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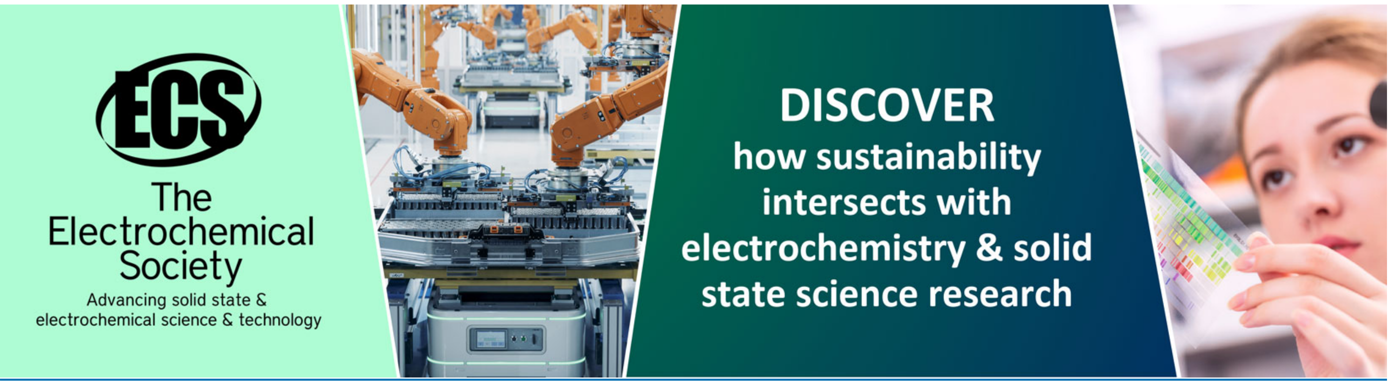

Molecular clouds HD/H_2 in the early Universe

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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 was 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 μm 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 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, ~ 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

$$\mathrm{H_2 + D^+ \rightarrow HD + H^+} \tag{1}$$

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 deexites 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, $S^{\rm HD}$ [11]. This function shows how photodestruction decreases as a function HD column density, $N_{\rm HD}$, relative to the unattenuated photodestruction rate $\chi D^{\rm HD}$, where χ is the UV field in the units of Draine field [12] and $D^{\rm HD} = 2.6 \times 10^{-11}\,\mathrm{s^{-1}}$ [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 χ we can write

$$F^{\rm HD} n_{\rm H_2} n_{\rm D^+} + R^{\rm HD} n_{\rm H}^{\rm tot} n_{\rm D} = \frac{1}{2}\chi D^{\rm HD} S^{\rm HD}(N_{\rm HD}) e^{-\tau_g} n_{\rm HD}, \tag{2}$$

where $F^{\rm HD} = 2 \times 10^9\,\mathrm{cm^3 s^{-1}}$ [1] is the chemical formation rate of HD in eq (1), $R^{\rm HD} = 6.3 \times 10^{-17}\,\mathrm{cm^3 s^{-1}}$ is the HD formation rate on the dust grains, τ_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 $\tau_g = \sigma_g(N_{\rm H} + 2N_{\rm H_2})$, where σ_g is the dust grain Lyman-Werner photon absorption cross section (in units $\mathrm{cm^2}$) per hydrogen nucleon [13]. σ_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 $1.9 \times 10^{21}\,\mathrm{cm^{-2}}$ [14].

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

$$n_{\rm D^+} = \frac{k}{k'} \frac{n_{\rm H^+} n_{\rm D}}{n_{\rm H}^{tot} + 2n_{\rm H_2} A} \tag{3}$$

where k and k' are the rates of direct and reversed charge-exchange reaction, respectively, $A = \frac{F^{\rm HD}}{2k'} - 1 \approx 0$ [1].

