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CHEMISTRY AND SMALL-SCALE STRUCTURE OF DIFFUSE AND TRANSLUCENT CLOUDS

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Abstract. The small, thin diffuse and translucent molecular clouds are excellent laboratories for studying the ways in which small-scale structure and interstellar chemistry affect each other. Variations of density or column density and chemical stratification can be found on scales as small as 0.01 pc. The origin of such structures and the evolutionary states of small clouds remain elusive.

Keywords : interstellar chemistry; molecular clouds

1. Introduction

Diffuse and translucent molecular clouds present special advantages for the investigation of the coupling between interstellar chemistry and small-scale structure in interstellar clouds. They also represent important test cases for developing theoretical tools needed to characterize the chemistry in larger, denser, star-forming regions. By diffuse clouds, we mean regions with line-of-sight visual extinction of $A_V \approx 1$ mag or less. The translucent clouds have $A_V \approx 1-5$ mag and often possess substantial abundances of various molecules. Both types of clouds are thin enough to be observed by means of optical absorption lines superimposed on the spectra of background stars, but thick enough in many cases to show detectable emission lines of molecules like CO at mm and sub-mm wavelengths. Typically the diffuse and translucent clouds are not directly involved in star formation. Many of these clouds are quite nearby, with fairly well determined distances $D \approx 50-200$ pc, so that rather small linear scales are resolvable in emission lines. For example, a 30'' antenna beam corresponds to 6000 AU (0.03 pc) at $D = 200$ pc. Absorption line measurements sample an even smaller scale dictated by the angular size of the background star : e.g., a star of radius $10 R_\odot$ at 500 pc isolates a cylinder through a

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cloud that is 0.04 AU across for a cloud distance of $D = 200$ pc. While the velocity resolution of radio measurements may routinely be 0.1 km s^{-1} , that of the optical spectra is rarely better than 3 km s^{-1} . This also raises basic questions about what is meant by an interstellar “cloud” : usually, a cloud is defined as a distinct velocity component. Counting the number of “clouds” along the line of sight may thus be seriously limited by instrumental resolution at optical wavelengths. In principle, the complementary information provided by radio and optical measurements may permit theories of molecule formation to be tested rigorously at the level of a factor of 2 or better in abundances. In practice, the interpretation can be complicated by subtle effects of small-scale structure. However, given enough observational information, we may be able to use the chemical information for indirect analyses of the internal structure.

The empirical definitions of diffuse and translucent clouds in terms of thickness (column density or extinction) allow quite different phenomena to be included in the same categories : small, isolated clouds; surface layers of giant molecular clouds; and high-latitude molecular clouds, for example. Translucent clouds are characterized by total hydrogen column densities $N_H \geq 10^{21} \text{ cm}^{-2}$. There may be a variety of origins and evolutionary states represented, which range from dissipating fragments of previous large clouds, to condensing pieces that are forming new larger structures. One unifying property is that ultraviolet starlight is likely to play an important role in the chemistry and thermal balance of all these clouds. Thus, translucent clouds embody most of the features that one expects in photodissociation regions (PDRs) in star-forming complexes where a molecular cloud surface is scorched by intense ultraviolet light from hot, young stars nearby (cf. Tielens and Hollenbach 1985), except that the ultraviolet fluxes and gas densities are typically lower. It is important to recognize that chemical stratification is a form of internal structure that can affect the thermal properties of the matter and that can sometimes mask physical stratification (variations in density and temperature).

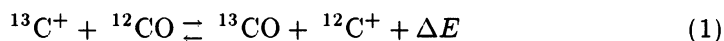
Owing to the deluge of new observational results, only recent results will be reviewed here. Langer (1990) has discussed velocity and density structure in diffuse clouds. Reviews of the chemistry of diffuse and translucent clouds include Dalgarno (1988), van Dishoeck and Black (1988a), and van Dishoeck (1990a,b).

