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THE KINETIC TEMPERATURE AND DENSITY OF THE SAGITTARIUS B2 MOLECULAR CLOUD FROM OBSERVATIONS OF METHYL CYANIDE

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ABSTRACT

From observations with the Bell Laboratories 7 m telescope of the K components of the CH_3CN $J = 4 \rightarrow 3$ rotational transition at 73.6 GHz, $6 \rightarrow 5$ transition at 110.4 GHz, and $7 \rightarrow 6$ transition at 128.7 GHz, a mean kinetic temperature of 85 ± 10 K and a mean H_2 density of $(1.1 \pm 0.5) \times 10^5$ cm^{-3} are deduced for the central 2′ of the Sgr B2 molecular cloud. Within the $K = 0$–4 ladders of CH_3CN in Sgr B2 the populations of the radiatively coupled J levels are relaxed, with a rotational temperature of approximately 16 K—similar to that of several linear molecules.

Subject headings: interstellar: molecules — molecular processes — nebulae: individual

I. INTRODUCTION

Nearly all our knowledge of the structure, temperature, and density of interstellar molecular clouds has been derived from observations of trace molecular constituents since H_2 and He, the dominant species, are exceedingly difficult to observe in cold regions of high obscuration. To illustrate how temperature and density can be determined from observations of a trace polar molecule, let us consider the simple case of such a molecule with optically thin rotational lines in a static, homogeneous cloud of kinetic temperature T_{kin} and neutral particle density $n \approx n(H_2)$, and let us assume that rotational excitation results only from collisional impact with H_2 and radiative interaction with the cosmic microwave background. Rotational populations will typically equilibrate on the scale of days, so statistical equilibrium is also a good assumption. In very diffuse or very dense clouds the rotational temperature T_{rot} of such a molecule is well defined, being equal at low density to 2.7 K, the background temperature, and at high density to T_{kin}; but at intermediate densities T_{rot} is not precisely defined, and level populations and line intensities in general depend in a complicated way on T_{kin} and $n(H_2)$. In principle it is possible to solve for these in terms of the observed line intensities if the matrix of collisional excitation rates or cross sections is known. In practice this inversion is often impossible—because collisional rates are poorly known, because of observational uncertainties, or because the assumption of cloud homogeneity is poorly satisfied. In attempting to carry out this inversion symmetric top molecules offer distinct advantages, as we will demonstrate by determining the temperature and density of the Sgr B2 molecular cloud from observations of methyl cyanide, CH_3CN.

In a symmetric top the rotational levels are labeled by J, the total angular momentum quantum number, and K, the quantum number for the projection of angular momentum along the symmetry axis. Rotational radiative transitions do not change K, so that the total population of one K ladder relative to another is determined only by collisions and is hence a function only of T_{kin}. Within a K ladder the populations radiatively relax and are thus a function of both T_{kin} and $n(H_2)$, but, with T_{kin} determined, the problem of finding $n(H_2)$ is considerably simplified.

These properties have been used previously to determine the temperature and density of Sgr B2 from observations of the $J = 6 \rightarrow 5$ transition in methyl cyanide (Solomon *et al.* 1971, 1973). For lack of data on additional J levels, these authors assumed that the distribution within each K ladder could be described by an effective rotational temperature, which they guessed to be about 5 K. The intensities observed in the different K ladders then implied $T_{kin} = 100$ K.

In this paper we present well calibrated observations of three CH_3CN rotational transitions, and with them we refine our knowledge of the temperature and density of the Sgr. B2 cloud. We first show that an approximate rotational temperature T_J that is much smaller than T_{kin} can be defined within the various K ladders. Relaxing this assumption, we then proceed to determine T_{kin} and $n(H_2)$ on the basis of statistical equilibrium alone by fitting a theoretical spectrum to the observational data. This calculation requires the rates for CH_3CN collisional excitation which have not yet been measured or

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explicitly calculated, but by using constraints imposed by molecular scattering theory and analogies with similar molecules we have been able to make reasonable estimates for these. Two sets of rates which are thought to span the range of likely values have been used to determine the sensitivity of our results to the collisional model.

