Retrieving physical conditions from interstellar H$_2$ emission lines: a non linear fitting technique

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Abstract. The importance of the formation pumping on the rovibrational level distribution of H$_2$ is revisited. A detailed comparison of different formation mechanisms on dust surfaces and in the gas-phase is carried out, and it is found that dust surface formation dominates the formation pumping. It is shown that formation pumping in a cold gas can mimic the excitation conditions found in hotter regions. The presence of a significant fraction of molecular hydrogen in very high rotational levels observed towards OMC-1 Peak 1 is explained by means of pumping by newly formed H$_2$ molecules and does not require high temperature gas.

1. Introduction

Dust grains conventionally provide a surface for the formation of H$_2$ from atomic hydrogen [11]. Although there is a general agreement about the process, the actual mechanism is not understood and the internal energy distribution of the nascent hydrogen molecule is unknown. Presumably some fraction of the bond energy, 4.476 eV, of H$_2$ is retained and subsequently redistributed as the H$_2$ molecule undergoes collisions in the interstellar gas. There have been experimental attempts to measure the degree of vibrational excitation of H$_2$ desorbed from surfaces [10], which support the prediction that a significant fraction of the newly formed H$_2$ is in vibrational and rotational excited levels of the ground electronic state. Classical molecular dynamics and fully quantum mechanical calculations have been carried out for H$_2$ formation on surfaces considered analogs of interstellar dust [3,2,17,24,5], but the results have been quite different particularly in the predicted vibrational distribution.

In the modelling exercise, various assumptions have been made. Black & Dalgarno (1976)[1] proposed that the H$_2$ formation energy is equipartitioned among the internal energy of the molecule, the kinetic energy of the molecule, and the internal energy of the grain lattice. They further assumed that the 1.5 eV of H$_2$ internal energy is distributed statistically among the rovibrational levels. Le Bourlot et al (1995)[13] considered the formation of H$_2$ in its highest vibrational level, $v = 14$ close to the dissociation threshold, with $J = 2$ and 3, weighted by the nuclear spin statistics. No energy is transferred to translation or to dust lattice modes. Duley & Williams (1986)[8] suggested a mechanism which differs from previous proposals in the method of stabilization of the reacting complex. The stabilization energy ($\sim 0.4$ eV) is transferred to a surface band, whose energy is that of the OH stretching vibration. The model predicts that the H$_2$ molecule on formation is ejected into the gas vibrationally excited ($v \leq 7$) but rotationally cool ($J = 0, 1$). Draine & Bertoldi (1986)[7] proposed a rovibrational distribution function that does not include the rotational degeneracy factor $2J + 1$ but includes a factor $1 + v$. The formation temperature is $T_f = 50,000$ K, the ortho-to-para ratio is 2.78, the mean vibrational
and rotational levels are 5.3 and 8.7, respectively. The deviation from the statistical thermal distribution function has been introduced to enhance the populations of high vibrational states relative to high rotational states. Detailed quantum mechanical calculations have shown that much of the H$_2$ should be produced in an excited state, with rovibrational and translational energy of the order of 1 eV [9,16].

Takahashi & Uehara (2001) [23] investigated the effects of formation pumping on the infrared H$_2$ emission spectra produced in a collisionless gas. These authors constructed formation pumping models for hydrogen molecules newly formed on icy mantles, carbonaceous and silicate dust, based on classical and quantum theoretical studies of molecular dynamics [17,22,9,16]. A more detailed model was presented by Tiné et al. (2003) [26], that predicted H$_2$ rovibrational emission line intensities for representative points in diffuse and dark interstellar clouds. Clear spectral signatures of H$_2$ formation on dust are evident in the resulting spectra.

Using ISO/SWS [20] obtained near- and mid-infrared spectra towards OMC-1 Peak 1, which contain a number of emission and absorption features, dominated by 56 H$_2$ rovibrational and pure rotational lines. Data analysis provide information on the average gas excitation over an unprecedented range (from $T_{ex} = 600$ K for the lowest rotational and vibrational states up to $T_{ex} \sim 3000$ K at level energies larger than $\Delta E_{vJ}/k > 14,000$ K). Although existing C-shock models have been able to provide results in excellent agreement with observational data up to level energies $\Delta E_{vJ}/k \leq 40,000$ K [14], they fail by a factor of five to reproduce the highest observed level ($v, J = (0, 27)$). Rosenthal, Bertoldi & Drapatz (2000) [20] suggested that a different mechanism (e.g. gas-phase routes) might be populating this level and possibly other high levels.

In this work we revisit the contribution of H$_2$ formation pumping to the population of the high-energy levels. We do not try to constrain a shock model of the emitting region observed by Rosenthal, Bertoldi & Drapatz (2000) [20], since this task is accomplished by existing C-shock models [14]. Instead, we present a detailed analysis of the possible role played by the H$_2$ formation process in the shaping of the very high energy level distribution.

