Discovery of a Perseus-like cloud in the early Universe

**H_i-to-H_2 transition, carbon monoxide and small dust grains at \(z_{\text{abs}} \approx 2.53\) towards the quasar J0000+0048**

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Received 23 June 2016 / Accepted 2 September 2016

**ABSTRACT**

We present the discovery of a molecular cloud at \(z_{\text{abs}} \approx 2.5255\) along the line of sight to the quasar SDSS J000015.17+004833.3. We use a high-resolution spectrum obtained with the Ultraviolet and Visual Echelle Spectrograph together with a deep multi-wavelength medium-resolution spectrum obtained with X-shooter (both on the Very Large Telescope) to perform a detailed analysis of the absorption lines from ionic, neutral atomic and molecular species in different excitation levels, as well as the broad-band dust extinction. We find that the absorber classified as a Damped Lyman-\(\alpha\) system (DLA) with \(\log N(\text{H}_1)\) (cm\(^{-2}\)) \(\approx 20.8 \pm 0.1\). The DLA has supersolar metallicity \(Z \approx Z_\odot\), albeit to within a factor of two to three) with a depletion pattern typical of cold gas and an overall molecular fraction \(f = 2N(\text{H}_2)/[2N(\text{H}_1) + N(\text{H}_1)] \approx 50\%\). This is the highest \(f\) -value observed to date in a high-\(z\) intervening system. Most of the molecular hydrogen arises from a clearly identified narrow \((b \sim 0.7\) km s\(^{-1}\)) cold component in which carbon monoxide molecules are also found, with \(\log N(\text{CO}) \approx 15\). With the help of the spectral synthesis code Cloudy, we study the chemical and physical conditions in the cold gas. We find that the line of sight probes the gas deep after the H\(\text{I}\)-to-H\(_2\) transition in a \(\sim 4-5\) pc-size cloud with volumic density \(n_0 \sim 80\) cm\(^{-3}\) and temperature of only 50 K. Our model suggests that the presence of small dust grains (down to about 0.001 \(\mu\)m) and high cosmic ray ionisation rate \((q_{\text{HI}} \sim \text{a few times } 10^{-15}\) s\(^{-1}\)) are needed to explain the observed atomic and molecular abundances. The presence of small gas is also in agreement with the observed steep extinction curve that also features a 2175 Å bump. Interestingly, the chemical and physical properties of this cloud are very similar to what is seen in diffuse molecular regions of the nearby Perseus complex, despite the former being observed when the Universe was only 2.5 Gyr old. The high excitation temperature of CO rotational levels towards J0000+0048 betrays however the higher temperature of the cosmic microwave background. Using the derived physical conditions, we correct for a small contribution \((0.3\) K) of collisional excitation and obtain \(T_{\text{CSH}}(z = 2.53) \approx 9.6\) K, in perfect agreement with the predicted adiabatic cooling of the Universe.

**Key words.** quasars: absorption lines – ISM: clouds – ISM: molecules – dust, extinction – cosmology: observations – cosmic background radiation

1. Introduction

The formation and evolution of galaxies is strongly dependent on the physical properties of the gas in and around galaxies. Indeed, the gas is the reservoir of baryons from which stars form and at the same time, it integrates the chemical and physical outputs from star-formation activity. The gas that is accreted onto galaxies has to cool down and go through different transitional processes that will determine its properties during its evolution before the final collapse that give birth to stars. Different phases are indeed identified in the interstellar medium, depending on the temperature and density and whether the matter is ionised or neutral (atomic or molecular). In their two-phase model, Field et al. (1969) showed that thermal equilibrium leads neutral gas to segregate into a dense phase, the cold neutral medium (CNM), embedded into a diffuse intercloud phase, the warm neutral medium (WNM). Detailed theoretical and numerical works (e.g. Krumholz et al. 2009; Sternberg et al. 2014) show that a
transition from H$_1$ to H$_2$ then occurs in the former phase, depending on the balance between H$_2$ formation on the surface of dust grains (e.g. Jura 1974b), and its dissociation by UV photons (e.g. Dalgarno & Stephens 1970), itself dependent on both self- and dust-shielding.

Observationally, UV absorption spectroscopy of Galactic clouds towards nearby stars reveal that the molecular fraction, $f = 2H_2/(2H_2 + H_1)$, sharply increases above a H$_1$ column density threshold of $5 \times 10^{20}$ cm$^{-2}$. A similar threshold has been found by Reach et al. (1994) from far-infrared emission studies of interstellar clouds, using dust as a tracer for H$_2$. Higher column-density thresholds were observed in the Magellanic Clouds (Tumlinson et al. 2002), which could be the consequence of a higher UV radiation field together with a lower metallicity in these environments. However, it is also possible that a significant fraction of the observed H$_1$ column density is actually unrelated to the atomic envelopes of the H$_2$-absorbing clouds (Welty et al. 2012), since N(H$_1$) is derived through unresolved 21-cm emission, while N(H$_2$) is measured in absorption.

This highlights the main difficulty in observing the transition regions: because molecular clouds have sizes of only a few tens to a few hundred parsec (e.g. Fukui & Kawamura 2010) it is very difficult to compare H$_2$ with its associated H$_1$ in the cloud envelope without also integrating nearby atomic gas. High spatial resolution (sub-pc) studies exist for nearby molecular clouds such as the Perseus cloud. Lee et al. (2012) observe relatively uniform H$_1$ surface density of $\Sigma_{H_1} \sim 6-8$ $M_\odot$ pc$^{-2}$ around H$_2$ clouds, in agreement with the theoretical expectations based on H$_2$ microphysics at solar metallicity, assuming CNM a priori (Krumholz et al. 2009) or not (Bialy et al. 2015).

Ideally, we would also like to study the atomic to molecular transition and the subsequent star formation over parsec scales in other galaxies. Observations of nearby galaxies have been possible at slightly sub-kpc resolution, revealing a saturation value around $\Sigma_{H_1} \sim 9$ $M_\odot$ pc$^{-2}$ (Bigiel et al. 2008). However, the observational techniques applied in the local Universe are not applicable yet in the distant Universe without a further strong loss of spatial resolution. Prescriptions of star-formation over galactic scales, such as the empirical relation between the molecular to atomic ratio and the hydrostatic pressure (e.g. Blitz & Rosolowsky 2006) are nevertheless available and can be used in evolution models of galaxies (e.g. Lagos et al. 2011), although this corresponds to an extrapolation at high redshift of a phenomenon observed in the local Universe. The increase of sensitivity in sub-mm astronomy has also permitted tremendous progress in recent years with detailed studies of the relation between molecular content and star formation at intermediate redshifts (e.g. Tacconi et al. 2013), although still limited to relatively bright and massive galaxies. In addition, observations of atomic gas through H$_1$ 21-cm emission (currently limited to $z < 0.4$, e.g. Catinella et al. 2008; Freudling et al. 2011; Fernández et al. 2016) will have to await future radio facilities such as the Square Kilometre Array.

At high redshift, information about gas in the Universe can be accurately obtained through absorption studies towards bright background sources. In particular, damped Lyman-$\alpha$ systems (DLAs, see Wolfe et al. 2005, for a review), with N(H$_1$) $\geq 2 \times 10^{20}$ cm$^{-2}$, trace the neutral gas in a cross-section weighted manner, independently of the luminosity of the associated object. DLAs have been conjectured to be originating from gas associated with galaxies, in particular since DLAs contain the bulk of the neutral gas at high redshift (e.g. Prochaska et al. 2005; Prochaska & Wolfe 2009; Noterdaeme et al. 2009b, 2012a) and their metallicity is increasing with decreasing redshift (e.g. Rao et al. 2006; Rafelski et al. 2012). While the dust production in the bulk of DLAs seems to be very low (Murphy & Bernet 2016), the excitation of atomic and molecular species indicates some ongoing star-formation activity (e.g. Wolfe et al. 2004; Srianand et al. 2005; Neeliman et al. 2015). This is also suggested by numerical simulations (e.g. Cen 2012; Bird et al. 2014) or semi-analytical models (e.g. Berr et al. 2016) but direct associations with galaxies remain difficult to establish, with only a few associations between intervening DLAs and galaxies revealed so far at $z > 2$ (Möller & Warren 1993; Möller et al. 2004; Fynbo et al. 2010; Kroger et al. 2012; Noterdaeme et al. 2012b; Bouché et al. 2013; Kashikawa et al. 2014; Hartoog et al. 2015; Srianand et al. 2016). Indeed, statistical studies show a low level of in-situ star formation (Rahmani et al. 2010; Fumagalli et al. 2015), although Ly-α emission has been detected through stacking in sub-samples with the highest H$_1$ column densities (Noterdaeme et al. 2014), suggesting the latter arise more likely from gas associated with galaxies at very small impact parameters.

Noterdaeme et al. (2015a) suggest that H$_2$ is more frequently found in high column density DLAs, but that the measured overall molecular fraction remains much lower than what would be expected from single clouds, even at the typically low metallicities of DLAs. This indicates that most of the observed H$_1$ column density along the line of sight is actually unrelated to the H$_2$ core and does not participate in its shielding (see also Noterdaeme et al. 2015b). This again marks the difficulty of distinguishing the H$_1$ envelope of molecular clouds from unrelated atomic gas along the same line of sight. Several methods have been developed to statistically derive the CMN fraction in DLAs. The low detection rate of 21-cm absorption in DLAs indicates high average spin temperatures and hence points to the fact that most DLAs are dominated by WNM (e.g. Kanekar et al. 2014). Neeliman et al. (2015) recently suggest that the bulk of neutral gas could be in the CMN for at least 5% of DLAs, based on the fine-structure excitation of singly ionised carbon and silicon. This further indicates that such clouds can be as small as a few parsecs. A small size of CMN clouds is also inferred from the lack of correspondence between 21-cm and H$_2$ absorption seen in DLAs (Srianand et al. 2012) and by the partial coverage of the background quasar’s broad line region by H$_2$-bearing clouds (e.g. Balashev et al. 2011).

