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# A SHOCK MODEL FOR INFRARED LINE EMISSION FROM H<sub>2</sub> MOLECULES

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Department of Physics, Yale University Received 1977 January 21; accepted 1977 April 14

#### ABSTRACT

We consider a shock model for the  $H_2$  infrared line emission detected in the Orion Nebula by Gautier *et al.* We solve the equations describing stationary gas flow and excitation of  $H_2$  in the radiative cooling region behind a shock. We find that, for the high densities needed to explain the observed line strengths, the populations of the vibration-rotation levels are nearly in LTE. By matching the calculated line strengths to the observations, we find that the acceptable values of shock velocity and upstream molecular density must be of order  $8 \le v_0 \le 21 \text{ km s}^{-1}$  and  $10^5 \le n_0 \le 10^6 \text{ cm}^{-3}$ .

Subject headings: infrared: sources — interstellar: molecules — nebulae: Orion Nebula — shock waves

### I. INTRODUCTION

Infrared emission in several lines of the fundamental and first-overtone vibration bands of molecular hydrogen has recently been observed in the Orion Nebula by Gautier et al. (1976), Grasdalen and Joyce (1976), and Beckwith et al. (1977). The relative strengths of the observed lines indicate a high excitation temperature for rotational levels within the first vibrational state. The lines seem to be optically thin and are probably from a hot shell of gas. We shall discuss the possibility that the infrared lines are from a shockheated region in a dense molecular cloud.

After submitting an earlier version of this paper, we received a preprint by Kwan (1977) in which he presented a similar model for the infrared  $H_2$  emission. There he pointed out the importance of dissociation of  $H_2$  in determining the shock structure. We have therefore revised our calculations to include this effect. We have also received a preprint from Hollenbach and Shull (1977) in which a similar model is discussed.

### II. REVIEW OF OBSERVATIONAL DATA

We review some facts from the observations which any model for the emission must explain.

First is the position, size, and shape of the emitting region. Gautier *et al.* (1976) detected the lines at the Becklin-Neugebauer object (BN) and at a position in the Kleinmann-Low nebula (KL) 10" S of BN. Grasdalen and Joyce (1976) mapped the emission and found that it covers a region about 30" by 1' extended along the NE-SW direction, centered 20" NW of BN. At the assumed distance of 460 pc the emission covers an area of  $\sim 2 \times 10^{34}$  cm<sup>2</sup>.

The surface brightness of the fundamental S(1) line was observed to be  $3 \times 10^{-3}$  ergs cm<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup> at BN by Gautier *et al.* and a maximum of  $7.2 \times 10^{-3}$  ergs cm<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup> by Grasdalen and Joyce. If we assume that the line is optically thin this implies a column density of molecules in the excited state with vibrational quantum numbers v = 1 and rotational quantum number J = 3 at maximum of about  $3 \times 10^{17}$  cm<sup>-2</sup>. Beckwith *et al.* (1977) detected the S(1) line from v = 2 to v = 1 at a maximum surface brightness of 0.1 times that of the S(1) line from v = 1 to v = 0.

The relative brightnesses of the lines of the 1-0 band were fitted with a thermal excitation law by Gautier *et al.* They find temperatures of 2500(+1500, -700) K for BN, and 1400(+1700, -600) K for the region in KL that they observed.

## III. POSSIBLE MODELS FOR THE EMISSION

Two explanations for the emission are considered. The first is the ultraviolet pumping model of Black and Dalgarno (1976). In this model UV radiation is absorbed in the Lyman and Werner bands of  $H_2$ , and then the molecules decay back to excited vibrational and rotational levels of the ground electronic state. Radiative cascade through these levels gives rise to infrared lines. This model predicts lines of comparable strength coming from vibrational levels higher than v = 1, contrary to observations, and also predicts different ratios for the v = 1 lines than observed. For gas densities above about  $10^4$  cm<sup>-3</sup> collisional deexcitation is important in determining the populations of the vibration-rotation levels. A modification of the Black and Dalgarno model which includes collisional

processes may be able to produce the line strengths observed. Such a model involves solving the formation-destruction equation for the molecules coupled with rate equations for the level populations, radiative transfer of the UV lines, and the energy balance equation. Our preliminary attempts make us uncertain of whether such calculations will give solutions close to the observations.

The second model which we consider is that of shock heating of a dense molecular cloud. In this case we find that a rather simple model can reproduce the observations closely.

