

THE 0.9–2.5 MICRON SPECTRUM OF COMET WEST 1976 VI

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ABSTRACT

The infrared spectrum of comet West 1976 VI, obtained during its 1976 apparition, is discussed and analyzed. The spectrum covers the region 0.9–2.5 μm at a resolution of 4.6 cm^{-1} . It is calibrated on a specific intensity scale ($\text{ergs s}^{-1}\text{ cm}^{-2}\text{ \AA}^{-1}\text{ sr}^{-1}$). The slope of the albedo curve shows a slight reddening from 0.9 to 2.0 μm and thermal emission longward of 2.0 μm . By fitting this curve, a color temperature of $500 \pm 50\text{ K}$ was obtained for the coma dust particles. No absorptions due to ices such as H_2O , NH_3 , CO_2 , CH_4 , H_2S , or NH_4HS could be seen. No emissions or absorptions from possible parent molecules were detected. Our spectra provide the first cometary detection of the triplet C_2 Ballik-Ramsay bands, as well as the first unambiguous detection of the singlet system of C_2 by the $\Delta v = 0$ transitions of the Phillips bands. Strong emissions from the red system of CN are also observed. Absolute luminosities are determined for all these bands, as well as column densities using a fluorescence model. Our observed intensity ratio of the triplet to singlet system in C_2 differs by a factor of 10–20 from statistical equilibrium predictions. A ratio of ~ 17 is deduced for the population of the triplet to that of the singlet state of C_2 . Our spectrum also serves as a valuable resource to photometric observers who wish to select filters in the infrared or to determine the contributions of cometary emissions to their broadband measurements.

Subject headings: abundances — comets — infrared: spectra — line identifications

I. INTRODUCTION

The analysis of cometary spectra in the infrared region above 1 μm can provide information on cometary ice absorptions, and emissions or absorptions by parent molecules. However, the weaker spectral flux of the comets and the lower detector sensitivity in this region make acquisition of their spectra difficult. For these reasons infrared observations of comets have so far been limited to photometry. Such photometry of the relatively bright comets has been obtained since 1966 by a number of observers (e.g., Becklin and Westphal 1966; Maas, Ney, and Woolf 1970; Rieke and Lee 1974; Ney and Merrill 1976; Oishi *et al.* 1978; A'Hearn, Dwek, and Tokunaga 1981). The throughput and multiplex advantages of Fourier spectroscopy offered hope that medium-resolution spectra of bright comets could be acquired.

Comet West provided such an opportunity, and we were able to obtain a spectrum of this comet with our interferometer (Larson and Fink 1975). Although comet West was considerably brighter than Kohoutek, it did not receive the same attention. Only a few spectra in the visible to $\sim 0.6\text{ }\mu\text{m}$ were reported for this comet (Chaubey 1978). One uncalibrated spectrum was obtained in the region 0.57–0.87 μm (Gary, Fountain, and O'Dell 1977); but it does not overlap our data and so does not permit direct intercomparison of the molecular transition strengths. Narrow-band photometry was car-

ried out by A'Hearn, Hanisch, and Thurber (1980), Schuster and Lopez (1976), and Cosmovici *et al.* (1978). Photometry from 0.5 to 20 μm was reported by Ney and Merrill (1976) and from 1 to 20 μm by Oishi *et al.* (1978). Analysis of these IR data showed that comet West was quite dust rich.

In this paper we describe our infrared data and present exploratory analyses of several topics. We investigate the comet's thermal emission spectrum and its solar reflection continuum, search for absorption features due to ices, search for emission and absorption features by parent molecules, and briefly discuss the observed emission features from molecular radicals in the coma. We derive approximate column densities for CN and C_2 , assuming a simple resonance fluorescence model. These calculations can be refined by including additional effects and employing more sophisticated fluorescence models. We feel, however, that this is beyond the scope of the present survey paper. More detailed analyses addressing additional topics are left to future papers.

II. OBSERVATIONS AND DATA REDUCTIONS

Comet West 1976 VI was observed during 1976 March 13–16 UT at the 1.5 m Catalina telescope of the University of Arizona Observatories. A log of the observations is presented in Table 1. The comet was observed at air masses between 1.8 and 3.5. An Idealab Fourier spec-

TABLE 1
COMET WEST OBSERVATIONAL PARAMETERS

Object	UT Date	Integration Time (s)	Air Mass	r (AU)	Δ (AU)	α^a
West	1976 Mar 13.5	1140	2.1	0.600	0.947	76°
West	14.5	2700	3.5	0.626	0.960	74°
West	14.5	780	2.2	0.626	0.960	74°
West	15.5	2040	3.5	0.651	0.973	73°
West	15.5	2940	2.3	0.651	0.973	73°
West	16.5	1710	2.8	0.676	0.986	71°
West	16.5	1590	2.3	0.676	0.986	71°
West	16.5	1020	1.8	0.676	0.986	71°
η Boo	14.3	960	2.1	...	...	...

