THE ASTROPHYSICAL JOURNAL, 208:458–467, 1976 September 1

H_2 IN EXPANDING CIRCUMSTELLAR SHELLS

DAVID HOLLENBACH
Department of Physics, University of Colorado at Colorado Springs
AND
SHIH-I CHU AND RICHARD MCCRAY*
Joint Institute for Laboratory Astrophysics, University of Colorado and National Bureau of Standards; and Department of Physics and Astrophysics, University of Colorado
Received 1975 December 22; revised 1976 February 13

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 H_2 in rotational levels $j = 0$–6 agree reasonably well with *Copernicus* ultraviolet observations of some early-type stars. The model explains why no H_2 features with column densities in the range 10^{15}–10^{18} cm^{-2} have been observed.

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

I. 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 H_2 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 $N(0) \geqslant 10^{17}$ cm^{-2}, the $j = 0, 1, 2$ levels are populated according to a Boltzmann distribution with $T \approx 90$ 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 1975*a*, *b*). For absorbing features with $N(0) \leqslant 10^{15}$ cm^{-2}, even the $j = 0, 1, 2$ levels are populated nonthermally. The absence of stars for which $10^{15} \leqslant N(0) \leqslant 10^{18}$ cm^{-2} appears to be statistically significant (Spitzer and Jenkins 1975).

Jura (1975*a*, *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 H_2. 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 R_g, atomic density n, and unshielded photoabsorption rate β_0 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 $T \approx 60$–100 K and $R_g \approx 1$–3×10^{-17} cm^3 s^{-1} as expected. The remarkable conclusion reached by Jura is that, for four of the eight stars analyzed which have optically thin H_2 [$\log N(0) \leqslant 14$] and for four of the nine stars which have optically thick H_2 [$\log N(0) \geqslant 19$], the H_2 cloud is exposed to an ambient ultraviolet intensity that exceeds the average interstellar value by a substantial factor ($\sim$5–30). Further, the gas pressure in the H_2 clouds in front of these stars exceeds the characteristic interstellar value $nT \approx 10^3$ cm^{-3} K typically by a factor of 10, and the clouds are rather thin ($\leqslant 1$ pc). The large inferred ultraviolet intensity requires the H_2 cloud to be within some 10–30 pc of the observed star. That, and the elevated gas pressure, suggest a causal connection between the H_2 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

* John Simon Guggenheim Memorial Foundation Fellow.

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_2 clouds with high β_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_2 molecules with the hydrodynamical theory of Castor, McCray, and Weaver to construct models for the time-dependent formation and excitation of H_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_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

$$R_s(t) = 26.6 L_w^{1/5} n_0^{-1/5} t_6^{3/5} \quad \text{pc} \tag{1}$$

and velocity

$$V_s(t) = 15.6 L_w^{1/5} n_0^{-1/5} t_6^{-2/5} \quad \text{km s}^{-1}\,, \tag{2}$$

where L_w is the power of the solar wind in units 10^{36} ergs s^{-1} ($L_w = 1.27$ for mass loss rate $10^{-6}\,M_\odot$ yr^{-1} and wind velocity 2000 km s^{-1}), n_0 (cm^{-3}) is the atomic density of the ambient interstellar medium, and t_6 is the age of the system in units 10^6 yr.

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

$$t_0 = 0.60 L_i L_w^{-1} n_0^{-1} \times 10^6 \quad \text{yr}\,, \tag{3}$$

where L_i is the stellar luminosity in ionizing photons in units 10^{48} 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 $T_s \approx 75$ K, at which radiative cooling by fine structure transitions and rotational excitation of H_2 becomes ineffective (cf. Dalgarno and McCray 1972). There may be significant temperature variation within the H I 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 $P_s = 1.3 m_H n_0 V_s^2$, where the factor 1.3 allows for 10 percent helium. We can write

$$P_s = (n_H + n_{He} + n_2)kT_s = (n - n_2)kT_s\,,$$

where $n = n_H + n_{He} + 2n_2$ is the total density and n_2 is the H_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

$$(n - n_2)/n_0 \approx (V_s/C_s)^2 \tag{4}$$

throughout the shell, where $C_s = (kT_s/1.3 m_H)^{1/2} = 0.690$ km s^{-1} for $T_s = 75$ 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:

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

III. FORMATION, DESTRUCTION, AND ROTATIONAL EXCITATION OF H_2

H_2 molecules are assumed to form on grains according to the theory of Hollenbach and Salpeter (1971) at a rate $R_g n n_H$, where we take $R_g = 2.5 \times 10^{-17}$ cm^3 s^{-1} (cf. Jura 1975*a*). 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 $F_g(j)$ given by Spitzer and Zweibel (1974).

