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# THE HEATING OF INTERSTELLAR CLOUDS BY VIBRATIONALLY EXCITED MOLECULAR HYDROGEN

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## ABSTRACT

We discuss the possibility that vibrationally excited  $H_2$  may be collisionally de-excited, so providing a heating mechanism for interstellar clouds which operates by coupling the stellar radiation to the gas. The majority of excitations in the Lyman and Werner bands of  $H_2$  return the molecules to the ground electronic state in a vibrationally excited level, the most favored being  $v'' = 7$ . We compare the heating rate obtained in this way with other mechanisms which have been postulated, and present the results of calculations of temperature as a function of depth into clouds of different densities. It appears that this mechanism is a significant one, which should be taken into account in detailed models of dense clouds.

## I. INTRODUCTION

There has been a continuing effort to understand the heating and cooling processes in the interstellar medium since Spitzer's classic papers (1948-50). The most recent review is that of Dalgarno and McCray (1972) who list a very large number of collisional processes contributing to cooling and discuss time-independent and time-dependent heating effects. This article presents a heating mechanism not considered hitherto, which may be applicable to dense interstellar  $H_2$  clouds. It can effectively couple stellar radiation  $\sim 1000\text{\AA}$  with the gas by the collisional de-excitation of vibrationally excited  $H_2$ .

## II. THE MECHANISM

It has been shown by Stecher and Williams (1967) that a significant fraction of all excitations in the  $H_2$  ( $v'' = 0$ ) Lyman bands by the absorption of  $\sim 1000\text{\AA}$  radiation results in destruction of the molecules because the cascade is into the vibrational continuum of the ground state. Accurate calculations by Dalgarno and Stephens (1970) show this fraction to be 23%. The remaining 77% of the Lyman band excitations, and all the Werner band excitations (for  $\lambda > 912\text{\AA}$ ) return the molecules to vibrationally excited bound levels in the electronic ground state. The initial distribution among these levels is known (Allison and Dalgarno 1969, Cartwright and Drapatz 1970),  $v''$  in the range 4 - 10 being most favored. Since  $H_2$  has no dipole moment, transitions between the vibrational levels of the ground state are forbidden. The vibrational transition probabilities are therefore very small; for example, the  $v'' = 1 \rightarrow v'' = 0$  transition has a rate  $8.56 \times 10^{-7} \text{ sec}^{-1}$  (Dalgarno, private communication, 1972). These values imply long radiative lifetimes, and so it is of interest to assess

the importance of collisional de-excitation of these levels. In such collisions, the vibrational energy removed is transformed into kinetic energy.

Formally, we may treat the problem by writing down the equation for the number density of  $H_2$  in any particular vibrational level in terms of absorption of radiation, and of relaxation by radiative and collisional processes. In equilibrium, there are fifteen coupled algebraic equations, from which the mean level populations may be determined. Then the heating function is given by the relaxation rates times the appropriate energy transfer.

Thanks to the work of Dalgarno and his associates much of the necessary data concerned with radiative processes is available. However, the collisional data is extremely poorly known, if at all. Most of that which exists refers only to the 0-1 band. Consequently, with the present level of knowledge the full set of equations cannot be solved. However, we assert that useful information can be obtained from a two-level system in which the lower level represents  $v'' = 0$ , and the upper level represents all  $0 < v'' \leq 14$ . We shall use a radiative rate for the upper level corresponding to the inverse of the radiative lifetime of the  $v'' = 7$  level and a mean energy released per relaxation collision equivalent to this level also. This assumes that relaxation is complete when it occurs.

