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CN, CH, AND CH^+ TOWARD ζ OPHIUCHI

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ABSTRACT

Observations with a resolution of 600,000 of interstellar absorption from the CN 3874.6 Å, CH 4300.3 Å, and CH^+ 4232.5 Å lines reveal several new features of the clouds along the line of sight toward ζ Oph. The CN line consists of two overlapping components which are similar to those seen in the CO pure rotational lines. The CH^+ line is well described by a single Gaussian line profile with FWHM of 3.5 km s^{-1}. The CH profile is a composite of a CN–like profile and a CH^+–like profile indicating for the first time that CH exists in two regions of very different character. The sharp lines seen in CH, CN, and CO are formed in two molecular clouds. The broad CH^+ and CH lines are attributed to shocked gas. However, models of MHD shocks account for the observed column density of CH^+–like CH, but not that of CH^+. In addition, the predicted velocity difference between (CH^+–like) CH and CH^+ is not observed.

Subject headings: interstellar: abundances — interstellar: molecules — stars: individual (ζ Oph)

I. INTRODUCTION

The problems of understanding the physical conditions in which molecules are formed and evolve in diffuse interstellar clouds have been actively pursued in recent times. The carbon-bearing diatomic molecules of CO, CN, CH, C_2, and CH^+ have received considerable attention (see the reviews by Federman 1987 and van Dishoeck and Black 1988). Except in the case of CO, the interpretations have relied heavily on observations of optical absorption lines seen in the spectra of bright stars behind diffuse clouds. These observations have typically been made using spectra resolutions ($\lambda/\Delta\lambda \leq 100{,}000$) that permit accurate measurements of the equivalent width but not of the profiles of the interstellar lines. In an attempt to improve on this situation, we are observing optical interstellar absorption lines at a resolution of 600,000 or 0.5 km s^{-1}. At this resolution, interstellar lines for most diffuse clouds are resolved. In this *Letter*, we report on our observations of CN, CH, and CH^+ in the clouds toward ζ Oph.

Previous observations by Hobbs (1973) come closest to the resolution employed in this work. Hobbs used a scanning Fabry-Perot spectrometer to observe the CH^+ 4232 Å line toward several stars. These observations had a resolution of about 300,000, or 1 km s^{-1}, and were probably adequate to resolve the majority of CH^+ lines. Since the typical width seen in the millimeter CO lines toward diffuse clouds is on the order of 0.5 km s^{-1}, the study of CN and CH requires considerably higher resolution. Black and van Dishoeck (1988) have discussed the value of high spectral resolution observations of molecular lines.

II. OBSERVATIONS

The observations reported here were obtained in 1989 May and August using the McDonald Observatory's 107 inch (2.71 m) telescope and the coudé spectrometer (Tull 1972). The spectrometer was used with an echelle grating in a high order in double pass, and a Tektronix CCD chip was employed as the detector. With a slit width of 100 μm, the spectral resolution was approximately 600,000 at the wavelengths we observed. Each pixel sampled between 1.5 and 1.7 mÅ of the spectrum, depending on the wavelength. This provided a slight oversampling of the instrumental profile (FWHM 6.8–7.8 mÅ) which, from observation of Th lines from a hollow cathode lamp, was shown to be determined by the slit width. Our analysis accounts for the instrumental profile by convolving the model multicomponent line profile with the instrumental (Gaussian) profile. The total optical depth (τ_λ) in the line at a given wavelength is the sum over the several components and the intensity profile is equal to exp ($-\tau_\lambda$). The profile of a component's absorption coefficient is assumed to be Gaussian. For each species, several 40 minute exposures were combined to form a single spectrum of 512 points from which a 150 pixel section of points was fitted to the model using a standard linearized least-squares procedure. The model also included a term to account for a linear continuum.

