

Atomic and molecular hydrogen in the circumstellar envelopes of late-type stars

A. E. Glassgold and P. J. Huggins *Physics Department,
New York University, 4 Washington Place, New York, NY 10003, USA*

Received 1982 July 14; in original form 1982 February 17

Summary. We discuss the distribution of atomic and molecular hydrogen in the expanding circumstellar envelopes of cool evolved stars. Our main concern is to evaluate the effects of photodestruction of H_2 by galactic UV radiation, including shielding of the radiation by H_2 itself and by dust in the envelope. One of the most important parameters is the H/H_2 ratio which is frozen out in the upper atmosphere of the star. For stars with photospheric temperatures $T_* \gtrsim 2500$ K, atmospheric models suggest that the outflowing hydrogen is mainly atomic, whereas cooler stars should be substantially molecular. In the latter case, photodissociation of H_2 and heavy molecules contribute to the atomic hydrogen content of the outer envelope. Our estimates indicate that atomic hydrogen is almost at the limit of detection in the C-rich star IRC + 10216, and may be detectable in warmer stars. Failure to detect it would have important implications for the general understanding of circumstellar envelopes.

1 Introduction

The circumstellar envelopes of cool evolved stars have recently become the subject of considerable observational attention. Line emission and absorption from the gas phase atoms and molecules as well as continuum radiation from the dust provide important information on a wide range of astrophysical processes, such as advanced stages of stellar evolution, nucleosynthesis, mass loss and grain formation (see e.g. Zuckerman 1980).

Despite this interest, relatively little theoretical analysis has been made of numerous physical and chemical processes which affect the circumstellar material. In a recent paper (Huggins & Glassgold 1982, hereafter referred to as Paper I), we discussed one such process, the photodestruction of heavy molecules in expanding carbon-rich envelopes induced by galactic ultraviolet radiation. Similar processes appropriate to oxygen-rich shells have been briefly discussed by Goldreich & Scoville (1976), Scalo & Slavsky (1980) and Jura & Morris (1981).

In this paper we focus on hydrogen in the circumstellar envelopes of cool stars. Our goal is to describe the partition into atomic and molecular hydrogen as a function of radial

distance in the envelope. The result is important because, being the most abundant species, the physical and chemical differences between H and H₂ affect the properties of the shell. Because the physical conditions in the stellar photosphere and the outer regions of the envelope differ so markedly, the problem is conveniently discussed in terms of characteristic regions within the envelope where different processes dominate. These include the thermal equilibrium between H and H₂ in the photosphere; the freezing-out of the abundances in the upper atmosphere of the star; possible formation of H₂ on warm grains at the inner edge of the dust shell; photodestruction of H₂ in the outer envelope — particularly the shielding of ultraviolet radiation by dust and by the Lyman band lines of molecular hydrogen; and the production of atomic hydrogen by photodestruction of heavy molecules. In Section 2 an overview of the problem is given; in Sections 3–6 specific processes in the different regions are discussed; and in Section 7 the results are discussed in terms of the observations.

2 General formulation of the hydrogen abundance problem

The physical picture we adopt is of a spherically symmetric envelope of dust and gas expanding from an evolved late-type star of photospheric temperature T_* . For simplicity we assume that the mass loss rate (\dot{M}) is constant and that the radial gas flow $v(r)$ tends to a constant (V) for large r , which implies an asymptotic density profile $n(r) \sim 1/r^2$. Typical parameters we have in mind are $T_* \approx 2000\text{--}3000\text{ K}$, $V \approx 5\text{--}30\text{ km s}^{-1}$, and \dot{M} in the range $1(-6) - 1(-4) M_\odot \text{ yr}^{-1}$.

The dimensions of the system can be crudely characterized by three radii: R_* , the photospheric radius of the star; $R_m(t)$, the outer boundary of the shell at time t ; and R_0 , where the dust begins to form and the wind speed approaches V . Our understanding of the physical conditions in the transition region, $R_* < r < R_0$, is limited, and we avoid using any but the most general information about it. Observations of the best studied circumstellar shell, that of IRC +10216 (Cohen 1979; Knapp *et al.* 1982; Kwan & Linke 1982; Zuckerman 1980) suggest envelope parameters $R_* \approx 1(14)\text{ cm}$, $R_0 \approx 3(15)\text{ cm}$, $R_m \sim 1(18)\text{ cm}$, $T_* \approx 2200\text{ K}$ and $\dot{M} \approx 1(-4) M_\odot \text{ yr}^{-1}$.

In Eulerian form, the differential equations for the number densities of atomic and molecular hydrogen, n_1 and n_2 , for prescribed steady flow $v(r)$ in the envelope are:

$$\left[\frac{\partial}{\partial t} + v \left(\frac{\partial}{\partial r} + \frac{2}{r} \right) + \frac{dv}{dr} \right] n = 0 \quad (2.1)$$

$$\left(\frac{\partial}{\partial t} + v \frac{\partial}{\partial r} \right) x_2 = P - D x_2 \quad (2.2)$$

where $n = n_1 + 2n_2$ is the total density of hydrogen nuclei, $x_2 = n_2/n$, and P and D specify appropriate production and destruction processes. The variable r may range over 4 orders of magnitude. Consequently, the terms contributing to P and D vary considerably and it is impossible to obtain a closed form solution satisfying the inner boundary condition. Our procedure is to simplify the rate equation (2.2) by keeping only the terms with the shortest time-scales. Solutions to the simplified equations can then usually be found and a global picture of the H/H₂ abundance obtained by assembling the solutions appropriate for each part of the shell.

In the following we discuss the solutions in the four regions illustrated schematically in Fig. 1:

- (1) The transition region, $R_* < r < R_0$, extending from the photosphere to the beginning of the dust shell. For cool stars the heavy atoms are mainly in the form of saturated

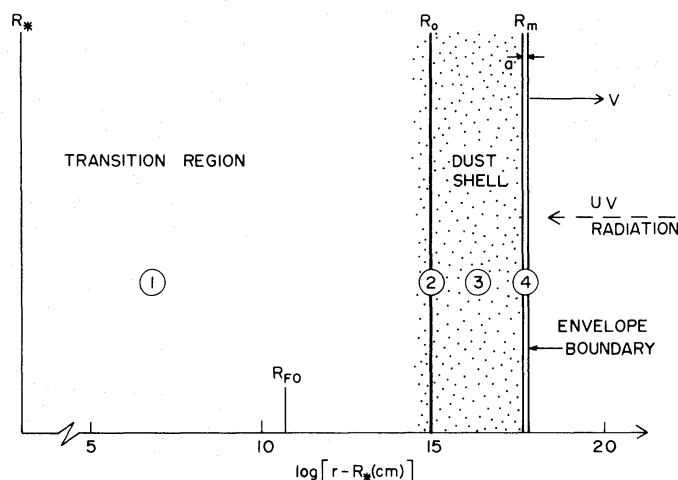


Figure 1. Schematic illustration of the regions important for the distribution of atomic and molecular hydrogen in a circumstellar shell. See Section 2 for discussion.

molecules, but hydrogen can be a mixture of atoms and molecules. Above the photosphere the temperature and density decrease so that the H/H_2 ratio becomes frozen in the upper atmosphere of the star.

(2) The inner surface of the dust shell, where the dust is fairly warm ~ 500 K and the gas density high $\sim 1(5) - 1(10) \text{ cm}^{-3}$. Here we consider whether H_2 can form on warm dust grains.