^a Phase angle (Sun-comet-Earth).

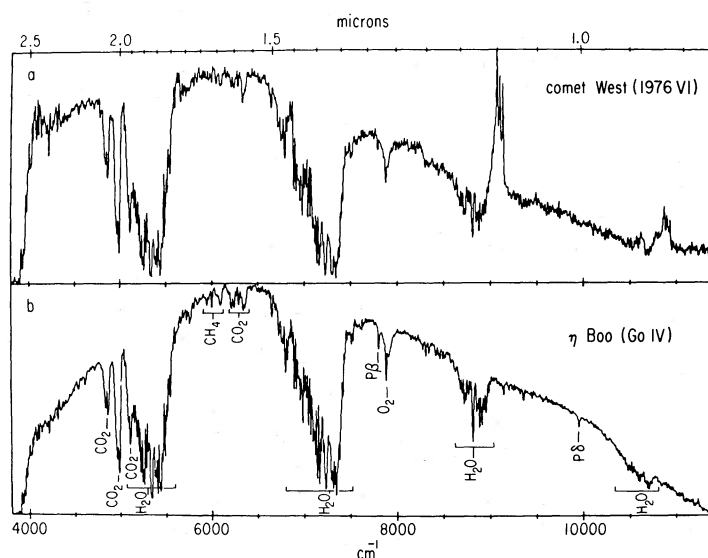


FIG. 1.—(a) The observed spectrum of comet West, for an air mass of 2.7, normalized to one at the maximum intensity. This spectrum includes atmospheric absorptions and the telescope and instrumental spectral responses. (b) The corresponding spectrum of the comparison star, η Boo, for an air mass of 2.1. Major telluric and stellar absorptions are labeled.

trometer (Larson and Fink 1975) with two InSb detectors was used to obtain spectra from 4000 to 11,400 cm^{-1} (2.5–0.88 μm) at a resolution of 4.6 cm^{-1} . A short-wave pass filter prevented radiation with $\nu < 4000 \text{ cm}^{-1}$ from being detected. Our 10" square aperture covered the four subnuclei (maximum separation $\sim 8''$), which were the result of the splitting of comet West only a few weeks earlier (Marsden 1976).

The raw interferograms were co-added into blocks of 168–670 individual scans having similar air mass. The resulting interferograms were transformed, and the spectra were averaged with appropriately assigned weights. The final spectrum has an average air mass of 2.7 and is displayed in Figure 1a. The solar-type star η Boo (G0 IV) was used as the comparison, and its interferograms were reduced in the same manner as those of the comet. The spectrum of η Boo at an air mass of 2.1 is shown in

Figure 1b. The major telluric absorptions and a few stellar lines are marked.

The ratio of comet West to the Sun is shown in Figure 2. Since the weights assigned to the individual comet spectra were chosen to optimize the signal-to-noise ratio, the final air mass was not as close to that of η Boo as desirable. This resulted in residual telluric bands in the ratio spectrum. The solar-type star η Boo tracks the colors of the Sun to within 3% from 0.9 to 2.5 μm . Although we consider this difference to be within the errors of IR photometry, we applied a 3% slope correction to the raw ratio of comet West/ η Boo. Thus the ratio in Figure 2 is the true albedo of comet West.

In order to make quantitative calculations of molecular column densities, it was necessary to determine a spectrum of comet West on an absolute flux scale. Our ratio spectrum corrected for the Sun's colors was con-

