THE ASTROPHYSICAL JOURNAL, 169:L39–L44, 1971 October 1

MICROWAVE DETECTION OF INTERSTELLAR FORMAMIDE

R. H. RUBIN AND G. W. SWENSON, JR.
University of Illinois Observatory

AND

R. C. BENSON, H. L. TIGELAAR, AND W. H. FLYGARE
Noyes Chemical Laboratory, University of Illinois, Urbana
Received 1971 August 6

ABSTRACT

Formamide was detected by its microwave emission from the $2_{11} \rightarrow 2_{12}$ rotational transition at ~4620 MHz in the direction of Sgr B2 and possibly Sgr A. There is evidence that all three of the $\Delta F = 0$ hyperfine components are present. The astronomical rest frequencies are in good agreement with laboratory measurements.

I. INTRODUCTION

Formamide (NH_2CHO), the simplest molecule containing the amide linkage, was detected in the direction of Sgr B2 at 6.5 cm. This is the first interstellar molecule found that contains H, C, N, and O all in the same molecule. The observations were made 1971 March 23 with the 140-foot telescope at the NRAO.[1] The molecule was detected by emission from its K-type doubling transition $2_{11} \rightarrow 2_{12}$. The rotational-energy levels of formamide exhibit hyperfine splitting due to the coupling of the electric-quadrupole moment of the ^{14}N nucleus with the electronic-charge distribution. For Sgr B2 the $F = 2 \rightarrow 2$ and $F = 1 \rightarrow 1$ hyperfine components were clearly resolved, while the strongest component, $F = 3 \rightarrow 3$, was blended with the H112α line. For Sgr A, since the bandpass did not include the $F = 2 \rightarrow 2$ component, the detection is less certain, but the $F = 3 \rightarrow 3$ line is probably present and blended with the H112α line.

II. LABORATORY MEASUREMENTS

The energy levels of the lowest rotational states in the absence of hyperfine splitting are shown in Figure 1. To the right of the energy-level diagram is a schematic indicating the hyperfine splittings of the 2_{11} and 2_{12} levels. Both $\Delta F = 0$ and $\Delta F = \pm 1$ transitions are allowed, but since the ($\Delta F = \pm 1$, $\Delta J = 0$)-transitions are about 3 times less intense than the weakest ($\Delta F = 0$, $\Delta J = 0$)-transition, only the $\Delta F = 0$ components are expected to be observed.

The rest frequencies of the $F = 2 \rightarrow 2$, $F = 3 \rightarrow 3$, and $F = 1 \rightarrow 1$ absorption transitions were measured in the laboratory, using a standard high-resolution microwave spectrometer employing 5-kHz Stark modulation (Flygare *et al.* 1969). The full widths at half-intensity were ~80 kHz. The measured rest frequencies are: $F = 2 \rightarrow 2$ 4617.118 $\pm$ 0.02, $F = 3 \rightarrow 3$ 4618.970 $\pm$ 0.02, and $F = 1 \rightarrow 1$ 4619.988 $\pm$ 0.02 MHz. There is excellent agreement between the experimental relative intensities of the above lines and the theoretical intensities of 23:42:15. The parameter $3(B - C)$ may be obtained from the measured $F = 1 \rightarrow 1$ and $F = 2 \rightarrow 2$ components and the centrifugal distortion correction of -123 kHz (Kurland and Wilson 1957). Thus, $3(B - C) =$ 4618.676 $\pm$ 0.02 MHz, which was obtained independently of the quadrupole coupling constants. The parameter $B - C$ is then 1539.559 $\pm$ 0.02 MHz, which is useful in calculating the rigid-rotor frequencies of $K = 1$ doublets in $^{14}NH_2CHO$.

