

HUBBLE SPACE TELESCOPE OBSERVATIONS OF C₂ MOLECULES IN DIFFUSE INTERSTELLAR CLOUDS¹

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ABSTRACT

Interstellar C₂ *F*-*X* (1342 Å) and *D*-*X* (2313 Å) bands in the spectrum of ζ Oph were detected using the Goddard High-Resolution Spectrograph on the *Hubble Space Telescope*. The total C₂ column density is $(1.79 \pm 0.06) 10^{13} \text{ cm}^{-2}$ for an adopted *f*-value of 0.0545 for the 2313 Å band of the Mulliken (*D*-*X*) system. Relative *f*-values for the 0–0 *F*-*X*, 0–0 *D*-*X*, and 2–0 *A*-*X* (Phillips) bands are derived by combining ultraviolet and near-infrared spectra: $f_{00}^{FX}/f_{00}^{DX} = 1.83 \pm 0.18$ and $f_{20}^{AX}/f_{00}^{DX} = 0.0226 \pm 0.0029$. For the Mulliken system, lines are detected up to a rotational level $J'' = 24$. The relative populations along the rotational ladder are shown to be consistent with the physical and environmental conditions suggested by other diagnostics. Interstellar C₂ molecules were detected towards ξ Per [$N(\text{C}_2) = (0.80 \pm 0.23) 10^{13} \text{ cm}^{-2}$] but not towards β¹, π, and ω¹ Sco [$N(\text{C}_2) \leq 0.17 \times 10^{13} \text{ cm}^{-2}$].

Subject headings: ISM: molecules — ISM: abundances — ISM: clouds

1. INTRODUCTION

The *Hubble Space Telescope* with the Goddard High-Resolution Spectrograph (GHRS) has reawakened interest in interstellar diffuse clouds by providing access to the ultraviolet where many atomic and molecular resonance transitions are to be found. This paper discusses ultraviolet observations of the C₂ molecule whose lowest rotational levels are an effective probe of a cloud's kinetic temperature and whose high rotational levels are sensitive to the gas density and the radiation field permeating the cloud. Interstellar C₂ molecules were discovered by Souza & Lutz (1977) who detected two absorption lines of the Phillips system's 1–0 band near 10145 Å in the spectrum of the highly reddened star Cyg OB2 No. 12. Subsequently, interstellar C₂ molecules have been detected toward less reddened stars using the weaker but more easily observed 2–0 and 3–0 bands of the Phillips system. This paper is concerned primarily with ultraviolet transitions of interstellar C₂ toward ζ Oph.

Very high resolution spectra of the optical absorption lines of CN and CH show that the molecules along the line of sight to ζ Oph reside in two velocity components or cool clouds separated by about 1 km s^{-1} (Lambert, Sheffer, & Crane 1990; Crawford et al. 1994). Observations of the CO $J = 1-0$ and $2-1$ emission lines at millimeter wavelengths (Le Boulrot, Gerin, & Perault 1989; Wilson et al. 1992) also show the presence of the same two clouds. The optical CH⁺ line shows a single broader profile suggesting that it is formed in warm (shocked?) gas. This warm gas also contains some CH radicals. It is presumed that the C₂ molecules along with the CN and CO molecules reside in the two cool clouds with a negligible fraction present in the warm gas.

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Interstellar C₂ towards ζ Oph was discovered by Chaffee & Lutz (1978) who detected one line of the 2–0 band of the Phillips system. (An earlier search by Lutz & Souza 1977 for lines of the 1–0 band proved unsuccessful but the upper limit on the C₂ column density was consistent with the measurement obtained by Chaffee & Lutz.) Snow (1978) reported a detection of a line of the 0–0 band of the Mulliken system at 2313 Å. Observations of the C₂ Phillips system have been reported by Hobbs & Campbell (1982), and Danks & Lambert (1983) for the 2–0 band near 8760 Å and by van Dishoeck & Black (1986a) for the 3–0 band near 7720 Å. The three sets of measurements are generally in agreement and define the relative populations of the even rotational levels of the C₂ molecule's ground state between $J = 0$ and $J = 14$. (The rotational ladder does not possess levels with odd values of J .) This paper reexamines interstellar C₂ in the ζ Oph clouds using high signal-to-noise spectra of the Mulliken 0–0 band at 2313 Å and the *F*-*X* 0–0 band at 1342 Å. The rotational ladder is now detected to $J = 24$. The observations provide the first accurate measurement of the relative *f*-values of the Phillips, Mulliken, and *F*-*X* systems. Interstellar C₂ molecules are also detected toward ξ Per. Upper limits to the C₂ column density are provided for three additional lines of sight.

2. OBSERVATIONS

There are two electronic transitions of the C₂ molecule from the electronic ground state ($X^1\Sigma_g^+$) which are accessible with *HST* and the GHRS: the Mulliken $D^1\Sigma_u^+ - X^1\Sigma_g^+$ system with its 0–0 band near $\lambda_{\text{air}} = 2313 \text{ Å}$ and the $F^1\Pi_u - X^1\Sigma_g^+$ system with its 0–0 band near $\lambda_{\text{vac}} = 1342 \text{ Å}$. Our observations of the former were made with an echelle grating (ECH-B) providing a resolution of about 90,000 when a star is observed through the small science aperture (SSA). The echelle grating (ECH-A) was unavailable for the observations of the *F*-*X* system. This was not a serious handicap as the grating G160M provides an adequate resolution and at a higher sensitivity than the echelle.

Since the rotational structure of the Mulliken band is well resolved, no information is lost by the inability to resolve the *F*-*X* band in which the rotational lines are more closely spaced.

The observing and reduction procedures were based on those used to observe the interstellar CO bands at high signal-to-noise (Lambert et al. 1994). The standard FP-SPLIT procedure of four subexposures separated successively by about 20 pixels was adopted. For both the ECH-B and G160M exposures the standard FP-SPLIT was executed at three slightly different central exposures so that the central portion of each bandpass was covered in 12 separate exposures with a given interstellar feature appearing at 12 different locations on the Digicon's photocathode. Standard IRAF tasks (e.g., STSDAS/FPSPLIT) were employed in correcting the observed sets of four FP-SPLIT spectra for the granularity of the photocathodes. The final spectrum was obtained by shifting and co-adding the three corrected spectra to obtain the final spectrum for a given band. As a check on the procedure, which is slightly less sophisticated than that discussed and employed by Lambert et al. (1994), it is noted that the measured S/N ratio from the continuum near 2313 Å in the ζ Oph spectrum agrees well with the S/N expected for this spectrum having a total count in the continuum of 40,000. Table 1 summarizes the available observations.

Interstellar lines are impressed upon the stellar spectrum containing broad absorption lines. Fortunately, the C₂ Mulliken lines fall in a region where the stellar continuum is quite smooth so that definition of the local continuum required to produce the "normalized" spectrum introduces no significant additional uncertainty into the measurement of a C₂ line's

equivalent width. The C₂ Mulliken band in the spectrum of ζ Oph in Figure 1 shows the expected *P* and *R* branches of a transition with great clarity. Figure 2 shows on an expanded scale three pairs of lines from the *P* and *R* branches. In combination these figures show that the rotational ladder of the C₂ ground state had been probed to *J*' = 24 which is an advance on the limit *J*' = 14 from observations of the Phillips system. Equivalent widths of the Mulliken lines are listed in Table 2. Wavelengths of the Mulliken lines were provided by G. Stark (1992, private communication). The mean width of the 17 strongest C₂ lines is Δλ(FWHM) = 0.027 ± 0.002 Å corresponding to a resolution λ/Δλ = 87,000, as expected of ECH-B with the small science aperture.² (The radial velocity estimated from the C₂ lines differs by about 5 km s⁻¹ from that of CN and other lines formed in the denser parts of the diffuse clouds. This difference is attributed to a systematic error in the measurement of the GHR spectra arising from the lack of a contemporaneous wavelength calibration.)