Because H$_2$-bearing systems are rare among the overall DLA population (e.g. Ledoux et al. 2003; Noterdaeme et al. 2008; Jorgenson et al. 2014), directly targeting H$_2$ (instead of blindly targeting H$_1$ gas) could provide a more efficient way to study the phase transition. Unfortunately, H$_2$ lines are located in the Ly $\alpha$ forest and are difficult to detect at low spectral resolution (except when the absorption is in the damped regime, Balashev et al. 2014). In turn, neutral carbon provides an excellent tracer of H$_2$ molecules (e.g. Snow & McCall 2006), since the ionisation energy of C$_1$ is close to that of H$_2$ photodissociation. Furthermore, several transitions are located out of the Ly $\alpha$ forest, making it possible to search for strong C$_1$ absorption even at low spectral resolution (see Ledoux et al. 2015). Such selection has led to the first detections of CO molecules in absorption at $z > 1.6$, which also opens the exciting possibility to directly measure the cosmic microwave background (CMB) temperature through the excitation of CO (Noterdaeme et al. 2011). In the two high redshift cases where H$_2$ lines are also covered, we measured overall molecular fractions of about 25% (Srianand et al. 2008; Noterdaeme et al. 2010), that is significantly higher than in other H$_2$-bearing DLAs, which generally have $f \sim 1\%$ or less (Ledoux et al. 2003).
In our quest for molecular-rich systems in the Sloan Digital Sky Survey-III (SDSS-III), we found a new case at $z_{\text{abs}} \approx 2.5$ towards the quasar SDSS J000015.17+004833.3 (hereafter J0000+0048) with strong C I absorption and a prominent 2175 Å bump, which we followed-up with the Very Large Telescope. The characteristics of this system in terms of molecular fraction, CO column density, and metallicity supersede all values measured in DLAs so far. A cold, molecule-bearing component is clearly identified, allowing us to perform an unprecedentedly detailed analysis of the chemical and physical conditions in the molecular cloud and to study the transition from the atomic to the molecular phase. We present our observations in Sect. 2, the absorption-line analysis of atomic, atomic and molecular species in Sect. 3. We discuss the metallicity and dust abundance in Sect. 4, the extinction in Sect. 5 and the physical conditions in the cloud in Sect. 6. We use CO to measure the cosmic microwave background temperature at $z = 2.53$ in Sect. 7. We search for star-formation activity in Sect. 8 and conclude in Sect. 9.

2. Observations and data reduction

2.1. UVES

High-resolution spectroscopic observations of J0000+0048 ($z_{\text{em}} \approx 3.03$) were carried out using the Ultraviolet and Visual Echelle Spectrograph (UVES; Dekker et al. 2000) mounted on the unit 2 of the 8.2 m Very Large Telescope (VLT) at Paranal observatory under two distinct ESO programmes 093.A−0126(A) in 2014 (P93) and 096.A−0354(A) in 2015 (P96). The former observations were all performed using the standard beam splitter with 390+564 setting at a slit width of 0.9″.

The latter (P96) were mostly performed with the same setting but with a narrower slit width of 0.7″ in the red arm, and attached Th-Ar calibration. We also observed the quasar $2 \times 4200$ s with central wavelength set to 760 nm in the red arm in order to extend the spectral coverage over the redshifted absorption position of useful metal species (Zn II, Fe II). These were taken with a 0.9″-wide slit. We used a CCD readout with $2 \times 2$ binning and set the slit position to parallactic angle for all the observations to minimise the effects of atmospheric dispersion. A summary of the observations is shown in Table 1.

The data were reduced using UVES Common Pipeline Library (CPL) data reduction pipeline release 6.5 using an optimal extraction algorithm (Horne 1986). We used 4th order polynomials to find the dispersion solution. The individual science exposures were shifted to the heliocentric-vacuum frame correcting for the observatory’s motion towards the line of sight at the exposure mid point, using the air-to-vacuum relation from Ciddor (1996).

All exposures taken with the BLUE arm were obtained using a 0.9″-wide slit and extracted onto a fixed wavelength grid with a pixel step of 2.5 km s$^{-1}$ which corresponds to the pixel size on the CCD. The spectrum of each echelle order was interpolated onto this global grid so that no further rebinning was required neither when merging orders of an exposure nor when combining different exposures. Similarly, exposures taken with the RED arm have higher resolution and smaller pixel sizes and were extracted onto a grid with a pixel step of 2.0 km s$^{-1}$.

Cosmic ray residuals and bad pixels were flagged using a semi-interactive procedure and the data quality was checked to remove a few failed exposures. Individual 1D extractions were then scaled and combined together into three final 1D spectra: a “blue” spectrum, with spectral resolution 6.30 km s$^{-1}$; a “red” spectrum with resolution ranging from 5.45 to 5.80 km s$^{-1}$ corresponding to all exposures taken with 0.9″ slit and a higher resolution “red” spectrum, with resolution 4.60–4.70 km s$^{-1}$, combining the 0.7″-wide slit exposures. The average S/N per pixel is about 8 at 4000 Å in the blue spectrum. The combined red spectrum has in turn $S/N \approx 20$ at 5300 Å.

2.2. X-shooter

Deep, medium-resolution spectroscopic observations of J0000+0048 over the full wavelength range from ~320 nm to ~2.25 μm were carried out at the VLT unit 3 using X-shooter under ESO programme 096.A−0924(B). We performed all observations using the Nodding mode and slit widths of 1.3″, 0.9″ and 1.2″ for the UVB, VIS and NIR arm, respectively, and a binning of 1 × 2. We used different slit position angles to maximise the spatial coverage around the quasar location. The log of observations is shown in Table 1.

Our X-shooter data reduction heavily relied on the pipeline supplied by ESO in its version 2.5.2 (Modigliani et al. 2010). For every position angle, we used the pipeline to apply a flat-field correction, order tracing and rectification of individual frames in each nodding position individually. In the UVB and VIS arms, the sky spectrum was subtracted using regions in the 11″-long X-shooter slit free of signal. In the NIR, the intensity of the sky spectrum is high so we used the frame taken at the alternate nodding position closest in time for background subtraction. Wavelength and flux calibrations were performed using arc lamp lines observed during daytime and the nightly spectrophotometric standard, respectively.

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Table 1. Log of observations.

<table>
<thead>
<tr>
<th>Programme ID</th>
<th>Setting/Mode</th>
<th>Slit widths (arcsec)</th>
<th>Observing dates</th>
<th>Exposure time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>093.A−0126(A)</td>
<td>390+564</td>
<td>0.9, 0.9</td>
<td>Aug. 2014</td>
<td>5 × 4800 s</td>
</tr>
<tr>
<td>096.A−0354(A)</td>
<td>390+564</td>
<td>0.9, 0.7</td>
<td>Oct.-Nov. 2015</td>
<td>6 × 4200 s</td>
</tr>
<tr>
<td>096.A−0354(A)</td>
<td>437+760</td>
<td>0.9, 0.9</td>
<td>Nov. 2015</td>
<td>2 × 4200 s</td>
</tr>
<tr>
<td>096.A−0924(B)</td>
<td>Nodding</td>
<td>1.3, 0.9, 1.2</td>
<td>Sep-Dec 2015, Aug 2016</td>
<td>8 × 2 × (1400, 1430, 3 × 480)</td>
</tr>
</tbody>
</table>

Notes. The different values for slit width correspond to different arms, ordered by increasing wavelength: BLUE, RED for UVES and UVB, VIS, NIR for X-shooter. The exposure times for X-shooter data are detailed as (number of OB) × (nodding positions) × (exposure time for a given position), with the NIR being sub-divided in 3 integrations (NDIT).
This process provided us with sky-subtracted, wavelength- and flux-calibrated 2D spectra. After cosmic-ray and bad-pixel detection using our own algorithm based on Laplacian-filter edge detection, we averaged these frames with variance weighting. This yielded a single frame per arm and position angle. We then obtained the 1D spectra by optimal extraction, where the appropriate weights along the spatial direction were derived using a Moffat-function fitted to the data. Finally, the spectra were corrected for Galactic foreground reddening (Schlafly & Finkbeiner 2011) and converted into a vacuum heliocentric reference frame. We checked the quality of the flux calibration by comparing the spectra against each other and found agreement within 15% in the UVB (and better in the other arms). Similarly, we found no evidence for significant chromatic slit losses in the data by comparing with accurate multi-band photometry (see Sect. 5).

Because X-shooter sits at the Cassegrain focus of the VLT, shifts in the wavelength solution by about 0.5 Å are not uncommon due to flexure (e.g. Bristow et al. 2011). This is particularly expected when observations are performed off the parallactic angle. Thanks to UVES observations of the same object, we indeed noticed and corrected for wavelength distortions in the UVB arm: we smoothed the UVES spectrum to X-shooter’s spectral resolution and cross-correlated the resulting spectrum with the X-shooter data over 200 Å chunks. The wavelength distortions were different for each observation but could be very well approximated by a linear function of wavelength (see also Chen et al. 2014). We thus corrected for this distortion before combining the individual 1D exposures. This led to an improvement of the wavelength calibration accuracy by a factor of more than ten compared to the pipeline results (Fig. 1) without losing spectral resolution in the final spectrum due to blurring effect. The combined X-shooter spectrum had a S/N ratio ∼35, 55 and 25 and resolution around 75, 32 and 35 km s$^{-1}$ in the UV, visual and near infrared, respectively.

3. Absorption line analysis

We detect metal absorption lines in the $z_{\text{abs}} = 2.525$ absorption system from various ionisation stages from high-ionisation species (e.g. C IV, Al III, see Fig. 2) and singly ionised species (Si II, Ni II, Zn II and Fe II) spread over roughly 400 km s$^{-1}$. We detect a narrow component at the extreme red edge of the profile in which we also detect neutral (Si I, Mg I, Cl I, C I) and molecular (H$_2$, CO) species. While the overall kinematic profile is interesting – with a large velocity extent and absorption strengths varying differently with velocity for different ions, suggesting galactic winds – we mostly focus on the molecular component in this paper. We used VPFIT (Carswell & Webb 2014) version 10.3 to model the absorption profiles using multi-component Voigt-profile fitting in order to obtain redshifts, Doppler parameters and column densities of different species.

During our analysis, we combined the two red UVES spectra into a single spectrum using an inverse variance weighting. In principle, the resulting spectral point spread function (SPSF) becomes the combination of the two Gaussian SPSF as done by Carswell et al. (2012). In practice, because we are using data from the same instrument with resolutions that differ by only 20%, the resulting SPSF can very well be approximated by a single Gaussian with resolution ranging from 5 to 5.25 km s$^{-1}$ over the region covered by both original spectra. We checked that fitting both red spectra simultaneously or using their combination provided consistent results. Therefore we here provide the results using the combined spectrum. For the particular case of CO, we tested this in more detail and also provide the simultaneous fit to the two sets of UVES data.

