

OBSERVATIONS OF FORMAMIDE AT 6 CM IN SAGITTARIUS B2

By J. C. RIBES,*† J. G. ABLES,* P. D. GODFREY,‡ and R. D. BROWN‡

[Manuscript received 21 August 1972]

Abstract

Six hyperfine components of the $2_{12}-2_{11}$ transition of formamide (NH_2CHO) have been measured in the laboratory. The multiplet was subsequently observed in emission in the direction of Sgr B2 with the 64 m telescope at Parkes. The relative frequencies and intensities of the three strongest components in the hyperfine structure are in excellent agreement with the laboratory measurement. Their Doppler shift corresponds to a radial velocity of 62 km s^{-1} .

I. INTRODUCTION

Rubin *et al.* (1971) have reported the detection of formamide (NH_2CHO) in Sgr A and Sgr B2, and the laboratory measurement of the frequency of the hyperfine structure lines $F = 2 \rightarrow 2$, $3 \rightarrow 3$, and $1 \rightarrow 1$ of the $2_{12}-2_{11}$ transition. The strongest line, $F = 3 \rightarrow 3$ at 4618.99 MHz , lies close to the hydrogen recombination line $\text{H } 112\alpha$ at 4618.79 MHz and was found to be blended with it in the Sgr B2 observation. The other two formamide lines were seen at a radial velocity of 62 km s^{-1} .

Here we report laboratory measurements of six hyperfine components of the formamide $2_{12}-2_{11}$ transition and the observation of the three strongest lines in Sgr B2. The $\text{H } 112\alpha$ line was effectively removed from the formamide profile by subtracting the observed profile of the adjacent $\text{H } 111\alpha$ recombination line. These observations are part of a molecular line search being conducted as a joint program between the Department of Chemistry of Monash University and the Division of Radiophysics of CSIRO.

II. LABORATORY MEASUREMENTS

Previous authors (Kurland and Wilson 1957; Costain and Dowling 1960) have measured and analysed the microwave spectrum of formamide at wavelengths of 3 cm and less to obtain the geometry, electric dipole moment, and nitrogen quadrupole-coupling hyperfine constants for the molecule. More recently, a study of the Zeeman effect in some of the microwave transitions has been reported (Flygare and Benson 1971). With the exception of the recent communication by Rubin *et al.* (1971) there appears to be no mention in the literature of a direct laboratory measurement of any formamide transition at wavelengths longer than 3 cm.

In principle, the molecular constants obtained from the analysis of the shorter wavelength microwave transitions could have been used to calculate the frequency and

* Division of Radiophysics, CSIRO, P.O. Box 76, Epping, N.S.W. 2121.

† Present address: Section d'Astrophysique, Observatoire de Paris, 92-Meudon, France.

‡ Department of Chemistry, Monash University, Clayton, Vic. 3168.

intensity of other lines at longer wavelengths but, in the case of formamide, published values of the quadrupole-coupling constants were considered insufficiently accurate to be of use in calculating the hyperfine splittings in the $2_{12}-2_{11}$ transition at 6 cm. We have therefore measured directly the absorption profile for the $2_{12}-2_{11}$ hyperfine multiplet (see Fig. 1(a)) using a conventional Stark-modulated waveguide spectrometer. The vertical lines below the experimental trace in Figure 1(a) indicate the theoretical line positions and relative intensities. These were obtained from a simple analysis of the hyperfine splittings in the experimental trace.