(3) The interior of the dust shell, where the physical properties resemble those in interstellar clouds. Here ultraviolet radiation from the surrounding interstellar medium can penetrate and dissociate H_2 , but the rate is diminished considerably by shielding by the molecules themselves and by grains.

(4) The outer edge of the dust shell where, within a characteristic length a , the shielding goes away and the dissociation rate tends to the ambient interstellar value.

3 Atomic hydrogen in the transition region between the photosphere and the dust shell

In the discussion of the H/H_2 ratio in circumstellar envelopes, the transition region between the photosphere and the bulk of the dust is the least tractable. There are two reasons for this. First, the outer atmospheric structure of cool stars is poorly known, and secondly, the physical processes (and consequent physical conditions) which drive the mass loss are highly uncertain. It is not known, for example, whether grain formation is the cause of, or merely the result of mass loss. Our discussion is therefore rather tentative. While this region is important for fixing the inner boundary condition for the remainder of the envelope, it constitutes only a small fraction of the total mass of an extended envelope.

3.1 FREEZE-OUT

The atmospheric structures of the coolest stars are rather poorly understood due primarily to the complex opacities contributed by the molecules which form at low temperatures. Based on available model atmospheres, thermal equilibrium calculations of abundances indicate that sufficiently cool stars may have comparable amounts of atomic and molecular hydrogen in their outer layers (Johnson, Beebe & Sneden 1975). Some examples of the run of abundance of atomic hydrogen, based on published atmospheres, are given in Fig. 2. The results for oxygen-rich (Fig. 2a) and carbon-rich (Fig. 2b) atmospheres are qualitatively

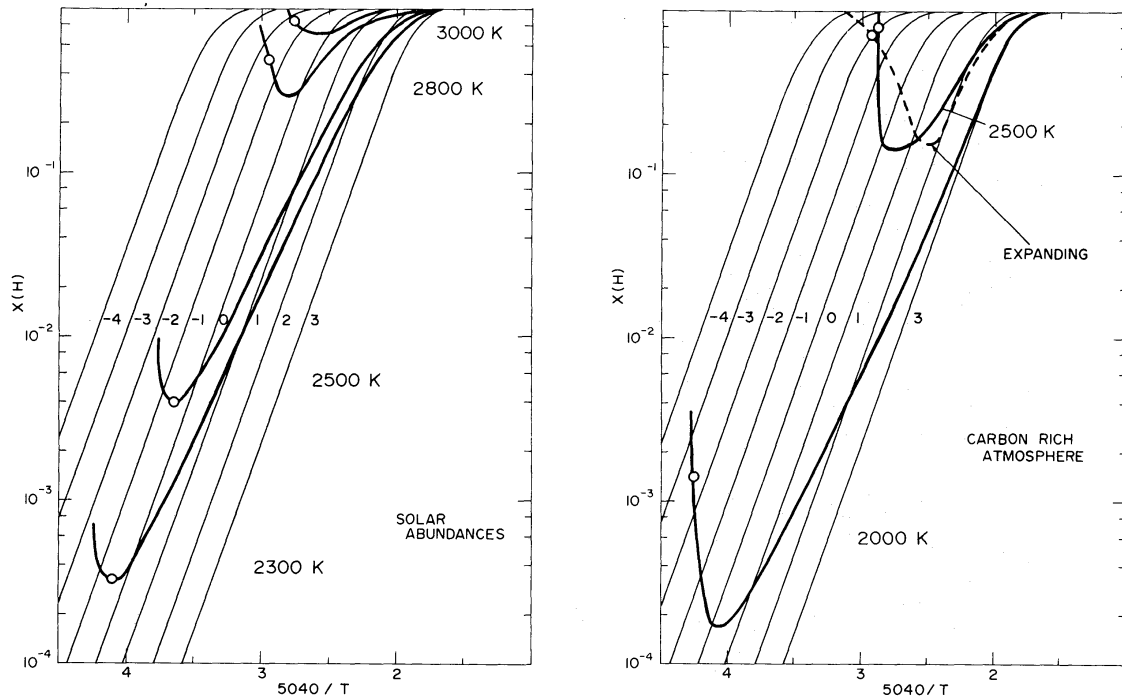
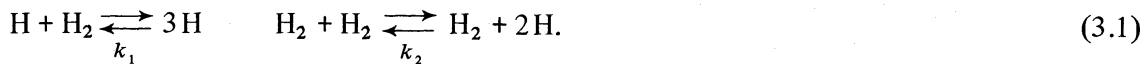


Figure 2. Thermal equilibrium abundance of atomic hydrogen. The light lines are a series of calculations at fixed pressure (labelled by $\log p$ in dyne/cm²). The heavy solid curves are runs of $x(\text{H})$ based on the static stellar atmospheres of Johnson (1974). (a) is for O-rich stars (solar abundances, $\log g = 1$) and (b) for C-rich stars ($\text{C/O} = 5$, $\log g = 1$) the dash curve is based on Lucy's (1976) calculation of an expanding atmosphere. The freeze-out points are indicated by open circles.

similar. In addition to the static models (Johnson 1974), results are shown for Lucy's expanding atmosphere (Lucy 1976) in Fig. 2(b). The run of atomic hydrogen is not very different from the static case for the same photospheric temperature, 2500 K. Fig. 2 indicates that temperature is the most important variable in determining equilibrium abundances in photospheric regions, and that the C/O ratio is a secondary factor.

For the p, T regime in question, the balance between H and H₂ is maintained by the reactions



The rate constants are well known (Jacobs, Giedt & Cohen 1967; Thoe 1978); for $T = 2000$ K, $k_1 \approx 2(-32)\text{ cm}^6\text{ s}^{-1}$ and $k_2/k_1 \sim 1/8$. From solutions of the rate equations derived from equation (3.1), the recombination time-scale is of order $2(30)\text{ s}(\text{n cm}^3)^{-2}$. Of course in equilibrium the forward and backward rates of the reactions (3.1) are equal.

At some point, which need not be specified exactly, radial motion of the gas must be initiated to feed the mass loss. Since details of this process are unknown, we merely adopt a characteristic dynamical time-scale for this process of $\sim 1(9)\text{ s} (= 1(14)\text{ cm km}^{-1}\text{ s}^{-1})$, which corresponds to gas motions at a few stellar radii which are a small fraction of the terminal outflow velocity. Under these conditions, three-body recombination ceases when $n \lesssim 1(11)\text{ cm}^{-3}$ ($\log P \sim -2$ or -3). In other words, H₂ freezes out at a value f_{FO} , determined by the condition $\tau_{\text{dy}} = \tau_{\text{rec}}$. These points are labelled FO in Fig. 2; they occur sufficiently far above the photosphere that most of the hydrogen in the stellar atmosphere is in thermal equilibrium. For very cool stars, $T_* \sim 2000$ K, $f_{\text{FO}} = 1$.

These considerations are barely altered by inclusion of H⁻ formation of H₂ (McDowell 1961; Dalgarno & McCray 1973): $\text{H}^- + \text{H} \rightarrow \text{H}_2 + \text{e}$. For carbon-rich model atmospheres at

$T_* = 3000, 2500$ and 2000 K, three-body formation dominates in the photosphere; the two mechanisms become comparable in the upper atmosphere where $\log P \sim -1$ or -2 , i.e. just before freeze-out occurs. Thus H^- formation may sustain chemical equilibrium beyond the point where three-body recombination can, in agreement with earlier considerations of this process in circumstellar shells (Clegg & Wootten 1980; Jameson & Williams 1981). The conclusion then stands, i.e. it is likely $f_{FO} \ll 1$ for $T_* \geq 2500$ K but, for $T_* \lesssim 2000$ K, f_{FO} will be very close to unity.

