Physical conditions in two high-redshift H$_2$-bearing GRB-DLAs, 120815A and 121024A.

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ABSTRACT
The gamma-ray burst (GRB) afterglows provide an unique opportunity to study the interstellar medium (ISM) of star-forming galaxies at high-redshift. The GRB-DLAs (damped Lyman-α absorbers) contain a large neutral hydrogen column density, N(H I), and are observed against the GRB afterglow. A large fraction of GRB-DLAs show presence of molecular hydrogen (H$_2$) which is an indicator of star-formation. Hence it is important to study those GRB-DLAs which have H$_2$ lines to decipher and understand their physical conditions. The GRB-DLAs 121024A and 120815A, situated at redshift 2.30 and 2.36 respectively, are two such important H$_2$-bearing GRB-DLAs. Besides H$_2$, these two GRB-DLAs also show many metal lines. In this work we have carried out a detail numerical study on the H$_2$ lines, as well as on those metal lines, in GRB-DLAs 121024A and 120815A self-consistently. We use the spectral synthesis code CLOUDY for this study. This modeling helps us to determine the underlying physical conditions which give rise such lines and hence to understand these two GRB-DLAs in much more detail than any other previous investigation. We find that the hydrogen densities for these two H$_2$-bearing DLAs are $\geq 60$ cm$^{-3}$. Moreover our study infers that the linear sizes are $\leq 17.7$ pc for these two GRB-DLAs, and the mean gas temperatures averaged over the cloud thickness, are $\leq 140$ K. Overall, we find that these two H$_2$-bearing GRB-DLAs are denser, cooler and smaller compared to those without H$_2$.

Key words: galaxies: high-redshift, galaxies: ISM, ISM: molecules

1 INTRODUCTION
Molecular hydrogen (H$_2$) is the first neutral molecule to be formed in the universe, and it is the most abundant and the main constituent of molecular clouds where star formation takes place (Burton 1992; Tielens 2005; Bigiel et al. 2008). Furthermore, H$_2$ controls most of the chemistry in ISM through its ionic or neutral form. In addition to these, level populations of H$_2$ in various levels can be used as tracers for physical conditions. For example, in the well-shielded H$_2$ gas the lower rotational levels of the ground state of H$_2$ are mostly collisionally dominated, hence they are in LTE, and can be used to infer gas temperature (Abgrall et al. 1992). Whereas, the higher levels are generally populated by non-thermal processes and can be used to estimate ambient radiation field (Draine & Bertoldi 1996; Shaw et al. 2005) and the cosmic ray ionisation rate of hydrogen (Tineé et al. 1997). As a result, H$_2$ spectra provide an excellent opportunity to probe star formation and chemical enrichment of galaxies ranging from local to high-redshift (z).

In Milky Way, a large neutral hydrogen column density N(H I) is in general associated with H$_2$ (Savage et al. 1977; Winkel et al. 2017; Marasco et al. 2017). Furthermore, H$_2$ controls most of the chemistry in ISM through its ionic or neutral form. In addition to these, level populations of H$_2$ in various levels can be used as tracers for physical conditions. For example, in the well-shielded H$_2$ gas the lower rotational levels of the ground state of H$_2$ are mostly collisionally dominated, hence they are in LTE, and can be used to infer gas temperature (Abgrall et al. 1992). Whereas, the higher levels are generally populated by non-thermal processes and can be used to estimate ambient radiation field (Draine & Bertoldi 1996; Shaw et al. 2005) and the cosmic ray ionisation rate of hydrogen (Tineé et al. 1997). As a result, H$_2$ spectra provide an excellent opportunity to probe star formation and chemical enrichment of galaxies ranging from local to high-redshift (z).

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ected against the GRB afterglow are called GRB-DLAs. The long GRBs, with a duration greater than two seconds, are believed to be originated from the core-collapsed supernova. Since massive stars are short lived and are located in star-forming regions of galaxies, it is apparent that GRBs are also associated with star-forming regions of a galaxy (Woosley 1993). An excellent review of GRB-DLAs in the Swift era is provided by Schady (2017).

To date, many QSO-DLAs and GRB-DLAs have been observed by several groups (Prochaska et al. 2001; Srianand et al. 2005a; Ledoux et al. 2009; Daniel et al. 2008; Toy et al. 2016; Ledoux et al. 2009; Heintz et al. 2019; Bolmer et al. 2019) etc. The GRB-DLAs are smaller in number than QSO-DLAs as GRBs are transitory in nature. However, the GRB-DLAs show larger N (HI) and higher metallicity than those of QSO-DLAs (Prochaska et al. 2007). Here, metallicity relative to solar is expressed as \[ \log[N(X)/N(H)] = \log[N(X)/N(H)]_{\odot} \] (with X = Zn, or Si, or S). It was also noticed by Cucchiara et al. (2015) that at high-z the average metallicity of QSO-DLAs decline at a faster rate than GRB-DLAs. In general, QSO-DLAs probe diffuse gas and hence they are not suitable to study star formation. On the contrary, since GRBs are located inside the galaxies, GRB-DLAs probe inner regions of galaxies (Fynbo et al. 2008), and consequently, GRB-DLAs are much suitable for studying star-forming regions. However, recent studies of extremely saturated DLAs (ESDLA) (Noterdaeme et al. 2014, 2015a; Balashev et al. 2017; Ranjan et al. 2018; Bolmer et al. 2019; Ranjan et al. 2020) indicate that ESDLAs likely represent the same population of the galaxies, probed by small impact parameters, and hence can probe star-forming regions. Furthermore, recently, a huge data is also available on GRB-DLA host galaxies up to a very high redshift (z ≈ 6) (Hartoog et al. 2015; Bolmer et al. 2019).