3.1. Atomic hydrogen

We determined the H I column density of the system by simultaneously fitting the continuum of the background quasar together with a Voigt profile to the damped Ly $\alpha$ absorption line. Higher-order Lyman lines were not usable due to blending with stronger damped H$_2$ lines (see Sect. 3.4). We used the X-shooter spectrum since it has much higher signal-to-noise ratio than the UVES spectrum in this region. Moreover the X-shooter spectrum is flux calibrated, making it easier to determine the continuum placement. We obtained $\log N$(H I) $= 20.8 \pm 0.1$. As expected, the UVES data is consistent with this value, see Fig. 3.

3.2. Metals

About twenty velocity components with a wide dynamical range of optical depths can be distinctly identified in the profiles of Si II
and Fe II thanks to several transitions spanning a range of oscillator strengths. We used these species together with Si I (whose 1807 Å transition is blended with Si II1808) to obtain a first solution for the component structure. We then included Ni II and Fe II and let the column densities vary freely while the Doppler parameters and redshifts were tied together for singly ionised species. The redshift and Doppler parameters for neutral species (Si I and Mg I) were kept independent.

A very narrow component \( (b = 0.6 \text{ km s}^{-1}) \) corresponding to the neutral and molecular species is clearly seen at the extreme red edge of the profiles of Si II1808 and Zn II12026, 2062 while much weaker in Fe II lines and not detected at all in Ni II (see the component at \( v = 0 \text{ km s}^{-1} \) in Fig. 4). This already indicates a high level of dust depletion since the later species are refractory while zinc is a volatile element (e.g. Pettini et al. 1997).

We use this narrow component \( (z = 2.52546) \) as the reference for the zero-velocity in all figures and discussions in the paper. We also note that we did not make any assumption on the velocity structure (that is, redshift and Doppler parameter) of this component and we fitted the molecular, atomic, and ionic species independently. The results from fitting the lines are shown in Fig. 4 and the corresponding parameters provided in Table 2. We measured total column densities of respectively \( \log N(C^+) = 20.80 \pm 0.10 \) and \( \log N(H_2) = 20.80 \pm 0.10 \) in that component, with \( b \sim 0.7 \text{ km s}^{-1} \). These values should be considered with great caution as the fit was sensitive to the initial guess, leading to uncertainties larger than an order of magnitude.

### 3.3. Neutral carbon

The strong C I absorption lines that were used to select the system from the low-resolution SDSS spectrum are resolved in our UVES spectrum into different components and different fine-structure levels. We detect all three fine-structure levels of neutral carbon’s ground state triplet \( (2s^22p^6P_{0,1,2}) \) in five components, the strongest of which (by a factor of more than a hundred in column density) is associated with the narrow component seen in both the low-ionisation metal profile and in molecular absorption \( (H_2 \text{ and CO}) \). We simultaneously fitted all components from the fine-structure levels \( (J = 0, 1, 2) \), here denoted C I, C I’, C I”, respectively, tying Doppler parameters and redshifts for a given velocity component. We note that while this decreases the number of free parameters, it is based on the reasonable assumption that the fine-structure levels share the same physical origin.

We used the lines at \( \lambda = 1500 \) and 1656 Å, located outside the Ly \( \alpha \) forest, to constrain the fit (see Fig. 6). Including other lines (e.g. C I1277, 1328) did not improve the constraints due to the blends, lower S/N and lower spectral resolution. The results are provided in Table 3.

### 3.4. Molecular hydrogen

The spectrum of J0000+0048 is crowded with very strong Lyman (\( B^1 \Sigma_g^+(\nu’)-X^1 \Sigma_g^+(0) \)) and Werner (\( C^1 \Pi_u(\nu’)-X^1 \Sigma_g^+(0) \)) lines from molecular hydrogen bluewards of 4000 Å (see Fig. 8). Since the X-shooter spectrum has a much higher S/N and an extended wavelength coverage in the blue compared to the UVES spectrum, we used both spectra for the analysis of \( H_2 \). After normalising the spectra using a spline function, the UVES spectrum was particularly useful to identify regions blended with intervening Ly \( \alpha \) absorption from the forest, which were subsequently excluded during the fitting process.

Because the first ionisation potential of carbon, 11.26 eV, is very close to that of \( H_2 \) dissociation, carbon is usually considered a good tracer of molecular hydrogen (e.g. Triandos et al. 2005). While there is no one-to-one correspondence, we can expect \( H_2 \) to be present in the five components in which C I is detected. Unfortunately, because the \( H_2 \) lines are strongly saturated, it was impossible to distinguish the several close components in their profile. We therefore measured only the total \( H_2 \) column density by modelling the absorption profile using a single velocity component. This model is dominated by the reddest narrow component, for which the C I column density is about two orders of magnitude higher than in the rest of the components. We tied together the redshifts for the different \( H_2 \) rotational levels, under the assumption that they arise from the same physical cloud. Absorption lines for the low rotational levels (\( J \leq 2 \)) are damped, meaning that the column density was well constrained while the
Fig. 4. Multi-component Voigt-profile fit to singly ionised species (red), overlayed on top of the normalised UVES data. Regions marked in blue correspond to species other than the one labelled; for example, the blue region in SiII λ1808 is due to absorption by SiII λ1807.

Fig. 5. Fit to the CII* λ1335 absorption profile (UVES data). The blue and green curves correspond to the contribution from each transition of the doublet. The top axis shows the relative velocity corresponding to the strongest transition (green, with $\lambda = 1335.7077$ Å rest-frame).

profile does not directly depend on (and therefore did not constrain) the Doppler parameter.

Figure 7 shows the excitation diagram of H$_2$, which presents the population in each rotational level against the energy of that level:

$$\frac{N(H_2, J')}{g(H_2, J)} = \frac{N(H_2, J)}{g(H_2, J)} e^{-E_{J'/J}/kT_{eff}},$$

where $E_{J'/J}$ is the energy difference between levels $J$ and $J'$, $g(H_2, J)$, $g(H_2, J')$ are the respective spin statistical weights and $T_{eff}$ is the excitation temperature. $T_{01}$ is generally considered as a very good indicator of the kinetic temperature of the gas at such high column density, where selective self-shielding is no longer at play and the low rotational levels are easily thermalised thanks to short collisional time-scales (Roy et al. 2006; Le Petit et al. 2006). In turn, the high rotational levels are characterised by a higher excitation temperature. This is expected and seen in interstellar clouds because of the very slow infrared relaxation after UV or formation pumping into high-$J$ levels. Moreover

Fig. 6. Fit to the neutral carbon lines (from UVES data). The green numbers below each plot indicate the fine structure level $J$ for each of the five detected C I components.

A82, page 6 of 24
collisional de-excitation becomes difficult at the high-\(J\) levels, where the level spacing becomes so large (several hundred cm\(^{-1}\)) that these amounts of energy cannot be transferred in collisions, particularly at the densities and temperatures seen in the ISM. This leads to the observed non-Boltzmann distribution. We also note that the observed excitation diagram corresponds to integrated values and that possible additional warmer components with lower \(N(H_2)\) will mostly contribute to the high-\(J\) levels.

We measured \(T_{\text{rot}}\) = 51 ± 2 K, which is lower than the value typically seen in \(H_2\)-bearing DLAs (Srianand et al. 2005, \(T \sim 150\) K), and closer to what is seen in our Galaxy, with an average of about 77 K (Rachford et al. 2002). The kinetic temperature \(T_{\text{kin}} \approx T_{\text{rot}}\) corresponds to a Doppler parameter for \(H_2\) of \(b_{\text{rot}} \approx 0.65\) km s\(^{-1}\) if we assume thermal broadening only. However, because turbulent broadening is also likely present, as indicated by similar Doppler parameters for much heavier species, this value should be considered as a lower limit to the line broadening. We were able to get a more realistic estimate of the Doppler parameter by quadratically adding this pure thermal value to the turbulent \(b\)-value seen for heavier species (for which \(b_{\text{rot}}\) is negligible, see Fig. 16) and obtained 

\[
b = \sqrt{b_{\text{th}}^2 + b_{\text{turb}}^2} \approx 1.0\ \text{km s}^{-1}.
\]

However, it has been observed in several \(H_2\)-bearing systems that the Doppler parameter can be an increasing function of the rotational level (e.g. Lacour et al. 2005; Noterdaeme et al. 2007; Albornoz Vásquez et al. 2014), possibly due to more turbulent than an warmer external layers where UV pumping of \(H_2\) is enhanced (Balashev et al. 2009). We therefore also performed a fit using a high \(b\)-value of 5 km s\(^{-1}\). The resulting parameters are provided in Table 4. We obtained a total column density of log \(N(H_2) = 20.43 ± 0.02\), which implies an overall molecular fraction of \(f = 2N(H_2)/(2N(H_2) + N(H_1)) \approx 0.46 ± 0.07\), that is the highest value measured to date in a quasar-DLA. This also corresponds to a strict lower limit to the molecular fraction in the cold component.

### 3.5. Deuterated molecular hydrogen

Several lines of deuterated molecular hydrogen are also detected in both the UVES and X-shooter spectra. However, HD lines are often blended with Ly \(\alpha\) forest or \(H_2\) absorption and are saturated in the low S/N ratio UVES spectrum but weak in the medium resolution X-shooter spectrum. We therefore used a different
fitting procedure based on a Markov chain Monte Carlo method. We considered L0R0, L4R0, L5R0, L6R0, L8R0 and W0R0, locally re-normalised, as well as L11R0 and L14R0 (covered only by X-shooter). We used two components with fixed redshifts (z = 2.525458 and z = 2.525348) corresponding to the strongest components seen in C1 and used C1 Doppler parameters as priors. The synthetic HD profiles in the UVES spectrum are shown in Fig. 9 together with the corresponding X-shooter profile. We only consider the total HD column density as being reasonably trustable, with log N(H2) = 16.64^{+0.16}_{-0.18}. This corresponds to HD/2H2 = (8.1^{+3.7}_{-2.9}) \times 10^{-5}, which is significantly higher than typical ratios observed in our Galaxy (Snow et al. 2008). Our inferred ratio is also higher than the primordial value estimated from D/I/H1 in low metallicity high-z DLAs ((D/H)I = (2.53 \pm 0.04) \times 10^{-5}; Cooke et al. 2014). While a high abundance of deuterium can possibly be explained by a strong supply of primordial gas (as suggested by Ivanichik et al. 2010), the molecular ratio observed here is more likely explained by chemical fractionation and charge exchange processes (Liszt 2015).

