Molecular clouds HD/H$_2$ in the early Universe

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Abstract. We present a simplified semi-analytical description of the relative HD/H$_2$ abundance in the cold neutral interstellar medium. With this description we were able to obtain three asymptotics of the relative HD/H$_2$ abundance and its dependence on physical parameters in the medium, namely, the number density of the gas, the intensity of the ultraviolet field, the cosmic ray ionization rate and metallicity. Our calculations in presented simple formalism are in the reasonable agreement with the calculations using the Meudon PDR code. We found that in the case of low metallicity and a higher cosmic ray ionization rate, the relative abundance of HD/H$_2$ is significantly enhanced, which can explain the observed difference between the local and high-z measurements of relative HD/H$_2$ abundance.

1. Introduction

It is well known that molecular hydrogen – the most abundant molecule in the Universe, predominantly resides in the cold interstellar medium of the galaxies. However, it is very hard to observe H$_2$ in emission, since it has zero dipole moment in the ground electronic state and therefore rotational-vibrational transitions in the ground state are forbidden. Therefore, other molecules with non zero dipole moment are used as the tracers of molecular gas. In contrast to H$_2$, its isotopologue, HD, has non zero dipole moment in the ground electronic state, hence the dominant transition at 112 $\mu$m between $J = 1$ and $J = 0$ rotational levels is permitted, and therefore HD can be in principle used to study dense molecular gas. Generally, HD is more suitable to study low metallicity ISM than CO, since the relative HD/H$_2$ abundance is not so sensitive to metallicity than CO/H$_2$. However, the exact dependence of HD/H$_2$ on metallicity and other physical conditions in the medium can be studied with numerical modelling of ISM (e.g., [1, 2]), but it is still poorly constrained observationally. The only available method now to directly measure HD/H$_2$ relative abundance is absorption line spectroscopy of the electronic transitions. Observations with the UV satellites telescopes (Copernicus and FUSE) found that the relative abundance of HD/H$_2$ molecules (measured in absorption towards bright stars in our Galaxy as the ratio of column densities) is significantly below the expected values from the D/H isotopic ratio and slightly depends on the column density of the absorber [3]. However, the systematical uncertainty dominates these measurements, since resolution of the UV spectra is not enough to resolve exact velocity structure of the absorber. Interestingly, that at high redshifts current instrumentation allow us to measure HD/H$_2$ abundance with much higher precision than local ones, since due to redshift resonant absorption lines are shifted in the optical band, where characteristic resolution is at least 3 times higher. Such resonant HD and H$_2$ absorption lines detected in the high-z quasars, are associated with so called Damped Lyman alpha systems (DLA) – absorption line systems of damped Lyman series H$\text{I}$ lines and associated metal lines,
that are thought to be associated with galaxies at high redshifts. The problem is that the cross section of the molecular gas is much lower than the atomic gas and therefore the fraction of H$_2$/HD-bearing DLAs is small, $\sim 4$ per cent [4]. Therefore, since the first detection of HD at high redshifts [5], only 14 HD/H$_2$ systems have been detected at $z > 2$ ([6, 7, 8, 9] and references therein). With advent of the techniques to preselect H$_2$-bearing DLAs for the follow up studies from Sloan Digital Sky Survey (see e.g. [10]), the rate of detection is significantly increased.

In this work we present the semi-analytical description of HD/H$_2$ transition which with new measurements from the follow up targets (Kosenko et al. in prep.) in future can be used as additional constraint on physical conditions.

2. Analytical description of HD/H$_2$ ratio

The equilibrium number density of HD molecules in the diffuse ISM is determined by balance of formation and destruction. Two main channels of HD formation are: gas-phase reaction

$$\text{H}_2 + \text{D}^+ \rightarrow \text{HD} + \text{H}^+ \quad (1)$$

and formation of HD on the surface of dust grains. The main channel of HD destruction is photodestruction, concerned with UV pumping in resonant lines of Lyman and Werner bands (it is very similar to H$_2$). A small fraction ($\sim 15\%$) of pumped HD molecules deexcites in the continuum of the ground electronic state, i.e. dissociates. While UV field penetrates into the cloud, HD lines in which pumping occurs become saturated (and also there can be additional dilution of the UV field by dust and H$_2$ and H$_i$ lines [11]) and UV pumping rate decreases, and therefore photodestruction reduced. It is well known shielding mechanism that regulates H$_i$/H$_2$ and D$_i$/HD transitions in the ISM and it is usually specified by self shielding function, $S_{\text{HD}}$ [11]. This function shows how photodestruction decreases as a function HD column density, $N_{\text{HD}}$, relative to the unattenuated photodestruction rate $\chi D_{\text{HD}}$, where $\chi$ is the UV field in the units of Draine field [12] and $D_{\text{HD}} = 2.6 \times 10^{-11} \text{s}^{-1}$ [1].