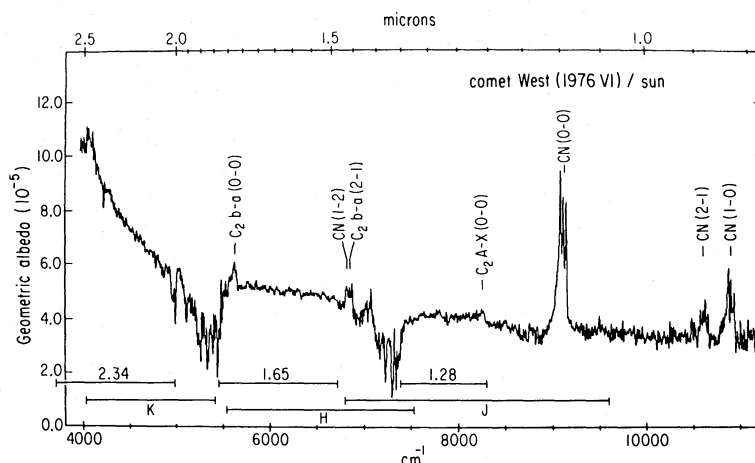


FIG. 2.—Albedo spectrum of comet West. Slight air mass mismatching resulted in residual telluric absorptions of H_2O and CO_2 . Major cometary molecular emissions are marked. Standard *JHK*-filter bandpasses of Johnson (1965) and Rieke (1982) and those used by Ney and Merrill (1976) are drawn below the spectrum.

verted to a relative flux distribution by first multiplying by the spectral distribution of the Sun as given by Arvesen, Griffin, and Pearson (1969). At the same time we inverted our ratio spectrum to a linear wavelength scale in μm to make it compatible with standard photometry. We used the *J* and *H* photometry of comet West by Ney and Merrill (1976) and by Oishi *et al.* (1978) to provide an absolute flux calibration. The first authors used a square $20''$ aperture, while the second used a $60''$ circular aperture. The continuum flux ratio from these two investigations agreed with the ratio of their aperture diameters, indicating that the continuum brightness of the coma followed a $1/\rho$ falloff reasonably well. We corrected the *H*-fluxes of Ney and Merrill (1976) to our $10''$ square aperture and interpolated their data to our observation date. This $1/\rho$ falloff used to obtain our absolute fluxes posed no problem for our results; however, we note that extrapolation of a $1/\rho$ brightness dependence to smaller sized apertures could present some problems. From our relative flux spectrum, the flux density F_H , in the *H*-filter passband, can be obtained by

$$F_H = K \int h(\lambda) R_H(\lambda) d\lambda.$$

Here, $R_H(\lambda)$ is the response curve of the *H*-filter (Ney 1982*a*), and $h(\lambda)$ is the height of our relative flux spectrum in arbitrary units. Comparison of F_H to the *H* flux density by Ney and Merrill (1976) determines the constant K and thus provides the absolute calibration sought. Both the *J* and *H* passbands gave consistent results. A similar result was obtained from an internal calibration method, though it was judged to be less accurate. It involved relating the peak interferogram levels per unit integration time of comet West and η Boo

to their respective spectra, and using the published photometry of η Boo (Johnson 1966). We divided the absolute flux by the solid angle used in these observations and obtained the mean specific intensity over our aperture, which is equivalent to the surface brightness for a uniform extended source. This quantity is plotted in Figure 3 as a function of wavelength.

III. DISCUSSION

The ratio spectrum of comet West to the Sun is displayed in Figure 2. Because the air mass for η Boo was somewhat smaller than the comet average, the spectrum shows spurious absorptions at the positions of the 1.4 and 1.9 μm water vapor bands and the triad of CO_2 bands near 2 μm . The continuum of the comet rises slightly from 10,000 to 5500 cm^{-1} . For $\nu < 5500 \text{ cm}^{-1}$, the continuum level increases sharply because of thermal emission from the dust particles in the coma. No obvious absorption features intrinsic to the comet either from solids or gases are seen.

Quite conspicuous, however, are a number of strong emission features in the comet's spectrum. All identified emissions originate from two species: CN and C_2 . The positions and identifications of the emissions are listed in Table 2. The CN emissions belong to the electronic-vibrational group from the upper state $A^2\Pi_i$ to the ground electronic state $X^2\Sigma_g^+$ ($A \rightarrow X$ transition). The strongest of these bands is the 0-0 transition at 9117 cm^{-1} , followed by the 1-0 transition at 10,904 cm^{-1} . The next series to the $v''=1$ state is represented by the 2-1 (10624 cm^{-1}) and 0-1 (7075 cm^{-1}) bands. The 1-1 transition (8862 cm^{-1}) is expected to be very weak and is not seen in our spectrum. The identification of the 0-2 (5059 cm^{-1}) band to the $v''=2$ level is doubtful in our data.

