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MOLECULE FORMATION IN FAST NEUTRAL WINDS FROM PROTOSTARS

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ABSTRACT

The processes that produce and destroy molecules in very high velocity winds from low-mass protostars are analyzed in the context of a time-dependent chemical model. Molecules such as CO and SiO can be formed in significant quantities even though the overwhelming fraction of hydrogen remains atomic. This result is in accord with recent detections in protostellar winds of CO and H I at velocities greater than 100 km s^{-1}. The conditions for substantial molecule formation are moderate mass-loss rate ($>10^{-6}$ $M_\odot$ yr^{-1}) and a temperature distribution that decreases fairly rapidly with distance from the protostar.

Subject headings: stars: circumstellar shells — stars: pre–main-sequence — stars: winds

I. INTRODUCTION

Molecular outflows are a common feature of star formation regions (e.g., Lada 1985) and are generally believed to consist of ambient material driven by the winds of embedded protostars. Several lines of evidence suggest that low-mass protostellar winds are mainly neutral (see the papers by Evans *et al.* 1987 and Natta *et al.* 1988 and references therein), which raises the possibility that molecule formation may occur in the primary wind. This question has not been previously discussed in any detail with the exception of Rawlings, Williams, and Cantó (1988), who concluded that substantial molecular abundances cannot be produced in the high-temperature winds of T Tauri stars with low mass-loss rates.

We consider formation and destruction processes for molecules in winds that emanate directly from protostars of moderate luminosity and calculate their abundances for a range of mass-loss rates and physical properties. We find that, under appropriate circumstances, large abundances of CO and other heavy molecules can be formed while hydrogen remains essentially atomic. Our results explain the recent observations of Lizano *et al.* (1988) who detected extremely high velocity H I and CO emission in the wind from HH 7–11. Additional detections of extremely high velocity CO have been reported by Koo (1989).

II. THE PHYSICAL MODEL

Our approach is to analyze molecular formation and destruction processes in a mass element of the wind as it travels away from the protostar and experiences varying physical conditions such as density, temperature, and radiation field. We adopt a simplified model for the wind suggested by recent observational and theoretical results and we assume that the wind originates directly from the protostar and that it is steady and spherically symmetric. We ignore interactions with ambient material that become important for understanding the large-scale structure of protostellar flows with typical dimensions of the order of 10^{16} cm. We represent the protostellar radiation field by a blackbody of temperature T_* and radius R_*, and consider a range of mass-loss rates $\dot{M}$. Little is known about the temperatures in protostellar winds, and we model $T(r)$ as follows: $T = T_0$ for $r < R_0$ and $T = T_0(R_0/r)^p$ for $r > R_0$, and then consider variations in the three parameters. We expect T to be large close to the protostar and then to fall rapidly with distance due to a variety of cooling processes; for adiabatic cooling alone, $p = 4/3$. The heating and cooling of protostellar winds of the type discussed by Shu *et al.* (1988) is being analyzed by Ruden, Glassgold, and Shu (1989). For purposes of comparing different models, we define a "standard case" suggested by HH 7–11: $\dot{M} = 3 \times 10^{-6}$ $M_\odot$ yr^{-1}, $V = 150$ km s^{-1}, $R_* = 5 \times 10^{11}$ cm, and $T_* = 5000$ K (Lizano *et al.* 1988), together with the temperature distribution parameters, $T_0 = T_*$, $R_0 = 2R_*$, and $p = 1$.

At first sight, it might seem difficult to form large molecular abundances in a fast wind emitted by a moderately hot protostar. Although the temperature and the density of the wind are large enough to promote chemical synthesis, e.g., by overcoming energy barriers, molecules are also rapidly destroyed under these conditions. Particularly crucial is the short time available for chemical synthesis, of the order of the initial dynamical (expansion) time $t_{\rm dy} = r/V \sim 10^5$ s. An analogous situation occurs in the formation of molecular hydrogen during the cosmological recombination epoch (Dalgarno and Lepp 1987). In both cases the density is high, the radiation field is strong, and time is of the essence.