TABLE 1

Ionizing Flux and Ultraviolet Photoabsorption Rate for Early-Type Stars

Spectral Type	T_{eff} (K)	L_i ($\times 10^{48}$ photons s^{-1})			$K = \beta_0 R^2$ ($\times 10^{-7}$ pc^2 s^{-1})		
	V	V	III	I	V	III	I
O4	50,000	88	88	88	69	76	76
O5	47,000	52	52	59	53	62	65
O6	42,000	18	22	36	31	38	51
O7	38,500	7.3	12	23	18	33	42
O8	36,500	3.9	8.0	20	13	31	53
O9	34,500	2.1	6.1	13	10	29	62
B0	30,900	0.44	0.88	3.4	6.9	16	64
B0.5	26,200	0.032	0.064	0.40	2.4	4.0	29
B1	22,600	3.3×10^{-3}	7.3×10^{-3}	0.058	0.73	1.45	12.7
B2	20,500	7.3×10^{-4}	1.8×10^{-3}	0.015	0.36	0.55	7.3
B3	17,900	7.3×10^{-5}	2.2×10^{-4}	3.7×10^{-3}	0.05	0.07	1.6

The molecules are destroyed at a rate 0.11 β_j, where β_j (s^{-1}) is the rate of photoabsorption in the Lyman bands from state j (Jura 1975*a*). 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 $p_{i,j}$ calculated by Black and Dalgarno (1975) and given in Table 1 of Jura (1975*a*).[1] 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 β_j is given by

$$\beta_j = S_j \beta_{0j} = S_j \sum_i \sigma_i(j) G_0(\nu_{ij}) , \tag{6}$$

where $\sigma_i(j) = 0.0265 f_i(j)$ cm^2 Hz is the integrated line absorption cross section of the ith Lyman (or Werner) band of the jth rotational level, and $f_i(j)$ is the corresponding oscillator strength, $G_0(\nu)$ is the ambient ultraviolet continuum field (cm^{-2} s^{-1} Hz^{-1}), and β_{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,

$$S_j \approx 4.2 \times 10^5 N_2(j)^{-1/2} , \tag{7}$$

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

$$G_0(\nu) \propto L_\nu / R_s(t)^2 ,$$

where L_ν is the luminosity spectrum of the central star. We have ignored the variation of L_ν with frequency over the corresponding wavelength range $\lambda = 930$–1130 Å and simply assumed that $G_0(\nu) \approx G_0(\lambda = 1000$ Å$)$, so that

$$\beta_{0j} = \beta_0 = K R_s(t)^{-2} \tag{8}$$

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 $< T_{eff} <$ 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 $\Delta M_{bol} \approx \pm 0.4$. 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.

[1] The indices i, j should be permuted in this table.

The time-dependent populations of H_2 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 ($T \approx 75$ K, $n \gtrsim 100\ \mathrm{cm}^{-3}$) almost all the H_2 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.,

$$n_{2,j} = n_2 \frac{g_j}{Q(T)} \exp(-E_j/kT), \tag{9}$$

where $g_0 = 1$, $g_1 = 9$, $g_2 = 5$, and $Q(T) = \sum_j g_j \exp(-E_j/kT)$ is the partition function. We have assumed that statistical equilibrium between the $j = 0$, 2 para states and the $j = 1$ ortho state of H_2 is established by proton interchange collisions (Dalgarno, Black, and Weisheit 1973). Therefore, to a good approximation the destruction rate $\beta_d n_2 = 0.11 \sum_j S_j \beta_{0j} n_{2,j}$ of all H_2 molecules can be written

$$\beta_d n_2 = 0.11 S(N_2) \beta_0 n_2 \tag{10}$$

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 $S(N_2)$ is given by

$$S(N_2) = 4.2 \times 10^5 N_2^{-1/2} Q(T)^{-1/2} \tilde{Q}(T), \tag{11}$$

where

$$\tilde{Q}(T) = \sum_{j=0}^{2} [g_j \exp(-E_j/kT)]^{1/2} \tag{12}$$

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

Now consider the fate of H_2 molecules in a thin shell of fixed mass and thickness $\delta x(t, t_1)$ that entered the circumstellar shell at time t_1 in a short time interval δt_1. The total number of atoms $\delta\mathcal{N}(t_1)$ in the shell is given by