Initially, Tumlinson et al. (2007) studied five GRB-DLAs but did not find H2 in spite of large N(H I). They concluded that this lack of H2 may be due to a combination of low metallicity and an FUV radiation field of 10-100 times the Galactic mean field. Later, Ledoux et al. (2009) observed seven \( z > 1.8 \) GRB afterglows with VLT/UVES but they also did not find H2 in their sample. They explained the lack of detected H2 through the low metallicities, low depletion factors, and moderate particle densities of these systems. Though Tumlinson et al. (2007) and Ledoux et al. (2009) differed regarding the FUV radiation field, they both agreed on the low metallicity of these systems. Ledoux et al. (2009) estimated a particle density of \( 5-15 \text{ cm}^{-3} \), a linear cloud size of \( 520^{+240} \text{-} 190 \text{ pc} \), and the kinetic temperature \( > 1000 \) K for these seven \( z > 1.8 \) GRB afterglows of their sample which did not show H2. Later Toy et al. (2016) observed a sample of 45 GRB-DLAs in the redshift range of 2 to 6 and they found that DLA counterpart star formation rates (SFRs) are not correlated with either redshift or H I column density.

However, some other GRB-DLAs, which harbour H2, were found, namely, GRB-DLA 80607, GRB-DLA 121024A, GRB-DLA 120815A and GRB-DLA 120327A at redshifts 3.03, 2.30, 2.36 and 2.8 (Sheffer et al. 2009; Friis et al. 2015; Krühler et al. 2013; D’Elia et al. 2014). Recently Bolmer et al. (2019) have observed 22 GRB-DLAs with VLT/X-shooter for \( z > 2 \). In their sample, they found H2 absorption lines in 6 out of these 22 GRB-DLAs, which also include GRB-DLA 121024A, GRB-DLA 120815A and GRB-DLA 120327A. They concluded that there is no lack of detected H2 for GRB-DLAs and the detection rate is much higher in GRB-DLAs than the QSO-DLAs. It has been noted that for GRB-DLAs with log N (H I) > 21.7, the detection of molecular hydrogen increases (Bolmer et al. 2019). The same increase in the detection rate at high HI is also seen in QSO-DLAs (Noterdaeme et al. 2015a; Balashev & Noterdaeme 2018). Earlier, such conversion of HI to H2 was analytically studied (Sternberg 1988; Sternberg et al. 2014), and observationally constrained for both low and high redshifts (Savage et al. 1977; Welty et al. 2016; Noterdaeme et al. 2015a; Balashev & Noterdaeme 2018). It is thus natural to ask whether the physical conditions of H2-bearing DLAs are quite different than those without H2, and if so, how to probe and then understand that. One of the plausible answers for detectable H2 could be the presence of dust grains, higher metallicity, and higher density. Dust grains are very important as their surfaces act as a catalyst for efficient H2 formation. As an example, it has been suggested by many observers (Srianand et al. 2005a,b) that the H2-bearing QSO-DLAs might have higher density and higher dust content compared to the non H2-bearing QSO-DLAs.

A detail numerical spectroscopic modeling of GRB-DLAs considering all the possible microphysics of H2 is thus quite crucial to determine the underlying physical conditions which give rise such lines, and hence to understand these systems which harbour H2. Previously, Whalen et al. (2008) had carried out a numerical simulation to understand the absence of H2 in GRB-DLAs. However, so far, no one has performed any detailed microscopic modelling of such systems which harbour H2. Previously, we successfully carried out several detail modelings of QSO-DLAs (Srianand et al. 2005a,b; Shaw et al. 2016; Rawlins et al. 2018) with detected H2 lines. Following that in this work, we employ the spectral synthesis code CLOUDY (Ferland et al. 2017) for a microscopic detail modelling with an aim to understand the physical conditions of H2-bearing GRB-DLAs.