The formation of the most easily detectable molecule, CO, occurs in three stages, starting with the synthesis of H_2, then OH, and finally CO. The first step involves the rare hydrogen ions, H^- and H_2^+, which are formed by radiative association,

$$e + \mathrm{H} \rightarrow \mathrm{H}^- + h\nu \,, \qquad (1)$$

$$\mathrm{H}^+ + \mathrm{H} \rightarrow \mathrm{H}_2^+ + h\nu \,. \qquad (2)$$

Molecular hydrogen is then produced mainly by

$$\mathrm{H}^- + \mathrm{H} \rightarrow \mathrm{H}_2 + e \,, \qquad (3)$$

$$\mathrm{H}_2^+ + \mathrm{H} \rightarrow \mathrm{H}_2 + \mathrm{H}^+ \,. \qquad (4)$$

The rates of the above reactions are well known (see Dalgarno and Lepp 1987). The ionization is produced by the photoionization of collisionally excited H atoms by the Balmer continuum radiation from the protostar. Our calculation of the ionization includes collisional excitation and de-excitation of the $n = 2$ level of H by electrons and H atoms and trapping of Lyα (in the Sobolev approximation) as well as photoionization and radiative recombination. In order to achieve a substantial H_2 abundance, the wind need only have a moderate ionization fraction ($\sim 10^{-3}$). Collisional dissociation becomes negligible when the wind temperature falls below 2000 K.

The synthesis of OH and CO proceeds mainly by

$$O + H_2 \rightarrow OH + H\,, \tag{5}$$

$$C + OH \rightarrow CO + H\,, \tag{6}$$

$$O + CH \rightarrow CO + H\,. \tag{7}$$

Again, significant abundances of OH and CO can only be achieved when the wind temperature decreases below the energy barriers of strong destruction reactions. The abundance of OH is ultimately limited by charge exchange ($H^+ + OH \rightarrow OH^+ + H$) followed by rapid dissociative recombination of OH^+ and by photodissociation. We have also included additional heavy element chemistry that produces CH, SiO, and related molecules. A full description of the wind chemistry will be given in a later paper in preparation.

The recombination of heavy atoms with IP < 13.6 eV and fractional abundances relative to hydrogen $> 10^{-5}$ (C, S, Si, Mg, Fe) is also important in producing significant molecular abundances. In the absence of dust, these elements shield the UV radiation that would otherwise dissociate the molecules. In particular cases, e.g., H_2 and CO, self-shielding also occurs, but the dominant sources of shielding below 1100 Å are C I and S I. However, OH is dissociated by UV radiation out to 2000 Å, and this band is only partially blocked by recombined atoms. The presence of several unrecombined ions such as Al^+ and Na^+ also affects the recombination of H^+ and thus the level of chemical activity.

Several crucial requirements for strong chemical synthesis emerge from this brief outline of the chemistry. First, the basically neutral wind must have a moderate ionization level, provided in our theory by photoionization of excited atomic hydrogen by Balmer continuum photons. Second, the temperature must drop below ~2000 K fairly rapidly, e.g., within $\sim 5R_*$. Third, the radiation that dissociates molecules must be shielded, either by the molecules themselves or by recombined heavy atoms.

III. RESULTS

Figure 1 illustrates the spatial variation of the abundances in our theory, obtained by integrating the time-dependent chemical rate equations for the standard case defined in § II. The integration is started with initial conditions appropriate to the photosphere. The H^+ ion relaxes very slowly whereas most of the other species relax rapidly, at least at the start of the integration. The figure shows that the abundances of H_2, OH, and CO increase significantly as T decreases beyond $2R_*$ and the destruction processes are turned off. The abundances of H_2 and CO then assume essentially constant values because their production routes also freeze out. On the other hand, OH continues to be destroyed by charge exchange with H^+ and eventually decreases to a very small abundance.

Hydrocarbon chemistry occurs in the model but C_2, the most abundant carbon-bearing molecule after CO, would probably be difficult to detect in this type of wind. The spatial distribution of the CH radical has a double peak due to the operation of two formation processes, $C + H_2 \rightarrow CH + H$ and $C + H \rightarrow CH + h\nu$. Very little of HCO^+ is produced ($< 4 \times 10^{-12}$).