Observations of the *F*-*X* band were obtained and reduced in the same way as those of the Mulliken 0-0 band. The *F*-*X* band falls in the short-wavelength wing of a blend of broad stellar O IV lines at λ_{vac} = 1342.992 and 1343.512 Å with a weaker separate line at 1338.612 Å also present in the stellar spectrum (Bromander 1969). Owing to the location of the *F*-*X* band in the stellar line and to the lower resolution of the G160M grating, definition of the local continuum is somewhat more uncertain than for the Mulliken 0-0 band. The *F*-*X*

² A precise determination of the instrumental profile may permit limits to be set on the apportionment of the C₂ molecules between the two clouds observed in CN and CO to be separated by 1.2 km s⁻¹. Calculated line widths increase by about 0.003 Å as the C₂ concentration in the second cloud is raised from 0% to 50%.

TABLE 1
OBSERVATION SUMMARY TABLE

Star	λ _c ^a	Root-name ^b	UT ^c (1992)	Counts ^d (Pixel)	T _{exp} ^e (s)
HD 1497571 (ζ Oph)	1329.7	z0xz0108	186.563	37046	217.6
	1331.2	z0xz0109	186.567	37185	217.6
	1334.1	z0xz010a	186.572	37077	217.6
	2312.0	z0xz010d	186.576	15082	217.6
	2312.5	z0xz010e	186.581	14999	217.6
	2313.0	z0xz010f	186.619	16143	217.6
HD 144217A (β ¹ Sco)	2312.0	z0xz0209	149.457	9530	108.8
	2312.5	z0xz020a	149.461	9316	108.8
	2313.0	z0xz020b	149.502	10559	108.8
HD 143018 (π Sco)	1329.7	z0xz0308	185.901	30728	108.8
	1331.2	z0xz0309	185.904	31767	108.8
	1334.1	z0xz030a	185.907	30136	108.8
	2312.0	z0xz030d	185.911	8300	108.8
	2312.5	z0xz030e	185.946	9294	108.8
	2313.0	z0xz030f	185.949	8714	108.8
HD 144470 (ω ¹ Sco)	2312.0	z0xz0409	186.092	10192	544.0
	2313.5	z0xz040a	186.103	12258	544.0
HD 24912 (ζ Per)	2312.0	z0xz0509	267.648	5256	326.4
	2313.0	z0xz050b	267.660	4928	326.4

^a Central wavelength in Å of spectra.
^b Unique name for data set in the HST archive.
^c UT time (day of year and decimal day of year 1992) at start of exposure.
^d Total counts in one pixel (one-quarter diode) summed over all sub-exposures. All stellar data were acquired with STEP-PATT = 5 in which sub-spectra are acquired at 1/4 diode magnetic deflections. Background spectra are built up using 6% of the total integration time.
^e Total exposure time in seconds.

TABLE 2
EQUIVALENT WIDTHS OF C₂ MULLIKEN LINES AND COLUMN DENSITIES OF INTERSTELLAR C₂ TOWARD ζ OPH

<i>J</i> '	LINE	W _λ (mÅ)	N(<i>J</i> ') ^a	
			Line	Mean
0.....	R(0)	1.76 ± 0.36	0.75 ± 0.15	0.75 ± 0.15
	R(2)	3.80 ± 0.42	3.00 ± 0.30	
2.....	P(2)	2.46 ± 0.40	2.70 ± 0.43	2.90 ± 0.24
	R(4)	4.04 ± 0.34	3.50 ± 0.27	
4.....	P(4)	3.00 ± 0.27	3.05 ± 0.27	3.27 ± 0.19
	R(6)	2.84 ± 0.28	2.37 ± 0.23	
6.....	P(6)	2.77 ± 0.34	2.67 ± 0.33	2.47 ± 0.19
	R(8)	2.31 ± 0.29	1.90 ± 0.25	
8.....	P(8)	2.15 ± 0.38	1.97 ± 0.34	1.92 ± 0.20
	R(10)	1.77 ± 0.30	1.43 ± 0.24	
10.....	P(10)	1.49 ± 0.33	1.30 ± 0.25	1.37 ± 0.17
	R(12)	1.44 ± 0.25	1.15 ± 0.17	
12.....	P(12)	1.17 ± 0.31	1.00 ± 0.26	1.11 ± 0.14
	R(14)	0.84 ± 0.24	0.66 ± 0.19	
14.....	P(14)	1.11 ± 0.27	0.94 ± 0.23	0.77 ± 0.15
	R(16)	0.85 ± 0.26	0.67 ± 0.20	
16.....	P(16)	0.67 ± 0.32	0.55 ± 0.24	0.62 ± 0.16
	R(18)	0.79 ± 0.20	0.62 ± 0.16	
18.....	P(18)	0.62 ± 0.37	0.51 ± 0.30	0.60 ± 0.14
	R(20)	0.64 ± 0.23	0.50 ± 0.18	
20.....	P(20)	0.58 ± 0.32	0.48 ± 0.20	0.49 ± 0.13
	R(22)	0.61 ± 0.26	0.48 ± 0.24	
22.....	P(22)	0.52 ± 0.23	0.42 ± 0.20	0.44 ± 0.15
	R(24)	0.47 ± 0.33	0.47 ± 0.26	
24.....	P(24)	0.36 ± 0.26	0.29 ± 0.21	0.32 ± 0.16
	R(24)	0.47 ± 0.33	0.47 ± 0.26	

^a Units: 10¹² cm⁻²

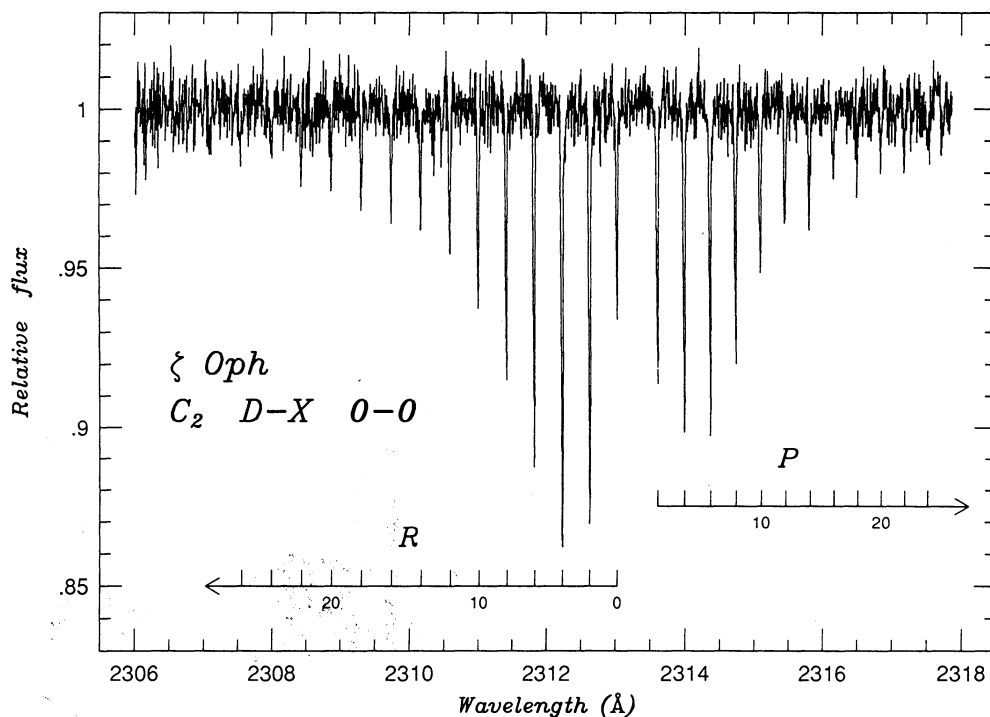


FIG. 1.—Spectrum of ζ Oph showing interstellar lines from the C₂ molecule's 0-0 band of the Mulliken system. Lines of the P and R branches are identified below the spectrum by the rotational quantum number J'' of the lower level.

