be 1 channel width.

^b With respect to associated $F = 2 \rightarrow 1$ transition normalized to 5.0.

^c Best fit to line wings.

^d Best fit to line peak.

scale to show the entire region used in the baseline fit. For this blend it was necessary to fix the line widths and centers of the Gaussians to the line widths and LSR velocities obtained from fits to the unblended H¹³CCCN profile. As the data in Table 3 indicate, HC₃N and its three ¹³C isomers are all well fitted by an 18.1 km s⁻¹ Gaussian line width. All three isomers exhibit a hyperfine ratio of approximately 5:3:1, which is the optically thin LTE value. The data in Table 3 also indicate that the relative strengths between the three ¹³C isomers of HC₃N are H¹³CCCN : HC¹³CCN : HCC¹³CN = $0.9 \pm 0.1 : 1.1 \pm 0.1 : 1$. Therefore, contrary to the results of CWW, we find that there is *no* evidence that the line intensities or widths vary among the three ¹³C isomers of HC₃N.

Indeed, Wolfsberg *et al.* (1979) have made a theoretical evaluation of the distribution of ¹³C in HC₃N at thermodynamic equilibrium. From their calculations we find that for an assumed kinetic temperature of 85 K (Cummins *et al.* 1983), H¹³CCCN:HC¹³CCN:HCC¹³CN = 0.9:0.9:1, suggesting that the relative fraction among the three ¹³C isomers of HC₃N in Sgr B2 should be small. At lower temperatures, Wolfsberg *et al.* predict that H¹³CCCN should be the least abundant, while HCC¹³CN should have the highest abundance among the three isomers. The small amount of fraction predicted by this simple calculation is completely consistent with our results.

Use of the $J = 1 \rightarrow 0$ transition as a ${}^{12}\text{C}/{}^{13}\text{C}$ probe is made difficult by the fact that HC₃N seems to be a weak maser in this source. If it is a weak maser, the gain of the maser will be proportional to the intensity of the hyperfine transition. This would imply that the $F = 0 \rightarrow 1$ hyperfine transition is the least affected by the weak maser effect. Using the measured $F = 0 \rightarrow 1$ intensities from HC₃N and H¹³CCCN, we find that ${}^{12}\text{C}/{}^{13}\text{C} = 11 \pm 2$. Note that if masing is important even in the $F = 0 \rightarrow 1$ transition, this derived ${}^{12}\text{C}/{}^{13}\text{C}$ ratio would be an upper limit. However, because the excitation and radiative transfer are obviously complicated, it is plausible that the $F = 2 \rightarrow 1$ transition is enhanced while the $F = 0 \rightarrow 1$ transition is diminished relative to its LTE strength. Thus, this ${}^{12}C/{}^{13}C$ isotope ratio should be used with caution.

This derived value for the carbon isotope ratio is slightly less than the values of 15-25 derived from observations of NH₂CHO (Lazareff, Lucas, and Encrenaz 1978), OCS (Goldsmith and Linke 1981), CH₃CN (Cernicharo et al. 1988), and H₂CO (Gardner, Ribes, and Cooper 1971; Gardner and Whiteoak 1979; Henkel et al. 1983; Wilson et al. 1976; Zuckerman et al. 1974). We should point out that in Henkel et al. a ¹²C/¹³C ratio (after correction for photon trapping) of 10 was derived, but was abandoned because of doubts surrounding the applicability of trapping corrections from the statistical equilibrium model to Sgr B2. With this they concluded that their uncorrected value of ~ 20 was more reasonable. We have also observed H₂CO and H₂¹³CO in Sgr B2 using the 43 m telescope at Green Bank and find that ${}^{12}C/{}^{13}C \approx 21$, with no correction for photon-trapping effects (Mangum et al. 1988). We have calculated the photon trapping correction to this isotope ratio by considering models of Sgr B2 using the large velocity gradient (LVG) approximation (de Jong, Chu, and Dalgarno 1975; Goldsmith, Young, and Langer 1983). Using the observed $2_{11} \leftarrow 2_{12}$ and $1_{10} \leftarrow 1_{11}$ antenna temperatures for H₂CO and H₂¹³CO from our observations and the work of Henkel et al. (1983), we find the photon trapping to be negligible.