The quantitative aspects of these conclusions depend sensitively on the precise details of model atmospheres of cool stars with expanding envelopes. Theoretical work of this type is still at a provisional stage, especially for the coolest stars. For this reason it is advisable to consider f_{FO} as an initial condition in analysing the further chemical evolution of the hydrogen after it leaves the star and reaches the regions where substantial amounts of dust and heavy molecules exist. The possibility of freeze-out of the H/H_2 ratio just above the photospheres of cool stars was already noted by Goldreich & Scoville (1976); they assumed $f_{FO} = 2/3$ in their discussion of the envelopes OH/IR stars. Freeze-out of hydrogen can affect significantly the results of chemical calculations of heavier species.

The density and temperature decrease in the expanding envelope lead to a general decrease in chemical activity. Once three-body and negative-ion formation of H_2 cease, the H/H_2 ratio remains fixed unless some one- or two-body reaction becomes operative. The most important one-body destruction process is dissociation by ultraviolet photons. Unless strong chromospheric UV radiation is present, photodissociation operates in the outer regions of the shell, as will be discussed in Section 4.

3.2 FORMATION OF H_2 ON DUST

Another one-body process may be important, formation of H_2 on the surface of dust grains, with rate equation

$$\left. \frac{dn_2}{dt} \right|_{\text{Gr form}} = R_{\text{Gr}} n_1 n. \quad (3.2)$$

The rate constant R_{Gr} is the product of several factors: grain surface area per unit volume, sticking probability, and the probability for an adsorbed H atom to produce an H_2 molecule (once formed, the recombination energy of 4.5 eV is sufficient to eject the molecule from the grain). The usual value of the rate constant (Spitzer 1978), $R_{\text{Gr}} = 2(-17) \text{ cm}^3 \text{ s}^{-1}$, is obtained by taking the last two factors to be $\sim 1/3$ and by determining the third factor from interstellar extinction. The characteristic time for H_2 formation on grains, $\tau_{\text{Gr}} = 1/R_{\text{Gr}}n$ is $\sim 1(9) \text{ yr } n^{-1}$ for the interstellar medium. If the rate for circumstellar envelopes is about the same, then the high densities in the inner regions of these shells could make $\tau_{\text{Gr}} < \tau_{\text{dy}}$. To determine whether grain formation of H_2 is relevant, we rewrite this inequality using $\tau_{\text{dy}} = r/v$, $n = C/r^2$ for steady mass loss, where

$$C = \dot{M}/4\pi m_H v = 3(37) \text{ cm}^{-1} \dot{M}_{-5}/v_{10} \quad (3.3)$$

and \dot{M} is the mass loss rate of hydrogen nuclei ($\dot{M}_{-5} = \dot{M}/1(-5) M_\odot \text{ yr}^{-1}$ and $v_{10} = v/10 \text{ km s}^{-1}$). The result is

$$r < b \equiv R_{\text{Gr}} C/v = 9(14) \text{ cm}^{-1} \dot{M}_{-5} v_{10}^{-2}. \quad (3.4)$$

In other words, thick circumstellar shells with $\dot{M}_{-5}/v_{10}^2 > 1$ will recombine atomic hydrogen at $r \sim 1(15) \text{ cm}$ if R_{Gr} has the optimum interstellar value. We now present reasons why this may be the case.

We divide the discussion of R_{Gr} into two parts, (1) the probability for sticking and recombination, and (2) the effective grain area per unit volume. For the interstellar medium, the theory of topic (1) has been dominated by the concept of a maximum or critical dust temperature T_{cr} for efficient formation. The key quantity is the evaporation time

$$t_{\text{evap}} = \nu_0^{-1} \exp(D/kT_d) \quad (3.5)$$

where D is the binding energy and ν_0 is the 'trial' rate, $\sim 1(12)\text{s}^{-1}$. For warm grains with mainly weak binding sites, t_{evap} could become so short that recombination does not occur. Although Hollenbach & Salpeter (1971) estimated $T_{\text{cr}} \sim 20\text{ K}$ (revised upwards to 25–40 K by Goodman 1978), they emphasized that impurities and defects could produce strong binding sites which would increase T_{cr} substantially. Barlow & Silk (1976) went even further by advocating that most sites were chemically absorbing, which raises D/k from ~ 1000 to $10\,000\text{ K}$.

The problem of hydrogen recombination on warm grains becomes critical for circumstellar shells because the dust is heated directly by the star. For concreteness we consider IRC+10216 where model fits to the infrared observations agree in the relevant region $r = 1(15)–1(16)\text{ cm}$ (Crabtree & Martin 1979; Mitchell & Robinson 1980; Rowan-Robinson & Harris 1982); the temperatures at these two positions are ~ 500 and 200 K , respectively.

It is an open question whether circumstellar dust at these temperatures can form H_2 efficiently. The answer depends sensitively on the physical properties of the newly formed dust. Warm grain formation of H_2 has been discussed by Hollenbach & McKee (1979), along the lines of the original investigation of Hollenbach & Salpeter (1971). For a reasonable fraction of impurity sites $\sim 1(-4)$, and $D/k \sim 800\text{ K}$ for physical adsorption (Goodman 1978), their considerations suggest $T_{\text{cr}} \sim 100\text{ K}$. If the bulk of the sites are chemically adsorbing (Barlow & Silk 1976), then the critical temperature would be higher, $\sim 300\text{ K}$.

On the basis of observations of Solar System particles, Adabi *et al.* (1976) suggested that interstellar grains have a microporous structure which increases their area as well as their adsorption potentials. These authors suggest that warm microporous grains provide a large and efficient surface for forming H_2 . This proposal, founded on laboratory studies of microporous substances, together with the trend of theoretical discussions, suggests that H_2 formation on circumstellar dust grains must be considered as a real possibility.

Hollenbach & McKee (1979) also considered the dependence of the sticking probability S on the incident gas speed. As long as the drift velocity of the grains relative to the gas does not become too large, i.e. $\geq 3\text{ km s}^{-1}$, $S \approx 0.2–0.4$ – not much different from earlier estimates of $1/3$. Grain collisions could also destroy the molecules in fast collisions (Goldreich & Scoville 1976) but, for H_2 , the required velocities $\sim 10\text{ km s}^{-1}$ are higher than expected for circumstellar shells. Previous theoretical models of C-rich shells (Kwan & Hill 1977) and O-rich shells (Goldreich & Scoville 1976) have used drift velocities of 2 and 9 km s^{-1} , respectively. Because the connection between drift velocity and stellar parameters is not yet well founded, it is reasonable to conclude that the sticking probability for H atoms is not negligible.

The other important factor in the rate constant R_{Gr} , the grain area per unit volume, is the product of the grain number density and mean surface density per grain. Again these properties are poorly understood, and both factors could be larger for new circumstellar grains as opposed to interstellar grains. For example, Adabi *et al.* (1976) note that microporous grains could have 100 times more surface area than would be expected on the basis of their linear dimensions.

