The effect of Lyman $\alpha$ radiation on mini-Neptune atmospheres around M stars: application to GJ 436b

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ABSTRACT
Mini-Neptunes orbiting M stars are a growing population of known exoplanets. Some of them are located very close to their host star, receiving large amounts of UV radiation. Many M stars emit strong chromospheric emission in the H I Lyman $\alpha$ line (Ly$\alpha$) at 1215.67 Å, the brightest far-UV emission line. We show that the effect of incoming Ly$\alpha$ flux can significantly change the photochemistry of mini-Neptunes’ atmospheres. We use GJ 436b as an example, considering different metallicities for its atmospheric composition. For solar composition, H$_2$O-mixing ratios show the largest change because of Ly$\alpha$ radiation. H$_2$O absorbs most of this radiation, thereby shielding CH$_4$, whose dissociation is driven mainly by radiation at other far-UV wavelengths ($\sim 1300$ Å). H$_2$O photolysis also affects other species in the atmosphere, including H, H$_2$, CO$_2$, CO, OH and O. For an atmosphere with high metallicity, H$_2$O- and CO$_2$-mixing ratios show the biggest change, thereby shielding CH$_4$. Direct measurements of the UV flux of the host stars are important for understanding the photochemistry in exoplanets’ atmospheres. This is crucial, especially in the region between 1 and $10^{-6}$ bars, which is the part of the atmosphere that generates most of the observable spectral features.

Key words: planets and satellites: general - planets and satellites: atmospheres

1 INTRODUCTION
Recent exoplanet surveys have discovered the first planets with sizes between 2 Earth radii ($R_{\text{Earth}}$) and 3.5$R_{\text{Earth}}$, the size of Neptune. These planets, known as mini-Neptunes, revolve around the M stars GJ 436b (Butler et al. 2004), GJ 1214b (Charbonneau et al. 2009), Kepler 26b and Kepler 321 (Borucki et al. 2011) and GJ 3470b (Bonfils et al. 2012). Since mini-Neptunes around M stars are expected to be abundant (Laughlin et al. 2004) and M stars are the most common stars in the solar neighborhood (Chabrier 2003), we expect that many more mini-Neptunes will be discovered in the near future.

Since M stars have low effective temperatures, the bulk of their flux is emitted in the optical and near IR. Inactive M stars have very low-photospheric–UV-continuum emission when compared to solar-type stars. Direct observations of active M dwarfs show a high flux in the far-UV (FUV 912–1700 Å) (Shkolnik & Barman 2014), and the percentage of total UV flux from the star in the H I Lyman $\alpha$ line (Ly$\alpha$) is between 37 and 75 per cent compared to 0.04 per cent for the Sun (France et al. 2013). While most of the stellar Ly$\alpha$ radiation is scattered or absorbed in the interstellar medium, Ly$\alpha$ is the brightest FUV emission line in the stellar spectrum seen by an exoplanet (France et al. 2013) which makes this emission line critical for atmospheric photochemistry.

While the effect of extreme-UV irradiation (EUV 200–911 Å) was studied for Earth-like (Lammer et al. 2011) and giant planets (Yelle 2004; Lammer et al. 2003; Lecavelier des Etangs et al. 2004; Yelle 2006; Murray-Clay et al. 2009; Koskinen et al. 2010; Sanz-Forcada et al. 2011; Lecavelier des Etangs et al. 2012) and the consequence of high FUV M star irradiation was explored for habitable planets’ atmospheres (Scalo et al. 2007; Buccino et al. 2007; Segura et al. 2010), the effect of FUV irradiation and especially Ly$\alpha$ flux on hot mini-Neptune atmospheres has not yet been evaluated. Solar Ly$\alpha$ radiation is known to have a strong impact on the photochemistry of the planets in our Solar System, and the effects of stellar Ly$\alpha$ radiation on the photochemistry of hot extrasolar planets are expected to be important, but such effects have not yet been quantified. In particular, the effect of Lyman-$\alpha$ radiation on the thermal profile in...
2 MODEL DESCRIPTION

