THE PHOTODISSOCIATION OF CO IN CIRCUMSTELLAR ENVELOPES

G. A. MAMON, A. E. GLASSGOLD, AND P. J. HUGGINS Department of Physics, New York University Received 1987 August 27; accepted 1987 November 2

ABSTRACT

We calculate the CO photodissociation rate for the unshielded interstellar medium using recent laboratory results which confirm that photodissociation occurs by way of line absorption. The new rate of 2×10^{-10} s⁻¹ is an order of magnitude larger than that used in earlier studies and requires that many situations in which CO photodissociation plays a role need to be reexamined. We demonstrate the effects of line photodissociation with calculations of the abundances of the CO photochain in the circumstellar envelopes of cool, evolved stars. For low mass-loss rate, optically thin envelopes, the large photodissociation rate leads to a CO distribution $\sim 10^{16}$ cm in extent; for thicker envelopes, strong line shielding leads to a much larger CO distribution with a steep falloff. These envelope sizes are considerably smaller than commonly discussed in the literature. We show how the results of the full theory can be simulated by a schematic model based on representative bands and provide a simple interpolation formula for the spatial variation of the CO abundance. The distribution of ¹³CO and the photodissociation products, C and C⁺ are also discussed. For ¹³CO, the selective photodissociation due to its lower abundance tends to be canceled by chemical fractionation. We discuss the important implications of these results for the ion-molecular chemistry of circumstellar envelopes and for observations of circumstellar CO, C, and C⁺.

Subject headings: molecular processes — stars: circumstellar shells

I. INTRODUCTION

In many astrophysical situations the transition from molecular to atomic gas occurs as a result of photodissociation. Carbon monoxide is one of the most important molecules in the study of interstellar and circumstellar matter, but in the past there has been no firm understanding of its photodissociation by the interstellar radiation field. Following a suggestion by Bally and Langer (1982), Morris and Jura (1983, hereafter MJ) and Glassgold, Huggins, and Langer, (1985, hereafter Paper I) investigated some of the consequences of CO photodissociation occurring through a line process rather than through a continuum process for circumstellar and interstellar matter, respectively. As a result of the recent laboratory measurements of the far-UV absorption and fluorescence cross sections by Letzelter et al. (1987), definitive calculations of the CO photodissociation rate can now be made, and the new photodissociation rate is significantly larger than previous estimates. Consequently, situations in which CO photodissociation plays an important role need to be reevaluated. A particular application discussed here is CO photodissociation in the circumstellar envelopes of cool, evolved stars undergoing substantial mass loss. Not only is CO an important diagnostic for these objects but, at least in the case of spherical envelopes, their simple geometry allows the relevant radiative transfer to be developed in a straightforward way.

It was pointed out in Paper I that the dissociating radiation is absorbed by CO itself ("self-shielding") and by other species such as atomic and molecular hydrogen, atomic carbon, and dust ("mutual shielding"). In the case of 13 CO, any near coincident lines of 12 CO provide additional shielding. In this paper we treat these processes in the context of the photochemical model (e.g., Huggins and Glassgold 1982a) in which the major molecular constituents of expanding red giant winds are destroyed by penetrating interstellar UV radiation. For present purposes we focus on the case of 12 CO and 13 CO and their dissociation products. Additional applications to circumstellar chemistry are investigated in companion papers on carbon-rich envelopes (Glassgold *et al.* 1987) and oxygen-rich envelopes (Mamon, Glassgold, and Omont 1987). In § II we review the underlying physics, particularly CO line photodissociation, and describe the basis of the model calculations for circumstellar envelopes. The results are described in § III for CO and in § IV for ¹³CO and the dissociation products, C and C⁺; the paper is concluded with a brief summary in § V.

II. THE CO PHOTODISSOCIATION RATE AND ITS APPLICATION TO CIRCUMSTELLAR ENVELOPES

The laboratory experiments of Letzelter *et al.* (1987) show that CO is photodissociated by a line process over the relevant wavelength range extending from the threshold (1120 Å) to the Lyman cutoff (912 Å). The upper limit to any continuum dissociation in this wavelength band is less than 1% of the total rate. Ignoring a small number of partially overlapping bands, the total photodissociation rate is the sum of contributions from individual bands,

$$G = \sum_{i} g_i \,. \tag{1}$$

For a typical unshielded region of the interstellar medium, the *i*th band contributes

$$g_i^{(0)} = 0.0265 K_i f_i 4\pi I(v_i) \, \mathrm{s}^{-1} \,, \tag{2}$$

where f_i is the absorption oscillator strength, K_i is the probability for dissociation, and I is the mean intensity of the interstellar radiation field (measured in photons cm⁻² s⁻¹ Hz⁻¹ sr⁻¹). Table 1 lists the dissociating bands for CO for $\lambda > 912$ Å (adapted from Table 1 of Letzelter *et al.* 1987). We have calculated the oscillator strengths, using their integrated cross sections (col. [3]), and the contribution of each band to the rate for the unshielded interstellar medium (col. [5]), using a fit to

