

Microwave Emission of the $2_{11} \rightarrow 2_{12}$ Rotational Transition in Interstellar Acetaldehyde

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Abstract

The $2_{11} \rightarrow 2_{12}$ transition of acetaldehyde at 3195.167 MHz has been observed in emission in Sgr B2 with the Parkes 64 m telescope. Comparison of the intensities of the $1_{10} \rightarrow 1_{11}$ and $2_{11} \rightarrow 2_{12}$ emission lines suggests that both transitions may be inverted.

Introduction

Gottlieb (1973) reported an emission line at 1065 MHz in Sgr B2 and Sgr A which was identified with a $1_{10} \rightarrow 1_{11}$ transition in acetaldehyde (CH_3CHO) on the basis of the agreement in radial velocity with other molecules observed in the galactic centre region. To provide spectroscopic confirmation of this we have observed the $2_{11} \rightarrow 2_{12}$ transition of CH_3CHO in Sgr B2 (G0.7-0.0) at a frequency of 3195 MHz. The rest frequency of the $2_{11} \rightarrow 2_{12}$ transition was measured in the laboratory in order to derive an accurate radial velocity for the interstellar emission.

Rest Frequency of $2_{11} \rightarrow 2_{12}$ Transition

The microwave spectrum of acetaldehyde at frequencies greater than 8 GHz was first analysed by Kilb *et al.* (1957). Although the molecule is not rigid, owing to internal rotation of the methyl group with respect to the remainder of the molecule, Kilb *et al.* found that for the $K_{-1} = 1$ Q -branch transitions the frequencies of lines for molecules in states with A -torsional symmetry are given by the usual rigid rotor formula with a minor correction for centrifugal distortion:

$$\nu = \nu_R + D_J J^2(J+1)^2,$$

where the centrifugal distortion coefficient D_J has the value -0.00285 MHz.

Kilb *et al.* (1957) gave only approximate values for the effective rotational constants b' and c that are needed to calculate the rigid rotor frequency ν_R for the $2_{11} \rightarrow 2_{12}$ line. A more accurate value of ν_R has been calculated by using the measured frequency of 1065.075 ± 0.005 MHz for the $1_{10} \rightarrow 1_{11}$ line given by Gottlieb (1973), since $\nu_R(2_{11} \rightarrow 2_{12})$ is exactly three times larger than $\nu_R(1_{10} \rightarrow 1_{11})$. This gives a calculated value for the rest frequency of the $2_{11} \rightarrow 2_{12}$ line of 3195.16 ± 0.02 MHz. Following the astronomical observation, the transition was measured in the laboratory at Monash University using a conventional Stark modulation microwave spectrometer. The measured frequency of 3195.167 ± 0.010 MHz is in good agreement with the previously calculated value.

Astronomical Observations

The Parkes 64 m telescope was equipped with a 9 cm parametric amplifier having a noise temperature of about 200 K. The telescope beam had a half-width of $6' \cdot 2$ arc. The methods of observation and reduction are described by Sinclair *et al.* (1973).

We detected the $2_{11} \rightarrow 2_{12}$ transition of acetaldehyde in the direction of Sgr B2 in an observing period from 13 to 17 December 1971 (Fourikis *et al.* 1971). The line profile in Fig. 1 was obtained using a 64-channel spectrometer with a filter bandwidth of 33 kHz, the integration time being 60 min; the telescope was directed at the position R.A. $17^{\text{h}} 44^{\text{m}} 13^{\text{s}} \cdot 3$, Dec. $28^{\circ} 25' \cdot 8$ (epoch 1950.0).

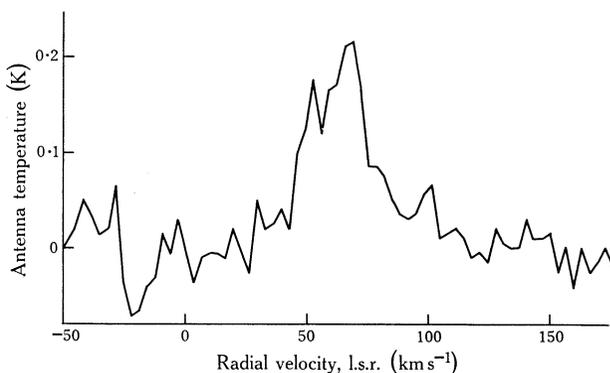


Fig. 1. Profile of the $2_{11} \rightarrow 2_{12}$ emission at 3195.167 MHz from acetaldehyde in Sgr B2, observed with the Parkes 64 m telescope. The channel bandwidth was 33 kHz.

