1986ApJ...307..332V

THE ASTROPHYSICAL JOURNAL, **307**:332–336, 1986 August 1

DETECTION OF THE (3, 0) PHILLIPS BAND OF INTERSTELLAR C_2 TOWARD ZETA OPHIUCHI[1]

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Received 1985 October 25; accepted 1986 January 17

ABSTRACT

Observations of the interstellar C_2 molecule in the (3, 0) Phillips band around 7720 Å are presented for the line of sight toward ζ Oph. Twelve weak C_2 lines with equivalent widths less than 0.6 mÅ, originating from rotational levels up to $J'' = 10$ are detected among a multitude of atmospheric oxygen lines. The measured C_2 column densities in the various rotational levels generally agree well with those found from observations of C_2 in the (2, 0) Phillips band around 8750 Å. Previous studies have yielded conflicting results for the temperature inferred from the populations of the lowest levels. Our observed C_2 rotational population distribution implies a low kinetic temperature, $T \approx 30$ K, and a relatively low but uncertain density, $n_H \approx 200$ cm^{-3}, in the center of the ζ Oph cloud.

Subject headings: interstellar: abundances — interstellar: molecules — stars: individual

I. INTRODUCTION

The interstellar C_2 molecule has been observed toward a number of reddened early-type stars. The C_2 observations are of particular interest since absorption lines arising from various rotational levels of the ground state of the molecule can be detected. Because C_2 has no dipole moment and thus lacks rapid radiative rotational transitions, the corresponding rotational populations are determined by a competition between collisional excitation and de-excitation, and radiative excitation through absorption into excited electronic states followed by infrared cascade (Chaffee *et al.* 1980). Comparison of the measurements with theoretical population distributions (van Dishoeck and Black 1982) generally allows the determination of the kinetic temperature and density in the line-forming regions. The temperature is constrained mainly by the observed column densities in the lower rotational levels, $J'' = 0$ and 2, the density by those in the higher levels $J'' > 4$.

Most observations of interstellar C_2 have been performed in the $A\,^1\Pi_u$–$X\,^1\Sigma_g^+$ Phillips system for which the transitions lie in the far-red, near-infrared part of the spectrum and can thus be observed from Earth. Although the first detection of interstellar C_2 was in the ($v' = 1$, $v'' = 0$) Phillips band at wavelengths around 10140 Å (Souza and Lutz 1977), recent observations have focused on measurements in the (2, 0) band at 8750 Å (e.g., Chaffee and Lutz 1978; Hobbs 1979, 1981; Chaffee *et al.* 1980; Hobbs and Campbell 1982; Danks and Lambert 1983; van Dishoeck and de Zeeuw 1984). The (2, 0) band lies conveniently in a wavelength region where there are virtually no atmospheric lines. Also, the Reticon detectors with which most observations are performed, are more sensitive below 9000 Å.

From each rotational level $J'' > 0$, three different lines, belonging to the P-, Q-, and R-branches, arise within one band. A comparison of the column densities derived from the individual lines thus provides an excellent check on the reliability of the results. Most of the O, B, and A type stars used for interstellar absorption-line studies exhibit a strong H I Paschen 12 line near 8750 Å, the redward wing of which typically provides a steep continuum for most of the C_2 R-branch lines with $J'' < 14$. Because of this problem of continuum placement, the equivalent widths of the (2, 0) R lines are generally less reliable than those of the strong Q and weak P lines with the same J''. For $J'' = 0$, however, only one line, the $R(0)$ line, exists. The accuracy of the inferred temperature for a particular line of sight is therefore limited mainly by the accuracy of the measured column density in $J'' = 0$ from the $R(0)$ line.

The temperature in the bulk of the primary component in front of the star ζ Oph has been the subject of considerable controversy. Values between 20 K (Black and Dalgarno 1977) and 60 K (Crutcher and Watson 1981; Wannier, Penzias, and Jenkins 1982) have been suggested. Since the C_2 molecules are thought to be located mainly in the central region of the cloud (van Dishoeck and Black 1986), an accurate determination of their rotational populations provides another measure of the temperature in the cloud. Observations of C_2 toward ζ Oph in the (2, 0) Phillips band have been performed most recently by Hobbs and Campbell (1982) and Danks and Lambert (1983). Although the two sets of observations agree reasonably well for most of the lines, they show unfortunate discrepancies for the $J'' = 0$ to $J'' = 2$ column density ratios. The measurements of Danks and Lambert imply a low temperature, $T \approx 25$ K, whereas the observations by Hobbs and Campbell suggest a higher temperature, $T \approx 50$ K. The earlier observations of the Mulliken system of C_2 by Snow (1978) at ultraviolet wavelengths also suggested a low temperature. An independent measurement of the C_2 $J'' = 0$ and 2 column densities toward ζ Oph is therefore certainly warranted.