TABLE 1	
 Distance Designed on C	\mathbf{n}

	PHOTODISSOCIATION BANDS OF CO								
Band ^a	λ (Å)	$f^{\mathbf{b}}$	$(\text{cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1})$	(s ⁻¹)					
1	1099.0	3.7 (-5)	5.8 (-8)	5.8 (-14)					
2*	1076.1	3.6 (-2)	5.4 (-8)	4.7 (-11)					
3	1063.1	2.8 (-3)	5.2 (-8)	2.3 (-12)					
4*	1051.7	2.5 (-3)	5.0 (-8)	3.2 (-12)					
5	1029.3	4.3 (-5)	4.5 (-8)	5.1 (-14)					
6	1017.9	4.4 (-5)	4.3 (-8)	4.9 (-14)					
7	1010.9	4.4 (-5)	4.1(-8)	4.8 (-14)					
8*	1002.5	7.9 (-3)	3.9 (-8)	8.2 (-12)					
9*	989.3	4.6 (-4)	3.5 (-8)	4.3 (-13)					
10*	985.6	1.5(-2)	3.4 (-8)	1.4 (-11)					
11	982.7	4.8(-4)	3.4 (-8)	4.3 (-13)					
12	977.5	1.8(-3)	3.2 (-8)	1.5 (-12)					
13	972.7	1.2(-2)	3.0 (-8)	9.3 (-12)					
14*	970.4	2.1(-2)	3.0 (-8)	1.6 (-11)					
15	968.9	1.2(-2)	2.9 (-8)	9.6 (-12)					
16*	968.4	7.7(-3)	2.9 (-8)	5.9 (-12)					
17	964.4	2.8(-3)	2.8 (-8)	2.0 (-12)					
18	960.5	2.6(-4)	2.6 (-8)	1.8 (-13)					
19*	956.1	1.3(-2)	2.4(-8)	8.7 (-12)					
20	949.9	2.2(-2)	2.2(-8)	1.3 (-11)					
21	948.4	2.8(-3)	2.1(-8)	1.6 (-12)					
22	946.3	7.6(-3)	2.0(-8)	4.1 (-12)					
23	941.1	2.6(-2)	1.8(-8)	1.2 (-11)					
24	939.9	2.1(-2)	1.7(-8)	9.7 (-12)					
25	935.7	3.8(-3)	1.5 (-8)	1.5 (-12)					
26	933.1	4.0(-2)	1.4(-8)	1.4 (-11)					
27	930.0	6.3(-3)	1.2(-8)	2.0 (-12)					
28	928.4	6.7 (-3)	1.1(-8)	1.9 (-12)					
29	925.8	1.6(-2)	9.4 (-9)	4.1 (-12)					
30	924.6	5.1(-3)	8.6 (-9)	1.2 (-12)					
31*	922.8	6.3(-3)	7.5 (-9)	1.3 (-12)					
32	917.3	2.8(-2)	3.8 (-9)	2.9 (-12)					
33*	915.8	9.9 (— 3)	2.8 (-9)	7.3 (-13)					
34	913.5	3.4(-2)	1.1(-9)	1.0(-12)					

^a Bands followed by an asterisk are assumed to correspond to 0–0 transitions with no isotope shift.

^b Bands 2, 3, and 13 have $K_i = 0.89$, 0.60, and 0.96, respectively. All other bands have $K_i = 1$.

Nort.—Parentheses indicate multiplication by the power of ten given within the parentheses.

the far-UV interstellar radiation field given by Jura (1974) (col. [4]). The total unshielded rate is then $G^{(0)} = 2.0 \times 10^{-10} \text{ s}^{-1}$, and the associated mean oscillator strength (weighted by the radiation field) is 0.0087. This rate is an order of magnitude larger than the earlier value based on a putative continuum process and used in chemical models of diffuse clouds. The rate $G^{(0)}$ is sensitive to the spectrum of the far-UV interstellar radiation field. For example, if the radiation field is represented by the flux at 1000 Å, $G^{(0)} = 3.7 \times 10^{-10} \text{ s}^{-1}$. For comparison and later applications, the photoionization rate for atomic carbon with the Jura radiation field is $G^{(0)}(C) = 3.4 \times 10^{-10} \text{ s}^{-1}$.

The basis for treating CO photodissociation in circumstellar envelopes has been given previously in Paper I and MJ. In particular, MJ developed the radiative transfer for a typical far-UV line that dissociates CO, using the Sobolev approximation. Consequently, we need only indicate here how to adapt the results of MJ to the full complement of bands measured by Letzelter *et al.* (1987) and to include appropriate mutual shielding (Paper I). For purposes of simplicity, we consider only the effects of the interstellar radiation field and ignore internal radiation sources. Fluorescent line radiation of H₂, induced by cosmic-ray secondary electrons (Prasad and Tarafdar 1983; Sternberg, Dalgarno, and Leep 1987), might add to the photodissociation of CO deep within the most massive and shielded envelopes.

Although the experiment of Letzelter et al. (1987) represents an important advance in the measurement of the CO photodissociation cross section, further measurements are needed to clarify the process. More recent experiments by Yoshino et al. (1987) at 20 times the spectral resolution indicate that the cross sections for some of the bands below 1000 Å may be larger than reported by Letzelter et al. The spectroscopic parameters of the upper states have not been established for most of the bands below 1000 Å. This affects our treatment of the radiation transfer within the circumstellar envelope which requires the Hönl-London factors for the rotational part of the oscillator strength. About one-half of the assignments for the states above 1000 Å are Σ and one-half are Π . In the absence of definitive information, we use the Hönl-London factors for Σ - Σ transitions, i.e., we do not treat *Q*-branch lines explicitly. This should lead to only small changes in the total CO photodissociation rate inside the circumstellar envelope.

We have also assumed that the line widths are small compared with that associated with the expansion velocity V. The preliminary results of Letzelter *et al.* indicate that some of the lines may be broader than this, in which case improvements to the Sobolev approximation should be implemented. Large line widths and other blending tend to introduce some aspects of continuum self-shielding into the problem, but it is unlikely that the qualitative conclusions of our calculations will be substantially altered by these effects. We ignore them here, pending additional experiments to better establish the photodissociation cross section.

Inside the circumstellar envelope the contribution of each band g_i is modified by optical depth effects and, in the Sobolev approximation, is given by

$$g_i = \langle \beta_i(r) \rangle \gamma_i(r) g_i^{(0)} , \qquad (3)$$

where $\langle \beta_i(r) \rangle$ is a mean escape probability and $\gamma_i(r)$ is the continuum attenuation factor for band *i*. The mean escape probability is an average over the rotational states involved in the transition, weighted by the populations of the initial states. In the Sobolev approximation, the escape probability for each transition is given by a simple function of the optical depth, as discussed in more detail in the Appendix. In evaluating equation (3) for each of the bands in Table 1, we have assumed for simplicity that the populations are given by a Boltzmann distribution with the excitation temperature $T_{ex}(r)$; later we vary $T_{ex}(r)$ to investigate the sensitivity of the results to this quantity. We also use the continuum factor of MJ,

$$\gamma_i(r) = \exp\left[-1.644\tau_c(\lambda_i)^{0.86}\right],$$
 (4)

where $\tau_c(\lambda_i)$ is the radial optical depth for continuum absorption at wavelength λ_i .