b) TMC-1

In the dark cloud TMC-1 we have measured the intensities of the three hyperfine transitions of HC₃N and present the results in Table 4 and Figures 2 and 3. To within measurement error, the hyperfine ratio at peak intensity is 5:3:1. The $F = 2 \rightarrow 1$ hyperfine transition of each of the three ¹³C isomers is present at the 2 σ level. In order to support the validity of this marginal detection, we have averaged the three $F = 2 \rightarrow 1$ ¹³C transitions together. The result of this averaging is shown in Figure 3. A Gaussian fit to this averaged profile yields $T_4 =$ 13 ± 4 mK. Given this result, we calculate ${}^{12}C/{}^{13}C = 61 {}^{+26}_{-16}$.

The fractionation calculations of Wolfsberg *et al.* (1979) indicate that in a cold cloud like TMC-1 there should be a significant amount of fractionation among the ¹³C isomers of HC₃N. Assuming a kinetic temperature of 10 K, one would expect the relative concentrations to be H¹³CCCN:HC¹³CCN:HCC¹³CN = 0.2:0.5:1. If these model predictions are correct, the averaging procedure used above becomes considerably more complicated. In any event, because of the low signal-to-noise ratio in our observations, we can neither support nor contradict this prediction.

TMC-1 is at essentially the same distance from the Galactic center as the Sun, i.e., 8 kpc. Evolutionary models for the Galaxy predict a positive ${}^{12}C/{}^{13}C$ gradient as a function of galactocentric radius (Audouze, Lequeux, and Vigroux 1975; Dearborn, Tinsley, and Schramm 1978). Our measurements are thus in line with such theories. Also, since the solar ${}^{12}C/{}^{13}C$ ratio is 89, and the Galaxy has had 5 billion years to enrich the interstellar medium with ${}^{13}C$, one would expect the carbon isotope ratio in TMC-1 to be less than the solar value.

The ${}^{12}C/{}^{13}C$ isotope ratio derived from our HC₃N observations is slightly larger than that derived from optical observations of CH⁺ toward five stars in the solar neighborhood (Hawkins and Jura 1987; ${}^{12}C/{}^{13}C = 43 \pm 4$). Given the complexity of the CH⁺ experiment, we feel that there is not substantial disagreement between the HC₃N and CH⁺ isotope ratios. Our HC₃N ${}^{12}C/{}^{13}C$ ratio is slightly lower than the





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1988ApJ...334..182M

		-				
Isomer	$F \rightarrow F'$	V _{LSR} ^a (km s ⁻¹)	FWHM ^a (km s ⁻¹)	T _A (mK)	I _{REL}	Comments ^b
		TM	/ IC-1			
HC ₃ N	$0 \rightarrow 1$ $2 \rightarrow 1$ $2 \rightarrow 1$ $1 \rightarrow 1$	6.11 6.11 6.11	0.54 0.54 0.54	222 ± 31 789 ± 22 898 ± 31	1.2 5.0	P GH P
H ¹³ CCCN	$1 \rightarrow 1$ $2 \rightarrow 1$	6.20	0.54	12 ± 7	5.0 5.0	P P
HC ¹³ CCN HCC ¹³ CN	$2 \rightarrow 1$ $2 \rightarrow 1$	6.20 6.20	0.50 0.50	12 ± 7 12 + 7	5.0 5.0	P
All ¹³ C	$2 \rightarrow 1$	6.20	0.44	12 ± 7 13 ± 4	5.0	GA
		Sg	gr A			
HC ₃ N	$0 \to 1$ $2 \to 1$ $1 \to 1$	50.61 50.61 50.61	23.91 23.91 23.91	50 ± 3 306 ± 3 140 ± 3	0.8 5.0 2.3	G G G
All ¹³ C	$2 \rightarrow 1$	50.61	23.91	<4	,	GA

TABLE 4 TMC-1 AND SAGITTARIUS A MEASURED LINE PARAMETERS

^a Standard error assumed to be one channel width.

