

OPTICAL OBSERVATIONS RELATED TO THE MOLECULAR CHEMISTRY IN DIFFUSE INTERSTELLAR CLOUDS

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ABSTRACT. Observations, which have been published since 1979, of molecular species in diffuse clouds will be discussed. Particular attention will be given to the ultraviolet measurements of CO with the Copernicus and IUE satellites and to ground-based optical measurements of CH, CH⁺, CN, and C₂. These data encompass large enough samples to test the chemical schemes expected to occur in diffuse clouds. Upper limits for other species (e.g., H₂O, H₂O⁺, and C₃) place restrictions on the pathways for molecular production. Moreover, analysis of the rotational distribution of the C₂ molecule results in the determination of the physical conditions of the cloud. These parameters, including density, temperature, and the intensity of the radiation field, are necessary for modeling the chemistry.

I. INTRODUCTION

Many measurements of absorption at ultraviolet and optical wavelengths from interstellar species have been obtained in recent years. This review paper deals with observations that bear on the chemistry of interstellar clouds, particularly diffuse clouds, and that have been published since 1979. For results before 1979, Snow's (1980) presentation at Symposium No. 87 of the IAU on interstellar molecules is recommended. Recent analyses of the chemistry, which are based on the new data, are discussed elsewhere in this volume by John Black.

The remainder of the present review addresses observational surveys in Section II, upper limits that place a significant constraint on chemical models in Section III, and recent advances and future prospects in Section IV.

II. ULTRAVIOLET AND OPTICAL SURVEYS

Since 1979, several surveys of molecular absorption from CO, CH, CH⁺, CN, and C₂ in diffuse clouds have been completed. Because of the important role that molecular hydrogen plays in the chemical schemes

for molecules containing heavy elements, the present review is generally restricted to observations of lines of sight studied by the Copernicus satellite for H_2 absorption [$E(B-V) < 0.4$]. When only $E(B-V)$ is known, the fraction of gas in atomic or molecular form is difficult to ascertain; the amount of absorption from H_2 (preferably) and/or H I is needed for this purpose. The observations toward directions where only $E(B-V)$ is available (such as those discussed in Dickman et al. [1983] and Tarafdar [1983]) will be especially useful in the near future because the High Resolution Spectrometer on the Hubble Space Telescope may provide necessary data on molecular hydrogen. Data toward moderately reddened stars associated with molecular material are discussed in Section IV.

Ultraviolet results for CO have been obtained with the Copernicus satellite (Federman, et al. 1980; Snow and Jenkins 1980) and with the International Ultraviolet Explorer satellite (Black 1980; Tarafdar and Krishna Swamy 1982). The data toward χ Ophiuchi (Frisch 1980) has been included in Fig. 1, as has that toward X Persei (Lien et al. 1980).

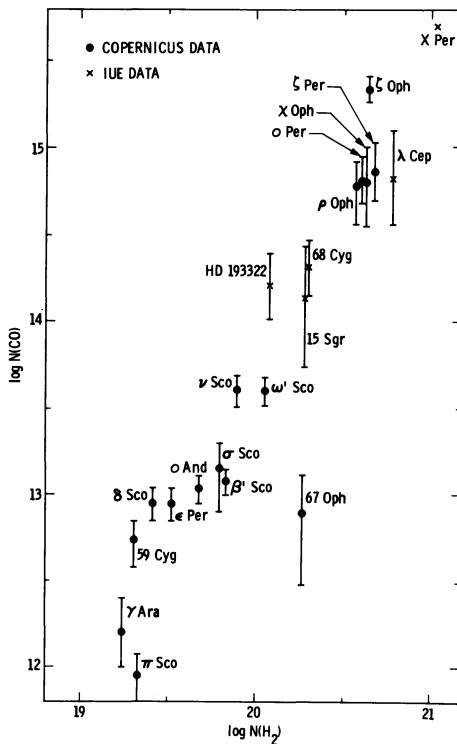


Figure 1. A log-log plot of the column density of CO versus the column density of H_2 . Directions with only an upper or lower limit on $N(CO)$ are not shown.

These data are plotted as column densities $N(\text{CO})$ against the column densities of H_2 , $N(\text{H}_2)$. This figure illustrates that $N(\text{CO})$ varies with $N(\text{H}_2)$ roughly linearly, but at most quadratically, as first pointed out by Federman et al. (1980). The dependence on $N(\text{H}_2)$ provides an understanding of the chemistry (see below). The data from the IUE satellite fills in the gap in $N(\text{CO})$ at 10^{14} cm^{-2} found in the similar figure of Federman et al. (1980), and the trend does not show a break, as suggested by these authors. A break in the trend could signify an alteration in the chemical processes for the gas phase scheme, such as a different production or destruction route. Also note that the data compiled in Fig. 1 are for several transitions of CO (A-X, B-X, C-X, and E-X), thus indicating that a consistent set of oscillator strengths have been chosen for interpreting the data.