2. Chemical Structure

The basic *chemical* structure of a small molecular cloud is thought to be governed by the processes that form and destroy the hydrogen molecule. Until a large fraction of the hydrogen is in the form of H_2 , very little molecular formation involving other elements can occur. H_2 molecules exposed to the general Galactic background of ultraviolet starlight are readily photodissociated on a time scale of the order of 10^3 years. The most efficient formation mechanism of H_2 , association of H atoms on grain surfaces, is still slow in absolute terms, and the molecular fraction, $f = 2n(\text{H}_2)/n_H$, in unshielded regions will usually be very low. Because

the photodissociation of H_2 is initiated by line absorptions (P. M. Solomon, as reported by Field *et al.* 1966), which begin to saturate at column densities as low as $N(H_2) \approx 10^{14} \text{ cm}^{-2}$, the molecules deeper into a cloud “feel” fewer line-core photons than do those near the boundary where the highest rates of absorption and dissociation occur. This effect is called *self-shielding* and has been described by Stecher and Williams (1967) and Federman *et al.* (1979). The line absorptions in H_2 are even more likely to lead to fluorescent excitation than dissociation (by a ratio of $\approx 6/1$), so that the destruction rate and abundance of H_2 are intimately linked to its excitation. A result of the depth-dependent balance between formation and destruction of H_2 is that the H_2/H abundance ratio varies over orders of magnitude through a diffuse or translucent cloud and the mean molecular weight, by approximately a factor of two. Detailed depth-dependent models of the excitation and abundance of H_2 in such clouds have been constructed by van Dishoeck and Black (1986) and Viala (1986). The transition from a fully atomic composition ($H/H_2 \gg 1$) to a largely molecular gas ($H/H_2 \leq 1$) is predicted to occur at an extinction $\Delta A_V \approx 0.1$ into a diffuse cloud (mean density \approx a few hundred cm^{-3}). This is substantiated by ultraviolet absorption observations of H_2 in diffuse clouds (Spitzer and Jenkins 1975, especially their Figure 4).

Carbon monoxide is one of the few other molecules whose abundance is limited by self-shielding ultraviolet line absorptions. Thus its abundance tends to be significant only when its column density exceeds the threshold for effective shielding. This threshold is only somewhat lower than the minimum column density for detection of its mm-wavelength emission lines. Because the abundances of carbon and oxygen in the interstellar gas are almost 10^4 times smaller than that of hydrogen, extinction by dust and absorption by overlapping lines of H_2 play a more important role in shielding the CO than does the dust in shielding the H_2 . The dissociating lines of CO are intrinsically broader than those of H_2 so that their natural widths may dominate their line broadening in the interstellar medium and thus lead to a less sharp transition layer than for H_2 . According to gas-phase theories of interstellar chemistry, CO arises from the basic oxygen cycle that generates OH, H_2O , and related ions, which react with carbon atoms or ions to produce CO^+ , HCO^+ , and CO; and from reactions that form simple hydrocarbons and hydrocarbon ions, CH , CH_2 , CH_3 , CH_2^+ , CH_3^+ , etc., which then react with oxygen to form HCO^+ and CO. The various isotopic varieties of CO can form similarly, but there is an additional, temperature-sensitive exchange reaction,



which enriches ^{13}C in ^{13}CO at low temperatures, because $\Delta E/k \approx 36 \text{ K}$. The photodissociation of CO is also partly isotope-selective (Bally and Langer 1982, Glassgold *et al.* 1985, van Dishoeck and Black 1988b). Thus we expect the $^{12}CO/^{13}CO$ abundance ratio to vary with depth through a cloud, following the growth of attenuation of ultraviolet starlight and responding to any gradients in temperature.

