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MODEL CALCULATIONS OF THE UV - EXCITED MOLECULAR HYDROGEN IN INTERSTELLAR CLOUDS

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ABSTRACT

We have calculated 2448 interstellar cloud models to investigate the formation and destruction of high rotational level H_2 according to the combinations of five physical conditions: the input UV intensity, the H_2 column density, cloud temperature, total density, and the H_2 formation rate efficiency. The models include the populations of all the accessible states of H_2 with the rotational quantum number J < 16 as a function of depth through the model clouds, and assume that the abundance of H_2 is in a steady state governed primarily by the rate of formation on the grain surfaces and the rates of destruction by spontaneous fluorescent dissociation following absorption in the Lyman and Werner band systems. The high rotational levels J = 4 and J = 5 are both populated by direct formation into these levels of newly created molecules, and by pumping from J = 0 and J = 1, respectively. The model results show that the high rotational level ratio $N(4)/N(0)$ is proportional to the incident UV intensity, and is inversely proportional to the H_2 molecular fraction, as predicted in theory.

Key words: ISM, H_2 Clouds, FUV, Molecular hydrogen

1. INTRODUCTION

The hydrogen molecule (H_2) is the most abundant molecule in the interstellar medium (ISM) and plays a central role in a variety of processes that significantly influence the chemical and physical state of the ISM (Spitzer 1978). Since H_2 in its ground electronic state has no permanent electric dipole moment, H_2 in quiescent interstellar clouds has been observed directly only by means of its ultraviolet absorption lines along lines of sight where the total visual extinction is A_v < 2 mag (Black & van Dishoeck 1987, hereafter BvD87). Systematic measures of the rich spectrum of H_2 in the far-ultraviolet (FUV) give the values of $N(J)$, the column density of H_2 molecules in the rotational level J of the ground vibrational and electronic state. The sum of these gives $N(H_2)$ which can be compared with the predictions of theories for H_2 formation and disruption. The rotational excitation depends on physical conditions in the clouds, and can be used to determine the cloud temperature T, the volume density n(H I) of neutral hydrogen, and $_0$, the probability per unit time that an H_2 molecule at the cloud surface absorbs a photon in any of the Lyman or Werner lines (Spitzer & Jenkins 1975). Evidently, β_0 is a measure of the ultraviolet radiation flux incident on a cloud (Spitzer 1978; Lee et al. 2000). For example, from $N(1)/N(0)$ one may infer the kinetic temperature of the clouds (Shull & Beckwith 1982). Also, Jura (1975) has shown that one can calculate *Rn,* the product of formation rate and density, and estimate β_0 from a comparison between the detailed numerical calculations and the observations of $N(4)/N(0)$, which is controlled by the optical pumping rate. Therefore, observations of the high-rotational level molecular hydrogen can provide the UV radiation field intensity around a cloud, which are not easy to obtain directly.

In this paper, we present H_2 cloud model calculation results of 2448 combinations of the 5 physical parameters: the input UV intensity I_{UV}, the H_2 column density H_2, cloud temperature T, total hydrogen density n_H, and the H_2

formation rate efficiency y_f, to analyze the relationship between the high rotational H_2 level ratio and above parameters. In Section 2, the H_2 model developed by BvD87 is described, and the input parameters for the calculation are introduced. In Section 3, the basic calculation results are described, and the relations between the molecular fraction and the high rotational H_2 level ratio are plotted under various physical conditions. In Section 4, we describe the conclusion.

2. MODEL CALCULATIONS

We have used the H_2 model program developed by van Dishoeck & Black (1986) and BvD87. The program considers the abundance and excitation of H_2 in plane-parallel clouds, includes all 211 bound levels of all vibrational levels, v = 0-14, of the $X^{1+}{}_g$ state of H_2 with J up to an arbitrary limit of 15, and treats explicitly the rates of all electronic transitions involving these levels. Photoionization out of excited H_2 levels with v = 4 is included explicitly, and the effect of direct photodissociation out of v = 3 is considered. It is assumed that the abundance of H_2 is in steady state governed primarily by the rate of formation on grain surfaces and the rates of destruction by spontaneous fluorescent dissociation following absorption in the $B^{1+}{}_g$ - $X^{1+}{}_g$ Lyman and $C^1{}_u$ - $X^{1+}{}_g$ Werner band systems. The equation of transfer is solved for 22445 absorption lines simultaneously with the equations of statistical equilibrium that describe the populations of 211 levels of $X^{1+}{}_g$ (v = 0-14, J = 15), 629 levels of $B^{1+}{}_g$ (v = 0-36, J = 16), and 476 levels of $C^1{}_u$ (v = 0-13, J = 16). The resultant model program generates the output results of dissociation and excitation rates, densities, and column densities of all vibrational, rotational levels of H_2 along the depth of the model cloud.

