

# H<sub>2</sub> formation and excitation in the diffuse interstellar medium

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**Abstract.** We use far-UV absorption spectra obtained with FUSE towards three late B stars to study the formation and excitation of H<sub>2</sub> in the diffuse ISM. The data interpretation relies on a model of the chemical and thermal balance in photon-illuminated gas. The data constrain well the  $nR$  product between gas density and H<sub>2</sub> formation rate on dust grains:  $nR = 1$  to  $2.2 \times 10^{-15} \text{ s}^{-1}$ . For each line of sight the mean effective H<sub>2</sub> density  $n$ , assumed uniform, is obtained by the best fit of the model to the observed  $N(J = 1)/N(J = 0)$  ratio, since the radiation field is known. Combining  $n$  with the  $nR$  values, we find similar H<sub>2</sub> formation rates for the three stars of about  $R = 4 \times 10^{-17} \text{ cm}^3 \text{ s}^{-1}$ .

Because the target stars do not interact with the absorbing matter we can show that the H<sub>2</sub> excitation in the  $J > 2$  levels cannot be accounted for by the UV pumping of the cold H<sub>2</sub> but implies collisional excitation in regions where the gas is much warmer. The existence of warm H<sub>2</sub> is corroborated by the fact that the star with the largest column density of CH<sup>+</sup> has the largest amount of warm H<sub>2</sub>.

**Key words.** ISM: molecules – ISM: clouds – ISM: lines and bands – ISM: individual objects: chameleon – ultraviolet: ISM – stars: individual: HD 102065, HD 108927, HD 96675

## 1. Introduction

The H<sub>2</sub> formation is a key process for the understanding of the thermal and density structure as well as the chemical evolution of the interstellar medium (ISM). The H<sub>2</sub> formation rate was first estimated through the modelling of the hydrogen recombination on dust surfaces (e.g. Hollenbach et al. 1971). Based on an analysis of Copernicus observations of atomic and molecular hydrogen in the local diffuse clouds, Jura (1975a) proposed an H<sub>2</sub> formation rate ( $R = 3 \times 10^{-17} \text{ cm}^3 \text{ s}^{-1}$ ) which corresponds to the Hollenbach et al. (1971) prediction for a total grain surface of  $10^{-21} \text{ cm}^2/H$  and a recombination efficiency of 0.5.

The excitation of the H<sub>2</sub> rotational levels from the ground state observed in absorption in the UV is a diagnostic of physical conditions. In diffuse clouds, the low  $J$  lines provide a measure of the gas temperature while the excitation of the  $J > 2$  levels is generally interpreted as a result of the fluorescence cascade following H<sub>2</sub> pumping by the UV radiation from the target stars. But collisional excitation in shocks driven by the star have also been considered.

Since the pioneering work of Black & Dalgarno (1976) on which the Jura analysis of Copernicus data is based, much progress has been made in the modelling of H<sub>2</sub> in space, in particular about the fluorescence cascade after UV pumping of electronic transitions and collisional deexcitation rates (Combes & Pineau des Forêts 2000). The *Far Ultraviolet Spectroscopic Explorer* (FUSE) is also now providing new

UV absorption observations of Galactic H<sub>2</sub> superseding the Copernicus observations by their sensitivity (Snow et al. 2000; Shull et al. 2000; Rachford et al. 2001). The topic of H<sub>2</sub> formation and excitation has also been revived by the observation of the mid-infrared transitions between the rotational levels of the vibrational ground state. These data have been used to estimate the H<sub>2</sub> formation rate in warm photo-dissociation regions at the surface of molecular clouds (Draine & Bertoldi 1999; Habart et al. 2002) where the gas and the dust are both warmer than in the diffuse ISM and thus where the H<sub>2</sub> formation efficiency or the processes involved might differ. ISO observations are not sensitive enough to detect the mid-IR H<sub>2</sub> line emission in the low to moderate column density lines of sight studied in the UV but they have allowed to detect an extended warm H<sub>2</sub> component away from star forming regions across the Galaxy (Verstraete et al. 1999) and in the edge-on galaxy NGC 891 (Valentijn & van der Werf 1999). The Galactic data has been interpreted as evidence for the existence of warm H<sub>2</sub> gas heated by the dissipation of kinetic turbulent energy.

