Constraining of physical conditions in the cold neutral medium using HD/H$_2$ relative abundance

D N Kosenko$^1$, S A Balashev$^1$

$^1$ Ioffe Institute, 26 Politekhnicheskaya st., St. Petersburg, 194021, Russia
E-mail: kosenkodn@yandex.ru, s.balashev@gmail.com

Abstract. We present constraints on physical conditions in diffuse HD/H$_2$-bearing molecular clouds using measured HD/H$_2$ column density ratio. We used recently published formalism that describes how this ratio changes with ultraviolet field intensity, number density and cosmic ray ionization rate. Out of them the most important parameter is the cosmic ray ionization rate, as it determines the chemistry in neutral medium and is still poorly constrained in ISM. Using the result of absorption line analysis in our Galaxy and in several high-redshift systems we found that value of cosmic ray ionization rate is $1.3^{+1.3}_{-0.5} \times 10^{-17}$ s$^{-1}$ in our Galaxy and is few $\times 10^{-18}$ s$^{-1}$ in DLAs at high redshifts.

1. Introduction

Interstellar medium (ISM) is one of the most important constituents of the galaxies. The interplay between ISM and stars controls the formation and evolution of galaxies, since ISM provides a raw material for the star-formation, whereas ongoing star-formation affects on the properties of ISM by various feedback process. Indeed stars produce UV photons, which determine the multiphase structure of the ISM, that consists of ionized, neutral and molecular phases. Additionally stars enrich the ISM with the metals and dust, which affect (along with the UV field) the thermal state of the ISM and determine the initial mass function for ongoing star-formation. Moreover, exploded supernovae – the product of star evolution, not only supply the ISM with the mechanical energy and sustain ISM turbulence, but also are the sites of the efficient production of the cosmic rays, which are one of the main constituents of the energy budget in the ISM. Additionally, cosmic rays determine the residual ionization fraction in the neutral and molecular phases, therefore control the chemistry in the cold ISM.

The cosmic ray ionization rate (CRIR) have been widely studied in our Galaxy over past several decades via different methods, but the obtained constraints range from few $10^{-18}$ to few $10^{-16}$ s$^{-1}$ (e.g. [1, 2, 3, 4, 5]). Moreover, different constraints for some systems contradict each other [5]. Therefore it is very important to determine CRIR with independent estimates. Recently, we have presented the formalism that describes how the relative abundance of molecular hydrogen and its isotopomer, deuterated hydrogen, H$_2$ and HD, respectively, (and also the column density ratios, $N_{\text{HD}}/N_{\text{H}_2}$ – a principal outcome of absorption line analysis) is defined by the metallicity and the physical conditions, namely, CRIR, number density and UV field [6]. The metallicity can usually be well measured using spectra of stars or quasars, which also can provide the robust measurements of $N_{\text{HD}}/N_{\text{H}_2}$. Recently it was shown that number density and UV field strength can be independently constrained by excitation of associated
neutral carbon, CI, and H$_2$ [7, 8] and hence $N_{\text{HD}}/N_{\text{H}_2}$ measurements provide the route for the determination of the CRIR. In this paper we applied the developed formalism to the measured relative abundance of HD and H$_2$ in our Galaxy towards nearby stars and in remote galaxies located on the line of the sight towards the quasars at high redshifts.

2. Method

We used our recently published formalism [6] to estimate physical conditions in the ISM using observed HD/H$_2$. In this formalism we consider the steady state plane-parallel diffuse cloud with metallicity $Z$, number density $n$, exposed by cosmic rays with ionization rate per hydrogen atom $\zeta$ and by beamed ultraviolet field with intensity $\chi$ (relative to Draine interstellar radiation field [9]) from one side. For simplicity we used fixed temperature $T = 100$ K, since the reaction rates have a little dependence on the temperature. Hence the ratio of column densities of HD to H$_2$ molecules, $N_{\text{HD}}/N_{\text{H}_2}$, can be obtained by solving the differential equation

$$\frac{dN_{\text{HD}}}{dN_{\text{H}_2}} = \frac{n_{\text{HD}}}{n_{\text{H}_2}} = 2\frac{D}{H} f_{\text{H}_2} \left(1 + \frac{1}{\beta_{\text{chem}} f_{\text{H}_2} + \beta_{\text{dust}}}ight)^{-1},$$

where $D/H$ is D to H isotopic ratio, $f_{\text{H}_2}$ is H$_2$ molecular fraction, which is a function of the physical parameters and H$_2$ column density, following the formalism presented by [10].