More information on the column densities may be obtained by observations of other bands in addition to the (2, 0) band. The (3, 0) band of the Phillips system lies near 7720 Å and its oscillator strength is only a factor of 2 smaller than that of the

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(2, 0) band (van Dishoeck 1983; Chabalowski, Peyerimhoff, and Buenker 1983). Detection of the stronger *R* and *Q* lines toward ζ Oph should therefore be feasible and might help to refine the inferred temperature in the center of the ζ Oph cloud.

II. OBSERVATIONS

Spectra in the wavelength region of the C_2 (3, 0) Phillips band were obtained with the ESO coudé echelle spectrograph fed by the 1.4 m coudé auxiliary telescope, using an unintensified Reticon detector of 1872 photodiodes cooled to 140 K (Enard 1981). The resolving power was set at 80,000 (97 mÅ), corresponding to an entrance slit width of 348 μm and a reciprocal dispersion of 2.4 Å per mm or 35 mÅ per pixel. The detector array was centered at 7720 Å, and covered the 7687–7753 Å range. This range includes all *R* lines of the (3, 0) band of practical interest, the *Q* lines for $J'' \leq 12$, and the *P* lines for $J'' \leq 10$. Nine exposures with an average integration time of 45 minutes were taken toward ζ Oph on three different nights between 1984 August 21 and 28, under conditions of average to good transmission and seeing. The total integration time was about seven hours. Flat-field lamp spectra were taken immediately before and after each stellar exposure and were used to normalize them after correction for readout noise. The reduced spectra were then co-added, taking into account the Earth's motion.

Although the wavelength region around 7720 Å is free of strong stellar lines, it is heavily contaminated by atmospheric lines of molecular oxygen, which may obscure the weak C_2 lines. Since the velocity of the Earth relative to ζ Oph changes during the year, it produces a shift in the wavelengths at which the C_2 lines appear relative to the positions of the stationary oxygen lines. Only at a certain time of year are most of the C_2 lines, including the *R*(0) and *Q*(2) lines, not directly obscured by oxygen lines. This fact was the main motivation for performing the observations in August even though ζ Oph can then be seen for only a small portion of the night. Three additional spectra in the (3, 0) band, with a total integration time of $2\frac{1}{2}$ hours, were taken at a less favorable time in 1985 March, when the most important C_2 lines for our purposes are blended with oxygen lines.

III. RESULTS

The summed spectrum of ζ Oph in the region of the C_2 (3, 0) Phillips band obtained in 1984 August is presented in Figure 1. Twelve absorption features belonging to the *P*, *Q*, and *R* branches and originating from levels up to $J'' = 10$ can be identified. Because of the smaller oscillator strength of the (3, 0) band, the interstellar C_2 features are very weak, and a factor of 4 longer integration times are needed to obtain the same accuracy as for lines in the (2, 0) band. The pattern of the stronger absorption lines in Figure 1 belongs to molecular oxygen in the Earth's atmosphere. These lines were used to establish the wavelength scale, based on the laboratory wavelengths of Babcock and Herzberg (1948). The measured positions of the C_2 lines then yield a heliocentric radial velocity of (-15.3 ± 1) km s^{-1}, in good agreement with $v_{\rm helio} = (-14 \pm 1)$ km s^{-1} obtained by Hobbs and Campbell (1982) and Danks and Lambert (1983) from observations of the C_2 (2, 0) band.