The species with the greatest potential for blocking of the CO bands are atomic and molecular hydrogen, but the possibilities for near coincidence of the transitions are different for the two species. The spacing of the Lyman transitions of atomic hydrogen is such that relatively few near coincidences with the CO bands occur. The Lyman and Werner bands of H₂ are roughly uniformly distributed over the 900–1100 Å region, and 11 of these lines with initial rotational quantum numbers in the range J = 0-2 coincide with the CO bands within 0.4 Å as do six others within 1 Å. In our treatment of H₂ blocking, we assume that the relevant (outer) parts of the envelope are

1988ApJ...328..797M

cool enough so that only the J = 0-2 lines of H₂ are significantly populated. The H₂ lines are highly saturated and one of them can effectively block a CO band even if it is several tenths of an angstrom away.

In this paper we consider circumstellar envelopes whose hydrogen is mainly molecular. This assumption is well justified for cool stars with photospheric temperatures less than 3000 K (Glassgold and Huggins 1983). The envelopes of such stars do have a small amount of atomic hydrogen (Glassgold and Huggins 1983), e.g., between 10^{17} and 10^{18} cm⁻² for IRC + 10216, but the amount is insufficient to produce very much blocking from the (atomic) Lyman lines. The situation would be very different for warmer stars, which are predominantly atomic and for diffuse interstellar clouds with $N(H) > 10^{19}$ cm⁻². It is also appropriate to ignore the shielding due to atomic carbon because the calculated column density and photoionization cross section satisfy the condition $N(C) \ll \sigma_{\rm ph}(C)^{-1} = 6 \times 10^{16}$ cm⁻².

The H_2 lines become so optically thick that absorption occurs in the radiative wings of the Lyman and Werner transitions. From the point of view of the CO lines, the blocking of the dissociating radiation by a nearby H_2 line can be included in the continuum factor of equation (4). Thus, the optical depth in this equation is a sum of contributions from dust and the wings of those Lyman and Werner lines which originate from the lowest rotational states of H_2 . Despite the strong blocking of many CO lines by H_2 , the effect on the total CO photodissociation rate inside a circumstellar envelope is only a quantitative one because the CO bands that are distant from H_2 lines still contribute ~ 50% of the total rate.

The isotope shift of the far-UV transitions of CO is substantial except for v = 0-0 transitions. Thus the shielding of ¹³CO by ¹²CO occurs only for 0-0 transitions, where the isotope shift is typically 0.01 Å (Paper I). Most of the ¹³CO bands are shifted by a large amount (>0.5 Å) (Eidelsberg 1987) and there is only a modest amount of mutual shielding of ¹³CO by the more abundant isotope.

The effects of the most important physical processes that enter into the above theory are illustrated in Figure 1. This shows the variation of the photodissociation rate of CO with radius for the case of a spherically symmetric envelope of steady mass-loss rate with parameters given in Table 2. The total photodissociation rate is given by the solid curve at the top, labeled "Total." Starting at the outside of the envelope, the rate decreases sharply near $r = 5 \times 10^{17}$ cm due to the onset of self-shielding. It then follows the linear law expected at intermediate distances on the basis of the optically thick limit of the theory for the model $1/r^2$ CO density distribution (see eq. [3] and the Appendix). The rate decreases even further at smaller distances due to dust shielding. By $r = 10^{16}$ cm, the

 TABLE 2

 Parameters for the Standard Model

Expansion velocity	$V = 15 \text{ km s}^{-1}$
Mass-loss rate (total hydrogen)	$M = 10^{-5} M_{\odot} \text{ yr}^{-1}$
Initial CO abundance ^a	$\begin{cases} x_0(^{12}\text{CO}) = 4 \times 10^{-4} \\ (^{13}\text{CO}) = 2 \times 10^{-6} \end{cases}$
	$(x_0(^{13}\text{CO}) = 8 \times 10^{-6})$
	$(r_0 = 9 \times 10^{10} \text{ cm})$
Temperature distribution ⁶ , $T = 14.6 \text{ K} (r/r_0)^{\varphi} \dots$	$\phi = -0.72, r < r_0$
	$(\phi = -0.54, r \ge r_0$
Dust shielding ^c , $\tau_c^{(a)} = d/r$	$d = 2.6 / \times 10^{10} \text{ cm}$

^a Relative to total hydrogen, $n(H) + 2n(H_2)$.

^b For $r > 1.92 \times 10^{18}$ cm, T = 2.8 K.

^c The value of *d* scales with \dot{M}/V .



FIG. 1.—Photodissociation rates as a function of radius for the standard model. The total rate is shown, with and without H_2 blocking, by the solid and the dashed curves, respectively. The contributions of representative, individual bands are labeled by the band wavelength in Å.

various shielding mechanisms have reduced the CO photodissociation rate by over 4 orders of magnitude.