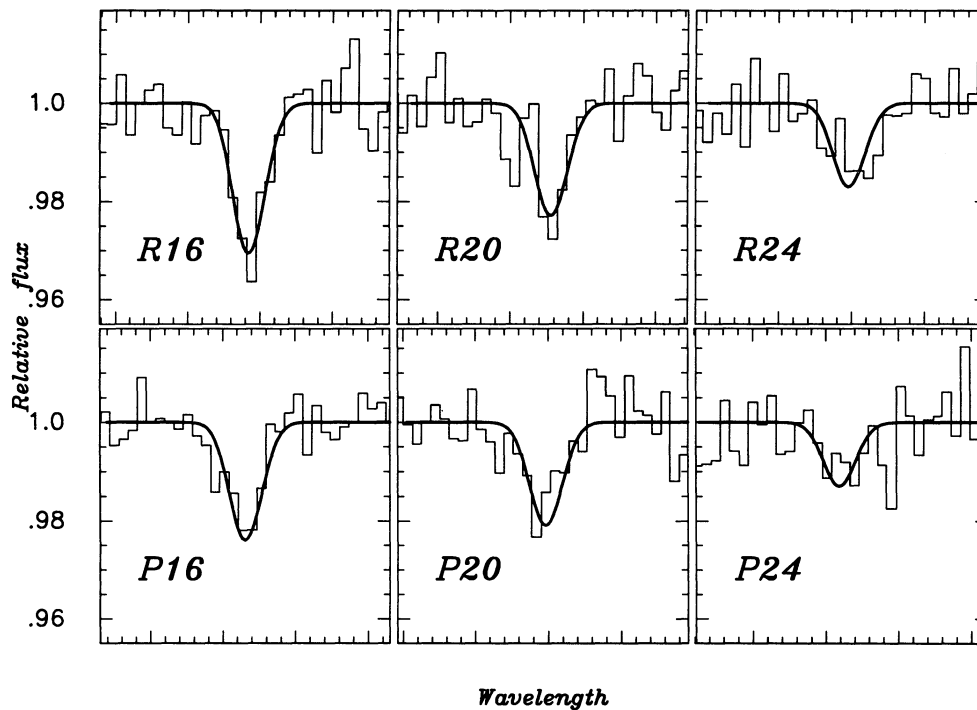


FIG. 2.—Selected C₂ lines from the spectrum shown in Fig. 1. Each panel shows 0.2 Å centered on the C₂ line.

band was also included on a spectrum recorded as part of a study of the interstellar CO bands (Lambert et al. 1994). These two independently observed and reduced spectra have been summed to produce the final normalized spectrum shown in Figure 3. Rotational structure is evident but because individual rotational lines are not resolved, the observed spectrum is converted to a C₂ column density through the application of a synthetic spectrum, as described below.

Interstellar atomic lines are present near 1342 Å in spectra of ζ Oph and π Sco. These are summarized in the Appendix. To a detection limit of about 0.3 mÅ in equivalent width, there are no other interstellar lines in the 2312 Å spectra.

3. INTERSTELLAR C₂ TOWARD ζ OPH

Interstellar C₂ molecules are detectable in absorption through transitions from the molecule's electronic ground state. Laboratory spectroscopy has revealed three such transitions: the Phillips system (*A* ¹Π_u–*X* ¹Σ_g⁺) in the near infrared, the Mulliken (*D* ¹Σ_u⁺–*X* ¹Σ_g⁺) system with its strongest band at 2313 Å, and the *F* ¹Π_u–*X* ¹Σ_g⁺ system with a 0–0 band at 1342 Å (Herzberg, Lagerqvist, & Malmberg 1969; Huber & Herzberg 1979). Although the present paper is concerned with the two ultraviolet transitions, reference is made to the Phillips system.

3.1. The Mulliken System

The strongest lines of the Mulliken 0–0 band are slightly saturated. A correction for saturation was made using the model of the two clouds derived from very high resolution profiles of optical CN and CH lines (Lambert et al. 1990). The specific model considers one cloud to have twice the C₂ column density of the other with a *b*-value of 0.35 km s^{−1} for the C₂-richer cloud and 0.30 km s^{−1} for the other cloud. Predicted line profiles in Figure 2 are based on the mean column

densities (Table 2) convolved with the instrumental profile derived for ECH-A observations of CO lines. For the strongest lines, the column density is underestimated by about 20% when saturation is ignored.

A standard expression relates the equivalent width of a weak line to the column density:

$$W_{\lambda} = \frac{\pi e^2}{mc^2} \lambda_{J'J''}^2 f_{J'J''} N(J''), \quad (1)$$

where $\lambda_{J'J''}$ is the wavelength and $f_{J'J''}$ is the *f*-value of the transition from a lower rotational level J'' having a column density $N(J'')$, and other symbols have their usual meanings. The *f*-value of the line is conveniently written as

$$f_{J'J''} = f_{v'v''} \frac{S_{J'J''}}{2J'' + 1}, \quad (2)$$

where $f_{v'v''}$ is the band *f*-value and $S_{J'J''}$ is the Hönl-London factor or rotational line strength—see Larsson (1983) for further discussion of $f_{v'v''}$, $f_{J'J''}$, and $S_{J'J''}$ and the conditions under which a line's *f*-value may be written as a product of a band *f*-value and a Hönl-London factor. For the Mulliken system $S = J'' + 1$ for the *R* branch and J'' for the *P* branch.

Column densities $N(J'')$ derived from the equivalent widths are given in Table 2. Equivalent widths were corrected for saturation before using equation (1). A value $f_{v'v''} = f_{00}^{DX} = 0.0545$ (see below) is adopted in equation (2). For $J'' \geq 2$ independent and consistent estimates of $N(J'')$ from the *P* and *R* lines are averaged to obtain the final values which are shown as a function of excitation energy in Figure 4. The levels $J'' = 0$ to 24 yield a combined column density of $(1.70 \pm 0.06) \times 10^{13}$ cm^{−2}. In order to complete the estimate of the column density with the populations of levels $J'' = 26$ and higher, a rotational temperature $T_{\text{rot}} = 785 \pm 30$ K was found from a fit to the