In this paper, we re-consider the question of H<sub>2</sub> formation and excitation in the diffuse ISM by analysing FUSE observations of three late B stars located behind the Chamaeleon clouds. IRAS images show that these stars unlike most earlier type stars usually observed in the UV are truly background field stars that do not interact with the matter responsible for the absorption and that do not contribute to the incident radiation field. These three stars were part of a larger sample of Chamaeleon lines of sight observed with IUE to correlate the UV extinction curve with changes in the dust size distribution

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**Table 2.** H<sub>2</sub> column densities (in cm<sup>-2</sup>) in the excited ( $J \geq 2$ ) levels, derived from a curve of growth analysis by assuming successively  $b = b_{\text{CH}}$  and  $b = b_{\text{CH}^+}$ , when available. It is likely that the true  $N(\text{H}_2)$  is intermediary or close to one of these two estimates.

	HD 102065		HD 108927	HD 96675	
$b_{\text{adopted}}$	1.9 km s <sup>-1</sup>	3.0 km s <sup>-1</sup>	2.2 km s <sup>-1</sup>	1.6 km s <sup>-1</sup>	2.2 km s <sup>-1</sup>
$N(\text{H}_2, J = 2)$	$2.6 \times 10^{18}$	$2.5 \times 10^{18}$	$1.7 \times 10^{17}$	$3.3 \times 10^{18}$	$3.4 \times 10^{18}$
$N(\text{H}_2, J = 3)$	$3.1 \times 10^{17}$	$1.1 \times 10^{17}$	$9.3 \times 10^{16}$	$1.7 \times 10^{17}$	$8.7 \times 10^{16}$
$N(\text{H}_2, J = 4)$	$5.6 \times 10^{16}$	$6.0 \times 10^{15}$	$1.5 \times 10^{15}$	$4.0 \times 10^{15}$	$1.4 \times 10^{15}$
$N(\text{H}_2, J = 5)$	$1.2 \times 10^{15}$	$4.5 \times 10^{14}$	$\leq 6 \times 10^{13}$	$\leq 2 \times 10^{14}$	

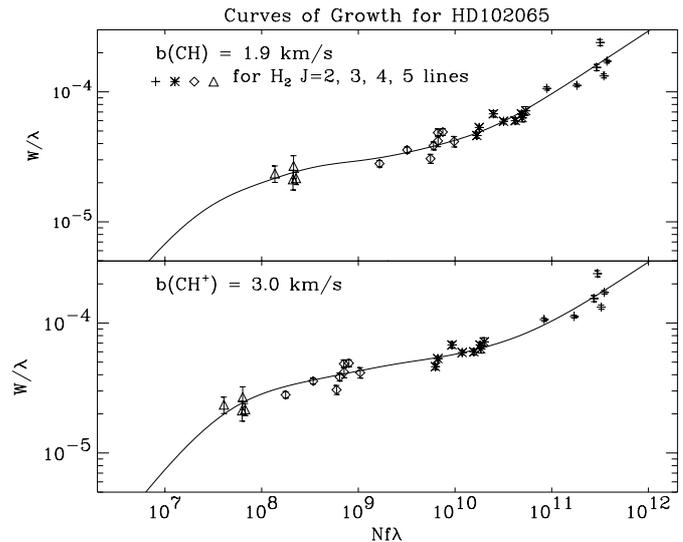
to the curve of growth corresponding to  $b(\text{CH})$  ( $b = 1.9 \text{ km}^{-1}$ , top) and  $b(\text{CH}^+)$  ( $b = 3.0 \text{ km}^{-1}$ , bottom). One must keep in mind that significant uncertainties can be attached to these column densities in case the velocity distribution of the excited H<sub>2</sub> gas is different from that of CH and CH<sup>+</sup>. However in view of the general good linear correlation of  $N(\text{CH})$  with  $N(\text{H}_2)$  at these column densities (Mattila 1986), and the correlations of  $N(\text{CH}^+)$  with excited H<sub>2</sub> column densities (see Sect. 4), it is likely that the  $J \geq 2$  column densities are intermediary or close to one of these two estimates.