Discussion

Radial velocity and line width

For a rest frequency of 3195.167 MHz the radial velocity at the peak of the line is $62 \pm 3 \text{ km s}^{-1}$. This value agrees well with velocities observed in Sgr B2 for many molecules, e.g. hydroxyl, formaldehyde, formamide, cyanoacetylene, thioformaldehyde (Sinclair *et al.* 1973) and methanimine (Godfrey *et al.* 1973). The radial velocity for the $1_{10} \rightarrow 1_{11}$ emission of acetaldehyde observed by Gottlieb (1973) was $58 \pm 10 \text{ km s}^{-1}$, which is close to the velocity $54 \pm 9 \text{ km s}^{-1}$ found for methanol (Radford 1972).

The line width at half-power for the $2_{11} \rightarrow 2_{12}$ transition of acetaldehyde corresponds to a velocity spread of approximately 24 km s^{-1} . This is comparable with the width of lines associated with other molecules in Sgr B2.

Column density of molecules

The column density $N_l L$ of molecules in the 2_{12} (lower) state is related to the optical depth $\tau(\nu)$ by

$$N_l L = \int N_l ds = \frac{3ck g_l}{8\pi^3 g_u \nu_{lu}^2 |\mu_{lu}|^2} \int \tau(\nu) d\nu, \quad (1)$$

where ν_{lu} is the transition frequency between the state u and the lower state l , $|\mu_{lu}|^2$ is the square of the dipole matrix element for the transition ($= (1.04 \text{ D}^*)^2$)

* 1 debye (D) = $3.336 \times 10^{-30} \text{ C m}$.

in this case) and T_e is the excitation temperature of the 2₁₁-2₁₂ doublet. When the optical depth is small, the brightness temperature of the line profile $\Delta T(\nu)$ is approximately equal to $(T_e - T_{bg})\tau(\nu)$, where T_{bg} is the brightness temperature of the continuum background, including the isotropic radiation of 2.7 K. Substitution into equation (1) then yields

$$N_l L = \frac{3ck g_l}{8\pi^3 g_u} \frac{T_e}{T_e - T_{bg}} \frac{1}{\nu_{lu}^2 |\mu_{lu}|^2} \int \Delta T(\nu) d\nu. \tag{2}$$

We assume that the size of the acetaldehyde cloud in Sgr B2 is the same as that of the cyanoacetylene cloud mapped by McGee *et al.* (1973), i.e. about 5' arc. If we also assume a beam efficiency of 0.8, the observed 2₁₁→2₁₂ emission profile corresponds to a column density of

$$N_l L = 3.5 \times 10^{14} T_e / (T_e - T_{bg}) \text{ molecules cm}^{-2}, \tag{3}$$

which rises from a minimum of 3.5×10^{14} molecules cm⁻² if $T_e \gg T_{bg}$ to very high values if $T_e \approx T_{bg}$. We shall explore possible values of T_e/T_{bg} in the next subsection.

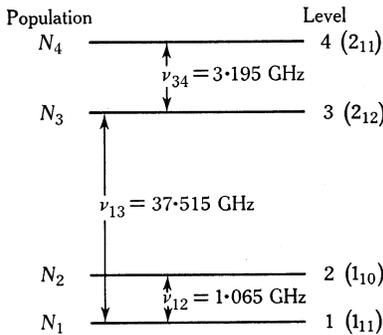


Fig. 2. Energy level scheme used for comparison of intensities of emission at 1.065 GHz (ν_{12}) and 3.195 GHz (ν_{34}).

Rotational excitation

Since the 2₁₁→2₁₂ line is observed in emission we know that T_e is greater than T_{bg} . It is likely that T_e will be comparable with the kinetic temperature in the Sgr B2 molecular cloud, which ranges from 12 K (from the CO observations of Penzias *et al.* 1971) to 60 K (from the NH₃ observations of Cheung *et al.* 1969). It is thus comparable with the continuum temperature of 50 K observed from Sgr B2 at a wavelength of 9 cm. A large fraction of the continuum is absorbed by the formaldehyde and hydroxyl molecules at $V \approx 60$ km s⁻¹ in the direction of Sgr B2, so that much of the continuum originates behind these molecules and therefore presumably also behind the acetaldehyde. However, observations of a single spectral line give little information about T_e or T_e/T_{bg} .