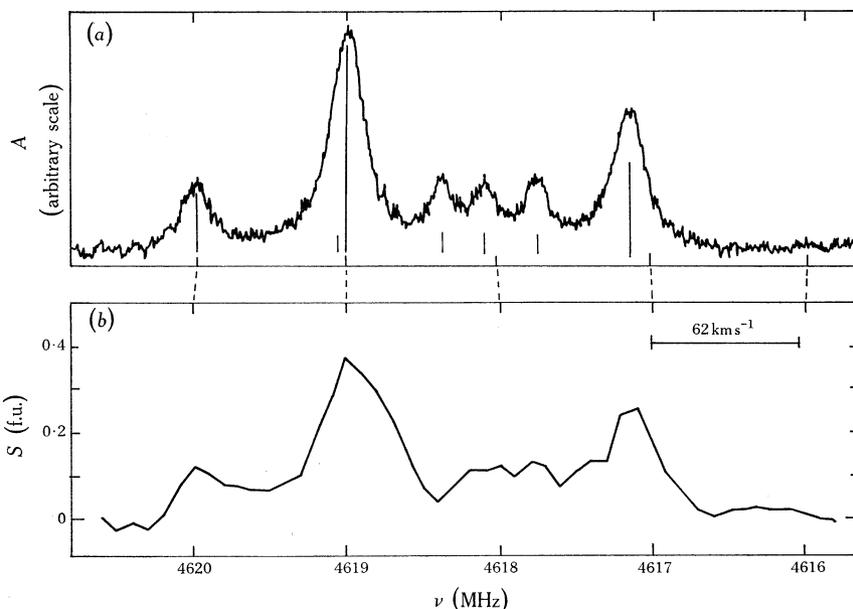


Fig. 1.—Microwave spectra of formamide at 6 cm shown as functions of rest frequency ν : (a) absorption A measured in the laboratory (the calculated position and relative intensity of each line are indicated by the position and size of a vertical bar below the profile); and (b) emission S in flux units ($1 \text{ f.u.} = 10^{-26} \text{ W m}^{-2} \text{ Hz}^{-1}$) derived from the Sgr B2 observations. The frequency shift used to bring about alignment with the laboratory measured profile (corresponding to a radial velocity of 62 km s^{-1} with respect to the local standard of rest) is indicated by the horizontal bar.

From Table 1 it is seen that the frequencies given by Rubin *et al.* (1971) for $\Delta F = 0$ are in good agreement with the present work. The calculated frequencies were computed using revised values for the formamide ^{14}N nuclear quadrupole-coupling constants χ_{aa} and χ_{bb} in the molecular plane, obtained from our analysis of the $2_{12}-2_{11}$ absorption. A comparison of the previously accepted values (Kurland and Wilson 1957) and the revised values is given below:

Kurland and Wilson (1957)	$\chi_{aa} = 1.9 \text{ MHz}$	$\chi_{bb} = 1.7 \text{ MHz}$
Present work	$\chi_{aa} = 1.94 \pm 0.03 \text{ MHz}$	$\chi_{bb} = 1.90 \pm 0.03 \text{ MHz}$

It is seen that in the present work the two constants were found to be almost equal.

This is consistent with the nitrogen atom being in a valence state which possesses trigonal symmetry about the out-of-plane direction c . Actually the bonding at the nitrogen has been shown to be slightly nonplanar (Costain and Dowling 1960). However, from the quadrupole-coupling data, the two hydrogen atoms at the nitrogen are apparently sufficiently close to the plane of the remainder of the molecule for the electric field gradient at the nitrogen nucleus to have axial symmetry about the c direction.

TABLE 1
LABORATORY PARAMETERS OF FORMAMIDE $2_{12}-2_{11}$ HYPERFINE MULTIPLET

$F \rightarrow F$	Theoretical relative intensity	Frequency (MHz)		
		Present measurements	Present calculations	Rubin <i>et al.</i> (1971) measurements
2→2	23·1	4617·14±0·02	4617·14	4617·12±0·02
2→3	5·2	4617·75±0·02	4617·75	—
2→1	5·0	4618·09±0·02	4618·09	—
3→2	5·2	4618·37±0·02	4618·37	—
3→3	41·5	4619·00±0·02*	4618·98	4618·97±0·02
1→2	5·0	—	4619·06	—
1→1	15·0	4620·01±0·02	4620·01	4619·99±0·02

* This component actually consists of the merged profiles of components $F = 3 \rightarrow 3$ and $F = 1 \rightarrow 2$.

III. INTERSTELLAR OBSERVATIONS

The observations were carried out on 13–15 July 1971 with the 64 m telescope at Parkes. The beamwidth was 4'·4 arc and linear polarization was accepted. The receiving system employed a cryogenic parametric amplifier, with an overall noise temperature on cold sky of less than 100 K, together with a 64-channel filter spectrometer (Batchelor *et al.* 1969). Filters with 100 kHz bandwidth were used.

As previously noted (Gardner *et al.* 1971), the telescope gain has a small periodic variation with frequency (of period 5·7 MHz) due to reflections between the apex of the dish and the feed platform. To reduce this instrumental baseline ripple, we obtained "off-source" profiles at a reference region, observed over the same zenith angle range as the source, and subtracted these from the "on-source" profiles.

On the assumption that the instrumental effect did not contain sharp features, the off-source profiles were smoothed over five channels before subtraction. In this way, for equal times on and off source, the contribution of the off-source noise to the final profile was reduced from 41% (without smoothing) to only 10%.