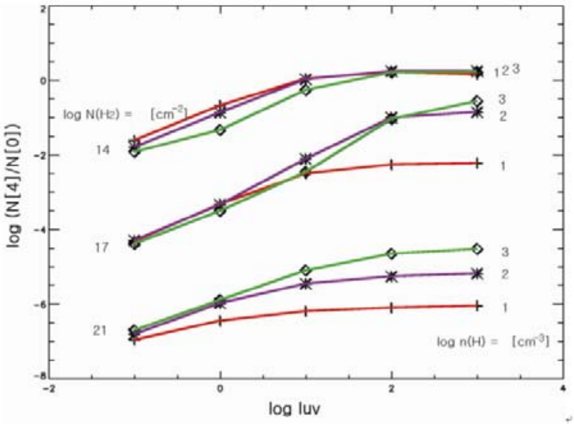
The model program requires several initial input parameters, such as the total hydrogen density n_H, cloud temperature T, total H_2 column density $N(H_2)$, the energy spectrum and the intensity of incident UV radiation field I_{UV}, H_2 formation rate efficiency parameter y_f, which is related with the formation rate as $R = 3 \times 10^{-18}\ T^{1/2}\ y_f$ (BvD87). I_{UV} is the enhancement factor compared with the mean interstellar value adopted by Draine (1978), i.e., (= 1000) = 4.5 x 10^{-8} photons cm^{-2} s^{-1} Hz^{-1}. For our model calculations, we have made each combination among these five parameters: n_H = (10, 10^2, 10^3, 10^4, 10^5) cm^{-3}, T = (10, 100, 200) K, $N(H_2)$ = (10^{14}, 10^{15}, 10^{16}, 10^{17}, 10^{18}, 10^{19}, 10^{20}, 10^{21}) cm^{-2}, I_{UV} = (10^{-1}, 10^0, 10^1, 10^2, 10^3, 10^4, 10^5), and y_f = (0.1, 1, 10). Total 2448 cloud models have generated valid results out of 2520 possible combinations. The remaining 72 cases such as n_H = 10 cm^{-3}, T = 10 K, $N(H_2)$ = 10^{14} cm^{-2}, I_{UV} = 10^4, and y_f = 10 do not make proper conditions for the interstellar clouds. We have followed the interstellar standard values described in BvD87 for the remaining parameters.

3. RESULTS AND ANALYSIS

3.1 High Rotational Level H_2 Ratio vs. Incident UV Intensity

The selective model results of the relation between I_{UV} and $N(4)/N(0)$ are shown in Figure 1 and 2 for two different set of parameters. In Figure 1, T and y_f are fixed while $N(H_2)$ and n_H are varied. Detailed parameter values are presented in the caption. It is obvious that $N(4)/N(0)$ is proportional to I_{UV}, although it is eventually saturated as I_{UV} becomes higher. This saturation limit results from the competition between grains and molecules for absorbing UV photons in the case of high $N(H_2)$ clouds (the lower group in Figure 1), and the exhaustion of low rotational level H_2 in the case of low $N(H_2)$ clouds (the upper group in Figure 1). In all cases, the line and continuum optical depths at 1000 are initially comparable when the ratio I_{UV}/n_H is of the order of unity (BvD87). Thus when $I_{UV}/n_H < 1$, line absorption completely dominates the attenuation of the UV radiation and most of the available photons dissociate and excite H_2, which produces the same $N(4)/N(0)$ ratios independent to the hydrogen density n_H. When $I_{UV}/n_H = 1$, however, some of the these photons are removed by the grains so that the efficiency of excitation of H_2 is reduced (Pak et al. 1998). This means that the presence of an intense UV radiation field will not yield the maximum $N(4)/N(0)$ ratio unless the density n_H is also large, which is easily seen in Figure 1.

On the contrary, $N(H_2)$ and n_H are fixed, while T and y_f are varied in Figure 2. A higher temperature increases the H_2 formation rate (BvD87) and thus has a larger $N(4)/N(0)$ ratio, especially when I_{UV} is low, because the grain temperature is governed mainly by the cloud temperature through collisions in that case. The effect of the H_2 formation rate coefficient y_f is dominant when I_{UV} becomes higher, because the competition between grains and molecules for the UV photons depends not only on I_{UV} and n_H but actually on the ratio $I_{UV}/[n_H\ y_f]$ (See equation (15) in BvD87). Hence, if I_{UV} is low, then changes in n_H and y_f



Finger 1. Model calculation results of the high rotational H_2 level ratio vs. the incident UV intensity when T = 100 K and y_f = 1. The plus, asterisk, and diamond symbols indicate n_H = 10, 100, and 1000 cm^{-3}, respectively.