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Substituting eq (3) into eq (2) and introducing

$$\beta^{\rm chem} = \frac{F^{\rm HD}\frac{k}{k'}n_{\rm H^+}}{\chi D^{\rm HD}S^{\rm HD}e^{-\sigma_g(N_{\rm H}+2N_{\rm H_2})}} \equiv \frac{\beta_0^{\rm chem}}{S^{\rm HD}e^{-\sigma_g(N_{\rm H}+2N_{\rm H_2})}} \tag{4}$$

$$\beta^{\rm dust} = \frac{2R^{\rm HD}n_{\rm H}^{\rm tot}}{\chi D^{\rm HD}S^{\rm HD}e^{-\sigma_g(N_{\rm H}+2N_{\rm H_2})}} \equiv \frac{\beta_0^{\rm dust}}{S^{\rm HD}e^{-\sigma_g(N_{\rm H}+2N_{\rm H_2})}}, \tag{5}$$

we can write

$$\frac{n_{\rm HD}}{n_{\rm D}} = \beta^{\rm chem}\frac{f_{\rm H_2}}{1+f_{\rm H_2}A} + \beta^{\rm dust} \tag{6}$$

The values of $\beta_0^{\rm chem}$ and $\beta_0^{\rm dust}$ are the values of $\beta^{\rm chem}$ and $\beta^{\rm dust}$ in the case of unattenuated UV field for HD, i.e. $S_{\rm HD} = 1$ and $\tau_g = 0$ and have a weak temperature dependence, that at typical temperature of the cold diffuse ISM, $T = 100\,{\rm K}$

$$\beta_0^{\rm chem} = 0.5\left(\frac{f_{\rm H^+}}{10^{-4}}\right)\left(\frac{n}{100\,{\rm cm^{-3}}}\right)\chi^{-1}, \quad \beta_0^{\rm dust} = 1.2\times10^{-4}\left(\frac{n}{100\,{\rm cm^{-3}}}\right)\chi^{-1}Z, \tag{7}$$

where $f_{\rm H^+}$ and Z are the ionization fraction and metallicity in the medium.

Using eqs (4)-(5) and taking into account that $n_{\rm D}+n_{\rm HD} = n_{\rm D}^{\rm tot}$ and $n_{\rm H_2}/n_{\rm H} = f_{\rm H_2}/2(1-f_{\rm H_2})$, here $f_{\rm H_2} = 2n_{\rm H_2}/\left(n_{\rm H}+n_{\rm H_2}\right)$ is H_2 molecular fraction we get

$$\frac{n_{\rm HD}}{n_{\rm H_2}} = 2\frac{\rm D}{\rm H}\frac{1}{f_{\rm H_2}}\left(\frac{1}{\beta^{\rm chem}\dfrac{f_{\rm H_2}}{1+f_{\rm H_2}A}+\beta^{\rm dust}}+1\right)^{-1}, \tag{8}$$

Since $f_{\rm H_2}$, $\beta^{\rm chem}$ and $\beta^{\rm dust}$ are the functions of $N_{\rm H_2}$ and $N_{\rm HD}$, so substituting $n_{\rm HD}/n_{\rm H_2} = {\rm d}N_{\rm HD}/{\rm d}N_{\rm H_2}$ we obtain differential equation. To solve this equation we should also specify the value of ionization fraction, which in the cold neutral medium will be dominantly the function of cosmic ray ionization rate, but also depends on the metallicity and the number density of the gas (Balashev in prep.).

Figure 1 shows the calculated $N_{\rm HD}(N_{\rm H_2})$ profiles for $n = 100\,{\rm cm^{-3}}$, $f_{H^+} = 10^{-4}$, $\chi = 1$ and $Z = 1$. We find the similar results with [1, 2], that $N_{\rm HD}/N_{\rm H_2}$ ratio can significantly vary with cloud depth and significantly depends on the ISM parameters (see figure 2).

3. Asymptotics

One can note from the figure 1 that there are evident asymptotical values of $N_{\rm HD}/N_{\rm H_2}$. In this section we will find the expressions for these asymptotics as the functions of the physical parameters of the cloud. Note that asymptotics we derive for the volume number densities $n_{\rm HD}/n_{\rm H_2}$ using eq (8), will be the same for the HD to H_2 column densities ratio.