More insight into the rotational excitation of the acetaldehyde is provided by a comparison of the 1₁₀→1₁₁ and 2₁₁→2₁₂ emission lines. For the four energy levels shown in Fig. 2 the ratio of the integrated profile intensities for the transitions between levels 4 and 3 and between levels 2 and 1 is, from equation (2),

$$\int \Delta T_{34}(\nu) d\nu / \int \Delta T_{12}(\nu) d\nu = \left(\frac{\nu_{34}}{\nu_{12}} \right)^2 \frac{|\mu_{34}|^2}{|\mu_{12}|^2} \frac{1 - T_{bg34}/T_{34}}{1 - T_{bg12}/T_{12}} \left[\frac{g_3}{g_1} \exp\left(-\frac{h\nu_{13}}{kT_{13}}\right) \right], \tag{4}$$

where T_{12} , T_{34} and T_{13} are the excitation temperatures T_e of the corresponding transitions. The quantity in square brackets is the population ratio N_3/N_1 ; the value of $h\nu_{13}/k = 1.8$ K. Equation (4) enables us to determine T_{ij}/T_{bgij} as a function of T_{13} . The value of T_{13} might be anywhere between the 2.7 K isotropic background temperature and the kinetic temperature of the cloud, but is probably closer to the latter, i.e. some tens of kelvins.

As before, we assume that the acetaldehyde cloud has a size of about 5' arc and that it is optically thin for the radio emission lines. From the Parkes observations at $\nu_{34} = 3195$ MHz and the Green Bank observations of Gottlieb (1973) at $\nu_{12} = 1065$ MHz (0.2 K emission on the 43 m telescope with a line width of 85 kHz), the left-hand side of equation (4) has the value 0.27 (assuming comparable efficiencies for the two telescopes). Substituting $(\nu_{34}/\nu_{12})^2 = 9$, $|\mu_{34}|^2/|\mu_{12}|^2 = 1/3$ and $g_3/g_1 = 5/3$ (Townes and Schawlow 1955), we find

$$\frac{1 - T_{bg34}/T_{34}}{1 - T_{bg12}/T_{12}} = 0.054 \exp\left(\frac{1.8}{T_{13}}\right). \quad (5)$$

We shall now consider the implications of equation (5) in several ranges of T_{ij}/T_{bgij} which could produce emission lines at both ν_{12} and ν_{34} .

(i) $T_{ij} \gg T_{bgij}$

For $T_{12} \gg T_{bg12}$ and $T_{34} \gg T_{bg34}$ we require $\exp(-1.8/T_{13}) = 0.054$, or $T_{13} = 0.6$ K. Although no observations have been made of the $2_{12} \rightarrow 1_{11}$ or $2_{11} \rightarrow 1_{10}$ transitions (ν_{13} or ν_{24}) in CH_3CHO , no case is known of a millimetre-wave transition with T_e below the isotropic background temperature of 2.7 K. We thus reject a solution which requires the ν_{13} (and ν_{24}) transitions to be cooled below 2.7 K.

For the more likely case of $T_{13} \geq 2.7$ K, we have the ratio $N_3/N_1 \geq 0.85$. From equation (4) we then see at once that for $T_{ij} > T_{bgij}$ the ratio on the left-hand side would exceed 2.6, compared with the observed ratio of 0.27. Thus the emission at ν_{12} is much too strong relative to that at ν_{34} to allow T_{ij} to be much greater than T_{bgij} .

(ii) $T_{ij} \approx T_{bgij}$

The variation of T_{34}/T_{bg34} with T_{12}/T_{bg12} which satisfies equation (5) is shown in Fig. 3a for various values of T_{13} . Over the whole range $2.7 \text{ K} < T_{13} < \infty$, the value of T_{34} is restricted to a narrow range a few per cent greater than T_{bg34} . What is shown by Fig. 3a is that the intensity at ν_{34} can be drastically reduced compared with case (i) if the excitation temperature T_{34} of this transition is nearly equal to the brightness temperature of the background continuum radiation at this frequency, namely ~ 50 K. If the levels are collisionally excited, the kinetic temperature would then have to be somewhat greater than 50 K. However, we would then expect T_{12} also to be about 50 K, much less than T_{bg12} at $\nu_{12} = 1065$ MHz (about 500 K), and this is contrary to the observation of emission from the $1_{10}-1_{11}$ doublet.

(iii) *Maser Emission (T_{ij} Negative)*

A high value of the integral of $\Delta T_{12}(\nu) d\nu$ could alternatively be explained by amplification of the strong continuum present at the observing frequency. This would require T_{12} to be negative. The necessary degree of inversion can be calculated from equation (5), with results as shown in Fig. 3b. When the $1_{10}-1_{11}$ transition is

strongly inverted ($|T_{12}|$ small) the 2₁₁-2₁₂ transition has also to be inverted (T_{34} negative). For a lower degree of inversion of the 1₁₀-1₁₁ transition, the observations can be fitted without inversion of the 2₁₁-2₁₂ transition but with high positive values of T_{34}/T_{bg34} .

