H₂ IN EXPANDING CIRCUMSTELLAR SHELLS

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ABSTRACT

Hydrogen molecules are formed in the thin dense shell of interstellar gas swept up by the expanding interstellar bubble around an early-type star with a strong stellar wind. The formation of molecules on grains is not in equilibrium with photodestruction. Theoretical calculations of the column densities of H₂ in rotational levels j = 0–6 agree reasonably well with Copernicus ultraviolet observations of some early-type stars. The model explains why no H₂ features with column densities in the range 10^{15}–10^{16} cm⁻² have been observed.

Subject headings: interstellar: molecules — molecular processes — stars: circumstellar shells — stars: early-type

1. INTRODUCTION

The Copernicus satellite has provided us with observations of interstellar molecular hydrogen absorbing ultraviolet Lyman bands from the background continuum of O and B stars. From observations of approximately 50 lines in the range 1030–1125 Å, Spitzer and Cochran (1973), Spitzer, Cochran, and Hirshfeld (1974), and Drake (cf. Spitzer and Jenkins 1975), have inferred column densities of H₂ in the j = 0 through j = 6 rotational levels of the ground electronic and vibrational state for each of approximately 30 stars. They found that, for absorbing features with j = 0 column densities N(0) > 10^{17} cm⁻², the j = 0, 1, 2 levels are populated according to a Boltzmann distribution with T ≈ 90 K, as would result from collisions in cool dense interstellar gas, but the j = 4, 5, 6 levels have a much greater population than that given by the Boltzmann distribution. (The j = 3 level is an intermediate case.) The higher j levels are evidently populated by the nonthermal processes of pumping by ultraviolet radiation in the Lyman and Werner bands and by formation of molecules in excited states on grains, followed by radiative cascade to the ground vibrational state (Black and Dalgarno 1973, 1976; Spitzer and Cochran 1973; Spitzer and Zweibel 1974; Jura 1975a, b). For absorbing features with N(0) < 10^{16} cm⁻², even the j = 0, 1, 2 levels are populated nonthermally. The absence of stars for which 10^{16} < N(0) < 10^{18} cm⁻² appears to be statistically significant (Spitzer and Jenkins 1975).

Jura (1975a, b) has interpreted the Copernicus observations in terms of a model in which a single cloud of uniform density and temperature contains a steady-state population of H₂. The higher rotational levels are populated nonthermally by ultraviolet pumping and formation on grains. The models are parametrized by the gas temperature T of the cloud, grain formation rate coefficient Rₙ, atomic density n, and unshielded photoabsorption rate βₜ which is proportional to the ambient ultraviolet radiation field in the Lyman bands. Models which are in good qualitative agreement with observations of individual stars have T ≈ 60–100 K and Rₙ ≈ 1–3 × 10⁻¹⁷ cm³ s⁻¹ as expected. The remarkable conclusion reached by Jura is that, for four of the eight stars analyzed which have optically thin H₂ [log N(0) < 14] and for four of the nine stars which have optically thick H₂ [log N(0) > 19], the H₂ cloud is exposed to an ambient ultraviolet intensity that exceeds the average interstellar value by a substantial factor (~5–30). Further, the gas pressure in the H₂ clouds in front of these stars exceeds the characteristic interstellar value nT ≈ 10³ cm⁻³ K typically by a factor of 10, and the clouds are rather thin (~1 pc). The large inferred ultraviolet intensity requires the H₂ cloud to be within some 10–30 pc of the observed star. That, and the elevated gas pressure, suggest a causal connection between the H₂ cloud and the star (Spitzer and Jenkins 1975).

What is the origin of these thin, dense clouds of relatively high pressure? Steigman, Strittmatter, and Williams (1975) have noted that the O and B stars that are used for interstellar ultraviolet absorption observations are the very stars that are observed to have large mass loss in strong stellar winds (Morton 1967; Smith 1970; Conti and Leep 1974), and that the stellar wind can have a profound dynamical influence on the interstellar gas surrounding

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the star. Therefore, the *Copernicus* observations have a strong selection effect toward measuring interstellar gas as affected by a strong stellar wind. Steigman, Strittmatter, and Williams showed that the wind would sweep up ambient interstellar gas into a thin expanding circumstellar shell, which would eventually include cool dense neutral gas. Castor, McCray, and Weaver (1975, 1976) have developed the idea of Steigman, Strittmatter, and Williams into a detailed model for the dynamics of a wind-driven circumstellar shell. We wish to suggest here that the H\textsubscript{2} clouds with high β\textsubscript{0} observed by the *Copernicus* satellite are in fact these expanding circumstellar shells.

In order to support this suggestion, we shall join the theory for formation, destruction, and rotational excitation of H\textsubscript{2} molecules with the hydrodynamical theory of Castor, McCray, and Weaver to construct models for the time-dependent formation and excitation of H\textsubscript{2} in these shells. In § II we briefly review the salient features of the dynamics of the shell and in § III we put the theory for H\textsubscript{2} formation and excitation into the dynamical framework. In § IV we describe detailed numerical results, and in § V we discuss the interpretation of the *Copernicus* ultraviolet observations in terms of these models.

II. WIND-DRIVEN CIRCUMSTELLAR SHELLS

According to Castor, McCray, and Weaver (1975), the wind-driven shell has radius

\[ R_d(t) = 26.6L_\odot^{1/5}n_0^{-1/5}t_9^{3/5} \text{ pc} \] (1)

and velocity

\[ V_d(t) = 15.6L_\odot^{1/5}n_0^{-1/5}t_9^{-2/5} \text{ km s}^{-1} \] (2)

where \( L_\odot \) is the power of the solar wind in units \( 10^{38} \text{ erg s}^{-1} \) (\( L_\odot = 1.27 \) for mass loss rate \( 10^{-6} M_\odot \text{ yr}^{-1} \) and wind velocity \( 2000 \text{ km s}^{-1} \)), \( n_0 \) (\( \text{cm}^{-3} \)) is the atomic density of the ambient interstellar medium, and \( t_9 \) is the age of the system in units \( 10^9 \text{ yr} \).