The measured equivalent widths obtained from the co-added spectra are presented in Table 1. In August, only the strong *Q*(4) line was obscured by the oxygen lines. Table 1 also includes the results obtained in 1985 March. Because of the shorter total integration time, these results are less reliable,

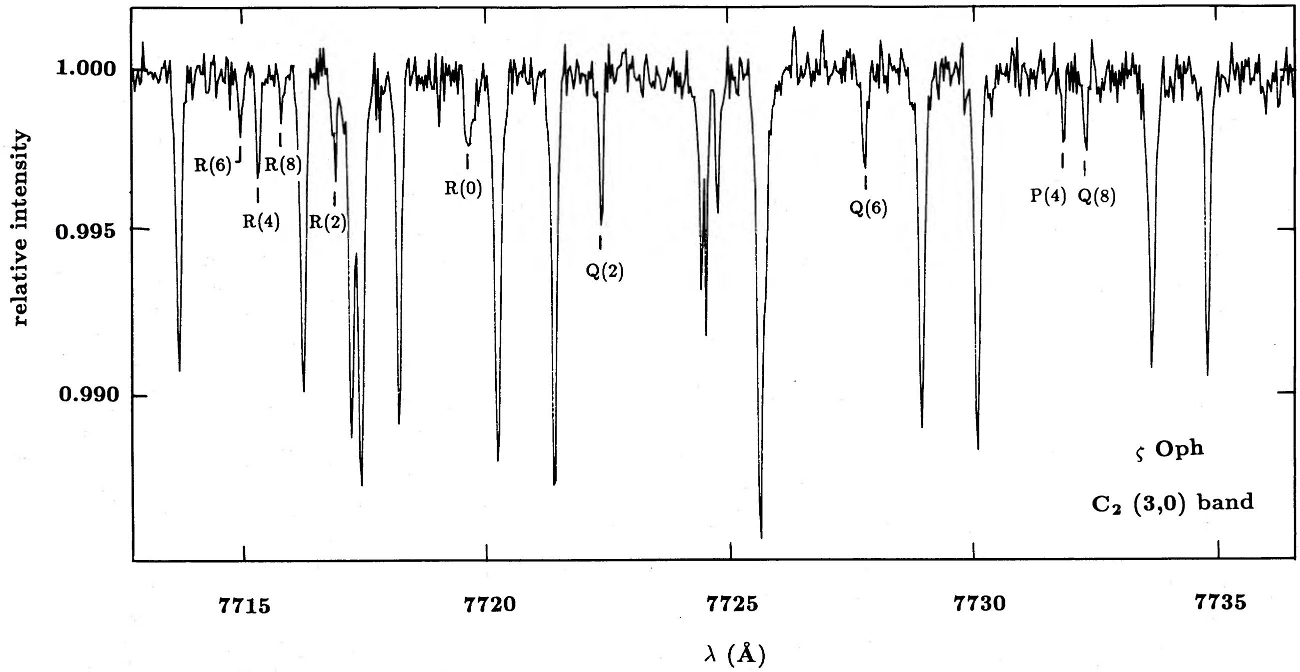

FIG. 1.—Spectrum of ζ Oph in the region of the (3, 0) Phillips band of C_2. Abscissa indicates wavelength with respect to a laboratory frame. Total integration time was seven hours, resulting in a spectrum with a signal-to-noise ratio greater than 1000 RMS in the continuum. The stronger features without identification in the spectrum belong to atmospheric molecular oxygen. The C_2 *Q*(4) line is lost in one of them. The oxygen line at 7724.6 Å is affected by a cosmic-ray hit. The *Q*(10) line has been detected longward of 7735 Å.