### 3. H<sub>2</sub> formation

#### 3.1. Determination of the $nR$ product

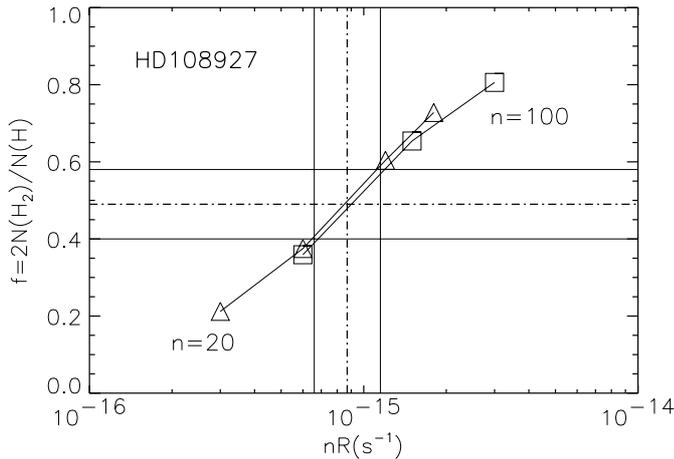
The local balance between H<sub>2</sub> formation and photo-dissociation can be written as:  $n(\text{HI}) nR = n(\text{H}_2) \beta_0 G S$ , where  $n(\text{HI})$ ,  $n(\text{H}_2)$ ,  $n$  are the atomic, molecular and total hydrogen densities ( $n = n(\text{HI}) + 2n(\text{H}_2)$ ),  $R$  the H<sub>2</sub> formation rate,  $\beta_0$  is the Solar Neighborhood value of the H<sub>2</sub> photo-dissociation rate in the absence of shielding,  $G$  is the radiation field value in Solar neighborhood units and  $S$  a shielding factor including dust extinction and H<sub>2</sub> self-shielding. For the stars studied here, the IRAS maps show that the stars do not heat the matter responsible for the absorption, we can thus assume that the stars do not contribute to the radiation field and we can take  $G = 1$  (Boulanger et al. 1994). For a constant  $n$ , integration over the line of sight leads to:  $nR = \frac{1}{2} \frac{f}{1-f} \beta_0 < S >$  where  $f$  is the molecular hydrogen fraction:  $f = 2N(\text{H}_2)/N_{\text{total}}$ , where  $N_{\text{total}}$ , the total column density is derived from the extinction,  $N_{\text{total}} = 5.8 \times 10^{21} E(B - V)$ , and  $< S >$  is the mean shielding factor. From this formula, one thus sees that the product  $nR$  can be derived from the measured molecular hydrogen fraction  $f$ .

Practically a model is necessary to determine the abundance and distribution of H<sub>2</sub> molecules over its ro-vibrational levels as a function of depth into the cloud and thereby derive the  $nR$  product from  $f$ . We have used an updated version of the stationary model developed by Abgrall et al. (1992) and Le Boulrot et al. (1993). The model assumes a semi-infinite plane parallel geometry and solves the equations of thermal and chemical balance iteratively as a function of depth into the cloud. Transfer in the H<sub>2</sub> lines (50 ro-vibrational levels are included in these calculations) and dust extinction are taken into account. The far UV extinction curves used in the models are specific for each star and present a wide variety in terms of 2200 Å bump and far UV rise. These curves are extrapolations



**Fig. 2.** Curves of growth for the excited levels of H<sub>2</sub>. The top plot shows the curve of growth for  $b(\text{H}_2) = b(\text{CH})$  and the bottom plot that for  $b(\text{H}_2) = b(\text{CH}^+)$ . The  $J > 1$  column densities listed in Table 1 have been derived by fitting the measurements of all  $J > 1$  levels together to both curves of growth respectively.

of fits to the IUE extinction curves performed by Boulanger et al. (1994). The chemical network includes 100 species and 775 reactions. To take into account UV penetration from two sides, we run models with half the total extinction and multiply all integrated column densities by two. For all calculations, we have assumed a constant gas density through the line of sight. Since we can assume  $G = 1$ , the model has only two free parameters, the gas density  $n$  and the product  $nR$ . The gas kinetic temperature is calculated in the model at each depth assuming local equilibrium between heating and cooling processes. The dominant heating process is the photo-electric effect on small grains. Heating by dissipation of turbulent kinetic energy is not included. Model results are shown in Fig. 3 for the line of sight towards HD 108927, where the computed H<sub>2</sub> fraction  $f$  is plotted versus the product  $nR$ . A comparison of the model results for  $n = 20$  and  $100 \text{ cm}^{-3}$  illustrates the density independence of the relationship. The horizontal lines in the figure represent the measured  $f$  with its error bar (from Table 1). The intersections of these lines with the model results define the range for  $nR$ . We have used the model to quantify the uncertainties on the product  $nR$  related to the line of sight extinction and the far-UV radiation field. We find that the error bar on the  $A_V$  measurement translates into an uncertainty of  $\pm 50\%$  on  $nR$ .