III. RESULTS

Inspection of the line profiles (Fig. 1) shows that the three molecules have dissimilar profiles. The CN line consists of a minimum of two components with relative strengths of about 2 to 1. By contrast, the CH^+ line has a much broader single Gaussian profile. Interpretation of the CH line is complicated by the fact that the Λ-type doubling is resolved at our resolution. However, the observed profile may be seen as a blend of the disparate CN and CH^+ profiles with the broad wings of the CH line arising from a CH^+–like component and the core of the CH line arising from a CN–like contribution consisting of two components. In this section, we discuss our detailed fits of the line profiles.

a) CN *Profile*

The observed profile of the CN $R(0)$ line at 3874 Å was fitted to a two-component Gaussian where each component consisted of two subcomponents corresponding to the $R_1(0)$ and the ${}^RQ_{21}(0)$ transitions separated by 3.5 mÅ and of relative

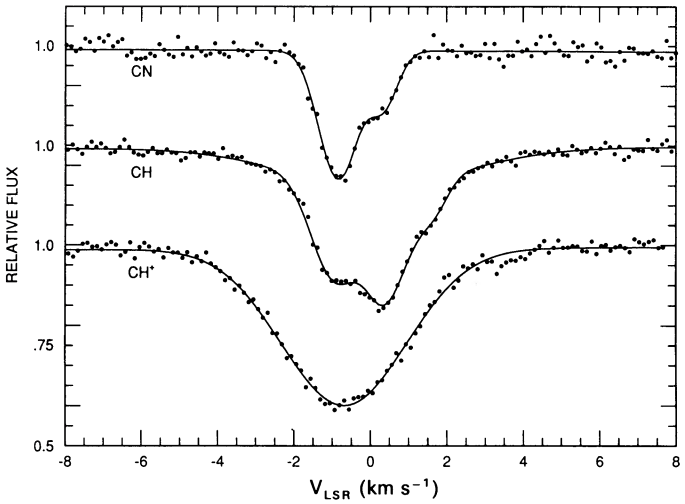

FIG. 1.—Profiles of the CN 3874 Å, CH 4300 Å, and CH^+ 4232 Å lines in the spectrum of ζ Oph. The CN and CH profiles have been shifted so that the stronger of the two narrow components is at $V_{LSR} = -0.79$ km s^{-1}, the velocity of the stronger CO component. The solid lines show the least-squares–fitted profiles.

strength $\frac{2}{3}$ and $\frac{1}{3}$. The velocity splitting between the two main components, as well as the widths and the heights of the components were free parameters in the fitting procedure. Table 1 lists the parameters we determined from observations obtained in 1989 August.

Observations of the CO pure rotation lines $J = 1$–0 and $J = 2$–1 toward ζ Oph have shown two and possibly more components. The presence of two components was seen first by Crutcher and Federman (1987). Of several recent studies, Le Bourlot, Gerin, and Perault (1989) obtained the highest spatial resolution with a FWHM of 23″ at the $J = 1$–0 line and 12″ at the $J = 2$–1 line. Table 1 compares the two-component Gaussian fits to the CN and the CO $J = 1$–0 lines. The CN components' separation matches well the CO results. It is somewhat surprising that the main CN component is broader than its CO counterpart. We presume that the very narrow beam (i.e., the stellar angular diameter) of the optical observations passes through cloudlets that are more turbulent than the average of the cloudlets contributing to the much broader beam of the CO observations. Le Bourlot *et al.* point out that the weak component's velocity and profile, unlike those of the main component, vary on small angular scales. Therefore, it is not surprising that the weak component may be sharper in the CN line. The small difference between the velocities of the CN and CO main components may not be real. Since our reference spectrum from a hollow cathode lamp probably does not illuminate the spectrometer in the same way as a star, a small velocity error is possible. In addition, the difference of 0.3 km s^{-1} is equivalent to an error in the CN line's adopted wavelength (Black and van Dishoeck 1988) of only 3.9 mÅ.