In relatively young systems the H \( \text{ii} \) region of the star includes the circumstellar shell; if so, the temperature in the shell is maintained at a typical H \( \text{ii} \) region value, \( T \approx 8000 \text{ K} \). By comparing equations (12) and (13) of Castor, McCray, and Weaver, we find that an H \( \text{ii} \) shell first forms after a time

\[ t_0 = 0.66L_\odot^{-1}n_0^{-1} \times 10^6 \text{ yr} \] (3)

where \( L_\odot \) is the stellar luminosity in ionizing photons in units \( 10^{38} \text{ s}^{-1} \). Once this happens, radiative cooling of interstellar gas swept up by the shell is rapid, so we may expect the temperature of the shell to drop rapidly to a value \( T_\ast \approx 75 \text{ K} \), at which radiative cooling by fine structure transitions and rotational excitation of H\textsubscript{2} becomes ineffective (cf. Dalgarno and McCray 1972). There may be significant temperature variation within the H \( \text{ii} \) shell, say, from 50–150 K, but we have not attempted to include this variation in our calculations.

The gas pressure in the shell is given by \( P_\ast = 1.3m_\text{p}n_0V_d^2 \), where the factor 1.3 allows for 10 percent helium. We can write

\[ P_\ast = (n_\text{H} + n_\text{He} + 2n_2)kT_\ast = (n - n_2)kT_\ast , \]

where \( n = n_\text{H} + n_\text{He} + 2n_2 \) is the total density and \( n_2 \) is the H\textsubscript{2} density in the shell. Here we have ignored the effect of a magnetic field; the possible importance of magnetic pressure will be discussed in § V. One can verify that the sound travel time through the shell is less than 0.05 times the age of the system, so that gas in the shell will be approximately in hydrostatic equilibrium with respect to the shock front. There is a slight pressure gradient in the shell due to deceleration of the front, but the pressure drops by less than 20 percent from the front to the inner boundary, and we have neglected this effect. Therefore, we can write

\[ (n - n_2)/n_0 \approx (V_d/C_\ast)^2 \] (4)

throughout the shell, where \( C_\ast = (kT_\ast/1.3m_\text{p})^{1/2} \approx 0.690 \text{ km s}^{-1} \) for \( T_\ast = 75 \text{ K} \).

It is convenient to write the equations for molecule formation in a frame of reference where the spatial coordinate \( x = 0 \) at the shock front and increases toward the star. Then, conservation of mass passing through the shock determines the location \( x(t, t_1) \) at time \( t \) of a gas atom that first entered the shell at time \( t_1 \):

\[ 4\pi R_d(t)^2 \int_{r_\text{shell}} n(x, t)dx = \frac{4\pi}{3} n_0[R_d(t)^3 - R_d(t_1)^3] . \] (5)

III. FORMATION, DESTRUCTION, AND ROTATIONAL EXCITATION OF H\textsubscript{2}

H\textsubscript{2} molecules are assumed to form on grains according to the theory of Hollenbach and Salpeter (1971) at a rate \( R_\text{m}n_\text{H} \), where we take \( R_\text{m} = 2.5 \times 10^{-17} \text{ cm}^3 \text{ s}^{-1} \) (cf. Jura 1975a). We assume that newly formed molecules, once they reach rotational states \( j \) of the ground vibrational state, are populated according to the formation distribution function \( F(j) \) given by Spitzer and Zweibel (1974).
### TABLE 1
IONIZING FLUX AND ULTRAVIOLET PHOTOABSORPTION RATE FOR EARLY-TYPE STARS

<table>
<thead>
<tr>
<th>Spectral Type</th>
<th>$T_{\text{eff}}$ (K)</th>
<th>$L_i$ ($\times 10^{44}$ photons s$^{-1}$)</th>
<th>$K = \beta_0 R^2$ ($\times 10^{-7}$ pc$^2$ s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>V</td>
<td>V</td>
<td>III</td>
</tr>
<tr>
<td>O4</td>
<td>50,000</td>
<td>88</td>
<td>88</td>
</tr>
<tr>
<td>O5</td>
<td>47,000</td>
<td>82</td>
<td>82</td>
</tr>
<tr>
<td>O6</td>
<td>42,000</td>
<td>18</td>
<td>22</td>
</tr>
<tr>
<td>O7</td>
<td>38,500</td>
<td>7.3</td>
<td>12</td>
</tr>
<tr>
<td>O8</td>
<td>36,500</td>
<td>3.9</td>
<td>8.0</td>
</tr>
<tr>
<td>O9</td>
<td>34,500</td>
<td>2.1</td>
<td>6.1</td>
</tr>
<tr>
<td>B0</td>
<td>30,900</td>
<td>0.44</td>
<td>0.88</td>
</tr>
<tr>
<td>B0.5</td>
<td>26,200</td>
<td>0.032</td>
<td>0.064</td>
</tr>
<tr>
<td>B1</td>
<td>22,600</td>
<td>$3.3 \times 10^{-5}$</td>
<td>$7.3 \times 10^{-5}$</td>
</tr>
<tr>
<td>B2</td>
<td>20,500</td>
<td>$7.3 \times 10^{-6}$</td>
<td>$1.8 \times 10^{-8}$</td>
</tr>
<tr>
<td>B3</td>
<td>17,900</td>
<td>$7.3 \times 10^{-8}$</td>
<td>$2.2 \times 10^{-8}$</td>
</tr>
</tbody>
</table>