$$f_{\text{H}_2} = \frac{2n_{\text{H}_2}}{n_H + 2n_{\text{H}_2}} = \frac{1}{1 + \frac{1}{4}\alpha S_{\text{H}_2}(N_{\text{H}_2}) e^{-\tau_g}},$$

where $S_{\text{H}_2}(N_{\text{H}_2})$ is H$_2$ self-shielding function, $\alpha$ is a ratio of H$_2$ photodissociation rate in the optically thin regime to the H$_2$ dust formation rate, $\tau_g$ is a dust opacity in the Lyman-Werner band [10]. Here $\alpha$ and $\tau_g$ are functions of $\chi$, $Z$, $n$, so they were varied during our following calculations. Dimensionless parameters $\beta_{\text{chem}}$ and $\beta_{\text{dust}}$ are

$$\beta_{\text{chem}} \approx 6 \times 10^{-3} \frac{n Z d}{\chi} \left(1 + 1.95 f_{\text{H}_2} \frac{8 \times 10^{-10} \zeta (1 - 0.95 f_{\text{H}_2})}{n Z^2 d^2 (1 + 0.15 e^{-1} \chi^{-1} n Z)} + 1 - 1\right),$$

$$\beta_{\text{dust}} \approx 1.2 \times 10^{-6} \frac{n Z}{\chi},$$

where $d$ is the depletion of carbon onto dust grains and it is a function of the metallicity (see e.g. [11]).

Equation (1) can be solved numerically, and then compared with observed ratio $N_{\text{HD}}/N_{\text{H}_2}$, and therefore provide constraints on the parameters, namely, metallicity, cosmic ray ionization rate, number density and UV field intensity. Among them the metallicity, $Z$, can be well estimated via metal absorption lines analysis in spectra, therefore for simplicity we fixed it to be the best fit value. Additionally, the recent results by [7] indicate that it is possible to constrain $n$ and $\chi$ from relative $J = 1/J = 0$ population of H$_2$ and relative population of neutral carbon (CI) fine structure levels, which both are tightly linked to HD abundance. To obtain constraints on the parameters, we used Markov Chain Monte Carlo (MCMC) method with affine sampler [12, 13]. For systems where the information was available we used constraints on $n$ and $\chi$ (from excitation of H$_2$ and CI) as priors. Since there were no constraints on $\zeta$, the determination of this parameter is the main outcome of this analysis.
3. Results

3.1. High-z systems
We searched for HD is 7 H$_2$-bearing DLAs detected in quasar spectra obtained by VLT/X-Shooter [7]. The detailed description of the measurements of HD abundance in these systems will be presented in Kosenko et al, in prep. We detected HD in only three out of these seven DLAs. The column density measurements, redshifts and metallicities are summarized in table 1. For $n$ and $\chi$ we used priors from [7]. We also added to the analysis already known DLA system at $z=2.786$ towards J 0843+0221 [14] with priors from [7]. The obtained 1d and 2d posteriors on the parameters in analysed systems are shown in Figure 1 and presented in table 1.

We could not constrain $\zeta$ in the system towards J 1236+0010 since uncertainty on $N_{HD}$ are too large; in the system towards J 0843+0221 we place only lower limit on $\zeta$.

3.2. Galaxy
We fitted all of the systems together to obtain “average” conditions in diffuse clouds in Milky Way; for calculations we used priors log $\chi = 0.7 \pm 0.3$ and log $n = 1.8 \pm 0.3$ [16] and fixed metallicity $Z = 0.7$ for all of the sightlines. Our fit results are $\zeta = (1.3^{+1.3}_{-0.5}) \times 10^{-17} \text{ s}^{-1}$, $\chi = 4.1^{+3.3}_{-1.4}$, $n_{H_2}^{tot} = 110^{+50}_{-50} \text{ cm}^{-3}$. The obtained posterior probability functions are shown in Figure 2 and curve for average parameters compared with measured HD and H$_2$ column densities is shown in Figure ??.

4. Discussion
We found that cosmic ray ionization rate in the analyzed high-z systems is few$\times10^{-18} \text{ s}^{-1}$, which is few times lower than the average $\zeta$ in Milky Way that we obtained. This can be naturally explained, since UV field intensity in these particular DLAs is found to be relatively low. Since it UV flux is likely correlates with CRIR, since both these parameters scaled with the star-formation, the lower CRIR values are expected for these DLAs. Additionally, it is worth mentioning that such method, based on HD/H$_2$ ratio, now is the only way to determine CRIR in the high-z galaxies probed by DLAs. Indeed the molecules used in local Universe, like OH, OH$^+$ and H$_2$O$^+$ technically are very hard to access in DLAs. This is partially due to the fact that high-z systems have on average lower metallicity and therefore O-bearing molecules are less abundant. In contrast, at lower metallicity HD abundance can be significantly enhanced [6].