IV. RESULTS

Figure 2(a) shows the observed profile on Sgr B2 resulting from 2½ hr integration on source and the same time off source. The observed frequencies have been reduced to rest frequencies, assuming a radial velocity of 62 km s⁻¹. The $F = 2 \rightarrow 2$ and $1 \rightarrow 1$ lines at 4617·13 and 4620·00 MHz respectively are clearly visible, while the stronger $F = 3 \rightarrow 3$ line at 4618·99 MHz is blended with the H 112 α line at 4618·79 MHz.

In order to separate the formamide emission from the H 112 α line, we observed during the same period the H 111 α line at 4744.183 MHz. Figure 2(b) shows the observed H 111 α profile (30 min on source and 30 min off source) together with a best-fit Gaussian curve having the parameters: central radial velocity, 59.2 km s⁻¹; half-intensity width, 50 km s⁻¹; and intensity, 0.69 f.u.*

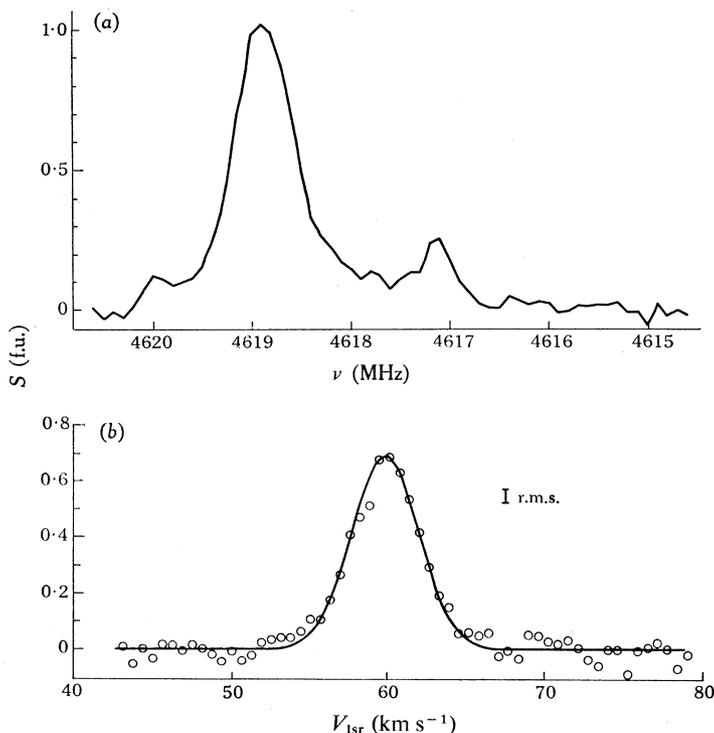


Fig. 2.—Observed 6 cm emission S in Sgr B2 from: (a) formamide and H 112 α , shown as a function of rest frequency ν on the assumption of a radial velocity V_{lsr} for the source of 62 km s⁻¹; and (b) H 111 α recombination line at 4744.183 MHz (open circles). In (b), the curve shows the Gaussian fit used in removing the H 112 α line and the error bar indicates the r.m.s. of the residuals.

A Gaussian curve with these parameters positioned at the H 112 α frequency was subtracted from the formamide observation. The resulting profile, with a frequency shift of 960 kHz, corresponding to a radial velocity V_{lsr} of 62 km s⁻¹ with respect to the local standard of rest is shown in Figure 1(b). The relative frequencies of the remaining lines are in good agreement with the laboratory spectrum of formamide (Fig. 1(a)). The radial velocity of 62 km s⁻¹ is characteristic of a number of molecular lines observed in Sgr B2.

Although one cannot give too much weight to the observed $F = 3 \rightarrow 3$ line because of the uncertainties of the H 112 α subtraction procedure, the general agreement with the laboratory measurement is excellent. This holds not only for the relative positions but also for the relative amplitudes of the three strongest lines.

* 1 flux unit (f.u.) = 10^{-26} W m⁻² Hz⁻¹.

The observed amplitude ratio for the lines (3→3) to (2→2) to (1→1) is 3·2 : 2·1 : 1 as compared with the laboratory value 3·1 : 2·1 : 1. The three weaker lines $F = 2 \rightarrow 3$, $2 \rightarrow 1$, and $3 \rightarrow 2$ are not individually visible in the Sgr B2 observation but the average intensity level at their position is approximately equal to the peak of the $F = 1 \rightarrow 1$ line, in agreement with the laboratory profile.