The molecules are destroyed at a rate 0.11 $\beta_0$, where $\beta_0$ (s$^{-1}$) is the rate of photoabsorption in the Lyman bands from state $j$ (Jura 1975a). The photodestruction fraction 0.11 is independent of the rotational state $j$ from which the Lyman photon is absorbed. The remaining 0.89 of the photons absorbed from state $j$ result in bound molecules which radiatively cascade back to the rotational state $i$ of the ground state with redistribution probabilities $p_{ij}$ calculated by Black and Dalgarno (1975) and given in Table 1 of Jura (1975a). In steady state, where photodestruction equals formation on grains, the population of the higher rotational levels is dominated by radiative pumping because a given molecule is radiatively pumped approximately 9 times before it is destroyed and another is formed.

The photoabsorption rate $\beta_j$ is given by

$$\beta_j = S_j \beta_{0j} = S_j \sum \sigma(j) G_0(n_0),$$

(6)

where $\sigma(j) = 0.0265f(j)$ cm$^2$ Hz is the integrated line absorption cross section of the $j$th Lyman (or Werner) band of the $j$th rotational level, and $f(j)$ is the corresponding rotational level, and $G_0$ is the ambient ultraviolet continuum field (cm$^{-2}$ s$^{-1}$ Hz$^{-1}$), and $\beta_{0j}$ is the unshielded photoabsorption rate from state $j$. (We have neglected ultraviolet extinction by dust.) The dimensionless parameter $S_j$ accounts for the self-shielding in optically thick lines of H$_2$. Jura (1974) shows that if the lines are on the square root part of the curve of growth,

$$S_j \approx 4.2 \times 10^6 N_2(j)^{-1/2},$$

(7)

where $N_2(j)$ is the column density in cm$^{-2}$ of molecules in state $j$.

We are primarily interested in the situation where the dominant ultraviolet radiation field comes from the central star. Therefore, we have

$$G_0(\nu) \propto L_\nu / R_\star(\nu)^2,$$

where $L_\nu$ is the luminosity spectrum of the central star. We have ignored the variation of $L_\nu$ with frequency over the corresponding wavelength range $\lambda = 930$–1130 Å and simply assumed that $G_\nu(\nu) \approx G_\nu(\lambda = 1000 \text{ Å})$, so that

$$\beta_{0j} = \beta_0 = KR_\star(t)^{-2}$$

(8)

is independent of rotational level $j$. The constant $K$ depends on stellar spectral type and luminosity class and has been calculated for model early-type stars using the effective temperature and radius scale of Panagia (1973) and the model stellar atmospheres for stars in the temperature range $30,000$ K $< T_{\text{eff}} < 50,000$ K given by Auer and Mihalas (1972). For the cooler stars B0.5 through B3, we have estimated $K$ from a blackbody calculation. The ultraviolet flux from O4 I to B0 I supergiants is roughly constant because the later-type supergiants have larger effective radii to offset their lower effective temperature. Table 1 lists the results of these calculations, as well as the stellar ionizing luminosity $L_i$ taken from Panagia (1973) which determines when an H I shell first forms according to equation (3). Stothers (1972) has listed the measured masses of early-type stars in binary systems; as a typical example, two O9 III stars with masses $19 M_\odot$ and $26 M_\odot$ are observed. This range in the mass of a given type is reflected in a range in the absolute luminosity of $\Delta M_\text{bol} \approx \pm 0.4$. Therefore, $L_i$ and $K$ in Table 1 are "average values" and are only accurate to a factor of 2 for a particular star. Unfortunately, it is not yet possible to estimate the wind power $L_w$ from first principles. A reasonable guess might be that $L_w = 1$ for an O7 star and that $L_w \propto L_i$, so that equation (3) yields $t_0 \approx 5 \times 10^6$ yr $n_0^{-1}$, independent of spectral type.

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1 The indices $i, j$ should be permuted in this table.
The time-dependent populations of H₂ molecules in an expanding circumstellar shell follow from coupled equations for formation, destruction, and rotational excitation of molecules in each \( j \) level. A major simplification of the equations results from the observation that at the temperatures and densities of interest (\( T \approx 75 \text{ K} \), \( n \approx 100 \text{ cm}^{-3} \)) almost all the H₂ molecules will be found in the \( j = 0, 1, \) and \( 2 \) levels. The population of these low levels are well approximated by Boltzmann statistics, i.e.,

\[
n_{2,j} \approx n_2 \frac{g_j}{Q(T)} \exp \left(-\frac{E_j}{kT}\right),
\]

where \( g_0 = 1, g_1 = 9, g_2 = 5 \), and \( Q(T) = \sum_j g_j \exp \left(-\frac{E_j}{kT}\right) \) is the partition function. We have assumed that statistical equilibrium between the \( j = 0, 2 \) para states and the \( j = 1 \) ortho state of H₂ is established by proton interchange collisions (Dalgarno, Black, and Weisheit 1973). Therefore, to a good approximation the destruction rate \( \beta_d n_2 \approx 0.11 \sum_j S_{j'} n_{2,j} \) of all H₂ molecules can be written

\[
\beta_d n_2 = 0.11 S(N_d) \beta_d n_2
\]

provided that the Lyman lines from the \( j = 0, 1, \) and \( 2 \) levels are on the square root part of the curve of growth. (This assumption is not necessarily true for the \( j = 2 \) level, but it is adequate, since the photodestruction rate from \( j = 2 \) is relatively unimportant.) The effective shielding factor \( S(N_d) \) is given by

\[
S(N_d) = 4.2 \times 10^{6} N_d^{-1/2} Q(T)^{-1/2} \tilde{Q}(T),
\]

and \( T \) is the (assumed constant) kinetic temperature of the molecular shell.