TABLE 1

THE CN 3874.6 Å LINE

QUANTITY[a]	MOLECULE	
	CN	CO
FWHM (component 1)	0.98 ± 0.06	0.60 ± 0.01
FWHM (component 2)	0.64 ± 0.13	0.86 ± 0.03
Velocity V_{LSR} (component 1)	−1.1 ± 0.2	−0.79 ± 0.01
Component separation	1.18 ± 0.06	1.18 ± 0.02
Relative strength[b]	0.29 ± 0.08	0.62 ± 0.04

[a] All quantities except the relative line strengths are expressed in km s^{-1}. Data for CO refer to the $J = 1$–0 line and are taken from Le Bourlot *et al.* 1989. The ratio of the strengths of the two components refers to integrated line strengths.

[b] The observed equivalent width is $W_\lambda = 7.4 \pm 0.2$ mÅ.

Langer, Glassgold, and Wilson (1987) observed the CO $J = 1$–0 line with a 1′.7 beam and deconvolved the line into three main components and one weak component. When we fitted the CN line to a three-component model, an adequate fit is obtained, but the required line widths are larger than the 0.50–0.58 km s^{-1} widths obtained by Langer *et al.* The additional components found by Langer *et al.* are probably artifacts of their larger beam size; Le Bourlot *et al.* clearly show that the velocity of their weak component varies on scales smaller than Langer *et al.*'s beam.

b) CH^+ *Profile*

The CH^+ at 4232 Å is very well fitted by a single Gaussian profile with a FWHM of 3.49 ± 0.09 km s^{-1}. The equivalent width from our observations is $W_\lambda = 23.1 \pm 0.3$ mÅ. The measured velocity of the CH^+ line is $V_{LSR} = -0.9 \pm 0.5$ km s^{-1} where the Moon provided the reference spectrum. We adopt $V_{LSR} = -0.7$ km s^{-1} (Lambert and Danks 1986). The rest wavelength of the CH^+ line was taken to be $\lambda_{air} = 4231.548$ Å (Carrington and Ramsay 1982).

c) CH *Profile*

We initially modeled the Λ-doubled CH line with CN–like components where the wavelengths of the Λ-doubled components separated by 0.0205 Å were taken from Black and van Dishoeck (1988). This attempt failed to fit the extended wings that are an obvious feature of the CH line profile. Then we increased the number of Gaussian components to six: four components ("CN–like") associated with the two clouds seen in the CN line each with Λ-doubled components and a pair of Λ-doubled components ("CH^+–like") associated with the broad CH^+ line. We assumed that the Λ-doubled components had the same width and strength and that the two CN–like velocity components had the same separation as found for CN and CO. Analyses of the CH B–X (0, 0) lines at 3879 and 3886 Å confirm our assumption that the upper and lower Λ-doubled ground state levels have very nearly equal populations (Jura and Meyer 1985; Palazzi, Mandolesi, and Crane 1988). All other parameters of the model were determined by the least-squares fitting procedure. The observed profile is fitted very well. Since the splitting of the CN–like components is comparable to the separation of the Λ-doubled components, the longer wavelength narrow core in Figure 1 is the deeper of the two cores. The line widths and velocities are given in Table 2 and compared with the values for CN and CH^+. The CH^+–like component is redshifted by 0.36 ± 0.10 km s^{-1} relative to the CN–like component. The relative strength of the CH^+–like and CN–like contributions is $R = 0.5 \pm 0.1$. The column density of the CH^+–like component is $N(CH) = 1.2 \times 10^{13}$ cm^{-2} with $N(CH)/N(CH^+) \simeq 0.35$ where the column densities are adapted from Danks, Federman, and Lambert (1984) and Lambert and Danks (1986). Observations of the CH 9 cm radio line (Liszt 1979; Willson 1981) with a 9′ beam previously showed evidence for the two sharp components but did not reveal a CH^+–like component.