2.1 Stellar flux

GJ 436 is an M3 dwarf ($T_{\text{eff}} = 3416$ K) with a radius $R_* = 0.455 R_{\odot}$ (von Braun et al. 2012). Its coronal flux ($\log L_X = 27.16 \pm 0.34$) is smaller than the mean for M dwarfs ($\log L_X = 27.6$), indicating a low activity corona for GJ 436 (Poppenhaeger et al. 2010). The first reconstructed Ly$\alpha$ emission line profile performed for GJ 436 was based on (HST/STIS) observations (Ehrenreich et al. 2011). Here we use the most recent UV spectral observation of GJ 436 from 1150 to 3140 Å (France et al. 2013), including the reconstructed Ly$\alpha$ emission line profile, which is 1750 ergs cm$^{-2}$ s$^{-1}$ at 0.03AU (France et al. 2013). The temperature structure of the exoplanet atmosphere is not known for most hot extrasolar planets, and different values lead to differences in the upper atmosphere-mixing ratios (Visscher & Moses 2011; Miguel & Kaltenegger 2014). Other important species like HCN and C$_2$H$_2$ are beyond the scope of this work and will be included in a future study. To characterize vertical-mixing processes in the atmosphere, we use a constant-eddy diffusion coefficient. Although this coefficient is difficult to constrain, results derived from comparisons between 1D and 3D models for HD 209458b show that the eddy-diffusion coefficient has values between $K_{ZZ} = 10^8$ and $K_{ZZ} = 10^{12}$ cm$^2$ s$^{-1}$ (Parmentier et al. 2013). Following these results, we adopt an intermediate value of $K_{ZZ} = 10^9$ cm$^2$ s$^{-1}$ in our calculations. Note that this value is not known for most hot extrasolar planets, and different values lead to differences in the upper atmosphere-mixing ratios (Visscher & Moses 2011; Miguel & Kaltenegger 2014). An exploration of extreme cases was performed by Miguel & Kaltenegger (2014) who showed that dissociation becomes less efficient as vertical mixing becomes stronger in the atmosphere which affects the atmospheric abundances and the effect of Ly$\alpha$ radiation in the atmosphere.

We obtained the temperature and pressure profiles from a radiative atmosphere model developed by for highly irradiated exoplanets by Guillot (2010) who found global mean thermal profiles comparable to detailed-atmospheric model calculations. The temperature structure of the exoplanet atmosphere as a function of the mean optical depth for thermal radiation ($\tau$) is given by equation 1 (Guillot 2010):

$$
\text{1 http://cos.colorado.edu/kevinf/muscles.html}
\text{2 www.uv-vis-spectral-atlas-mainz.org}
$$
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We use $\gamma = 0.05$ which provides a good match to the thermal structures retrieved from observations of GJ 436b [Stevenson et al. 2010; Madhusudhan & Seager 2011; Moses et al. 2013] and GCMs models [Lewis et al. 2010]. The planet’s internal temperature ($T_{\text{int}}$) is usually adopted as 50 K for old mini-Neptunes [e.g. Miller-Ricci & Fortney 2010], but GJ 436b has a high eccentricity [e=0.146 von Braun et al. 2012] which implies a potentially tidally heated exoplanet [Agundez et al. 2014]. We therefore adopt
Photodissociation of atmospheric molecules occurs mostly in the upper atmosphere. This process is typically a one-way reaction which means that the probability of recombination and subsequent photon emission is negligible, thereby maintaining chemical disequilibrium in this region of the atmosphere.

All major species in mini-Neptune atmospheres considered in our model have a dissociation energy corresponding to wavelengths shorter than 2800 Å — H₂O (dissociation energy 5.17 eV, equivalent to 2398 Å), CO₂ (5.52 eV or 2247 Å), CH₄ (4.55 eV or 2722 Å), H₂ (4.52 eV or 2743 Å) and CO (11.14 eV or 1113 Å). Therefore, UV radiation dominates the photochemistry in mini-Neptune atmospheres.

Fig. 3 shows the absorption cross sections as a function of wavelength for the most abundant molecules in the mini-Neptune atmospheres considered in this paper: H₂ (green) (Backx et al. 1979), H₂O (black) (Mota et al. 2004), CO (brown) (Sun & Weissler 1953), CH₄ (blue) (Lee et al. 2000), CH₃O (red) (Hueslett & Berkowitz 2014; Venot et al. 2013). Fig. 3(a) shows the region between 1200 and 2100 Å, and a larger region (between 200 and 2100 Å) is shown in Fig. 3(b).

Fig. 3 shows that H₂O and CH₄ have higher cross sections between 1000 and 1400 Å and are especially susceptible to Lyα radiation from the host M star. Because of its short wavelength for dissociation, CO does not dissociate in response to FUV radiation, but has two peaks at 1332 and 1474 Å corresponding to the excitation of the various excited states of the molecule. CO₂ is a strong absorber at short wavelengths (λ < 1200 Å, maximum at 900 Å), but CO₂ does not have a high cross section in the FUV. Even though H₂ has a small cross section in the FUV, it becomes a strong absorber at short wavelength (λ < 1200 Å) in exoplanet atmospheres because of its high abundance. Thus H₂ shields other molecules from very shortwave radiation.