Our calculation incorporates detail microphysics both at atomic and molecular levels including collisional physics and line shape theory. In this work we choose following two systems: GRB-DLAs 121024A and 120815A, and study them self-consistently. We select these two GRB-DLAs as they have higher molecular fraction with log(f) = -1.14 ± 0.15 and -1.4, respectively, and so will serve our purpose best to distinguish H2-bearing from non-H2-bearing GRB-DLAs. In addition to H2, these two DLAs show numerous metal lines together with the rest frame UV absorption lines of H2. Along with H2 lines, above mentioned extra lines are also modeled self-consistently in our calculation.

This article is organized as below: in section 2 we give details of our calculation using CLOUDY. Detail of micro-physics incorporated in our calculation is also provided. In section 3 we present the findings from this study, first providing results for GRB-DLA 120815A and then for GRB-DLA 121024A. Summary and conclusions are presented in section 4.
2 CALCULATIONS

CLOUDY is a self-consistent stationary micro-physics code based on \textit{ab initio} calculation of thermal, ionisation, and chemical balance of non-equilibrium gas and dust exposed to a source of radiation. It predicts column densities of various atomic and molecular species and resultant spectra covering the whole range of EM radiation and vice versa using a minimum number of input parameters. It has a state-of-the art detailed H$_2$ network (Shaw et al. 2005) embedded which is very helpful for modelling environments with H$_2$. The H$_2$ network includes 301 rovibrational levels within the ground electronic state and also the rovibrational levels within the lowest six excited electronic states.

Here, we briefly discuss the main formation and destruction processes of H$_2$ that are implemented inside CLOUDY and affect the H$_2$ level populations. Since the formation process of H$_2$ is exothermic and the resulting energy for such process is close to its dissociation energy, H$_2$ formation does not simply take place in gas phase by interaction of two H atoms. It requires a mechanism to take away some of the formation energy to form a stable H$_2$ molecule. In a dusty environment, dust plays the role to share that formation energy. As a result, H$_2$ is mainly formed on dust grain surfaces where dusts can act as a catalyst and take away some of the formation energy. In a dust-free environment, H$_2$ can still form through an exchange reaction of H with H$^-$ (Launay et al. 1991) and H$_2'^+$ (Kristic 2002) but the reaction rates are smaller. The main destruction and excitation mechanism for H$_2$ is the photoexcitation. In this process, H$_2$ absorbs Lyman and Werner band photons and gets excited to higher electronic levels. Of these excited populations, 10-15% comes down to the continuum of ground electronic state and get dissociated. The rest populates higher vibrational levels of the ground electronic state (Abgrall et al. 1992). Besides this, the formation process is exothermic, hence the dust grains also play a crucial role in the distribution of level population of newly formed H$_2$ on dust grain surfaces (Black & van Dishoeck 1987; Le Bourlot et al. 1995; Draine & Bertoldi 1996; Takahashi & Uehara 2001). Note that deep into the cloud, excitation by secondary electrons produced by cosmic ray is also an important H$_2$ level excitation mechanism (Tine{é} et al. 1997). All these above mentioned processes are incorporated inside CLOUDY and details are given in Shaw et al. (2005) and Gay et al. (2012). It is well known that depending on the nuclear spin orientations, H$_2$ can be in one of the two quantum states, namely, ortho or para. In an ortho state, the nuclear spins are aligned parallel, whereas in a para state, they are anti-parallel. Note that radiative transitions are not possible between ortho and para states of the ground electronic level and only reactive collisions with H$^0$, H$^+$, and H$^+$ (Sun & Dalgarno 1994; Gerlich 1990; Le Bourlot 1991) are capable to make transitions between these quantum states. In our H$_2$ network, CLOUDY includes both reactive and non-reactive collisions. For details, see (Shaw et al. 2005).

2.1 Modelling

For all the models that we incorporated in this work, we assume a plane-parallel constant pressure gas exposed to radiation. We vary a few free parameters, as will be discussed below, to match the predicted column densities with the observed column densities of various atoms, ions and state specific H$_2$. The chosen radiation field has three components: a meta-galactic radiation at appropriate redshift (Haardt & Madau 2012), a synchrotron radiation (power-law continuum) arising from GRB afterglow and a blackbody radiation from \textit{in situ} star formation. Our GRB-DLA models are similar to our previous QSO-DLA models (Srianand et al. 2005a; Shaw et al. 2016; Rawlins et al. 2018) except that here we have an additional synchrotron radiation arising from GRB afterglows. While the gas is exposed to UV radiation from everywhere it is exposed to GRB afterglow only from one side.

In the current CLOUDY set up, it is not possible to consider both two-sided and one-sided radiation fields simultaneously in a same model. Hence we consider following two cases separately: Case 1, where we assume that the gas cloud is irradiated from both sides; and Case 2: where we assume that the gas cloud is irradiated from one side. We present our results for both the cases. The models presented here show that this does not effect the conclusions. However, it need to be noted that the geometry of the cloud is unknown and might be unknowable. The time history of the cloud is not known and we are also using a stationary code. These can also affect the results.