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

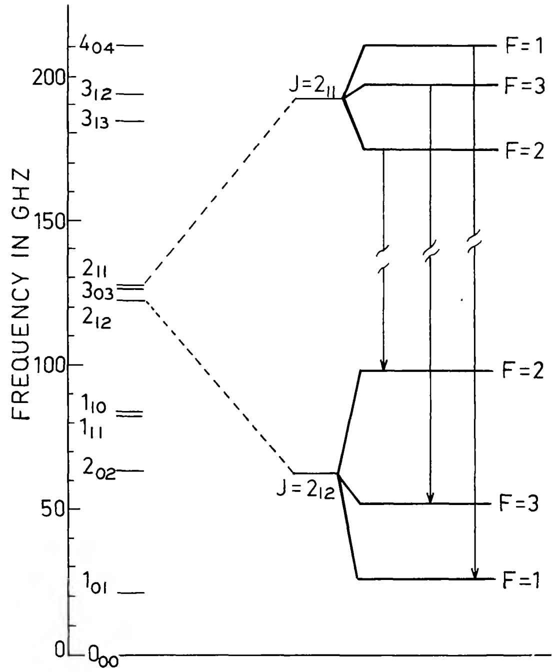

FIG. 1.—Lowest rotational-energy levels for formamide. Hyperfine splittings for the 2_{12} and 2_{11} levels are shown in the inset. The $\Delta F = 0$ transitions are indicated.

III. ASTRONOMICAL OBSERVATIONS

Observations were made with the cooled TRG 6-cm parametric amplifier and the NRAO 413-channel digital autocorrelation receiver. We observed in the total power (nonswitched) mode. The system temperature on cold sky was $\sim 70°$ K, the aperture efficiency was ~ 50 percent, and the half-power beam width (HPBW) was $\sim 6\rlap{.}'5$. We used the autocorrelator as two separate 192-channel receivers (parallel operation) effectively to increase the integration time. Observations were predominantly made with a 5-MHz bandpass, but some data for Sgr B2 were obtained with a 10-MHz bandpass. The ratio of observing time on-source to off-source was 5 to 1. By appropriately shifting the local oscillator frequency in successive on-source measurements, we were effectively smoothing the off-source measurements when forming the difference spectra of on-off.

Figures 2 and 3 show spectra for Sgr B2 and Sgr A, respectively. In each case the telescope was pointed at the peak of the continuum emission. The velocity and frequency scales are with respect to the local standard of rest. The "standard" molecular-cloud velocities correspond to a frequency of 4620 MHz. These spectra were smoothed to a resolution of 104 kHz by using a weighting function which is nearly the equivalent of cosine weighting of the autocorrelation function. In Figure 2 the data collected using a 5-MHz bandpass have been averaged with those obtained using a 10-MHz bandpass. The arrows indicate, from left to right, rest frequencies for the lines He112α, formamide $F = 1 \rightarrow 1$, formamide $F = 3 \rightarrow 3$, H112α, and formamide $F = 2 \rightarrow 2$. For Sgr B2, the integration time on source for a radial velocity with respect to the local standard of rest, $V_{\rm LSR} \lesssim 180$ km s^{-1}, was 140 min, while for larger velocities it was 50 min. For Sgr A, the total time on source was 100 min.

The rest frequency of the H112α line is 4618.790 MHz, only 180 kHz lower than that for the formamide $F = 3 \rightarrow 3$ line. Hence, our spectra must be interpreted with the possibility that the $F = 3 \rightarrow 3$ line is blended with the H112α line. In Figure 2 the positions of the formamide lines and the H112α and the He112α (4620.672 MHz) lines

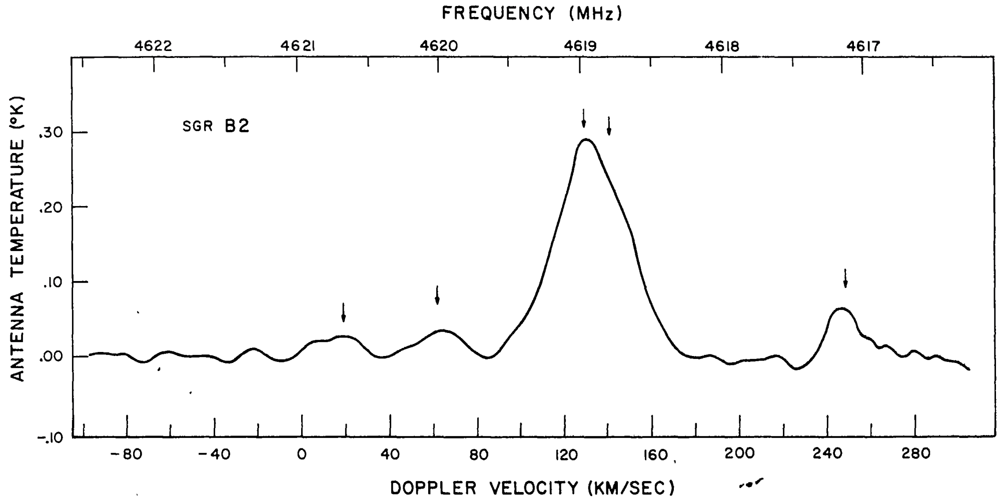

FIG. 2.—Spectrum for Sgr B2. Velocity and frequency scales are such that the molecular-cloud velocity relative to the local standard of rest (62 km s^{-1}) corresponds to a frequency of 4620 MHz. *Arrows*, from left to right: frequencies for the lines He112α, formamide $F = 1 \rightarrow 1$, $F = 3 \rightarrow 3$, H112α, and formamide $F = 2 \rightarrow 2$. Formamide frequencies are those measured in the laboratory.