$$\delta\mathcal{N}(t_1) = 4\pi R_s(t)^2 \delta N(t, t_1) = 4\pi R_s(t_1)^2 n_0 V_s(t_1) \delta t_1, \tag{13}$$

where $\delta\mathcal{N} = n\delta x$ is the column density of all atoms in the thin shell. We can then write the equation for formation and destruction of H_2 molecules in this thin shell as follows:

$$\frac{d}{dt}[R_s(t)^2 \delta N_2(t, t_1)] = R_g R_s(t)^2 \delta N(t, t_1) n_H(t, t_1) - 0.11 S[N_2'(t, t_1)] \beta_0(t) R_s(t)^2 \delta N_2(t, t_1), \tag{14}$$

where $\delta N_2 = n_2 \delta x$ is the column density of H_2 molecules in the thin shell and

$$N_2'(t, t_1) = \sum_{t' \leq t_1} \delta N_2(t, t') \tag{15}$$

is the column density of molecules *interior* to the shell under consideration. We may use equation (4) and the definitions of δN_2 and δN to find

$$n_2(t, t_1) = n_0 \left[\frac{V_s(t)}{C_s}\right]^2 \left[\frac{\delta N_2(t, t_1)}{\delta N(t, t_1) - \delta N_2(t, t_1)}\right] \tag{16}$$

and

$$n_H(t, t_1) = n_0 \left[\frac{V_s(t)}{C_s}\right]^2 \left[\frac{0.9\delta N(t, t_1) - 2\delta N_2(t, t_1)}{\delta N(t, t_1) - \delta N_2(t, t_1)}\right]. \tag{17}$$

It is now possible to calculate the time evolution of H_2 molecules in the circumstellar shell from t_0 to t_{max} by starting with the first H I shell $\delta\mathcal{N}(t_0)$ that forms, and solving the coupled set of equations (14) and (15) by adding another shell $\delta\mathcal{N}(t_0 + k\delta t)$ to the system at each successive time step, where $k = \{1, 2, 3 \ldots k_{max} = (t_{max} - t_0)/\delta t\}$.

Given the densities $n_2(j)$ of H_2 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

$$\frac{d}{dt} n_2(j') \approx 0 \approx R_g n n_H \tilde{F}_g(j') + \beta_0(t) \sum_j S_j[N_2'(j)] \tilde{p}_{j'j} n_2(j) + \bar{n} \sum_j C_{jj'} n_2(j) - \left(A_{j'} + \bar{n} \sum_j C_{j'j}\right) n_2(j'), \tag{18}$$

where $A_{j'}$ is the radiative decay rate of state j', $nC_{j'j}$ represents the de-excitation rate from state j' to state j due