2.2 Input parameters

In this work, we use the dimensionless ratio of hydrogen-ionising photon $Q(H)$ (s$^{-1}$) to total-hydrogen densities $n(H)$ (cm$^{-3}$) in order to quantify the radiation field, and denote it by ionisation parameter, $\chi$, as,

$$\chi = \frac{Q(H)}{4\pi r_0^2 c n(H)}. \quad (1)$$

Here $r_0$ and $c$ are the separation (cm) between the center of the source of ionizing radiation and the illuminated face of the cloud, and the speed of light, respectively.

We consider both graphite and silicate grains in the calculations with MRN (Mathis et al. 1977) size distribution over ten size bins in the range 0.005 to 0.25 micron (ISM grains). For MRN grains, the grain size distribution varies as $a^{-3.5}$, where $a$ is the radius of the grain. Besides that, dusts provide heating through photoelectric heating, as well as it shields interior regions of molecular cloud from far-ultraviolet (FUV) radiation. The detail grain physics included in CLOUDY was described in van Hoof et al. (2004). It has been observed that dust is correlated with metallicity, and in general, metallicity is anti-correlated with redshift. It is believed that Fe is strongly depleted on dust grains whereas Zn is not depleted. Hence, one can estimate the metallicity and dust-to-gas ratio with the help of Zn/H and Fe/Zn ratios (Prochaska & Wolfe 2002). In our models, both metallicity and dust-to-gas ratio are derived using column densities of Zn, Fe and equation no. 1 from Prochaska & Wolfe (2002).

As mentioned earlier, cosmic ray affects the level populations of H$_2$ via secondary electrons which are produced by cosmic ray ionisation (Tine{é} et al. 1997). However, the cosmic ray ionisation rate is not the same along all line-of-sights (Indriolo et al. 2007; Shaw et al. 2008a). Since not much is
known on the cosmic ray ionisation rate at high-redshift, we consider this rate as a free parameter in our models.

We also treat the total hydrogen density, which includes all forms of hydrogen bearing chemical species, as a free parameter in our models. To be noted that CLOUDY requires at least one suitable stopping criterion for each model and it will stop calculations at some depth of the cloud depending on the stopping criterion. These stopping criteria vary depending on particular observed quantities that one match with. For all our case 2 models, we consider the observed total H\textsubscript{2} column densities as the stopping criterion, i.e., CLOUDY will continue its calculation till a depth of the cloud where the predicted total H\textsubscript{2} column density matches well with the corresponding observed value. Whereas, for case 1, we stop the model at a depth in the cloud where the total H\textsubscript{2} column density equals half of the observed H\textsubscript{2} column density. Finally we multiply our predictions by 2 to mimic the situation where the cloud is irradiated from both sides.

A built-in optimization program, based on phymir algorithm (van Hoof 1997), which calculates a non-standard goodness-of-fit estimator $\chi^2$ and minimises it by varying input parameters, is employed to identify the best model. Sometimes, to reach to the final model of a calculation, a few parameters are fine tuned so that the observed data can be matched maximally. This optimisation program is user friendly and has been utilised extensively in many previous works (Ferland et al. 2013; Srianand & Petitjean 2000; Shaw et al. 2006; Rawlins et al. 2018; Shaw & Bhattacharyya 2019).

In this work, using various parameters as discussed above, our main focus is to model the observed state-specific H\textsubscript{2} column densities self-consistently together with other observed column densities of ionic, atomic and molecular species to understand the underlying physical conditions which play pivotal roles to generate them. Below we discuss our findings.

3 RESULTS

In this section, results and main findings are elaborated. First GRB-DLA 120815A is discussed in detail, followed by GRB-DLA 121024A.

3.1 GRB-DLA 120815A

For the GRB-DLA 120815A, H\textsubscript{2} lines were first detected at $z = 2.36$ by Krühler et al. (2013). They observed the line-of-sight using X-shooter at VLT. H\textsubscript{2} absorption lines were observed in the rest frame Lyman and Werner bands (11.2–13.6 eV) which have been shifted to optical band due to redshift and hence could be easily observed by X-shooter which is an optical telescope. They reported H\textsubscript{2} column densities for the first four rotational levels of ground state. The neutral carbon and H\textsubscript{2} gets photo-dissociated by photons of the same energies, and hence the neutral carbon generally co-exists with H\textsubscript{2} (Noterdaeme et al. 2007, 2018; Jorgenson et al. 2009). As expected, the neutral carbon was also observed in this GRB-DLA. Beside H\textsubscript{2}, they also detected various metal lines, such as Zn, S, Si, Mn, Fe, Ni in their first ionisation states. The observed metallicity ([Zn/H]) and dust depletion ([Zn/Fe]) were found to be -1.15 ± 0.15 and 1.01 ± 0.10, respectively. Using these the dust-to-gas ratio is calculated to be ≈ 0.06 of the local ISM value, and is used in our models. They also found the broadening parameter of the H\textsubscript{2} lines to be $8.7 ± 0.6$ km s\textsuperscript{-1}. In our model, we fix the microturbulence/broadening parameter to the observed value 8 km s\textsuperscript{-1}.