The dashed curve gives the total CO photodissociation rate when H₂ line blocking is ignored. Over most of the interior of the envelope, H₂ blocking reduces the photodissociation rate by only a factor of 2 or 3, because a substantial number of CO bands are not blocked. It is interesting that some H₂ blocking occurs even at $r = 10^{18}$ cm in this model, which implicitly assumes that the hydrogen content of the envelope is completely molelcular out to infinity. For an envelope of finite age t, the H₂-H transition near the outer edge (r = Vt) will make the total rate approach the unshielded value, $G^{(0)} = 2 \times 10^{-10}$ s^{-1}

The other curves in Figure 1 give the contributions of a selection of individual CO bands labeled by their wavelengths in angstroms. The properties of the bands in Table 1 help explain the variation of these partial dissociation rates with radius. Thus dissociating band 2 at 1076.1 Å has a large dissociation oscillator strength (0.032) and is strongly self-shielded. It is the single most important band, contributing 23% of the total rate at the outside of the envelope but, because of selfshielding, only 1% in the interior. The variation of the rate for band 2 is typical of the stronger bands which dominate the total photodissociation rate. Band 34 at 913.5 Å is also strongly dissociating, but it contributes little to the total rate because the interstellar radiation field is very small near the Lyman cutoff. Band 8 at 1002.5 Å is moderately strong but it is very effectively blocked by a closely coincident H₂ line. Bands 1 (1099 Å) and 11 (983 Å) are both weak and are not close to any H₂ lines; the former is hardly self-shielded because its oscillator strength is very small (3.7×10^{-5}) and plays a dominant role in the inner part of the envelope.

10

III. THE DISTRIBUTION OF CO

We now present the results of the theory of the photodissociation of circumstellar CO in terms of the actual distribution of the CO abundance, defined as the ratio of CO density to the total hydrogen densty $[n_{\rm H} = n({\rm H}) + 2n({\rm H}_2)]$. The abundance of CO can be calculated accurately in terms of the simplest photochain (Huggins and Glassgold 1982a),

$$CO \xrightarrow{hv} C \xleftarrow{hv} C^+, \qquad (5)$$

in which the backward arrow signifies radiative recombination. The neglect of other reactions is justified by more complete chemical studies (Glassgold et al. 1987; Mamon, Glassgold, and Omont 1987). The results for a standard model will be discussed first; the physical parameters are given in Table 2. We use two power laws to fit the calculations by Kwan and Linke (1982) of the kinetic temperature of IRC +10216 in the outer envelope, and cut it off at 2.8 K, the temperature of the cosmic background radiation.

In Figure 2 we compare the spatial variation of CO with and without line shielding. The curve labeled S is the standard calculation (Table 2) which includes all the important shielding processes discussed in § II. In comparison with the case where the only shielding of the dissociating UV radiation is by dust, the CO distribution for the standard case differs substantially in two ways: the CO distribution is shifted outward (by more than a factor of 5) and it decreases more rapidly in the transition region. Inclusion of H₂ blocking shifts the CO distribution outward by 30%. Dust plays a minor role in the presence of strong line shielding. For the standard case, the dust optical depth is only ~ 0.2 in the CO transition region.



FIG. 2.—The spatial distribution of the CO abundance for the standard case (S) of Table 2. Variational calculations are shown for the cases of no line shielding ("Dust"), no H₂ blocking, and reduced excitation temperature.

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800

No. 2, 1988

The variation of the CO abundance distribution with massloss rate, keeping all other parameters fixed, is shown in Figure 3. In the limit of very small \dot{M} , the distribution approaches that of "free decay" (Huggins and Glassgold 1982*a*),

$$x = x_0 = \exp\left[-V/G^{(0)}\right].$$
 (6)

With increasing \dot{M} , dust and especially self-shielding become important, and both the size of the distribution and the steepness of its decline increase. If the size of the distribution is defined by the position where x(CO) has decreased by a factor of 2, $r_{1/2} \propto (x_0 \dot{M})^{0.6}$, reminiscent of the scaling of the OH peak in the H₂O photochain (Huggins and Glassgold 1982b).

The excitation of the CO levels in any given circumstellar envelope depends on a number of factors including the gas kinetic temperature and density, the infrared and cosmic background radiation fields, and photon trapping. Increasing the rotational excitation temperature T_{ex} tends to decrease the effective opacity of the absorbing transitions and to reduce the self-shielding of the envelope. For simplicity in the present calculations, we assume that the levels are thermalized at the kinetic temperature, i.e., $T_{ex} = T_k$. In order to investigate the sensitivity of the results to T_{ex} , we have also done calculations with $T_{ex} = 0.5T_k$. These two cases should bracket most situations. The results of setting $T_{ex} = 0.5T_k$ for the standard model are shown in Figure 2; the shifts in the curves are slight. Thus the results are not very sensitive to the level populations.

The curves in Figure 3 for intermediate values of \dot{M} should be considered rather provisional in view of our ignorance of the CO excitation properties in these envelopes. For low and intermediate mass-loss rates, $\dot{M} < 10^{-6} M_{\odot} \text{ yr}^{-1}$, the excitation of the CO levels is strongly affected by the IR flux from the star and inner dust shell, thereby diminishing the dependence of the photodissociation rate on the kinetic temperature. Of course, for very small \dot{M} , the envelopes are almost optically thin and the photodissociation rate is independent of excitation. The excitation and thermal properties of these envelopes deserves further study, but this is beyond the scope of the present paper.

The results shown in Figures 2 and 3 have been obtained from a detailed theory that includes individual treatment of the many bands of CO and the lines of molecular hydrogen as well as the effects of dust. We now discuss two simpler, but approximate, treatments that should be useful in both theoretical modeling and the analysis of observational data. In earlier discussions of CO line self-shielding (e.g., MJ and Paper I), a schematic model was used in which the ensemble of dissociating bands was replaced by a number of identical bands. Now that the physical properties of the bands have been measured, we can investigate whether this approach is a good approximation. The ensemble of CO bands is represented by N_e identical bands of wavelength $\langle \lambda \rangle$, dissociation oscillator strength $\langle f_d \rangle$, and effective total unshielded photodissociation rate G_e . Using $\langle \lambda \rangle = 1000$ Å (the results are insensitive to this value), the approximation is specified by any pair of the quantities G_e , $\langle f_d \rangle$, and N_e ; the third is directly related to the others by equations (1) and (2). We find that the schematic model can reproduce the CO abundance distribution to a high degree of accuracy; the difference would barely be visible in the plots used in this paper. For the standard model and $G_e = G^{(0)} = 2$ $\times 10^{-10}$ s⁻¹, $\langle f_d \rangle = 0.029$ or $N_e = 12$; the reduction of N_e from 34 to 12 comes from H₂ blocking and the fact that the transition region is determined mainly by the stronger CO bands with $\langle f_d \rangle \sim 0.01$. (Deep inside the envelope, even very weak bands contribute to the total rate, but their effect on the abundance CO is negligible because the dissociation rate is already very small.) The parameters of the schematic model do not change much when the mass-loss rate is changed. Its main limitation is that the abundance of C⁺ becomes inaccurate



FIG. 3.—The CO abundance distribution for a range of mass-loss rates (units M_{\odot} yr⁻¹). All other parameters are the same as in Table 2.