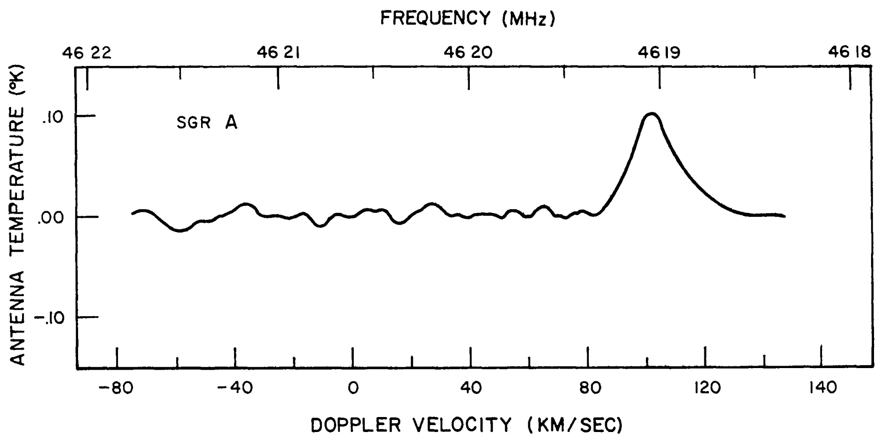

FIG. 3.—Spectrum for Sgr A. Velocity and frequency scales are such that the molecular-cloud velocity relative to the local standard of rest (40 km s^{-1}) corresponds to a frequency of 4620 MHz.

are indicated by arrows, if we assume the "standard" molecular-cloud velocity for Sgr B2, $V_{\rm LSR} = 62$ km s^{-1}. There have been several measurements made for Sgr B2 of the H109α line (5008.923 MHz). The most recent, and the observation with the most integration time (Ball *et al.* 1971), yields the following parameters: line temperature $T_l = 0.27 \pm 0.03°$ K, line-width at half intensity $\Delta\nu_l = 900 \pm 84$ kHz, and $V_{\rm LSR} = 57 \pm 5$ km s^{-1}. Assuming Doppler broadening, we obtain an expected width of 828 kHz for the H112α line by scaling the width of the H109α line. Because of possible non-LTE effects, it is difficult to extrapolate the H112α-line temperature from the H109α value. For this reason and the additional reason that the absolute calibrations of the line-antenna temperatures are uncertain, we assume the H112α-line temperature is 0.27° K. Scaling $T_l = 0.07°$ K for the $F = 2 \rightarrow 2$ line by the theoretical relative intensities, $T_l \sim 0.13°$ K for the $F = 3 \rightarrow 3$ line. We assume $\Delta\nu_l = 260$ kHz for the $F = 3 \rightarrow 3$ line, the same as that for the $F = 2 \rightarrow 2$ line. For the lines measured in this paper, we estimate the uncertainties in T_l to be $\pm 0.02°$ K, in $\Delta\nu_l$ to be ± 30 kHz, and in $V_{\rm LSR}$ to be ± 4 km s^{-1}.

Taking into account the difference in radial velocities, we have superimposed the $F = 3 \rightarrow 3$ and H112α lines assuming Gaussian line shapes with the parameters mentioned above. The resulting blend has a width of 630 kHz and a peak temperature of 0.38° K, in good agreement with the observed profile, which has $T_l = 0.30°$ K and $\Delta\nu_l = 600$ kHz. Agreement in antenna temperature is rather fortuitous because there are considerable uncertainties in the absolute calibration between different observations. However, the agreement in line width indicates that our interpretation of the blended feature is reasonable. Furthermore, there is clear asymmetry in this blended line. The He112α line appears to be present in Sgr B2 with $T_l \sim 0.03°$ K. This is the first detection of a helium recombination line in this source.