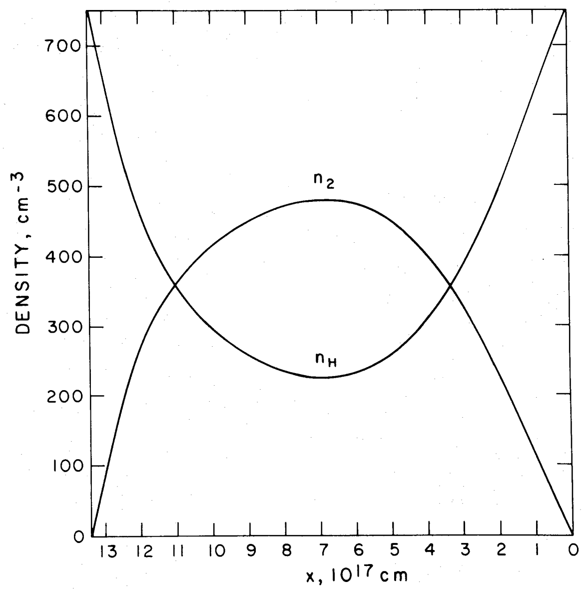

FIG. 1a

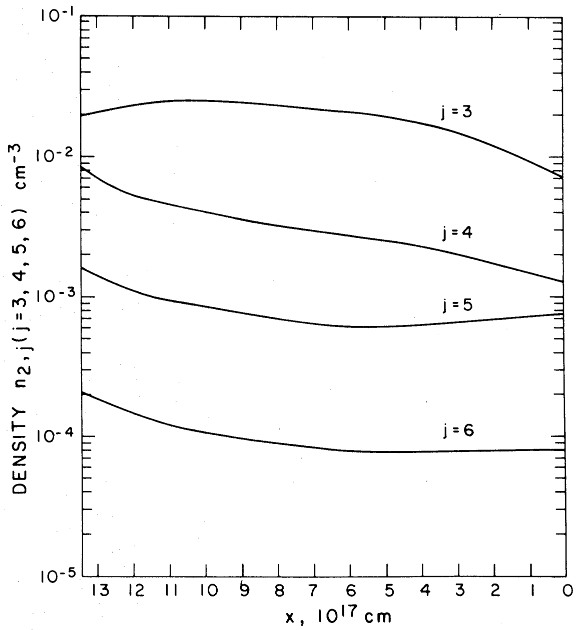

FIG. 1b

FIG. 1a.—Distribution of hydrogen atom density n_H and total hydrogen molecule density n_2 through the shell at $t = 5.06 \times 10^6$ yr. The interior of the shell is on the left-hand boundary at $x = 1.34 \times 10^{18}$ cm.

FIG. 1b.—Distributions of hydrogen molecule densities in excited rotational levels j = 3, 4, 5, and 6 through shell at $t = 5.06 \times 10^6$ yr.

to collisions with atoms and molecules, $\bar{n}C_{j'j} = n_H C_{j'j}(H) + n_2 C_{j'j}(H_2)$, and $\bar{n}C_{jj'}$ is the analogous collisional excitation rate from state j to j'. We have defined

$$\tilde{p}_{j'j} = \sum_{j'' \geq j}' p_{j'j''}$$

and

$$\tilde{F}_g(j') = \sum_{j'' \geq j'}' F_g(j'') ,$$

these sums being restricted to even (odd) j'' for para (ortho) hydrogen. We ignore the collisional de-excitation rate $n_p C_{j'j}(p)$ 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 $S_j[N_2(j)]$ are, of course, functions of (t, x) or of (t, t_1). 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 $C_{13}(H) = 1.0 \times 10^{-16}$ cm^3 s^{-1} and $C_{13}(H_2) = 0.2 \times 10^{-16}$ cm^3 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 $L_w = 0.127$, $L_i = 2.1$, and $K = 1.0 \times 10^{-6}$ s^{-1} pc^2, roughly appropriate for an O9.5 V star, and $n_0 = 80$ cm^{-3}. Figures 1a and 1b show the distribution of molecules $n_{2,j}(x)$ through the shell at $t = 5.06 \times 10^6$ yr, at which time $R_s(t) = 19.5$ 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 $v \approx n_0 V_s / n$, where $n \approx n_0 (V_s/C_s)^2$ 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

$$n_2(x) \approx 0.9 R_g n^2 (t - t_0) ,$$

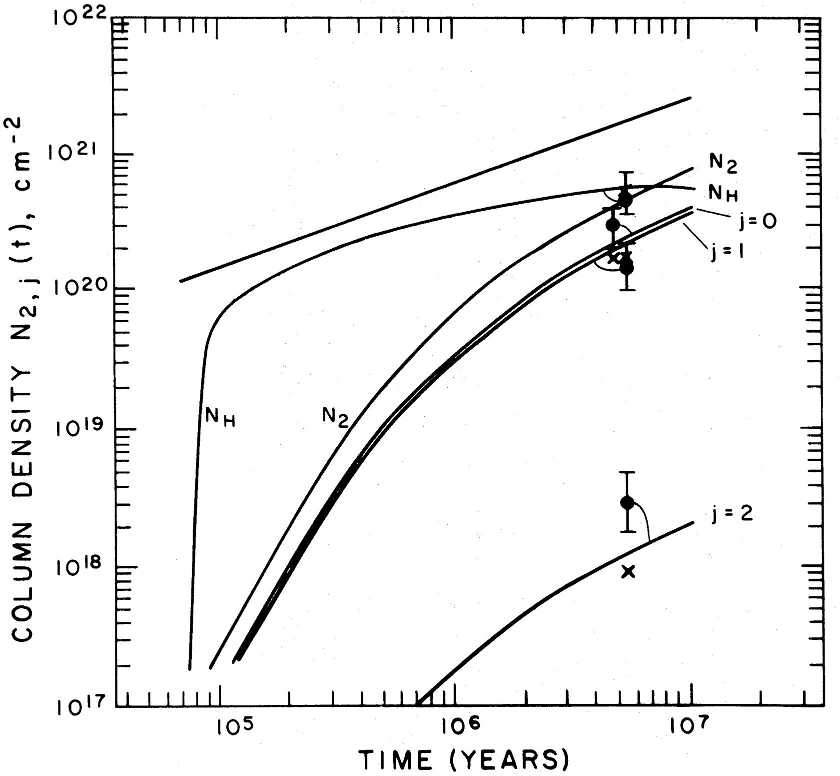

FIG. 2a.—Column densities N_H of hydrogen atoms, N_2 of total hydrogen molecules, and $N_{2,j}$ of molecules in $j = 0, 1, 2$ versus time t. Points with error bars are *Copernicus* ultraviolet observations of ζ Oph, and X's are results of a model by Jura for ζ Oph.