II. OBSERVATIONS

Our observations of the millimeter-wave spectrum of methyl cyanide in Sgr B2 were made with the 7 m telescope of the Bell Laboratories in Holmdel, New Jersey, between 1978 January and 1980 February. Observations were made in single sideband mode with a spectral resolution of 1 MHz. The method of hot and cold load calibration and of filtering are described by Goldsmith (1977). Position switching to a spot free of emission was also used. The best spectra were obtained of the $6 \rightarrow 5$ rotational transition at 110.4 GHz and the $7 \rightarrow 6$ transition at 128.7 GHz, with integration times of 1.8 and 3.9 hours, respectively, and a somewhat poorer spectrum of the $4 \rightarrow 3$ transition at 73.6 GHz was obtained in an integration of 30 min. The observational data are shown in Figure 1; T_R^* is the antenna temperature corrected for beam efficiency, atmospheric attentuation, ohmic losses, and spillover (Kutner and Ulich 1981). The beamwidth and efficiency of the 7 m antenna at the respective frequencies are given in Table 1.

By analogy with other molecules of similar complexity (such as HNCO and HC_3N) we expected that CH_3CN would be extended in Sgr B2 on the scale of the Bell antenna beam, and we have shown from a limited map of the $6 \rightarrow 5$ transition that this expectation is correct. In particular observations were made 2′ (one beamwidth at this frequency) N, E, S, and W of the central position; the antenna temperature averaged over these points was about half that found at the central position.

III. ANALYSIS

We have analyzed the data in terms of two excitation models, the first a simple two-temperature model very similar to that used by Solomon *et al.* (1971; see also Hollis *et al.* 1981), and the second a full statistical equilibrium calculation. In both cases we assumed that the source is homogeneous over the observed region. Although we have determined by limited mapping that the methyl cyanide emission comes from an extended region, we cannot preclude the possibility of structure on a scale smaller than our beamwidth. All transitions were assumed to be optically thin, consistent with the largest calculated optical depth being less than 0.1.

Methyl cyanide has relatively low frequency vibrational modes, and Sgr B2 is a known far-infrared source, so it is important to consider the possible effect of vibrational pumping on level populations. The infrared color temperature of Sgr B2 at wavelengths less than 100 μm is approximately 32 K (Gateley *et al.* 1978); the lowest frequency vibrational mode of CH_3CN, $\nu_8 = 365$ cm^{-1}, is well to the blue of the peak in the infrared intensity and will therefore provide the fastest pump