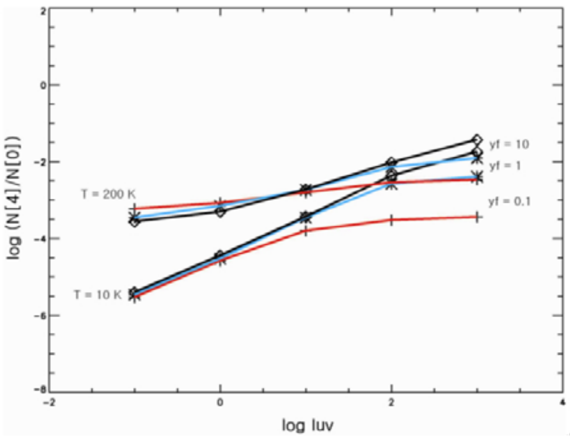


Figure 2. Model calculation results of the high rotational H_2 level ratio vs. the incident UV intensity when n_H = 10^3 cm^{-3} and $N(H_2)$ = 10^{18} cm^{-3}. The plus, asterisk, and diamond symbols indicate y_f = 0.1, 1, and 10, respectively.

make little differences in the resulting N(4)/N(0) ratios.

3.2 Molecular Fraction vs. Incident UV Intensity

The average column density-weighted molecular fraction f is defined to be

$$f = \frac{\Sigma 2N(\mathrm{H_2})}{\Sigma[N(\mathrm{HI})+2N(\mathrm{H_2})]} \qquad (1)$$

for the quantitative analysis of the model results. Equilibrium between the formation of H_2 with a rate coefficient R (in cm^{-3} s^{-1}) and the photodestruction of H_2 with rate D (in s^{-1}) in an interstellar cloud (Jura 1975) can be expressed as

$$Rn_{\mathrm{H}}n(\mathrm{H\,I}) = Dn(\mathrm{H_2}) \qquad (2)$$

If we assume an optically thin and homogeneous cloud (Jura 1974; Tumlinson et al. 2002), then

$$f = \frac{2Rn(\mathrm{H\,I})}{D} \qquad (3)$$

where f is the molecular fraction defined above. Since the photodestruction rate D is proportional to the interstellar radiation field (Jura 1974) and $N(4)/N(0)$ is also proportional to the incident UV intensity as described in the previous section, equation (3) can be expressed as following:

$$f \sim \frac{2Rn(\mathrm{H\,I})}{I_{\mathrm{UV}}} \sim \frac{Rn(\mathrm{H\,I})}{N(4)/N(0)} \qquad (4)$$

Note that n(H I) can be approximated to n_H when f << 1. Thus, the observed molecular fraction can be used to derive the cloud density n_H, if $N(4)/N(0)$ and R are obtained.

3.3 High Rotational Level H_2 Ratio vs. Molecular Fraction

If we assume f << 1 and take logarithm of equation (4), then

$$\log f \sim \log R + \log n_{\mathrm{H}} - \log\frac{N(4)}{N(0)} \qquad (5)$$

i.e. log f is linearly decreased with log $N(4)/N(0)$. To verify the relation, we have plotted our model results in Figure 3 with the variations of n_H, while y_f, and T (therefore R) are fixed. See the figure caption for the detailed parameter values. It is obvious in Figure 3 that the slope of each line is about -1 on average. The effect on the line constant of each physical parameter is the same as in the previous section.

4. CONCLUSION

A plane parallel H_2 model developed by BvD87 is used to

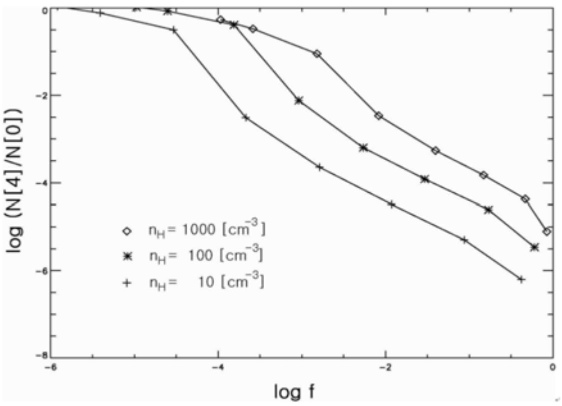


Figure 3. Model calculation results of log *f* vs. log *N*(4)/*N*(0). Three lines indicates different hydrogen density (n_H = 10, 100, and 1000 cm^{-3}) when T = 100 K, y_f = 1, and I_{UV} = 10.

investigate the ultraviolet-excited high rotational level H_2 in interstellar clouds. Total of 2448 synthetic model calculations with 5 independent physical parameters successfully reproduce the linear relation between the high rotational level ratio *N*(4)/*N*(0) and the incident UV intensity I_{UV}, and detailed influences caused by other parameters such as the hydrogen density, H_2 column density, cloud temperature *T*, and molecular formation rate coefficient y_f. Assuming a steady state between H_2 formation and destruction in a cloud, a simple theoretical equation predicts that the molecular fraction *f* is inversely proportional to the incident UV intensity I_{UV}, hence to the high rotational level ratio *N*(4)/*N*(0). Model simulations show that log *f* is linearly decreased with log *N*(4)/*N*(0), and n_H, y_f, and *T* can be determined by the position of the line in the plot.

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