TABLE 1

MEASURED EQUIVALENT WIDTHS[a] AND DERIVED COLUMN DENSITIES[b] FOR INTERSTELLAR C_2 TOWARD ζ OPH

			(3, 0) BAND[c]				(2, 0) BAND	
			W_λ		$N(J'')$		$N(J'')$	
J''	LINE	λ[d] (Å)	March	August	March	August	DL[e]	HC[f]
0......	$R(0)$	7719.329	O_2[g]	(0.38 ± 0.10)	O_2	(0.96 ± 0.20)	0.8	0.6
2......	$P(2)$	7725.819	O_2	...	O_2	...	...	...
	$Q(2)$	7722.095	(0.60 ± 0.15)	(0.56 ± 0.05)	(3.03 ± 0.75)	(2.83 ± 0.25)	2.0	2.1
	$R(2)$	7716.528	(0.25 ± 0.15)	(0.33 ± 0.10)	(1.58 ± 1.00)	(2.09 ± 0.63)	1.8	3.5
4......	$P(4)$	7731.663	(0.21 ± 0.10)	(0.23 ± 0.05)	(3.19 ± 1.50)	(3.49 ± 0.75)	2.8	...
	$Q(4)$	7724.219	(0.50 ± 0.10)	O_2	(2.53 ± 0.50)	O_2	3.0	2.6
	$R(4)$	7714.944	(0.20 ± 0.10)	(0.36 ± 0.05)	(1.52 ± 0.75)	(2.73 ± 0.62)	2.8	...
6......	$P(6)$	7738.737	0.15:	0.1:	2.0:	1.3:	2.5	...
	$Q(6)$	7727.557	(0.53 ± 0.10)	(0.48 ± 0.05)	(2.67 ± 0.50)	(2.42 ± 0.25)	2.1	2.4
	$R(6)$	7714.575	0.15:	(0.29 ± 0.07)	1.2:	(2.38 ± 0.57)	2.0	4.8
8......	$P(8)$	7747.037	...	<0.2	...	<2.4	1.3	...
	$Q(8)$	7732.117	(0.25 ± 0.10)	(0.31 ± 0.05)	(1.26 ± 0.5)	(1.57 ± 0.25)	1.7	3.3
	$R(8)$	7715.415	(0.20 ± 0.10)	(0.14 ± 0.05)	(1.72 ± 0.8)	(1.21 ± 0.43)	1.5	...
10......	$Q(10)$	7737.904	0.15:	(0.30 ± 0.10)	0.8:	(1.51 ± 0.50)	1.1	...
	$R(10)$	7717.470	<0.2	<0.2	<1.8	<1.8	1.2	1.2
12......	$Q(12)$	7744.900	<0.2	...	<1	...	0.9	...
	$R(12)$	7720.748	<0.2	<0.2	<1.8	<1.8	...	<0.9
14......	$Q(14)$	7753.141	...	...	...	...	0.7	...

[a] In mÅ.

[b] In 10^{12} cm^{-2}.

[c] Data of August are most reliable.

[d] Rest wavelengths in standard air.

[e] Danks and Lambert 1983; the estimated error is ~15%.

[f] Hobbs and Campbell 1982; the estimated error is ~25%.

[g] Line was masked by atmospheric oxygen lines.

especially for the weaker lines with $W_\lambda \lesssim 0.3$ mÅ. Also, in March the important $R(0)$ line was lost in the oxygen lines, and the $Q(2)$ line was superposed on two oxygen lines.

Since the equivalent widths of the strongest lines are only 0.5 mÅ, the possible presence of previously unknown weak telluric features or diffuse interstellar bands with equivalent widths of 0.1–0.2 mÅ may significantly influence the results (Meyer and Jura 1984). In particular, the $R(0)$ line appears somewhat broader in Figure 1 than the other weak lines. In principle, the problem with weak atmospheric features may be clarified by performing observations at different times of year. Unfortunately, the $R(0)$ line was obscured completely by oxygen lines during the second set of observations in March. Observations of the unreddened early-type star κ Sco did not show a pronounced feature at the position of the $R(0)$ line. Nevertheless, the equivalent width of the $R(0)$ line listed in Table 1 was obtained taking into account a weak underlying line with $W_\lambda \approx 0.1$–0.2 mÅ.

Column densities were obtained from the equivalent widths under the assumption of a linear relationship (van Dishoeck and de Zeeuw 1984), using the theoretical oscillator strength of the (3, 0) band $f_{30} = 7.5 \times 10^{-4}$ (van Dishoeck 1983). The resulting column densities for a particular level J'' derived from the P, Q, and R lines generally agree well within the estimated (2 σ) errors, although the $R(2)$ line appears both in August and in March somewhat weak compared with the $Q(2)$ line. The measured column densities of Danks and Lambert (1983) and Hobbs and Campbell (1982) derived from the (2, 0) band observations are included in Table 1. In order to be consistent with the (3, 0) band results, the published column densities were rescaled to the theoretical oscillator strength $f_{20} = 1.7 \times 10^{-3}$ (van Dishoeck 1983). If the experimentally inferred oscillator strengths (Erman *et al.* 1982; Davis *et al.* 1984; Bauer *et al.* 1985) for both the (2, 0) and (3, 0) bands were employed, all column densities in Table 1 would have to be multiplied by a factor of about two.