Without entering into details of the HD chemistry, we note that the reaction D^+ + H2 → HD + H^+ is fast and can lead to an increase of HD compared to H2. If we call f_{HD}/HD = HD/(HD + DI) the fraction of deuterium in molecular form, then we have

\[ \frac{HD}{2H2} = \left( \frac{D}{H} \right) \frac{f_{HD}}{f_{I}}. \]  

Assuming an intrinsic primordial value\(^1\), the high HD/H2 ratio can be explained for f_{HD}/f_{I} = 3.2, which naturally requires that the cloud cannot be fully molecular. This is indeed what we conclude from modelling the physical conditions in the cloud (Sect. 6). We however caution that a high-resolution spectrum with high S/N ratio is necessary to better take into account blends with the Ly-α forest and confirm our measurement.

\(^1\) We do not take into account astiration of the order of 0.1 dex due to the high metallicity and redshift of our system (see Dvorkin et al. 2016).

### Table 5. Neutral chlorine fitting parameters.

<table>
<thead>
<tr>
<th>z_{abs} (km s^{-1})</th>
<th>b (km s^{-1})</th>
<th>log N(C1)</th>
<th>b (km s^{-1})</th>
<th>log N(C1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.52500</td>
<td>6.5 ± 1.3</td>
<td>13.00 ± 0.06</td>
<td>6.6 ± 1.2</td>
<td>13.00 ± 0.06</td>
</tr>
<tr>
<td>2.52536</td>
<td>4.8 ± 1.5</td>
<td>13.03 ± 0.10</td>
<td>4.9 ± 1.1</td>
<td>13.04 ± 0.06</td>
</tr>
<tr>
<td>2.52546</td>
<td>0.8 ± 0.6</td>
<td>14.55 ± 1.92</td>
<td>0.7^a</td>
<td>14.63 ± 0.29</td>
</tr>
<tr>
<td>Total</td>
<td>14.58 ± 1.81</td>
<td></td>
<td>14.65 ± 0.27</td>
<td></td>
</tr>
</tbody>
</table>

**Notes.** (a) Fixed value (see text).

### 3.6. Neutral chlorine

Chlorine is known to be tightly linked with H2 thanks to rapid chemical reactions (e.g. Jura 1974a). In our Galaxy, observations of clouds with log N(H2) > 19 using the Copernicus satellite have revealed a clear correlation between the column density of both species (Mooney et al. 2012). Recently, Balashev et al. (2015) have used a sample of known H2-bearing DLAs to show that this relation stands at high redshifts and down to ten times lower column densities. Here, only one absorption line of neutral chlorine, ClIλ1347 is covered and not blended in our spectrum. Three components, that match those seen in the neutral carbon profile, are detected and used to constrain the column densities, while those associated to the weakest C1 components are below our detection limit. This again indicates that H2 should actually be present in more than one component, although too close to be distinguished within the damped profile of the strong, cold component. Unfortunately, the column density of neutral chlorine in that component is poorly constrained due to this line being in the intermediate regime with a strong dependence on the Doppler parameter. Therefore, the Voigt profile fit, with all parameters kept free, lead to a very high uncertainty in the column density. However, we can make the reasonable assumption that the Doppler parameter should be close to that of other species for this component. Since chlorine is expected to arise from the H2-bearing gas but with a much higher atomic mass, its thermal broadening should be negligible and its Doppler parameter close to that of other “heavy” species. Assuming b = 0.7 km s^{-1} (see Fig. 16), we obtained a very satisfactory fit with log N(ClI) = 14.6 ± 0.3 in the narrow component. We also fitted ClI assuming a more relaxed constraint on b. Taking b to be in the range 0.6–0.8 km s^{-1}, gave log N(ClI) = 14.43–14.89 with a similar uncertainty of 0.3 dex. This sets the overall uncertainty to about 0.4 dex. The results are shown in Fig. 10 and Table 5, where we also provide the fitting results leaving the Doppler parameter totally free, for completeness.

### 3.7. Neutral sulphur

Because the first ionisation potential of sulphur is 10.36 eV, neutral sulphur is only expected to be found in very shielded regions. To our knowledge, only a handful detections of S1 have been reported so far in DLAs, all associated to a molecular absorber featuring CO (Srianand et al. 2008) and/or strong H2 absorptions (Milutinovic et al. 2010; Balashev et al. 2011). Here, we detect S1 absorption lines with log N(S1) = 14.85 ± 0.18 in our UVES spectrum from five transitions in a single narrow (b = 0.50 ± 0.07 km s^{-1}) component, see Fig. 11. This suggests that S1 can be used as a tracer for CO (Nota et al., 2010), just like the presence of C1 implies that of H2. However, because S1 lines have similar strengths and are located in the same spectral region as CO lines, this is of little practical use to identify...
CO systems. Still, S\textsc{i} can be helpful in determining the velocity structure of multi-component CO absorption systems (e.g. Srianand et al. 2008; Noterdaeme et al. 2009a).

3.8. Neutral magnesium and neutral sodium

Neutral magnesium (Mg\textsc{i}) is detected in five transitions in our UVES spectrum (see Fig. 12). We clearly detect two components and possibly two additional weak components. The main component, again corresponding to the molecular one at $v = 0$ km s\textsuperscript{-1}, contains more than 80% of the total column density with log $N$(Mg \textsc{i}) = 14.1 $\pm$ 0.1. Interestingly, the hidden saturation of this component with very small Doppler parameter ($b = 0.86 \pm 0.1$ km s\textsuperscript{-1}) is directly evidenced by its relative strength compared to the second strongest component: both these components have similar observed optical depth for Mg \textsc{i}\textsc{I}2026, but the former is also seen in transitions with much smaller oscillator strengths.

We also detect the Na\textsc{i}λλ1589.1,5897 doublet in the NIR X-shooter spectrum. The non-Gaussian profile indicates that several components are present, although blended at the achieved spectral resolution (around $R \sim 8500$). We therefore used the velocity decomposition of Mg\textsc{i} obtained at high spectral resolution, that is, the redshifts and Doppler parameters of Na\textsc{i} were fixed to the value previously determined for Mg\textsc{i} and only the column density was allowed to vary. This assumption led to a good fit of the observed Na\textsc{i} absorption features (Fig. 13). We obtained a column density in the main component of log(Na\textsc{i}) = 15.0 $\pm$ 0.3 with a large fitting uncertainty due to the line being much narrower than the resolution element. We note that the value is very dependent on the exact normalisation and that the first ionisation potential of sodium (5.14 eV) is even lower than that of magnesium (7.65 eV), meaning that Na\textsc{i} may arise from deeper regions in the cloud. This means that Na\textsc{i} column densities should be considered with great caution until a high resolution infra-red spectrum is obtained. Using the empirical correlation observed in the Milky Way between Na\textsc{i} equivalent width and $E(B-V)$ from Poznanski et al. (2012), we expect $A_V \sim 0.3$ for their implicitly assumed $R_V = 3.1$. This is consistent with the value obtained in Sect. 5.

3.9. Carbon monoxide

We detect CO absorption lines from ten bands, belonging to two systems: the $\Lambda^1\Pi(v'')-\chi'\Sigma^+(0)$ for $v'' = 0$ to 8 and the $d^3\Delta(5)-\chi'\Sigma^+(0)$ inter-band system, see Fig. 14. We also tentatively detect the $e^1\Sigma^-\chi'\Sigma^+$ system, although the lines remain too weak to be significant (Fig. 15). Rotational levels are unambiguously detected from $J = 0$ to $J = 3$. The $J = 4$ lines are at the noise level for most bands, but included in the fit. We used the updated molecular data summarised in Dap\`a et al. (2016). Accurate wavelengths were obtained through calibration by laser and VUV synchrotron studies (Salumbides et al. 2012; Niu et al. 2013, 2015), while oscillator strengths and damping

Fig. 8. Portion of X-shooter UVB spectrum (black) around the H\textsc{i} lines, with the best-fit synthetic spectrum for H\textsc{i} absorption (with $b = 1$ km s\textsuperscript{-1}) in red. Horizontal blue segments connect rotational levels (short tick marks) from a given Lyman (L) or Werner (W) band, as labelled above. H\textsc{i} Ly-β and Ly-γ from the DLA are indicated as red dashed profiles. The green profile corresponds to HD lines.
constants were carefully re-evaluated taking into account an updated perturbation analysis. We did not consider the v′ = 5 AX system, which was completely blended with the extended Si IV.1393 absorption. Similarly, a large region of the (2−0) absorption band is contaminated by unrelated absorption and ignored during the fitting. Finally, the (6−0) band is also partially blended with smooth absorption from the Ly α forest, but the latter was well modelled using a single component. We therefore included this band and left the intervening Ly α parameters free during the fitting process. The other CO bands are apparently free from blending. We tied together the Doppler parameter and redshift for the different rotational levels. We were therefore left with seven free parameters for CO: b, z and the column densities for the 5 detected rotational levels. We obtained a satisfactory fit with a global χ^2 = 1.1, shown as the red profile in Fig. 14, with z = 2.525467, b = 0.7 km s^{-1} and obtained a total CO column density of almost 10^{13} cm^{-2}, which is the highest value measured among high-z quasar absorption systems to date. We further tested the robustness of our measurement. The details of this analysis are shown in the appendix.

From the non-detection of $^{13}$CO lines, we also constrain the isotopic ratio $^{12}$CO/$^{13}$CO to be higher than 40, assuming the same Doppler parameter, redshift and excitation temperature for both molecules. This is comparable with values in the solar neighbourhood ($^{12}$CO/$^{13}$CO ∼ 70; Sheffer et al. 2007), meaning that a measurement of the CO isotopic ratio at high-z should be possible in the near future. This is particularly interesting since the isotopic ratio seems to be anticorrelated with N(CO) in the Galaxy, indicating $^{13}$CO enhancement through chemical fractionation in the denser and colder regions (e.g. Sonnentrucker et al. 2007).