3.1. Highly shielded region $f_{H_2} \to 1$.

In that case the dependence on $\beta^{\rm chem}$ and $\beta^{\rm dust}$ is vanished in eq (8) and we get

$$\frac{n_{\rm HD}}{n_{\rm H_2}} = 2\frac{\rm D}{\rm H}, \tag{9}$$

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.

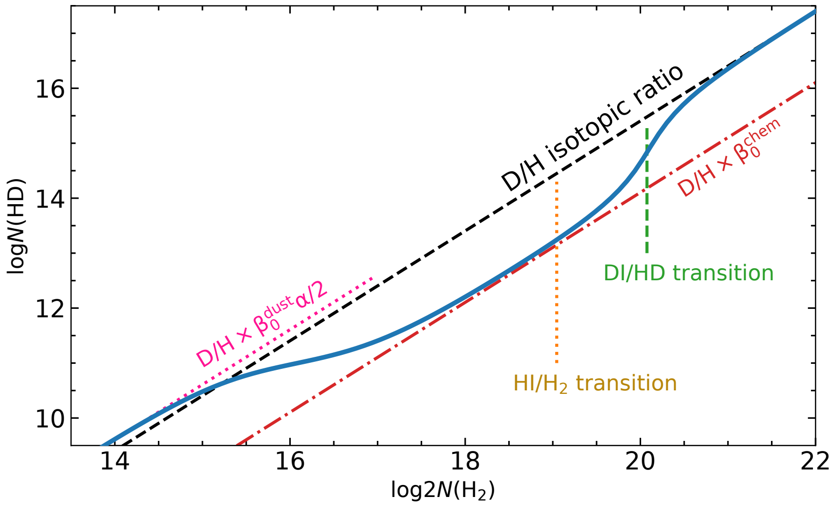

Figure 1: $\log N(\mathrm{HD})$ as function of $\log N(\mathrm{H_2})$. Solid blue curve is the solution of eq (8), magenta dotted line is asymptotic on the edge of the cloud (12), red dashed line is asymptotic in the case of unattenuated field neglecting formation of HD on dust (11), green dashed line shows $\mathrm{H_2}$ column density at which D/HD transition occurs (13), orange dotted line shows $\mathrm{H/H_2}$ transition point [15].

3.2. Unattenuated UV field.
In this limit $S^{\mathrm{HD}} \to 1$ (and hence $\log N_{\mathrm{HD}} \lesssim 14$). For the typical parameters of the ISM this condition automatically gives $\tau_g \to 0$ and we can obtain another asymptotic of HD to $\mathrm{H_2}$ ratio

$$\frac{n_{\mathrm{HD}}}{n_{\mathrm{H_2}}} = 2\frac{\mathrm{D}}{\mathrm{H}}\frac{1}{f_{\mathrm{H_2}}}\left(\frac{1+f_{\mathrm{H_2}}A}{\beta_0^{\mathrm{chem}} f_{\mathrm{H_2}} + \beta_0^{\mathrm{dust}}} + 1\right)^{-1} \tag{10}$$

Since $\beta_0^{\mathrm{dust}} \ll \beta_0^{\mathrm{chem}}$ for the typical conditions in the diffuse molecular ISM, β_0^{chem} term in the denominator will dominate in intermediate molecular fraction regions and will give

$$\frac{n_{\mathrm{HD}}}{n_{\mathrm{H_2}}} = 2\frac{\mathrm{D}}{\mathrm{H}}\beta_0^{\mathrm{chem}} \approx \frac{\mathrm{D}}{\mathrm{H}}\left(\frac{f_{\mathrm{H^+}}}{10^{-4}}\right)\left(\frac{n}{100\,\mathrm{cm^{-3}}}\right)\chi^{-1}, \tag{11}$$

while β_0^{dust} only can play role in the very surface of the clouds, where we can take $f_{\mathrm{H_2}} = \frac{4}{\alpha}$ (where $\alpha = \frac{\chi D^{\mathrm{H2}}}{R^{\mathrm{H2}} n_{\mathrm{H}}^{\mathrm{tot}}}$ [13]) and consequently

$$\frac{n_{\mathrm{HD}}}{n_{\mathrm{H_2}}} = 2\frac{\mathrm{D}}{\mathrm{H}}\frac{\beta_0^{\mathrm{dust}}}{f_{\mathrm{H_2}}} = \frac{\mathrm{D}}{\mathrm{H}}\beta_0^{\mathrm{dust}}\alpha = \frac{\mathrm{D}}{\mathrm{H}} \cdot \frac{R^{\mathrm{HD}} D^{\mathrm{H_2}}}{2R^{\mathrm{H_2}} D^{\mathrm{HD}}} \approx \frac{\mathrm{D}}{\mathrm{H}}. \tag{12}$$