### IV. SHOCK MODEL

We consider the steady flow of a plane shock wave in a cloud of uniform density. The parameters shock velocity  $v_0$ , initial gas density  $n_0$ , and fraction of hydrogen in molecular form f, determine the radiation emitted in the cooling zone behind the shock front. The total power per unit area transferred to the gas is proportional to  $\mu n_0 v_0^3$ , where  $\mu$  is the mean particle mass. The initial postshock temperature is proportional to  $\mu v_0^2/k$ . The emission seen from the shock is from gas along the line of sight through the cooling region, and therefore from gas at different temperatures. We will show how the surface brightness of the lines, the excitation temperature observed, and the relative strength of the overtone S(1) line determine the range of parameters  $n_0$  and  $v_0$ .

The basic equations of gas dynamics describing a plane shock have been given by Cox (1972). They are used in the following form:

$$\rho v = \rho_0 v_0 \quad \text{(continuity)} \,, \tag{1}$$

$$p + \rho v^2 = p_0 + \rho_0 v_0^2$$
 (momentum), (2)

$$\rho \frac{d}{dt} \left( \frac{\gamma}{\gamma - 1} \frac{p}{\rho} + \frac{1}{2} v^2 + f_{\text{H}_2} \frac{U}{\mu} \right) + n^2 \Lambda = 0 \quad \text{(energy)},$$
(3)

$$\frac{1}{v}\frac{d}{dt}(n_{\rm H_2}v) = -n_{\rm H_2}D \quad \text{(dissociation)}. \tag{4}$$

Time is measured as it moves with a gas parcel passing through the cooling zone behind the shock front. The preshock values of gas density, mass density, velocity, and pressure are  $n_0$ ,  $\rho_0$ ,  $v_0$ , and  $p_0$ , respectively, and the postshock values are n,  $\rho$ , v, and p. We define  $\gamma$  as the ratio of specific heats including only translational degrees of freedom ( $\gamma = 5/3$ ). The internal energy per molecule, U, is calculated by summing the product of level population and level energy over the vibration-rotation distribution function. The fraction of molecules at each point in the gas is denoted by  $f_{\rm H_2}$ . We take the abundance of He to be 0.1. The cooling function in ergs cm<sup>3</sup> s<sup>-1</sup> is  $\Lambda$ ,  $n_{\rm H_2}$  is the density of  $H_2$ , and the dissociation rate in s<sup>-1</sup> is D. For a strong shock  $(v_0 \gg v_{\rm sound})$  p is much greater than  $p_0$  and, using the ideal gas law, we reduce equations (1)–(4) to two

equations for the dimensionless densities  $u \equiv \rho/\rho_0$  and  $w_{\rm H_2} \equiv n_{\rm H_2}/n_0$ :

$$\frac{du}{dt} = \frac{(w^2 u^2 \Lambda / \mu_0 v_0^2) - f_{\text{H}_2}(u^2 - u)(f_{\text{H}_2} C_v + \epsilon) D}{(2.5 u - 4) + f_{\text{H}_2} C_v (u - 2)}, \quad (5)$$

$$\frac{dw_{\rm H_2}}{dt} = w_{\rm H_2} \left( \frac{1}{u} \frac{du}{dt} - D \right) \,, \tag{6}$$

where we have defined  $\mu_0$ , the preshock particle mass;  $w=n/n_0$ , the dimensionless density;  $\epsilon\equiv U/kT$ , the dimensionless internal energy; and  $C_v\equiv (dU/dT)/k$ , the dimensionless specific heat.

Field et al. (1968) have considered the structure of the radiatively cooling region of a shock in a cloud with H<sub>2</sub> present. They calculated the emission in the rotation lines of the lowest vibrational state and in fine-structure lines of heavier elements. They estimated that the emission and cooling due to the vibrationally excited states was small, and therefore ignored it. However, using collision rates which one of us has calculated (Chu 1977), we find that at high densities and temperatures the vibrational lines are quite important.