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deep within the envelope. As long as $x(C^+) > 10^{-7}$ however, the errors are usually considerably less than 50%. For applications to detailed chemical modeling, we suggest the use of $\langle f_d \rangle = 0.035$, which improves the fit to the C⁺ distribution at the expense of a slightly less accurate representation of the CO distribution.

On the basis of this validation of the schematic model, we recommend its use in many astrophysical applications where the accuracy of the complete multiband theory is not required. This procedure has already proved useful in chemical modeling of circumstellar envelopes (Glassgold *et al.* 1987; Mamon, Glassgold, and Omont 1987) and in a detailed study of CO in IRC +10216 (Huggins, Olofsson, and Johansson 1987). We expect that appropriate schematic models can also be developed for interstellar clouds.

If only the distribution of CO is of interest, it is possible to represent the results of the full theory even more simply by generalizing an approximate form of the CO abundance distribution derived by MJ in the optically thick limit of the Sobolev theory of line self-shielding,

$$x = x_0 (1 - r^2 / r_c^2) , (6)$$

$$r_{c} = \left(\frac{3x_{0}\,\dot{M}/m_{\rm H}}{4\pi V N_{\rm h} \langle 4\pi I K \lambda^{-1} \rangle}\right)^{1/2}\,,\tag{7}$$

where the quantity in angle brackets is an average over the N_b bands. The singular behavior of equation (6) near the cutoff radius is an artifact that arises from the assumption that the bands are optically thick, whereas they actually become optically thin in the limit $r \rightarrow r_c$ and $x \rightarrow 0$. Examination of the numerical solutions of the full theory shows that the real transition is continuous and that the contributing bands have a wide range of optical depths. Nevertheless equations (6) and (7)

express some qualitative aspects of the correct solution. For example, equations (6) and (7) imply that $r_{1/2} = 2^{-1/2} r_c \propto \dot{M}^{1/2}$, whereas the numerical solution typically gives $r_{1/2} \propto \dot{M}^{0.6}$, which is not too different. However, the characteristic size of the CO envelope is overestimated by equation (7). For example, in the standard case (Table 2), with $N_b = 34$ and $\langle 4\pi I K \lambda^{-1} \rangle = 2.6 \times 10^{-3}$ cm⁻³ Hz⁻¹ s⁻¹, equation (7) gives $r_{1/2} = 3.7 \times 10^{17}$ cm, significantly larger than the value in the complete theory (for the comparable case of no H₂ blocking), where $r_{1/2} = 1.8 \times 10^{17}$ cm. This discrepancy increases with decreasing mass-loss rate.

It is possible to obtain an improved fit to the CO abundance distribution by modifying equation (6) as

$$x = x_0 [1 - (r/r_c)^b]$$
(8)

and treating b and r_c as empirical parameters; 20% accuracy can be obtained in this way. A much better fit can be obtained with the formula

$$x = x_0 \exp\left[-\ln 2(r/r_{1/2})^{\alpha}\right],$$
 (9)

which does not have a sharp cutoff. As shown in Figure 4, the quality of the fits is high as long as x/x_0 is larger than 0.05. The best-fit parameters are shown in Figure 5 as a function of mass-loss rate for the standard velocity of 15 km s⁻¹ (solid curves) and $\frac{1}{2}$ and 2 times this value (short and long-dashed curves, respectively). For convenience in applications, numerical values of the parameters are given in Table 3. It is apparent that the slopes of the $r_{1/2}$ versus \dot{M} curves increase with \dot{M} . A good approximation for the mass-loss rate range, $10^{-6}-10^{-4}$ M_{\odot} yr⁻¹ is $r_{1/2} \propto \dot{M}^{0.6}$. In the limit of vanishing \dot{M} , $r_{1/2}$ approaches a constant, in keeping with the fact that the size of the abundance distribution is now determined by $V/G^{(0)}$ (Huggins and Glassgold 1982a).



FIG. 4.—Fit of equation (9) for the CO abundance distribution (dashed curves) compared with the full theory (solid curves) for a range of mass-loss rates. All other parameters are the same as in Table 2.

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802

1988ApJ...328..797M



FIG. 5.—Variation of the fitting parameters in equation (9) with mass-loss rate for three values of the expansion velocity, V = 7.5 (short-dashed curve), 15 (solid curve) and 30 km s⁻¹ (long-dashed curve). The top three curves show α and the bottom three show $r_{1/2}$. All other parameters are the same as in Fig. 2.

One important result of the above calculations is that the characteristic sizes of the CO envelopes are significantly smaller than previous estimates, and this can effect the interpretation of observation of circumstellar CO. For example, in analyzing CO survey data, Knapp and Morris (1985) and Wannier and Sahai (1986) used the old value of the CO photo-dissociation rate and a two-band approximation (following