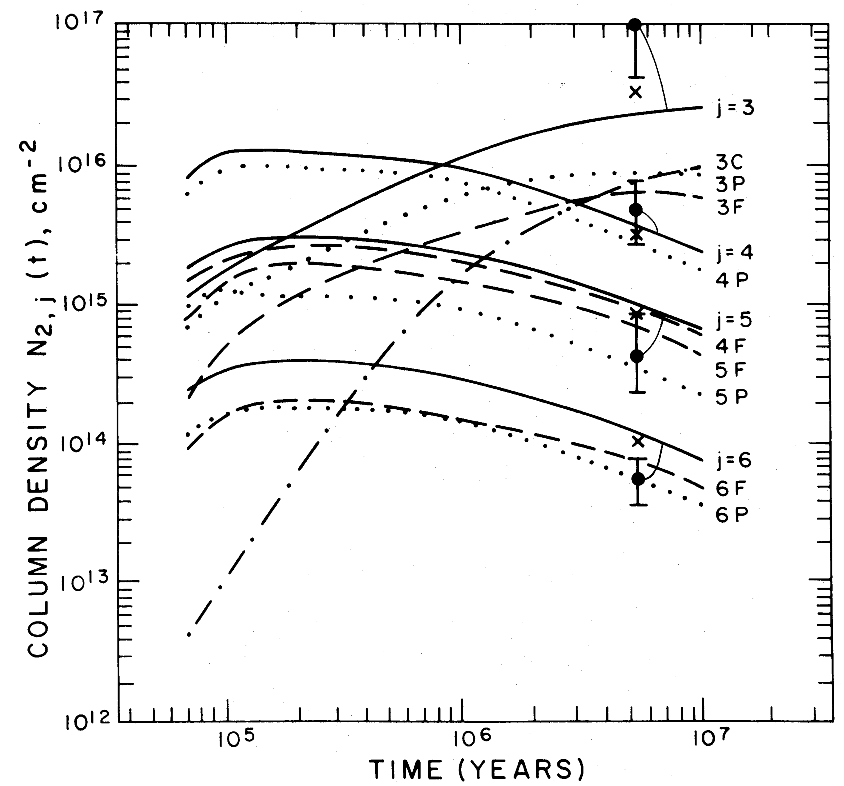

FIG. 2b.—Column densities N_{2j}, of hydrogen molecules in excited rotational levels $j = 3$, 4, 5, and 6 versus time t. *Solid curves*, total column densities. *Dashed curves*, contributions due to formation on grains (*F*). *Dotted curves*, contributions due to radiative pumping (*P*). *Dot-dash curve*,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

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

$$n_2(x) \approx 0.9 R_g n_0^2 V_s^5 C_s^{-6} x \tag{19}$$

in the outer part of the shell. Since the higher levels are populated primarily by formation here, we have

$$A_j n_j(x) = 0.9 R_g n^2 \tilde{F}_g(j) ,$$

or

$$n_j(x) \approx 0.9 R_g n^2 \tilde{F}_g(j) A_j^{-1} , \tag{20}$$

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 H_2 density in this region:

$$n_2(x) \approx 0.81 \frac{R_g^2 n_0^4 [v_s(t)/C_s]^8 Q(T)}{2[4.6 \times 10^4 \beta_0(t)]^2 \tilde{Q}(T)^2} (D - x) . \tag{21}$$

Except for a very thin surface layer where the Lyman bands are all optically thin, equation (21) is valid provided that $2n_2/n \ll 1$ and that the photodestruction lifetime of molecules in the shell is short compared with the age of the shell, or that $0.11\beta_0(t)S(N_2)t \gg 1$.