### III. THE TWO-LEVEL SYSTEM

For this system instead of fifteen equations, we obtain

$$\frac{d}{dt} n(H_2^*) = \alpha \beta n(H_2) - \alpha^* \beta^* n(H_2^*) - A n(H_2^*) - R n(H_2^*) \quad (1)$$

where  $n(H_2^*)$  represents the number density of vibrationally excited  $H_2$  molecules and  $n(H_2)$  that of  $H_2$ ,  $v'' = 0$  molecules. The rate of excitation from the X,  $v'' = 0$  state is  $\beta$ , and the fraction of all excitations returning to an X,  $v'' > 0$  bound

state is  $\alpha$ . In a similar way,  $\alpha^*\beta^*$  represents the fraction of all excitations of  $H_2^*$  not returning as  $H_2^*$ . This term includes direct photodissociation and photoionization of  $H_2^*$  which can occur in the interstellar medium (Stecher and Williams 1967). The symbols A and R represent the radiative relaxation (Einstein A-value) and the collisional relaxation ( $H_2^* \rightarrow H_2$ ) processes, respectively. Equation (1) assumes that  $n(H_2)$  is constant in time, i.e. that the production and destruction rates for  $H_2$  are equal. The mechanism may also be valid in non-steady situations. In equilibrium

$$n(H_2^*)/n(H_2) = \alpha\beta/(A + R + \alpha^*\beta^*) \quad (2)$$

and the heating rate is now

$$\dot{Q} = \epsilon_0 n(H_2^*) R$$

i.e.

$$\dot{Q} = n(H_2) \alpha\beta \epsilon_0 \left\{ \frac{R}{A + R + \alpha^*\beta^*} \right\} \quad (3)$$

where  $\epsilon_0$  is the mean energy released in the relaxation. It is convenient to discuss the term in the curly brackets separately from the rest of equation (3). Therefore, we introduce the notation

$$\xi = R/(A + R + \alpha^*\beta^*) \quad (4)$$

for the factor containing all the relaxation terms. This represents the coupling between the radiation energy and heat energy in the gas.

#### IV. RELAXATION PROCESSES

(a) Electrons - Vibrational excitation in slow e- $H_2$  collisions has been studied experimentally (Ehrhardt et al. 1968, Trajmar et al. 1969, and in particular, near the  $v'' = 1$  vibrational excitation threshold, Burrow and Schulz 1969) and also theoretically (Henry, 1970). From the relations between the excitation and de-excitation cross-sections

(Seaton 1958) we find the  $v'' = 1 \rightarrow v'' = 0$  de-excitation cross-section is  $\sim 2 \times 10^{-17} \text{ cm}^2$  for any thermal energy which is much less than the vibrational energy. We therefore, adopt for electrons:

$$\langle \sigma_{\text{coll}} u_{\text{coll}} \rangle_{1 \rightarrow 0, e} \approx 10^{-10} \text{ cm}^3 \text{ s}^{-1}, \quad (5)$$

while recognizing that the corresponding rate for higher  $v'' \rightarrow v'' - 1$  transitions may be faster.

(b) Atoms and Molecules - Takayanagi (1963) has reviewed the subject of collisionally induced vibrational transitions and presents criteria which make it clear that - under conditions appropriate to the present discussions - such transitions are unlikely. The existing evidence supports this view.

Relaxation of  $\text{H}_2^*$  in collision with  $\text{H}_2$  is very slow; measured times are on the order of  $10^{16}/n(\text{H}_2)$  seconds at room temperature and even longer at lower temperatures (Kiefer and Lutz, 1966; DeMartini and Ducuing, 1966). Relaxation of  $\text{H}_2^*$  by atoms H and He has been examined theoretically. For example, Micha and Rotenberg (1970) have considered He,  $\text{H}_2$  collisions. They find cross-sections which are negligible for our purpose. The case of H-atom relaxation is made slightly more favorable by the possibility of exchange,  $\text{H} + \text{H}_2^* \rightarrow \text{H}_2 + \text{H}$ , enabled by tunnelling through the appropriate barrier. Truhlar and Kupperman (1970) have used an appropriate  $\text{H}_3$  surface and find that the probability of a non-adiabatic collision is greater than 1/2 for a relative translational energy of some tenths of an eV.