At first we believed the line in Figure 3 for Sgr A was solely the $F = 3 \rightarrow 3$ transition (Rubin *et al.* 1971). Our conclusion was made on the basis of the nonappearance of the H109α line to a limit $T_l < 0.05°$ K (Reifenstein *et al.* 1970) and the narrow width of the feature, $\Delta\nu_l = 273$ kHz. The value of T_l is 0.1° K. Recently, Ball *et al.* (1971) have measured the H109α line in Sgr A and found $T_l = 0.077° \pm 0.01°$ K, $\Delta\nu_l = 501 \pm 84$ kHz, and $V_{LSR} = 19 \pm 5$ km s^{-1}. If we scale the H109α-line width by assuming Doppler broadening, we obtain $\Delta\nu_l = 463 \pm 77$ kHz for the H112α line. The observed peak corresponds to $V_{LSR} = 24$ km s^{-1} if we assume this is the H112α line only. This is in agreement with Ball *et al.*'s value of 19 ± 5 km s^{-1}. On the other hand, if this is just the $F = 3 \rightarrow 3$ line, then the velocity is 35 km s^{-1}, which is in good accord with the molecular-cloud velocity of 40 km s^{-1}. However, to explain the narrow line, it is necessary that the molecular line be present. The difference in rest frequencies of the H112α and $F = 3 \rightarrow 3$ line corresponds to a velocity separation of 12 km s^{-1}, while the difference in velocities of the recombination-line source (19 km s^{-1}) and the molecular-cloud source (40 km s^{-1}) is 21 km s^{-1}. Therefore, a line profile in which the $F = 3 \rightarrow 3$ line peaks at a velocity 9 km s^{-1} higher than the H112α line is consistent with the narrow feature observed and with the individual velocities of the ionized hydrogen and molecular sources. Again, the antenna temperature cannot be given much weight in this analysis, due to uncertainties in the absolute calibrations. Of course, observation of the $F = 2 \rightarrow 2$ component in the future would definitely confirm the presence of formamide.

We found no evidence of a formamide line in the following objects: W3 (continuum), W3(OH), Ori A, Ori B, the dust cloud L134, W49, W51, and DR 21. It is difficult to state limits, because the strongest line is, in most cases, lost in the recombination line.

IV. DISCUSSION

The central optical depth of the overall $2_{11} \rightarrow 2_{12}$ transition in the absence of hyperfine splitting is given by

$$\tau = \frac{2(\ln 2)^{1/2}\lambda^2 A_{ul}}{8\pi^{3/2}\Delta\nu_l} \frac{g_u}{g_l}\left(N_l - \frac{g_l}{g_u} N_u\right), \tag{1}$$

where $\Delta\nu_l$ is the full width of the line at half-intensity, A_{ul} is the Einstein coefficient for spontaneous emission (2.5×10^{-9} sec^{-1}), N_l and N_u are the column densities in the lower (2_{12}) and upper (2_{11}) states, respectively, and g_l and g_u are the statistical weights of the lower and upper states, respectively. Using Boltzmann statistics, we may write equation (1) as

$$\tau = \frac{2(\ln 2)^{1/2}\lambda^2 A_{ul}}{8\pi^{3/2}\Delta\nu_l} \frac{g_u}{g_l} N_l\left[1 - \exp\left(-\frac{h\nu}{kT_R}\right)\right], \tag{2}$$

where T_R is the rotation temperature (we assume that the excitation temperature equals the rotation temperature) and ν is the frequency of the $2_{11} \rightarrow 2_{12}$ line.

The quantity N_l can be related to the total population column density, N, through the rotational partition function Q_R by the following expression:

$$N_l = \frac{N g_l \exp\left(-E_l/kT_R\right)}{Q_R}\,, \tag{3}$$

where E_l is the energy of the lower level (2_{12}). For an asymmetric top, Q_R is given by the expansion (Gordy, Smith, and Trambarulo 1953),

$$Q_R = \left[\frac{\pi}{ABC}\left(\frac{kT_R}{h}\right)^3\right]^{1/2} \exp\left[h(B+C)/8kT_R\right]\left[1 + \frac{1}{12}\left(1 - \frac{B+C}{2A}\right)\frac{h(B+C)}{2kT_R} + \ldots\right], \tag{4}$$

where A, B, and C are the rotational constants (Costain and Dowling 1960). In the case of formamide, the above expansion may be truncated after the first term.