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

$$\sum_{j'=0}^{3} \tilde{p}_{j,j'} \beta_0(t) S_{j'}(N_{2j'}) n_{2j'}$$

is linearly proportional to the destruction rate $0.11\beta_0(t)S(N_2)n_2$, which in turn equals the formation rate $R_g n^2$ in this region, we may write

$$n_{2,j} \approx 0.9 R_g n^2 [\tilde{F}_g(j) + \tilde{p}_{e,j}(T)] A_j^{-1} , \tag{22}$$

where the equilibrium radiative pumping probabilities, defined by

$$\tilde{p}_{e,j}(T) \approx \sum_{j'=0,2 \text{ or } 1,3} \tilde{p}_{j,j'} [g_{j'} \exp(-E_{j'}/kT)]^{1/2} / [0.11 \tilde{Q}(T)] \tag{23}$$

are weak functions of temperature and have the values $\tilde{p}_{e,j}(75 \text{ K}) = 1.26$, 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 j 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 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 H_2 column density is given approximately by

$$N_2(t) \approx \frac{2.25 \times 10^{-2} R_g^2 n_0^4 [V_s(t)/C_s]^4 R_s(t)^2}{[4.6 \times 10^4 \beta_0(t)]^2} \left\{1 - \left[\frac{R_s(t_0)}{R_s(t)}\right]^3\right\}^2 Q(T) \tilde{Q}^{-2}(T) \propto t^2 \left[1 - \left(\frac{t_0}{t}\right)^{9/5}\right]^2 . \tag{24}$$

When the shell becomes thicker it may happen, particularly if the ultraviolet radiation field is not strong, that the distribution of H_2 through most of the shell is described by equation (19). If so, the H_2 column density is given approximately by

$$N_2(t) \approx 0.05 R_g n_0^2 \frac{V_s(t) R_s(t)^2}{C_s^2} \left(1 - \left[\frac{R_s(t_0)}{R_s(t)}\right]^3\right)^2 \propto t^{4/5} \left[1 - \left(\frac{t_0}{t}\right)^{9/5}\right]^2 . \tag{25}$$

However, once the shell becomes mostly molecular the H_2 column density is given approximately by

$$N_2(t) \approx 0.15 n_0 R_s(t) \propto t^{3/5} . \tag{26}$$

In general, the column density of H_2 is given approximately by

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

The results of detailed calculations for $N_2(t)$ in our model for the shell around ζ Oph are shown in Figures 2*a* and 2*b*. The total column density $N = N_{\text{H I}} + N_{\text{H II}} + N_2 + N_{\text{He}}$ is shown as the solid line with slope 3/5. Before

$t_0 = 6.25 \times 10^5$ yr, according to equation (3), the shell is entirely H II and there are no hydrogen atoms or molecules. After a very short time interval, $(t - t_0) = 4.7 \times 10^4$ yr, the atomic hydrogen column density in the shell rises to $N_{\rm H\,I} = 7.0 \times 10^{19}$ cm^{-2} and the molecular column density rises to $N_2 = 3.0 \times 10^{17}$ cm^{-2}. By this time the distribution of H_2 molecules in the shell is like that shown in Figure 1, which corresponds to $t = 5.60 \times 10^6$ 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 2*b* shows the column densities $N_{2,j}(t)$ 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 $N_{2F,j}(t)$ 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 $R_g n 4\pi R_s^2 N_{\rm H} \tilde{F}_g(j)$ and the total number of radiative decays per second in the shell is given by $4\pi R_s^2 N_{2F,j} A_j$. Equating these rates and using equations (4) and (5), we find

$$N_{2F,j}(t) \approx 0.3 R_g n_0^2 \frac{\tilde{F}_g(j)}{A_j} \frac{R_s(t) V_s(t)^2}{C_s^2} \left[1 - \left(\frac{t_0}{t}\right)^{9/5}\right], \tag{27}$$

which decreases roughly as $t^{-0.2}$ for $t \gtrsim 2t_0$. 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

$$N_{2F,j}(t) \approx 0.45 n_0 V_s(t) \frac{\tilde{F}_g(j)}{A_j}, \tag{28}$$

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

$$N_{2P,j}(t) \approx \frac{4.6 \times 10^4 \beta_0(t)}{A_j} N_2(t)^{1/2} Q(T)^{-1/2} \tilde{Q}(T) \tilde{P}_{e,j}(T) \tag{29}$$

which has the time dependence $N_{2P,j}(t) \propto t^{-0.8}$ if the shell is mostly atoms and $t \gtrsim 2t_0$ (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 molecule 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

$$R_F(j', j) \equiv N_{2F,j'}(t)/N_{2F,j}(t) = \tilde{F}_g(j') A_j / [\tilde{F}_g(j) A_{j'}]$$

and, specifically, $\log R_F(6, 4) = -1.16$ and $\log R_F(5, 4) = -0.18$, using the $F_g(j)$'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

$$R_P(j', j) \equiv N_{2P,j'}(t)/N_{2P,j}(t) = [\tilde{F}_g(j') + \tilde{p}_e(j')] A_j / [\tilde{F}_g(j) + \tilde{p}_e(j)] A_{j'},$$