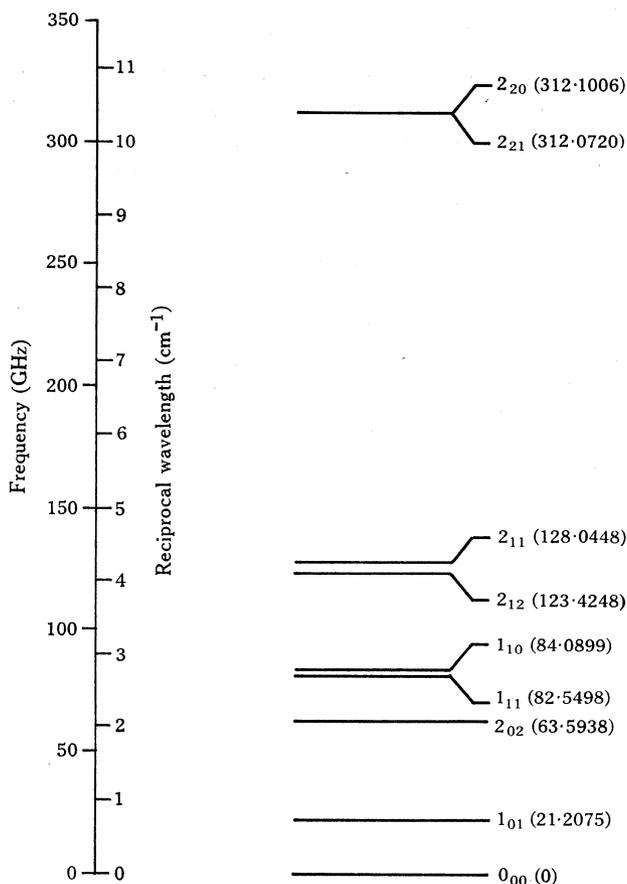


Fig. 3.—Energy levels of the lower rotational states of formamide. The values in parentheses are frequencies (GHz) computed from a rigid rotor model.

V. DISCUSSION

Formamide (NH_2CHO) is a prolate asymmetric top molecule with Ray's parameter $\kappa = -0.95$. In this respect it closely resembles formaldehyde (HCHO) with $\kappa = -0.96$ but, while the latter has two molecular symmetry planes, formamide has none. Consequently, allowed electric dipole transitions occur between very many more rotational levels in formamide than in formaldehyde and there are no metastable rotational levels or noncombining manifolds of rotational levels in the former, in contrast to the situation in formaldehyde (Snyder *et al.* 1969). The energies for the lower rotational states of formamide are shown in Figure 3. The energies are about one-third of those for the corresponding levels in formaldehyde.

Considering spontaneous radiation only, the relative probability of a formamide molecule in the 2_{11} level emitting in the $2_{11}-1_{10}$ transition at 43955 MHz to that of the same level emitting in the observed $2_{11}-2_{12}$ transition is of the order of the third power of the frequency ratio (i.e. ~ 860). Consequently, in the absence of strongly competing nonradiative processes, the $2_{11}-1_{10}$ emission should be readily detectable in Sgr B2.

VI. ACKNOWLEDGMENTS

The authors wish to thank Mr. J. G. Crofts for his assistance in measuring the laboratory microwave absorption frequencies. They are much indebted to Dr. F. F. Gardner for his guidance and support at all stages of this program. The Monash authors (P.D.G. and R.D.B.) acknowledge support of the work by a grant from the Australian Research Grants Committee.

VII. REFERENCES

- BATCHELOR, R. A., BROOKS, J. W., and SINCLAIR, M. W. (1969).—*Proc. Instn Radio electron. Engrs Aust.* **30**, 39.
- COSTAIN, C. C., and DOWLING, J. M. (1960).—*J. chem. Phys.* **32**, 158.
- FLYGARE, W. H., and BENSON, R. C. (1971).—*Molec. Phys.* **20**, 225.
- GARDNER, F. F., RIBES, J. C., and COOPER, B. F. C. (1971).—*Astrophys. Lett.* **9**, 181.
- KURLAND, R. J., and WILSON, E. B., JR. (1957).—*J. chem. Phys.* **27**, 585.
- RUBIN, R. G., SWENSON, G. W., JR., BENSON, R. C., TIGELAAR, H. L., and FLYGARE, W. H. (1971).—*Astrophys. J. Lett.* **169**, L39.
- SNYDER, L. E., BUHL, D., ZUCKERMAN, B., and PALMER, P. (1969).—*Phys. Rev. Lett.* **22**, 679.