Figures 11 and 12 of van Dishoeck and Black (1988) illustrate the depth-dependent variations of abundances of the isotopic varieties of CO in model clouds: the fractionation effects described above are significant at extinctions $\Delta A_V = 0.5 - 1$ mag, but depend sensitively on such parameters as the total density, the overall gas-phase carbon abundance, and the intensity of ultraviolet starlight. The growth of the total CO abundance is also sensitive to these parameters and is a steep function of depth. These effects emphasize the apparent structure in CO emission line maps: e.g., a 20% increase in H₂ column density can produce a factor of 2–3 increase in the column density of CO. If, in addition, there is a gradient in the density $n(\text{H}_2)$, the observable CO line intensity can be enhanced far out of proportion to the variations in density alone. Because the CO in translucent clouds is often just at the thresholds both of self-shielding and of detectable rotational line emission, it is very difficult to infer variations in physical parameters from apparent fluctuations in measurable intensities.

The reason for reviewing briefly this gas-phase chemistry is to reinforce the expectation that especially the small diffuse and translucent clouds are chemically stratified. Moreover, this chemical stratification is a form of small-scale internal structure, particularly as regards the abundances and excitation of molecules like ¹²CO and ¹³CO that are commonly used to trace the extent and internal structure of molecular clouds. Note also that this chemistry governs the abundances of the principal forms of carbon: C⁺, C, and CO, which are major coolants of the gas and which include the major electron donor and a dominant ion, C⁺. A thorough understanding of the chemistry and its variation with position inside a cloud is thus necessary for a complete description of the thermal properties of the gas (major coolants) and the coupling of the gas to magnetic fields (dominant ions and sources of electrons).

The identity of the principal ion and the coupling of gas, dust, and magnetic fields may be complicated by the chemical effects of large molecules such as polycyclic aromatic hydrocarbons (PAHs). These large molecules are probably very effective at capturing electrons and at neutralizing a variety of positive ions (Omont 1986; Lepp and Dalgarno 1988). In dense, dark clouds, the negative ion, e.g. PAH⁻, may be the most abundant charged species. Even in diffuse clouds, it will affect the atomic ionization balance measurably (Lepp *et al.* 1988), if the interstellar PAH abundance is 1–10% of the total carbon. In the absence of PAHs, the principal ions would tend to be C⁺, H⁺, H₃⁺, HCO⁺, H₃O⁺, etc., which all have charge/mass ratios at least 10 times larger than that of a 50-atom PAH⁻ ion. The consequences of a high abundance of charged, large molecules like PAH⁻ for coupling of gas to magnetic fields merit further consideration. The effects of PAHs on the chemistry and propagation of MHD shock waves in molecular clouds have been considered recently by Pineau des Forêts, Flower, and Dalgarno (1988) and Flower, Heck, and Pineau des Forêts (1989).

There are some fundamental, unresolved questions already lurking behind the facile discussion above. It is conventionally assumed that chemical abundances

in diffuse and translucent clouds are in steady state. Is this a good assumption? It was pointed out above that an important limiting time-scale is the lifetime of H_2 , which is only $\approx 10^3$ y at a typical cloud boundary; however, the effect of self-shielding can lengthen this to 10^7 y in the center of a diffuse cloud. The lifetime of a hydrogen atom against catalysis on a grain surface to form H_2 can also be long: $10^7(30/T)^{1/2}(200/n_H)$ y, where T and n_H are the kinetic temperature and total density of hydrogen nuclei, respectively. This latter chemical time-scale is comparable to the sound-crossing time for a cloud of total thickness $A_V \approx 1$ mag: $5 \times 10^6 A_V(30/T)^{1/2}(200/n_H)$ y. These estimates suggest that chemical time-scales involving the dominant species can be long compared with relevant dynamical, evolutionary scales. However, once the H_2 abundance even approaches its steady-state value, most other molecular abundances rapidly achieve steady state on time scales of $10^3 - 10^4$ years. Wagenblast and Hartquist (1988, 1989) have considered time-dependent effects on the abundance and excitation of H_2 in diffuse clouds. Tarafdar *et al.* (1985) have performed elaborate computations of the combined chemical and dynamical evolution of diffuse clouds, but have started from the presumption that diffuse structures collapse to form denser clouds. In all cases, time-dependent effects on structure and chemistry and their consequences for the evolution of small clouds are just beginning to be explored in detail. It seems obvious that initial conditions must affect the future development of these structures, but it is not so clear that observable properties can provide clues to what those initial conditions were.