TABLE 3 FIT PARAMETERS OF CO DISTRIBUTION

 Ň	$v = 7.5 \text{ km s}^{-1}$		$v = 15 \text{ km s}^{-1}$		$v = 30 \text{ km s}^{-1}$	
$(M_{\odot} \text{ yr}^{-1})$	<i>r</i> _{1/2}	α	<i>r</i> _{1/2}	α	r _{1/2}	α
1 (-8)	7.50 (15)	1.71	9.01 (15)	1.39	1.39 (16)	1.20
2(-8)	9.79 (15)	1.81	1.05 (16)	1.46	1.48 (16)	1.23
5(-8)	1.49 (16)	1.96	1.40 (16)	1.60	1.71 (16)	1.31
1(-7)	2.12 (16)	2.09	1.85 (16)	1.74	2.01 (16)	1.39
2(-7)	3.10 (16)	2.22	2.54 (16)	1.89	2.49 (16)	1.51
5(-7)	5.23 (16)	2.38	4.05 (16)	2.09	3.55 (16)	1.71
1 (-6)	7.91 (16)	2.51	5.95 (16)	2.24	4.88 (16)	1.88
2(-6)	1.21 (17)	2.66	8.88 (16)	2.39	6.94 (16)	2.05
5(-6)	2.14 (17)	2.90	1.54 (17)	2.61	1.15 (17)	2.29
1(-5)	3.35 (17)	3.07	2.35 (17)	2.79	1.72 (17)	2.47
2 (-5)	5.31 (17)	3.26	3.65 (17)	2.96	2.61 (17)	2.66
5(-5)	9.99 (17)	3.51	6.67 (17)	3.20	4.63 (17)	2.89
1 (-4)	1.64 (18)	3.71	1.07 (18)	3.39	7.26 (17)	3.07

Notes.—These parameters refer to the distribution given in equation (9). The units of $r_{1/2}$ are cm. Parentheses indicate multiplication by the power of ten given within the parentheses.

MJ) which yields envelope sizes that are typically a factor 5 times larger than given here for the same envelope parameter. Application of the new theory indicates that mass-loss rates inferred by these earlier analyses need to be increased in those cases where the angular size of the telescope beam is comparable to, or larger than, the CO envelope. This new result also resolves the problem raised by the above authors concerning the lack of double-peaked spectra in sources whose intensities indicate that the emission is optically thin. These effects have been discussed for the case of α Ori (Huggins 1987), where it was deduced that the source size was significantly smaller than suggested by earlier theory; this result is confirmed by the present results. The prescription given above for calculating the CO envelope size should enable CO survey data to be interpreted consistently in accord with the new theory of CO photodissociation.

IV. THE DISTRIBUTION OF C, C^+ , AND ¹³CO

The products of the CO photochain, C and C⁺, are important for circumstellar chemistry and are potentially useful observational probes of the outer regions of the envelopes. Figure 6 shows the spatial variation of the abundances for the standard case. Relative to the predictions of the simplest theory with only dust shielding (Huggins and Glassgold 1982*a*), the main changes are the shift of the CO-C⁺ transition to larger distances and the sharpening of the various abundance distributions. The transition is predominantly from CO to C⁺: the peak abundance of neutral carbon, $x_n(C)$, is always 1988ApJ...328..797M



FIG. 6.—The complete CO photochain for the parameters of Table 2

small compared with x_0 , the initial abundance of CO. The ratio $x_p(C)/x_0$ does increase with decreasing mass-loss rate but, even for $\dot{M} = 10^{-8} M_{\odot} \text{ yr}^{-1}$, $x_p(C)/x_0$ is only 0.25. The spatial distribution of neutral carbon is characterized by a long recombination tail that is sensitive to the temperature in the outer envelope. The radial column density of neutral carbon is typically of order $2 \times 10^{15} \text{ cm}^{-2}$ and fairly independent of \dot{M} . The detection of the emission in the fine structure lines of C is expected to be difficult in IRC + 10216 because of the problems in exciting the lines far from the star (Omont 1986).

The abundance of C⁺ decreases very rapidly going into the interior of the envelope. The details of its spatial distribution are quite important for the ionization of the envelope and for ion-molecule chemistry, particularly in O-rich circumstellar envelopes where CO is essentially the only source of C⁺ (Mamon, Glassgold, and Omont 1987). The detection of the 158 μ m far-infrared line or the radio recombination lines of C⁺ would be of great interest as further tests of the photochemical model, and sensitive new detection systems may make such observations feasible in the near future.

The measurement of the relative abundances of the mass 12 and 13 isotopes of carbon is of considerable importance for understanding stellar evolution. Radio observations of the isotope ratio for several circumstellar envelopes have been carried out (see, e.g., Knapp and Chang 1985). For the C-rich envelope IRC + 10216, the most accurate determination of the ${}^{12}C/{}^{13}C$ ratio, 50^{+6}_{-4} , is based on the optically thin lines of several molecules (Kahane *et al.* 1987). Chemical fractionation appears to be unimportant for on-source isotope ratio measurements in IRC + 10216 because a single isotope ratio is appropriate for all of these molecules. Measurements for other envelopes are generally less accurate, but the ratios for O-rich envelopes are smaller on average than for C-rich envelopes (Knapp and Chang 1985).

The demonstration that ion-molecule reactions are oper-

ative in circumstellar envelopes (Nejad, Millar, and Freeman 1984; Glassgold, Lucas, and Omont 1986) suggests that chemical fractionation of CO occurs through the well-known exchange reaction (Watson, Anicich, and Huntress 1976),

$${}^{13}C^{+} + {}^{12}CO \rightarrow {}^{12}C^{+} + {}^{13}CO$$
, (10)

which is exothermic by ~35 K. Below this temperature, the backward reaction is suppressed and production of ¹³CO from ¹²CO is favored. On the other hand, "selective photodissociation" (Bally and Langer 1982) favors ¹²CO because the lower abundance of ¹³CO produces relatively less self-shielding and more photodissociation of ¹³CO. The competition between these processes in interstellar clouds was investigated in Paper I with a schematic treatment of CO photodissociation. Using the new photodissociation rate and the theory described in § II, it is now possible to obtain more definitive results on the chemical and photo fractionation of CO in circumstellar envelopes.

We have calculated the abundances for both the ^{12}CO and ^{13}CO photochains, linking the two by the fractionation reaction equation (10). The properties of this reaction have been well established by laboratory experiments and we follow Paper I in fitting the temperature dependence of the forward and backward rate coefficients given by Langer *et al.* (1984). The unshielded photodissociation rates of ^{12}CO and ^{13}CO are the same, as are the rate coefficients for radiative recombination. According to Table 1, nine ^{13}CO bands coincide with ^{12}CO bands and are strongly shielded. In treating the case of overlapping ^{12}CO and ^{13}CO bands, we replace the optical depth for each isotope by the sum. However, the blocked bands contribute only 30% of the unshielded dissociation rate and so the effect of ^{12}CO blocking is only a quantitative one.