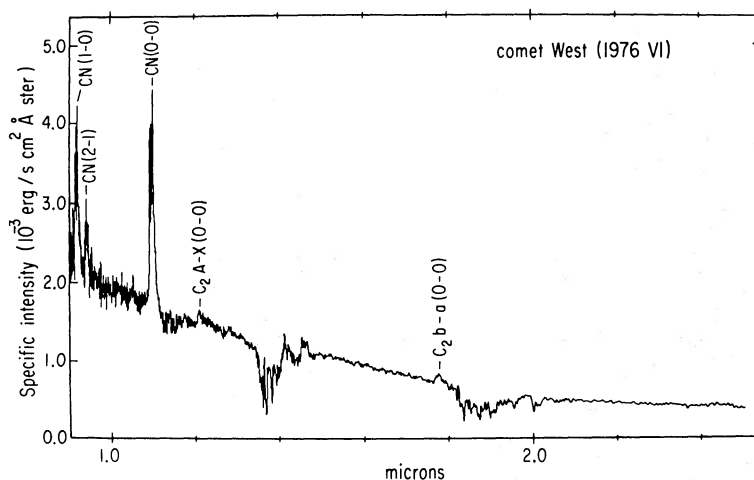


FIG. 3.—Absolute flux spectrum of comet West on a linear wavelength scale. Several prominent molecular emissions are labeled.

TABLE 2
EMISSION FEATURES IN COMET WEST

OBSERVED POSITION BAND CENTER		LISTED POSITION BAND HEAD (cm ⁻¹)	SPECIES	TRANSITION	
(cm ⁻¹)	(μm)			Electronic	Vibrational (v' → v'')
4050	(2.47) ^a	...	unassigned	...	...
5630	(1.78)	5632.7	C ₂	b → a	(0 → 0)
6850	(1.46)	6846.0	CN	A → X	(1 → 2)
		6888.4	C ₂	b → a	(2 → 1)
7050	(1.42)	7075.0	CN	A → X	(0 → 1)
		7080.8	C ₂	b → a	(1 → 0)
7812	(1.28) ^a	...	unassigned	...	...
8260	(1.21)	8268.2	C ₂	A → X	(0 → 0)
8482	(1.18)	8506.5	C ₂	b → a	(2 → 0)
9110	(1.10)	9117.4	CN	A → X	(0 → 0)
10480	(0.954) ^a	...	unassigned	...	...
10620	(0.942)	10624.3	CN	A → X	(2 → 1)
10895	(0.918)	10904.5	CN	A → X	(1 → 0)

^aEmission is marginally above the noise level.

Two types of band systems are observed for the C₂ molecule, the singlet Phillips band system $A\ ^1\Pi_u \rightarrow X\ ^1\Sigma_g^+$ ($A \rightarrow X$) and the triplet Ballik-Ramsay system $b\ ^3\Sigma_g^- \rightarrow a\ ^3\Pi_u$ ($b \rightarrow a$). This paper reports the first observation of the Ballik-Ramsay C₂ bands in a comet. The Phillips band transitions 3-0, 4-1, and 5-2 have been reported in comet Bradfield 1979 X by Danks and Dennefeld (1981), while the 3-0 band has been reported in comet Tago-Sato-Kosaka 1969 IX by O'Dell (1971).

However, both of these data sets suffer from severe blending by cometary CN and NH₂ bands and by telluric OH emissions. In our IR spectrum the (0-0) Phillips band at 8268 cm⁻¹ is clearly free from blends. Thus our data represent the first time that C₂ transitions from the singlet and triplet systems have been observed unblended in one spectrum. This has important ramifications for the relative populations of these two systems, as is discussed below.

a) The Thermal Emission Spectrum

Although only a small portion of the thermal emission spectrum is seen in Figure 2, a blackbody color temperature could be determined. The solar reflected light from 9000 to 5500 cm^{-1} can be represented quite closely by a straight line. It was extrapolated to wave-numbers below 5500 cm^{-1} and subtracted from the observed intensity of the comet. The resulting spectral energy distribution of the thermal emission was normalized to 1 at 4000 cm^{-1} and is plotted in Figure 4, in units of power/($\text{cm}^2 \text{ cm}^{-1}$). Also plotted in Figure 4 are the thermal emission curves, all normalized to 1 at 4000 cm^{-1} , for blackbody temperatures from 300 to 700 K. The discrimination between these curves is quite good. The observed thermal emission spectrum follows a blackbody curve quite closely, and a color temperature of 500 ± 50 K was determined.