The width of the CH^+–like component of the CH line is

TABLE 2

THE CH 4300 Å LINE

QUANTITY ($km\ s^{-1}$)	MOLECULES		
	CH[a]	CN	CH^+
FWHM (CN-like: component 1)	1.25 ± 0.04	0.98 ± 0.06	...
FWHM (CN-like: component 2)	0.74 ± 0.13	0.64 ± 0.13	...
FWHM (CH^+-like)	5.2 ± 0.4	...	3.49 ± 0.09
V_{LSR}(CN-like)	-0.6 ± 0.2	-1.1 ± 0.2[b]	...
V_{LSR} (CH^+-like)	-0.2 ± 0.2[c]	...	-0.9 ± 0.5[d]

[a] The observed equivalent width is $W_\lambda = 19.7 \pm 0.2$ mÅ.

[b] The CO lines give $-0.79 \pm 0.01\ km\ s^{-1}$.

[c] The least-squares estimate of the separation is V_{LSR} (CH^+-like) $- V_{LSR}$ (CN-like main component) $= 0.36 \pm 0.10\ km\ s^{-1}$, where this quantity is unaffected by the systematic errors that may affect the determinations of V_{LSR}.

[d] Lambert and Danks 1986 obtained $-0.7\ km\ s^{-1}$.

larger than the width of the CH^+ line. The CN line shows no sign of a broad CH^+-like component. The widths of the CH line's CN-like components are slightly larger than those of the CN line's components. On the assumption that the CN and CH CN-like widths are determined by a combination of small-scale turbulence and thermal broadening, we find temperatures and turbulent velocities (FWHM) of (340 ± 60 K, $0.6 \pm 0.1\ km\ s^{-1}$) and (80 ± 40 K, $0.5 \pm 0.2\ km\ s^{-1}$) for the components 1 and 2, respectively. The turbulent velocities are representative of values found in small molecular clouds from observations of millimeter lines (Myers 1983).

IV. MOLECULE FORMATION IN A SHOCK

Since the key reaction $C^+ + H_2 \rightarrow CH^+ + H$ is endothermic, interstellar CH^+ molecules are believed to be formed in hot gas behind shocks propagating through diffuse clouds (Elitzur and Watson 1978). OH production is controlled in part by an endothermic reaction ($O + H_2 \rightarrow OH + H$). For hydrodynamic shocks, the predicted ratio of column densities $N(OH)/N(CH^+) \approx 10$ (Elitzur and Watson 1980) is much greater than some observed ratios: $N(OH)/N(CH^+) \sim 1.7$ for ζ Oph (van Dishoeck and Black 1988). Production of OH is suppressed relative to CH^+ in magnetohyrodynamic (MHD) shocks where the ionized plasma may drift relative to the neutral gas (Draine 1980). The chemistry behind MHD *C*-shocks has been studied by Draine and colleagues (Draine and Katz 1986*a*, *b*; Draine 1986; Wardle and Draine 1987) and by Pineau des Forêts *et al.* (1986, 1987) and Monteiro *et al.* (1988). Quantitative differences between the two studies are due in part to differences in the reaction schemes and rates including the treatment of H_2 photodissociation (Flower *et al.* 1988).

Here, we test predictions of the velocities and profiles of CH and CH^+ lines from shocked gas. Predictions are taken from Draine and Katz (1986*a*, *b*) and Draine (1986). Predictions for a $10\ km\ s^{-1}$ shock show that the CH^+ profile is nearly Gaussian, but the CH profile is quite markedly non-Gaussian and appreciably broader than the CH^+ line. The former prediction is confirmed by our observations. Since the shock's contribution to the CH profile is blended with the narrower contributions from other sources, it is difficult to determine its profile. On the assumption that the profiles are Gaussian, observed line widths of CH and CH^+ are similar to those of the 10 km s^{-1} shock: $\Delta v(km\ s^{-1}) = 3.2$ (predicted) and 3.5 (observed) for CH^+ and $\Delta v = 5.7$ (predicted) and 5.2 (observed) for CH. The line widths (σ) are a combination of thermal (σ_T) and kinematic (σ_K) terms where $\sigma^2 = \sigma_T^2 + \sigma_k^2 \cos^2\theta$ and θ is the angle between the line of sight and the perpendicular to the shock front. Since σ(CH) is dominated by σ_k but the two components contribute about equally to $\sigma(CH^+)$, the ratio $\Delta v(CH)/\Delta v(CH^+)$ offers a means of measuring θ. Although predicted CH profiles are needed, comparison of the observed ratio and estimates of σ_k and σ_T suggest the ζ Oph shock is approximately perpendicular to the line of sight ($\theta \sim 0°$).