4. D I/HD transition

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

$$\beta^{\mathrm{chem}}\frac{f_{\mathrm{H_2}}}{(1+f_{\mathrm{H_2}}A)} + \beta^{\mathrm{dust}} = 1. \tag{13}$$

Since $\beta^{\mathrm{dust}} \ll 1$, the chemical formation of HD determines this transition and the $N_{\mathrm{H_2}}$ column density at which it occurs can be derived from

$$f_{\mathrm{H_2}} \approx \chi\left(\frac{f_{\mathrm{H^+}}}{10^{-4}}\right)^{-1}\left(\frac{n}{100\,\mathrm{cm^{-3}}}\right)^{-1} S^{\mathrm{HD}} e^{-\sigma_g(N_{\mathrm{H}}+2N_{\mathrm{H_2}})}. \tag{14}$$

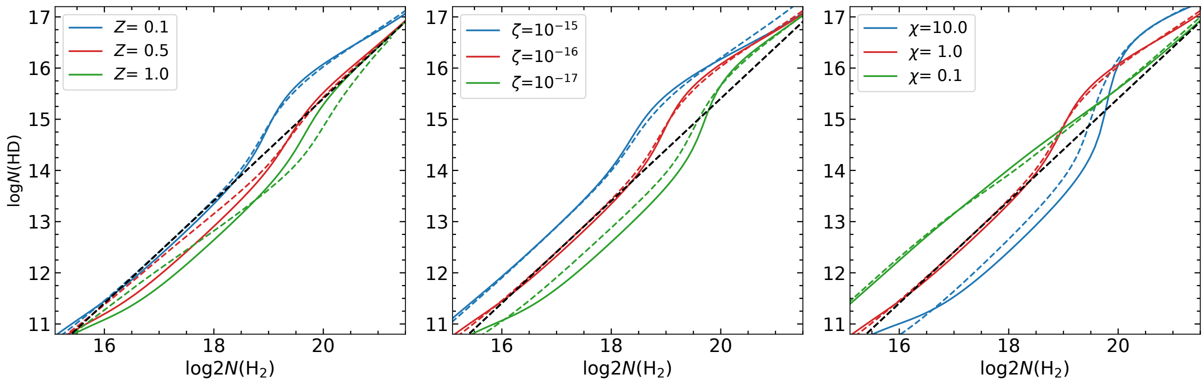

Figure 2: Dependence of HD on H_2 column densities for different values of metallicities (left, with fixed $\chi = 1$, $\zeta = 10^{-16}$ s^{-1}), cosmic ray ionization rate (central, with fixed $\chi = 1$, $Z = 0.1$) and UV field intensity (right, with fixed $\zeta = 10^{-16}$ s^{-1}, $Z = 0.1$). Solid colored curves show solution of eq (8), while the dashed colored curves are results from calculation by *Meudon PDR* code.

Taking into account that $f_{\rm H_2} = 1/2$ formally determines H I/H_2 transition we can set that D I/HD transition will occur at lower penetration depth into the cloud if

$$\chi \left(\frac{f_{\rm H^+}}{10^{-4}}\right)^{-1} \left(\frac{n}{100\,{\rm cm}^{-3}}\right)^{-1} S^{\rm HD} e^{-\tau_{\rm tran}} \lesssim \frac{1}{2}, \qquad (15)$$