Allowing a reasonable barrier shape, we find that a cross-section of  $\sim 10^{-19} \text{ cm}^2$  would be appropriate under the relevant conditions. We conclude that such interactions are unimportant compared to electrons. But it is possible that in some extreme situations they may be important. We, therefore, present the number densities of some de-exciting agents at which collisional and radiative de-excitation rates ( $\sim 10^{-7} \text{ s}^{-1}$ ) are equal. For  $\text{H}_2$ , H, e, p these number densities are  $\sim 10^{10}$ ,  $10^7$ ,

$10^3$  and  $10^2 \text{ cm}^{-3}$ , respectively.

## V. DISCUSSION OF THE FACTOR $\xi$

From the vibrational transition probabilities supplied by A. Dalgarno (private communication 1972), the mean cascade rate  $A$  which we should insert in (4) is  $3 \times 10^{-7} \text{ s}^{-1}$ . From (5) we adopt for  $R$

$$R = 10^{-10} n(e) \quad (6)$$

The other term in  $\xi$  is  $\alpha^* \beta^*$ . The information required to calculate  $\alpha^*$ , the fraction of excitations of  $\text{H}_2^*$  not returning to  $\text{H}_2^*$ , is available (Allison and Dalgarno 1969, Dalgarno and Stephens 1970, Cartwright and Drapatz 1970) and we present in Table I the fractions for each vibrational level, for the Lyman and Werner bands, including only those transitions for which  $\lambda > 912 \text{ \AA}$ . We choose a mean  $\alpha^*$  to be 0.2. The rate of excitation in the Lyman and Werner bands from  $\text{H}_2^*, \beta^*$ , will be larger than  $\beta$  since (with due allowance for rotational branching) 42 times as many levels are involved. The amount of  $f$ -value associated with each  $v''$  level is approximately the same. We shall assume  $\beta^* \simeq 42\beta$ . In the optically thin case, the lifetime of an  $\text{H}_2$  molecule in a typical interstellar radiation field is  $\sim 10^{10} \text{ s}$  (Stecker and Williams 1967). This means that  $\alpha\beta \simeq 4 \times 10^{-10} \text{ s}^{-1}$  and from this we calculate that  $\alpha^*\beta^*$  in the optically thin case is  $\sim 4 \times 10^{-9} \text{ s}^{-1}$ . Allowance for direct photodissociation of  $\text{H}_2^*$  increases this to  $\sim 5 \times 10^{-9} \text{ s}^{-1}$ . In most situations, therefore, we may write  $\xi = 3 \times 10^{-4} n(e)$  and the difficulty lies in the choice of  $n(e)$  for the situation considered (Pottasch 1972).

## VI. THE HEATING RATE

The heating rate is now given by

$$\mathcal{H} = n(\text{H}_2) \alpha \beta \epsilon_0 \xi \quad (7)$$

in which extinction and line absorption problems are all contained in  $\beta$ . We calculate extinction due to the grains at a rate of 3 magnitudes per kiloparsec of the mean interstellar medium (Stecker 1969), assuming a constant gas/



dust ratio. There is also competition for the  $\sim 1000\text{\AA}$  radiation by the photoionization of carbon, which has a threshold at 11.1 eV and a nearly constant cross section of  $1.1 \times 10^{-17} \text{ cm}^2$  over the first few eV of absorption (Bates and Seaton 1949). Werner (1970) has shown how the fractional abundance of carbon varies with depth inside clouds of various densities on the assumption that the electron density arises solely from the photoionization of carbon. This assumption may be in error. The line widths as a function of column density are from Cartwright and Drapatz (1970). We choose  $\epsilon_0 = 5 \times 10^{-12} \text{ erg}$ . In any given situation we may now evaluate  $\epsilon_0$ .

## VII. OTHER HEATING MECHANISMS

Besides the familiar suggestions of cosmic rays and X-rays (see e.g. Dalgarno and McCray 1972) as heat sources for the interstellar medium, and the recent idea of Watson (1972) concerning grains, there are a number of other heating mechanisms which may be significant. These have in common with the  $\text{H}_2^*$  heating rate the ability to couple stellar radiation energy to the gas as distinct from cosmic or X-ray energy. They depend on photodissociation and photoionization of molecules and ions. In general, each such event will release several eV into the gas. This process may be so efficient at using relatively low energy continuum radiation, that the rate-limiting mechanism is usually the formation rate of the relevant species.