4. Metallicity and dust depletion

4.1. Metallicity in the atomic and molecular gas

In this section, we briefly discuss the metallicity in the different phases. We denote the abundance of a species M relative to hydrogen as

$$[M/H] = \log(N(M)/N(H)) - \log(N(M)/N(H))_\odot,$$

where solar abundances are taken from the photospheric values of Asplund et al. (2009). H corresponds to the total hydrogen, that is, including both neutral (H) and molecular (H$_2$) forms. From our absorption line analysis, we infer...
We cannot measure the H I column density in individual components, we can expect that the metallicity in the cold component is at least as high as in the rest of the profile and obtain a more realistic lower limit. We assume

\[ [\text{Zn/H}]_c \geq [\text{Zn/H}]_{\text{overall}}, \]

where the index \( c \) stands for “cold”, that is, associated to the molecule-bearing gas. The molecular fraction in the cold component, \( f_c = 2N(H_2)/(2N(H_2) + N(HI)) \), can then be expressed as

\[ f_c \geq f \frac{N(\text{Zn II})_{\text{overall}}}{N(\text{H II})_c} = 0.54. \]

Conversely, if we assume that the cold component is fully molecular (i.e. \( f_c = 1 \)), we get an upper-limit to the metallicity in that component, \([\text{Zn/H}]_c < 0.7 \pm 0.5\), while the lower-limit to the metallicity in the warm gas is \([\text{Zn/H}]_w > -0.2\) (see Sect. 3.2).

Because chlorine is associated to the H₂-bearing gas, its abundance can also be used to constrain the metallicity of the latter using the relation from Balashev et al. (2015)

\[ [\text{Cl/H}] = [\text{Cl/H}_2] + \log f, \]

where

\[ [\text{Cl/H}_2] = \log \left( \frac{N(\text{Cl})}{2N(H_2)} \right) - \log \left( \frac{\text{Cl}}{\text{H}} \right)_\odot. \]

We measured \([\text{Cl/H}_2] \sim 0.4 \pm 0.3\) using the fit with fixed Doppler parameter for the main component. The lower limit to the molecular fraction \( f > 0.46\) (see Sect. 3.4) then implies \([\text{Cl/H}] > 0.05 \pm 0.3\) in the cold component. This is a conservative limit on the metallicity since several studies have argued for some depletion of chlorine, by about a factor of two (e.g. Mooney et al. 2012, and references therein). The abundance of chlorine is therefore consistent with the super-solar metallicity derived from zinc and phosphorus, assuming an intrinsic solar ratio. We also note that assuming a uniform metallicity across the different components implies that about 95% of H₂ resides in the main component.

### 4.2. Dust abundance from depletion of refractory elements

Ledoux et al. (2003) have revealed the existence of a relation between the presence of molecular hydrogen and both the overall metallicity (see also Petitjean et al. 2006) and the observed depletion factors in DLAs, that is, the probability to detect H₂ is higher when the relative abundances of metals (or dust) are high. Noterdaeme et al. (2008) further show that the column density of H₂ is strongly related to that of dust, quantified by the column density of iron missing from the gas phase \((N(\text{Fe}_{\text{dust}}))\), Vladilo et al. 2006). However, the metallicity and depletion factors are only indicative of the average values over the whole absorption path probed by the DLA while the \(N(\text{Fe}_{\text{dust}}))\) corresponds to an integrated value. Indeed, metals probe gas over a wide range of physical conditions, making it generally difficult
to associate a given metal component to a molecular one. Still, it has been possible to show that abundance ratios along the velocity profiles tend to show an enhanced depletion factor at the velocity where H$_2$ is detected (Rodríguez et al. 2006).

The system towards J0000+0048 presents an excellent opportunity to study this further, since the metal profile presents a well defined narrow component corresponding to the molecular gas. Figure 17 presents the observed depletion factors (Si, Ni and Fe relative to Zn) component by component. The three patterns follow well each other, indicating that the abundance ratios are mainly dictated by depletion onto dust grains, rather than differential nucleosynthesis. As expected, the cold narrow component presents a high level of dust depletion, indicating that this component has a high relative amount of dust. However, a dusty component does not necessarily have a high integrated column density of dust, which will be more naturally related to the column density (and hence detectability) of molecular species. We therefore computed the column density of iron locked into dust grains component by component. The cold, molecule-rich component becomes clearly visible and likely responsible for most of the extinction of the background quasar (see next section). We also notice a secondary peak at $v = -40$ km s$^{-1}$. Interestingly, this corresponds to the location of a neutral chlorine component, which also likely harbours H$_2$ molecules, though with a lower column density. This suggests that neutral chlorine could be directly used as a “high-resolution” tracer of dust within a DLA.
in the data reduction. We included photometry in the K-band from the UKIRT Infrared Deep Sky Survey (UKIDSS) and in band 1 from the Wide-Field Infrared Survey Explorer (WISE). We were not able to include the redder bands from WISE, since the quasar template at this redshift only covers part of band 2 at 4.6 μm. We observed an offset between the UKIDSS photometry and the SDSS and iWISE photometry. This is most plausibly due to variability of the quasar between the different epochs of observation. In order to correct for this offset, we scaled the spectrum to the z-band of the SDSS photometry and subsequently scaled the four UKIDSS bands to match the synthetic photometry calculated from the scaled spectrum.

The template of Selsing et al. was then smoothed with a Gaussian kernel (σ = 7 pixels) to prevent the noise in the template to falsely fit noise peaks in the real data. In order to take into account the uncertainty in the template, we convolved the errors on the spectrum with the uncertainty estimate from the template.

We then fitted the template to the data using 9 free parameters: 7 parameters to describe the extinction curve shape, a freely varying amount of dust, A_V, and an arbitrary scale since we do not know the intrinsic brightness prior to reddening.

5.1. Parametrisation of the extinction law

We used a slightly modified version of the formalism from Fitzpatrick & Massa (2007, hereafter, FM2007):

\[
k(\lambda - V) = E(\lambda - V)/E(B - V) = c_1 + c_2 x + c_3 D,
\]

where

\[
D = \left(\frac{x^2}{(x^2 - x_0^2)^2 + x^2 \gamma^2}\right)^{1/3}
\]

and x = λ_0 refers to inverse wavelength in units of μm⁻¹ at the absorber rest-frame. This corresponds to a linear component for the whole UV range (defined by c_1 and c_2) plus a 2175 Å bump, parametrised by c_3, x_0 and \gamma. FM2007 also consider a far-UV curvature component parametrised by c_4 at wavelengths shorter than c_5 (their Eq. (2)). We did not consider this component here (i.e., we set c_4 = 0) because we did not have enough data in the FUV. Moreover, the quasar template is more uncertain at very short wavelengths. In addition, preliminary fits to the data indicated that c_4 was poorly constrained and fully consistent with 0. We therefore excluded this parameter in the following analysis to simplify the fit without loss of generality.

In the infrared (IR), we used the power-law prescription of FM2007 assuming the correlation between k_IR and R_V, thus yielding an extinction curve of the form (Eq. (7) of FM2007):

\[
k(\lambda - V) = (-0.83 + 0.63 \times R_V) \times x^{1.84} - R_V.
\]

Since this part of the extinction curve is beyond the spectral coverage, we chose to reduce the two original IR parameters by including the correlation between k_IR and R_V. We used a spline interpolation as in FM2007, in the optical range using one anchor point in the optical to ensure a correct normalisation in the V-band. In order to obtain a smooth and continuous transition between the various parts, we included two anchor points in the UV and two in the IR. We used the UV points U_1 and U_2 as defined in FM2007 at 2600 and 2700 Å, respectively. In the IR, we anchored the spline at 0.75 and 1.0 μm⁻¹ (similar to the I_4 and I_5 points of FM2007).
Finally, we converted the extinction curve from the original formulation in terms of $E(\lambda - V)$ to use $A_V$:

$$A_V/A_I = \frac{1}{R_V} E(\lambda - V)/E(B - V) + 1.$$  \hfill (11)

5.2. Fitting the extinction

We fitted the parameters using a Markov chain Monte Carlo approach as implemented in the python package emcee (Foreman-Mackey et al. 2013). This way we were able to include priors and parameter boundaries in a straightforward way. The shape parameters for the 2175 Å bump, $x_0$ and $\gamma$, were given quite strong priors, since these parameters are generally observed to be very well behaved in many different environments (Fitzpatrick & Massa 1990; Gordon et al. 2003). As priors on the two parameters, we used the average values from Gordon et al. (2003), $x_0 = 4.57\pm0.01$ and $\gamma = 0.94\pm0.02$.

In order to give the photometry a more appropriate weight compared to the densely sampled spectral data, we calculated an effective number of pixels per filter. We calculated this quantity by integrating the filter transmission curves scaled to a maximum of 1, and interpolated onto a grid with the same sampling as the spectral data. This way, “pixels” with high transmission are weighted more than “pixels” with low transmission. The uncertainty for each filter was then divided by the square of this number.

The chain was initiated with 100 walkers located at initial locations around the best-fit from a quick χ² minimisation. We then ran the chain for 1200 iterations and discarded the first 600 as burn-in. From the posterior distributions we obtained the best-fit parameters stated in Table 7. We furthermore provide the inferred $A_{\text{bump}}$, which measures the strength of the 2175 Å bump. This quantity is defined in the following way:

$$A_{\text{bump}} = \frac{\pi c_3}{(2yR_V)} \times A_V.$$  

The best solution is shown in Fig. 18 where the reddened template is plotted on top of the spectral and photometric data. In Fig. 19, we show the inferred extinction curve. For comparison, we also show the average extinction curves towards the Small Magellanic Cloud (SMC) and Large Magellanic Cloud supershell (LMC2) from Gordon et al. (2003) as well as a Milky-Way extinction curve for the $R_V$ measured towards the B-type star ζ Per by Cardelli et al. (1989).

The uncertainty quoted on the $A_V$ from the best fit only includes the formal statistical error. This error is not fully representative as it does not take into account the intrinsic variations of the UV slope of the quasar. The slope of the quasar might vary with respect to the used template spectrum, which would lead us to infer a wrong amount of extinction. We have estimated this systematic effect on our best-fit $A_V$ by varying the slope of the used quasar template, by multiplying the template with a power-law normalised at 5500 Å. We note that this approach is only a rough approximation since the quasar shape is poorly described by a single power-law at all wavelengths. However, from about 1200 Å to 1 μm in the quasar rest-frame, this is a reasonable approximation. For each variation in the intrinsic slope, we fitted the data again. In this fitting procedure, we kept the extinction curve parameters fixed, since varying the intrinsic slope and $R_V$ simultaneously leads to a completely degenerate fit with non-physical fit parameters.