The optical depth is related to the line-antenna temperature, T_l, by

$$T_l = \eta(T_R - T_C - 3)\tau \tag{5}$$

for an optically thin line if we assume that a uniform cloud fills the beam. For the present observations, the beam efficiency η is $\sim$0.8 and for Sgr B2 the continuum temperature T_C is $\sim$10° K. The 3° K arises from the cosmic-background temperature. In order to estimate N from our observations of formamide, it is necessary to introduce a hyperfine dilution factor in equations (1) and (2) to obtain an appropriate τ for use in equation (5) with the antenna temperature of a specific hyperfine line. As was mentioned in § III, from the resolved $F = 2 \rightarrow 2$ component we scaled its line temperature by the theoretical relative intensity of the hyperfine components to obtain $T_l \sim 0.13$° K for the $F = 3 \rightarrow 3$ line. The appropriate hyperfine dilution factor for the $F = 3 \rightarrow 3$ line is 0.42 when account is taken of the $\Delta F = \pm 1$ transitions as well as those with $\Delta F = 0$.

Assuming $T_R = 50$° K, we obtain $\tau(F = 3 \rightarrow 3) = 0.0044$, hence justifying the optically thin treatment. Using this value of τ and equations (2)–(4) including hyperfine dilution, we find $N = 2.2 \times 10^{16}$ cm^{-2}. For $T_R \gtrsim 50$° K, N varies roughly as $T_R^{3/2}$. A conservative lower limit to N may be derived by assuming that all the formamide is in the 1_{10} state. Then for $|T_R| \sim 50$° K, $N \sim 4 \times 10^{11}$ cm^{-2}.

Maser-type action in the emission lines of NH_2CHO may be indicated by the small $\Delta\nu_l$ of 17 km s^{-1} in Sgr B2 as compared with 26.3 km s^{-1} for H_2CO (Zuckerman *et al.* 1970), 35 $\pm$ 7 km s^{-1} for CH_3OH (Ball *et al.* 1970), and 58 km s^{-1} for CO (Penzias, Jefferts, and Wilson 1970). However, the formamide line width is comparable to the 19 km s^{-1} for HC_3N (Turner 1971) and 13 km s^{-1} for SiO (Wilson *et al.* 1971).

Another explanation for different line widths for the above molecules could be variations in the spatial extent and, hence, in the Doppler broadening of the lines. Thus, the line-width comparison is inconclusive until other K-doubling and $\Delta J = \pm 1$ transitions are measured.

We wish to express our thanks to George Behrens for his assistance with the equipment and to Dr. John Ball for transmitting his and his colleagues' recombination-line observations. We also thank Dr. David Buhl and Anthony Willis for assistance in processing the data. It is a pleasure to acknowledge support of this project from NSF grants GP 23579 and GP 12382X.

REFERENCES

Ball, J. A., Gottlieb, C. A., Lilley, A. E., and Radford, H. E. 1970, *Ap. J.* (*Letters*), **162**, L203.
———. 1971 (private communication).
Costain, C. C., and Dowling, J. M. 1960, *J. Chem. Phys.*, **32**, 158.
Flygare, W. H., Hüttner, W., Shoemaker, R. L., and Foster, P. D. 1969, *J. Chem. Phys.*, **50**, 1714.
Gordy, W., Smith, W. V., and Trambarulo, R. F. 1953, *Microwave Spectroscopy* (New York: John Wiley & Sons).
Kurland, R. J., and Wilson, E. B., Jr. 1957, *J. Chem. Phys.*, **27**, 585.
Penzias, A. A., Jefferts, K. B., and Wilson, R. W. 1970, *Ap. J.*, **165**, 229.
Reifenstein, E. C. III, Wilson, T. L., Burke, B. F., Mezger, P. G., and Altenhoff, W. J. 1970, *Astr. and Ap.*, **4**, 357.
Rubin, R. H., Swenson, G. W., Benson, R. C., Tigelaar, H. L., and Flygare, W. H. 1971, *I.A.U. Circular No. 2319.*
Turner, B. E. 1971, *Ap. J.* (*Letters*), **163**, L35.
Wilson, R. W., Penzias, A. A., Jefferts, K. B., Kutner, M., and Thaddeus, P. 1971, *Ap. J.* (*Letters*), **167**, L97.
Zuckerman, B., Buhl, D., Palmer, P., and Snyder, L. E. 1970, *Ap. J.*, **160**, 485.