It thus appears likely that the observed intensity of the 1065 MHz emission from acetaldehyde in Sgr B2 requires maser amplification to explain the unexpectedly high intensity relative to that at 3195 MHz. The latter transition may also be inverted. The rotational excitation of the molecule cannot be specified more closely until observations have been made of the 2₁₂-1₁₁ and 2₁₁-1₁₀ transitions near 8 mm wavelength.

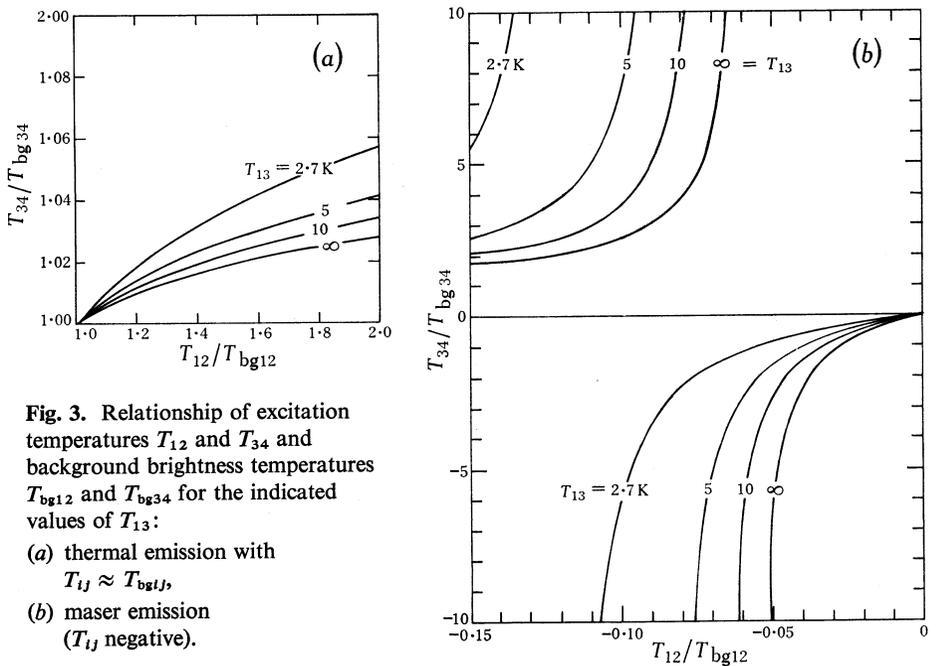


Fig. 3. Relationship of excitation temperatures T_{12} and T_{34} and background brightness temperatures T_{bg12} and T_{bg34} for the indicated values of T_{13} :

- (a) thermal emission with
 $T_{1j} \approx T_{bg1j}$,
(b) maser emission
(T_{1j} negative).

Acknowledgment

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References

- Cheung, A. C., Rank, D. M., Townes, C. H., Knowles, S. H., and Sullivan, W. T. (1969). *Astrophys. J.* **151**, L13.
 Fourikis, N., Sinclair, M. W., Brown, R. D., Godfrey, P. D., and Blackman, G. (1971). I.A.U. Circular No. 2379.
 Godfrey, P. D., Brown, R. D., Robinson, B. J., and Sinclair, M. W. (1973). *Astrophys. Lett.* **13**, 119.
 Gottlieb, C. A. (1973). In 'Molecules in the Galactic Environment' (Eds M. A. Gordon and L. E. Snyder), p. 181 (Wiley-Interscience: New York).
 Kilb, R. W., Lin, C. C., and Wilson, E. B. (1957). *J. chem. Phys.* **26**, 1695.
 McGee, R. X., Newton, Lynette M., Batchelor, R. A., and Kerr, A. R. (1973). *Astrophys. Lett.* **13**, 25.
 Penzias, A. A., Jefferts, K. B., and Wilson, R. W. (1971). *Astrophys. J.* **165**, 229.

- Radford, H. E. (1972). *Astrophys. J.* **174**, 207.
- Sinclair, M. W., Fourikis, N., Ribes, J. C., Robinson, B. J., Brown, R. D., and Godfrey, P. D. (1973). *Aust. J. Phys.* **26**, 85.
- Townes, C. H., and Schawlow, A. L. (1955). 'Microwave Spectroscopy', 698 pp. (McGraw-Hill: New York).

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