We conclude from this discussion of H_2 formation on warm circumstellar grains that the rate constant may be large enough to alter significantly the initial molecular fraction f

entering the envelope. Given this possibility, it is of interest to determine the variation in f due to grain formation. Assuming that the gas enters the part of the dust shell where $r > R_0$ with H_2 fraction f_{FO} , and that the wind has reached terminal speed, the Lagrangian form of equation (2.2), with $D = 0$ and P determined by equation (3.2), becomes

$$\frac{d}{dr} \ln x_1(r) = -b/r^2 \quad (3.6)$$

where b was defined in equation (3.4). The radial coordinate is related to the travel time by $r - R_0 = Vt$. For constant b , the solution is

$$x_1(r) = (1 - f_{FO}) \exp [b/r - b/R_0]. \quad (3.7)$$

The asymptotic form is controlled by the factor $\exp(-b/R_0)$; substantial conversion requires $b/R_0 \gtrsim 2$ or 3. More generally the characteristic length $b \propto R_{Gr} \dot{M} v^{-2}$ can vary, so equation (3.7) is only useful where the r^{-2} variation in density dominates. To illustrate the use of (3.7), we assume $T_{cr} \sim 200$ K. On the basis of the dust temperature profiles for IRC+10216, we expect the H_2 forming region of the dust shell to begin at $R_0 > 1(15)$ cm, and probably $\sim 1(16)$ cm. In order to obtain substantial conversion b must be at least as large and, from equation (3.7), this requires mass loss rates $\gtrsim 1(-4) M_\odot \text{ yr}^{-1}$. On the other hand, if grains as warm as 500 K are effective in forming H_2 , b could be the actual inner radius of the dust shell and the minimum mass loss rate required for conversion to H_2 could be of the order of $1(-5) M_\odot \text{ yr}^{-1}$.

It is important to reiterate how uncertain our understanding is of the transition region. The above discussion of freeze-out is a good example, in that our estimates of f_{FO} depend on the least reliable part of the model atmosphere calculations. Closely related is the question of whether the upper atmospheres of cool stars with thick circumstellar shells possess chromospheric regions. There is evidence that α Ori, an M2 supergiant, has a chromosphere (Lambert & Snell 1975; Wischniewski & Wendkar 1981; Linsky & Haisch 1979; Strickland & Sanner 1981). In this case the passage through the warm, partially ionized chromosphere alters the H/H_2 ratio, e.g. by H_2 formation of H^- and photodestruction by chromospheric UV radiation. The situation is further complicated by the possible occurrence of shocks, either in the stellar atmosphere or in the outer envelope (Cohen 1980). Further general discussion of these phenomena is probably unwarranted until more is known about the transition region.

4 The interior of the shell

By the time the gas has reached distances $r > b$ (defined in 3.4), all chemical activity will have ceased except for photodissociation. In analysing photodissociation, we have explicitly in mind the most interesting case of the more massive envelopes around cooler stars, for which the bulk of the hydrogen gas entering this region will be in molecular form as described in Section 3. Solutions for other cases can be developed by adopting appropriate boundary conditions. For $r \ll R_m$, photodestruction will be very slow, simply because there is so much gas to shield the incident UV radiation. With increasing r , the column density to the outside, $N(r) = C/r$ decreases, and eventually the photodestruction time becomes comparable to dynamical time-scale r/V .

Molecular hydrogen is destroyed by UV radiation in the 912–1108 Å wavelength band by a two-step process originally proposed by Solomon (Field, Somerville & Dressler 1966; Stecher & Williams 1967). For typical values of the galactic radiation field, the dissociation rate is $G_0 = 6(-11) s^{-1}$. The corresponding time-scale $\tau = 1/G_0 = 1.67(10) s = 528 \text{ yr}$ is

shorter than the typical ages of the envelopes of interest here, so photodissociation of H_2 does occur in regions of small or moderate shielding.

In addition to continuum shielding by dust grains and by the most abundant heavy molecules, the dominant shielding occurs in the Lyman band transitions themselves.* Ignoring formation processes, and using $v(r) \approx V$, we write the rate equation (2.2) as

$$\left(\frac{\partial}{\partial t} + V \frac{\partial}{\partial r}\right) x_2(r, t) = -\frac{1}{\tau} J[N_2(r, t)] \exp[-N(r)/N_{\text{sh}}] x_2(r, t). \quad (4.1)$$

The quantity $J \leq 1$ is the self-shielding function introduced by Hollenbach, Werner & Salpeter (1971) and applied to diffuse clouds by Federman, Glassgold & Kwan (1979); N_{sh} is an effective column density for continuum absorption by dust grains, heavy interstellar molecules, and other neutral species. For purposes of simplicity we retain only dust absorption because the other species make only a quantitative difference, especially in view of the fact (to be demonstrated below) that H_2 line self-shielding dominates.† The column densities $N_2(r, t)$ and $N(r, t)$ are along a radius from r to the shell edge, e.g.

$$N_2(r, t) = \int_r^{R_m} dr' n_2(r', t). \quad (4.2)$$

In equation (4.1) and the following, the use of exponential dust attenuation and a plane parallel slab approximation for J can be justified in terms of the large optical depth of the shell.

The solution of equations (4.1) and (4.2) is carried out in two stages subject to the boundary condition:

$$f[R_m(t), t] = f_1 \exp\left(-\frac{Vt - R_1}{\tau}\right) \quad (4.3)$$

where R_1 is a position in the inner shell considerably further out than $r = b$ (i.e. where essentially all reactions except photodestruction have ceased) and f_1 is the fraction of molecular hydrogen in the gas after freeze-out in the upper photosphere and any modification at $r = b$. In the first part of the solution, given here, we develop an approximation valid throughout most of the envelope for $r > R_1$ except close to the outer boundary. The surface region is dealt with in Section 5.

We consider positions sufficiently far inside the shell that the Lyman band lines are so optically thick that photodissociation occurs in the radiative wings of the lines. For expansion velocities $V \sim 10 \text{ km s}^{-1}$, this means $N_2(r, t) \gtrsim 1(19) \text{ cm}^{-2}$. Using the approximate form $N = C/r$, and assuming $f_1 = 0(1)$ so that $N_2(r, t) \approx N(r, t)/2$, we find that this condition is satisfied throughout the shell except near its outer edge. The radiative wings approximation for the self-shielding is then appropriate

$$J \approx (\mathcal{M}/N_2)^{1/2} \quad (4.4)$$

with $\mathcal{M} = 6.743(11) \text{ cm}^{-2}$, N_2 replaced by $\frac{1}{2}N = C/2r$.

Under the stated approximations, we recast equation (4.1) into Lagrangian form

$$\frac{d}{dt} \ln f(t, u) = -\frac{1}{\tau} \left[\frac{\mathcal{M}}{C} r(t, u) \right]^{1/2} \exp[-C/N_{\text{sh}} r(t, u)]. \quad (4.5)$$

* If all the molecules are in the lowest ortho- and para-rotational states ($J = 0, 1$), there are 60 Lyman band transitions in the relevant band pass. The Werner band transitions play a negligible role in dissociation.

† Similarly we ignore line absorption by heavy molecules, radicals and atoms.