For a shallower slope (by +0.2 dex), we obtained a best-fit $A_V$ of 0.12 mag. Conversely, for a steeper slope (smaller by −0.2 dex), we recovered a larger best-fit value of $A_V = 0.34$ mag. This change in slope is consistent with the average spread of intrinsic slopes observed in the literature (Vanden Berk et al. 2001; Krawczyk et al. 2015). Although the different slopes provide acceptable fits to the data, the best fit is obtained with the original quasar template.

As mentioned above, changing the slope of the template will inevitably change the slope of the recovered extinction curve. Although we cannot fit these two quantities together, we can require the fit to reproduce a value of $R_V$ consistent with an average Milky Way sight-line ($R_V = 3.1$), which is obtained for a change in slope of +0.04 dex, which in return yields a best-fit $A_V$ of 0.17 mag.

6. Modelling of the physical conditions in the cold cloud

In this section, we aim at understanding the structure of the cold gas by modelling the physical conditions using the version c13 of the spectral simulation code Cloudy (last described in Ferland et al. 2013). This code performs a self-consistent calculation of the thermal, ionisation and chemical balance of both the gas and dust exposed to a radiation source, with a full treatment of H₂ introduced by Shaw et al. (2005). The cloud was assumed to be old enough for all physical processes to be in steady state.

6.1. Geometry and turbulence

We considered a plane-parallel geometry with radiation illuminating both surfaces of the cloud. Such geometry has been successfully used to reproduce the physical conditions in typical interstellar clouds (e.g. van Dishoeck & Black 1986). We considered constant density models and stopped the calculation when reaching the observed H₂ column density (instead of N(H1)) whose measurement encompasses the whole profile). While H₂ is also likely present in more than one component, most of it should be found in the main cold component in which CO is also found. We considered a turbulent broadening of 0.7 km s⁻¹, as derived from the Doppler parameter of heavy elements, see Fig. 16. This is mostly important for its effect on the CO self-shielding with a negligible effect on H₂ due to the strong damping wings.

6.2. Incident radiation field and cosmic rays

The Haardt-Madau ionising UV background from both galaxies and quasar (see Haardt & Madau 2012) was included at the absorber’s redshift, and so was the CMB radiation. We also considered the presence of a local source of UV radiation by adding a blackbody radiation with a temperature of $T = 40{,}000$ K, to simulate the presence of hot stars. We parametrised the intensity
Fig. 18. Combined 1D X-shooter spectrum of J0000+0048 in black. The data has been replaced by the continuum over the Ly α forest. The yellow squares indicate the photometry in $u$, $g$, $r$, $i$, $z$, $Y$, $J$, $H$, $K$, and $W1$ bands (left to right). The uncertainty on the photometry is smaller than the extent of the square marker. The blue line shows the unreddened, smoothed template by Selsing et al. (2016), and the red line indicates the same template reddened by the best-fit extinction curve by an amount of $A_V = 0.23$. The red shaded area marks the strength of the 2175 Å bump. The upper edge of the shaded region corresponds to an extinction curve with no 2175 Å bump.

Fig. 19. Extinction curve as function of inverse wavelength at the rest-frame of the DLA normalised to the $V$-band extinction $A_V$. The grey line shows the full X-shooter spectrum divided by the template of Selsing et al. (2016). The black regions indicate the wavelength regions used in the fit, and the two black squares indicated the photometry in the $K$ and $W1$ bands. The red, solid line shows the best fit extinction curve, a clear 2175 Å bump is observed in the data. For comparison, the extinction curves from Gordon et al. (2003) are shown as solid blue (SMC), and grey dotted (LMC2) lines. The dashed line corresponds to a Milky-Way extinction law with the single parameter, $K_0$, corresponding to ζPer (Cardelli et al. 1989). A full derivation of the extinction curve towards this star is not available.

of this blackbody radiation by $\chi$, the ratio of the assumed incident blackbody radiation to the Habing (1968) field (compared in the range 0.44 to 1 Ryd). Since we aimed at understanding primarily the conditions in the cold cloud, we took into account the attenuation of the incident radiation after it went through neutral gas, removing photons between 1 to 4 Ryd. Cosmic rays were also included as they play a major role inside molecular regions, becoming the main source of ionisation and impacting the ion-molecule chemistry in the cold gas. Indeed, the cosmic ray ionisation rate, $\zeta_{\text{H}}$, is generally deduced from the abundance of chemical ions in our own Galaxy, where it is also found to vary by a large amount between different regions (e.g. Federman et al. 1996). We note however that this remains an active area of research, with more recent studies pointing towards an average Galactic value one order of magnitude higher than previously found (see e.g. Indriolo et al. 2007).

6.3. Abundances

We set the metal abundances to 2.5 times solar, as derived from the abundance of undepleted zinc, and assumed intrinsic solar ratio for all species. We applied the observed depletion factor for iron and silicon, which were observed in their dominant ionisation stages. Since we had no measurement of the total abundance of other species, we applied the default depletion values for the cold medium in the Galactic disc as compiled in Table 7.7 of the Hazy1 documentation of Cloudy.

6.4. Model with standard Galactic grains

As a first test, we started modelling the cloud using a canonical Milky-Way ISM dust grain mixture, with an abundance scaled to the metallicity, that is, we set the dust grain abundance 2.5 times the Galactic ISM value. Instead of running large grids of parameters, we varied the main input parameters individually and studied their effect on the predicted column densities. These parameters were: total hydrogen volumic density ($n_H$), strength of UV field ($\chi$) and cosmic ray ionisation rate $\zeta_{\text{H}}$. 

P. Noterdaeme et al.: A Perseus-like molecular cloud at $z_{\text{abs}} = 2.5$ towards J0000+0048
The initial density was mostly determined by matching the observed relative population of the C1 fine structure level with the computed ionisation, chemical and thermal balance. We note that the density of different colliders is calculated self-consistently across the cloud. We found that densities in the range 40–100 cm$^{-3}$ predict C1 ratios consistent with the ones observed. In turn, the CO/C1 ratio was strongly under-predicted by a factor of about 30. This issue has also been raised by Sonnentrucker et al. (2007), who note that most published models of translucent clouds predict less CO than observed for a given $N$(H$_2$). We found that decreasing $\chi$ did not help (as similarly concluded by Bensch 2006, when modelling the emission from the dark cloud Barnard 5 in the Perseus complex). Shaw et al. (2008) show that the CO column density increases almost linearly with $\xi_{\text{H}}$; however, increasing $N$(CO) this way led to a strong overproduction of C1 in our modelling. We therefore had to re-evaluate our initial assumptions but found that varying other parameters such as the shape of the incident UV field or the geometry of the cloud did not help either.

### 6.5. Model with small dust grains

Interestingly, the abundances of most molecular and neutral species observed at $z_{\text{abs}} = 2.5$ towards J0000+0048 are very similar to those observed in the Perseus cloud along $\zeta$Per, which has successfully been modelled by Shaw et al. (2008). These authors use a higher number of small grains compared to a standard mixture to approximate the observed $R_V$ and $E(B-V)$. The $\zeta$Per extinction curve is also quite similar to that observed towards J0000+0048, although the latter has a steeper UV slope, probably indicating a smaller average grain size. Small grains seems indeed to be a key ingredient to increase the column density of CO with respect to that of carbon and molecular hydrogen. In other words, a higher total surface of grains favours CO production without going too deep into the cloud. Shaw et al. (2008) also highlight the need of increased grain surface area to reproduce the CO column density towards SDSSJ1439+1117 (Srianand et al. 2008).

We therefore moved to a second series of models, using a dust grains size distribution containing more small grains. Typically, the distribution for each grain type (graphite and silicates) is parametrised as a single power law with the form $dn/da \propto a^{-n}$, where $n$ is the number of grains with radius in the range $[a, a + da]$. Nozawa & Fukugita (2013) have shown that a graphite-silicate model can reproduce well the range of extinction curves seen in the Milky-Way and Small Magellanic Cloud with a remarkably constant power law index $q \approx 3.5 \pm 0.2$, with a cut-off at small ($a_{\text{min}} \approx 0.05$ $\mu$m) and large ($a_{\text{max}} \approx 0.2$–0.3 $\mu$m) grain radii. These authors note that they could not determine well the small grain cutoff due to lack of data at short wavelengths, but that these have little effect on other parameters anyway. We therefore fixed $q = 3.5$ and found that a silicate-graphite mixture with a silicate-graphite ratio increased by 40% compared to canonical ISM mixture, together with $a_{\text{min}} = 0.001$ $\mu$m and $a_{\text{max}} = 0.15$ $\mu$m for both grain types, reproduced well the extinction curve derived in Sect. 5. In addition, we verified that the abundances of different metals locked into the grains were consistent with the observed metallicity for the assumed depletion pattern to within 0.1 dex, or better.

Using the small-grains model, we were able to reproduce most of the column densities to within 0.4 dex or better for most neutral, ionised, and molecular species, see Table 9, for $\chi = 0.5$ and $\xi_{\text{H}} = 2.5 \times 10^{-15}$ s$^{-1}$ (Table 8). The column density of Mg I remains however over-predicted by about 0.8 and the high rotational levels of H$_2$ are under-predicted. It is likely that the actual depletion of magnesium is much higher than assumed here (see De Cia et al. 2016). Indeed, for the high volumic density and molecular fraction estimated here, we can expect an order of magnitude stronger depletion of magnesium (see Jensen & Snow 2007), in which case the model perfectly matches the observations. Finally, most of the column density in the high-$J$ levels of H$_2$ could arise mostly from an additional warmer component, which is not modelled here. We also note that the predicted visual extinction ($A_V \approx 0.7$) is higher than what we derived through SED fitting or seen towards $\zeta$Per, but within a reasonable factor, given the uncertainties on the measurement and on the intrinsic quasar brightness.