This temperature is quite close to that of ~ 520 K determined by Campins and Rieke (1982) from the color index between 4.8 and 3.5 μm . They used an aperture of $\sim 8''$, similar to ours. Our temperature is somewhat higher than the color temperature of 425 ± 30 K obtained by Ney and Merrill (1976), who used a larger aperture and gray-body fit to their data. In general the measured color temperatures cannot be simply equated to the grain temperature, and different regions of the spectrum will give different color temperatures (Krishna Swamy and Donn 1968, 1979; Mukai 1977; Campins and Hanner 1982). For this reason, and also because of the larger aperture, which includes a different particle size distribution (Oishi, Okuda, and Wickramasinghe 1978), the far-IR data of Ney and Merrill are expected to be different from ours. For particle sizes of $\sim 0.5 \mu\text{m}$ or larger and a temperature near ours, the measured color temperature and the actual grain temperature are essentially indistinguishable (Krishna Swamy and Donn 1968, 1979; Mukai 1977; Campins and Hanner 1982). Our 500 K can therefore be equated to the grain temperature and compared with models for different grain sizes and composition given in Campins and Hanner (1982). We find that grains with a very low visible absorption coefficient (i.e., an imaginary index of refraction $k \leq 0.03$) are definitely excluded. This would eliminate pure silicate and pure ice particles. No definite conclusion can be reached for larger absorption coefficients since we cannot distinguish between the effects of particle size and absorption coefficient.

b) The Solar Reflection Continuum

The ratio spectrum of comet West in Figure 2 should be quite close to the true albedo of the comet for the region of solar reflected light. The spectrum shows a slight rise, or reddening, from 10,000 to 5500 cm^{-1} by a factor of 1.58. This is a continuation of a reddening trend starting at $\sim 5000 \text{ \AA}$, which we have observed for a number of comets (Johnson, Fink, and Larson 1983).

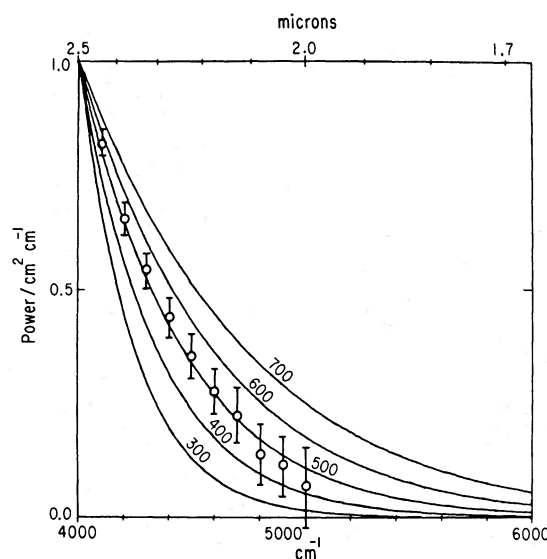


FIG. 4.—Thermal component of comet West's continuum spectrum normalized to 1 at 4000 cm^{-1} . A number of blackbody functions from 300 to 700 K are shown for comparison. The best fit is 500 ± 50 K.

This reddening could be due either to the scattering nature of the grains or to the grain composition. At present we have no means of distinguishing between the two cases.

From the measured surface brightness of the comet I_c , a geometric albedo p can be estimated by

$$p = \frac{I_c}{F_\odot} \pi r^2,$$

where r is the distance of the comet from the Sun in AU, and $F_\odot$ is the solar flux at 1 AU. At 8000 cm^{-1} we obtain $p = 4.1 \times 10^{-5}$, indicating that we are looking at a coma of particles rather than a solid surface. Since the average scattering cross section of the particles is quite model dependent, we did not derive a particle column density.

A number of broadband IR observations of comets have been carried out (Ney 1982*b*; Rieke and Lee 1974). In their analysis they assumed that the effect of cometary emissions within the IR filter passbands was negligible. We have marked on Figure 2 the effective wavelengths and the spectral passbands of the standard JK filters of Johnson (1965), the H filter of Rieke (1982), and the 1.28, 1.65, and 2.2 μm filters of Ney (1982*a*). The most significant contribution to the continuum occurs in the J filter, where we estimate that about 5% of the cometary flux is due to CN and C_2 emissions, although the strengths of emission features may vary considerably as a function of heliocentric distance, and from comet to comet (A'Hearn and Millis 1980). We suggest that our spectrum of comet West can

serve as a guide to the degree of contamination expected or to the selection of filters which more clearly separate the continuum and the emission features.

c) Search for Features Due to Ices and Parent Molecules

The presence of H₂O ice and other volatile ices is essential to Whipple's (1950) icy conglomerate model of a cometary nucleus. The search for the spectral signatures of such ices was therefore one of the prime motivations in obtaining the present spectrum of comet West. Unfortunately, the spectrum (Fig. 2) showed no absorption features due to ices. Considering the high grain temperatures found in the previous section, this result is not surprising in retrospect. Theories of the vaporization of icy grains from an icy conglomerate-type nucleus (Delsemme and Miller 1971) predict that the maximum extension of the icy grain halo (with grain radii $\leq 1 \mu\text{m}$) at a heliocentric distance of about 0.65 AU is only a few hundred kilometers.