The Lagrangian coordinate has been chosen as the particular time instant u when a mass element crosses the spherical shell R_{1n} ; by time t it will have reached the position $r(t, u) = R_1 + V(t - u)$. We can reduce equation (4.5) to quadrature by integrating over $dr_\mu = Vdt$ for fixed u and using the boundary condition $f(u, u) = f_1$:

$$\ln f(t, u)/f_1 = -\frac{1}{V\tau} (\mathcal{M}/C)^{1/2} \int_{R_1}^{r(t, u)} dr' r'^{1/2} \exp(-d/r') \quad (4.6)$$

where

$$d = C/N_{\text{sh}} \quad (4.7)$$

characterizes continuum absorption by dust in an expanding envelope; near $\lambda = 1000 \text{ \AA}$, $N_{\text{sh}} = 5.8(20) \text{ cm}^{-2}$ for interstellar dust. The result (4.6) holds for $r(t, u) < R_m(t)$. We usually suppress the argument (t, u) and write f as a function of r .

In analysing equation (4.6), it is useful to define the exponential integral-like function

$$D(x) \equiv \int_x^\infty ds \exp(-s) s^{-5/2} \quad (4.8)$$

which has the following limiting forms:

$$D(x) \rightarrow \frac{2}{3} x^{-3/2} \quad x \rightarrow 0; \quad D(x) \rightarrow \exp(-x) x^{-5/2} \quad x \rightarrow \infty. \quad (4.9)$$

An approximate solution in the outer shell can now be given

$$\ln f(r)/f_1 = -\alpha [D(d/r) - D(d/R_1)] \quad (4.10)$$

where

$$\alpha = \frac{d}{V\tau} \left[d / \left(\frac{C}{\mathcal{M}} \right) \right]^{1/2}. \quad (4.11)$$

We can obtain a qualitative understanding of the solution by considering the case $R_1 \ll d$. The second term of equation (4.10) is then negligible according to the asymptotic form of D in equation (4.9). This case is realized for moderate to large mass loss rates, say $\dot{M} \gtrsim 1(-6) M_\odot \text{ yr}^{-1}$, according to equation (4.7). For positions $d \ll r \ll R_m$, dust shielding is unimportant and the variation in the H_2 abundance due to self-shielding of the Lyman band lines is given by

$$\ln f(r)/f_1 \cong -\frac{2}{3} \frac{(\mathcal{M}/C)^{1/2}}{V\tau} r^{3/2}. \quad (4.12)$$

On the other hand, for $R_1 \ll r \ll d$, we obtain from equation (4.9)

$$\ln f(r)/f_1 \cong -\alpha \exp(-d/r) \left(\frac{d}{r} \right)^{-5/2} \quad (4.13)$$

which expresses the effects of line and dust shielding. Exact representations of the solution (4.10) are given in Figs 3 and 4. As we will verify in Section 5, this is essentially the exact solution to the problem, with only small corrections occurring near the boundary surface $r = R_m(t)$.

In Fig. 3 we illustrate the solution (4.10) for parameters suggested by IRC +10216: $\dot{M} = 4(-5) M_\odot \text{ yr}^{-1}$ and $V = 16 \text{ km s}^{-1}$; the parameters in our theory are: $d = 1.29(17) \text{ cm}$, $C/2\mathcal{M} = 1.11(26) \text{ cm}$ and $\alpha = 2.34(-4)$. This is a log-log plot of $1-f$, where $1-f$ is the abundance of atomic hydrogen resulting from the photodissociation of H_2 . The initial

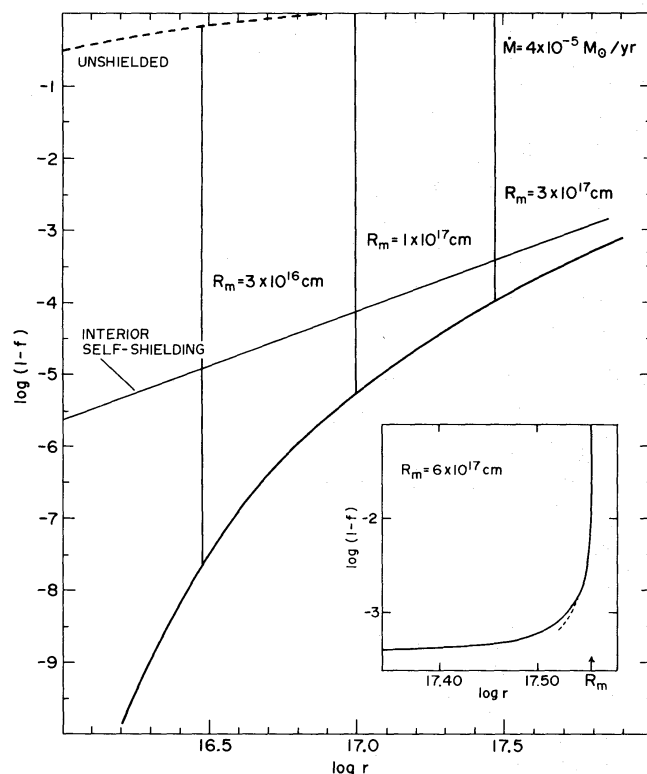


Figure 3. The molecular hydrogen run in the interiors of three shells of different ages, $t = 600, 1800$ and 6000 yr, corresponding to outer radii of $0.3, 1.0$ and $3.0(17)$ cm, given as $\log(1-f)$ versus $\log r$. The parameters are suggested by IRC + 10216: $\dot{M} = 4(-5) M_{\odot} \text{ yr}^{-1}$ and $V = 16 \text{ km s}^{-1}$. The heavy solid curve is the interior solution equation (4.10); the dashed line at the top is for no shielding. The H_2 abundance in the interior of the shell is given by the solid curve for $r < R_m(t)$ and by the heavy vertical line connecting it with the dash curve. There is no discontinuity in slope at R_m ; the insert shows the smooth transition on a small scale for the case $R_m = 6(17)$ cm.

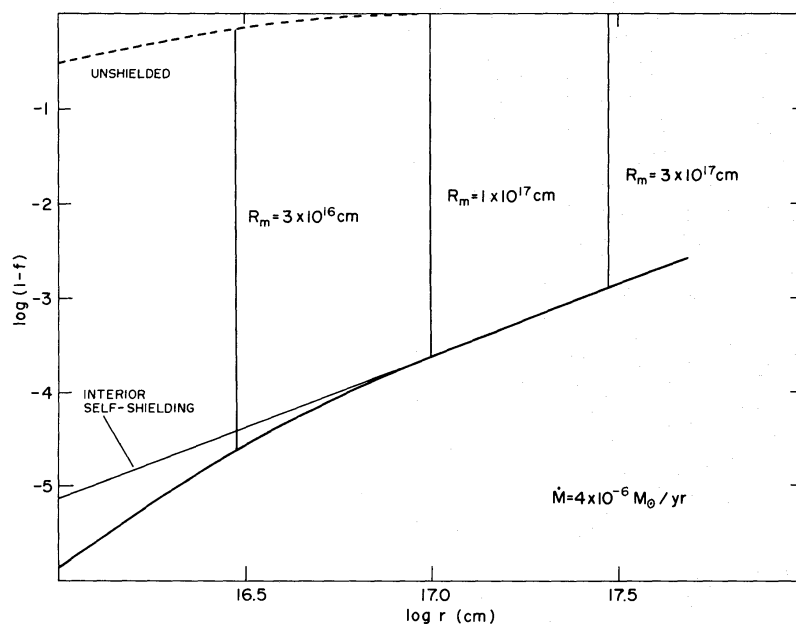


Figure 4. $\log(1-f)$ versus $\log r$ for the three shells in Fig. 3, except the mass loss rate has been reduced by 10: $\dot{M} = 4(-6) M_{\odot} \text{ yr}^{-1}$.

abundance has been chosen as $f_1 = 1$. Shells of three ages are shown, and their boundaries are indicated by heavy vertical lines. At the top of the figure, the abundance variation for unshielded decay $f(r)/f_1 = \exp(-r/V\tau)$, is represented by a dashed line. The heavy line at the bottom is the solution (4.10). Thus a shell of finite age is represented by the heavy curve for $r < R_m$ and the vertical line at $r = R_m$ connecting it with the curve for unshielded decay. As will be shown below, the transition does not have a discontinuity in slope but occurs smoothly over a very small distance. The insert for $R_m = 6(17)$ cm shows the transition region for an old shell, as derived in Section 5. For the younger shells the transition thickness is too small to be visible in the figure.