As mentioned previously, in our model we consider that radiation consists of a meta-galactic background at $z = 2.36$, a blackbody radiation from an $n_{\text{iso}}$ star formation and a power law continuum due to afterglow. Krühler et al. (2013) found a power law slope of -0.78 as the best-fit value. Furthermore, recently, Li et al. (2018) have published a large catalogue of multi-wavelength GRB afterglows with spectral indices of 70 GRBs, and they have mentioned -0.78±0.01 as the spectral index for GRBs 120815A. Based on these facts, we choose -0.8 as the spectral index for GRB. As an example, in Fig.1 we plot all the components of the SED for GRB-DLA 120815A (case 1). The corresponding UV field is equivalent to 7 Habing. Case 2 also has the similar features with corresponding UV field 6.6 habing. In Table 1 we list the model parameters corresponding to our best model and the second and third columns represent Case 1 and Case 2, respectively. In case 1, our model predicts a hydrogen density of $440$ cm\textsuperscript{-3}. Whereas, for case 2 the predicted hydrogen density is lower, 230 cm\textsuperscript{-3}. For other elements, whose lines were observed, we vary their abundances in our model to match their observed values while keeping the abundances of other elements at 0.07 of the ISM value. Final values of metal abundances of Zn, S, Si, Fe, Ni, Cr and Mn, that we obtain are: $\text{Zn} = 0.06$ of the local ISM value, and is used in our models.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Element & Case 1 & Case 2 \\
\hline
Zn & $0.06$ & $0.06$ \\
S & $0.07$ & $0.07$ \\
Si & $0.07$ & $0.07$ \\
Mn & $0.07$ & $0.07$ \\
Fe & $0.07$ & $0.07$ \\
Ni & $0.07$ & $0.07$ \\
Cr & $0.07$ & $0.07$ \\
Mn & $0.07$ & $0.07$ \\
\hline
\end{tabular}
\caption{Metal abundance for GRB-DLA 120815A in case 1 and case 2.}
\end{table}
from our best fit model, match well with the observed data (within the observed error bars) by Krühler et al. (2013). In addition to these, we also predict the abundances of C, O, N and Mg. Krühler et al. (2013) have measured the A addition to these, we also predict the abundances of C, O, N (within the observed error bars) by Krühler et al. (2013). In addition reported by Indriolo et al. (2007). In Table 2 we compare observable amount of OH and OH ties in two different columns. To be noted that in addition significant contribution to the observed species, observable amount of OH and OH § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § § Section 1 – 10 (2020)
described all the possible excitation and de-excitation processes of the hyperfine levels related to 21 cm transition, as incorporated by CLOUDY. It includes collisional excitations and de-excitation by H, and incorporates by CLOUDY. It includes collisional excitations and de-excitation processes for this source. In the grain photoelectric heating, a dust grain absorbs a FUV photon and emits energetic electrons which heats up its surrounding region by collisions. We find that the grain photoelectric heating diminishes deep inside the cloud as FUV decreases inside the cloud. On the other hand, fractional heating by cosmic ray ionisation increases as one moves inside the cloud. The dominant coolants are found to be O I and C II lines.

We would like to emphasis here that for both cases we find the GRB-DLA 120815A is denser, smaller, and cooler than that reported by Ledoux et al. (2009) for GRB-DLAs in their first ionised state. The reported metallicity ([Zn/H]) and dust depletion ([Zn/Fe]) are observed to be $-0.6\pm0.2$ and $0.85\pm0.04$, respectively. Using these the dust-to-gas ratio is calculated to be $0.2$ of the local ISM value.

Though the component wise column densities were reported for metal lines, the component wise H$_2$ and H I column densities were not provided. Hence, we add up the three H$_2$-bearing components and consider them as a single component, and try to decipher the physical conditions of this stratified component. They have mentioned that the total H I column density for this stratified component is $10^{21.6}$ cm$^{-2}$. In this calculation we use the metallicity and dust-to-gas ratio to the observed value. Friis et al. (2015) used $-0.9\pm0.0$ as the spectral index for the GRB afterglow. In addition to this, Li et al. (2018) also observed $-0.86\pm0.01$ as the spectral index for GRB 121024A. Keeping the observed value in mind, we fix the slope for the power law continuum to $-0.9$. Similar to our study of previous DLA, here also in our calculations we consider Case 1 and 2. The individual components of the SED have similar features as shown in Fig. 1. The equivalent UV fields are 15 and 28 Habing for cases 1 and 2, respectively. Below we presents our results for these two cases.