The molecular contribution to the cooling is due to energy loss by dissociation and infrared radiation. The radiative cooling function is given most precisely by a sum over all pairs of molecular levels of the difference in collision rates up and down multiplied by the energy difference of the levels. Using the collision rates, and Einstein A values kindly provided by Dr. John Black, we find that for densities above about 10<sup>4</sup> cm<sup>-3</sup> the collisional de-excitation rates are greater than the radiative for the vibration-rotation transitions. For  $n_0 \gg 10^4$  cm<sup>-3</sup> the cooling time for the gas after the shock passes will be much longer than the collision times in and out of each level. We can assume in this case that the level populations are given by Boltzmann factors, and write the radiative cooling as a sum of all the infrared line emission from the molecules in LTE:

$$\Lambda_{r} = \frac{f_{\rm H_2}}{n} \sum_{i} \sum_{j \le i} n_i A_{ij} E_{ij} . \tag{7}$$

Here  $n_i$  is the population of the *i*th level;  $A_{ij}$  the Einstein A coefficient for the transition between levels i and j; and  $E_{ij}$  the energy difference of the *i*th and jth levels;  $n_i$  is given by

$$n_i = g_i Z^{-1} \exp(-E_i/kT),$$
 (8)

where  $g_i$  is the statistical weight of the *i*th level, and Z is the partition function. The dissociation cooling is calculated from the dissociation rate and energy by

$$\Lambda_d = \frac{f_{\rm H_2}}{n} DE_d \,. \tag{9}$$

The internal energy and specific heat are calculated using a Boltzmann distribution. We have included levels for v=0 to 7 and J=0 to 10 in the calculation of  $\Lambda_{\tau}$ ; and v=0 to 14 and J=0 to 20 for the thermodynamic functions  $\epsilon$  and  $C_v$ . Vibrational energy levels

are taken from Herzberg and Howe (1959) and rotational constants are from Herzberg (1950). The calculated values of  $\epsilon$  and  $C_v$  are sensitive to the number of levels used and the energies of these levels. We find, however, that a reasonable variation of the parameters used to calculate the thermodynamic functions changes the results of the model calculations by less than 5%.

The jump condition at the shock front is determined as usual by conservation of mass, momentum, and energy flux, assuming that the internal equilibrium distribution is realized before the gas begins to cool. Shock-tube experiments at temperatures up to 7000 K indicate that this should be accurate when considering the dissociative cooling rate (Hurle, Jones, and Rosenfeld 1969). For a gas in which all the hydrogen is in H<sub>2</sub>, we find that the jump in density across the shock front ranges from 6.2 to 7.7 for shock velocities between 8 and 21 km s<sup>-1</sup>. This corresponds to a range in effective specific heat ratio of 1.3 to 1.4.

Kwan (1977) has indicated the influence of collisional dissociation on the temperature structure and emission of the shocked gas. We find the dissociation to be important for shock velocities greater than  $12 \text{ km s}^{-1}$ . The primary effect is to cool the gas very rapidly to 5000 K and thereby decrease the IR line emission from the hotter regions when  $v_0 > 12 \text{ km s}^{-1}$ .

emission from the hotter regions when  $v_0 \ge 12~{\rm km~s^{-1}}$ . Various experiments on dissociation of  $H_2$  by  $H_2$  and by H give rates that differ greatly in magnitude and in temperature dependence. The highest temperature at which the rates have been measured is 8000 K (Breshears and Bird 1973), and significant differences occur when extrapolating the rates of the different experiments to temperatures above 10,000 K. The most recent work is that of Breshears and Bird; their results agree closely with theory by Shui (1973). We have used the following rates from Breshears and Bird for dissociation of  $H_2$  by  $H_2$  and H:

$$k_d^{\text{H}_2} = 5.48 \times 10^{-9} \exp(-53,000/T) \text{ (cm}^3 \text{ s}^{-1}), (10)$$
  
 $k_d^{\text{H}} = 3.52 \times 10^{-9} \exp(-43,900/T) \text{ (cm}^3 \text{ s}^{-1}). (11)$ 

The rates are different from those used by Kwan (1977), and we have examined the effect of this difference on the results by doing model calculations using Kwan's rates also.

The total cooling due to atomic fine-structure transitions and due to the vibration-rotation lines of

CO is less than about 10% of the  $H_2$  cooling, and has not been included in our calculation.

Our assumption of Boltzmann distribution in the vibration-rotation levels depends on comparing the collisional de-excitation rates with the radiative rates for  $H_2$ . Table 1 shows some typical  $H-H_2$  reactive and  $H_2-H_2$  inelastic collision rates for a temperature of 1000 K. Our  $H-H_2$  vibrational de-excitation rates are substantially larger at high temperature than those used by Kwan (1977). We note that the collisional de-excitation of  $H_2$  by  $H_2$  is dominated by those near-resonant V-R and V-V transitions in which the energy defect is small. Einstein A values are typically  $2 \times 10^{-7} \, \mathrm{s}^{-1}$  for the  $\Delta_v = 1$  quadrupole transitions.