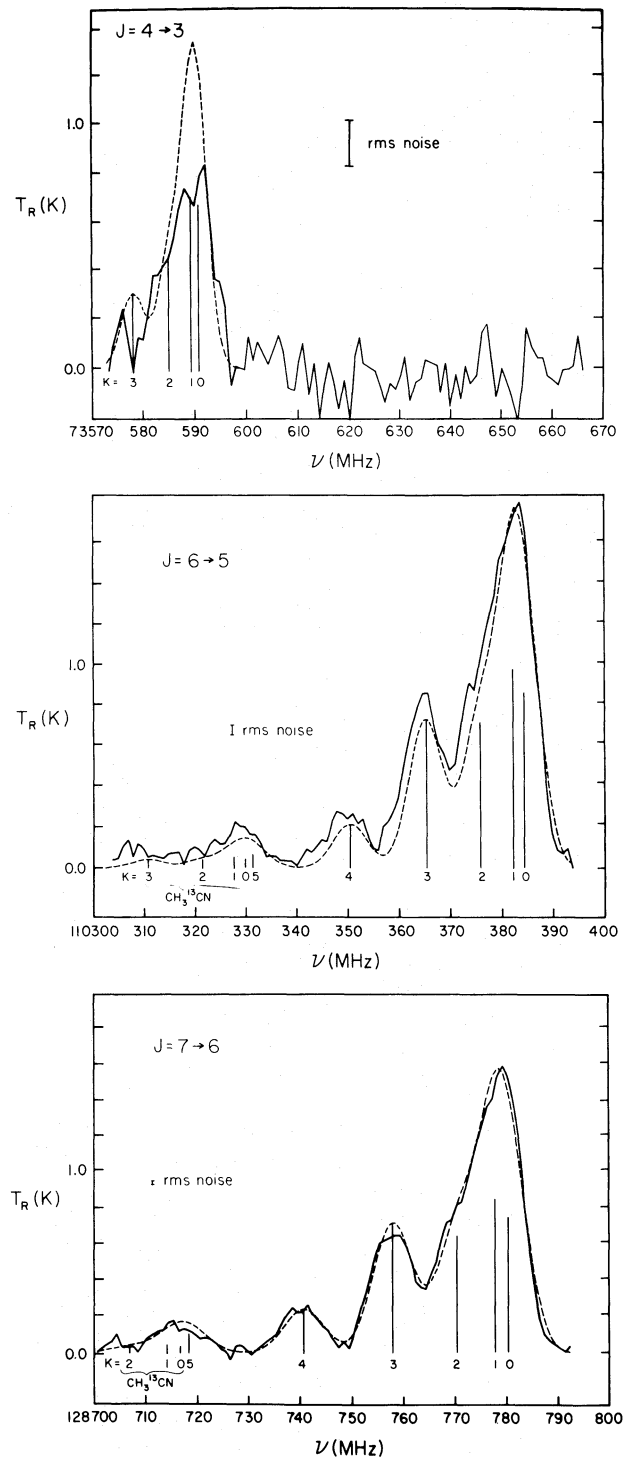

FIG. 1.—The observed methyl cyanide spectra (*full lines*) are compared with predicted spectra (*broken lines*) obtained from the least squares fit statistical equilibrium calculation (using collision rate set 1). The predicted spectra are obtained by assuming Gaussian line shapes for each transition whose calculated frequency and intensity are indicated by the vertical lines. The ordinate is antenna temperature corrected for beam efficiency.

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TABLE 1

BEAM WIDTH AND EFFICIENCY OF THE 7 m TELESCOPE

Frequency (GHz)	Full Beam Width at Half-Intensity (arcmin)	Beam Efficiency
73	2.9	0.95
110	1.9	0.79
128	1.6	0.72

rate. The absolute oscillator strengths for CH_3CN have not been measured. To provide an upper limit, we have assumed a dipole derivative of 25 esu $g^{-1/2}$, which can be compared with the value of 4 esu $g^{-1/2}$ measured for the analogous CCN bending mode in HC_3N (Deguchi *et al.* 1979) or 11 esu $g^{-1/2}$ for the strong bending mode in CO_2 (Person *et al.* 1981). Subject to 32 K blackbody radiation, vibrational excitation of this transition will occur at a rate of 3×10^{-7} s^{-1}, which is at least two orders of magnitude slower than collisional excitation of the ground rotational levels at the density we deduce for Sgr B2. Vibrational radiative excitation of CH_3CN can therefore be ignored.

a) *Two-Temperature Model*

The observational data, Figure 1, were least squares fitted with overlapping Gaussians to obtain the intensity of each transition and a value for source linewidth Δv and source velocity with respect to the local standard of rest v_{LSR}. The intensities were then fit with a two-temperature excitation model, where T_{kin} describes the distribution of total population among K ladders, and T_J describes the population distribution within each K ladder and is assumed independent of K. The best fit gives $T_{kin} = 81$ K, $T_J = 16$ K, and a CH_3CN column density of 1.4×10^{14} cm^{-2}. Intensities predicted by this model are compared with the experimental values in Figure 2. With these two temperatures, and with an estimate for the collisional cross section, one can estimate $n(H_2)$ within the context of a two-level system. Adopting a cross section of 2×10^{15} cm^2, as in the earlier studies, we find $n(H_2) = 2 \times 10^6$ cm^{-3}.

One difficulty with this approach is that separation of the overlapping $K = 0$ and $K = 1$ transitions requires an initial guess for T_{kin} and also the (not unreasonable) assumption that $N_A = N_E$, where N_A and N_E are the column densities in A ($K = 0, 3, 6, \ldots$) and E ($K = 1, 2, 4, 5, \ldots$) symmetry species, respectively. Another possible problem is the assumption that the population distribution within the K ladders can be described by a single effective temperature, T_J, and that this is independent of K. To circumvent these restrictions and to find $n(H_2)$ in a more direct manner, we undertook a statistical equilibrium calculation using the model described next.

b) *Statistical Equilibrium Model*

This model uses the equations of statistical equilibrium with collision rates dependent on the quantum numbers of each transition to solve for the excitation temperature (and hence intensity) of each spectral line as a function of T_{kin} and $n(H_2)$. Assuming a Gaussian line shape, the actual spectrum can be predicted from this information plus five additional parameters—N_A, N_E, Δv, v_{LSR}, and the ratio of CH_3CN to $CH_3{}^{13}CN$. (The last parameter