The CH and CH^+ lines from the shock are predicted to differ in radial velocity: $\Delta V = |V_{LSR}(CH^+) - V_{LSR}(CH)| \sim 3 \cos\theta\ km\ s^{-1}$, approximately independent of shock speed for those shocks that produce the necessary amount of CH^+. The sign of the velocity difference depends on the shock's direction: CH^+ is blueshifted relative to CH for shocks approaching the observer. The observed velocity difference of $\Delta V = -0.5$ km s^{-1} is in sharp disagreement with the prediction $\Delta V \sim 3$ km s^{-1} for $\cos\theta \sim 1$ implied by the line widths. Mere inspection of Figure 1 shows that the velocity of the CH component responsible for the broad wings cannot be displaced by as much as 3 km s^{-1}. This discrepancy may indicate that the ion-neutral drift velocities are smaller than predicted across the shock or that the CH molecules are formed preferentially for reasons of chemistry at the rear of the shock where the drift velocities are small, or that *C*-shocks are inappropriate.

Further tests of the *C*-shock models are possible if the preshock and cool postshock gas can be identified from among the several components identified in the optical absorption or radio emission lines. Crutcher's (1975) analysis of high-resolution profiles of the NaD lines (Hobbs 1969), the K I 7699 Å line (Hobbs 1974), and the Ca II K line (Marshall and Hobbs 1972) led to five velocity components at $V_{LSR} = -13.3$, -2.8, -0.3, $+1.8$, and $+4.5\ km\ s^{-1}$. Slightly different velocities were given by Hobbs (1973). The $-13.3\ km\ s^{-1}$ component is probably unrelated to the complex near $V_{LSR} = 0\ km\ s^{-1}$ (Frisch and York 1987). The $+1.8\ km\ s^{-1}$ component, which contains more ionized gas than either the $+4.5$ or $-2.8\ km\ s^{-1}$ components (Morton 1975), seems an unlikely candidate for either the post- or preshock gas.

The $-0.3\ km\ s^{-1}$ component which is the dominant contributor to the Na I, K I, CH, CN, CO, and other lines is generally identified with the cold compressed postshock gas (Elitzur and Watson 1980; Draine 1986). The CN, CH and CO profiles show that the $-0.3\ km\ s^{-1}$ component consists of two components. Identification of the $-0.3\ km\ s^{-1}$ component as single is based on observations of the K I line (Hobbs 1974), but these were at a resolution that was probably insufficient to resolve the line into two components separated by $1.2\ km\ s^{-1}$. Large-scale mapping in the CO $J = 2$–1 line around ζ Oph led Barrett, Solomon, and Mooney (1989) to suggest that the line of sight to ζ Oph intersects the overlapping edges of two molecular clouds. Then, the -0.8 and $+0.4\ km\ s^{-1}$ components identified in molecular lines and suspected in the neutral atomic lines may arise from quiescent gas in these molecular clouds and be unrelated to a shock. Certainly, our derived temperature and turbulent velocity for the two components are compatible with an identification with approximately normal molecular clouds.