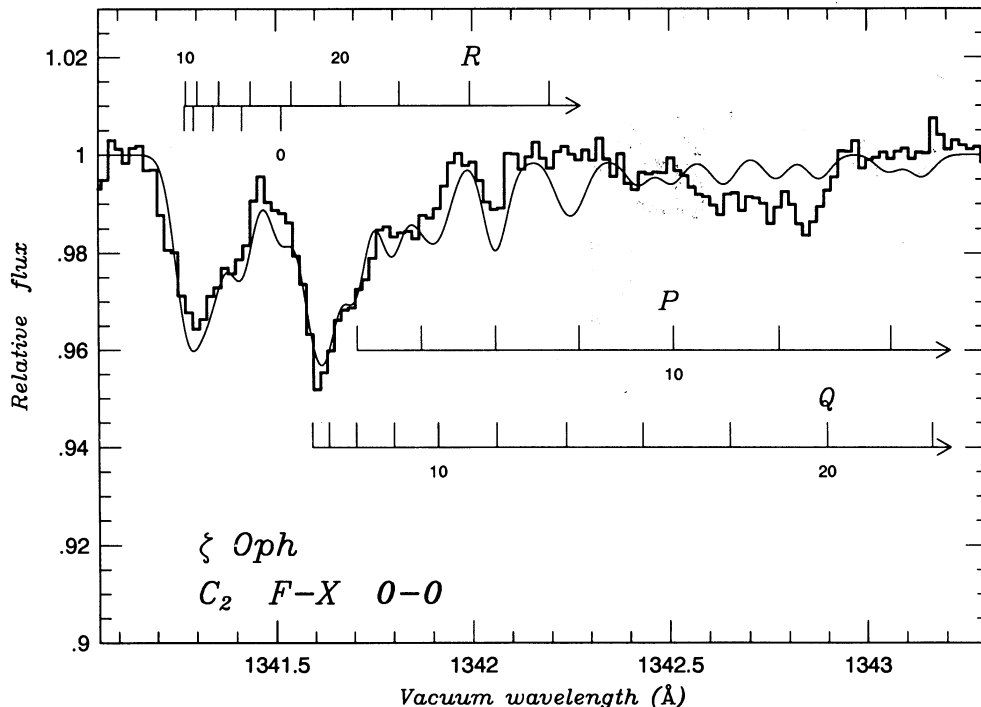


FIG. 3.—Spectrum of ζ Oph showing interstellar lines from the C₂ molecule's 0–0 band of the *F*–*X* system. Locations of the *P*, *Q*, and *R* branches are identified by the rotational quantum number J'' of the lower level. A synthetic spectrum computed as described in the text is represented by the solid line.

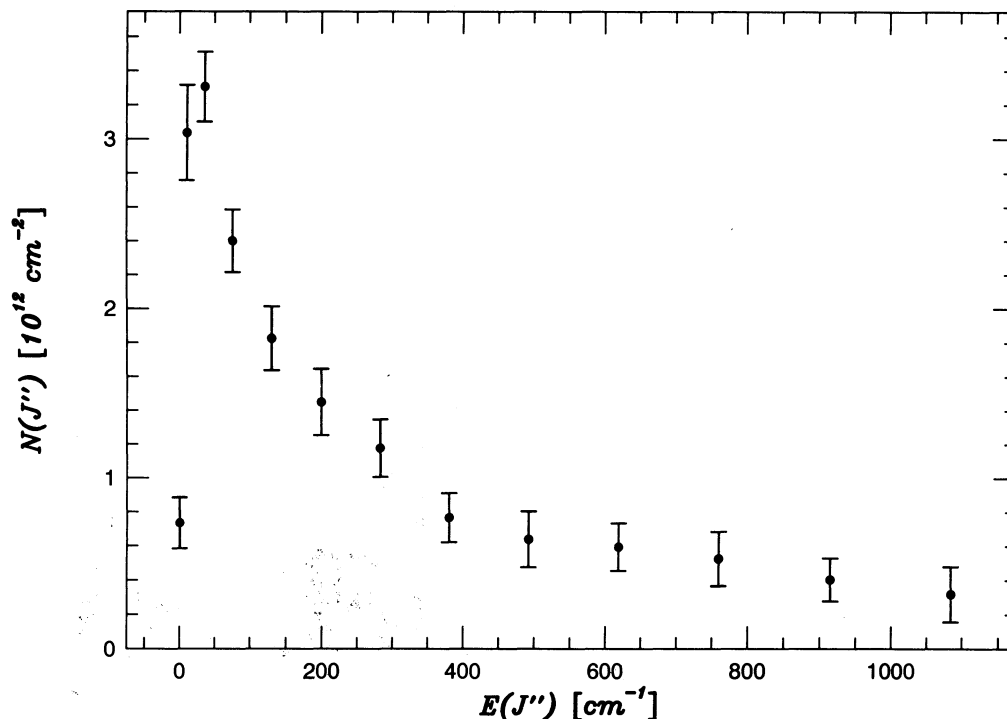


FIG. 4.—Column densities of the rotational levels of the C_2 molecule's ground electronic state, as derived for the vibrational level $v'' = 0$ from the spectrum shown in Fig. 1.

levels $J'' = 16$ – 24 . Then, if this T_{rot} is assumed, the levels $J'' = 26$ and higher are estimated to contribute $(0.09 \pm 0.02) \times 10^{13} \text{cm}^{-2}$ or 5% to the column density of C_2 . The total column density of C_2 is then $(1.79 \pm 0.06) \times 10^{13} \text{cm}^{-2}$. (A similar procedure applied at $J'' = 14$, the limit of observations of the Phillips system, shows that the correction for unobserved levels is then 8%.)

The present observations of the Mulliken system toward ζ Oph were preceded by Snow's (1978) report of the $R(0)$ line in spectra acquired with the *Copernicus* satellite. Snow's equivalent width (3.2 mÅ) is almost twice that reported here. For the $R(2)$ line, Snow set an upper limit to the equivalent width of 2.6 mÅ which is smaller than the present measurement of 3.8 mÅ. These discrepancies with the *Copernicus* results seem puzzling but must be judged in light of Snow's detection of an unidentified interstellar line between the $R(0)$ and $R(2)$ lines. This "apparent feature" was measured to have an equivalent width of "nearly 4 mÅ, or about 3 times the probable error" but on the present spectra there is no line at the measured wavelength. Since the upper limit to the equivalent width of 0.35 mÅ is a factor of 10 smaller than Snow's reported value, it is necessary to conclude that the systematic errors afflicting the *Copernicus* spectra were underestimated.

3.2. The F - X System

Herzberg et al.'s (1969) laboratory investigation of the C_2 molecule's spectrum in the vacuum ultraviolet led to the discovery of the $F^1\Pi_u-X^1\Sigma_g^+$ system through its 0–0 and 1–0 bands with R branch band heads at 1341.3 and 1314.0 Å, respectively. Wavelengths of rotational lines in the stronger 0–0 band were measured with an accuracy of about a few mÅ from $J'' = 10$ to $J'' = 38$ with almost identical coverage of the P , Q , and R branches. Molecular constants for the upper and lower states derived by Herzberg et al. are used here to predict

the wavelengths of the low J'' lines not resolved or measured in the laboratory spectra.

Detection of interstellar C_2 via the F - X bands was first achieved by Lien (1984) who detected the 0–0 and perhaps also the weaker 1–0 band in *IUE* spectra of X Per. Attempts to detect the F - X 0–0 band in the spectrum of ζ Oph through use of the *Copernicus* satellite were unsuccessful: Morton (1975) set an upper limit of 5.2 mÅ on the equivalent width of the $R(0)$ line and Snow (1976) subsequently refined the upper limit to 1.32 mÅ. The present spectra (Fig. 3) clearly show the band with the expected partial resolution of its rotational structure. The measured equivalent width of the feature containing the low- J'' R lines is 6.0 mÅ, which exceeds Snow's upper limit by a factor of about 5. The equivalent width of the band is 13.5 mÅ.