Now consider the fate of H₂ molecules in a thin shell of fixed mass and thickness \( \delta x(t_1) \) that entered the circumstellar shell at time \( t_1 \) in a short time interval \( \delta t_1 \). The total number of atoms \( \delta N'(t_1) \) in the shell is given by

\[
\delta N'(t_1) = 4\pi R_d(t)^2 \delta N(t, t_1) = 4\pi R_d(t_1)^2 n_0 V_d(t_1) \delta t_1,
\]

where \( \delta N' \) is \( n \delta x \) is the column density of all atoms in the thin shell. We can then write the equation for formation and destruction of H₂ molecules in this thin shell as follows:

\[
\frac{d}{dt} [R_d(t)^2 \delta N_d(t, t_1)] = R_d R_d(t)^2 \delta N(t, t_1) n_0 V_d(t_1) - 0.11 S[N_d(t, t_1)] \beta_d(t) R_d(t)^2 \delta N_d(t, t_1),
\]

where \( \delta N_d = n_2 \delta x \) is the column density of H₂ molecules in the thin shell and

\[
N_d(t, t_1) = \sum_{t < t < t_1} \delta N_d(t, t')
\]

is the column density of molecules interior to the shell under consideration. We may use equation (4) and the definitions of \( \delta N_d \) and \( \delta N \) to find

\[
n_d(t, t_1) = n_0 \left[ \frac{V_d(t)}{C_e} \right]^2 \left[ \frac{\delta N_d(t, t_1)}{\delta N(t, t_1) - \delta N_d(t, t_1)} \right]
\]

and

\[
n_d(t, t_1) = n_0 \left[ \frac{V_d(t)}{C_e} \right]^2 \left[ 0.9 \delta N(t, t_1) - 2 \delta N_d(t, t_1) \right].
\]

It is now possible to calculate the time evolution of H₂ molecules in the circumstellar shell from \( t_0 \) to \( t_{\text{max}} \) by starting with the first H I shell \( \delta N'(t_0) \) that forms, and solving the coupled set of equations (14) and (15) by adding another shell \( \delta N'(t_0 + k \delta t) \) to the system at each successive time step, where \( k = \{1, 2, 3 \ldots k_{\text{max}} = (t_{\text{max}} - t_0)/\delta t\} \).

Given the densities \( n_d(j) \) of H₂ in the \( j = 0, 1, 2 \) levels it is then possible to find the populations of the \( j' = 3, 4, 5, 6 \) levels. Since the radiative decay times of these excited levels are very short compared with the age of the circumstellar shell, their populations are very well approximated by local steady-state equations of the form

\[
\frac{d}{dt} n_{d}(j') \approx 0 \approx R_d n_d(t) \beta_d(j') + \beta_d(t) \sum_j S_{j'j} n_d(j) + \alpha \sum_j C_{j'} n_d(j) - \left(A_{j'} + \alpha \sum_j C_{j'}\right) n_d(j'),
\]

where \( A_{j'} \) is the radiative decay rate of state \( j' \), \( nC_{j'} \) represents the de-excitation rate from state \( j' \) to state \( j \) due
to collisions with atoms and molecules, \( \bar{n}C_{j'j} = n_R C_{j'j}(H) + n_p C_{j'j}(H_2) \), and \( \bar{n}C_{j'j} \) is the analogous collisional excitation rate from state \( j \) to \( j' \). We have defined

\[
\bar{p}_{j'j} = \sum_{j' \neq j} P_{j'j}
\]

and

\[
\bar{F}_q(j') = \sum_{j' \neq j} F_q(j'),
\]

these sums being restricted to even (odd) \( j' \) for para (ortho) hydrogen. We ignore the collisional de-excitation rate \( n_C C_{j'j}(p) \) due to protons, since we expect \( n_p \ll 10^{-2}n \) throughout most of the circumstellar shell. In equation (18) all the densities \( n \) and \( S_j[N_d(j)] \) are, of course, functions of \( (t, x) \) or of \( (t, t_j) \). Since radiative pumping and collisional excitation among the higher \( j' \) levels is negligible, it is a good approximation to take the radiative pumping sum over \( j \) in equation (18) to include only \( j = 0, 2 \) for \( j' = 4 \) and \( j' = 6 \), and to include only \( j = 1 \) for \( j' = 3 \), and \( j = 1, 3 \) for \( j' = 5 \). In practice the only significant collision processes are those between \( j = 1 \) and \( j' = 3 \), for which we have used rate coefficients at \( 75 \) K \( C_{10}(H) = 1.0 \times 10^{-16} \) \( \text{cm}^3 \text{s}^{-1} \) and \( C_{10}(H_2) = 0.2 \times 10^{-16} \) \( \text{cm}^3 \text{s}^{-1} \), estimated from Dalgarno, Henry, and Roberts (1966) and Allison and Dalgarno (1967). The de-excitation rate coefficients \( C_{31}(H) \) and \( C_{31}(H_2) \) can be calculated from the detailed balancing relation.