Two recent publications dealing with CH observations at 4300 \AA are those by Federman (1982a) for directions predominantly in the Northern Hemisphere and by Danks, Federman, and Lambert (1984) for directions mainly in the Southern Hemisphere. The combined set of measurements, which were acquired with Reticon detectors, introduce little dispersion among the values of $N(\text{CH})$ for a given $N(\text{H}_2)$, thereby showing the inherent stability and reproducibility of photoelectric detectors. The column density of CH varies linearly with that of H_2 , as expected from the gas phase chemical models (Danks, et al. 1984).

The linear dependence of CH with H_2 is a consequence of the predominance of photochemistry in diffuse clouds; for each stage of the chemistry for neutral molecules, another factor of density (n) and optical depth [$\exp(\tau)$] enters into the chemical rate equation. The CH radical is the first neutral carbon molecule formed in the chemical scheme (a first stage molecule) and thus varies linearly with H_2 . Similar arguments apply to the roughly quadratic variation of CO with H_2 (i.e., CO forms via reactions involving the neutral molecule OH - CO is a second stage molecule), as well as the cubic dependence of CN on H_2 ($\text{CH} \rightarrow \text{C}_2 \rightarrow \text{CN}$). The data for C_2 does not span a large enough range in $N(\text{H}_2)$ to test any correspondence with H_2 ; the models predict a quadratic dependence.

Because the absorption lines are weaker for CN and C_2 (equivalent widths $W_\lambda \leq 1 \text{ m\AA}$), the amount of data is somewhat limited at this time. Much of the existing data were obtained with photoelectric detectors. The most comprehensive survey of CN near 3875 \AA at present is that of Federman, Danks, and Lambert (1984). They found that $N(\text{CN})$ varies as the third power of $N(\text{H}_2)$. This observational result is consistent with the models of gas phase chemistry which show that CN forms during the third stage of the chemical networks. For C_2 , two recent surveys (Danks and Lambert 1983; van Dishoeck and de Zeeuw 1984) supplement the data for several individual lines of sight (Hobbs 1981 for α Persei; Hobbs 1979 and Chaffee et al. 1980 for ζ Persei; Hobbs and Campbell 1982 for ζ Ophiuchi). The above measurements were of the 2-0 Phillips band at $\lambda 8760$; Lien (1985) measured absorption from the F - X transition toward X Persei with the IUE satellite. These molecular carbon data only sample clouds with $N(\text{H}_2) \sim 4 \times 10^{20} \text{ cm}^{-2}$ and, therefore, are of limited value in analyzing the gas phase chemistry. Because the

column density of C_2 in rotational levels with $J > 10$ has been measured, C_2 has proven to be an excellent means of determining the physical conditions within the diffuse cloud, such as density, temperature, and radiation field intensity (cf. van Dishoeck and Black 1982). The physical conditions are necessary parameters for accurate chemical modeling of the clouds.

Although the steady-state gas phase models of the chemistry in diffuse clouds reproduce the trends seen in data for CO, CH, and CN, as well as the total amounts of these molecules and C_2 for a given $N(H_2)$, the models fail with CH^+ . Elitzur and Watson (1978; 1980) suggested that shocks may play a role in the formation of CH^+ by allowing the endothermic reaction $C^+ + H_2 \rightarrow CH^+ + H$ to proceed at the elevated temperatures behind the shock. Federman (1980; 1982a,b) showed that CH^+ data verify the consequences of the model involving shocks. These consequences are 1) that there is a shift in the velocity of line center between CH^+ and CH because the two molecules form in different parts of the flow and 2) that $W_\lambda(CH^+)$ is proportional to both the amount of shift in velocity and the Doppler parameter of the CH^+ line because these indicate the temperature of the shocked gas. Federman (1982a) showed that approximately half the lines of sight that he studied showed evidence for the shift in velocity. Figure 2 amplifies that fact by showing all the available data relating to the