**Fig. 3.** Determination of the  $nR$  product from the H<sub>2</sub> fraction  $f$  for HD 108927. The triangles and square symbols represent model calculation for  $n = 20$  and  $100 \text{ cm}^{-3}$ , respectively.

An uncertainty of a factor 2 on the far-UV radiation field intensity, which is a reasonable assumption, translates into an error-bar of the same amplitude on  $nR$ . We thus consider that within the framework of the model, a factor of 2 is the magnitude of the error-bar on  $nR$ . Additional systematic errors could be coming from the simplifying assumptions made in the model. These are of course impossible to quantify.

The  $nR$  values derived for the three stars are listed in Table 3. Their scatter is of a factor of 2, comparable to the uncertainty on the individual measurements. Jura (1975b) had found a much larger scatter with values from  $5 \times 10^{-16}$  to  $3 \times 10^{-14} \text{ s}^{-1}$ . The dispersion of Jura's values might be partly due to changes in the  $G$  value among the lines of sight towards the very luminous stars observed by Copernicus.

### 3.2. Determination of $R$ from the H<sub>2</sub> density estimate

To determine the H<sub>2</sub> formation rate  $R$  one must complement the  $nR$  values with an estimate of the gas density  $n$ .

The gas density  $n$  is the second free parameter of the model. Density governs the cooling rate and the assumption of thermal balance makes the gas density and temperature uniquely related at each depth once the external radiation field is given. Any tracer of the gas temperature is therefore also a tracer of the density. We thus determine the gas density by fitting the model to the column density ratio of the two first levels,  $N(J = 1)/N(J = 0)$ , known to be an indicator of temperature. Figure 4 illustrates the best fits, corresponding to the density values indicated in each diagram. Note that in the model the temperature is not uniform, its value is determined at each depth by the thermal balance. The temperature  $T_B$  indicated in Fig. 4 is that of the shown Boltzmann distribution corresponding to the  $N(J = 1)/N(J = 0)$  ratio value.

The  $R$  values derived for the three lines of sight, based on these density estimates are listed in Table 3. This determination of  $n$  assumes that the ortho to para H<sub>2</sub> ratio is at its equilibrium value and is therefore very sensitive to the temperature, which is itself, within the assumption of thermal balance, very

**Table 3.** H<sub>2</sub> formation rate  $R$  from the product  $nR$  and the density  $n$  estimated from  $N(\text{H}_2, J = 1)/N(\text{H}_2, J = 0)$ .

Etoile	HD 102065	HD 108927	HD 96675
$nR \text{ (s}^{-1}\text{)}$	$2.3 \times 10^{-15}$	$0.87 \times 10^{-15}$	$2.0 \times 10^{-15}$
$n \text{ (cm}^{-3}\text{)}$	50	28	50
$R \text{ (cm}^3 \text{s}^{-1}\text{)}$	$4.5 \times 10^{-17}$	$3.1 \times 10^{-17}$	$4.0 \times 10^{-17}$