^b P = antenna temperature determined from peak of line; G = all line parameters determined from Gaussian fit to line; GA = Gaussian fit after Hanning smoothing to average of all ¹³C isomers; GH = Gaussian fit after Hanning smoothing.

value of ~ 80 derived from recent observations of CO and ¹³CO toward the star ζ Oph (Langer, Glassgold, and Wilson 1987). Langer, Glassgold, and Wilson suggest, though, that this slightly larger ¹²C/¹³C may be affected by enhancement of ¹²CO by self-shielding of the far-UV dissociating radiation (Glassgold, Huggins, and Langer 1985) and fractionation. Last, the ¹²C/¹³C ratio derived from our HC₃N observations is twice as large as found previously using H_2CO (Evans et al. 1975) and DCO⁺ (Guélin, Langer, and Wilson 1982). Evans et al. have suggested that their measurements may need to be increased by a factor of 2 to take photon trapping into account. Guélin, Langer, and Wilson suggest that their low value may be due to chemical enhancement of ¹³C in the DCO⁺ molecule.

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c) Sgr A

In Figure 4 and Table 4 we present our HC₃N results for the Galactic center source Sgr A. The measured hyperfine intensity ratio is 6.2 ± 0.4 : 2.8 ± 0.2 : 1. It has been suggested that this slightly non-LTE hyperfine ratio is due to the effects of weak maser emission in the $J = 1 \rightarrow 0$ transition (Walmsley et al. 1986). If this transition were weakly masing, we might also expect to observe a shift in the velocity of peak emission from that observed in the higher-J transitions. Observations of the $J = 2 \rightarrow 1$, $J = 10 \rightarrow 9$, $J = 12 \rightarrow 11$, and $J = 15 \rightarrow 14$ transitions by Walmsley et al. (1986) indicate that these higher-J transitions peak near 49 km s⁻¹. We find that the velocity of the $J = 1 \rightarrow 0$ transition coincides with higher-J transitions. This, coupled with the near-LTE hyperfine ratio and Gaussian line shapes found in the $J = 1 \rightarrow 0$ transition, suggest that the masing is so weak, if present, that it can be safely ignored.

There is no hint of a detection of the $F = 2 \rightarrow 1$ hyperfine transition of any of the three ¹³C isomers of HC₃N. The rms noise was typically 6-8 mK in the regions containing the lines. Averaging the $F = 2 \rightarrow 1$ regions of the spectra for the three ¹³C isomers and force-fitting a Gaussian with a line width

equal to that derived from our HC₃N observations of Sgr A lead to an amplitude of 2 ± 2 mK. Using upper limits of between 4 and 8 mK (which represents the Gaussian amplitude plus 1 σ and 3 σ , respectively) suggests that ${}^{12}C/{}^{13}C \gtrsim 38-75$. While we feel that this result, as with all upper limits, should be viewed with some suspicion, there seems little doubt that the value is higher than that in Sgr B2.

Our measured ¹²C/¹³C limit for Sgr A is higher than values found using other molecules. Using H₂CO, Whiteoak and Gardner (1972) and Gardner and Whiteoak (1979) derive ¹²C/ ${}^{13}C \approx 13$, while Wilson *et al.* (1976) derive ${}^{12}C/{}^{13}C > 13$. Neither measurement was corrected for photon trapping, which would raise these calculated ${}^{12}C/{}^{13}C$ ratios. Frerking et al. (1980) and Wannier, Linke, and Penzias (1981) have used $^{12}C^{34}S/^{13}C^{32}S$ and $H^{12}C^{15}N/H^{13}C^{14}N$, respectively, to study the C, S, and N double isotope ratios in Sgr A. Assuming a terrestrial value of 23 for the ³²S/³⁴S ratio, the results of Frerking et al. imply ${}^{12}C/{}^{13}C \approx 33$. The Wannier, Linke, and Penzias results, using the terrestrial ¹⁴N/¹⁵N ratio of 269, imply ${}^{12}C/{}^{13}C < 12$.