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

Since the $\tilde{F}_g(j)$'s are very uncertain parameters, depending on unknown processes on grain surfaces, our numerical values for the $R_F(j', j)$'s are not particularly significant. What is significant is that the equilibrium models require the observed $R(6, 4)$ to be the same for every H_2 cloud, regardless of grain formation rate R_g, gas density n, or unshielded photodestruction rate β_0. Further, $R(6, 4)$ is very weakly dependent on cloud temperature T. [The ratio $R(5, 4)$ 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 $R(6, 4)$ 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 $R(6, 4)$ tends toward $R_p(6, 4)$; later, formation dominates the population of the higher j levels and $R(6, 4)$ tends toward $R_F(6, 4)$. However, in this particular model the ratio $R(6, 4)$ has not yet changed much. At $t = 5.60 \times 10^6$ yr we have $R(6, 4) = -1.50$. The fact that the observed ratio for ζ Oph, $R(6, 4) = -2.13 \pm 0.28$ (Spitzer, Cochran, and Hirshfeld 1974), is outside the range defined by $R_p(6, 4) = -1.60$ and $R_F(6, 4) = -1.16$ suggests that the formation distribution function $F_g(j)$ 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 $n \gtrsim 10^2$ cm^{-3}. Therefore, the column density $N_{2,3}(t)$ is not well approximated by equations (25)–(27), which do not include the effects of collisions. Figure

2*b* shows that the $N_{2,3}(t)$ curve differs markedly from the $N_{2,j\geqq 4}(t)$ 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 $N_{2,3}(t)$ curve toward the Boltzmann value, which would be parallel to the $N_{2,j<3}(t)$ curves of Figure 2*a*.

We may characterize the column density $N_{2,3}(t)$ by an excitation temperature $T_{31} = 844[\ln(7N_{2,1}(t)/3N_{2,3}(t)]^{-1}$. In the example shown $T_{31} = 116$ K at $t = 2.70 \times 10^5$ yr and $T_{31} = 80$ K at $t = 10^7$ 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_{31} above T_K. As time proceeds, the relative importance of radiative pumping decreases rapidly; therefore T_{31} approaches T_K. As the shell becomes less dense, radiative decay of $j = 3$ becomes comparable with collisional de-excitation, and eventually T_{31} will drop below T_K. In a model with high ambient density n_0 such as the example shown, T_{31} stays close to T_K. In a model with lower ambient density, T_{31} starts out with a value well above T_K and decreases with time more rapidly.

V. DISCUSSION

The parameters R_g, T, n_0, and K of the model shown in Figures 1*a* and 1*b* and Figures 2*a* and 2*b* were chosen to fit the observations of H_2 in front of the O9.5 V star ζ Oph (Spitzer *et al.* 1973; Spitzer, Cochran, and Hirshfeld 1974). Our model at $t = 5.06 \times 10^6$ yr agrees reasonably well with the observations shown on Figures 2*a* and 2*b*. The internal structure of the shell at this time is shown in Figures 1*a* and 1*b*.

Also shown in Figures 2*a* and 2*b* are the results of a steady-state model by Jura (1975*b*) which agrees equally well with the observations. The parameters used by Jura to fit the observations of this star are $R_g = 3.3 \times 10^{-17}$ cm^3 s^{-1}, $n = 700$ cm^{-3}, $T = 75$ K, and $\beta_0 = 5.0 \times 10^{-9}$ s^{-1}, while we have $R_g = 2.5 \times 10^{-17}$ cm^3 s^{-1}, $T = 75$ K, $n = 836$ cm^{-3} and $\beta_0 = 2.65 \times 10^{-9}$ s^{-1} at $t = 5.06 \times 10^6$ 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 $j = 5$.

As in the case of ζ 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 ζ Oph. Another defect of both Jura's theory and ours is that the calculated column densities $N_{2,3}$ 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 that inferred from the ratio $N_{2,2}/N_{2,0}$ 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):

$$n'/n_0 \approx 2.5 n_0^{1/2}(B_0/3 \times 10^{-6}\ \text{gauss})^{-1}[V_s(t)/10\ \text{km s}^{-1}]\,, \tag{30}$$

where B_0 is the ambient interstellar magnetic field. For example, in our model for ζ Oph at 5.06×10^6 yr, an ambient magnetic field of $B_0 = 3 \times 10^{-6}$ gauss would limit the compression ratio n'/n_0 to a factor of ~5 instead of the factor ~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 (1975*b*), many of the stars observed with rotationally excited H_2 are runaway stars. If so, the large ($|V_* - V_{\text{gas}}| \approx 20$–50 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 ($V_s \approx |V_* - V_{\text{gas}}|$) 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 $16 \lesssim \log N_2 \lesssim 18$. 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 10^7 yr.