Silicon provides a good illustration of heavy element chemistry. We find that a large fraction (25% in Fig. 1) is processed into SiO at about $5R_*$ where the gas is fairly warm. This molecule is formed by the analog of equation (6) with C replaced by Si. A substantial amount of silicon and other heavy elements may form dust at larger distances (Ruden, Glassgold, and Shu 1988). The recombination of many of the heavy atoms, notably C, Si, and S, ensures significant shielding of the radiation that dissociates molecules.

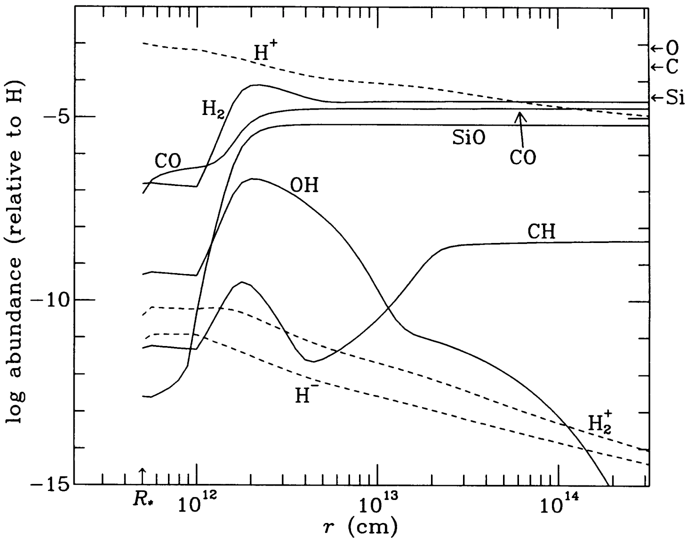

FIG. 1.—Abundance relative to H of observable molecules and progenitor ions vs. distance. The standard parameters used in the calculation are $\dot{M} = 3 \times 10^{-6}\ M_\odot\ \mathrm{yr}^{-1}$, $V = 150\ \mathrm{km\ s}^{-1}$, $R_* = 5 \times 10^{11}$ cm, $T_* = T_0 = 5000$ K, $R_0 = 2R_*$, and $p = 1$. Ionic abundances are shown by *dashed* curves. The essentially atomic nature of the wind can be seen by comparing these abundances with the initial values of the dominant species, H (unity), C, O, and Si (shown by arrows at the right).

The general properties of the results depend most sensitively on the mass-loss rate and on the temperature distribution. Figure 2 shows that the freeze out abundance of CO is a rapidly increasing function of mass-loss rate, varying roughly as $\dot{M}^{3/2}$ for the standard case (*solid curve*). A substantial fraction of the available carbon is converted into CO for $\dot{M} \sim$

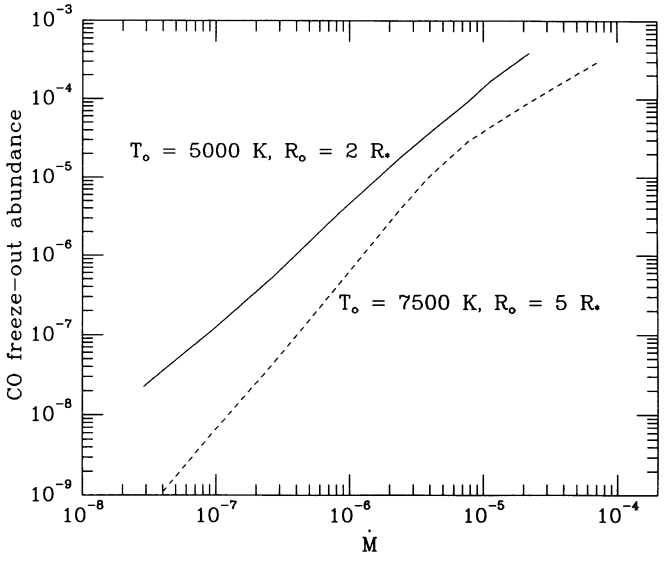

FIG. 2.—Freeze-out abundance of CO vs. mass-loss rate. The *solid* curve is for the standard parameters used in Fig. 1. For the *dashed* curve, the temperature parameters have been changed to $T_0 = 7500$ K and $R_0 = 5R_*$ in order to illustrate the sensitivity to the temperature distribution.