IV. RESULTS

The results of a typical calculation are shown in Figures 1 and 2. In this case the assumed parameters were \( L_x = 0.127 \), \( L_t = 2.1 \), and \( K = 1.0 \times 10^{-6} \) \( \text{s}^{-1} \) \( \text{pc}^2 \), roughly appropriate for an O9.5 V star, and \( n_0 = 80 \) \( \text{cm}^{-3} \). Figures 1a and 1b show the distribution of molecules \( n_{j'j}(x) \) through the shell at \( t = 5.06 \times 10^6 \) yr, at which time \( R_d(t) = 19.5 \) pc according to equation (1). The interior boundary of the shell is at \( x = D = 1.34 \times 10^{18} \) cm on the left-hand side. The relative populations of the \( j = 0, 1, 2 \) levels are fixed throughout the shell according to the assumed Boltzmann distribution with \( T = 75 \) K.

We can understand the distribution of molecules in the outer part of the shell as follows. Shocked interstellar gas flows into the shell from the outside \( (x = 0) \) with velocity \( v \simeq n_v V_v/n \), where \( n \simeq n_d(V_d/C_d)^2 \) according to equation (4), provided that the gas is mostly atomic. Here the formation rate of molecules is much greater than the destruction rate, so

\[
n_d(x) \approx 0.9R_d^2 v^2(t - t_0),
\]
Fig. 2a.—Column densities $N_H$ of hydrogen atoms, $N_2$ of total hydrogen molecules, and $N_{2, j}$ of molecules in $j = 0, 1, 2$ versus time $t$. Points with error bars are Copernicus ultraviolet observations of $\zeta$ Oph, and X’s are results of a model by Jura for $\zeta$ Oph.

Fig. 2b.—Column densities $N_{2, j}$ of hydrogen molecules in excited rotational levels $j = 3, 4, 5$, and 6 versus time $t$. Solid curves, total column densities. Dashed curves, contributions due to formation on grains ($F$). Dotted curves, contributions due to radiative pumping ($P$). Dot-dash curve, contribution to $j = 3$ from collisional excitation ($C$). Points with error bars are Copernicus ultraviolet observations of $\zeta$ Oph; X’s are results of a model by Jura for $\zeta$ Oph.

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where \((t - t_0) \approx x/v\), assuming plane-parallel flow. Therefore,

\[
n_2(x) \approx 0.9 R \xi n_0^2 V_s \xi C_\xi^{-6} x \tag{19}
\]
in the outer part of the shell. Since the higher levels are populated primarily by formation here, we have

\[
A_p n_2(x) = 0.9 R \xi n_0^2 \bar{F}_3(j),
\]
or

\[
n_2(x) \approx 0.9 R \xi n_0^2 \bar{F}_3(j) A_j^{-1},
\]

which is approximately independent of \(x\) for \(j \geq 4\). The \(j = 3\) level is an intermediate case, since both collisions and formation affect its population.

Molecules in the interior of the shell on the left-hand boundary of Figure 1 are exposed to a strong ultraviolet flux from the central star. Here the photodestruction of molecules is in equilibrium with formation, and Figure 1 shows that \(n_2\) is approximately linear with \((D - x)\) in this region. Following Jura (1974), Appendix 1, we derive from equations (11) and (14) an approximate law for the \(\text{H}_2\) density in this region:

\[
n_2(x) \approx 0.81 \frac{R \xi n_0^2 [\bar{v}_e(t)/C_3]^3 q Q(T)}{2[4.6 \times 10^{4} R \xi n_0^2]^{3} \bar{Q}(T)^{2}} (D - x). \tag{21}
\]

Except for a very thin surface layer where the Lyman bands are all optically thin, equation (21) is valid provided that \(2 n_2/n \ll 1\) and that the photodestruction lifetime of molecules in the shell is short compared with the age of the shell, or that \(0.11 \bar{b}_0(t) S(N_2)t \gg 1\).

The population of the \(j \geq 4\) levels in this interior layer are dominated by radiative pumping. Since the radiative pumping rate

\[
\sum_{j=0}^{9} \bar{b}_{j,0} b_0(t) S_1(N_2)t n_2 t
\]
is linearly proportional to the destruction rate \(0.11 \bar{b}_0(t) S(N_2) n_2\), which in turn equals the formation rate \(R \xi n_0^2\) in this region, we may write

\[
n_2(t) \approx 0.9 R \xi n_0^2 [\bar{F}_3(j) + \bar{b}_e(T)] A_j^{-1},
\]

where the equilibrium radiative pumping probabilities, defined by

\[
\bar{b}_e(T) \approx \sum_{j=0, 2, or 4, 5, 6} \bar{b}_{j,1} g_j \exp \left(-E_j/kT\right)^{1/2}/[0.11 \bar{Q}(T)]
\]
are weak functions of temperature and have the values \(\bar{b}_e(T)(75 K) = 1.26, 0.54,\) and \(0.22,\) respectively, for \(j = 4, 5, 6\). By comparing equations (20) and (23), we find that the populations of the higher levels on the inside of the shell, where radiative pumping dominates, exceed those on the outside of the shell, where formation dominates, by factors 7.67, 2.19, and 2.78, respectively, for \(j = 4, 5, 6\).