As Table 1 shows, the column densities obtained from the (3, 0) band results are generally consistent with those measured by Danks and Lambert in the (2, 0) band. The largest discrepancy is found for the column density in $J'' = 2$ as derived from the $Q(2)$ line. The equivalent width of the $Q(2)$ line in March may easily have been overestimated, since the line appeared just in between two closely spaced oxygen lines. In August, however, the $Q(2)$ line was not contaminated by oxygen lines and its equivalent width was consistently ~0.5–0.6 mÅ for each of the exposures. Also, the $Q(2)$ line clearly appears stronger in the spectrum than, for example, the $Q(6)$ line, for which the derived column density agrees well with that found by Danks and Lambert. The discrepancy for the $Q(2)$ line could be resolved if the ratio of oscillator strengths f_{20}/f_{30} were slightly overestimated. However, the measured equivalent widths of the (2, 0) lines of Danks and Lambert, combined with those of the corresponding (3, 0) lines, imply a ratio of band oscillator strengths $f_{20}/f_{30} = (2.1 \pm 0.4)$, in harmony with the theoretical ratio $f_{20}/f_{30} = 2.2$ (van Dishoeck 1983). The accuracy with which the C_2 potential curves and the variation of the A–X transition moment with internuclear distance are known allows a possible error in the theoretical ratio of only 5%. Note also that even the strongest (2, 0) line measured by Danks and Lambert is on the linear part of the curve of growth (within 10% of derived column density) for any value of the Doppler parameter $b > 0.12$ km s^{-1}, which corresponds to a temperature for thermal broadening alone of $T > 21$ K. Another possible solution would be the presence of a weak feature with $W_\lambda \approx 0.1$ mÅ underlying also the $Q(2)$ line in August. The column density derived from the $R(2)$ line agrees well with the measurements of Danks and Lambert, but is considerably lower than that found by Hobbs and Campbell. In fact, Hobbs and Campbell appear to have overestimated substantially the equivalent widths of all R lines which lie on the steep part of the stellar Paschen feature. They also overestimated the equivalent width of the $Q(8)$ line, because they probably did not recognize that at their experimental resolution of 0.25 Å, the absorption feature at 8773 Å is a blend of the $Q(8)$ and $P(4)$ lines, with the equivalent width of the $P(4)$ line at least half of that of the $Q(8)$ line. In the (3, 0) band the $Q(8)$ and $P(4)$ lines are well separated. The column density in $J'' = 0$ obtained from the (3, 0) band observations is, even taking into account the possibility of a weak underlying feature, slightly larger than those found by Danks and Lambert and Hobbs and Campbell.

The wavelength region covered in the spectra of the (3, 0) Phillips band includes the K I line at 7698 Å. This interstellar line appears very strongly in the spectra with an equivalent width $W_\lambda = (62 \pm 1)$ mÅ, somewhat less than $W_\lambda = (69 \pm 6)$ mÅ measured by Chaffee and White (1982).

IV. DISCUSSION

The best estimates of the column densities in $J'' = 0$ and 2 from the (3, 0) band observations, $N(0) = (0.9 \pm 0.2) \times 10^{12}$ cm^{-2} and $N(2) = (2.4 \pm 0.4) \times 10^{12}$ cm^{-2}, lead to a population ratio $N(0)/N(2) \approx (0.37 \pm 0.07)$. The measurements of Danks and Lambert (1983) give $N(0)/N(2) \approx (0.40 \pm 0.07)$, where it should be noted that *each* of their individual sets of observations obtained on three different nights yields this ratio within a very narrow range. The ratio based on the published averaged column densities of Hobbs and Campbell, $N(0)/N(2) \approx 0.23$ must be discarded, since their averaged column density in $J'' = 2$ is strongly influenced by the measured equivalent width of the $R(2)$ line, which is too large. Taking only their column density in $J'' = 2$ as obtained from the $Q(2)$ line into account, the measured ratio is $N(0)/N(2) \approx 0.29$. This latter value, which is probably a safe lower limit to the $N(0)/N(2)$ column density ratio, would correspond to a kinetic temperature of 40 K if the C_2 rotational population distribution were thermal. Since the radiative excitation processes in C_2 contribute efficiently to the populations of the higher rotational levels, the actual kinetic temperature in the C_2 line-forming region will be less than 40 K.