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$10^{-6}\ M_{\odot}\ \mathrm{yr}^{-1}$; the conversion is complete for $\dot{M} \sim 3 \times 10^{-5}\ M_{\odot}\ \mathrm{yr}^{-1}$. The degree of conversion also depends on the parameters characterizing the temperature distribution, increasing for fixed T_* with decreasing R_0 and T_0 and with increasing p (the slope of the temperature fall-off). However, the difference between the value $p = 1$ used in the figures and $p = 4/3$ (adiabatic) or 2/3 are less than a factor of 2. If the gas is heated to high temperatures out to several R_*, the degree of molecular synthesis is reduced significantly. This is illustrated by the *dashed* curve in Figure 2 for which the gas temperature is 7500 K out to $5R_*$. Similarly, if the gas starts to cool immediately on leaving the photosphere, it is increased.

By adopting a blackbody spectrum we may have overestimated the protostellar UV flux, as is found in the case of T Tauri stars (Bertout, Basri, and Bouvier 1988). If the protostar and disk meet in a strong accretion shock, sufficient UV radiation may be emitted to compensate for the blanketing produced in the protostellar atmosphere. If a UV excess does exist, it is unlikely to affect our main result because of the strong shielding of the far-UV radiation by the recombined atoms (C, S, Si, etc.).

Both the physical basis and the results of our model differ with Rawlings, Williams, and Cantó (1988) who considered low mass-loss ($1.4 \times 10^{-9}\ M_{\odot}\ \mathrm{yr}^{-1}$) and high temperature (up to 20,000 K) winds suggested by the Hartmann, Edwards, and Avrett (1982) model of T Tauri stars. In light of the dependence of molecular synthesis on mass-loss rate and wind temperature discussed above, it is not surprising that they obtain very small molecular abundances. Our work also differs in the underlying ionization mechanism and in the values adopted for various rate constants, especially photodestruction rates for H^- and H_2^+, which Rawlings *et al.* appear to have underestimated by at least one order of magnitude.

IV. DISCUSSION

Our results are in qualitative agreement with the limited observational data available on extremely high velocity winds from low-mass protostars and suggest a number of further observational investigations. In particular they explain the detection by Lizano *et al.* (1988) of CO and H I at velocities of 150 km s^{-1} in HH 7–11. One remarkable aspect of our results is that a substantial fraction of the heavy elements can be processed into molecules while hydrogen remains almost completely atomic (see Fig. 1). Our result that little HCO^+ is produced in the wind also agrees with the detection of this ion at substantially lower velocities than CO and H I (Lizano *et al.* 1988). These authors interpret the observed HCO^+ as being excited and possibly produced by the collision of the very high speed protostellar wind with more slowly moving or stationary gas.

Our calculations suggest at least one other molecular radio diagnostic of extremely high velocity protostellar winds, SiO. Because it is formed close to the protostar, an SiO maser may be formed. A search for CH is also in order. Although we have not yet completed our analysis of the sulfur chemistry, SO may be another diagnostic possibility. The atomic character of the wind also suggests that the far-infrared fine-structure transitions of O I are potentially important diagnostics of this type of wind. However, KAO observations of the 63 μm line of O I in protostellar winds (Cohen *et al.* 1988) indicate that significant improvements in sensitivity will be required for this purpose. The 309 and 607 μm lines of C I may, however, be observable with existing or planned submillimeter telescopes. Of course substantial opportunities remain to observe the high-velocity wings of protostellar winds in the various lines of CO. Our result, that the abundance of CO increases as $\dot{M}^{3/2}$, indicates, however, that extremely high velocity CO formed directly in protostellar winds will be difficult to detect if the mass-loss rate is much below our standard value.

In conclusion, we have shown on the basis of well-established molecular physics that heavy molecules can be formed efficiently in extremely high velocity protostellar winds while hydrogen remains almost completely atomic. The sensitivity of the atomic and molecular abundances to conditions at the base of the wind suggests that they can provide useful diagnostics for the physical conditions in this region and may thereby place constraints on the mechanisms which generate protostellar winds.

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