The evolution of the \(\text{H}_2\) column density in the shell can be understood as follows. The distribution of molecules through the interior of a newly formed shell is described by equation (21). It therefore follows that the \(\text{H}_2\) column density is given approximately by

\[
N_2(t) \approx \frac{2.25 \times 10^{-2} R \xi n_0^2 [V(t)/C_3]^4 R(t)^2}{[4.6 \times 10^{4} R \xi n_0^2]^{3}} \left(1 - \frac{R(t)}{R(t_0)}\right)^{3} Q(T) \bar{G}_2(T) \alpha t^{2/3} \left(1 - \frac{t_0}{t}\right)^{3/5} t^{3/5} . \tag{24}
\]

When the shell becomes thicker it may happen, particularly if the ultraviolet radiation field is not strong, that the distribution of \(\text{H}_2\) through most of the shell is dominated by equation (19). If so, the \(\text{H}_2\) column density is given approximately by

\[
N_2(t) \approx 0.05 R \xi n_0^2 C_3 \xi V(t)/R(t)^2 \left(1 - \frac{R(t)}{R(t_0)}\right)^{3} \alpha t^{2/3} \left(1 - \frac{t_0}{t}\right)^{3/5} t^{3/5} . \tag{25}
\]

However, once the shell becomes mostly molecular the \(\text{H}_2\) column density is given approximately by

\[
N_2(t) \approx 0.15 n_0 R(t) \alpha t^{3/5} . \tag{26}
\]

In general, the column density of \(\text{H}_2\) is given approximately by

\[
N_2(t) = \min \{\text{eq. (24)}, \text{eq. (25)}, \text{eq. (26)}\} .
\]

The results of detailed calculations for \(N_2(t)\) in our model for the shell around \(\zeta\) Oph are shown in Figures 2a and 2b. The total column density \(N = N_{\text{H}1} + N_{\text{H}11} + N_2 + N_{\text{He}}\) is shown as the solid line with slope 3/5. Before
t_0 = 6.25 \times 10^6 \text{ yr}, according to equation (3), the shell is entirely H_2 and there are no hydrogen atoms or molecules. After a very short time interval, (t - t_0) = 4.7 \times 10^4 \text{ yr}, the atomic hydrogen column density in the shell rises to N_{H_2} = 7.0 \times 10^9 \text{ cm}^{-2} and the molecular column density rises to N_{H_2} = 3.0 \times 10^{17} \text{ cm}^{-2}. By this time the distribution of H_2 molecules in the shell is like that shown in Figure 1, which corresponds to t = 5.60 \times 10^6 \text{ yr}, and the shell is mostly molecular. The relative populations of the j = 0, 1, 2 column densities are set according to the assumed Boltzmann distribution.

Figure 2b shows the column densities N_{2j}(t) of the excited levels j \geq 3. Here the solid curves are the total column densities for each j, and the dashed curves labeled F, P, C are the separate contributions due to formation, radiative pumping, and collisional excitation, respectively. These curves can also be understood in a simple way. First, consider the contributions N_{2j}(t) due to nonequilibrium formation. If the shell is mostly atomic hydrogen, the total number of molecules formed per second in levels j \geq 4 is given by R_pn^4 \pi R_p^2 N_{H_2} P_j(t) and the total number of radiative decays per second in the shell is given by 4\pi R_p^2 N_{2j}(t) A_j. Equating these rates and using equations (4) and (5), we find

$$N_{2p_j}(t) \approx 0.3 R_p n_0^2 \frac{P_j(t)}{A_j} \frac{R_0^2 V(t)}{C_s^2} \left[ 1 - \left( \frac{t}{t_0} \right)^{3/5} \right]$$

which decreases roughly as t^{-0.3} for t \geq 2t_0. This behavior changes when the shell becomes mostly molecular, in which case the total number of molecules formed with j \geq 4 is proportional to the rate at which the shell sweeps up hydrogen atoms. In that case we find

$$N_{2p_j}(t) \approx 0.45 n_0 V(t) \frac{P_j(t)}{A_j}$$

which decreases as t^{-0.4}.

Similarly, we may calculate the contributions (P) to the j \geq 4 column densities due to radiative pumping by equating the total number of molecules in the shell pumped to j \geq 4 per second to the rate of radiative decays to obtain

$$N_{2p_j}(t) \approx \frac{4.6 \times 10^4 P_j(t)}{A_j} N_{d}(t)^{3/4} Q(T)^{-1/2} \frac{P_j(t)}{A_j}$$

which has the time dependence N_{2p_j}(t) \propto t^{-0.8} if the shell is mostly hydrogen and t \approx 2t_0 (cf. eq. [25]), and N_{2p_j}(t) \propto t^{-0.9} if the shell is mostly molecules.

By considering ratios of column densities of rotationally excited H_2 we may remove uncertain parameters from consideration and learn more about the molecular formation process. For example, if nonequilibrium formation on grains is the dominant source of excited H_2, we find from equations (27) and (28) that the ratio

$$\frac{R_d(j', j)}{N_{2p_j}(t)/N_{2p_j}(t)} = \frac{P_d(j', j)}{A_j} \frac{P_d(j', j)}{A_j}$$

and, specifically, log R_d(6, 4) = -1.16 and log R_d(5, 4) = -0.18, using the F_d(j')'s given by Spitzer and Zweibel (1974). If, on the other hand, formation of H_2 on grains is in steady state with ultraviolet photodissociation in the cloud under consideration, the corresponding ratio would be

$$\frac{R_d(j, j')}{N_{2p_j}(t)/N_{2p_j}(t)} = \frac{P_d(j')}{A_j} + \frac{P_d(j')}{A_j}$$

and we find log R_d(6, 4) = -1.60 and log R_d(5, 4) = -0.72. [Jura's (1975b) results show log R_d(6, 4) \approx -1.50 and log R_d(5, 4) \approx -0.55 for every case.]