Therefore in the steady state assumption and plain parallel geometry, when one side of the cloud is exposed by the unattenuated UV field with strength $\chi$ we can write

$$F_{\text{HD}} n_{\text{H}_2} n_{\text{D}^+} + R_{\text{HD}} n_{\text{H}^+} n_{\text{D}} = \frac{1}{2} \chi D_{\text{HD}} S_{\text{HD}}(N_{\text{HD}}) e^{-\tau_g} n_{\text{HD}}, \quad (2)$$

where $F_{\text{HD}} = 2 \times 10^9 \text{cm}^3\text{s}^{-1}$ [1] is the chemical formation rate of HD in eq (1), $R_{\text{HD}} = 6.3 \times 10^{-17} \text{cm}^3\text{s}^{-1}$ is the HD formation rate on the dust grains, $\tau_g$ is the optical depth attributed with attenuation of the UV field by dust, which can be expressed as a function of the total hydrogen column density $\tau_g = \sigma_g(N_{\text{H}} + 2N_{\text{H}_2})$, where $\sigma_g$ is the dust grain Lyman-Werner photon absorption cross section (in units cm$^2$) per hydrogen nucleon [13]. $\sigma_g$ is a function of the dust-to-gas ratio, i.e. usually linearly scaled with metallicity and its typical value in the Milky Way (for solar metallicity) is $1.9 \times 10^{21} \text{cm}^2$ [14].

In the diffuse ISM abundance of D$^+$ is mainly defined by the charge-exchange reaction H$^+ + \text{D} \leftrightarrow \text{D}^+ + \text{H}$ and by reaction (1) and hence

$$n_{\text{D}^+} = \frac{k}{k'} n_{\text{H}^+} n_{\text{D}} n_{\text{H}_2} A \quad (3)$$

where $k$ and $k'$ are the rates of direct and reversed charge-exchange reaction, respectively, $A = \frac{F_{\text{HD}}}{2\chi} - 1 \approx 0$ [1].
In that case the dependence on \( \beta \)

3.1. Highly shielded region

In that case the dependence on \( \beta \) and \( \beta_{\text{dust}} \) is vanished in eq (8) and we get

\[
\frac{n_{\text{HD}}}{n_{\text{H}}} = 2 \frac{D}{H} \frac{f_{\text{H}}}{f_{\text{H}} + 1} \left( \frac{1}{\beta_{\text{chem}} + \frac{f_{\text{H}}}{f_{\text{H}} + 1}} \right)^{-1},
\]

i.e. all D is in HD molecules. Note, that here we neglect other reactions, e.g. destruction of H\(_2\) and HD by cosmic rays and chemical destruction of HD in eq (1) reversed reaction, which can maintain not unit molecular fractions in shielded parts of the clouds.
3.2. Unattenuated UV field.

In this limit $S_{\text{HD}} \to 1$ (and hence $\log N_{\text{HD}} \lesssim 14$). For the typical parameters of the ISM this condition automatically gives $\tau_g \to 0$ and we can obtain another asymptotic of HD to H$_2$ ratio

$$\frac{n_{\text{HD}}}{n_{\text{H}_2}} = 2 \frac{D}{H} \frac{1}{f_{\text{H}_2}} \left( \frac{1 + f_{\text{H}_2}A}{\beta_0^{\text{chem}} f_{\text{H}_2} + \beta_0^{\text{dust}}} + 1 \right)^{-1} \tag{10}$$

Since $\beta_0^{\text{dust}} \ll \beta_0^{\text{chem}}$ for the typical conditions in the diffuse molecular ISM, $\beta_0^{\text{chem}}$ term in the denominator will dominate in intermediate molecular fraction regions and will give

$$\frac{n_{\text{HD}}}{n_{\text{H}_2}} = 2 \frac{D}{H} \frac{\beta_0^{\text{chem}}}{f_{\text{H}_2}} \approx D \frac{f_{\text{H}_2}^{10^{-4}}}{\left( n_{100 \text{ cm}^{-3}} \right)} \chi^{-1} \approx D \frac{\chi R_{\text{HD}}^2}{R_{\text{H}_2}^3} \approx \frac{D}{n_{\text{tot}}} \chi, \tag{11}$$

while $\beta_0^{\text{dust}}$ only can play role in the very surface of the clouds, where we can take $f_{\text{H}_2} = \frac{4}{\alpha}$ (where $\alpha = \frac{\chi R_{\text{HD}}^2}{n_{\text{tot}}}$ [13]) and consequently

$$\frac{n_{\text{HD}}}{n_{\text{H}_2}} = 2 \frac{D}{H} \frac{\beta_0^{\text{dust}}}{f_{\text{H}_2}} = 2 \frac{D}{H} \frac{\beta_0^{\text{dust}}}{f_{\text{H}_2}} \approx 2 \frac{D}{2 R_{\text{H}_2}^3} \approx \frac{D}{n_{\text{tot}}} \chi \approx \frac{D}{n_{\text{tot}}} \chi. \tag{12}$$

4. DI/HD transition

The processes of HD formation and destruction obviously imply that $n_{\text{HD}}$ is gradually increasing to the cloud center from some low value to $n_{\text{tot}}^D$, i.e. it is increasing function of the column density. Conversely, $n_D$ is decreasing from $n_{\text{tot}}^D$, hence there is the transition point between DI and HD, which formally can be specified as $n_D = n_{\text{HD}}$, or $f_{\text{HD}} = 1/2$. Using eq (6) we can write the condition for DI/HD transition as

$$\beta^{\text{chem}} \frac{f_{\text{H}_2}}{1 + f_{\text{H}_2}A} + \beta^{\text{dust}} = 1. \tag{13}$$