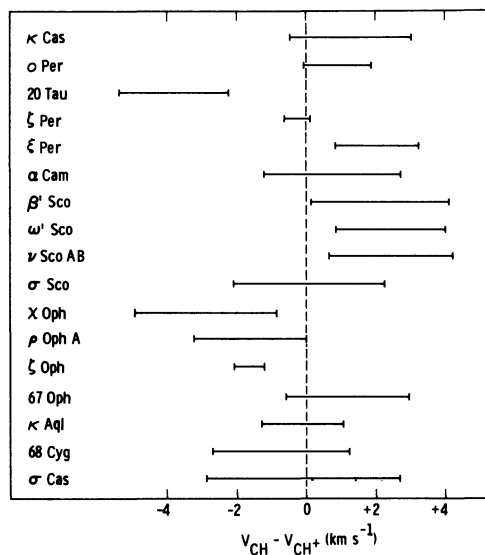


Figure 2. The differences in the velocity at line center for CH and CH^+ . The rest wavelength of Carrington and Ramsay (1982) for CH^+ has been used.

shift in velocity, including the data of Chaffee (1975) for ρ Ophiuchi A and ζ Ophiuchi and of Frisch (1979) for χ Ophiuchi. These data use the most recent determination of the wavelength for the CH^+ line at 4243.548 \AA (Carrington and Ramsay 1982).

As an alternative to shocks producing the required temperatures, White (1984) suggested that the CH^+ formed near the Pleiades through the high temperatures resulting from enhanced photoelectric heating and molecular hydrogen dissociation. His results are based on the fact that the interstellar gas near the Pleiades is quite close to the stars (cf. Jura 1977; Federman 1982b). Most recently, Danks and Lambert (1985) have shown that $N(\text{CH}^+)$ has the strongest correlation with the column density of the upper rotational levels of H_2 , a result first suggested by Frisch and Jura (1980). The results of Danks and Lambert (1985) are the strongest evidence that CH^+ is produced in gas with high temperatures; the cause of the elevated temperatures is not clear for all the observed directions, however.

III. UPPER LIMITS

Upper limits are of importance because they can place constraints on the chemical models. Smith and Snow (1979) set upper limits to the amount of H_2O toward several lines of sight with data taken with the Copernicus satellite. They compared the results with the amount of OH measured at ultraviolet wavelengths. The results are consistent with gas phase schemes involving ion-molecule reactions. In particular, H_2O is less than 10% of OH, indicating that OH preferentially forms from the dissociative recombination of H_3O^+ (Herbst 1978). Another way of testing the oxygen-based chemistry is by searching for intermediate species in the network. Smith, Schempp, and Federman (1984) set upper limits to the amount of absorption from the A - X electronic transition of H_2O^+ for several directions. The most stringent limits were set for the gas toward ζ Ophiuchi; the data are consistent with the predictions of the ion-molecule schemes. Federman and Trauger (1985, unpublished) have reduced the upper limit toward ζ Oph by a factor of 4 ($W_\lambda \leq 0.05 \text{ m\AA}$ [3σ]). The $N(\text{H}_2\text{O}^+)$ is less than $3 \times 10^{11} \text{ cm}^{-2}$. This limit is interesting because the chemical models require approximately this much H_2O^+ to reproduce the observed amount of OH; a second source of OH may therefore be necessary. The shock chemistry that reproduces the observed abundance of CH^+ probably produces the additional OH through the endothermic reaction $\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$. Accurate velocities for the OH absorption are needed to verify this hypothesis.

Clegg and Lambert (1982) obtained upper limits for C_3 from measurements of $\lambda 4050$ in several diffuse clouds, including ζ Per and ζ Oph. Their limits for the cloud toward ζ Oph are consistent with chemical models [$N(\text{C}_3) < 0.1 N(\text{C}_2)$], although the photodissociation rate has not been measured for C_3 .