The spectrum of comet West (Fig. 2) showed no absorption features due to ices of H₂O (1.5, 1.65, 2.0 μm), NH₃ (1.6, 2.0, 2.2 μm), CO₂ (1.44, 2.0 μm), CH₄ (1.17, 1.4, 1.7, 2.3 μm), H₂S (1.6, 2.0 μm), and NH₄HS (1.5, 1.7, 2.2 μm) (Fink and Sill 1982). For these bands with $\lambda \geq 1.8 \mu\text{m}$ we determine an upper limit to the ratio of the transmission at the band center to that of the nearby continuum. For all ices except CO₂ we set an upper limit of 3% absorption at the band center; for CO₂ it is 5% because of blending with telluric features. Our 10" (7100 km) aperture included contributions from the four subnuclei, their icy halos, and the surrounding dust coma. Assuming that the icy halo extended to a radius of ~ 300 km for each of the four subnuclei, the icy grains could cover at most 2.3% of our aperture, which is consistent with our nondetection of any ices.

The spectral signatures of ices can also be considerably weakened if the ice grains are small (Hanner 1981) or if they are contaminated by dark material (Clark 1981). Hanner calculated that if the icy grains are pure H₂O ice with radii greater than 1 μm , then the 2.0 μm features would have a depth of about 20%. The spectrum presented in Figure 2 thus rules out a substantial ice halo of pure H₂O ice, but we cannot exclude a large halo of small ice grains or dirty ice grains or a condensed halo of large particles.

Our spectrum in Figure 2 shows no evidence for emission or absorption by parent molecules. We have searched for four representative molecules in our spectra: NH₃, CH₄, N₂O, and H₂S. These molecules were selected because they have bands in relatively clear regions from 1 to 2.5 μm and because we had laboratory spectra available for these molecules. The most likely parent molecule, water vapor, could not be probed because of the strong telluric interference.

The positions of the bands utilized for each molecule are listed in Table 3. Next follows an estimate of the average limiting equivalent width, relevant both to emission and absorption. The transitions of the various bands for each molecule exhibited comparable strengths except for the 2.20 μm CH₄ Q-branch, which was somewhat weaker. To within the accuracy possible for upper limits, the use of an average limiting equivalent width is therefore quite adequate. Unfortunately, band strengths for the listed transitions are not readily available. To obtain an estimate of these strengths we used laboratory absorption measurements that were generated for our upper limit determinations for Io (Fink, Larson, and Gautier 1976). These are applicable to comet West, because the Io spectrum had a similar signal-to-noise ratio and spectral resolution. The laboratory amounts, in cm-amagat, corresponding to the upper limits of the equivalent width are given in the last column of Table 3.

If the limiting equivalent widths in Table 3 are interpreted in terms of absorption, the corresponding laboratory amount of absorber can be converted in a straightforward manner to column densities of the order of 10^{19} molecules cm^{-2} . A rough calculation, however, shows that expected emission intensities should be $\sim 10^5$ times those for absorption. This factor arises primarily because of the small total cross section of the light scattered back to us by the coma particles. This cross section can be estimated as $\sim 10^{-5}$ from the continuum albedo of Figure 2. Thus, in absorption by backscattered sunlight, only about 10^{-5} of the total cross section occupied by the parent molecules is sampled.

From the above consideration, an upper limit to the column densities of $\sim 10^{14}$ molecules cm^{-2} can be estimated for the parent molecules in Table 3. A more precise value for this upper limit would require a more detailed fluorescence calculation employing proper transition probabilities. This is beyond the scope of this paper. The number of daughter molecules which could be expected within our aperture is roughly equal to the number of parent molecules times the ratio of the scale length of the daughter divided by that of the parent. The latter ratio is usually within an order of magnitude of unity. Thus an upper limit of $\sim 10^{14}$ cm^{-2} for the parents agrees reasonably well with representative measured column densities for daughters of $\sim 10^{13}$ cm^{-2} (cf. Table 4).

d) The Molecular Emission Features

Applying a simple fluorescence model, our measured emission intensities in Table 4 were used to estimate the total number of emitters contributing within our aperture. We assume the coma to be optically thin and an upper level (u) to be populated from a lower level (l) by absorption of sunlight. The total luminosity L_{ul} , from a column of unit cross section perpendicular to our line of