We list our best model parameters for these cases in the second and third columns of Table 4. The abundances of the elements, whose lines have been observed, are varied to match their observed values. The predicted hydrogen density is 100 cm$^{-3}$ and 60 cm$^{-3}$ for case 1 and case 2, respectively. Beside hydrogen density, the ionisation parameter for the

### Table 3. Variation in column densities of GRB-DLA 120815A (in dex) for variation of different input parameters (Case 1).

| Species | $\Delta n$(H) | $\Delta n$(grain) | $\Delta \log(\chi)$ |
|---------|----------------|-------------------|---------------------|
|         | power law      | power law         | power law           |
|         | 0.3 dex        | 0.3 dex           | -0.3 dex            |
| H I     | 0.02           | -0.30             | -0.20               |
| Mg I    | -0.01          | -0.35             | 0.04                |
| Ni II   | -0.07          | -0.38             | -0.22               |
| Zn II   | 0.01           | -0.28             | -0.20               |
| C I     | -0.02          | -0.32             | -0.04               |
| Fe II   | 0.01           | -0.28             | -0.22               |
| Mn II   | 0.01           | -0.28             | -0.21               |
| S II    | 0.02           | -0.28             | -0.22               |
| CO      | 0.10           | 0.21              | 0.27                |
| OH      | 0.08           | 0.22              | 0.05                |
| OH$^+$  | 0.01           | -0.10             | 0.25                |
| HCl     | 0.03           | -0.06             | 0.03                |
| H$_2$O  | 0.14           | 0.39              | 0.21                |
| H$_2$O$^+$ | 0.85       | 0.14              | -0.13               |
| H$_3^+$ | 0              | 0.18              | 0                   |
| H$_2$(0) | -0.03         | -0.05             | 0.07                |
| H$_2$(1) | 0             | 0.01              | -0.03               |
| H$_2$(2) | 0.10          | 0.16              | -0.20               |
| H$_2$(3) | 0.24          | 0.13              | -0.31               |

3.2 GRB-DLA 121024A

In this section, we present our findings for another H$_2$-bearing GRB-DLA: GRB-DLA 121024A. The first trigger of GRB-DLA 121024A was reported in 2012. Later, Friis et al. (2015) observed numerous absorption and emission lines spanned over five components. However, H$_2$ was detected in only three out of five components (c+d+e) in rest frame Lyman and Werner band. They derived H$_2$ in its lowest four rotational states of the ground vibrational level ($J = 0, 1, 2, 3$). However, CO ($<14.4$) was not detected even though H$_2$ was detected. In addition to these, many metal lines of the metals Fe, Ni, Cr, Mn, Ca, Zn were present in their first ionised state. The reported metallicity ([Zn/H]) and dust depletion ([Zn/Fe]) are observed to be $-0.6\pm0.2$ and $0.85\pm0.04$, respectively. Using these the dust-to-gas ratio is calculated to be $0.2$ of the local ISM value.

Though the component wise column densities were reported for metal lines, the component wise H$_2$ and H I column densities were not provided. Hence, we add up the three H$_2$-bearing components and consider them as a single component, and try to decipher the physical conditions of this stratified component. They have mentioned that the total H I column density for this stratified component is $10^{21.6}$ cm$^{-2}$. In this calculation we use the metallicity and dust-to-gas ratio to the observed value. Friis et al. (2015) used $-0.9\pm0.02$ as the spectral index for the GRB afterglow. In addition to this, Li et al. (2018) also observed $-0.86\pm0.01$ as the spectral index for GRB 121024A. Keeping the observed value in mind, we fix the slope for the power law continuum to $-0.9$. Similar to our study of previous DLA, here also in our calculations we consider Case 1 and 2. The individual components of the SED have similar features as shown in Fig. 1. The equivalent UV fields are 15 and 28 Habing for cases 1 and 2, respectively. Below we presents our results for these two cases.

We list our best model parameters for these cases in the second and third columns of Table 4. The abundances of the elements, whose lines have been observed, are varied to match their observed values. The predicted hydrogen density is 100 cm$^{-3}$ and 60 cm$^{-3}$ for case 1 and case 2, respectively. Beside hydrogen density, the ionisation parameter for the
powerlaw continuum also differs for these two cases. Our best model for case 1 and case 2 predicts value of $A_V \approx 0.65$ and 0.54, respectively. This value is consistent with $A_V = 0.9 \pm 0.3$ as measured by Friis et al. (2015). Our best models predict the cosmic ray ionisation rate for hydrogen $0.36 \times 10^{-16}$ s$^{-1}$, same for both the cases.

In the fourth and fifth columns of Table 5 we compare our predicted column densities with the observed data for case 1 and case 2, respectively. As can be seen that our predicted column densities match very well with the observed values within the observed error bars. Previously Friis et al. (2015) reported column densities for two different cases, the grain photoelectric heating is found to be the main source of heating, whereas the main sources of cooling for case 1.

For the one-sided radiation field model, the predicted size of the GRB-DLA 121024A to be nearly 16 parsec for case 1. For both the cases, the grain photoelectric heating is found to be the main source of heating, whereas the main sources of cooling for case 1. Temperature and $H^0/H_{total}$, $H^+/H_{total}$, $2H_2/H_{total}$ are plotted as a function of distance into GRB-DLA 120815A (Case 2). The temperature axis is shown in the right.