We have further checked our assumption of Boltzmann equilibrium by solving a differential equation for the population of a single level of  $H_2$  along with the cooling equation. This equation is solved assuming that all other levels are populated according to LTE. This technique indicates the density at which we expect departures from equilibrium to become important, and we find that for  $n_0 \ge 10^4$  the level populations are essentially in LTE. Kwan (1977) does not reach this conclusion, and solves rate equations for the vibrational level populations. This is understood to be a result of the smaller H-H<sub>2</sub> vibrational de-excitation rates which he uses.

Assuming that  $H_2$  molecules are formed on dust grains at a rate  $\approx 10^{-17}~n_0~\rm cm^{-3}$  (Hollenbach, Werner, and Salpeter 1971), we find that the typical formation time for the molecules is much greater than the cooling time of a shock in a dense cloud. We therefore do not include formation of  $H_2$  in our model. By comparing the formation time to a typical cloud collapse time of  $\approx (G\mu n_0)^{-1/2}$ , we find that for clouds of density greater than  $10^2~\rm cm^{-3}$  most of the hydrogen should be in the form  $H_2$ , provided there is not a strong UV field present, which would dissociate the molecules. The Copernicus observations (Spitzer et al. 1973) show that there exists a large fraction of molecules in clouds of density  $\sim 10^3~\rm cm^{-3}$ . Since our models all have density approximately  $10^5~\rm cm^{-3}$ , we assume that all the hydrogen is in molecules.

Using the described function for  $\Lambda$  we integrate equations (5) and (6) for a range of parameters  $v_0$  and  $n_0$  along with the level populations to get the total column densities of the excited  $H_2$  levels. The strengths of the infrared emission lines are calculated from the column densities of the excited levels and the Einstein

TABLE 1
TYPICAL H<sub>2</sub> COLLISION RATES AT 1000 K

Collision Process	Rate (cm <sup>3</sup> s <sup>-1</sup> )	Energy Transfer*
$\begin{array}{c} H+H_2(v=1,J=3) \rightarrow H_2(v=0,J=3)+H \dots \\ H_2(0,0)+H_2(1,3) \rightarrow H_2(0,0)+H_2(0,3) \dots \\ H_2(0,0)+H_2(1,3) \rightarrow H_2(0,5)+H_2(0,4) \dots \\ H_2(0,5)+H_2(1,3) \rightarrow H_2(0,7)+H_2(0,7) \dots \\ H_2(2,0)+H_2(0,0) \rightarrow 2H_2(1,0) \dots \end{array}$	$\begin{array}{c} 1.8 \times 10^{-12} \\ 3.3 \times 10^{-14} \\ 5.2 \times 10^{-11} \\ 3.2 \times 10^{-10} \\ 7.0 \times 10^{-12} \end{array}$	(V-T) (V-T) (V-R) (V-R) (V-V)

<sup>\*</sup> Energy modes:  $V \equiv \text{vibrational}$ ,  $T \equiv \text{translational}$ ,  $R \equiv \text{rotational}$ .

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A values. Temperature and density profiles through the cooling zone are similar to Kwan's Figure 1, except that our initial temperatures are larger since we include He in the gas composition. The thickness of the cooling region behind the shock where the excited H<sub>2</sub> is found is typically  $3 \times 10^{12}$  cm for  $n_0 = 10^5$  cm<sup>-3</sup> and  $v_0 = 10$  km s<sup>-1</sup>.

#### V. RESULTS AND DISCUSSION

We define "rotational excitation temperatures" from the column densities of the rotational levels J and J' in v = 1 by  $T_{1;J,J'} \equiv [k \ln (N_{1,J}/N_{1,J'})]^{-1} \Delta E_{JJ'}$ , where  $\Delta E_{JJ'}$  is the energy difference between the levels J and J', and  $N_{1J}$  is the column density of level v =1,J. These temperatures are not true excitation temperatures as would be defined from local populations of molecules in excited states relative to those in the ground state. Even though the gas at any point is in LTE, the temperatures as defined above may be different for each pair of levels since the column densities, being integrals of the level populations through the cooling zone of the shock, are weighted to higher temperature regions for the higher levels. We find, however, that  $T_{1:J,J'}$  depends only weakly on J and J'. For example, for  $v_0 = 10 \text{ km s}^{-1}$ ,  $T_{1:0,5} =$ 1.2  $T_{1;0,1}$ . Therefore, we may represent the relative column densities of the first five rotational levels in v = 1 by a single, average excitation temperature,