TABLE 3
DETECTION LIMITS FOR FOUR POTENTIAL PARENT MOLECULES

Molecule	Bands Used (μm)	Equivalent Width Limit (cm^{-1})	Corresponding Laboratory Amount (cm-amagat)
NH_3	1.98 } 2.25 }	6	0.40
CH_4	1.67 } 2.20 } 2.32 } 2.37 }	4	0.40
N_2O	2.11 } 2.26 }	1	0.90
H_2S	1.59	5	24

TABLE 4
EMISSION-BAND LUMINOSITIES AND COLUMN DENSITIES

SPECIES	TRANSITION		POSITION (cm^{-1})	$L_{v'v''}$ (ergs $\text{s}^{-1} \text{cm}^{-2}$) ($= 4\pi I_{v'v''}$)	$\frac{L_{v'v''}}{L_{0-0}}$	PREDICTED FLUORESCENCE RATIOS $L_{v'v''}/L_{00}$	COLUMN DENSITY $N(\text{molecules cm}^{-2})$
	Electronic	Vibrational ($v' \rightarrow v''$)					
CN	$A \rightarrow X$	0-0	9117.4	3.65	1.00	1.00	10.4×10^{12}
	$A \rightarrow X$	1-1	8862.1	< 0.11	< 0.03	0.04	...
	$A \rightarrow X$	0-1	7075.0	... ^a	...	0.31	...
	$A \rightarrow X$	1-2	6846.0	$< 0.37^b$	< 0.10	0.13	...
	$A \rightarrow X$	1-0	10904.5	1.64	0.45	0.55	7.6×10^{12}
	$A \rightarrow X$	2-1	10624.3	0.54	0.15	0.14	10.2×10^{12}
	$A \rightarrow X$	3-2	10344.7	< 0.07	< 0.02	0.014	...
C_2	$b \rightarrow a$	0-0	5632.7	0.91	1.00	1.00	6.2×10^{12}
	$b \rightarrow a$	1-1	5462.8	... ^a	...	0.11	...
	$b \rightarrow a$	2-2	5293.8	... ^a	...	0.004	...
	$b \rightarrow a$	0-1	4014.7	$< 0.23^c$	< 0.24	0.12	...
	$b \rightarrow a$	1-0	7080.8	< 0.06	< 0.06	0.46	...
	$b \rightarrow a$	2-1	6888.4	$< 0.37^b$	< 0.4	0.16	...
	$b \rightarrow a$	2-0	8506.5	< 0.06	< 0.06	0.009	...
C_2	$A \rightarrow X$	0-0	8268.2	0.17	0.18 ^d	1.59 $\rightarrow$ 3.63 ^d	0.37×10^{12}

^aBlended with telluric H_2O .

^bBlending of C_2 $b \rightarrow a$ (2-1) and CN $A \rightarrow X$ (1-2).

^cAt edge of bandpass.

^dFrom a theoretical model by Krishna Swamy and O'Dell 1981.

sight and for a particular vibrational emission band, is then given by

$$\frac{L_{ul}}{h\nu_{ul}} = c\rho(\nu_{lu})N_l B_{lu}(1 - \sigma_D) \frac{A_{ul}}{\sum_{l'} A_{ul'}}. \quad (1)$$

Here, h is Planck's constant; c is the velocity of light; $\rho(\nu_{lu})$ is the solar energy density at the comet at the absorption frequency ν_{lu} ; N_l is the population in the

lower state; and B_{lu} and A_{ul} are the Einstein coefficients for absorption and spontaneous emission, respectively. The fraction $A_{ul}/\sum_{l'} A_{ul'}$ is the relative transition probability for our particular transition as compared to all possible transitions out of this level. The collisional de-excitation coefficient is σ_D , which we shall take to be zero in the rarified medium of the coma.

Since the comet is an extended source, our measured specific intensity (ergs $\text{s}^{-1} \text{cm}^{-2} \text{sr}^{-1}$) is equal to the surface brightness of the comet. Assuming it to be

uniform over our aperture, the total luminosity is obtained by simply multiplying by 4π . The luminosities of the observed CN and C_2 bands corresponding to a column of unit cross section are listed in Table 4. We also list the ratios of the CN band luminosities to that of the CN (0–0) transition. The C_2 band luminosities are normalized to that of the C_2 Ballik-Ramsay (0–0) band.

The solar energy density was determined from Labs and Neckel (1968). We calculated the relative transition probabilities and Einstein B -coefficients for the CN $A \rightarrow X$ bands from oscillator strengths reported by Lambert (1968).¹ We used these factors with the CN band luminosities to compute CN column densities listed in the last column of Table 4.