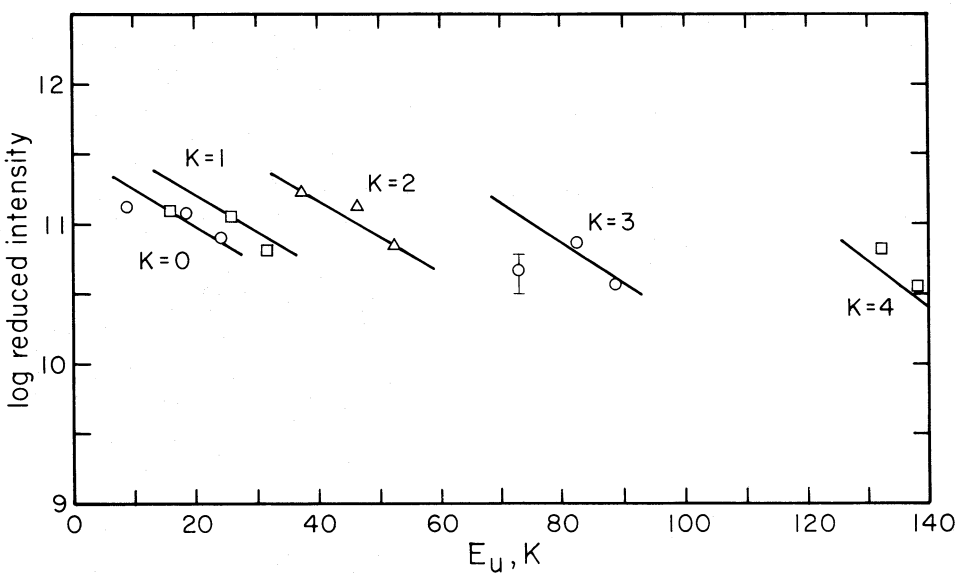

FIG. 2.—Observed methyl cyanide line intensities are compared with predictions of the two-temperature model. The log of the corrected antenna temperature divided by the oscillator strength (Linke, Frerking, and Thaddeus 1979) is plotted as a function of the energy of the upper spectroscopic level. Experimental data are indicated by open symbols; except for $K = 3$, $J = 4 \rightarrow 3$, the error bars are smaller than the symbols. The model predicts that within each K ladder the points will lie on the indicated line segments; the slope of these lines is determined by the effective rotational temperature T_J.

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is needed since transitions of $CH_3{}^{13}CN$ are blended with $K = 5$ transitions of CH_3CN.) All seven parameters were varied in a nonlinear least squares program to obtain the best fit to the data. The small hyperfine splittings due to the nitrogen nuclear quadrupole were found to have a negligible effect on the spectral fits. Noise in the $J_U = 4$ spectrum was much greater than that in the $J_U = 6$ and 7 spectra, and the data were weighted in the fit by the inverse of the square of rms noise in each spectrum.

Since neither laboratory data nor specific theoretical calculations for CH_3CN–H_2 collisions exist, the rates were estimated from analogous systems for which calculations are available, taking into account constraints from molecular scattering theory as described in the Appendix. Two sets of rates were chosen that are believed to span the likely range of uncertainty. Comparison of results from these two sets should provide an indication of the sensitivity of derived parameters to the uncertainty in collision rates.

Best fit parameters from this model are given in Table 2. In all cases the formal uncertainties in the parameters given by the least squares fitting program were much less than the spread due to uncertainties in the collision rates. The fits to the spectra are quite good as can be seen in Figure 1, the results obtained with rate set 1. The fit with rate set 2 is nearly identical, although the best fit parameters are somewhat different.

A potential difficulty with this approach is the possibility that the data do not contain enough information to warrant a seven parameter fit, in which case the values obtained might not be physically meaningful. Several factors suggest that this has not occurred. First, the values obtained for Δv, v_{LSR}, and $CH_3CN/CH_3{}^{13}CN$ are in good agreement with measurements on other molecules in this source. Second, the least squares correlation matrix indicates that the parameters that describe the line shape: Δv and v_{LSR}, are only weakly coupled to those that describe intensities via statistical equilibrium: T_{kin}, $n(H_2)$, N_A, and N_E; hence, the former cannot be correcting for deficiencies in the model. Finally, a fit was made with only three parameters, T_{kin}, $n(H_2)$, and the total CH_3CN column density, by setting $N_E = N_A$, $^{12}C/^{13}C = 20$, $\Delta v = 20.7$ km s^{-1}, and $v_{LSR} = 59.7$ km s^{-1}; $n(H_2)$ and $N_A + N_E$ were essentially the same as for the seven-parameter fit, but T_{kin} was lower by about 8 K. This constrained fit provided noticeably poorer agreement with the observed spectrum.