We found the cosmic ray ionization rate in diffuse clouds of Milky Way to be $\zeta \approx (1.3^{+1.3}_{-0.5}) \times 10^{-17} \text{ s}^{-1}$. We note that this value is obtained assuming the similar physical conditions towards all sightlines in the Galaxy. However, it is evident, that UV field and CRIR can have significant dispersion from one line of sight to another, even for these measurements that were mostly

### Table 1: Physical conditions in the systems

| Target          | $z$       | log $Z$  | log $N_{H_2}$ | log $N_{HD}$ | log $\chi$  | log $n_{H_2}^{tot}$ | log $\zeta$ |
|-----------------|-----------|---------|---------------|--------------|--------------|---------------------|-------------|
| J 0858+1749     | 2.625241  | $-0.63^{+0.02}_{-0.02}$ | 19.72$^{+0.02}_{-0.02}$ | 14.85$^{+0.05}_{-0.05}$ | $0.1^{+0.2}_{-0.2}$ | $1.8^{+0.1}_{-0.1}$ | $-17.3^{+0.1}_{-0.1}$ |
| J 1236+0010     | 3.03292   | $-0.58^{+0.04}_{-0.03}$ | 19.76$^{+0.04}_{-0.03}$ | 15.96$^{+0.14}_{-0.05}$ | $0.4^{+0.2}_{-0.4}$ | $1.6^{+0.5}_{-0.6}$ | $-17.9^{+0.6}_{-0.5}$ |
| J 2347−0051     | 2.587971  | $-0.82^{+0.05}_{-0.03}$ | 19.44$^{+0.01}_{-0.02}$ | 14.39$^{+0.14}_{-0.21}$ | $-0.4^{+0.04}_{-0.04}$ | $2.0^{+0.5}_{-0.5}$ | $-17.6^{+0.6}_{-0.5}$ |
| J 0843+0221     | 2.78650   | $-1.52^{+0.08}_{-0.10}$ | 21.21$^{+0.02}_{-0.02}$ | 17.35$^{+0.15}_{-0.34}$ | $1.2^{+0.2}_{-0.2}$ | $2.8^{+0.1}_{-0.1}$ | $-17.3^{+0.5}_{-0.2}$ |
| Galaxy          | 0         | $-0.15$ | set of measurements | $0.6^{+0.3}_{-0.2}$ | $2.1^{+0.2}_{-0.2}$ | $-16.9^{+0.5}_{-0.2}$ |

Figure ??
DLA at $z=2.588$ towards J 2347-0051

DLA at $z=2.588$ towards J 2347-0051

DLA at $z=3.033$ towards J 1236+0010

DLA at $z=3.033$ towards J 1236+0010

Figure 1: The marginalized posterior probability functions for CRIR, UV field strength and number density, obtained from fitting measured $N_{\text{HD}}/N_{\text{H}_2}$ in the systems at high redshifts. The diagonal panels on each subplot indicate 1d posterior function, where the blue shade area corresponds to 0.68 confidence level. The non-diagonal panels show the 2d posterior function, where dark and light blue regions correspond to 0.68 and 0.95 confidence levels.

obtained for the $\sim 1 - 4 \text{ kpc}$ distance around the Sun [15]. Indeed, some absorption systems can be located near star-forming regions and/or supernovae remnants, where the cosmic ray ionization rate and/or intensity of the UV field can be significantly enhanced. Indeed similar to UV field, CRIR decreases within a galaxy at large distances from the accelerator at least as $d^{-2}$ due to losses in interactions and effects of particle propagation [17, 18, 19]. This can induce additional systematic uncertainty in reported value.
5. Conclusion
We applied a recently published simple semi-analytical formalism based on HD formation and destruction balance equation to constrain physical properties in the HD/H$_2$–bearing diffuse molecular clouds using measured HD and H$_2$ column densities. We have analysed physical properties in three new and one already known DLA systems found in the spectra of distant quasars and estimated average conditions in diffuse molecular clouds in our Galaxy. We found that CRIR in DLAs at high redshifts are few \( \times 10^{-18} \) s$^{-1}$. We obtained “average” CRIR in Milky Way to be \( \zeta = (1.3^{+1.3}_{-0.5}) \times 10^{-17} \) s$^{-1}$.

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Figure 2: The same as in the Figure 1, but obtained by fitting $N_{\text{HD}}/N_{\text{H}_2}$ measured along 41 sightlines in our Galaxy [15].

HD vs H$_2$: squares are data measured in our Galaxy [15], circles are data measured at high redshifts, black curve is a solution of equation (1) with best parameters for systems in Milky Way, thin blue lines calculated at the parameters drawn from the corresponding posterior function.
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