The molecules listed above, however, have emission distributions that peak at $V_{LSR} \approx 42 \text{ km s}^{-1}$, while the HC₃N emission peaks near 50 km s⁻¹. It appears, then, that the HC₃N in Sgr A traces gas at a different radial velocity than H₂CO, CS, and HCN.

We should also point out that even though Sgr A and Sgr B2 are both Galactic center molecular clouds, with similar physical characteristics, they apparently have significantly different ¹²C/¹³C ratios. One possible explanation for this difference could be that there are chemical differences between the two clouds which cause ¹³C to be enhanced relative to ¹²C, or vice versa. Given the current state of interstellar chemistry, we cannot explore this alternative. Advances in the theories of cvanopolyyne formation will, it is hoped, shed some light on the chemical differences between these two Galactic center clouds.

No. 1, 1988

1988ApJ...334..182M



Velocity (km s⁻¹)

FIG. 2.—The $J = 1 \rightarrow 0$ transitions of HC₃N, H¹³CCCN, HC¹³CCN, and HCC¹³CN in TMC-1. Note that the spectra for the three ¹³C isomers are displayed with the same velocity scale.

d) Other Sources

Table 5 lists the results of our HC_3N observations of other Galactic molecular clouds. All of the upper limits are nondetections. At least at this transition, none of these sources are good candidates for ¹³C determinations.

IV. THE HC₃N $J = 1 \rightarrow 0$ TRANSITION: A WEAK MASER?

Ever since its initial detection is Sgr B2, the $J = 1 \rightarrow 0$ transition has been known to exhibit a non-LTE hyperfine ratio. Two arguments have been used to explain this result: (1) superposition of up to four distinct velocity components along the line of sight (McGee, Newton, and Butler 1975) and (2) weak maser emission (Morris *et al.* 1976; CWW). Below we discuss each of these suggestions separately in order to reach a consistent conclusion as to the nature of this transition.

a) The Four-Component Model

McGee, Newton, and Butler (1975, hereafter MNB) made observations of the $J = 1 \rightarrow 0$ transition of HC₃N in Sgr B2 using the Parkes 64 m radio telescope (beam size 2.4). They

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1988ApJ...334..182M

Vol. 334



FIG. 3.—The $F = 2 \rightarrow 1$ hyperfine components of the $J = 1 \rightarrow 0$ transition of HC₃N and its ¹³C isomers in TMC-1. The spectrum for the ¹³C isomers was created by averaging the H¹³CCCN, HC¹³CCN, and HCC¹³CN spectra in Fig. 2. Note that both spectra in this figure are displayed on the same velocity scale.

were able to detect all three hyperfine transitions at resolutions ranging from 0.39 to 1.29 km s⁻¹. Using their 1.29 km s⁻¹ results, they fitted four Gaussian curves to the main $(F = 2 \rightarrow 1)$ hyperfine component of the $J = 1 \rightarrow 0$ transition. MNB also fitted a four velocity component model to a 6 cm H₂CO profile obtained at Parkes (velocity resolution ~2 km s⁻¹, beam size 4.1) in order to check the results of the fourcomponent fit to their HC₃N profile. They found that a good fit to the H_2CO profile was obtained when they used the same central velocities (to within the errors) as were used in the HC_3N four-component fit, but that they had to double the line widths obtained from the HC_3N four-component fit.