IV. RECENT ADVANCES AND FUTURE PROSPECTS

During the last couple of years results utilizing modern photoelectric detectors (Reticons; CCDs; etc.) and improved spectrometers have been published. One exciting area of current research is the measurement of weak absorption lines, especially from moderately reddened directions associated with molecular material. For example, Hobbs, Black, and van Dishoeck (1983) and Lutz and Crutcher (1983) have obtained C_2 spectra toward several stars, including HD 29647 which is behind the outer envelope of the Taurus Molecular Cloud - 1 (TMC1). These authors find that the lowest rotational levels of C_2 have excitation temperatures significantly lower than the excitation temperatures toward less reddened stars. Additional ways of utilizing data from weak lines have been reported. Meyer and Jura (1984;1985) have determined the temperature of the cosmic background radiation at millimeter wavelengths through measurements of the three lowest rotational levels of CN; they found a temperature of 2.7 K. Hawkins, Jura, and Meyer (1985) determined the $^{13}C/^{12}C$ ratio toward ζ Oph from measurements of CH^+ and found a ratio (~ 45) consistent with that determined from UV observations of CO using the Copernicus and IUE satellites (Wannier, Penzias, and Jenkins 1982). Vanden Bout and Snell (1980), however, found a slightly larger ratio (~ 75) from CH^+ measurements. The differences between the two CH^+ measurements are attributed to the different Doppler parameters used to determine the amount of saturation and the slight differences in the measured equivalent widths. Other studies have been reported of the measurements of absorption lines below 4000\AA for stars in Taurus (HD 29647, Crutcher 1985) and Ophiuchus (e.g., HD 147889, Crutcher and Chu 1985; Cardelli and Wallerstein 1985). Through estimates of the amount of H_2 in the gas toward the stars in Ophiuchus, Cardelli and Wallerstein found that the linearity between $N(CH)$ and $N(H_2)$ continues for $N(H_2) > 10^{21} \text{ cm}^{-2}$, while the cubic relationship between $N(CN)$ and $N(H_2)$ becomes less steep for the moderately reddened lines of sight. The results of Cardelli and Wallerstein are consistent with gas phase models of the chemistry because chemical destruction terms play an increasingly important role for moderately reddened lines of sight. Since the CH radical is produced during the first stage of chemical processing, it is expected to be less sensitive to the chemical destruction terms. (CN is formed during the third stage.) Moreover, Crutcher and Lutz (1985) and van Dishoeck and Black (1985) have used the red sensitivity of silicon photoelectric detectors to obtain interstellar spectra of the Red System of CN near $\lambda 9140$ and $\lambda 7900$, respectively, toward highly reddened stars ($A_V \leq 7 \text{ mag.}$). Previously, only the Violet System near $\lambda 3875$ had been observed in interstellar gas.

At least three exciting avenues for future research in the ultraviolet and visible portions of the spectrum can be enumerated. One involves using optical techniques to study the composition of molecular clouds, as is evident from some the results recently published. Another involves the High Resolution Spectrometer (HRS) on the Hubble Space Telescope. This instrument will have the resolving powers similar or better than the spectrometer onboard the Copernicus

satellite and will be used to measure absorption lines toward stars fainter than was possible with either the Copernicus satellite or the IUE satellite. The HRS will be capable of measuring absorption lines, for example, from H₂, as well as H₂O and OH for studies of the chemistry of oxygen-bearing species. Last, the improved sensitivity of detectors will enable measurements of very weak lines.

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DISCUSSION

GUELIN: Can you make some comments about the connection between CO vs A_V relation in the diffuse clouds and in envelopes of dense clouds as obtained from radio observations?

FEDERMAN: In diffuse clouds with $A_V < 1$, one has to be a bit careful, as there is a lot of gas in atomic form which does not play any role in the chemistry. But when you get to $A_V > 1$, especially $A_V > 2$, there is probably very nearly direct correspondence between A_V and H_2 and so the trend should continue to what I showed; it might be a bit more steep as you get to more reddened line, but the trend should continue.

JACKSON: The oscillator strength of the CN red system is now well determined. I have made lifetime measurements on the $v' = 0$ level of the $A^2\Pi$ state and T. Slander has made measurements on the $v' = 1$ to 7 levels. The observed lifetimes agree with the ab initio calculations from Sweden.

WILLIAMS: I refer to your definition of 1st, 2nd and 3rd stage molecules. The observations are concerned with column densities, whereas your explanation is given in terms of local density. Does this mean that in your view, local and column densities are related?

FEDERMAN: My diffuse cloud models, which include thermodynamic balance, indicate density and temperature gradients. The difference between surface and core is only a factor of 2 or 3; thus, local and column densities may be equated to a good approximation.

IRVINE: What does recent data show on the $^{13}\text{C}/^{12}\text{C}$ ratio in diffuse clouds?

JURA: Isabel Hawkins has essentially finished her Ph.D. thesis of obtaining spectra of CH^+ absorption lines with the Reticon detector at the coude focus of the Lick Observatory 120" telescope. For 5 stars, the results indicate that $n(^{12}\text{CH}^+)/n(^{13}\text{CH}^+)$ is between 40 and 45. This indicates that $[^{12}\text{C}]/[^{13}\text{C}]$ is also between 40 and 45.

PANDE: Have any attempts been made to determine the turbulent velocity fields and kinetic temperatures from the line profiles of various species observed by you in molecular clouds?

FEDERMAN: The thermal width of absorption lines from molecules in diffuse clouds is about 1 km s^{-1} . The observations show wider lines, but the source of the additional width is not known.