Models of MHD shocks (Draine and Katz 1986*a*; Pineau des Forêts *et al.* 1986) show that the CH^+ and CH molecules are destroyed at the downstream edge of the shock. It has yet to be demonstrated that CH can be resynthesized in the postshock gas. The problem may be acute. In Draine's model of the

line of sight to ζ Oph, the dense postshock gas is followed by a photoionization front and the H II region around ζ Oph. In short, the postshock gas may not be revealed by molecular lines and is not necessarily to be identified with the −0.3 km s^{-1} component(s). Draine (1986) identifies the +4.5 km s^{-1} (+5.5 km s^{-1} in his paper) as preshock gas and the postshock gas with the −0.3 km s^{-1} (+0.4 km s^{-1} in his paper) component. His preferred model predicts $V_{LSR}(CH^+) = +0.6$ km s^{-1} and $V_{LSR}(CH) = +2.9$ km s^{-1} for a shock propagating toward the Sun at 9 km s^{-1} at an angle of 40° to the line of sight. These predicted velocities and their separation are in disagreement with our observations. We suggest that the postshock gas may be the −2.8 km s^{-1} component which contributes a strong NaD line. Then, for a shock directly along the line of sight, Draine's model predicts $V_{LSR}(CH^+) = -1.9$ km s^{-1} and $V_{LSR}(CH) = +1.1$ km s^{-1}. The agreement with the observed velocities is not improved, but optimization of the chemical reaction network, shock speed, structure, and inclination to the line of sight may lead to some improvement.

Van Dishoeck and Black (1988) draw attention to a common problem of the MHD shock models: they demand H_2/H ratios of near unity in the preshock gas, but H_2 molecules can only be shielded from photodissociation in relatively thick clouds, and, hence, it would seem that the preshock gas should be revealed by strong lines of Na I etc., but this is not observed in ζ Oph and other lines of sight. The region of the shock containing CH^+ and CH is so thick that it may subtend a large angle on the sky. At the distance (140 pc; Draine 1986) of ζ Oph, the molecule-rich region subtends 20″ (Draine and Katz 1986*a*) to 60″ (Pineau des Forêtes *et al.* 1986) for a shock transverse to the line of sight. Then, for modest angles of inclination, the line of sight is fed by a shock that is propagating into a molecular cloud over quite a broad front. Then a shock at a moderate angle to the line of sight can propagate into a region rich in H_2 molecules while the line of sight takes a short path through the cloud.

The relative abundances of CH and CH^+ are apparently accounted for by Draine's (1986) favored model for ζ Oph which predicts $N(CH)/N(CH^+) \simeq 0.3$ where the observed ratio is 0.35. The model predicts less CH^+ (by a factor of 2) than is observed. However, this prediction is based on an incorrect identification of the principal products from the photodissociation of CH^+ (Flower *et al.* 1988), and when corrected, the predicted CH^+ density is reduced such that it is a factor of 6 less than is observed. Monteiro *et al.* (1988), who discuss MHD shocks in which the previously neglected photodissociation of H_2 is taken into account, find that a model with a 9 km s^{-1} shock predicts quite well the observed rotational excitation of H_2 and the CH column density, but fails by a factor of 4 to predict sufficient CH^+. They conclude that "current MHD shock models do not enable the presence of a shock along the line of sight to ζ Oph to be convincingly demonstrated."

Our high-resolution spectra of the CN 3874 Å line shows that the CN molecules reside in the two quiescent clouds responsible for the CO emission. The CH^+ 4232 Å line has a broad Gaussian profile suggesting that it is formed in a shock. For the first time, we show that the CH line at 4300 Å is formed partly in the quiescent molecular clouds and partly in the shock. The latter component of the CH line is, as predicted, broader than the CH^+ line, but the predicted velocity difference between CH and CH^+ from the MHD shock is not observed. Furthermore, published models of MHD shocks appear unable to account for the observed column density of CH^+ without violating other observational constraints such as the CH and OH column densities and the rotational excitation of H_2 molecules.

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