Some observations of translucent (cf. Jannuzi *et al.* 1988), high-latitude (Maganani, Blitz, and Mundy 1985; Keto and Myers 1986), and tiny (Knapp and Bowers 1988) molecular clouds indicate that the masses are too small for these clouds to be in virial equilibrium given their apparent sizes and velocity dispersions. The implications are that gravity does not completely control their structure and that they may be subject to rapid dissipation or other structural changes. Some observed features of the high-latitude clouds may have a natural explanation in terms of collisions between cloud condensations (Keto and Lattanzio 1989).

Even complicated theoretical models often make embarrassingly simple assumptions about the velocity field and about variations of density and temperature. Plane-parallel slabs or spheres with uniform (or uniformly varying) physical parameters are most common. How much difference does it make to our theoretical description of a cloud if, for example, it is filamentary with a turbulent velocity field and a non-Gaussian, high-velocity kinematic component? The chemical effects of "hot" atoms and ions (i.e., those with excess kinetic energy compared with mean thermal values) have been investigated in a few cases (Adams *et al.* 1984; Yee *et al.* 1987; Brown *et al.* 1990), but only in the microscopic sense in which the excess translational energy results from specific chemical reactions. The high abundance of widespread CH^+ in diffuse clouds remains a puzzle for interstellar chemistry, in part because C^+ ions do not react directly with H_2 unless they have excess translational energy of 0.4 eV or more. It should be noted that if a fraction 10^{-8} of all

C^+ in a diffuse cloud were translationally “hot”, then the CH^+ abundance could be explained. It seems not completely unreasonable that a macroscopic component of hot atoms and molecules might exist in molecular clouds, especially in view of the observational evidence of intermittent turbulence on all scales (Falgarone and Phillips 1990). Whether or not such a hot component could affect observable abundances has not been explored yet. One way in which the turbulence could be chemically important is through mixing of dense and dilute gas (Boland and de Jong 1982, Chièze and Pineau des Forêts 1989).

This consideration raises another fundamental question : at what scale do microscopic and macroscopic phenomena overlap? This may be of practical importance if the characteristic scale of overlap is large enough to have observable effects. Almost all descriptions of chemical reaction rates in the interstellar medium assume Maxwellian velocity distributions and corresponding thermal reaction rate coefficients : for this assumption to be valid, particle motions must be able to be thermalized on a small, microscopic length scale. Consider, for example, the thermalization of photoelectrons in a diffuse cloud. The mean excess kinetic energy of the electron produced by



is $\langle E \rangle = 0.87 \text{ eV} \gg kT$ in typical Galactic starlight. These electrons lose energy and become thermalized in collisions with thermal electrons and with abundant neutrals like H and H_2 . At the densities $n(e) \approx 0.1$ and $n(H_2) \approx 300\text{--}1000 \text{ cm}^{-3}$ characteristic of translucent clouds (Black and van Dishoeck 1990), the thermalization time and corresponding mean-free path are $\approx 10^5 \text{ s}$ and $10^{12} - 10^{13} \text{ cm}$, respectively. This suggests that one cannot assume an ensemble of interstellar electrons to be fully thermalized on scales much smaller than 1 AU. If intermittent turbulent motions persist to such scales, they may add to the complexity of non-Maxwellian tails in the “microscopic” speed distributions. Similarly, highly reactive positive ions may always be more likely to undergo reactions before suffering enough elastic encounters to become thermalized.