 $T_{\rm exc}$ . We may also define "vibrational excitation temperatures" from the column densities of the J=3 levels in v=2 and 3 relative to v=1. We have, for example,  $T_{1,2}\equiv [k\ln{(N_{1,3}/N_{2,3})}]^{-1}(E_{2,3}-E_{1,3})$ , where  $E_{1,3}$  and  $N_{1,3}$  are the energy and column density in the level v=1, J=3. We use J=3 as a reference since these levels give rise to the strong S(1) lines. Vibrational excitation temperatures defined with respect to v=0 are not as meaningful since the populations in v=0 are not observable in the same spectral region.

Figure 1 shows the immediate postshock temperature  $T_{\rm kln}$ ,  $T_{\rm exc}$ ,  $T_{1,2}$ , and  $T_{1,3}$  versus shock velocity. We have also shown as dashed curves the functions  $T_{\rm exc}$ ,  $T_{1,2}$ , and  $T_{1,3}$  obtained by using Kwan's dissociation rates.

Using  $T_{\rm exc}$ , the absolute strength of the S(1) line, and the observed ratio of surface brightness of the fundamental and overtone S(1) lines, we find the range of allowable parameters. This is illustrated in Figure 2 for molecular fraction f=1.0. The upper and lower limiting curves for  $n_0$  are set by requiring the surface brightness of the fundamental S(1) line to be in the range  $1.8 \times 10^{-3} \le I \le 7.2 \times 10^{-3}$  ergs cm<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup>.

The low-velocity limit is set by the requirement that  $T_{1,2}$  be  $\leq 1900$  K. This limit is approximately  $v_0 \geq 8$  km s<sup>-1</sup>. The high-velocity limit is  $v_0 \approx 21$  km s<sup>-1</sup>, above which the molecules are destroyed before the shock cools. For shocks of velocity greater than 21 km s<sup>-1</sup> the gas cools slowly by radiation from atoms and CO molecules (Kwan 1977).

We see from Figure 1 that shock velocities over a wide range give nearly the same relative strength of

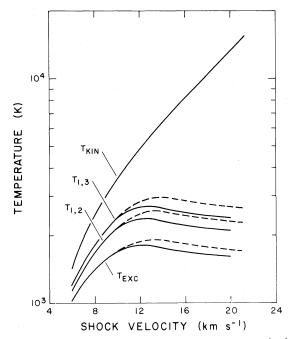


Fig. 1.—Immediate postshock temperature,  $T_{\rm kin}$ , excitation temperatures  $T_{1,2}$  of v=2 relative to v=1;  $T_{1,3}$ , of v=3 relative to v=1; and  $T_{\rm exc}$ , of relative column densities of rotational levels within v=1 versus shock velocity  $v_0$ ; assuming molecular fraction f=1 and no magnetic field. Dashed lines indicate the excitation temperatures calculated by using Kwan's (1977) dissociation rates.

the observed lines. We conclude that a shock with velocity between 8 and 21 km s $^{-1}$  and appropriate density as indicated in Figure 2 can produce the  $\rm H_2$  emission observed in Orion.

From Figure 1 we predict that for such a shock the excitation temperature fitted to the first five rotational levels of v=1 will lie between 1600 K and 2000 K, a range more restricted than the observational limits set by Gautier *et al.* (1976). We also estimate the surface brightness of the 3–0 S(1) line at 8151 Å using  $T_{1,3}$  from Figure 1. We find that, at the BN object, this line should have surface brightness between  $1.8 \times 10^{-6}$  and  $1.2 \times 10^{-5}$  ergs cm<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup>, depending on the actual shock velocity.

An upper limit to the surface brightness of the 3-0 S(1) line of  $2.6 \times 10^{-7}$  ergs cm<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup> in the region of maximum IR emission has been set by Traub (1977). If we assume that the absence of this line is due to extinction, the minimum extinction needed at  $2\mu$  is 0.7 mag. This implies an extinction of 7 mag in the visual band (cf. Aannestad and Purcell 1973). The presence of this extinction is not unexpected in the Orion region; however, it does require that the  $2\mu$  lines be formed with at least twice the observed power.