TABLE 2

PROPERTIES OF THE SAGITTARIUS B2 MOLECULAR CLOUD

Property	Collision Model 1	Collision Model 2
T_{kin} (K)	88.7	92.1
$n(H_2)$ (cm^{-3})	1.6×10^5	6.2×10^4
N_A (cm^{-2})	6.3×10^{13}	6.2×10^{13}
N_E (cm^{-2})	7.9×10^{13}	7.7×10^{13}
Δv (km s^{-1})	21.0	21.1
v_{LSR} (km s^{-1})	59.5	59.6
$CH_3CN/CH_3{}^{13}CN$	19.8	20.2

The relative column densities for A and E symmetry species found in the statistical equilibrium calculations are somewhat unexpected. In thermal equilibrium at finite temperatures $N_A/N_E \geq 1$ with the high temperature limit of unity being a good approximation even at 80 K. Although it is possible that the nonthermal (less than unity) ratio we find does, in fact, reflect an interesting physical phenomenon, we are unable to suggest any plausible mechanism. We therefore believe that this result reflects systematic errors, for example, reabsorption of $K = 0$ intensity by cold foreground gas. Unfortunately, the derived T_{kin} is sensitive to assumptions about the N_A/N_E ratio. As discussed above, fixing this ratio at the plausible value of unity in the statistical equilibrium fit lowers T_{kin} by 5–10 K. The lower value of T_{kin} obtained in the simpler two-temperature model also appears largely to reflect the assumption that $N_A/N_E = 1$. We estimate however that systematic errors are unlikely to amount to more than 10 K, and we accordingly adopt $T_{kin} = 85 \pm 10$ K.

From the standpoint of statistical equilibrium, it is instructive to reconsider the validity of the two-temperature model. Its fundamental assumption is that all levels within a K ladder share a common excitation temperature T_J. In Figure 3 we show the variation of T_{ex} with J_U that has been obtained from statistical equilibrium calculations. Although there is strong variation for low J_U, for intermediate and high J_U, T_{ex} is approximately constant, and dependence on K is small. Further, this qualitative behavior is not sensitive to the choice of collision rates. The present observational study is mainly based on $J_U = 6$ and 7, and it is noteworthy that the statistical equilibrium model has optimized T_{kin} and $n(H_2)$ so that T_{ex} is approximately 17 K for both of these levels. This is illustrated in Figure 4 which shows the variation of T_{ex} as a function of $n(H_2)$. It is hence not surprising that the two temperature model yields a very similar effective rotational excitation temperature, $T_J = 16$ K. The distribution between different K ladders is determined by essentially the same physical parameter, T_{kin}, in both models, and both yield similar values. Determination of the CH_3CN column density requires assumptions about the distribution of population among the unobserved levels, the two models giving somewhat different results; however, the effect here is rather small with agreement to better than 10%. On the other hand the two-level assumption needed to obtain $n(H_2)$ within the context of the two-temperature model is poor, and $n(H_2)$ is overestimated by more than an order of magnitude. Figures 3 and 4 suggest that the addition of data for lower J_U transitions would make analysis by the simpler two temperature model less reliable; it would also place stronger demands on the statistical equilibrium model including the need for more accurately known collision rates.

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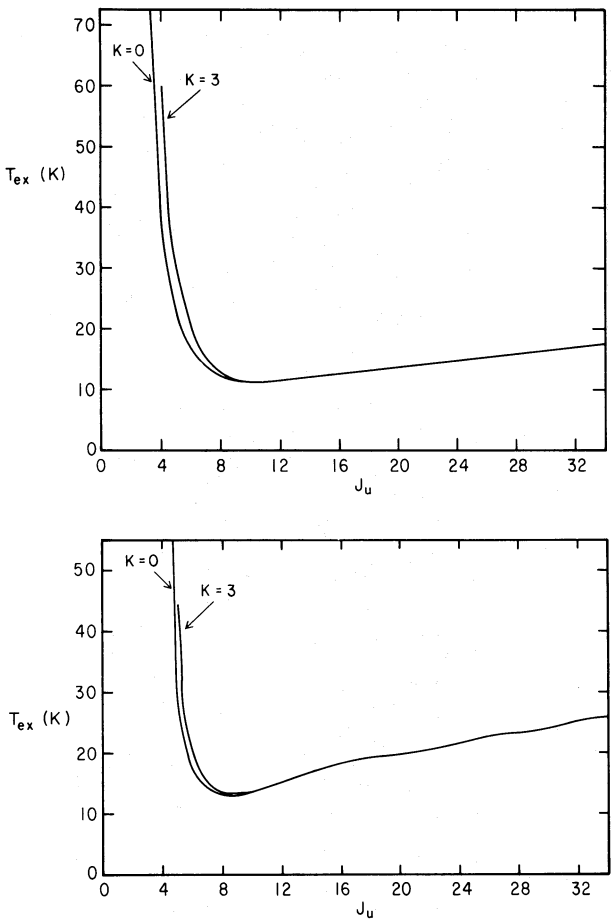

FIG. 3.—Excitation temperatures calculated from the statistical equilibrium model are shown as a function of J_U. Upper and lower plots correspond to the two different assumptions for the collision rates; in each case the values of T_{kin} and $n(H_2)$ are fixed by the least squares fit to the data. Excitation functions for the $K = 1$ and $K = 2$ ladders, which are not shown, fall in between those for the $K = 0$ and $K = 3$ ladders.