We have attempted to fit our HC_3N profile with their four Gaussian component model. The fit to our data was fair but was not as good as our two-component models. We have also made the same comparison as MNB by fitting a four Gaussian



FIG. 4.—The $J = 1 \rightarrow 0$ transition of HC₃N in Sgr A

1988ApJ...334..182M

No. 1, 1988

TABLE 5

MEASURED LINE PARAMETERS FOR OTHER SOURCES					
Source	Isomer	$F \rightarrow F'$	V_{LSR} (km s ⁻¹)	T _A ^a (mK)	
тмс-2	HC ₁ N	$0 \rightarrow 1$	+ 6.4	35 ± 38	
	HC ₃ N	$2 \rightarrow 1$		173 ± 38	
	HC ₃ N	$1 \rightarrow 1$		121 ± 38	
	H ¹³ CCCN	$2 \rightarrow 1$	•••	<37	
	HC ¹³ CCN	$2 \rightarrow 1$		< 37	
	HCC ¹³ CN	$2 \rightarrow 1$	••••	< 34	
L1544	HC ₃ N	$2 \rightarrow 1$	+ 7.3	<40	
Orion-KL	HC ₃ N	$2 \rightarrow 1$	+ 8.6	<128	
L183 4N	HC ₂ N	$2 \rightarrow 1$	+2.6	126 ± 10	
	H ¹³ CCCN	$2 \rightarrow 1$		<12	
	HC ¹³ CCN	$2 \rightarrow 1$		<12	
	HCC ¹³ CN	$2 \rightarrow 1$		<12	
ρ Oph B	HC ₃ N	$2 \rightarrow 1$	+ 3.8	<100	
W31C	HC ₃ N	$2 \rightarrow 1$	+ 0.0	<98	
W33	HC ₃ N	$2 \rightarrow 1$	+ 33.8	<69	
L778	HC ₃ N	$2 \rightarrow 1$	+9.9	<41	
B335	HC ₃ N	$2 \rightarrow 1$	+ 8.7	< 37	
DR21 (OH)	HC ₃ N	$2 \rightarrow 1$	-4.0	< 36	
N7538 (OH)	HC ₃ N	$2 \rightarrow 1$	-61.7	< 38	
S162	HC ₃ N	$2 \rightarrow 1$	-44.7	< 38	

^a All values at peak intensity.

component model to an unpublished 2 cm H_2CO profile obtained by us at the NRAO 43 m radio telescope. Using the same fit parameters as MNB used for H_2CO , we were unable to obtain a good fit to our 2 cm H_2CO profile. A twocomponent fit to our 2 cm H_2CO profile, though, yields an excellent fit with central velocities of 64.9 and 81.3 km s⁻¹ and line widths of 16.6 and 11.9 km s⁻¹, respectively.

MNB obtained hyperfine ratios ranging from 6:2:1 to 16:5:1. This would indicate that all four velocity components are exhibiting some non-LTE radiative transfer effect in the HC₃N $J = 1 \rightarrow 0$ transition. The sense of the difference from LTE suggests weak maser amplification of the background continuum source (see below). One of the distinguishing properties of a masing spectral line is a narrowing of the line with respect to its normal Doppler-broadened shape. There is then no reason to expect these four velocity components to be Gaussian in form. We conclude, then, that the four-component model is not a good description of the velocity structure we see in Sgr B2.

b) The Weak Maser Model

Morris *et al.* (1976) have argued that the $J = 1 \rightarrow 0$ transition is weakly masing by noting the following: (1) Statistical equilibrium calculations for HC₃N predict a population inversion in the $J = 1 \rightarrow 0$ transition for $10^3 \leq n_{\text{TOT}} \leq 10^5$ cm⁻³ and $T_k > 10$ K. (2) $N(\text{HC}_3\text{N}) \approx 10^{16}$ cm⁻² in the $J = 1 \rightarrow 0$ transition, a value ~ 100 times that derived from observations of the optically thin higher-J transitions. (3) The observed hyperfine ratio (10:4:1) deviates from its LTE value of 5:3:1 in the same sense that would be expected if a weak maser was occurring. (4) The velocity of peak emission for the $J = 1 \rightarrow 0$

transition is higher than that observed for the other HC_3N transitions. This is consistent with the $J = 1 \rightarrow 0$ transition being a weak maser, since the velocity along the path of highest gain through the cloud does not necessarily correspond to the velocity of maximum thermal emission in the higher-J transitions. Our observations support these conclusions.