This observation is also evidence against a model in which the infrared emission lines are the result of ultraviolet pumping. If the assumed UV source is a star external to the cloud, such as  $\theta'$  Ori C, the UV continuum cannot penetrate to the emitting region. If,

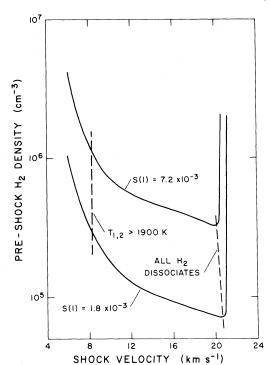


Fig. 2.—Range of parameters velocity  $v_0$  and initial density no, to match  $H_2$  infrared observations for case with f = 1. The low-velocity cutoff is for  $T_{1,2} \ge 1900$  K. The high-velocity cutoff is the velocity above which all the molecules are destroyed. The density limits at each velocity are set to match maximum and minimum contours on Grasdalen's map.

on the other hand, the assumed UV source is buried within the cloud, we estimate that the interstellar dust that absorbs most of the UV continuum will produce an infrared continuum which is roughly an order of magnitude brighter than observed (Rieke, Low, and Kleinmann 1973).

A magnetic field has two effects on the shock flow. The first is to reduce the total power of the shock which goes into thermal energy of the gas. This can be compensated for in our model by increasing  $v_0$  so that the initial postshock temperature is constant as we increase the magnetic field. The second effect is to inhibit the compression in the cooling region. This does not affect the  $H_2$  emission for  $T_{\rm kin} \leq 5000$  K since the vibrational cooling dominates, and is independent of density. For  $T_{\rm kin} > 5000$  K the dissociation cooling is important and is linear on the density. Thus a strong magnetic field will decrease the relative importance of dissociative cooling. However, the dissociation is most important at the highest temperatures when the density has not yet increased greatly, and therefore the inhibition of compression due to a magnetic field will not significantly alter our conclusions. Field et al. (1968) have discussed the effects of magnetic fields on the gas flow in greater detail.

We conclude that a shock with suitable parameters can produce the observed emission. We now discuss a possible source of such a shock. Since there is no obvious infrared or radio continuum centered on the H<sub>2</sub> line-emitting region, we are forced to look elsewhere in the vicinity. The obvious candidate is the Trapezium star  $\theta^1$  Ori C, an O7 star of luminosity  $\sim 10^5 L_{\odot}$  that is some 0.25 pc SE of the emitting region. As Hollenbach and Shull (1977) have pointed out, it is difficult to understand such a high shock velocity in terms of an ionization front, because such a model would require the ionized gas to have an emission measure orders of magnitude greater than observed.

Another possibility is that the shock is driven by a stellar wind from  $\theta^1$  Ori C. Castor, McCray, and Weaver (1975) have presented a theory for the development of an expanding shell of gas driven by a stellar wind. Snow and Morton (1977) find evidence that  $\theta^1$  Ori C does have such a wind. We find from the theory of Castor et al. that a stellar wind with a mass loss rate  $\dot{M}_w \approx 10^{-5} M_{\odot} \text{ yr}^{-1}$  and terminal velocity  $V_w \approx 2000 \text{ km s}^{-1}$  will drive a shock to a distance 0.25 pc in a medium of ambient density  $n_0 = 6 \times 10^5 \text{ cm}^{-3}$  in a time  $t = 1.5 \times 10^4 \text{ yr}$ , and at that time the shock will have a velocity  $v_0 = 8 \text{ km s}^{-1}$ . These parameters are in the range necessary to explain the H<sub>2</sub> emission according to Figure 2, but the required stellar wind mass loss rate is uncomfortably large. Perhaps the discrepancy is due to density inhomogeneities in the original gas distribution around the Trapezium stars, or perhaps the shock is generated by some as yet unexplained phenomenon associated with star formation in this region.

We thank Dr. John Black for sending us unpublished Einstein coefficients of hydrogen molecules, Dr. Gary Grasdalen for communicating results to us before publication, and Dr. Harm Habing for helpful discussions. This work was supported by the National Science Foundation through grant number AST 75-23590 to the University of Colorado. One of us (S.-I C.) wishes to acknowledge the support by the National Science Foundation grant PHY 74-09408-A02 through which part of this work was done at Yale University.

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