More information on the physical conditions in the ζ Oph cloud can be obtained by comparing the measured column density ratios for all levels with theoretical population distributions (van Dishoeck and Black 1982; van Dishoeck 1984). The theoretical distributions are characterized by the kinetic temperature T and the combination of parameters $n_c \sigma_0/I_R$, where n_c is the density of C_2 collision partners in the cloud, $n_c = n(\mathrm{H}) + n(\mathrm{H}_2)$, I_R is a scaling factor for the radiation field in the far-red relative to the radiation field adopted by van Dishoeck and Black, and σ_0 is the cross section for collisional de-excitation. Data of high quality permit both the temperature and the excitation parameter $n_c \sigma_0/I_R$ to be determined. For any temperature $T < 40$ K, the observed level distributions as derived from both the (3, 0) and (2, 0) band measurements are found to agree well with theory for $n_c \sigma_0/I_R \approx (3 \pm 1) \times 10^{-14}$ cm^{-1}. Figure 2 illustrates the comparison between the observed and theoretical population ratios for $T = 30$ K.

For $n_c \sigma_0/I_R \approx 3 \times 10^{-14}$ cm^{-1}, the observed $N(0)/N(2)$ column density ratio is best fitted by $T \approx 20$–25 K (see the tables by van Dishoeck 1984), the measured $N(4)/N(2)$ and $N(6)/N(2)$ ratios by a somewhat higher temperature $T \approx 35$ K. The kinetic temperature in the center of the ζ Oph cloud, as inferred from the C_2 observations, is therefore $T \approx (30 \pm 10)$ K. This temperature agrees well with $T = 22$ K found in the center of the model of the ζ Oph cloud by Black and Dalgarno (1977), which was based on an interpretation of the observed rotational population of the H_2 molecule. Recent improved models of the ζ Oph cloud (van Dishoeck and Black 1986) also have $T \approx 20$–25 K in the center of the cloud. The predicted C_2 column-averaged temperature in these models is ~ 10 K higher than the central temperature. The higher temperature $T \approx 60$ K suggested by Crutcher and Watson (1981) and Wannier *et al.* (1982) was based mainly on observations of the ^{13}CO/^{12}CO column density ratio. As discussed by van Dishoeck and Black (1986), the CO column-averaged temperature in the models is higher than those of the H_2 and C_2 molecules, so that these observations may not be in conflict with the low temperature inferred in this work.

The derived excitation parameter $n_c \sigma_0/I_R \approx 3 \times 10^{-14}$ cm^{-1} implies $n_c \approx 150$ cm^{-3}, if $I_R \approx 1$ and $\sigma_0 \approx 2 \times 10^{-16}$ cm^2 is assumed (van Dishoeck and Black 1986). The corresponding hydrogen nuclei density $n_\mathrm{H} = n(\mathrm{H}) + 2n(\mathrm{H}_2) \approx 225$ cm^{-3}, is significantly smaller than $n_\mathrm{H} = 2500$ cm^{-3} found in the center of the ζ Oph model of Black and Dalgarno (1977), but agrees well with the density $n_\mathrm{H} \approx 200$ cm^{-3} inferred by Crutcher and Watson (1981). The new models of the ζ Oph cloud (van Dishoeck and Black 1986) which reproduce a wide variety of observations also indicate low densities $n_\mathrm{H} \approx 200$–600 cm^{-3} in the center of the cloud, although the actual value is still uncertain by a factor of at least 2.

The total C_2 column density in the observed levels $J'' \leq 14$ is $\sim 1.2 \times 10^{13}$ cm^{-2}. Adding to this the populations in the higher levels as estimated from the best-fitting model, the total C_2 column density toward ζ Oph is $(1.5 \pm 0.2) \times 10^{13}$ cm^{-2}, if the theoretical oscillator strengths are employed. If the experimental oscillator strengths are used, the inferred column density is a factor of 2 larger.