where $\tau_{\rm tran}$ is H I/H_2 transition optical depth [15]. The derived D I/HD and H I/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) D I/HD transition takes place at the lower penetration depth of the cloud, than H I/H_2 transition and consequently $N_{\rm HD}/2N_{\rm H_2}$ ratio can be higher than isotopic D/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 $n_{\rm H}^{tot} = 100\,{\rm cm}^{-3}$ and fixed temperature, $T = 100\,$K. The base model has metallicity $Z = 0.1$, the scaling factor of UV field $\chi = 1$ and the cosmic ray ionization rate $\zeta = 10^{-16}\,{\rm s}^{-1}$. Then we varied independently Z, χ and ζ in ranges (0.1, 0.5, 1), (0.1, 1, 10) and (10^{-15}, 10^{-16}, $10^{-17}\,{\rm s}^{-1}$), 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 $f_{\rm H_2} = 0.5$ (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 $N_{\rm HD}/N_{\rm H_2}$ 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 HD/H_2 ratios. These changes can essentially explain systematic difference between HD/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 HD/H_2 ratio, which can be evidently explained by a wide expected dispersion of the physical conditions at high-z DLAs. Since HD/H_2 ratio is sensitive to variation of the physical conditions (Z, T, $n_{\rm H}^{\rm tot}$, χ, ζ), it can be used to constrain

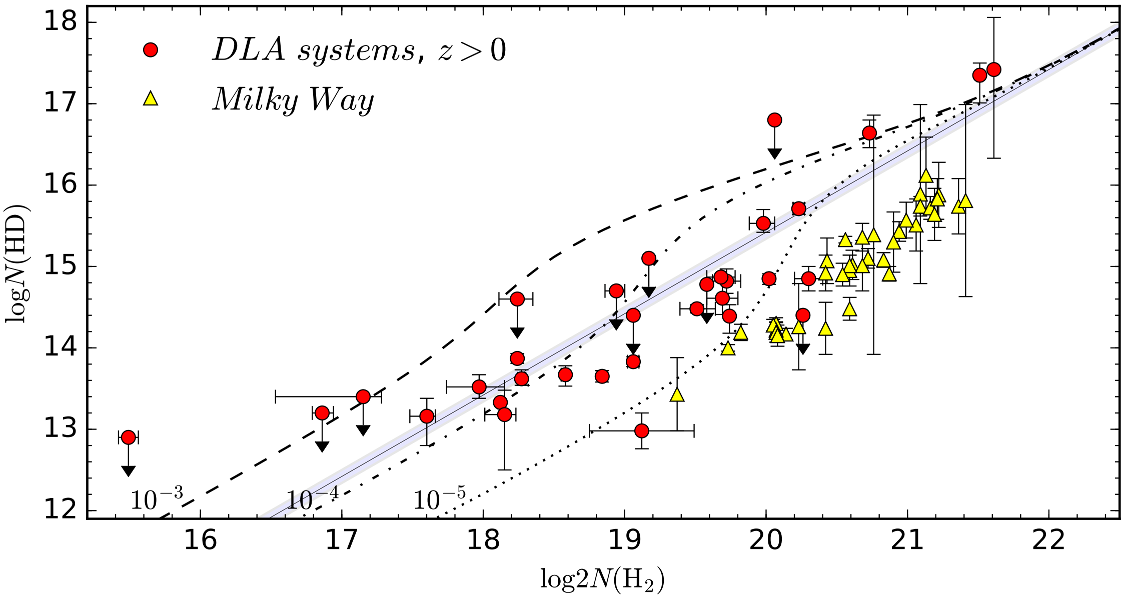

Figure 3: Relative abundance of HD and H_2 molecules measured in our Galaxy and high redshifts. Dashed, dashed-dotted, and dotted curves correspond to solutions of eq.(8) for $f_{H^+} = 10^{-3}$, 10^{-4}, 10^{-5}, respectively, with fixed $Z = 0.1$, $\chi = 1$, $n = 100\,\mathrm{cm}^{-3}$ and T = 100 K.

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 I 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 $\chi = 1$, $Z = 0.1$, $n_{\rm H}^{\rm tot} = 100$ cm^{-1} that are 'typical' for high-z DLAs. We can see that variation of ionization fraction alone can explain the observed dispersion of the HD/H_2 ratio measured at high-z DLAs.

Acknowledgments
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