Figure 7*a* shows the spatial distribution of 12 CO and 13 CO with and without fractionation for the standard case (Table 2), which assumes an initial isotope ratio of 50. Without fractiona-







805

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806

tion (dashed curves), the transition from ¹³CO to ¹³C⁺occurs at a much smaller radius than the corresponding transition for the more abundant isotope—simply because the smaller abundance of ¹³CO produces less self-shielding. When fractionation is included (solid curve), however, substantial amounts of ¹³CO are produced in the ¹²CO transition region and the two distributions become very similar. In other words, fractionation undoes the effects of selective photodissociation. The sizes of the CO distributions can be simply characterized by the onehalf radius, defined by $x(r_{1/2})/x_0 = \frac{1}{2}$. For small values of \dot{M} ($< 5 \times 10^{-6} M_{\odot} \text{ yr}^{-1}$), $r_{1/2}(^{13}\text{CO}) < r_{1/2}(^{12}\text{CO})$, whereas for large values of \dot{M} ($> 5 \times 10^{-6} M_{\odot} \text{ yr}^{-1}$), $r_{1/2}(^{13}\text{CO}) >$ $r_{1/2}(^{12}\text{CO})$. However, the difference between the sizes of the ¹²CO and ¹³CO distributions is always small, no more than 10% or 20%.

Some of these effects can be seen more clearly in Figure 7b, which plots the abundance ratio of the CO isotopes as a function of distance, again with (solid curves) and without (dashed curves) fractionation. For purposes of clarity, the results for small mass-loss rates are not shown. Without fractionation, the ratio of ${}^{12}CO$ to ${}^{13}CO$ becomes very large as soon as the ${}^{13}CO{-}^{13}C^+$ transition is reached. This increase is halted by fractionation at a characteristic distance which depends on the mass-loss rate and the temperature distribution. Fractionation reduces the ¹²CO/¹³CO ratio significantly below its initial value, but only in the tenuous, outer parts of envelopes, where ¹³CO is difficult to detect. At intermediate distances, where both isotopes can be detected, the theory predicts modest increases in the isotope ratio by up to 20%. For IRC + 10216, the theory predicts an essentially constant ¹²CO/¹³CO ratio out to 3×10^{17} cm (100" for a distance of 200 pc). Existing measurements of isotope ratios for this envelope have been restricted to on-source observations. It is important to emphasize that the predicted constancy of the ${}^{12}CO/{}^{13}CO$ isotope ratio in IRC + 10216 is due to the cancellation of strong selective photodissociation (associated with line self-shielding) by strong chemical fractionation.

The results shown in Figure 7 are largely independent of the initial isotope ratio, $R_0 = {}^{12}\text{CO}/{}^{13}\text{CO}$. When R_0 is varied over the range 5-80 (or greater) keeping $x_0(CO)$ fixed, the ¹²CO photochain is hardly changed. The shapes of the ${}^{13}CO$ and ${}^{13}C^+$ distributions are only slightly altered, but their absolute values are shifted according to the new value of R_0 . The distribution of ¹³C is affected at intermediate distances but, when R_0 is changed from 5 to 80 for example, the renormalized distributions differ by no more than a factor of 3. The general insensitivity of the distributions to the initial isotope ratio, other than an overall scaling of the ¹³CO photochain, can be understood in terms of the relevant physical processes and the assumption that $R_0 \ge 1$. At very small distances from the star, there are essentially no carbon ions and the two photochains are independent of one another. At very large distances, the assumption $R_0 \gg 1$ implies that the relatively small abundance of ${}^{13}C^+$ does not alter the recombination of either ${}^{12}C^+$ or ¹³C⁺. Over much of the intermediate range of distances, both the forward and backward rates of equation (10) are fast enough that the fractionation process is equilibrated and the two transitions are locked together.

The above calculations suggest that the CO isotope ratio varies significantly only in the outer parts of circumstellar envelopes where it would be difficult to measure. The effects of selective photodissociation and fractionation might be detected more readily through their effect on species synthesized by ion-molecule reactions initiated by the C⁺ ion. The ${}^{12}C^{+}/{}^{13}C^{+}$ ratio is generally much less than R_0 before the CO to C⁺ transitions are complete, i.e., C⁺ is fractionated to a significant degree. The most obvious candidates for indirect fractionation by C⁺ are hydrocarbon molecules with three carbon atoms such as C₃H and C₃H₂ which are formed by reactions of C⁺ and acetylene. In O-rich circumstellar envelopes, the small ${}^{12}C^{+}/{}^{13}C^{+}$ ratio should have a significant effect on the relative abundances of the HCO⁺ isotopes. In this connection, it should also be mentioned that, when R_0 becomes as small as 5, ${}^{13}C^{+}$ makes an important contribution to the electron density.

The CO isotope problem can be analyzed with the help of the schematic model of CO photodissociation discussed in § III. However, the lower abundance of ¹³CO requires the use of a larger oscillator strength, e.g., for the standard parameters $\langle f_d(^{13}CO) \rangle = 0.072$ compared with $\langle f_d(^{12}CO) \rangle = 0.029$. The increase is largely due to the enhanced importance for the rarer isotope of H₂ blocking relative to self-shielding.

V. CONCLUSION

Carbon monoxide is one of the most important constituents of interstellar and circumstellar matter. Its abundance in diffuse interstellar clouds and in the transition regions of dense clouds and circumstellar envelopes is dictated by photodissociation. However, the physics of CO photodissociation by UV radiation has only recently been understood through the new measurements of its absorption and fluorescence cross sections by Letzelter *et al.* (1987). Thus it is now possible to put the theory of these regions on a sound basis.