Since the F_d(j')'s are very uncertain parameters, depending on unknown processes on grain surfaces, our numerical values for the R_d(j', j)'s are not particularly significant. What is significant is that the equilibrium models require the observed R_d(6, 4) to be the same for every H_2 cloud, regardless of grain formation rate n, gas density n, or unshielded photodestruction rate P_d. Further, R_d(6, 4) is very weakly dependent on cloud temperature T. The ratio R_d(5, 4) is a less reliable indicator, since it depends on the ortho-para ratio, which involves additional physical processes. Our dynamical models involve a changing combination of radiative pumping and nonequilibrium formation, so that R_d(6, 4) is not constant. Early in the development of the system, when the circumstellar shell is near the central star, radiative pumping tends to be more important relative to formation, and R_d(6, 4) tends toward R_d(6, 4); later, formation dominates the population of the higher j levels and R_d(6, 4) tends toward R_d(6, 4). However, in this particular model the ratio R_d(6, 4) has not yet changed much. At t = 5.60 \times 10^6 \text{ yr} we have R_d(6, 4) = -1.50. The fact that the observed ratio for \xi Oph, R_d(6, 4) = -2.13 \pm 0.28 (Spitzer, Cochran, and Hirshfeld 1974), is outside the range defined by R_d(6, 4) = -1.60 and R_d(6, 4) = -1.16 suggests that the formation distribution function F_d(j) may be significantly different from that given by Spitzer and Zweibel (1974).

The j = 3 level plays an important diagnostic role because, unlike the higher j levels, its population is significantly influenced by collisions with atoms and molecules at densities n \approx 10^2 \text{ cm}^{-3}. Therefore, the column density N_{2j}(t) is not well approximated by equations (25)-(27), which do not include the effects of collisions. Figure

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2b shows that the $N_{\text{a}2}(t)$ curve differs markedly from the $N_{\text{a}2,\text{e}2}(t)$ curves in that it increases with time, while the others decrease. This behavior can be understood qualitatively in terms of collisions tending to drive the $N_{\text{a}2}(t)$ curve toward the Boltzmann value, which would be parallel to the $N_{\text{a}2,\text{e}2}(t)$ curves of Figure 2a.

We may characterize the column density $N_{\text{a}2}(t)$ by an excitation temperature $T_{\text{a}2} = 844\ln(7N_{\text{a}2}(t)/3N_{\text{a}1}(t))^{-1}$. In the example shown $T_{\text{a}2} = 116\text{ K}$ at $t = 2.70 \times 10^8\text{ yr}$ and $T_{\text{a}1} = 80\text{ K}$ at $t = 10^9\text{ yr}$. This behavior can be understood as follows. At early times, when the shell is thin and close to the star, radiative pumping is the dominant source of $j = 3$, and this effect elevates $T_{\text{a}2}$ above $T_K$. As time proceeds, the relative importance of radiative pumping decreases rapidly; therefore $T_{\text{a}2}$ approaches $T_K$. As the shell becomes less dense, radiative decay of $j = 3$ becomes comparable with collisional de-excitation, and eventually $T_{\text{a}2}$ will drop below $T_K$. In a model with high ambient density $n_0$ such as the example shown, $T_{\text{a}2}$ stays close to $T_K$. In a model with lower ambient density, $T_{\text{a}2}$ starts out with a value well above $T_K$ and decreases with time more rapidly.

V. DISCUSSION

The parameters $R_\odot$, $T$, $n_0$, and $K$ of the model shown in Figures 1a and 1b and Figures 2a and 2b were chosen to fit the observations of H$_2$ in front of the O9.5 V star $\zeta$ Oph (Spitzer et al. 1973; Spitzer, Cochran, and Hirshfeld 1974). Our model at $t = 5.06 \times 10^6\text{ yr}$ agrees reasonably well with the observations shown on Figures 2a and 2b. The internal structure of the shell at this time is shown in Figures 1a and 1b.

Also shown in Figures 2a and 2b are the results of a steady-state model by Jura (1975b) which agrees equally well with the observations. The parameters used by Jura to fit the observations of this star are $R_\odot = 3.3 \times 10^{-6}$ cm$^3\text{ s}^{-1}$, $n = 700\text{ cm}^{-3}$, $T = 75\text{ K}$, and $\beta_0 = 3.0 \times 10^{-10}\text{ s}^{-1}$, while we have $R_\odot = 2.5 \times 10^{-7}\text{ cm}^3\text{ s}^{-1}$, $T = 75\text{ K}$, $n = 836\text{ cm}^{-3}$, and $\beta_0 = 2.65 \times 10^{-9}\text{ s}^{-1}$ at $t = 5.06 \times 10^6\text{ yr}$. Our model has higher gas density but the same fraction of molecules to atoms because the molecule formation has not had time to come to equilibrium with photodissociation. Our model has a somewhat lower radiation field because we have ignored ultraviolet continuum absorption by dust and because the molecule formation process plays a relatively greater role in populating the higher $j$ levels, especially $j = 5$.

In the case of $\zeta$ Oph we can construct circumstellar shell models for other early-type stars which agree reasonably well with the observations in most cases. But we find, as did Jura, that significant discrepancies remain. We have already mentioned the problem with $R(6, 4)$ in $\zeta$ Oph. Another defect of both Jura’s theory and ours is that the calculated column densities $N_{\text{a}2}$ tend to be less than the observed values.

There are a number of possible explanations for these discrepancies. One important fact is that the observed lines for $j = 2$ and $j = 3$ in these stars tend to lie on the flat part of the curve of growth, so that the inferred column densities in these levels are most sensitive to assumptions such as that of constant temperature throughout the H$_2$ shell. Also, the assumption of statistical equilibrium between the populations of ortho- and para-H$_2$ with the same kinetic temperature as inferred from the ratio $N_{\text{a}2,\text{d}}/N_{\text{a}2,\text{g}}$ is suspect. Since ortho-para transitions are caused by proton exchange collisions (Dalgarno, Black, and Weisheit 1973), and there are likely to be more protons near the surfaces of the molecular cloud where the temperature may be significantly greater than in the interior, it seems reasonable that there might be more ortho-H$_2$ than a single temperature model would predict. Also, if some H$_2$ molecules are formed in regions of the shell where there are very few protons, the ortho-para ratio may remain high there, reflecting the ratio upon formation on grains.