There are several additional arguments which lend some support to the weak maser model. If we assume that the excitation temperature is the same for all three hyperfine transitions, we can calculate the optical depth in the $J = 1 \rightarrow 0$ transitions:

$$\frac{T_A(F=2\to 1)}{T_A(F=1\to 1)} = \frac{1-\exp(-0.56\tau)}{1-\exp(-0.33\tau)}.$$

Using the best-fit values for T_A obtained by Gaussian fitting to the peak and line wings of the $F = 2 \rightarrow 1$ transition (see Table 3) yields $\tau = -3.2 \pm 0.3$ for the optical depth τ in the $J = 1 \rightarrow 0$ transition. This would imply that the optical depth in the $F = 2 \rightarrow 1$ hyperfine component is ~ -1.8 , which would amplify the background continuum source ($T_C \sim 11$ K) to more than an order of magnitude above our observed T_A . It appears, then, that either the beam filling factor is <0.01 or, more likely, our assumption that the excitation temperature is the same for the three hyperfine components is not valid. This would occur if the $F = 2 \rightarrow 1$ transition is inverted and masing weakly.

Since a weak maser can cause a spectral line to be narrowed with respect to its intrinsic Doppler-broadened width, one might expect to see this in the $F = 2 \rightarrow 1$ transition. Our observations are consistent with there being a small amount of narrowing in this transition (see Table 3). The amount of expected narrowing, though, is proportional to $(-\tau)^{-1/2}$, indicating that the small optical depths observed and the complex velocity structure in the source probably conspire to mask any narrowing of the $F = 2 \rightarrow 1$ transition. We cannot therefore conclude that the slightly non-Gaussian profile of the $F = 2 \rightarrow 1$ transition is caused by maser narrowing.

Given the arguments above, we feel that it is highly probable that the $J = 1 \rightarrow 0$ transition is exhibiting weak maser emission in Sgr B2.

The physical process which produces this inversion, however, remains somewhat elusive. Goldsmith (1972) has investigated various models for the collisional excitation of CO under typical molecular cloud conditions. He found that a population inversion can occur in the $J = 1 \rightarrow 0$ transition when the selection rules for collisional transitions in linear molecules become such that hard collisions, instead of dipole collisions, dominate. The inversion occurs because the hard collisions take molecules to higher-J states, from which they cascade downward via spontaneous emission. Since the spontaneous emission coefficient for a transition from J to J - 1 is proportional to $J^4/(2J + 1)$, the spontaneous emission rate for the $J = 2 \rightarrow 1$ transition will be 9.6 times that of the $J = 1 \rightarrow 0$ transition, which can cause the J = 1 level to become overpopulated with respect to the J = 0 level for a specific range of density and temperature. This behavior has not been identified in the more common linear molecules (such as CO, CS, and HCN) because the optical depths in the transitions observed are high enough so that the excitation of the molecule is moderated by interaction with the ambient radiation field. This does not seem to be the case with HC_3N , leading one to believe that this mechanism may be causing the anomaly in the $J = 1 \rightarrow 0$ transition in Sgr B2.

V. CONCLUSIONS

1. The $J = 1 \rightarrow 0$ transitions provide no direct evidence for isotopic fractionation in Sgr B2, in contrast to an earlier suggestion of such fractionation.

2. Since its discovery, the HC₃N $J = 1 \rightarrow 0$ transition has been suspected to be a weak maser in Sgr B2. Our data give additional support for that view.

3. Taking masing naively into account, we find ${}^{12}C/$ ${}^{13}C = 11 \pm 2$ for Sgr B2. The ratios are 61^{+28}_{-16} for TMC-1 and \gtrsim 38–75 for Sgr A. This result for Sgr A, if taken seriously, suggests either that there are strong source-to-source varia-

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tions in ${}^{12}C/{}^{13}C$ or that the ${}^{13}C$ isomers of HC₃N are strongly enhanced in some sources and not in others.

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