Since the rotational structure is not cleanly resolved, the F - X band is analyzed using a synthetic spectrum. The populations of the rotational levels provided by the Mulliken system are adopted. The two-cloud model was assumed. The predicted spectrum was smoothed with the instrumental profile, a Gaussian with a width (FWHM) of 16km s^{-1} (Lambert et al. 1994). The f -value of the F - X band was adjusted to get the optimum fit to the observed band profile. Figure 3 shows this fit corresponding to $f_{00}^{FX} = 0.10 \pm 0.01$ for $f_{00}^{DX} = 0.0545$ and $N(\text{C}_2) = 1.79 \times 10^{13} \text{cm}^{-2}$ from the Mulliken system. Inspection of Figure 3 shows that the synthetic spectrum does not fit the observations as well as might have been expected. Particularly obvious discrepancies occur at 1342.0, 1342.2 and from 1342.5 to 1342.9 Å. At 1342.0 Å the synthetic spectrum which is primarily influenced by the $P(6)$ and $Q(12)$ lines is too strong. The $P(8)$ line with small contributions from $Q(14)$ and $R(26)$ determines the absorption at 1342.2 Å which appears to be absent from the observed spectrum; the line is seen in neither of the two spectra which have been summed to give the observed spectrum in Figure 3. Between 1342.5 and 1342.9 Å,

the observed spectrum shows considerably more absorption than predicted. These anomalies are puzzling. One possibility is that the granularity on the photocathode is not entirely removed by the reduction procedures. Of course, there may be weak and as yet unidentified interstellar lines responsible for the anomaly at 1342.5–1342.9 Å. The stellar absorption lines may not have smooth profiles, as assumed here in setting the local continuum. Overlooked blends of photospheric lines will introduce errors into the adopted local continuum and, hence, into the $F-X$ band's profiles. One recalls the irregular profiles of the He I 6678 Å line reported by Vogt & Penrod (1983) and attributed by them to nonradial oscillations of ζ Oph. These must be present in the ultraviolet stellar absorption lines with a separation between points of above-average and below-average absorption of 0.5–1.0 Å. Then, these expected irregularities as undulations of the normalized continuum might account quite well for the mismatch between the synthetic and observed spectra. Perhaps, the effects of the nonradial oscillations are more severe for the O IV lines at 1342 Å than for lines of lower stages of ionization. These effects are unlikely to make observed spectra taken at different times differ in similar ways from the synthetic spectrum. A final possibility is that the relative $f_{J,J''}$ -values are not given by equation (2). Since the $F^1\Pi_u$ state has a shallow potential curve with a potential maximum between the equilibrium internuclear separation and the dissociation limit (Bruna & Grein 1994), it is possible that there is a significant vibration-rotation interaction such that $f_{J,J''}$ is not separable into $f_{v,v'}$ and $S_{J,J''}$. A complete absence of individual lines is unlikely to be attributable to this effect because Herzberg et al. (1969) did not report intensity anomalies.

3.3. Rotational Excitation of C₂

Observed populations along the rotational ladder are summarized in Table 3 from the present observations of the Mulliken system and published observations of the Phillips system. Column densities are normalized to that for $J'' = 2$ in order to factor out differences in the adopted f -values of the bands. At a glance, it is seen that the four sets of observed column densities define the same distribution. Upper limits for $J'' = 12$ by Hobbs & Campbell (1982) and van Dishoeck & Black (1986a)

are only slightly lower than the observed column densities reported here and by Danks & Lambert (1983). The measurement for $J'' = 4$ by Danks & Lambert lies outside the range shown by the other measurements.

The C₂ molecule's rotational ladder, in sharp contrast to that of a heteronuclear molecule like CN or CO, has significant population to high J'' levels. This difference between homonuclear and heteronuclear molecules arises because the electric dipole pure rotational transitions in the ground electronic state are forbidden for C₂ but allowed for CN or CO. Populations along the C₂ ladder reach equilibrium under the combined influences of collisional excitation and de-excitation, pumping driven by electronic transitions (primarily the Phillips system), and electric quadrupole transitions down the rotational ladder and intersystem transitions between levels of the ground (singlet) state and the lowest triplet (lower level of the Swan system) state. Our analysis draws on the theoretical work of van Dishoeck & Black (1982) because they considered levels up to $J'' = 20$, which comes closest to the limit set by the GHRS observations ($J'' = 24$). Other studies of excitation of C₂ include Le Bourlot, Roueff, & Viala (1987).

Under conditions of high gas density and weak radiation field in the near-infrared, the rotational ladder reaches equilibrium at the gas kinetic temperature T_k ; the excitation temperatures $T_{J,2}$ given by the relative populations of the levels $J'' = J$ and $J'' = 2$ are all equal to T_k . As the ratio of collisional excitation to radiative excitation (primarily via the Phillips system) declines, the rotational ladder relaxes to a higher excitation temperature set by the color temperature of the interstellar radiation field such that $T_{J+1,2} > T_{J,2} > T_{J-1,2}$ and $T_{J,2} > T_k$ for all $J > 2$. The populations of the two lowest rotational levels ($J'' = 0$ and 2) give the best approximation to T_k . The observed relative population of the $J'' = 0$ and 2 levels is $N_0/N_2 = 0.26 \pm 0.05$ or $T_{0,2} = 60(+\infty, -15)$ K. The levels J'' from 16 to 24 give, as noted above, a much higher rotational temperature of $T_{rot} = 785$ K. This temperature is much lower than the interstellar radiation field's color temperature, indicating that the competition between collisional and radiative excitation has no clear winner.

Van Dishoeck & Black (1982) predicted populations for three values of the parameter that measures the competition between collisional de-excitation and radiative excitation. This latter parameter is $E = n\sigma_0/I$ where n is the gas density [$n = n(\text{H}) + n(\text{H}_2)$], σ_0 is the (assumed) constant cross section for all de-excitations $J + 2 \rightarrow J$ by either an H atom or an H₂ molecule, and I is a scaling factor to be applied to the interstellar near-infrared radiation field adopted by van Dishoeck & Black. Predictions of the rotational population for $J'' = 0$ to 20 for $E = 10^{-12}$, 10^{-13} , and 10^{-14} at $T_k = 20, 45, 60$, and 100 K were tabulated by van Dishoeck & Black. Observed (Mulliken) populations and theoretical predictions for $E = 10^{-13}$ and 10^{-14} at $T_k = 20$ and 60 K are compared in Figure 5 in the customary plot where the slope of a best-fitting straight line is inversely proportional to the excitation temperature. At $E = 10^{-14}$ radiative excitation controls the rotational population which is a maximum at $J'' = 16$ for $T_k = 60$ K. Quite obviously, the $E = 10^{-14}$ predictions which are insensitive to T_k do not fit the observations: the high J'' levels have a much lower population than predicted. Predictions for $E = 10^{-13}$ also do not fit the observations: the high J'' levels have a much higher population than predicted.