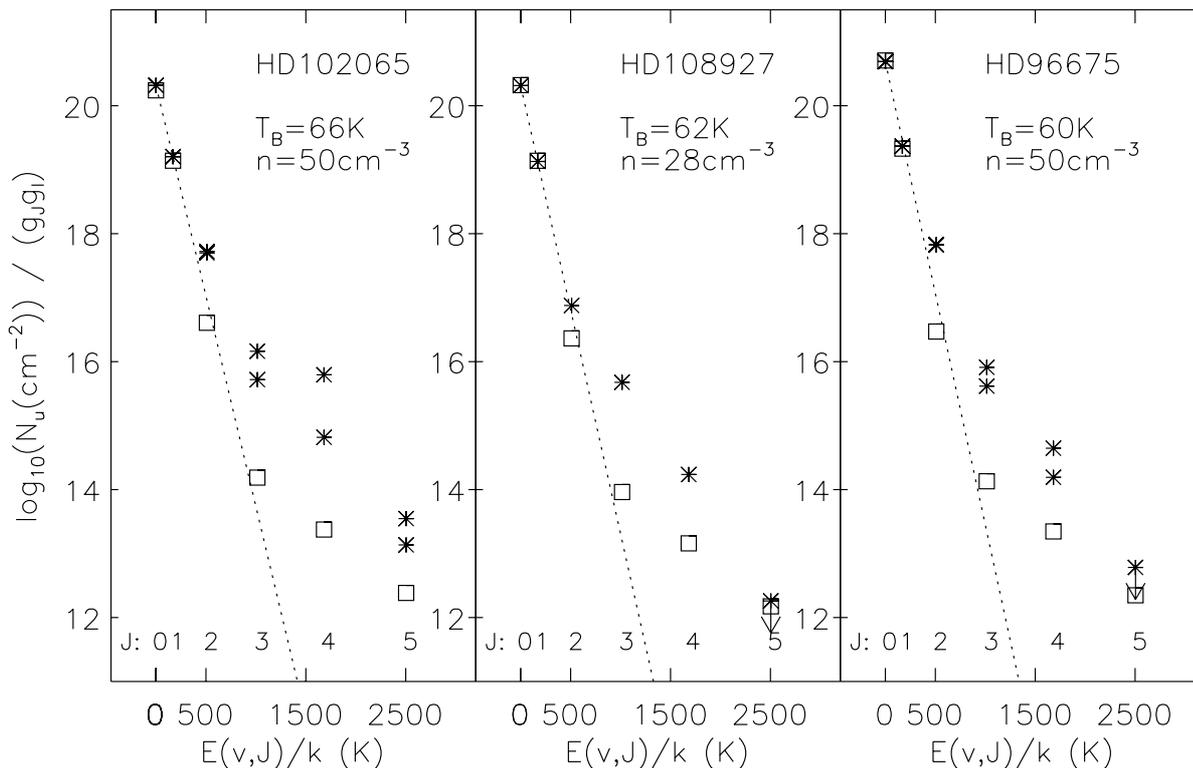
sensitive to the gas density. Within the model framework, the H<sub>2</sub>  $J = 1$  and 0 column density ratio constrains density within about 20%, an uncertainty smaller than that on the product  $nR$ . The uncertainty on  $R$  is thus governed by the uncertainty on  $nR$ : about a factor of 2.

The values of  $R$  for the three lines of sight are close to each other and close to the values found by Jura (1975a) but with significantly lower uncertainties. Note nevertheless that the derivation of  $R$  from  $nR$  is valid within the hypothesis that the density is homogeneous in the molecular gas. This might not be the case. Indeed, for HD 102065 for which we have been able to derive three other independent density estimates from the comparison of model calculations and measured quantities (namely  $N(\text{C I})$ ,  $N(\text{CH})$  and the C I fine structure level population from Gry et al. 1998), there is a scatter of a factor of three among the four density estimates. This scatter might well reflect a density inhomogeneity along the line of sight but could also result from other model shortcomings, in particular in our understanding of the chemistry in diffuse clouds.

The  $nR$  values directly translate into an H<sub>2</sub> formation timescale of  $1/(nR) \sim 2 \times 10^7$  yrs. For the three stars it is a few times larger than the dynamical timescale ( $\sim 10^6 L(\text{pc})/b(\text{km s}^{-1})$  yrs) set by turbulent motions on the scales of the absorbing clouds ( $L = N/n \sim 10$  pc). The model tells us that the photodissociation timescale is larger than the H<sub>2</sub> formation timescale especially in the shielded layers of the cloud (the dissociation timescale goes from about  $3 \times 10^7$  yrs to about  $3 \times 10^8$  yrs for  $A_V$  from 0.3 to 1). On the other hand the timescale of ortho to para conversion through proton exchange reactions with protonated ions (e.g. H<sup>+</sup> and H<sub>3</sub><sup>+</sup>, Gerlich 1990) is much shorter ( $0.2$  to  $2 \times 10^5$  yrs). Consequently, the observed H<sub>2</sub> abundance may not correspond to the equilibrium value between formation and destruction and by assuming equilibrium in our interpretation we could be overestimating  $R$  and the  $nR$  product. Study of a larger sample of stars could reveal scatter in the  $R$  and  $nR$  values reflecting various states of evolution.