The photodissociation of a diatomic molecule XY of dissociation energy D by radiation of energy E gives a heat gain (E-D). The fastest production rates via radiative association are  $\sim 10^{-16} \text{ cm}^3 \text{ s}^{-1}$  (Julienne and Krauss 1972) and thus the greatest heating rate that can be obtained is  $\sim 10^{-28} n(X)n(Y) \text{ erg cm}^{-3} \text{ s}^{-1}$ . Grain surface reactions may improve this rate somewhat. This is unlikely to be significant in dense clouds.

Photodetachment in negative ions also provides a possible heat source. Using the radiative attachment rate of de Jong (1972)

for H+e we find a heating rate  $\sim 10^{-30} T n(H)n(e) \text{ erg cm}^{-3} \text{ s}^{-1}$  which clearly has little significance in dense clouds but may be important in the intercloud region.

In section III we emphasized that allowance should be made for direct photodissociation of  $H_2^*(v \geq 3)$ . Each such photodissociation supplies heat and using III we estimate a heating rate of  $\sim 10^{-24} n(H_2) \text{ erg cm}^{-3} \text{ s}^{-1}$  in the optically thin case at the edge of clouds. In the interior this rate falls off quickly since two photons are required to make it work. But this rate may be significant in low density clouds where a high  $H_2$  production rate exists.

#### VIII. DISCUSSION OF THE SIGNIFICANCE OF THE HEATING RATE

To determine the significance of  $\mathcal{H}(H_2^*)$  we compare it with other heating rates which have been suggested. All of these heating rates fall off with depth. There is considerable doubt that the lower energy cosmic rays penetrate denser clouds at all (Solomon and Werner 1971). X-rays of 1/4 keV are absorbed with an optical depth of unity in a column density of  $6 \times 10^{19} \text{ cm}^{-2}$ . The grain mechanism of Watson competes directly for the photons operating the  $\mathcal{H}(H_2^*)$  mechanism. Because the modes of decrease are complicated, we first show in Table II heating rates at zero depth into clouds for the various processes. The rate  $\mathcal{H}(H_2^*)$  is given for an incident flux of  $10^6 \text{ photons cm}^{-2} \text{ s}^{-1} \text{ \AA}^{-1}$  the optically thin case, and on the assumption that  $n(e) = n(C^+)$ , a minimum case. Clearly, these zero depth rates are not very meaningful in an absolute sense but this table shows that-especially in denser regions - the heating rate  $\mathcal{H}(H_2^*)$  must be considered.

A clearer and perhaps more realistic way to assess the importance of  $\mathcal{H}(H_2^*)$  is to couple it with a cooling rate to obtain a temperature at various depths in a cloud ignoring all other heating mechanisms. We present the results of these calculations in Table III. The incident radiation from at  $\sim 1000 \text{ \AA}$  was assumed to be  $10^6 \text{ photons cm}^{-2} \text{ s}^{-1} \text{ \AA}^{-1}$ .

The cooling rates are taken from Dalgarno and McCray (1972) and include cooling due to excitation in C, C<sup>+</sup>, O, CO, CN and H<sub>2</sub> by e and by H<sub>2</sub>. However, the rates quoted must be modified for the high density regions considered here due to collisional de-excitation of these species [cf. Bahcall and Wolf 1968]. In the calculation of  $\mathcal{J}^f(\text{H}_2^*)$  the equivalent widths of Cartwright and Drapatz (1970) were used, and allowance was made for extinction and the photoionization of carbon, the electron density being assumed to arise solely from this process. Thus we have a minimum  $\mathcal{J}^f(\text{H}_2^*)$  ignoring possible electrons from other sources. We also include temperatures which would be obtained if  $n(e)$  were 30 times greater. Finally, we show the temperatures which would be obtained if heavy atoms were depleted by sticking to grains in the manner suggested by Field, Goldsmith, and Habing (1969). The depletion factor is 10 times, and the effect is to reduce the cooling rate. The temperatures are given at various depths within the cloud measured from the edge, the incident flux of radiation being chosen as  $10^6 \text{ photons cm}^{-2} \text{ s}^{-1} \text{ \AA}^{-1}$  in the relevant wavelength range. Note that these temperatures are not precise calculations, but are a measure of the importance of  $\mathcal{J}^f(\text{H}_2^*)$ .