We see in Fig. 3 that the molecular hydrogen is very effective in shielding the interior of the shell. To demonstrate the dominant role of self-shielding, we also plot the case of no continuum absorption, equation (4.12), as the thin solid line in the middle of Fig. 3.

Fig. 4 illustrates the effect of reducing the mass loss rate by a factor of 10 while keeping all other parameters the same. Because of the non-linear properties of the shielding, $1-f$ increases by several orders of magnitude and reaches the $1(-3)$ level near the shell boundary. The most dramatic change is the decrease in the relative contribution of dust as compared to line shielding.

5 The transition at the surface of the circumstellar shell

The above theory breaks down near the boundary $r = R_m(t)$ for several reasons. First we have replaced N_2 by $N/2$ in the self-shielding factor in equation (4.1). Secondly we have ignored the existence of the boundary by using the approximation C/r for the column density to the outside, rather than $C(1/r - 1/R)$. Another possible source of error is the use of the radiative wings approximation for J in the surface region where the abundance of H_2 must tend to the surface value equation (4.3). We begin the investigation of the surface region with the exact Eulerian equation (4.1) and the differential form of equation (4.2). We ignore the shielding by continuum absorption (justified *a posteriori* by the small transition thickness in most cases) and replace the abundance by the density $n_2 = xn$:

$$\left[\frac{\partial}{\partial t} + V \left(\frac{\partial}{\partial r} + \frac{2}{r} \right) \right] n_2(r, t) = - \frac{1}{\tau} J[N_2(r, t)] n_2(r, t) \quad (5.1)$$

$$n_2(r, t) = - \frac{\partial}{\partial r} N_2(r, t). \quad (5.2)$$

We make the Galilean transformation

$$\rho = R_1 + Vt - r = R_m(t) - r \quad (5.3)$$

substitute (5.2) into (5.1), carry out the proper transformations to obtain a second-order equation for $N'_2(\rho, t) = N_2(r, t)$,

$$\left[\frac{\partial}{\partial t} + 2 \frac{V}{R_m(t)} + \frac{1}{\tau} J(N'_2) \right] \frac{\partial N'_2}{\partial \rho} = 0. \quad (5.4)$$

To integrate this equation, we transform the third term using the relation between the self-shielding factor J and the equivalent width W for each line (Federman *et al.* 1979):

$$J_i(N'_2) dN'_2 = (h_i \sigma_i)^{-1} dW(N'_2) \quad (5.5)$$

where $\sigma_i = f_i(\pi e^2/mc)$ and h_i is the fraction of H_2 in the lower state of transition i . The

function J which appears in equation (5.4) is an average over all Lyman band lines. Defining a particular mean equivalent width:

$$w(N_2') = \left\langle \frac{1}{h_i \sigma_i} w_i(N_2') \right\rangle \quad (5.6)$$

and integrating equation (5.3) with the boundary condition $N_2'(0, t) = 0$, we obtain this equation for the column density:

$$\left[\frac{\partial}{\partial t} + 2 \frac{V}{R_m(t)} \right] N_2'(\rho, t) = -\frac{1}{\tau} w[N_2'(\rho, t)]. \quad (5.7)$$

This first-order partial differential equation cannot be integrated easily, even for $\rho \ll R_m$, unless w has a simple functional form. A solution can be constructed, however, by piecewise approximation of w by power laws, $w = kN^n$ (with $n = 1, 0$ and $1/2$ for column densities defining, respectively, the linear, flat and square-root portions of the curve of growth):

$$N_2'(\rho, t) = u^{-2} \left\{ (1-n) \left[f(\rho) - \frac{k}{3-2n} u^{3-2n} \right] \right\}^{1/1-n} \quad (5.8)$$

where $u = R_m(t)/V\tau$ and $f(\rho)$ is a function to be determined from boundary conditions; this solution is valid only for $\rho \ll R_m(t)$.

For diffuse interstellar clouds, the radiative wings approximation ($n = 1/2$) is appropriate because the H–H₂ transition is large, $\sim 5(20) \text{ cm}^{-2}$ (Federman *et al.* 1979). For circumstellar shells, however, the transition region (in which f ranges from the boundary value in equation 4.3 to the interior value f_1) is too small to be consistent with the radiative wings approximation. The flat portion of the curve of growth is appropriate, and we use the approximation (when the optical depth is greater than two) based on a Gaussian line shape:

$$w \cong 260 \left[\frac{\pi e^2}{mc} \right]^{-1} N_2^n, \quad n = 0.15. \quad (5.9)$$

The use of a Gaussian line shape is justified by the very small size of the transition layer, which makes any effect of the velocity gradient in the expanding envelope negligible. The magnitude of the velocity dispersion is probably determined by turbulence, which might be large near the outer boundary of the envelope. Of course little is known about the physical conditions near the edge of the shell, which may be affected by the interaction of the expanding envelope with the interstellar medium.

We next invoke the proper boundary condition. Keeping ρ fixed, we consider an earlier time $t_1 \ll t$ when $f[R_m(t) - \rho, t_1] = f_1$; the initial value for the H₂ column density is then

$$N_2'(\rho, t) = \frac{1}{2} \frac{C}{R_m(t)^2} \rho. \quad (5.10)$$

Equation (5.8) finally becomes

$$N_2'(\rho, t) = \frac{f_1}{2} \frac{C}{R_m(t)^2} a(t) \{ [\rho/a(t)]^{1-n} - 1 \}^{1/1-n} \quad (5.11)$$

where

$$a(t) = \left(\frac{1-n}{3-2n} \right)^{1/1-n} \frac{v_{\text{rms}}}{\bar{\lambda}} \left[1.53(-3) \frac{\pi e^2}{mc} \frac{f_1}{2} \frac{C}{(V\tau)^2} \right]^{-1} \\ \times \{ [R_m(t)/V\tau]^{3-2n} - [R_m(t_1)/V\tau]^{3-2n} \}^{1/1-n} \quad (5.12)$$

is a new length characterizing the surface region. Inserting appropriate numerical factors, and ignoring the second term in equation (5.12), we find that

$$a(t) = 3.49(13) \text{ cm} \left(\frac{\bar{v}_{\text{rms}}}{\text{km s}^{-1}} \left/ V_{10}^{0.18} \dot{M}_{-5} f_1 \right. \right) R_m(t)^{3.18} \quad (5.13)$$

measuring R_m in units of 1(17) cm. Despite the rough cubic dependence, this parameter remains quite small even for old shells with $R_m \sim 1(18)$ cm.