Since $\beta^{\text{dust}} \ll 1$, the chemical formation of HD determines this transition and the $N_{\text{H}_2}$ column density at which it occurs can be derived from

$$f_{\text{H}_2} \approx \chi \left( \frac{f_{\text{H}_2}^{10^{-4}}}{10^{-4}} \right)^{-1} \left( \frac{n_{100 \text{ cm}^{-3}}}{100 \text{ cm}^{-3}} \right)^{-1} S_{\text{HD}} e^{-\sigma_\gamma (N_{\text{H}_2} + 2 N_{\text{H}_2})}. \tag{14}$$
Taking into account that \( f_{\text{H}_2} = 1/2 \) formally determines \( \text{H}_1/\text{H}_2 \) transition we can set that \( \text{D}_1/\text{HD} \) transition will occur at lower penetration depth into the cloud if

\[
\chi \left( \frac{f_{\text{H}_2}^+}{10^{-4}} \right)^{-1} \left( \frac{n}{100 \text{ cm}^{-3}} \right)^{-1} S_{\text{HD}} e^{-\tau_{\text{tran}}} \lesssim \frac{1}{2},
\]

where \( \tau_{\text{tran}} \) is \( \text{H}_1/\text{H}_2 \) transition optical depth [15]. The derived \( \text{D}_1/\text{HD} \) and \( \text{H}_1/\text{H}_2 \) transitions are shown by vertical dashed and dotted lines in figure 1, respectively. It is worth mentioning, that in case of low metallicity (0.1 of solar) \( \text{D}_1/\text{HD} \) transition takes place at the lower penetration depth of the cloud, than \( \text{H}_1/\text{H}_2 \) transition and consequently \( N_{\text{HD}}/2N_{\text{H}_2} \) ratio can be higher than isotopic \( \text{D}/\text{H} \) ratio.

5. Comparison with Meudon

We used Meudon PDR code (http://ism.obspm.fr) [16] to check our result. We assumed slab of the gas irradiated by beamed Draine radiation field from the observers side and calculated several isochoric models with \( n_{\text{H}_2}^{\text{tot}} = 100 \text{ cm}^{-3} \) and fixed temperature, \( T = 100 \text{ K} \). The base model has metallicity \( Z = 0.1 \), the scaling factor of UV field \( \chi = 1 \) and the cosmic ray ionization rate \( \zeta = 10^{-16} \text{ s}^{-1} \). Then we varied independently \( Z, \chi \) and \( \zeta \) in ranges \((0.1, 0.5, 1), (0.1, 1, 10) \) and \((10^{-15}, 10^{-16}, 10^{-17} \text{ s}^{-1}) \), respectively. To compare our calculations with Meudon results we set the ionization fraction in Eq (8) to be the same as in Meudon results at the \( f_{\text{H}_2} = 0.5 \) (the ionization fraction varies in the cloud and this choice corresponds to a kind of average value). In figure 2 we can see that Meudon calculations are in good agreement with our calculations, and that \( N_{\text{HD}}/N_{\text{H}_2} \) ratio changes significantly with variation of these parameters.

6. Discussion

From figure 2 one can see that the difference in the physical conditions, namely, lower metallicity and higher cosmic ray ionization rate resulted in the relatively higher \( \text{HD}/\text{H}_2 \) ratios. These changes can essentially explain systematic difference between \( \text{HD}/\text{H}_2 \) ratios in our Galaxy [3] and high-z DLAs (Kosenko in prep), that we show in figure 3. However, from figure 3 we can see that there is quite large dispersion of the observed \( \text{HD}/\text{H}_2 \) ratio, which can be evidently explained by a wide expected dispersion of the physical conditions at high-z DLAs. Since \( \text{HD}/\text{H}_2 \) ratio is sensitive to variation of the physical conditions \((Z, T, n_{\text{H}_2}^{\text{tot}}, \chi, \zeta)\), it can be used to constrain
the combination of these parameters. However, the metallicity can be well measured from metal lines. Number density, temperature and UV field can be constrained from the population of C$^1$ fine structure or H$_2$ rotational levels (Balashev et al. in prep.). Therefore with proper detailed analysis of associated DLAs, HD/H$_2$ ratio can be used to constrain the ionization fraction in the cold neutral ISM. In figure 3 we show an example how HD/H$_2$ abundance changes with the variation of ionization fraction for fixed $\chi = 1$, $Z = 0.1$, $n = 100$ cm$^{-3}$ and $T = 100$ K.

Figure 3: Relative abundance of HD and H$_2$ molecules measured in our Galaxy and high redshifts. Dashed, dashed-dotted, and dotted curves correspond to solutions of eq.(8) for $f_{H^+} = 10^{-3}$, $10^{-4}$, $10^{-5}$, respectively, with fixed $Z = 0.1$, $\chi = 1$, $n = 100$ cm$^{-3}$ and $T = 100$ K.

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