The standard chemical models have been tested against detailed observations of specific lines of sight, such as the classical diffuse cloud toward ζ Oph. In general, it is found that the abundances of molecules like CH, CN, C_2 and CO are consistent with the quiescent gas-phase chemistry, but that CH^+ is most likely formed as a result of a MHD shock propagating into the cloud. An important recent advance has been the achievement of 0.5 km s^{-1} resolution in observations of the molecular absorption lines of CH, CH^+ , and CN toward ζ Oph (Lambert, Sheffer, and Crane 1990), which permit *direct* tests of the relative importance of MHD shocks and quiescent chemistry : surprisingly, not only the CH^+ , but also part of the CH may be produced in a (shock-)heated layer. There are many ways in which small-scale structures and chemistry can affect each other through the propagation of MHD shocks in predominantly neutral clouds. There is by now a vast literature on this subject, a review of which is beyond the scope of this paper (see reviews of

Draine 1987, and Hartquist *et al.* 1990). Such shocks have been suggested to play a major role in the chemistry of high-latitude clouds (Magnani, Blitz and Wouterloot 1988), but little observational evidence has been found to support this picture (de Vries and van Dishoeck 1988; Magnani and Siskind 1990, Penprase *et al.* 1990). In general, the chemistry in high-latitude clouds resembles very much that found in translucent clouds.

3. Observations and Interpretations

The small-scale structure of diffuse and translucent clouds can be revealed by high-resolution spatial and/or spectral observations. Recent observations of molecular absorption lines at optical wavelengths with velocity resolutions of 0.5–3.0 km s⁻¹ have revealed much more complicated distributions of cloud components than was previously recognized (Jenkins *et al.* 1989; Lambert *et al.* 1990): several components spaced less than 1 km s⁻¹ are found in some cases, whereas weak components with nearly thermal line widths have been revealed in others. Such studies have been complemented by improved measurements of atomic constituents in many of the same clouds (e.g., Joseph and Jenkins 1990; Hobbs and Welty 1990). Emission line studies of diffuse and translucent clouds at mm/submm wavelengths have exposed complicated structures both on the plane of the sky and in radial velocity (e.g., Langer *et al.* 1987; Crutcher and Federman 1987; LeBourlot *et al.* 1989; Jannuzi *et al.* 1988; Magnani *et al.* 1985, 1990; Keto and Myers 1986; Knapp and Bowers 1988; van Dishoeck *et al.* 1991; Gredel *et al.* 1991). These measurements have spawned efforts to improve the interpretation and theoretical modeling (e.g., Jannuzi *et al.* 1988; van Dishoeck *et al.* 1991) and to refine the treatment of spectroscopic data in cases where intrinsic blending occurs at the same scale as astronomical velocity structure (Black and van Dishoeck 1988). It is important to note that optical absorption line measurements are much more sensitive to *very small* column densities ($N(\text{H}_2) \approx 10^{14} \text{ cm}^{-2}$) and thus can reveal a more diffuse, atomic component along the line of sight, whereas mm observations are limited to clouds with $N(\text{H}_2) \gtrsim 5 \times 10^{20} \text{ cm}^{-2}$.

Similar structure has been seen at the level of 0.02 pc in a molecular cloud of relatively low average column density by Falgarone and Pérault (1988). They interpret small-scale fluctuations in intensity of CO line emission as fluctuations of density. These fluctuations appear to be correlated in both space and velocity and, according to Falgarone and Pérault, are related to the turbulent velocity field of the cloud.

A recent study of the high-latitude translucent cloud toward HD 210121 (Gredel *et al.* 1991) also reveals considerable structure on both small and large scales, as shown in Figure 1. This contour map of peak antenna temperature in CO $J = 1-0$ displays several prominent peaks and small-scale brightness fluctuations within them, very sharp boundaries (notably along the southwestern edge), and large contrasts in brightness between the peaks and the large interior regions of weak