## 4. Warm H<sub>2</sub> gas

The excitation diagrams of Fig. 4 show that the H<sub>2</sub> column densities derived from the observations for  $J > 2$  are all significantly higher than the model values. This is true for our two determinations of H<sub>2</sub> column densities, the highest based on the Doppler parameter of CH and the lowest based on that of CH<sup>+</sup> (see Sect. 2). This means that H<sub>2</sub> excitation by UV pumping and H<sub>2</sub> formation on grains as computed with the model does not account for the  $J > 2$  H<sub>2</sub> column densities. With the model, we checked on HD 102065 that to populate these



**Fig. 4.** H<sub>2</sub> excitation diagrams. The asterisks represent the measured column densities listed in Table 1 for  $J = 0$  and  $J = 1$  and in Table 2 for the higher  $J$  levels within the two assumptions  $b(\text{H}_2)_{\text{ex}} = b(\text{CH})$  (higher values) and  $b(\text{H}_2)_{\text{ex}} = b(\text{CH}^+)$  (lower values). The squares represent the model that best fits the  $J = 0$  and  $J = 1$  observations and corresponds to the density indicated. The dashed line is the Boltzmann distribution for the temperature  $T_B$  corresponding to the observed  $N(J = 1)/N(J = 0)$  ratio.

levels by UV pumping alone (with no collisional deexcitation) we would have to increase the radiation field to a  $G$  value of 17 to reproduce the column densities derived with  $b(\text{CH})$  and to a  $G$  value of 9 to reproduce the column densities derived with  $b(\text{CH}^+)$ . Such values are clearly incompatible with the IRAS dust data because no enhanced IR dust emission is found at the position of the stars and the ratio between the 100  $\mu\text{m}$  cloud brightness and extinction is within the range of values observed over the high Galactic sky. We have checked also that we cannot reproduce the measured  $J = 2$  level populations even if all the H<sub>2</sub> binding energy (4.48 eV) is transformed in H<sub>2</sub> internal excitation.

We thus infer the existence of warm gas along the three lines of sight, where the  $J > 2$  H<sub>2</sub> levels are populated by collisional excitation. This statement relies on the validity of the H<sub>2</sub> column densities determinations. In the absence of any direct information, one cannot exclude that the H<sub>2</sub> velocity distribution is broader than that of both CH and CH<sup>+</sup> and consequently that even the lowest set of values in Table 2 are larger than the true H<sub>2</sub> column densities. However, we consider unlikely that the H<sub>2</sub> velocity distribution could be such that there is no need for warm H<sub>2</sub> gas because the detection of CH<sup>+</sup> in the direction of both HD 96675 and HD 102065 where it has been looked for is an independent evidence for the existence of a warm H<sub>2</sub> component along these lines of sight. If one considers only collisional excitation, the H<sub>2</sub> excitation temperature is lower than the true gas temperature for densities below the critical densities of each level. The temperature of the warm gas thus needs

to be at least equal to the H<sub>2</sub> excitation temperature derived from the  $J = 3$  to 5 levels, i.e. between 200 and 240 K for the three stars.

Our conclusion about H<sub>2</sub> excitation at  $J > 2$  levels differs from a common interpretation of UV H<sub>2</sub> absorption lines (e.g. Jura 1975b) where it is assumed that the high  $J$  levels are mainly populated by pumping through UV photons of the target stars. For our sample of stars we are able to rule out this interpretation, because the FUSE sensitivity allowed us to observe late B stars which do not interact with the absorbing matter, thus lines of sight for which the UV radiation field strength is constrained to be close to the mean Solar Neighborhood value.

The existence of warm H<sub>2</sub> gas within the diffuse ISM has been considered along many lines of sight to account for the observed column densities of CH<sup>+</sup>. The observed abundance of CH<sup>+</sup> is a well known problem of interstellar chemistry. The only efficient path for CH<sup>+</sup> formation is the highly endothermic (4640 K) reaction between C<sup>+</sup> and H<sub>2</sub>. Further, CH<sup>+</sup> is efficiently destroyed by reaction with H<sub>2</sub> once it is formed. One thus considers that CH<sup>+</sup> only exists in significant abundance where the molecular gas is warm. Away from hot stars, localized volumes of warm gas can be created and sustained by dissipation of the gas kinetic energy. Formation of CH<sup>+</sup> have been quantitatively investigated in the specific cases where dissipation occurs within MHD shocks (e.g. Flower & Pineau des Forêts 1998) or coherent vortices in MHD turbulence (Joulain et al. 1998). In these models the temperature of the warm gas and the ratio between CH<sup>+</sup> and warm H<sub>2</sub> column

**Table 4.** Abundance of excited H<sub>2</sub> gas.  $N(\text{H}_2)_{\text{ex}}$  (in cm<sup>-2</sup>) is the sum of the  $J = 3$  to 5 column densities from Table 1. The last column (ISO) refers to an infrared observation of a long line of sight through the Galaxy (from Falgarone et al. 2002).