The sparseness of van Dishoeck & Black's table of predicted populations makes interpolation uncertain. It appears, how-

TABLE 3

RELATIVE (ADJUSTED) POPULATIONS OF THE ROTATIONAL LADDER FOR $X^1\Sigma_g^+(v=0)$

J''	$5N(J'')/(2J'' + 1)N(2)^a$			
	This Paper	H&C	D&L	vD&B
0.....	1.28(0.28) ^b	1.14(0.56)	1.97(0.41)	1.78(0.40)
2.....	1.00(0.12)	1.00(0.23)	1.00(0.08)	1.00(0.08)
4.....	0.63(0.06)	0.51(0.15)	0.84(0.19)	0.53(0.08)
6.....	0.33(0.04)	0.49(0.19)	0.41(0.07)	0.35(0.04)
8.....	0.19(0.03)	0.24(0.07)	0.24(0.05)	0.16(0.02)
10.....	0.11(0.02)	0.11(0.06)	0.14(0.03)	0.13(0.04)
12.....	0.076(0.012)	<0.068	0.091(0.034)	<0.074
14.....	0.046(0.009)	...	0.057(0.033)	...
16.....	0.032(0.009)
18.....	0.028(0.007)
20.....	0.021(0.006)
22.....	0.017(0.006)
24.....	0.011(0.006)

^a H&C = Hobbs & Campbell 1982; D&L = Danks & Lambert 1983; vD&B = van Dishoeck & Black 1986.

^b 1.28(0.28) = 1.28 ± 0.28.

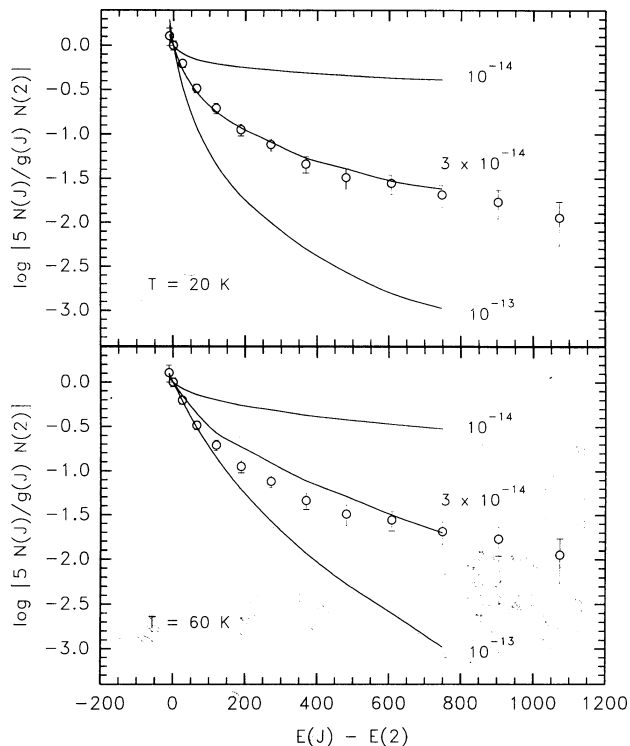


FIG. 5.—Observed and predicted relative populations of rotational levels in the C_2 ground ($v'' = 0$) state. The energies $E(J) - E(2)$ have units of cm^{-1} . The predictions are for the indicated kinetic temperatures and $E = n\sigma_0/I = 10^{-13}$, 3×10^{-14} , and 10^{-14} .

ever, that predictions for $E \approx 3 \times 10^{-14}$ provide a fair fit to the observations (Fig. 5). The best overall fit to the $J'' = 0$ – 20 populations is provided by a T_k between 20 and 45 K and $E = 3 \times 10^{-14}$. Figure 5 shows predictions for $T_k = 20$ and $E = 3 \times 10^{-14}$ which fit the observations for $J'' \gtrsim 2$ but fail marginally to account for the relative populations of $J'' = 0$ and 2: $N(0)/N(2) = 0.26 \pm 0.05$ is observed but 0.34 predicted. Approximate error bounds are 20 to 80 K for T_k and $\pm 50\%$ for E . Selection of this fit assumes that the two (or more) parcels of C_2 molecules along the line of sight have very similar conditions. A range of alternative solutions are possible: $T_k = 60$ K with $E = 10^{-13}$ for low J'' with addition of a component for high J'' with $E = 3 \times 10^{-14}$ at $T_k \sim 20$ – 100 K gives a reasonable fit to the observations.

An estimate of E is convertible to an estimate of the gas density provided that an assumption is made concerning the factor I , the scaling factor for the near-infrared radiation field, and the cross section σ_0 . Most previous (detailed) chemical models (van Dishoeck & Black 1986b; Viala, Roueff, & Abgrall 1988) for the gas towards ζ Oph suggest a more intense ultraviolet radiation field than the ambient interstellar one; presumably, the proximity of the clouds to ζ Oph is responsible for the enhancement. The argument for an enhanced radiation field is driven by the observed populations of high-lying rotational levels of H_2 which it is assumed are populated by pumping via ultraviolet transitions. There are, however, other ways of populating the high-lying levels of H_2 , e.g., interstellar shocks (Draine 1986) and newly formed H_2 molecules are rotationally hot upon ejection from the surface of a grain (Wagenblast 1992). An analysis of C_2 and CN densities in clouds (Federman et al. 1994) suggests no need to

enhance the ultraviolet radiation field. On the assumption that the spectrum of the radiation field is approximately that adopted by van Dishoeck & Black (1982), an indication that the ultraviolet fluxes were appropriately described implies that $I = 1$ for the near-infrared field.

With an assumption about the cross section σ_0 , it is possible to use the estimate of E with $I = 1$ to obtain an estimate of the average density n . Van Dishoeck & Black (1982) estimate $\sigma_0 = 2 \times 10^{-16} \text{ cm}^{-2}$. All levels are fitted with $n = 85$ – 225 cm^{-3} for $T_k \approx 30$ K when E is divided by 1.5, as suggested by van Dishoeck & Black (1982); these estimates of n would be about a factor of 2 lower if the theoretical estimates of excitation cross sections of Lavendy et al. (1991) and Robbe et al. (1992) were used. Since the amounts of atomic and molecular hydrogen are expected to be similar along the line of sight to ζ Oph, the total gas density, $n_t = n(\text{H}) + 2n(\text{H}_2)$, is approximately 50% larger than n . Thus, n_t is approximately 125–350 cm^{-3} . These results for the gas density are similar to estimates from the chemistry of C_2 and CN ($n_t = 400 \text{ cm}^{-3}$, Federman et al. 1994), the isotopic fractionation and rotational excitation of CO, and the excitation of the ground state fine structure of the neutral carbon atoms ($n_t = 100$ – 200 cm^{-3} , Sheffer et al. 1992; Lambert et al. 1994).

An intriguing possibility exists should $T_k = 60$ K for the gas sampled by C_2 . Then absorption from low and high J'' levels originates in material with somewhat different gas densities: for low J'' (≤ 6), $n = 175$ – 350 cm^{-3} , and $n_t = 275$ – 525 cm^{-3} , while for high J'' , $n = 125$ – 225 cm^{-3} and $n_t = 200$ – 350 cm^{-3} . The picture that emerges is one in which the bulk of the C_2 and CN molecules appear to be in a “dense” clump, which is revealed by considerations of the chemistry (Federman et al. 1994) and the analysis of the low-lying rotational levels of C_2 . The clump appears to be surrounded by a region containing ^{12}CO , C I atoms, and probably CH and OH. (The OH distribution in molecular cloud envelopes was studied by Wannier et al. 1993 who found the OH emission and abundance to peak in the vicinity of the transition from atomic to molecular hydrogen.) The high-lying levels of C_2 , as well as the ^{13}CO come from an intermediate region where the flux (i.e., I) is not much different than in the “dense” clump. The presence of an enhancement in ^{12}CO relative to ^{13}CO (Sheffer et al. 1992; Lambert et al. 1994) indicates that ^{12}CO shields itself from ultraviolet (dissociating) radiation more effectively than ^{13}CO and so ^{12}CO is probably widely spread across the clouds. Perhaps the clump and its envelope correspond to the two clouds revealed by profiles of the optical CN and the millimeter CO lines.