2. The model

2.1. Associative detachment

We constructed models of thermally excited H$_2$, in which the H$_2$ level populations result from formation pumping, radiative decay, collisional excitation and de-excitation. The approach is similar in many respects to those developed by Sternberg & Dalgarno (1989) [21] and Draine & Bertoldi (1996) [7]. The details of the model are reported in [4].

The presence of large column densities of H$_2$ in low levels of excitation suggests the coexistence of two different emitting regions in the ISO/SWS field of view. We summarize the characteristics of the shocked region by two layers at different kinetic temperatures and densities and adopted the set of physical parameters suggested by Rosenthal, Bertoldi & Drapatz (2000) [20] (see also [4]).

Following the suggestion by Rosenthal, Bertoldi & Drapatz (2000) [20], we firstly explore the possibility that gas-phase formation pumping might be efficient in populating highly excited rovibrational levels. In fact, although the recombination of H atoms absorbed onto grains produces much more H$_2$ than any gas-phase process, the associative detachment mechanism involving atomic hydrogen and the negative ion H$^-$ can be efficient under particular conditions [15,6]. In particular, the associative detachment reaction produces H$_2$ molecules preferentially in highly excited rovibrational levels, which then cascade towards the ground vibrational state by quadrupole radiative transitions. We hence include in the formation rate the additional contribution of the associative detachment channel.

The results of our computations show that the inclusion of the associative detachment process in the molecular pumping does not alleviate the problem posed by the existence of a high degree
The ionization fraction is \( x_e = 10^{-3} \). (a) \( T_k = 200 \text{ K} \). (b) \( T_k = 800 \text{ K} \).

of excitation [4]. In Fig. 1a, b we show the ratios of gas-phase and surface formation rates of \( \text{H}_2 \) \( (\kappa_{vJn} - R\delta_{vJnH}) \) for individual energy levels for the two layers. It is evident that gas-phase formation is much less efficient than surface catalysis which dominates the production pumping of newly formed molecules.

2.2. Surface pumping models
Recently, Meyer et al. (2001) [16] studied the associative desorption of \( \text{H}_2 \) on a graphite surface via an Eley-Reidel mechanism under conditions relevant to the interstellar medium. In the Eley-Reidel mechanism the second incident gas-phase \( \text{H} \) atom collides with the first \( \text{H} \) atom chemisorbed on the surface. Meyer et al. (2001) [16] used a time-dependent wave packet method and a newly developed potential, treating three degrees of freedom quantum mechanically. The product \( \text{H}_2 \) molecule appears less vibrationally excited than supposed previously on the basis of two-dimensional simulations. Most molecules have \( v \leq 2 \), but newly formed molecules have significant rotational excitation that peaks at about \( J = 15 \). The fraction of bond energy retained as internal energy of the molecule is approximately one third, and up 40-50% of the total energy can appear as translational energy. The remaining fraction is taken up as dust lattice excitation. Thus, surface formation pumping may be important in populating high rotational states of the ground vibrational level. This possibility is explored in this section.

We present results for a number of formation pumping models and some thermal profiles for the two gas layers mimicking the emitting region towards Orion OMC-1 Peak 1. In producing best-fit results we exploit a non-linear fitting technique, i.e. the Levenberg-Marquard method through the minimization of a \( \chi^2 \) merit function with respect to free parameters in their acceptable ranges (see [4,18,19] for details) We consider formation pumping models in which the acquired internal energy, \( T_i \), is statistically distributed among the energy levels (model A: \( f_1 = 2J + 1, f_2 = \Delta E_{vJ}/T_i \)). To enhance the populations of high-\( v \) states with respect to high-\( J \) states we consider also formation pumping functions with \( f_1 = v + 1 \) (model B). Thus,
Figure 2. Upper panels: excitations diagrams for class B (left side) and class C best-fit models (right side). Model column densities ($\Delta$) are compared with observational data (○). Lower panels: Residuals normalised to the observational data.

The models proposed by Black & Dalgarno (1976) is a class A model in the case of equipartition of energy between internal energy of the product molecule, translational degrees of freedom and dust lattice modes, while a class B model with $T_f = 50,000$ K corresponds to the pumping profile suggested by Draine & Bertoldi (1996) [7]. Finally, we include in the calculations the two vibration-rotation distributions of Takahashi & Uehara [23] for H$_2$ newly formed on icy mantles, carbonaceous dust, and silicate dust (models C).