IV. DISCUSSION

We have demonstrated the utility of symmetric top molecules like methyl cyanide as probes of the kinetic temperature and density in interstellar clouds. In particular we have analyzed observations of Sgr B2 on the assumption of statistical equilibrium, employing reasonable estimates for the collision rates. As anticipated, because the rotational K ladders are connected by collisional but not by radiative transitions, their relative populations provide a measure of T_{kin} that is largely independent of the collisional rates. Within each K ladder, on the other hand, the populations among different J levels can radiatively relax and are very far from thermalized at the indicated Sgr B2 density of about 10^5 cm^{-3}. An interesting quasi equilibrium, however, does exist for these levels: the excitation temperatures of adjacent levels are nearly equal, so that populations are approximately characterized by a rotational temperature, $T_J \approx 15$–20 K $\ll T_{kin}$, and this is nearly the same for the different K ladders. The extent of radiative relaxation—the difference between T_{kin} and T_J—then provides a measure of the density, albeit one that reflects uncertainties in the collision rates.

In general our detailed statistical equilibrium results justify use of the simple two-temperature model for obtaining T_{kin} adopted by Solomon *et al.* (1971) and recently revived by Hollis *et al.* (1981). However, validity of this model for conditions substantially different from those found here remains to be tested. While this model gives a reasonable estimate for T_{kin} from symmetric top data, the further assumptions needed to determine $n(H_2)$ are found to be poor. It is clear that a full statistical equilibrium calculation will always provide a better quantitative description. If well calibrated data for low as well as high J values are available this simpler model is expected to be less reliable. In that case better information about collision rates for use in a statistical equilibrium calculation will also be desirable.

The greatest uncertainty in our analysis probably lies in the assumption of a homogeneous molecular cloud—a point already noted in connection with the N_A/N_E ratio obtained from the statistical equilibrium model. Another indication that inhomogeneity may be important occurs in the fit to the $J = 4 \rightarrow 3$ data. Statistical equilibrium calculations for a homogeneous cloud predict that the excitation temperature should increase sharply for lower transitions, but the $J = 4 \rightarrow 3$ data do not clearly show this. Unfortunately, these data are so noisy that we cannot state with great confidence that they contradict the adopted model. Nonetheless, the trend agrees with a model that has, e.g., lower excitation foreground material. It is clear that better data for lower transitions are important for a more precise analysis, and that the physical parameters derived here must be regarded as averages over the 2′ beam of the Bell telescope. In order to estimate the errors that might be introduced by our neglect of small scale structure, we have considered the extreme assumption of a point-like source. In that case, T_{kin} decreases by about 25%, $n(H_2)$ decreases by about a factor of 3, the CH_3CN column density increases by nearly an order of magnitude, and the ratio of $^{12}C/^{13}C$ species increases by about 25%.

It is interesting that a number of molecular transitions observed in Sgr B2 all appear to be described by excitation temperatures of about 10–20 K. Although this might be interpreted as thermalization at a kinetic temperature in this range, the present methyl cyanide results suggest that such is not the case. More likely, these are further examples of quasithermal equilibrium similar to that found here for the J levels within each K ladder; this may be a quite common phenomenon under conditions of low excitation.

Finally, we compare our results with values derived for the Sgr B2 molecular cloud from other observations. The kinetic temperature of about 85 K that we obtain is in reasonable accord with the estimate of 100 K derived from earlier methyl cyanide observations