3.4. The f -Values of the C_2 Systems

An interstellar cloud serves as an absorption tube from which relative f -values of the three C_2 systems may be derived. The GHRs spectra provide directly the ratio $f_{00}^{AX}/f_{00}^{DX} = 1.83 \pm 0.18$. The published measurements of the 2–0 Phillips system’s lines toward ζ Oph give $f_{20}^{AX}/f_{00}^{DX} = 0.0226 \pm 0.0029$.

The Mulliken system is chosen as the calibrator to convert these relative f -values to absolute f -values. Bruna & Wright’s (1992) prediction from a detailed ab initio calculation is $f_{00}^{DX} = 0.0546$ which is in remarkably close agreement with an earlier ab initio prediction $f_{00}^{DX} = 0.0544$ by Chabalowski, Peyerimhoff, & Buenker (1983). Although the impression that these theoretical results are accurate to better than 1% is probably not sustainable on scrutiny by an expert, it does seem that $f_{00}^{DX} = 0.0545$ to within about 10%. Bruna & Wright point out

that their prediction for the radiative lifetime of the upper ($D^1\Sigma_u$) state of the Mulliken system is 14.6 ns for the vibrational level $v' = 0$ which agrees well with a measurement of 14.6 ± 1.5 ns reported by Smith (1969) and is fairly close to the value of 18.1 ± 1.0 ns obtained by Curtis, Engman, & Erman (1976). A shock-tube study of C₂ emission (Cooper & Nicholls 1975, 1976) yielded $f_{00}^{DX} = 0.017$ which is not in agreement with the ab initio predictions but Bruna & Wright argue that Cooper & Nicholls may have confused emission from the Mulliken system with that from another (Freymark) system. In what follows, $f_{00}^{DX} = 0.0545$ is adopted.

With this value, one obtains $f_{00}^{FX} = 0.10 \pm 0.01$ where the uncertainty does not include a contribution of perhaps 10% from f_{00}^{DX} . A recent ab initio calculation gives $f_{00}^{FX} = 0.095 \pm 0.009$ (Bruna & Grein 1994) in good agreement with our estimate.

Perhaps, the most interesting use of the relative f -values derived from these spectra of ζ Oph lies in the implied values of the f -values for the Phillips system. The above ratio of f -values gives $f_{20}^{AX} = (1.23 \pm 0.16) \times 10^{-3}$ where, as before, the uncertainty does not include a contribution from f_{00}^{DX} . The estimate of f_{20}^{AX} is in good agreement with a recent ab initio prediction of $f_{20}^{AX} = 1.44 \times 10^{-3}$ (Langhoff et al. 1990) for which an accuracy of about 5% was suggested. Astrophysical confirmation of the ab initio results is also provided by an analysis of solar lines of the C₂ Swan system 0–0 band and Phillips system 0–0 and 1–0 bands which give the same solar carbon abundance to within 10%–15% on adoption of Langhoff et al.'s f -values for the Phillips bands and the accurate experimentally determined f -value of the Swan system's 0–0 band—see Grevesse et al. (1991) for a discussion of the solar C₂ lines and other indicators of the photospheric carbon abundance. Comparison of the Swan and Phillips lines removes uncertainties due to the adopted model solar atmosphere and the dissociation energy of the C₂ molecule.

The pleasing agreement between the “astrophysical” and ab initio f -values for the Phillips system is in contrast with the disagreement between these values and recent laboratory measurements. The disagreement has been aired previously and, hence, a summary will suffice here. Measurements of the radiative lifetime of the $A^1\Pi_u$ state reported by Bauer et al. (1985) and Bauer et al. (1986) are longer than predicted by about 50%–100% depending on the vibrational level. The differences exceed the experimental measurement errors; note Bauer et al. (1986) used laser-induced fluorescence which is usually a very reliable way to measure radiative lifetimes. Bruna & Wright (1991) suggest that in Bauer et al.'s source, the population of the $A^1\Pi_u$ state was replenished through collisional transfers from a longer lived state. A likely candidate for the latter was suggested. However, Gong et al. (1994) have measured the radiative lifetime of that candidate and found its lifetime to be slightly shorter than Bauer et al.'s measured values for the $A^1\Pi_u$ state. Thus the particular suggested route for replenishment cannot apparently account for the discrepancy between the predicted and measured radiative lifetimes of the $A^1\Pi_u$ state.

Another source of a conflict with the ab initio predictions for the Phillips system is the relative measurement of the Swan and Phillips f -values by Davis et al. (1984), who measured absorption lines provided by a column of C₂ molecules in a high-temperature furnace. The measured ratios in combination with the value of f_{00} (Swan) suggested by Grevesse et al. (1991) give $f_{00}^{AX} = (1.66 \pm 0.06)10^{-3}$ and $f_{10}^{AX} = (2.05 \pm 0.04)10^{-3}$.

These values are smaller than those predicted by Langhoff et al. ($f_{00}^{AX} = 2.28 \times 10^{-3}$ and $f_{10}^{AX} = 2.38 \times 10^{-3}$) and are inconsistent with the values deduced from the solar C₂ Swan and Phillips lines.

The present observations of the interstellar ultraviolet C₂ lines confirm that independent ab initio calculations of Mulliken and Phillips systems' f -values are correct to within about 10%. It would seem that laboratory measurements of the radiative lifetime of the $A^1\Pi_u$ state overestimate the true lifetime by an amount exceeding the published errors of measurement.

3.5. Other Lines of Sight

Column densities of interstellar molecules are generally quite well correlated. Since the other lines of sight (ξ Per, β^1 , π and ω^1 Sco) penetrate interstellar clouds in which molecules have lower column densities than through ζ Oph's clouds, one expects, as is found, the C₂ ultraviolet bands to be much weaker than in the spectrum of ζ Oph. Federman et al. (1994) present a compilation of molecular column densities and show that, for example, the C₂ and CH column densities are quite well correlated. The chemical reaction network thought responsible for the C₂–CH correlation is presented and discussed by Federman et al. (1994). The correlation may be used to predict the C₂ column densities expected for the other four observed lines of sight.

CH column densities for the quartet taken from Federman et al.'s compilation are in order of decreasing magnitude: $\log N(\text{CH}) = 13.04$ (ξ Per), 12.51 (ω^1 Sco), 12.28 (β^1 Sco), and <11.7 (π Sco). Examination of the C₂–CH correlation suggests a C₂ column density for ξ Per in the range of $\log N(\text{C}_2) = 12.6$ –13.2. Individual rotational lines of the Mulliken 0–0 band are present but equivalent widths are uncertain. Our strategy for improving the S/N ratio was to co-add individual lines, specifically averaging the eight lines— $R(2)$ through $R(8)$ and $P(2)$ through $P(8)$ —which are the strongest in the spectrum of ζ Oph. This “average” C₂ line is clearly seen above the reduced noise (Fig. 6) with an equivalent width of 1.58 ± 0.45 mÅ.³ A fit to the averaged C₂ profile for ξ Per is made using the three-cloud model derived by Crane et al. (1994) from a high-resolution profile of the CH 4300 Å line. Small adjustments were made to the relative column densities of the three clouds; i.e., the C₂/CH was not assumed to be the same for all clouds. The marked asymmetry of the C₂ profile closely resembles that of the CH profile. A total column density $N(\text{C}_2) = (8.0 \pm 2.3) \times 10^{12} \text{ cm}^{-2}$ is obtained on the likely assumption that the rotational excitation of C₂ along the two lines of sight is similar. This column density, which is the lowest yet measured for C₂ along any line of sight, is in reasonable agreement with the prediction of $3.4 \times 10^{12} \text{ cm}^{-2}$ from chemical arguments in Federman et al. (1994) and lies within the range of the extrapolation of their C₂–CH correlation.