The formation temperatures are taken in the range $5,000 \leq T_f \leq 50,000$ K, although very high formation temperatures are unlikely because some fraction of the formation energy is lost to overcome the grain surface potential and some possibly goes into translational kinetic energy. Gas kinetic temperatures are $T_k = 100$, 200 and 300 K for the cooler slab, while in the warmer region $T_k = 600, 800$ K. We consider $\mathcal{L} = 8$ adjustable parameters, i.e. the set $\mathcal{R}$, $n_H$, $\gamma_{12}$, and $N_2$, for each gas layers.

In order to obtain the best model description of the Orion OMC-1 peak 1 observational data [20] we selected models having a normalized $\chi^2_n = \chi^2/N_{0,3} \leq 1 \times 10^{-5}$ (where $N_{0,3}$ is the column density of the level $v, J = (0, 3)$), and plausible physical parameters. The more likely thermal configurations found with this analysis are $T_k = 100$ and 600 K, and $T_k = 100$ and 800 K. Under these circumstances, at least for formation pumping models of type A and B, the H$_2$ formation rate $\mathcal{R}$ is always slower in the warmer slab than in the colder one.

Figs.2(a-b) show the excitation diagrams for the selected best class B and class C formation pumping models. In the lower panels, the residuals of column densities $R_{vJ} = |N_{vJ}(\text{mod}) - N_{vJ}(\text{obs})|/N_{vJ}(\text{obs})$ are displayed. These models provide results in overall reasonably good agreement with data. They fail in reproducing very high pure rotational states and show subthermal excitation of levels in excited vibrational manifolds.

In Fig.3 we show the excitation diagram for the selected best model, which is a class A model with $T_f = 15,000$ K. With the exception of energy levels of excited vibrational
manifolds (in particular $v = 1$), that are underpopulated with respect to the observational values, the agreement between modelled and observational data is in general satisfactory (cf lower panel in Fig.3). The observational errors are not shown in Fig.3, except than in the $v, J = (0, 27)$ case, since they are of the order of the circle radius. It is evident that the highest rotational states detected, $v, J = (0, 23)$ and $(0, 27)$, are perfectly reproduced. The population of these states does not require high temperature gas and it is a clear signature of the surface formation pumping. No model with a different formation pumping function can populate effectively these states. Moreover, only class A models with formation temperatures in the range $10,000 \, \text{K} \leq T_f \leq 20,000 \, \text{K}$ can accomplish this task. In Fig.3 we have also plotted the upper limits to the column densities of other very high energy rotational levels given in Rosenthal, Bertoldi & Drapatz (2000) [20] together with the results of a C-shock model of this region presented by Le Bourlot et al. (2002) [14]. It is interesting to note that these upper limits are suggestive of the existence of an high excitation tail ($T_{\text{ex}} \geq 3,000 \, \text{K}$) in the OMC-1 H$_2$ excitation diagram. These peculiar excitation conditions are present in our model results shown in Fig.3.

Finally, we would like to briefly discuss the offsets between the $v = 0$ and $v = 1$ populations, which is also found in Rosenthal, Bertoldi & Drapatz (2000) [20], but which does not occur in the observations. In a shock wave the sudden rise of translational temperature is not immediately
followed by an increase in the vibrational temperature, whose relaxation time is typically longer. Vibrational non-equilibrium therefore may arise due to rapid quasi-resonant vibration-vibration energy transfer between molecules. We have attempted to empirically simulate vibrational non-equilibrium inserting a damping factor in the de-excitation rates of energy levels in excited vibrational states. Although we obtained a better agreement with observational data, the overall description of $v > 0$ populations is not satisfactory and it requires a detailed treatment, e.g. by direct Monte Carlo simulation. Interesting enough, the damping factor does not produce appreciable modifications in the distribution of pure rotational levels.

3. Conclusions
The results of the present calculations suggest that H$_2$ formation on dust grain surfaces constitutes an important pumping channel and should be included in the modelling procedure. In particular, in the cold gas surface formation pumping dominates the populations of level $J \geq 20$. The distribution profile of very high energy levels is strongly affected by the assumed surface pumping function and depends particularly on the formation temperature. The large unexpected population of the energy level $v, J = (0, 27)$ is a clear signature of the surface formation process. The population of the energy level $v, J = (0, 27)$, and possibly those of other very high energy states, scales linearly with both the total cold H$_2$ column density and the total H$_2$ surface formation rate $R$. It is not clear how to discriminate among formation mechanisms, e.g. between Eley-Reidel and Langmuir-Inshealwood schemes, and among suggested surface pumping functions (excited vibrational levels are probably out of equilibrium). However, the (relatively) unbiased adopted fitting technique suggests that the H$_2$ formation energy is equipartitioned among the internal energy of the molecule, the kinetic energy of the molecule, and the internal energy of the grain lattice.

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