### Table 4. Physical parameters of GRB-DLA 121024A using CLOUDY.

| Physical parameters | best values | best values |
|---------------------|-------------|-------------|
|                      | Case 1      | Case 2      |
| Power law: log($x$)  | -3.3        | -2.8        |
| Black body: Temp (log K), log($x$) | 4.9, -2.5   | 4.9, -2.5   |
| Density n(H) (cm$^{-3}$) | 100         | 60          |
| Cosmic ray ionisation rate ($10^{-16}$ s$^{-1}$) | 0.4         | 0.4         |
| [Fe/H]               | -1.6        | -1.6        |
| [Mg/H]               | -1.0        | -1.0        |
| [Ca/H]               | -2.6        | -2.6        |
| [Zn/H]               | -0.9        | -0.9        |
| [Ni/H]               | -1.5        | -1.5        |
| [Mn/H]               | -1.8        | -1.8        |
| [Cr/H]               | -1.4        | -1.4        |

### Table 5. Comparison of observed and predicted column densities GRB-DLA 121024A (in log scale) using CLOUDY.

| Species | observed | observed | predicted | predicted |
|---------|----------|----------|-----------|-----------|
|         | b=10 ($\chi^2$) | b=1 ($\chi^2$) | b=1 ($\chi^2$) | b=1 ($\chi^2$) |
|         | Case 1 | Case 2 | Case 1 | Case 2 |
| H I     | 21.6    | 21.77   | 21.69    | 21.90     |
| H$_2$   | 19.90   | 19.90   | 19.90    | 19.90     |
| Mg I    | <13.86  | 13.65   | 13.44    | 13.44     |
| Ni II   | 14.47 ± 0.06 | 14.54    | 14.45    | 14.45     |
| Zn II   | 13.74 ± 0.04 | 13.52    | 13.43    | 13.43     |
| Ca II   | 12.40 ± 0.12 | 12.40    | 12.37    | 12.37     |
| Fe II   | 15.58 ± 0.03 | 15.63    | 15.55    | 15.55     |
| Mn II   | 13.47 ± 0.03 | 13.51    | 13.43    | 13.43     |
| Cr II   | 13.97 ± 0.03 | 14.03    | 13.94    | 13.94     |
| CO      | –       | 10.93   | 11.26    | 11.26     |
| HCl     | –       | 12.28   | 12.18    | 12.18     |
| H$_2$(0)| 19.7    | 19.7    | 19.69    | 19.63     |
| H$_2$(1)| 19.2    | 19.3    | 19.47    | 19.55     |
| H$_2$(2)| 16.1    | 18.3    | 17.72    | 17.83     |
| H$_2$(3)| 16.0    | 18.2    | 17.21    | 17.83     |
| H$_2$(total)| 19.8 | 19.9 | 19.90 | 19.90 |
Table 6. Variation in column density of GRB-DLA 121024A (in dex) for variation in different input parameters (Case 1).

| Species | $\Delta n(H)$ | $\Delta$grain | $\Delta \log(\chi)$ | power law |
|---------|----------------|----------------|----------------------|-----------|
|         | 0.3 dex        | 0.3 dex        | -0.3 dex             | -0.3 dex  |
| H I     | 0.02           | -0.31          | -0.15                |           |
| Mg I    | 0.02           | -0.37          | -0.06                |           |
| Ni II   | 0.01           | -0.31          | -0.15                | -0.31     |
| Zn II   | 0.02           | -0.30          | -0.15                |           |
| Ca II   | 0.04           | -0.35          | -0.01                |           |
| Fe II   | 0.02           | -0.33          | -0.15                |           |
| Mn II   | 0.03           | -0.29          | -0.15                |           |
| Cr II   | 0.02           | -0.30          | -0.15                |           |
| CO      | 0.16           | 0.71           | -0.16                | 0.02      |
| HCl     | 0.01           | 0.08           | 0.15                 |           |
| H$_2$(0)| -0.03          | -0.16          | 0.02                 |           |
| H$_2$(1)| 0.04           | 0.18           | -0.10                |           |
| H$_2$(2)| 0.06           | 0.17           | -0.15                |           |
| H$_2$(3)| 0.26           | 0.03           | -0.29                |           |

Figure 4. Temperature and $H^0/H_{total}$, $H^+ / H_{total}$, $2H_2/H_{total}$ are plotted as a function of distance into GRB-DLA 121024A (Case 1). The temperature axis is shown in the right. This plot shows half of the cloud. The other half is just the reflection of this portion.

Figure 5. Temperature and $H^0/H_{total}$, $H^+ / H_{total}$, $2H_2/H_{total}$ are plotted as a function of distance into GRB-DLA 121024A (Case 2). The temperature axis is shown in the right.