The insert to Fig. 3 illustrates this solution using

$$f(r, t) = f'(\rho, t) = \left[\frac{\rho}{a(t)} \right]^{-n} \left\{ \left[\frac{\rho}{a(t)} \right]^{1-n} - 1 \right\}^{n/1-n}. \quad (5.14)$$

This expression vanishes at $\rho = a(t)$ and then increases with increasing ρ ; it is valid only for $\rho \ll R_m$, and eventually increases too much. The solid curve, calculated for $R_m = 6(17)$ cm and $v_{\text{rms}} = 5 \text{ km s}^{-1}$ is an interpolation between equation (5.13) and the interior solution, equation (4.10). This illustration shows how the abundance makes a smooth transition over a very small distance, in this case $\sim 1(17)$ cm.

6 Photodestruction of heavy molecules

The photodestruction of heavy molecules is another source of atomic hydrogen, as has been noted by Lafont, Lucas & Omont (1981) for the case of IRC+10216. The basis for this effect is given in Paper I, which deals explicitly with the photodestruction of heavy molecules, taking account shielding by dust and H_2 molecules. The details can be found in Appendix B of Paper I.

For illustration we consider IRC+10216 where $x(\text{C}_2\text{H}_2) = 1(-5)$, taking into account new f values (Ridgway & Hall 1976). We find that $x_{\text{HM}}(\text{H})$ increases rapidly for $r \gtrsim d(\text{C}_2\text{H}_2)$ – the characteristic dust shielding parameter for the photodestruction of C_2H_2 (defined in a similar way to the corresponding parameter for H_2 in equation 4.7). As r increases beyond $d(\text{C}_2\text{H}_2)$, $x_{\text{HM}}(\text{H})$ will approach $2x_1(\text{C}_2\text{H}_2)$, i.e. every C_2H_2 molecule will eventually be destroyed and produce two H atoms. For IRC+10216, for example, we expect $x_{\text{HM}}(\text{H})$ to reach $\sim 2(-5)$ beyond $r = 1(17)$ cm.

7 Discussion and summary

Two important conclusions can be drawn immediately from Sections 2–6: (1) the H/H_2 ratio in a circumstellar shell can vary dramatically with radius, and (2) it is very sensitive to the temperature of the central star and the mass loss rate.

The complexity of the abundance variation arises from the great range in physical conditions which can occur. In our highly idealized picture, we considered freeze-out in the stellar atmosphere; catalysed formation of H_2 molecules; slow, shielded photodestruction in the bulk of the envelope; and some photoproduction of atomic hydrogen from heavy molecules. The true situation may be further complicated by other processes which we have not considered, e.g. high speed shocks.

Two extreme cases help simplify the issues. For the hotter stars $T_* \gtrsim 3000 \text{ K}$ it seems likely that the hydrogen entering the bulk of the envelope after freeze-out will be atomic, and will remain so unless recombination occurs. Considering our uncertain understanding of the physical and chemical properties of circumstellar grains, this last possibility should be left open. For the coolest stars $T_* \lesssim 2000 \text{ K}$ with thick shells, the bulk of the envelope will be in molecular form except for a very thin shell at the outer edge of the envelope.

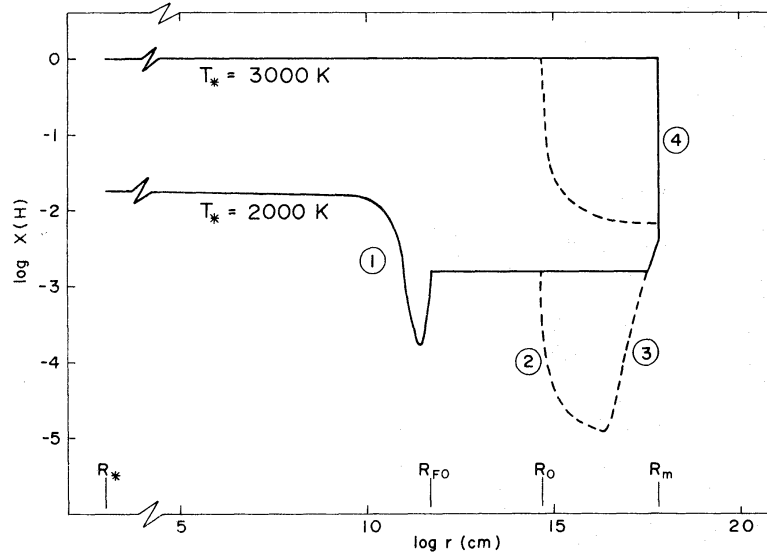


Figure 5. A schematic representation of the atomic hydrogen distribution for two thick circumstellar shells ($R_m = 6.3(17)$ cm and $\dot{M} = 4(-5) M_\odot \text{ yr}^{-1}$) but different photospheric temperatures. The four regions are the same as in Fig. 1. The dash curve shows the effect of efficient H_2 formation on warm grains. The solid curves are without this formation mechanism. For $T_* = 3000$ K the envelope is atomic, whereas for $T_* = 2000$ K the envelope is essentially molecular. In the latter case the H_2 abundance remains at the freeze-out level until photodestruction of H_2 become effective at the outer edge.

Intermediate cases may show a rich variety in structure, depending on stellar temperature and atmospheric structure and on the possibilities for grain catalysis. Some possibilities for the variation in the H/H_2 ratio with radius are shown schematically in Fig. 5.

Zuckerman, Terzian & Silverglate (1981, hereafter ZTS) have recently attempted to detect 21-cm emission from atomic hydrogen in envelopes around a variety of evolved stars using the Arecibo antenna (FWHM 3.2 arcmin). Their best limits were for the cool carbon star IRC+10216, for which an upper limit to the column density of $6(18) \text{ cm}^{-2}$ was obtained; this leads to an upper limit for the mass of atomic hydrogen $M_{\text{I}}(\text{IRC}+10216) < 1.1(31) \text{ gr}$. As a fraction of the total hydrogen mass M_{H} , this is $M_{\text{I}}/M_{\text{H}} < 0.012$, where we estimate $M_{\text{H}} = \dot{M} R_m / V = 0.94(33) \text{ gr}$ for a constant mass loss rate of $\dot{M} = 4(-5) M_\odot \text{ yr}^{-1}$, $R_m = 6(17) \text{ cm}$ (using a distance of 220 pc) and $V = 16 \text{ km s}^{-1}$.

We now compare this result of ZTS with the model given in this paper. There are five contributions to the atomic hydrogen content of IRC+10216, which arise from: (1) the photospheric layers, (2) injection into the envelope without recombination, (3) photodissociation of H_2 in the interior of the dust shell, (4) photodissociation of H_2 in the thin surface region and (5) photodestruction of heavy molecules.

According to Johnson *et al.* (1975), a typical column density for a cool, carbon-rich star with $\log g = 0$ is $N(\text{H I}) \sim 1(24) \text{ cm}^{-2}$. Adopting a stellar radius $R_* \sim 1(14) \text{ cm}$ (Cohen 1979), this gives $M_{\text{I}*} \approx 2.1(29) \text{ gr}$ for the photospheric H I , i.e. a fraction $M_{\text{I}*}/M_{\text{H}} = 2.2(-4)$ using the above mass estimate. Of course 21-cm emission from this warm H I will be beam diluted to $T_{\text{B}} \sim 2000 \text{ K}$ $(R_*/R_{\text{beam}})^2 \sim 2(-4) \text{ K}$, e.g. well below the sensitivity of the ZTS experiment.