V. CONCLUSIONS

Observations of C_2 in the (3, 0) band around 7720 Å have been presented and used to provide additional support for the suggestion of a low temperature in the center of the principal cloud toward ζ Oph. The region of the (3, 0) band has the advantages over the (2, 0) band region around 8750 Å that the R lines are not superposed on a stellar feature and that the $Q(8)$ and $P(4)$ lines are well separated. The main disadvantage of the (3, 0) band region is the presence of the atmospheric lines so that most of the C_2 lines can only be measured during a specific period of time for a particular line of sight. Also, because of the smaller oscillator strength of the (3, 0) band compared with the (2, 0) band, the lines are very weak. This implies not only that substantially longer integration times are needed for the (3, 0) band, but also that care should be taken of the possible presence of weak atmospheric features or diffuse interstellar bands underlying the C_2 features. Nevertheless, if additional independent information on the C_2 column densities, especially in $J'' = 0$ is needed, observations of the (3, 0) band may be of use. The oscillator strengths of the (v', 0) bands

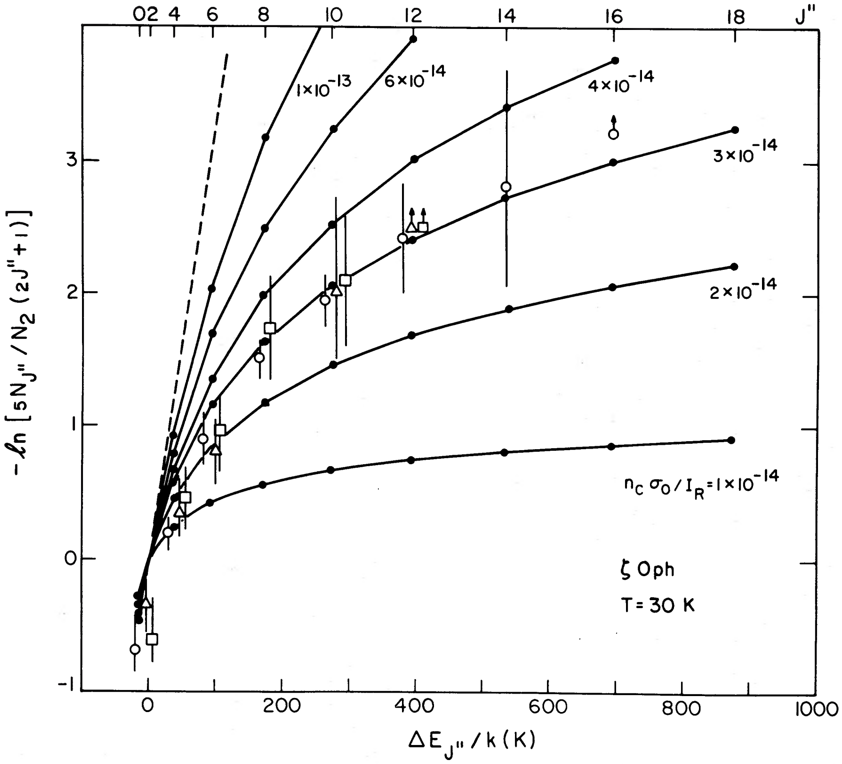

FIG. 2.—Theoretical relative rotational populations of C_2 as functions of the excitation energy (or rotational quantum number J''). The filled dots (●) connected by solid curves were calculated for a kinetic temperature $T = 30$ K and several excitation parameters $n_c \sigma_0/I_R$ (in cm^{-1}). Dashed line indicates the thermal distribution at 30 K. Observed column density ratios in the ζ Oph cloud are indicated by various symbols. Square (□): this work, (3, 0) band observations; circle (○): Danks and Lambert (1983), (2, 0) band observations; triangle (△): Hobbs and Campbell (1982), (2, 0) band observations, excluding the $R(2)$, $R(6)$, and $Q(8)$ lines.

with $v' > 3$ are decreasing very rapidly with increasing v' (van Dishoeck 1983), so that observations of them will not be feasible with the present detectors. On the other hand, the oscillator strengths of the (1, 0) band around 10140 Å and the (0, 0) band around 12100 Å are a factor of 2 larger than that of the (2, 0) band. The wavelength region around the (1, 0) band is free of strong atmospheric features, whereas the region around the (0, 0) band may be slightly inferior. With improvements in the sensitivity of detectors at $\lambda \gtrsim 1$ μm these bands may be more suitable for further observations, especially for thicker interstellar clouds.

The authors are grateful to the staff of the European Southern Observatory for assistance.

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