In conclusion, it is remarkable that our model reproduces fairly well the observed quantities with the small number of parameters considered. Further fine-tuning of the parameters could still be performed, and other parameters previously fixed could be varied. For example, a harder UV flux, with black-body temperature of $T \sim 60\,000$ K increases the CO column density by about 0.07 dex (hence a better agreement) while changing little the other predicted values. However, such fine-tuning is not the purpose of this paper, given the other uncertainties (in particular on the metallicity) and assumptions involved. We also remind that the true geometry of the cloud and its density profile is likely more complex than assumed. Lastly, we note that the chemistry of CO is an evolving research field. At the low densities of the ISM, CO can be formed through different paths and sequences of reaction. For example, radiative association between C$^+$ and H$_2$ (or with a much lower efficiency with H$^+$) leads to C$+$, which then reacts with O to produce CO. Several chemistry networks (such as hydrogen-oxygen) are initiated by cosmic rays, hence their importance in controlling the production of CO. However, as discussed by Goldsmith (2013), other physical phenomena such as shock heating (Elitzur & Watson 1978) or Alfvén waves (e.g. Federman et al. 1996; Visser et al. 2009) can also raise the temperature of the gas, leading to an increase of CO abundance. Finally, dissipation of energy from supersonic turbulence can deeply modify the chemistry of the gas (Goddard et al. 2009).

### Table 8. Cloudy input parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_H$</td>
<td>80 cm$^{-3}$</td>
</tr>
<tr>
<td>$\xi_{\text{H}}$</td>
<td>$2.5 \times 10^{-15}$ s$^{-1}$</td>
</tr>
<tr>
<td>$\chi$</td>
<td>0.5</td>
</tr>
<tr>
<td>turbulence</td>
<td>0.7 km s$^{-1}$</td>
</tr>
<tr>
<td>Metallicity$^a$</td>
<td>2.5 $Z_\odot$</td>
</tr>
<tr>
<td>log (C/H)</td>
<td>$-3.57$</td>
</tr>
<tr>
<td>log (O/H)</td>
<td>$-3.13$</td>
</tr>
<tr>
<td>log (Na/H)</td>
<td>$-6.06$</td>
</tr>
<tr>
<td>log (Mg/H)</td>
<td>$-4.70$</td>
</tr>
<tr>
<td>log (Si/H)</td>
<td>$-5.49$</td>
</tr>
<tr>
<td>log (Cl/H)</td>
<td>$-6.50$</td>
</tr>
<tr>
<td>log (Fe/H)</td>
<td>$-6.50$</td>
</tr>
<tr>
<td>log (Ni/H)</td>
<td>$-7.38$</td>
</tr>
</tbody>
</table>

Notes. $^a$ Abundance for all species except those listed below. The gas-phase abundance for the listed depleted species correspond to the same intrinsic metallicity after applying the depletion factors described in the text.
Table 9. Comparison of observed and predicted values in the cold component.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Observed value</th>
<th>Model prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>H I</td>
<td>&lt;20.9</td>
<td>20.7</td>
</tr>
<tr>
<td>CO</td>
<td>14.95 ± 0.05</td>
<td>14.72</td>
</tr>
<tr>
<td>C I</td>
<td>16.22 ± 0.07</td>
<td>16.40</td>
</tr>
<tr>
<td>C I, J = 0</td>
<td>16.10 ± 0.08</td>
<td>16.19</td>
</tr>
<tr>
<td>C I, J = 1</td>
<td>15.54 ± 0.14</td>
<td>15.93</td>
</tr>
<tr>
<td>C I, J = 2</td>
<td>14.67 ± 0.11</td>
<td>15.04</td>
</tr>
<tr>
<td>Si I</td>
<td>14.85 ± 0.18</td>
<td>14.53</td>
</tr>
<tr>
<td>Cl I</td>
<td>14.63 ± 0.29</td>
<td>14.50</td>
</tr>
<tr>
<td>Mg I</td>
<td>14.10 ± 0.10</td>
<td>14.92</td>
</tr>
<tr>
<td>Na I</td>
<td>15.00 ± 0.30</td>
<td>14.51</td>
</tr>
<tr>
<td>T01 (K)</td>
<td>51 ± 2</td>
<td>56</td>
</tr>
</tbody>
</table>

Notes. (a) Except for T01, all quantities correspond to column densities expressed in log (cm⁻²). (b) See text for the apparently strong mismatch between model and observations.

6.6. Characteristics of the cloud

The top panel of Fig. 20 shows the abundances of neutral atomic hydrogen, molecular hydrogen, neutral chlorine and carbon monoxide relative to the total amount of hydrogen as a function of the depth into the cloud. Only half of the profile is shown, the other half being symmetric with the assumed geometry. We find a total cloud size to be about 4 pc along the line of sight. The line of sight passes quickly through a sharp H I-to-H₂ transition, which is very well traced by neutral chlorine and after which the H₂ molecular fraction stays constant at about 50%. This incomplete conversion is due to destruction of H₂ in the cloud centre, inside the self-shielding layer (see also Liszt 2015).

The abundance of CO starts to be significant immediately after the H I-to-H₂ transition. Indeed the chemical networks leading to the formation of CO with H₂ as starting point are much more efficient than those starting with atomic hydrogen (see Goldsmith 2013). In addition, H₂ participates in the shielding of CO, through a few but important overlaps with FUV CO electronic bands (e.g. Glassgold et al. 1985; van Dishoeck & Black 1988; Bensch 2006; Visser et al. 2009). The abundance of C I does not vary much inside the molecular cloud, and does not directly follow H₂ nor CO. This is due to the abundance of C I being mostly determined by the ionisation and recombination balance. In addition, neutral carbon does not benefit from H₂ shielding nor participate directly in the molecules chemistry (which rather involve C⁺). The fact that C I is considered a tracer for H₂ is therefore more indirect: C I probes the conditions that favour the presence of H₂, without locally following the latter within layers of a given molecular cloud.

The temperature (central panel) varies slowly between ~70–80 K and 48 K towards the center of the cloud, in agreement with the average temperature measured from the column densities in the first H₂ rotational levels. Indeed, we predict T₀₁ ~ 56 K, very close to the measured value. Photoelectric effect on dust grains is the main heating source in the external layers on the cloud while cosmic rays become the main heating source in the cloud center. Heating by H₂ photo-dissociation contributes for a small fraction to the total heating and naturally decreases after the H I-to-H₂ transition. Cooling is in turn largely dominated by [C II]157 μm emission. The model predicts log N(C II) = 15.64. Unfortunately, we cannot test this prediction since the measurement is affected by a large uncertainty.

7. Temperature of the cosmic microwave background at z = 2.53

Srianand et al. (2008) and Noterdaeme et al. (2011) have shown that the excitation of CO at high redshift is largely dominated by the CMB radiation, that is, that other excitation processes such as collision are negligible, in which case T_C (CO) = T_CMB. More recently, Sobolev et al. (2015) estimate a correction to apply if we do take into account collisional excitation with hydrogen atoms and H₂ molecules. The correction depends almost linearly on the total volumic density and on the kinetic temperature. In addition, since the main collision partner is H₂, the correction increases with the molecular fraction. Using f = 0.5, T = 50 K and n_H₂ = 80 cm⁻³, their Eq. (7) implies an excess temperature of ΔT = 0.3 K. Applying this correction to the observed CO excitation temperature towards J0000+0048 (T_C (CO) = 9.3 ± 0.6 K; see Fig. 21) we obtained T_CMB (z = 2.53) = 9.6 ± 0.6 K in excellent agreement with the expected CMB temperature in the standard hot Big-Bang theory (T_CMB = T_0 (1 + z) = 9.61 K). Using the statistical equilibrium radiative transfer code RADEX A82, page 17 of 24
Our Cloudy model predicts $T_{\text{ex}}(\text{CO}) = 10$ K when the expected CMB radiation field at $z = 2.53$ is included, in agreement with the observed temperature. To test further the effect of the CMB radiation, we ran a model setting the CMB background temperature to the value measured at $z = 0$ instead ($T_0 = 2.726$ K, Fixsen 2009), while keeping all other parameters the same as previously. This model predicts a CO excitation temperature of 3.8 K, that is derived from the predicted population of the first three rotational levels since higher rotational levels do not follow the Boltzmann distribution anymore. The predicted temperature would then be similar to that seen in diffuse Galactic environments (Burgh et al. 2007) but about 10σ away from the measured value towards J0000+0048. We note that the difference between CMB temperature and CO excitation temperature tends to vanish at high redshift, where excitation by CMB becomes strongly dominant over collisional excitation.

Our result suggests ways to improve the constraints on the evolution of the CMB temperature at high redshift. From the distribution of the CO rotational levels alone, any departure from the Boltzmann distribution will be due to non-CMB (presumably collisional) processes. This means that a measurement remains uncertain achievable with future high resolution spectographs on extremely large telescopes. This will therefore need to be carefully evaluated.

Cyanogen (CN) is known to be an even better thermometer of the CMB temperature, with negligible contribution from collisions. Very accurate measurements have been performed using absorption spectroscopy towards nearby stars, including observations towards ζ Per (e.g. Roth & Meyer 1995; Ritchey et al. 2011). The similarity with our line of sight provides a good hope that CN lines will also be detectable in systems like J0000+0048. Indeed, a strong correlation between $N(\text{CO})$ and $N(\text{CN})$ is observed in our Galaxy (e.g. Fig. 18 of Sonnentrucker et al. 2007), with $N(\text{CN})$ of a few times $10^{12}$ cm$^{-2}$ at the CO column density of our system. However, obtaining high S/N and resolution in the NIR where the CN $J 3875$ lines are redshifted is technically challenging. In the case of J0000+0048, the lines unfortunately fall in a region of low transmission due to water vapour in the atmosphere. This means that the search for similar molecular systems at high redshift (for example, $z \sim 2.5$–3.5 for the CN lines to be redshifted in the $H$-band) needs to be continued. The CMB contribution for such systems will also be higher and their constraint on the evolution of CMB temperature stronger.

8. Direct search for star-formation activity

Motivated by the similarity between this absorbing cloud and the local ISM, we searched for the emission associated with active star formation. The main indicator of star formation, available to us in the data at hand, is the nebular emission lines from the photo-ionised gas in the vicinity of young stars. The most prominent of these lines in the rest-frame UV and optical are the two principal Balmer lines ($\text{H}_\alpha$ and $\text{H}_\beta$) and the two doublets from singly and doubly ionised oxygen ($[\text{O} \text{II}] \lambda \lambda 3726, 3728$ and $[\text{O III}] \lambda \lambda 4959, 5007$), which at the redshift of the DLA fall in the NIR spectrum from X-shooter. Unfortunately the H$\alpha$ line falls in the last order of the NIR spectrum, which is corrupted by strong sky background. We therefore searched for emission from the DLA counterpart using the following lines: $\text{H}_\beta$, $[\text{O III}]$, and $[\text{O III}]$. However, we did not detect emission from any of the lines.