	HD 102065	HD 108927	HD 96675	ISO
$N(\text{H}_2)_{\text{ex}}$	$1.7 - 3.7 \times 10^{17}$	$1.0 \times 10^{17}$	$0.9 - 1.7 \times 10^{17}$	$7.7 \times 10^{18}$
$A_V$	0.67	0.68	1.1	18
$\frac{N(\text{H}_2)_{\text{ex}}}{A_V}$	$2.5 - 5.4 \times 10^{17}$	$1.5 \times 10^{17}$	$0.8 - 1.6 \times 10^{17}$	$4.3 \times 10^{17}$

densities depends strongly on local physical conditions (e.g. shock velocity, gas density, magnetic field value). The addition of H<sub>2</sub> excitation studies provides a mean to constrain these models and can thus help understand the physics of kinetic energy dissipation in the diffuse ISM.

For each line of sight we have computed and listed in Table 4 a total column density of excited H<sub>2</sub> gas ( $N(\text{H}_2)_{\text{ex}}$ ) by summing the column densities in the  $J = 3$  to 5 levels. The range of values corresponds to the two assumptions used for the determination of H<sub>2</sub> column densities (see Sect. 2). The fact that CH<sup>+</sup> must form in warm H<sub>2</sub> gas makes us consider the lowest value of  $N(\text{H}_2)_{\text{ex}}$ , those obtained for the CH<sup>+</sup> Doppler parameter, to be the most realistic estimate. For HD 108927, in the absence of CH<sup>+</sup> observation only the higher estimate is listed. Note that in all cases the excited H<sub>2</sub> gas represents a very small fraction of the total gas. We have not attempted to separate the respective contributions of UV pumping in the cold gas and truly warm gas to the column densities of excited H<sub>2</sub>. The excitation diagrams in Fig. 4 show that UV pumping is always a minor contribution.

Based on Copernicus data, Frisch & Jura (1980) suggested a correlation between the column densities of H<sub>2</sub> in the  $J = 5$  level and CH<sup>+</sup>. They pointed out that CH<sup>+</sup> is particularly abundant in regions with large amounts of rotationally excited H<sub>2</sub>. This result has been confirmed by Lambert & Danks (1986) who compared the column densities  $N(\text{CH}^+)$  and  $N(\text{H}_2, J)$  for the rotational levels  $J = 0 - 5$  in a larger sample of sight-lines. They concluded that the rotationally excited H<sub>2</sub> is a tracer for those hot H<sub>2</sub> molecules that initiate CH<sup>+</sup> formation. Both lines of sight of our study, HD 102065 and HD 96675, for which the CH<sup>+</sup> column density is known, fit within the dispersion of the Lambert & Danks (1986) correlation diagrams. Note that the Lambert & Danks' sample consist of luminous stars for which one cannot exclude that the excited H<sub>2</sub> gas results from the interaction (UV pumping and shock) of the star with its surrounding medium. Further sight-lines such as those considered here, for which this possibility can be excluded, are needed to physically discuss the correlation between CH<sup>+</sup> column densities and warm H<sub>2</sub> in relation with existing models of CH<sup>+</sup> formation.

One Galactic line of sight not crossing any known star forming region has been observed with the mid-IR spectrometer on board of the Infrared Space Observatory (ISO). This observation lead to the detection of three pure rotational lines of the H<sub>2</sub> ground state (Verstraete et al. 1999; Falgarone et al. 2002). The H<sub>2</sub> populations inferred from these detections are

compared with our FUSE results in Table 4. The  $N(\text{H}_2)_{\text{ex}}/A_V$  ratio for the long line of sight through the Galaxy is a factor 5 and 2 higher than the lower estimates listed for HD 96675 and HD 102065. We thus find along these two sight-lines a fraction of warm H<sub>2</sub> gas close to the mean Galactic value derived from the ISO observation. The presence of warm H<sub>2</sub> thus seems to be a general characteristics of the diffuse ISM.

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