The calculated ratios of the CN band luminosities agree quite well with prediction from a fluorescence model. We point out that since the Einstein B -coefficients for absorption in the violet CN bands are about 10 times as strong as those for the red CN band, cascading from the higher $B^2\Sigma_u^+$ state can be an important contribution to the level populations. To determine which effect is more important would require a fluorescence calculation including the complete CN system, which is beyond the scope of this paper. Furthermore, the combined errors in absolute calibration, exact emitter field of view, and, above all, transition probabilities can easily cause errors in column densities by a factor of 2–3 or more. Thus the simple fluorescence model is probably adequate to obtain approximate column densities. For example, for the CN violet bands of comet West at the same heliocentric distance, A'Hearn and Millis (1980) reported a CN column density of $\sim 1.2 \times 10^{12}$ molecules cm^{-2} . Our CN column density is a factor of ~ 10 higher, but the aperture of A'Hearn and Millis was ~ 15 times our diameter. The two measurements are therefore in reasonable accord with a $1/\rho$ decrease in column density.

Probably one of the most significant results of our paper is the observation of bands arising from both the singlet and triplet systems of C_2 . Until the work of Ballik and Ramsay (1963), it had been supposed that the lowest triplet state, a $^3\Pi_u$, was the ground electronic state of C_2 . Ballik and Ramsay showed that this state was actually 610 cm^{-1} above the real ground state, $X^1\Sigma_g^+$ of the singlet system. For C_2 , singlet to triplet transitions are forbidden. In the formation of free radicals from parent molecules in a cometary environment, the daughter's energy state depends on the angular momentum state of the parent's ground state and that of the other fragment(s). In addition, the C_2 bond in the parent may dictate whether the C_2 daughter radical will

be formed in a singlet or triplet state. It is quite possible, therefore, that the daughter C_2 species could be formed in some energy level other than the singlet ground state. Observations of the C_2 singlet-to-triplet ratio at different nuclear distances as well as a range of heliocentric distances could lead to knowledge of the C_2 parent and C_2 production mechanism. The Swan bands of the triplet system provide some of the strongest features in cometary spectra, while the Phillips bands have not been detected reliably (O'Dell 1971; Krishna Swamy and O'Dell 1979). Our spectrum of comet West exhibits the same phenomena. The Ballik-Ramsay bands from the triplet system are much stronger than the Phillips bands of the singlet system.

Calculations have been published by Krishna Swamy and O'Dell (1977, 1979, 1981) for an equilibrium fluorescence model of C_2 , incorporating a considerable number of levels and also including a hypothetical singlet-triplet ground-state interaction. Their predicted ratio for the $\Delta v = 0$ transition of the Phillips transition to the $\Delta v = 0$ triplet Ballik-Ramsay system ranges from 1.6 to 3.6 depending on their assumed coupling constant. Our measured intensity ratio is 0.18 (Table 4). The predicted value is thus off by a factor of 10–20, showing that there are serious deficiencies in the model calculations. Since a full statistical equilibrium calculation failed to account for our observed intensities, we used a simple fluorescence model to determine a population ratio of ~ 17 for the triplet to the singlet state of C_2 . The C_2 relative transition probabilities and Einstein B -coefficients were computed from the Franck-Condon factors of Nicholls (1965) and the electronic transition moments of Cooper and Nicholls (1975). The C_2 column densities in the triplet state were similar to those found for CN.

Without having access to the details of Krishna Swamy and O'Dell's calculation, we believe the large discrepancies in their calculations are caused by their assumption of coupling between the ground state of the singlet system $X^1\Sigma_g^+$ and the ground state of the triplet system $a^3\Pi_u$. As Ballik and Ramsay have pointed out, this interaction is not allowed by the selection rules for perturbations. The mechanism proposed by Ballik and Ramsay involves coupling between the $X^1\Sigma_g^+$ ground state of the singlet system and the $b^3\Sigma_g^-$ excited state of the triplet system, which is allowed because both are g states. This interaction has actually been observed by Ballik and Ramsay. In this mechanism, molecules are trapped in the triplet system because of the rapid decay of the $b^3\Sigma_g^-$ excited state to the $a^3\Pi_u$ state. It would be of great interest to calculate the details of this trapping mechanism as proposed by Ballik and Ramsay to see whether it can explain the observed intensity ratios.

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¹A more recent determination of CN $A \rightarrow X$ oscillator strengths has been reported by Sneden and Lambert (1982), but their incomplete array of oscillator strengths prevented us from calculating relative transition probabilities. We note that there is less than a 20% difference between the relative oscillator strengths of Lambert (1968) and Sneden and Lambert (1982).

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