Even with the strategy of summing the eight most probable strongest lines, C₂ is not detected toward β^1 Sco, π Sco, and ω^1 Sco: $N(\text{C}_2) \leq 1.7 \times 10^{12} \text{ cm}^{-2}$ is obtained. This upper limit

³ The averaged line profile for ζ Oph has an equivalent width of 3.04 ± 0.30 mÅ and appears to have weak broad wings. Deconvolution gives a width (FWHM) of about 10 km s^{-1} . This component, if real, may originate in the same gas that provides the weak broad wings to the CH⁺ 4232 Å line discovered by Crane, Hegyi, & Lambert (1991). Alternatively, the ζ Oph profile may have a weak sharp component redshifted by 6 km s^{-1} with respect to the main component.

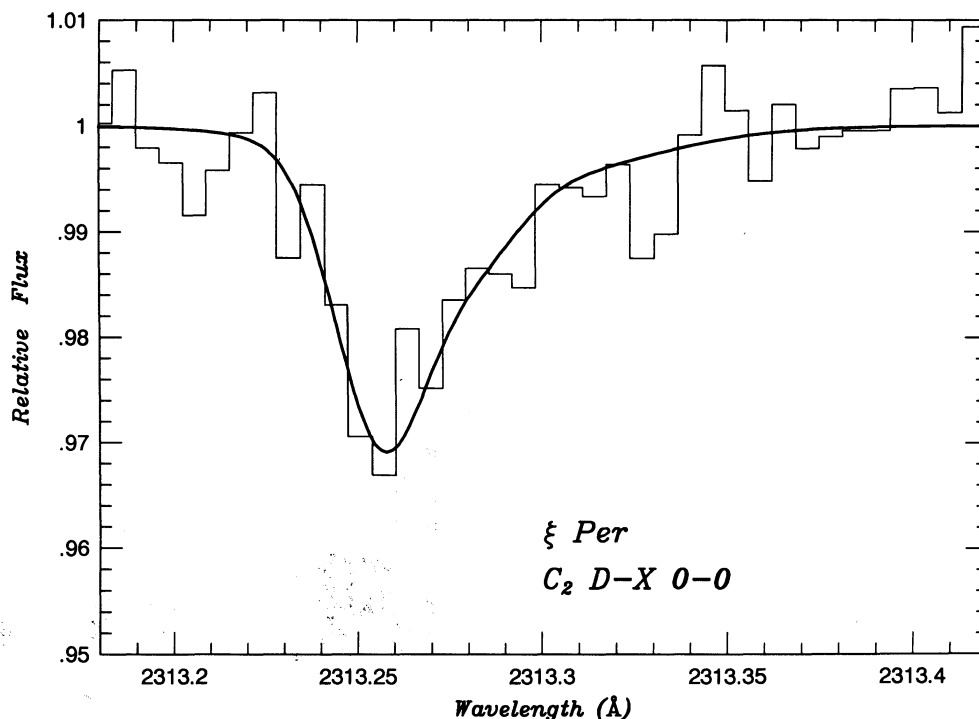


FIG. 6.—The averaged observed C_2 profile (histogram) for ξ Per obtained as described in the text. The predicted profile (solid line) corresponds to the column density $N(C_2) = 8.0 \times 10^{12} \text{ cm}^{-2}$.

for ω^1 Sco with the highest CH column density of the trio is at the lower end of the range of C_2 column densities predicted from extrapolation of the C_2 -CH correlation to the low CH column densities for these lines of sight. This result may suggest a steepening of the C_2 -CH correlation for regions of clouds most transparent to ultraviolet (dissociating) radiation. The upper limit is also consistent with the prediction of $7 \times 10^{11} \text{ cm}^{-2}$ based upon the chemical model described by Federman et al. (1994) with $n \sim 150 \text{ cm}^{-3}$. The model reveals that ultraviolet radiation indeed controls the amount of C_2 for this sight line.

4. CONCLUDING REMARKS

Interstellar C_2 molecules along the line of sight to ζ Oph were discovered by Chaffee & Lutz (1978) who detected a single line from the 2-0 band of the Phillips system. This discovery was followed by more extensive measurements by

others of the Phillips system. The present GHRIS spectra extend investigation of these C_2 molecules to ultraviolet bands from the Mulliken and the $F-X$ systems. Accurate relative f -values for the three systems are derived. It is to be noted that these “astrophysical” relative values are in fine agreement with the predictions from recent ab initio calculations. The observation of the Mulliken system shows lines from rotational levels with $J = 0-24$. The relative populations are shown to be explained by the excitation mechanism described by van Dishoeck & Black (1982) operating under environmental and physical conditions now expected for ζ Oph’s clouds.

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APPENDIX

ATOMIC LINES NEAR 1330 Å

The exposures (see Table 1) of ζ Oph and π Sco near 1330 Å include several atomic lines. These lines, which were identified using the convenient finding list compiled by Morton (1991), are listed in Table 4. No attempt has been made to search for lines close to the detection limit. For ζ Oph, a line of P III at 1334.813 Å is present; the line’s equivalent width and radial velocity confirm estimates off an independent spectrum by Federman et al. (1993). Equivalent widths measured for ζ Oph include contributions from the two principal clouds at heliocentric radial velocities of -15 and -27 km s^{-1} . A second Cl I line must be present but blended with one of the very strong C II lines: the Cl I line at 1335.726 Å has an f -value about 20% that of the line at 1347.240 Å. In addition to the atomic lines, two ^{12}CO bands from the $A^1\Pi-X^1\Sigma^+$ system are present in the ζ Oph spectrum: $W_\lambda = 32 \pm 1$ and $26 \pm 1 \text{ mÅ}$ for the 7-0 and 8-0 bands, values consistent with previous measurements (Lambert et al. 1994; Wannier, Penzias, & Jenkins 1982, respectively).

TABLE 4
 ATOMIC LINES NEAR 1330 Å

SPECIES ^a	LINE (Å)	f-VALUE ^b	W _λ (mÅ)			
			ζ Oph			
			HST ^c	C ^d	π Sco ^e	
S I.....	1316.543	3.45(-2) ^e	19	17.8	1 ^f	
	.615	6.16(-3)				
	.622	4.11(-4)				
Ni II.....	1317.217	1.46(-1)	12	
C I.....	1328.833	5.80(-2)	50	52 ± 6	8	
	C I*.....	1329.085				1.93(-2)
		.100				2.42(-2)
C I**.....	.123	1.45(-2)	58	60 ± 5	...	
	1329.578	4.34(-2)				
	.601	1.45(-2)				
C II.....	1334.532	1.28(-1)	202	189 ± 2	225	
C II*.....	1335.663	1.28(-2)	141	140 ± 4	159	
	.708	1.15(-1)				
	1347.240	1.18(-1)				
Cl I.....	1347.240	1.18(-1)	27	20.3	15	

^a C I ≡ C(2p² ³P₀), C I* ≡ C(2p² ³P₁), C I** ≡ C(2p² ³P₂), C II ≡ (2p² ²P_{1/2}⁰), and C II* ≡ C II(2p² ²P_{3/2}⁰).

^b From Morton 1991.

^c Uncertainty of ± 1 mÅ.

^d C ≡ Copernicus; see Morton 1975.

^e 3.45(-2) ≡ 0.0345.

^f Identification uncertain.

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