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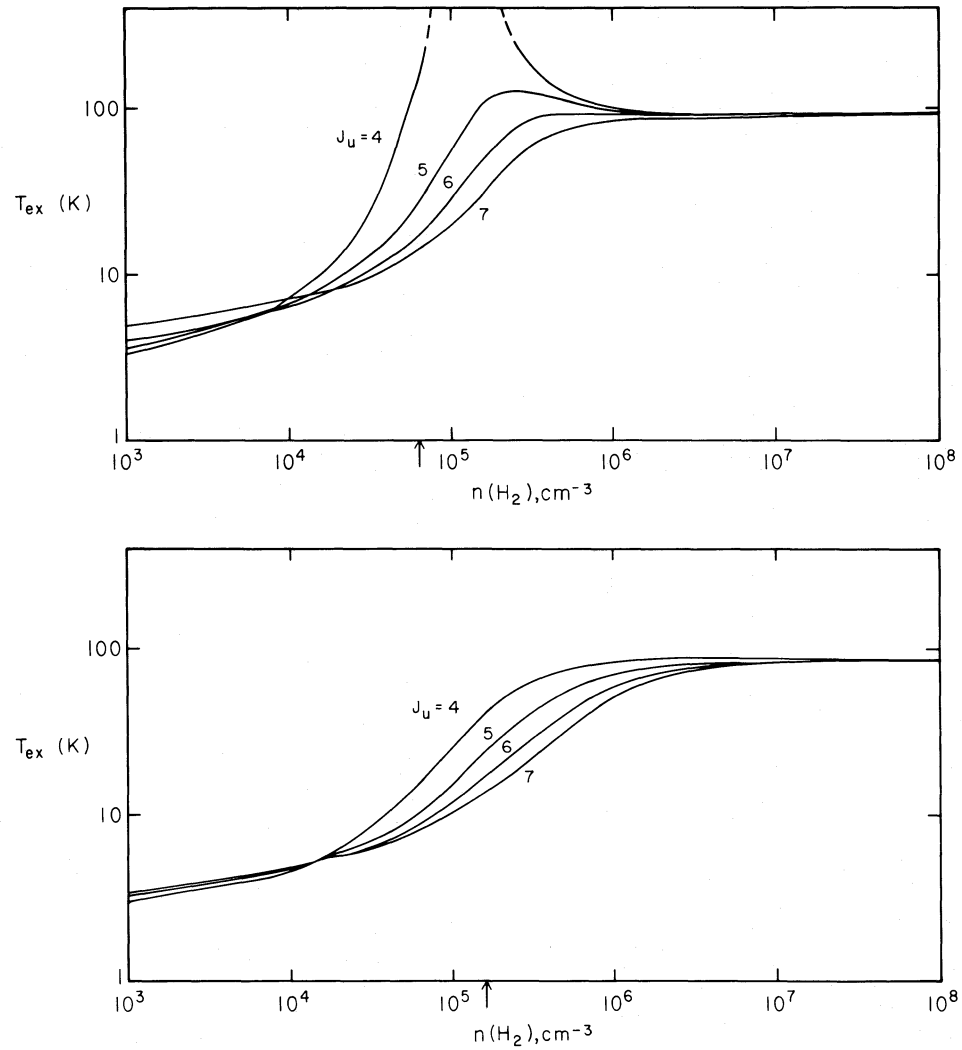

FIG. 4.—Excitation temperatures in the $K = 0$ ladder calculated from the statistical equilibrium model are shown as a function of $n(H_2)$. Upper and lower plots correspond to the two different assumptions for the collision rates. In each case T_{kin} has been set at its best fit value, and the best fit value for $n(H_2)$ is indicated by an arrow on the abscissa.

(Solomon *et al.* 1973). Recent observations of another symmetric top, methyl acetylene, however, suggest a somewhat lower value of $T_{kin} = 47 \pm 6$ K (Hollis *et al.* 1981). The source of this discrepancy is not clear although it might reflect small scale structure in the source. Our estimate $n(H_2) = 10^5$ cm^{-3} is somewhat more subject to uncertainties in the collision rates than the other derived parameters, but the credibility of this value is enhanced by its consistency with detailed analyses of CS (Linke and Goldsmith 1980) and OCS (Goldsmith and Linke 1981). The ratio of $^{12}C/^{13}C$ isotopic variants is in excellent agreement with values found for HC_3N (Wannier and Linke 1978) and OCS (Goldsmith and Linke 1981).

APPENDIX

To calculate rotational populations in statistical equilibrium requires knowledge of the matrix of state-to-state collisional excitation rates. There is little experimental data for most molecular collisions, and none for CH_3CN–H_2; fairly accurate rates have been obtained theoretically for simple systems such as CO–H_2, H_2CO–H_2, and NH_3–He, but such calculations have not been done for CH_3CN–H_2. However, experience suugests that collisional rates vary with enough regularity for similar molecules that it should be possible to make reasonable estimates.