On the other hand, the model does not explain the observations of optically thin H_2 with $\log N_2 \lesssim 16$ in front of some early-type stars. The interpretations of these observations (Jura 1975*a*) 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 naïve assumption that H_2 is formed at a rate $R_g'n^2$ 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 $R_g' \approx R_g$. In the optically thin limit the resulting H_2 column density in our model is given by

$$N_2(t) = \frac{1}{3}\frac{R_g' R_s(t) n_0^2}{\beta_0(t)}\frac{V_s(t)^2}{C_s'^2}\,. \tag{31}$$

For example, equation (31) gives $N_2(t) = 5.4 \times 10^{12} n_0 t_6\ \mathrm{cm}^{-2}$ if we assume the parameters $R_g' = 3 \times 10^{-17}$, $L_w = 0.127$, $K = 3.3 \times 10^{-8}\ \mathrm{s}^{-1}\ \mathrm{pc}^2$, and $C_s' = 10\ \mathrm{km\ s}^{-1}$ 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).

This work was partially supported by National Science Foundation grant GP-39308X and by National Aeronautics and Space Administration grant NSG 7128 through the University of Colorado. Part of this work was done by D. H. at the University of California, Berkeley, Astronomy Department and supported there by National Aeronautics and Space Administration grant NGR-05-003-578, thanks to the hospitality of Dr. J. Silk.

REFERENCES

Allison, A. C., and Dalgarno, A. 1967, *Proc. Phys. Soc.*, **90**, 609.
Auer, L. H., and Mihalas, D. 1972, *Ap. J. Suppl.*, **24**, 193.
Black, J. H., and Dalgarno, A. 1973, *Ap. J. (Letters)*, **184**, L101.
———. 1976, *Ap. J.*, **203**, 132.
Castor, J., McCray, R., and Weaver, R. 1975, *Ap. J. (Letters)*, **200**, L107.
———. 1976, to be published.
Conti, P. S., and Leep, E. M. 1974, *Ap. J.*, **193**, 113.
Dalgarno, A., Black, J. H., and Weisheit, J. C. 1973, *Ap. Letters*, **14**, 77.
Dalgarno, A., Henry, R. J. W., and Roberts, C. S. 1966, *Proc. Phys. Soc.*, **88**, 611.
Dalgarno, A., and McCray, R. 1972, *Ann. Rev. Astr. and Ap.*, **10**, 375.
———. 1973, *Ap. J.*, **181**, 95.
Hill, J. K., and Silk, J. 1975, *Ap. J.*, **198**, 299.
Hollenbach, D. J., and Salpeter, E. E. 1971, *Ap. J.*, **163**, 155.
Hollenbach, D. J., Werner, M. W., and Salpeter, E. E. 1971, *ibid.*, p. 165.
Jura, M. 1974, *Ap. J.*, **191**, 375.
———. 1975*a*, *ibid.*, **197**, 575.
———. 1975*b*, *ibid.*, p. 581.
Morton, D. C. 1967, *Ap. J.*, **150**, 535.
Panagia, N. 1973, *A.J.*, **78**, 929.
Smith, A. M. 1970, *Ap. J.*, **160**, 595.
Spitzer, L., Jr., and Cochran, W. D. 1973, *Ap. J. (Letters)*, **186**, L23.
Spitzer, L., Jr., Cochran, W. D., and Hirshfeld, A. 1974, *Ap. J. Suppl.*, **28**, 373.
Spitzer, L., Jr., Drake, J. F., Jenkins, E. B., Morton, D. C., Rogerson, J. B., and York, D. G. 1973, *Ap. J. (Letters)*, **181**, L116.
Spitzer, L., Jr., and Jenkins, E. B. 1975, *Ann. Rev. Astr. and Ap.*, **13**, 133.
Spitzer, L., Jr., and Morton, W. A. 1976, *Ap. J.*, **204**, 731.
Spitzer, L., Jr., and Zweibel, E. G. 1974, *Ap. J. (Letters)*, **191**, L127.
Steigman, G., Strittmatter, P. A., and Williams, R. E. 1975, *Ap. J.*, **198**, 575.
Stothers, R. 1972, *Ap. J.*, **175**, 431.

SHIH-I CHU and RICHARD MCCRAY: Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, CO 80309

DAVID HOLLENBACH: Department of Astronomy, University of California, Berkeley, CA 94720