The transfer of the UV radiation that dissociates CO longward of the Lyman cutoff depends on whether the dissociation occurs by a line or continuum process. The new experiments show that it is lines that dominate, and so the radiation transfer must deal with over 30 CO absorption bands and numerous, nearly coincident lines of atomic and molecular hydrogen. Using the results of Letzelter et al., we find that the CO photodissociation rate in the interstellar medium is $2.0 \times 10^{-10} \text{ s}^{-1}$. an order of magnitude larger than the rate used in the past. The new rate and a treatment of the radiative transfer and shielding are used to develop a theory for the CO abundance in the circumstellar envelopes of cool, evolved stars, and results are presented on the spatial variation of CO, C, and C⁺. As shown in §§ III and IV, these distributions play important roles in determining the observational properties of circumstellar envelopes. Detailed demonstrations of the significance of the new theory of CO photodissociation are given in separate papers dealing with the distribution of CO in IRC +10216 (Huggins, Olofsson, and Johansson 1987) and with circumstellar chemistry (e.g. Mamon, Glassgold, and Omont 1987).

Although substantial progress has been made in understanding the photodissociation of CO on the basis of recent laboratory measurements, considerable additional work still needs to be done. Further experiments are required to identify the spectroscopic properties of the upper states and to measure the widths of the lines. Depending on the precise outcome of these experiments, more accurate treatments of the radiation transfer in circumstellar envelopes may then be required. Considerations similar to those discussed in this paper are also important for the modeling of interstellar clouds (Bally and Langer 1982; Paper I; van Dishoeck and Black 1987). For No. 2, 1988

1988ApJ...328..797M

example, the recent comprehensive chemical models of diffuse interstellar clouds (e.g., van Dishoeck and Black 1986; Viala, Abgrall, and Roueff 1987) are likely to have difficulty in accounting for the measured column densities of CO when the new and larger CO photodissociation rate is used, and new ways of synthesizing CO may be called for.

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APPENDIX

NOTE ON THE MEAN ESCAPE PROBABILITY

The basis for the calculation of the CO photodissociation rate is the mean escape probability introduced in equation (3). In this Appendix we outline its calculation for circumstellar envelopes undergoing steady mass loss. Photodissociation occurs following the absorption of a photon in a transition in which the electronic, vibrational, and rotational quantum numbers change, and we represent such a transition symbolically as $lJ \rightarrow uJ'$. We refer to the set of transitions that occur with fixed values of the initial and final electronic and vibrational quantum numbers as a band and label the band by i = (l, u).

The oscillator strength for the transition $lJ \rightarrow uJ'$ factors into

$$f_{lJ,uJ'} = f_{l,u} f_{J,J'} .$$
 (A1)

For absorption from the ground state of CO, $f_i \equiv f_{l,u}$ is tabulated in Table 1 and the nonvanishing (normalized) Hönl-London factors are $f_{J,J+1} = (J+1)/(2J+1)$ and $f_{J,J-1} = J/(2J+1)$. The probability for finding the initial rotational state J is specified by a normalized distribution P(J). As discussed in the text, we represent P(J) with a Boltzmann distribution rather than calculating it self-consistently.

The mean escape probability is defined by

$$\langle \beta_i \rangle = \sum_{JJ'} P_J f_{J,J'} \beta_{IJ,uJ'} , \qquad (A2)$$

i.e., in terms of the normalized distribution function, $P_J f_{J,J'}$. Following MJ, the escape probability for transition $lJ \rightarrow uJ'$ is approximated simply as

$$\beta_{IJ, uJ'} = f(3/2\tau_{IJ, uJ'}), \tag{A3}$$

where

$$f(x) = (1 - e^{-x})x^{-1}$$
(A4)

and the optical depth is

$$\tau_{IJ, \, uJ'} = P_J f_{l, \, u} f_{J, \, J'} (\pi e^2 / mc) \lambda_{IJ, \, uJ'} V^{-1} C x(r) r^{-1} , \qquad (A5)$$

where m is the electron mass, $\lambda_{IJ, uJ'}$ is the wavelength, and x(r) is the CO abundance at radial distance r. This expression is based on the usual formula for the hydrogen density in an envelope with steady mass-loss rate \dot{M} and expansion velocity V,

$$n_{\rm H} = C r^{-2} \tag{A6}$$

and

$$C = \dot{M} (4\pi m_{\rm H} V)^{-1} . \tag{A7}$$

In the interior of the envelope, where x(r) is constant, the fact that the optical depth is large and inversely proportional to r implies that the mean escape probability and the dissociation rate vary linearly with r, as long as the effects of dust can be ignored.

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808

1988ApJ...328..797M

MAMON, GLASSGOLD, AND HUGGINS

Note added in proof.—As noted above in §§ II and III, large line widths and line blending could introduce aspects of self-shielding that are outside of the theory of radiation transfer used in this paper, which is based on the Sobolev approximation and the assumption that the lines are well separated. We have made a preliminary study of this possibility by representing those bands that appear to be very broadened as uniform absorption continua. According to the qualitative analysis of Viala, Letzelter, Eidelsberg, and Rostas (Astr. Ap., in press [1988]), 13 CO dissociating bands appear to have extremely short lifetimes ($\leq 10^{-12}$). When these bands are treated as dissociating continua, spread over the width of the band, the abundance distributions of the CO photochain are altered somewhat but they retain the essential properties described in this paper. The size of the CO distribution is reduced by $\sim 40\%$ due to the fact that the generally smaller continuum absorption allows the dissociating radiation to penetrate further into the envelope. This effect enhances the conclusion emphasized in the text that the new understanding of CO photodissociation implies considerably smaller circumstellar envelopes than previously considered. Of course this discussion of broadened lines is highly simplified and the conclusions must be regarded as tentative. A more complete investigation must await definitive, highresolution laboratory studies of the far-UV spectrum of CO.

A. E. GLASSGOLD, P. J. HUGGINS, and G. A. MAMON: Department of Physics, New York University, 2 Washington Place, New York, NY 10003