Considerable simplification occurs when the rotational energy intervals are small relative to the collisional energy,

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for then the entire matrix of collisional rates can be expressed in terms of a few fundamental rates, $Q(L, K)$, that are simply related to excitation out of the lowest $J = K = 0$ level. For a symmetric top these rates are:

$$R(JK \to J'K') = (2J' + 1) \sum_{L=|J-J'|}^{J+J'} \begin{pmatrix} J' & L & J \\ K' & K - K' & -K \end{pmatrix}^2 Q(L, |K - K'|) , \tag{A1}$$

the large bracket being a $3-j$ symbol (Green 1979). This formula assumes that K ranges over both positive and negative values, though levels which differ only in the sign of K are degenerate and are not spectroscopically distinguished. It is therefore convenient to combine the populations in degenerate levels, limit K to nonnegative values, and use rates that have been averaged over initial and summed over final K degeneracies.

Equation (A1) is often found to be a rather good approximation for downward transitions even when the rotational energy spacings (as at present) are appreciable with respect to the collisional energy; and rates for the corresponding upward transitions can then be obtained from detailed balance. It is then necessary to estimate only a rather small set of fundamental rates $Q(L, K)$. For other systems where detailed ab initio calculations are available, these are found to depend mainly on simple geometric properties of the collision systems. The $Q(L, 0)$ correspond to collisions which do not change the K quantum number and are expected to be similar to excitation of a linear molecule; OCS (Green and Chapman 1978) was chosen as an analogous system with similar geometrical parameters. Because of the threefold symmetry axis the $Q(L, K)$ are nonzero only if K (which corresponds to changes of the projection of J on the symmetry axis) is an integral multiple of three. The only system with similar symmetry for which detailed calculations have been performed is NH_3, and these suggest that the $Q(L, K)$ decrease rather slowly with K. Experimental data recently obtained for CH_3F–He in an expanding supersonic molecular beam indicate that relaxation within a K ladder is only two to three times faster than relaxation across K ladders—consistent with the rates adopted here (Gough 1982).

Based on these analogies and experience with other systems the two sets of $Q(L, K)$ listed in Table 3 have been adopted with the intention of spanning the extremes of reasonable behavior, the $Q(L, K)$ in the first set decreasing rather sharply with L and those in the second decreasing slowly, and hence favoring multiple quantum excitation. Because collisional excitation competes with radiative relaxation satisying the selection rule $\Delta J = \pm 1$, it is found that high ΔJ collisions can have an important qualitative effect on statistical equilibrium (Goldsmith 1972). Comparison of results using these two sets of collision rates should therefore give a reasonable estimate of the sensitivity to errors in the assumed rate constants.

Because the inferred H_2 density scales with the total collision rate, both sets of rates have been scaled so that the total rate into the lowest level is the same; it was chosen from an estimate of the geometric cross section and

TABLE 3

FUNDAMENTAL COLLISION RATES, $Q(L, K)$

		Collision Model	
L	K	1	2
1	0	3.39×10^{-10}	2.18×10^{-10}
2	0	1.69×10^{-10}	2.18×10^{-10}
3	0	1.35×10^{-10}	2.08×10^{-10}
4	0	1.02×10^{-10}	1.97×10^{-10}
5	0	6.77×10^{-11}	1.75×10^{-10}
6	0	3.39×10^{-11}	1.53×10^{-10}
7	0	1.35×10^{-11}	1.31×10^{-10}
8	0	0.0	1.09×10^{-10}
9	0	0.0	8.74×10^{-11}
10	0	0.0	6.55×10^{-11}
11	0	0.0	4.37×10^{-11}
12	0	0.0	3.93×10^{-11}
13	0	0.0	1.09×10^{-11}
3	3	2.37×10^{-10}	1.56×10^{-10}
4	3	1.02×10^{-10}	6.68×10^{-11}
5	3	4.74×10^{-11}	3.12×10^{-11}
6	3	2.03×10^{-11}	1.34×10^{-11}
7	3	6.77×10^{-12}	4.46×10^{-12}
6	6	6.77×10^{-11}	4.46×10^{-11}
7	6	3.39×10^{-11}	2.23×10^{-11}
8	6	6.77×10^{-12}	4.46×10^{-12}

NOTE.—$Q(L, K)$ in $cm^3\ s^{-1}$.

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is likely to be correct to within a factor of two. Microwave pressure broadening data for CH_3CN by H_2 which could provide an accurate value for this total rate are unfortunately not available.

Finally, it has been assumed that the downward collision rates are independent of kinetic temperature. This has been found to be an adequate approximation for other systems in the temperature range of interest here.

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