The second and third contributions are from the interior of the dust shell and are given by ($c = C/2m$)

$$M_{\text{Ish}} \approx 4\pi C R_m m_{\text{H}} \left[(1-f_1) + \frac{1}{15} R_m^{3/2} f_1 / V \tau c^{1/2} \right]. \quad (7.1)$$

As discussed in Sections 3 and 4, the second term, arising from photodissociation, may be smaller than the initial H abundance $1-f_1$ even for stars as cool as $T_* \sim 2000$ K. For IRC + 10216 we estimate

$$M_{\text{Ish}}(\text{IRC} + 10216) \approx 0.944(33) \text{ gr} [(1-f_1) + 1.6(-4)f_1] \quad (7.2)$$

where the coefficient is the total amount of hydrogen. For the model atmosphere J 24 of Johnson (1974) with $T_* = 2000$ K, it is interesting that $1-f$ does become as small as $1.7(-4)$, but the freeze-out value is 10 times larger. For Cohen's value $T_* \approx 2300$ K, the freeze-out abundance is probably ~ 0.01 . Of course the surface temperature of IRC + 10216 is not known precisely and the model atmospheres are uncertain. To summarize, the mass of photodissociated hydrogen is $\sim 1.5(29)$ gr, and the mass surviving from the photosphere could be as much as $1(31)$ gr.

The fourth contribution from the envelope edge is $M_{\text{Itr}} = 4\pi C a m_{\text{H}}$. Using equation (5.13) we estimate $M_{\text{Itr}}(\text{IRC} + 10216) \sim 1.9(29)$ gr – about the same as the photodissociated hydrogen in the interior. The atomic hydrogen arising from the photodestruction of hydrocarbons is $1.9(28)$ gr, and is less important than photodissociation of H_2 .

In comparing these estimates with the ZTS, we note that their upper limit $M_1 < 1.1(31)$ gr is ~ 20 times larger than the mass of atomic hydrogen produced by the photodissociation of all hydrogen-bearing molecules, which we estimate to be $5.5(29)$ gr. However, the atomic hydrogen surviving from the photosphere, if not reformed in the inner dust shell, could be as much as $1(31)$ gr if $T_* \approx 2300$ K and if the provisional stellar atmospheres are roughly correct. This suggests that atomic hydrogen is almost at the limit of detection in circumstellar shells of cool carbon-rich stars like IRC + 10216, and presently detectable in somewhat warmer stars with $T_* \gtrsim 2500$ K and similarly high mass loss rates. Failure to detect 21-cm emission would imply that either recombination does occur on warm grains, or that stellar atmosphere calculations now available are in serious error.

Clearly it would be of great interest to detect atomic hydrogen in circumstellar envelopes and, in view of the complexity of the radial distribution of H/H_2 , high sensitivity interferometric measurements are called for. (We understand that such searches are underway.) By such means the contributions of the photospheric layers could be separated from the photodissociated hydrogen in the envelope, and the role of recombination in the inner dust shell could be evaluated. The study of the atomic and molecular hydrogen distributions in circumstellar shells offers interesting opportunities for understanding the outer layers of cool, evolved stars and their enshrouding envelopes.

Acknowledgments

This research has been supported in part by NASA grant NGR-33-016-196 (to AEG) and an Alfred P. Sloan Fellowship and a grant from the Research Corporation (to PJH).

References

- Abadi, H. Joshi, P., Ramadurai, S. & Wickramasinghe, N. C., 1976. *Nature*, **263**, 214.
- Barlow, M. & Silk, J., 1976. *Astrophys. J.*, **207**, 131.
- Clegg, R. E. S. & Wootten, A., 1980. *Astrophys. J.*, **240**, 1.
- Cohen, M., 1979. *Mon. Not. R. astr. Soc.*, **186**, 837.
- Cohen, M., 1980. *Astrophys. J.*, **238**, L214.
- Crabtree, D. R. & Martin, P., 1979. *Astrophys. J.*, **227**, 900.
- Dalgarno, A. & McCray, R. M., 1973. *Astrophys. J.*, **181**, 95.
- Federman, S. R., Glassgold, A. E. & Kwan, J., 1979. *Astrophys. J.*, **227**, 466.

- Field, G. B., Somerville, W. B. & Dressler, A. J., 1966. *A. Rev. Astr. Astrophys.*, **4**, 226.
- Goldreich, P. & Scoville, N., 1976. *Astrophys. J.*, **205**, 144.
- Goodman, F. O., 1978. *Astrophys. J.*, **226**, 87.
- Hollenbach, D. & McKee, C. F., 1979. *Astrophys. J. Suppl.*, **41**, 555.
- Hollenbach, D. & Salpeter, E. E., 1971. *Astrophys. J.*, **163**, 155.
- Hollenbach, D., Werner, M. W. & Salpeter, E. E., 1971. *Astrophys. J.*, **163**, 155.
- Huggins, P. J. & Glassgold, A. E., 1982. *Astrophys. J.*, **252**, 201.
- Jacobs, T. A., Giedt, R. R. & Cohen, N., 1967. *J. Chem. Phys.*, **47**, 54.
- Jameson, P. V. & Williams, D. A., 1981. *Astrophys. Space Sci.*, **75**, 341.
- Johnson, H. R., 1974. *NCAR Tech. Note TN/STR-95*, January 1974.
- Johnson, H. R., Beebe, R. F. & Sneden, C., 1975. *Astrophys. J.*, **280**, 29.
- Jura, M. & Morris, M., 1981. *Astrophys. J.*, **251**, 181.
- Knapp, G. R., Phillips, T. G., Leighton, R. B., Lo, K. Y., Wannier, P. G. & Huggins, P. J., 1982. *Astrophys. J.*, **252**, 616.
- Kwan, J. & Hill, F., 1977. *Astrophys. J.*, **215**, 781.
- Kwan, J. & Linke, R., 1982. *Astrophys. J.*, **254**, 587.
- Lafont, S., Lucas, R. & Omont, A., 1982. *Astr. Astrophys.*, in press.
- Lambert, D. L. & Snell, R. L., 1975. *Mon. Not. R. astr. Soc.*, **172**, 272.
- Linsky, J. L. & Haisch, B. M., 1979. *Astrophys. J.*, **229**, L27.
- Lucy, L. B., 1976. *Astrophys. J.*, **203**, 75.
- McDowell, M. R. C., 1961. *Observatory*, **81**, 240.
- Mitchell, R. M. & Robinson, G., 1980. *Mon. Not. R. astr. Soc.*, **190**, 669.
- Ridgway, S. & Hall, D. N. B., 1976. *Nature*, **264**, 345.
- Rowan-Robinson, M. & Harris, S., 1982. *Mon. Not. R. astr. Soc.*, **200**, 197.
- Scalo, J. M. & Slavsky, D. B., 1980. *Astrophys. J.*, **239**, L73.
- Spitzer, L., 1978. *Physical Processes in the Interstellar Medium*, John Wiley, New York.
- Stecher, T. P. & Williams, D. A., 1967. *Astrophys. J.*, **149**, L29.
- Stickland, D. J. & Sanner, F., 1981. *Mon. Not. R. astr. Soc.*, **197**, 791.
- Thoe, J., 1978. *A. Rev. Phys. Chem.*, **29**, 223.
- Wischniewski, E. & Wendkar, H. J., 1981. *Astr. Astrophys.*, **96**, 102.
- Zuckerman, B., 1980. *A. Rev. Astr. Astrophys.*, **18**, 263.
- Zuckerman, B., Terzian, Y. & Silverglate, B., 1980. *Astrophys. J.*, **241**, 1014.