For each PA, we first subtracted the quasar trace in the 2D spectrum using a similar approach as described in Krogager et al. (2013) in order to search for the faint emission lines. In the following, we have combined the observations taken with a same position angle. We used an elliptical extraction aperture to search for the lines. In the spatial direction, we used a semi-minor axis of 400 km s$^{-1}$ around the expected location given from the redshift of the DLA. However, we observed no flux in any of the PAs. We derived the detection limits for the $[\text{O III}]$ line by adding 100 co-emission line profiles with various line fluxes (drawn randomly in log-space between $1 \times 10^{-18}$ and $1 \times 10^{-16}$ erg s$^{-1}$ cm$^{-2}$), line widths (drawn randomly between 50 and 350 km s$^{-1}$), and line strength ratio for the two transitions of the doublet (randomly drawn between 0.35 and 1.5; see Seaton & Osterbrock 1957). Each model line profile (assumed to be Gaussian) was convolved with the spatial broadening function, determined from the spatial profile of the quasar trace, to create a 2D line model. We subsequently added noise to the 2D line model according to the noise model from the 2D spectrum. For each realisation, we extracted the flux and noise within the elliptical aperture mentioned above. This resulted in a robust limit on the detectable flux within the aperture, given the fact that we do not know the intrinsic line width of the

Fig. 21. CO excitation diagram. The solid line gives the best fit to the rotational population using a Boltzmann distribution, with the associated uncertainty shown as dashed line.
depletion and extinction as well as the molecular content of this cloud. Our main findings are the following:

(1) The absorption system is characterised by super-solar metallicity (about 2.5 $Z_\odot$). Although the uncertainty on this value is large (by a factor of about 2–3), it is much higher than the metallicities seen in the overall population of H1-selected DLAs at this redshift (see e.g. Rafelski et al. 2012). The observed depletion of refractory elements is typical of cold gas in the Galactic disc and peaks at the location where molecular gas is found. Higher spectral resolution data would be desirable to constrain better the amount of metals in this very narrow component ($b \sim 0.7 \, \text{km} \, \text{s}^{-1}$).

(2) The DLA has a molecular fraction reaching almost 50% overall, being the largest value measured till now in a high-$z$ absorption system, for a total neutral hydrogen column density of log $N$(H) = 20.8. This corresponds to a neutral gas surface density of $\Sigma_{\text{HI}} \approx 5 \, M_\odot \, \text{pc}^{-2}$ and a molecular hydrogen surface density $\Sigma_{\text{H}_2} \approx 4.4 \, M_\odot \, \text{pc}^{-2}$. These surface densities are very similar to what is seen across the Perseus molecular cloud from high spatial resolution emission observations (Lee et al. 2012), despite the H1 and H2 surface densities being measured directly along a pencil beam line of sight in our study while derived from dust maps in the latter. This also shows that H1-to-H2 transition in our high-$z$ system is likely following the same physical processes as in our Galaxy.

(3) We further used the different molecular and atomic species to constrain the actual physical conditions in the cold gas with the help of the spectral synthesis code Cloudy. We found that the column densities can be well reproduced by a cloud with density around $n_1 \sim 80 \, \text{cm}^{-3}$ immersed into a moderate UV field, similar to the local interstellar radiation field. We showed that a high cosmic ray ionisation rate together with the presence of small dust grains – consistent with the depletion pattern, the steep extinction curve, and presence of a $2175 \, \text{Å}$ bump – can explain the high CO fractional abundance. The model also predicts a kinetic temperature around 40 K, in perfect agreement with that derived from the excitation of H2. The CO abundance rises immediately after the H1-to-H2 transition, thanks to the efficient chemistry paths involving H2, together with pre-shielding of CO. About half of the hydrogen remains in atomic form in the cloud interior, well inside the H1-to-H2 transition layer, due to H2 destruction by cosmic rays. This can also explain the high HD/2H2 ratio through chemical enhancement of HD compared to H2. We must however keep in mind that, in addition to cosmic rays, several other processes heating the gas can also enhance the production of CO (Goldsmith 2013) and that our model suffers from uncertainties in several input parameters, such as the metallicity. The detection of more molecular species in this system, together with comparison

<table>
<thead>
<tr>
<th>PA (deg)</th>
<th>$F([\text{O II}])$ $(10^{-17} , \text{erg} , \text{s}^{-1} , \text{cm}^{-2})$</th>
<th>SFR $(M_\odot , \text{yr}^{-1})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>&lt;4.0</td>
<td>&lt;22</td>
</tr>
<tr>
<td>−150</td>
<td>&lt;3.0</td>
<td>&lt;16</td>
</tr>
<tr>
<td>−60</td>
<td>&lt;3.8</td>
<td>&lt;21</td>
</tr>
<tr>
<td>+60</td>
<td>&lt;4.3</td>
<td>&lt;24</td>
</tr>
<tr>
<td>combined</td>
<td>&lt;1.9</td>
<td>&lt;9.9</td>
</tr>
</tbody>
</table>

9. Summary

In this work, we presented the detection and detailed analysis of an exceptional molecular absorber at $z_{\text{abs}} = 2.53$ towards the quasar J0000+0048, being one of the very few absorption systems featuring CO absorption lines known to date (see Noterdaeme et al. 2011, and references therein; Ma et al. 2015). Using both high resolution and multiwavelength spectroscopic observations, we derived the chemical composition, dust
of different codes (e.g. the Meudon PDR code, Le Petit et al. 2006) should break degeneracies between parameters such as dust abundance and cosmic ray rate and lead to a better understanding of the physical processes at play. Our study suggests that the presence of strong C1 lines, detectable at low spectral resolution (as in Ledoux et al. 2015), is a good indicator for high molecular hydrogen column density (in self-shielded regime), but this (or directly detecting damped H2 lines as in Balashev et al. 2014) is not a sufficient condition to get CO in detectable amounts. Since small grains seem to play a crucial role in the production of CO, selecting systems that, in addition to C1, also present a steep extinction curve and/or the presence of a 2175 Å bump should significantly increase the probability to detect CO.

(4) While our study shows that the line of sight towards J0000+0048 has chemical and physical characteristics similar to those found in diffuse molecular regions of the Perseus cloud, we have shown that the former absorbing cloud is immersed into a warmer cosmic microwave background radiation. We derived the temperature of the CMB radiation at the absorbing redshift from the excitation of CO lines, correcting for a small temperature excess due to collisional excitation. The temperature we obtained is in perfect agreement with the adiabatic cooling expected in the standard hot Big-Bang theory, $T_{\text{CMB}}(z) = T_0 \times (1+z)^{-0.14}$ is 9.6 K at $z = 2.53$.

Final remarks: the discovery presented here was facilitated by the discovery presented here was facilitated by the discovery presented here was facilitated by the SDSS web site is provided by the Alfred P. Sloan Foundation, the Participating Institutions, the French Participation Group, the German Participation Group, Brookhaven National Laboratory, Carnegie Mellon University, University of Florida, the French Participation Group, the German Participation Group, Harvard University, the Instituto de Astrofísica de Canarias, the Michigan State/Notre Dame/JINA Participation Group, Johns Hopkins University, Lawrence Berkeley National Laboratory, Max Planck Institute for Astrophysics, Max Planck Institute for Extraterrestrial Physics, New Mexico State University, New York University, Ohio State University, Pennsylvania State University, University of Portsmouth, Princeton University, the Spanish Participation Group, University of Tokyo, University of Utah, Vanderbilt University, University of Virginia, University of Washington, and Yale University.

References
Bouché, N., Murphy, M. T., Kacprzak, G. et al., 2013, Science, 341, 50
Appendix A: Robustness of the CO measurement

When estimating best-fit parameters, VPIT takes as input the normalised spectrum and the resolution provided by the user. This means that continuum placement uncertainties and errors due to the knowledge of the spectral point spread function (SPSF) are not reflected in the error estimates.

We tested the effect of SPSF uncertainties by refitting the data, using a range of spectral resolution from 4.75 to 5.25 km s\(^{-1}\). The resulting parameters remain well within their associated fitting uncertainty, with total column density varying by only ±0.05 dex, excitation temperature (see Fig. 21) varying by \(\Delta T_{\text{ex}} \sim 0.1\) K and Doppler parameter basically unchanged (\(<2\%\)). We also fitted the two red spectra simultaneously, instead of combining them (Fig. A.1). The results are also very close to what we get from the combined spectrum, as can be seen from the blue and red error bars in Fig. A.2, with a slight improvement in the \(\chi^2\) = 1.03 probably thanks to the better evaluated SPSF.

To estimate the effect of continuum placement uncertainties, we independently renormalised each region around CO absorption bands by randomly modifying the local continuum slope and intercept, following their respective normal error distribution. The distribution of CO column densities, Doppler parameter and excitation temperature obtained for hundred realisations of this “shaky” continuum procedure is shown in Fig. A.2. Clearly, the effect of continuum placement uncertainty is well within the error estimates from fitting the lines but highlights the correlation between \(b\), \(N\) and \(T_{\text{ex}}\). For example, a smaller Doppler parameter will result in a higher column density and a lower excitation temperature. It can also be seen from this figure that the most deviant points generally also have the highest \(\chi^2\)-values.
Fig. A.1. Voigt-profile fit to the CO absorption bands, labelled in blue in each panel. The left (resp. right) panels correspond to data taken with the 0.9″ (resp. 0.7″) slit. Rotational levels from $J = 0$ to $J = 3$ are indicated as green tick marks. The panel above each region shows the residual, with the blue line indicating the ±1σ interval, and the orange regions that used to constrain the fit.
Fig. A.2. Effect of continuum placement uncertainties on the total CO column density, excitation temperature and Doppler parameter. The histograms represent the distributions of log $N$(CO), $T_{\text{ex}}$(CO) and $b$ for 100 realisations where the continuum for each fitting region has been modified independently and randomly. The colour of each point indicates the reduced $\chi^2$ that varies from 1.08 (darkest) to 1.23 (lightest). The blue (resp. red) error bar corresponds to the best fit value using the combined UVES spectrum (resp. both UVES spectra fitted simultaneously).