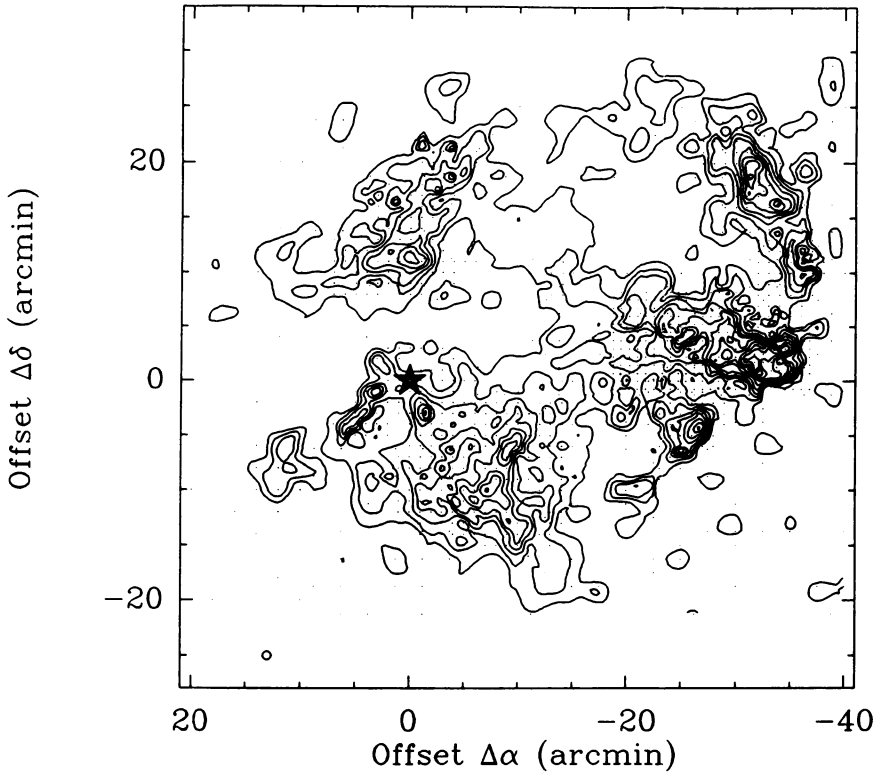


Fig. 1. Map of the peak T_A^* in $^{12}\text{CO } J=1-0$ in the high-latitude translucent cloud toward the star HD 210121. The lowest contour is $T_A^*=1$ K, and the increment between subsequent contours is 0.5 K. Map coordinates are offsets in arcmin from the star (from Gredel *et al.* 1991).

emission. Measurements of intensities of different lines have been used to estimate densities, temperatures, and abundances in parts of this cloud. The cloud appears to occupy an interesting regime of parameter space in which the abundance of CO has begun to be significant, but in which most of the carbon is still in atomic form. As discussed above, this is just the circumstance in which small variations in local conditions (e.g. density or total hydrogen column density) can produce very large fluctuations in line-of-sight CO column density (and hence in observable CO line intensity). Therefore, Gredel *et al.* suggest that much of the apparent small-scale structure in this cloud reflects fluctuations in line-of-sight column density of CO, rather than large variations in density, since no significant differences in molecular excitation are found between various positions in the cloud. On the other hand, weak evidence is found for a small density gradient across one clump from observed variations in the CO excitation. As a general conclusion, it is not trivial to distinguish density variations from variations in other properties, since in

the diffuse and translucent clouds, large fluctuations in observable intensities can result from small changes in physical properties.

Another method of finding small-scale structure involves the use of background stars in resolvable binaries (Meyer 1990) or in globular clusters (Bates *et al.* 1990, Langer *et al.* 1990) to map variations in interstellar absorption lines on angular scales of the order of arcseconds. Toward one nearby binary system, Meyer (1990) finds evidence of interstellar structure on scales less than 2000 AU. It is perhaps even more significant that Meyer finds no evidence of such structure in 5 other lines of sight. Some observational evidence exists for structures as small as 10^{14} – 10^{15} cm in the general interstellar medium (Fiedler *et al.* 1987, Diamond *et al.* 1989) based on interferometric measurements of radio sources at centimeter wavelengths.