It is clear from the cases considered that the heating from H<sub>2</sub><sup>\*</sup> is confined to the edges of clouds, as is the heating from any other suggested mechanisms. The central temperatures of dense regions must therefore be very low indeed. The relatively high temperatures at the edges of clouds will provide a confining pressure for clouds which are not gravitationally bound. The temperatures obtained are not inconsistent with observations (Heiles 1971) and this fact supports the view that heating by H<sub>2</sub><sup>\*</sup> is an important mechanism in dense clouds.

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TABLE I

$\alpha_{v''}^*$  represents the fraction of all excitations in the Lyman and Werner bands not returning to groundstate  $H_2^*$ , for each level  $v''$

$v''$	$\alpha_{v''}^*$ (Lyman)	$\alpha_{v''}^*$ (Werner)	$v''$	$\alpha_{v''}^*$ (Lyman)	$\alpha_{v''}^*$ (Werner)
1	0.19	0	8	0.16	0.05
2	0.21	0.03	9	0.17	0.03
3	0.16	0.01	10	0.17	0.02
4	0.17	0.02	11	0.15	0.05
5	0.18	0.06	12	0.14	0.08
6	0.18	0.02	13	0.18	0.15
7	0.16	0.02	14	0.34	0.51

$\alpha_{v''}^*$  is calculated from data in Allison and Dalgarno (1969), Dalgarno and Stephens (1970), and Cartwright and Drapatz (1970).

TABLE II

Approximate Heating Rates at Zero  
Depth into  $H_2$  Clouds ( $\text{erg cm}^{-3} \text{s}^{-1}$ )

$\gamma$ ( $H_2^*$ )	$2 \times 10^{-27} n^2(H_2)$
Cosmic Rays	$5 \times 10^{-27} n(H + H_2)$
X-Rays	$2 \times 10^{-26} n(H + H_2)$
Photodetachment from grains	$10^{-26} n(H + H_2)$
Photodestruction of $XH$ , maximum (formed in radiative association)	$10^{-33} n(H + H_2)$
Photodestruction of $XY$ , maximum (formed in radiative association)	$10^{-35} n^2(H + H_2)$
Photodetachment of $H^-$	$10^{-30} T n(H)n(e)$
Photodissociation of $H_2^*(v'' \geq 3)$	$10^{-24} n(H_2)$

(but see discussion in VII)

TABLE III

Temperatures at Selected Depth Within  $H_2$  Clouds of  
Different Densities Heated Solely by  $H_2^*$

Depth(cm)	$n(H_2) = 10^2$	Depletion	No Depletion
$1 = 10^{18}$	high $n(e)$	19	14
	low $n(e)$	12	8
$1 = 10^{19}$	high $n(e)$	15	11
	low $n(e)$	9	$<<10$
	$n(H_2) = 10^3$		
$1 = 10^{17}$	high $n(e)$	25	14
	low $n(e)$	13	8
$1 = 10^{18}$	high $n(e)$	12	8
	low $n(e)$	$<<10$	$<<10$
	$n(H_2) = 10^4$		
$1 = 10^{16}$	high $n(e)$	65	24
	low $n(e)$	18	13
$1 = 10^{17}$	high $n(e)$	$<<10$	$<<10$
	low $n(e)$	$<<10$	$<<10$

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Temperatures calculated to be more than a few degrees less than  $10^0 K$  are written  $<<10^0 K$ , since the cooling curve is not particularly accurate at these temperatures.

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