4 SUMMARY AND CONCLUSIONS

GRB afterglows provide an unique opportunity to study the interstellar medium of star-forming galaxies at high-redshift. Observationally many GRB-DLA show H$_2$, the main constituent of molecular clouds where star formation takes place. However, till date there is no detail study, incorporating quantum mechanical microphysics, on these systems to model H$_2$ lines. In this work for the first time we carry out such a study using spectral synthesis code CLOUDY, by modelling the observed column densities (Friis et al. 2015) of GRB-DLA 121024A and GRB-DLA 120815 (Krühler et al. 2013) self-consistently. We select these two specific H$_2$-bearing GRB-DLAs, situated at redshifts 2.30 and 2.36 respectively, as they have substantially large H$_2$ molecular fraction. While the gas is exposed to UV radiation from everywhere it is exposed to GRB afterglow only from one side. Since the current CLOUDY setup does not allow to include both one-sided and two-sided radiation field simultaneously in a given model, we consider two cases separately. In Case 1, we assume that the gas cloud is irradiated from both sides, whereas in Case 2 we assume that the gas cloud is irradiated from one side. We present results for both the cases. The first number in the parenthesis represents Case 1 and the second number represent Case 2, respectively. We will follow this convention throughout.

- The total hydrogen density, consisting of ionised and atomic hydrogen together with all the hydrogen bearing molecules, are found to be (440, 230) and (100, 60) cm$^{-3}$ for GRB-DLAs 120815 and 121024A, respectively. Earlier, Ledoux et al. (2009) estimated a particle density of 5-15 cm$^{-3}$ for seven z > 1.8 GRB afterglows of their sample which did not show H$_2$. Hence, our findings strongly suggest that the total hydrogen densities of H$_2$-bearing GRB-DLAs are higher than that of without H$_2$ GRB-DLAs. This finding is also very much consistent with the recent observation of Bolmer et al.
We find that the 21 cm spin temperature is higher and conversion of H I to H2 occurs there.

- Earlier, Ledoux et al. (2009) estimated a linear cloud size of 520×248 pc for GRB-DLAs lacking H2. Here we find that linear sizes of H2-bearing GRB-DLAs, 120815A and 121024A, are (9.8, 17.7) and (16, 13) pc, respectively. Taking together this also suggests that the linear sizes of H2-bearing GRB-DLAs are smaller than that without H2 GRB-DLAs. Noterdaeme et al. (2018) had also concluded that H2-bearing QSO-DLAs have small physical extent.

- Ledoux et al. (2009) estimated that the kinetic temperatures of the metal-poor H2 lacking GRB-DLAs are more than 1000 K. Our results suggest that the gas temperatures of H2-bearing GRB-DLAs are lower than that of GRB-DLAs without H2.

- The higher density, lower temperature and smaller physical extension as mentioned above suggests that the H2-bearing GRB-DLAs trace the cold neutral phase of the ISM.

- Most of the heating to the environment of these systems is contributed by photoelectric heating.

- Most of the cooling of these systems is contributed by O I and C II lines.

- We find $A_v$ values (0.32, 0.31) and (0.65, 0.54) for GRB-DLAs 120815 and 121024A, respectively. $A_v > 0.1$ for both the sight lines are consistent with the measurement of Bolmer et al. (2019).

- The cosmic ray ionization rate for hydrogen along the lines of sight for GRB-DLAs 120815 and 121024A are $(1.9×10^{-16}, 1.9×10^{-16})$ s$^{-1}$ and $(0.4×10^{-16}, 0.4×10^{-16})$ s$^{-1}$, respectively.

- The predicted column densities match very well with observed data except for the H2 ($J = 2$) level for GRB-DLA 120815A. In case of GRB-DLAs 121024A, Case 1 predicts H2 ($J = 0, 1$) levels better whereas Case 2 predicts H2 ($J = 2, 3$) levels better. Hence, only the temperature of these sources are constrained by the H2 ($J = 0, 1$) levels.

- Besides the observed species, the best model for GRB-DLA 120815A predicts OH and OH$^+$ column densities to be more than $10^{13}$ cm$^{-2}$. It will be interesting if this prediction gets verified by future observations.

- We find that the 21 cm spin temperature is higher than the gas kinetic temperature for both these sources, though observationally the 21 cm absorption line has not been found yet for none of them. It is to be noted that similar trend had also been observed for the QSO-DLA at redshift 1.78 along Q1333+ (Chengalur & Kanekar 2000; Cui et al. 2005). In future, 21 cm absorption can be observed for GRB-DLAs using LOFAR or SKA.

In future, following this study, we will investigate more such H2-bearing DLAs, some of which have recently been observed (Bolmer et al. 2019). It will be interesting to find whether our results also hold in general for all other H2-bearing DLAs. That may help us to gain significant insights into the physical conditions of these important astrophysical systems and to understand why they possess molecular hydrogen, the main constituent of molecular clouds where star formation takes place. That will be an important contribution to the physics of star formation at high-red shift.

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