Complementary optical and radio observations of molecular clouds have been discussed by Crutcher (1985), Crutcher and Chu (1985), Jannuzi *et al.* (1988), van Dishoeck and Black (1989), van Dishoeck *et al.* (1991), and Gredel *et al.* (1991) among others. In simplest terms, the optical absorption line measurements provide one-dimensional information through a narrow cylinder of matter along the line of sight to a well placed background star. Species with weak lines, e.g. C₂, show little or no effect of saturation; therefore, the column densities are directly proportional to measured equivalent widths (integrated intensities). A more complicated curve-of-growth analysis is required to interpret strong, saturated absorption lines like those of CN. On the other hand, emission line measurements typically refer to 30''–60'' antenna beams that average over all smaller-scale structure. In the case of CO lines, the beam-averaging is often non-linear in the sense that the lines are saturated and the radiative transfer within the cloud is, in principle, non-local. Recent observations of C₂ absorption and CO emission in the same translucent clouds yield somewhat discordant results for the densities that partly control the rotational excitation in both species (van Dishoeck *et al.* 1991). Intensity ratios for 3 transitions of ¹²CO and 1 transition of ¹³CO suggest hydrogen densities of the order of 10^3 cm⁻³ that are systematically higher than those, 200–500 cm⁻³, indicated by the measured rotational populations of C₂. There are several possible explanations. One is chemical stratification: the CO and C₂ may be distributed differently with respect to gradients of density and temperature. A second lies in the distribution of density fluctuations with respect to the quite different effective "beam sizes" of the absorption and emission measurements. A third possibility is that the treatment of the CO line formation has not been sophisticated enough to represent correctly the nature of the velocity field and small-scale density fluctuations. In order to characterize the possible effects of chemical stratification, chemical models were constructed in which density and temperature were allowed to vary in discrete steps subject only to observational constraints on total column densities (van Dishoeck *et al.* 1991). It was found that the hydrogen density, weighted by the distribution of CO could be several times larger than the density weighted by the distribution of C₂ along a line of sight through the model, but only when ultraviolet starlight is incident on both sides of the plane parallel model. For model clouds illuminated

on one side only, the situation can be reversed: C_2 is preferentially concentrated in the denser regions.

The CN molecule has been observed in diffuse and translucent clouds both by optical absorption line and millimeter emission line methods. Analysis of the excitation of CN excludes densities higher than $n(H_2) \approx 3 \times 10^3 \text{ cm}^{-3}$ on scales ranging from 10^{-3} to 60 arcsec in a sample of these clouds (Black and van Dishoeck 1990), and generally yields values consistent with the C_2 excitation. High quality CN absorption line data also provide measurements of the Doppler parameter b characterizing the saturation of the strongest lines. This value can be compared with that derived from CO or $^{13}\text{C}O$ mm observations, thus providing further information on the internal structure of the cloud (Gredel, van Dishoeck and Black 1991).

Another observed feature of translucent and high-latitude molecular clouds is that they often show asymmetrical, flat-topped, or possibly even centrally reversed profiles in CO emission lines. Theoretical calculations of line profiles formed in model clouds that have gradients of density, temperature, and CO abundance can reproduce the qualitative appearance of some of the complex profiles. Indeed, small central reversals can appear in such models whether the radiative transfer is treated according to the Sobolev approximation (large velocity gradients) or in a micro-turbulent description (van Dishoeck *et al.* 1991). Sometimes it may be difficult to distinguish such effects from multiple velocity components or profiles resulting from colliding clumps (Keto and Lattanzio 1989). The ominous implication of such calculations is that even in small clouds the observable line profiles are related to internal structure and chemical stratification in such a complicated way that it may be difficult—if not impossible—to infer much about the structure from the profiles!

4. Summary

Rapid advances in observational techniques and sensitivities have made it possible to observe very small-scale structure in nearby diffuse and translucent molecular clouds. Although these clouds are usually not directly implicated in the formation of stars, they provide important test cases for understanding the relationships among cloud structure (variations of density and temperature), chemistry, and turbulence. Every improvement in observation and in theoretical interpretation seems to increase the degree of apparent complexity! Studies of the smallest structures in the smallest clouds raise fundamental questions about chemical processes and about distinctions between microscopic and macroscopic phenomena.

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