The most likely reason for the discrepancies between theory and observations is that single component models are greatly oversimplified. The work of Spitzer and Morton (1976) shows that there are likely to be a number of components containing H$_2$ along the line of sight to the observed stars. Therefore, we must emphasize that the agreement of our model with the observations is likely to be fortuitous.

Furthermore, in our idealized models we have ignored a number of possibly important effects, such as interstellar magnetic fields and relative motion between the star and the interstellar gas. If the H I shell is sufficiently ionized that the magnetic field remains frozen to the gas, the compression of gas parallel to the lines of force is limited to a factor (Spitzer and Morton 1976):

$$n'/n_0 \approx 2.5n_0^{1/4}(B_0/3 \times 10^{-6}\text{ gauss})^{-1}|V_d(t)/(10\text{ km s}^{-1})|,$$

(30)

where $B_0$ is the ambient interstellar magnetic field. For example, in our model for $\zeta$ Oph at $5.06 \times 10^6\text{ yr}$, an ambient magnetic field of $B_0 = 3 \times 10^{-6}\text{ gauss}$ would limit the compression ratio $n'/n_0$ to a factor of $\sim 5$ instead of the factor $\sim 10$ that we obtained by neglecting the field.

The effects of motion of the star through the gas may be even more significant. As noted by Jura (1975b), many of the stars observed with rotationally excited H$_2$ are runaway stars. If so, the large ($|V_d - V_{\text{gas}}| \approx 20-50\text{ km s}^{-1}$) relative velocity between the star and the interstellar gas can greatly modify the hydrodynamic structure of the system. As will be described by Castor, McCray, and Weaver (1976), in that case the stellar wind pushes a conical shock front ahead of the star. The shock can then be considerably stronger ($V_d \approx |V_d - V_{\text{gas}}|$) and cause a correspondingly greater compression ratio (cf. eqs. [4] and [30]), so that the observed high density sheets may occur in a medium of lower ambient density $n_0$.

Perhaps this latter point is the best possibility to resolve the difficulty, pointed out by Spitzer and Morton (1976), in obtaining a high compression ratio with an ambient magnetic field. Spitzer and Morton suggested that
the \( H_2 \) might be formed in the shock around an expanding \( H_2 \) region, but they had difficulty in obtaining a high compression ratio in this way and they could not account for outward moving sheets around runaway stars. It will be interesting to apply our analysis of the formation and rotational excitation of \( H_2 \) in more realistic models for shocked \( H \) I.

Nevertheless, we consider our present model an attractive one because it accounts for a number of observations in a natural way. For example, it explains why the \( H_2 \) should be found in thin, dense sheets with gas pressure and ambient ultraviolet radiation field substantially greater than the average interstellar values. The elevated pressure is the ram pressure of the expanding shell, and the high ultraviolet radiation indicates that the shell is near the star. Further, as Spitzer and Morton have remarked, the \( H_2 \) component with the most negative velocity is the one with the high populations in \( J \geq 4 \), as would be expected with an expanding circumstellar shell.

Another success of our model is that it explains the absence of \( H_2 \) features with column densities \( 16 \leq \log N_2 \leq 18 \). As in the example shown, the column density \( N_2 \) jumps to \( \log N_2 \approx 18.5 \) in a time scale of order \( 10^5 \) yr after the circumstellar shell first traps the ionization front. This sudden transition is a typical behavior for all expanding shells and is independent of the magnitude of the ambient density \( n_0 \). Therefore, the probability of catching a circumstellar shell at a time when the \( H_2 \) shell is just beginning to form and has column density \( \log N_2 < 18.5 \) is of order \( 10^{-2} \), assuming that the observed stars have average lifetimes of \( 10^5 \) yr.

On the other hand, the model does not explain the observations of optically thin \( H_2 \) with \( \log N_2 \leq 16 \) in front of some early-type stars. The interpretations of these observations (Jura 1975a) suggests that these \( H_2 \) features are also associated with gas near the observed stars. According to our model, the expanding circumstellar shell in these systems is entirely within the \( H \) II region of the star, so that molecules cannot be formed there by grain catalysis of \( H \) I.

It is questionable whether molecules can form on grains in \( H \) II regions (cf. Hollenbach and Salpeter 1971). However, we have noticed that the naive assumption that \( H_2 \) is formed at a rate \( R'_2 n^2 \) as a result of protons sticking to grains, neutralizing, and combining with other hydrogen atoms on grain surfaces gives \( H_2 \) column densities in the right range if \( R'_2 \approx R_n \). In the optically thin limit the resulting \( H_2 \) column density in our model is given by

\[
N_2(t) = \frac{1}{3} \frac{R'_2 R_1(t) n_0^2}{\beta_0(t)} \frac{V(t)^2}{C'_0^2}.
\]  

(31)

For example, equation (31) gives \( N_2(t) = 5.4 \times 10^{12} n_0 \) cm\(^{-2}\) if we assume the parameters \( R'_2 = 3 \times 10^{-17} \), \( L_w = 0.127 \), \( K = 3.3 \times 10^{-8} \) s\(^{-1}\) pc\(^{-2}\), and \( C'_0 = 10 \) km s\(^{-1}\) for an \( H \) II shell with \( T = 8000 \) K. This last point is highly speculative; the \( H_2 \) may form by an entirely different physical process (cf. Dalgarno and McCray 1973; Hill and Silk 1975).

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