EUV radiation is not included here because it is absorbed in the upper atmosphere and does not reach pressures in the range described in this paper. Note that the fate of Lyα photons as they travel through the extended H-rich thermosphere is not yet clear as this radiation could be significantly scattered by H in the planet’s extended thermosphere (Lavvas et al. 2011; Koskinen et al. 2010) (see Section 5.2). A more detailed model of the extended upper at-
mosphere and atmospheric escape is beyond the scope of this paper.

Observations of GJ 436b’s atmosphere indicate a CO-rich and CH$_4$-poor atmosphere (Stevenson et al. 2013; Madhusudhan & Seager 2011; Knutson et al. 2014). This composition can be explained by adopting high metallicities, between 230 to 2000 x solar (Moses et al. 2013). We therefore explore the effect of high FUV, and especially Ly$\alpha$, flux on mini-Neptune atmospheres, for solar (Section 3.1.1) and high metallicity (Section 3.1.2) atmospheric composition.

3.1 Effect of high Ly$\alpha$ flux

3.1.1 Atmospheres with solar metallicities

In Fig. 4(a) we show how the photolysis rates of the molecules most susceptible to dissociation by Ly$\alpha$ flux (H$_2$O, CO$_2$ and CH$_4$) change in the atmosphere for different irradiation scenarios: GJ 436b irradiated by 1000 x Ly$\alpha$, 100 x Ly$\alpha$, 10 x Ly$\alpha$, and 1 x Ly$\alpha$, where n x Ly$\alpha$ is the reconstructed Ly$\alpha$ flux for GJ 436b multiplied by the factor n [see Fig. 1(b)]. The photolysis rate of species i ($r_i$) is proportional to the concentration of the species ($n_i$) and the photodissociation coefficient ($J_i$, shown in Fig. 4(b)) which depends only on the flux ($F$) and the cross section of the species ($\sigma_i$), as shown in equations (2) and (3) (Yung & Demore 1999):

$$r_i(z) = J_i(z) n_i(z),$$

$$J_i(z) = \int \sigma_i(\lambda) F(z, \lambda) d\lambda.$$

The H$_2$O concentration is higher than CH$_4$ and CO$_2$ (see Fig. 5(a)) and, therefore, has higher photolysis rates. H$_2$O absorbs most of the FUV radiation, becoming optically thick to radiation when $\lambda < 2000 \text{ Å}$ at $\sim 0.08$ bars. Lower photolysis rates at higher pressures are due to radiation at longer wavelengths ($2000 < \lambda < 2400 \text{ Å}$).

Fig. 4(b) shows that high values of the Ly$\alpha$ flux (1000, 100, and 10 x Ly$\alpha$) lead to more radiation at higher pressures in the atmosphere, thereby increasing the H$_2$O, CO$_2$ and CH$_4$ photolysis rates.

Figs. 5(a) - 5(b) show mixing ratios vs. pressure of the most abundant species in GJ 436b’s atmosphere with solar composition for four scenarios: 1000 x Ly$\alpha$ (small dotted), 100 x Ly$\alpha$ (dotted), 10 x Ly$\alpha$ (dots and dashes) and 1 x the reconstructed Ly$\alpha$ flux (solid line). For all species, mixing ratios in the four cases are the same for higher pressures, where photodissociation processes are not efficient, but start to deviate from equilibrium values when photodissociation of molecules occurs, mostly in the upper observable atmosphere (P < $10^{-5}$ bars).

Since GJ 436b is a cool planet with a T$_{eq}$ $\sim$ 640 K (assuming that the albedo=0), CH$_4$ is the most abundant carbon compound up to $10^{-4}$ bars for solar composition. At lower pressures, it is oxidized, and its abundance decreases rapidly. The CH$_4$ photolysis rate changes significantly with increasing Ly$\alpha$ flux (see Fig. 4(a)), as shown by the difference between the two extreme Ly$\alpha$ fluxes (1000 and 1 x Ly$\alpha$) being two orders of magnitude at $5 \times 10^{-5}$ bars, leading to different mixing ratios at lower pressures.

H$_2$O, which is the most abundant gas after He and H$_2$, starts to dissociate at $10^{-4}$ bars for 1000 x Ly$\alpha$, at $5 \times 10^{-5}$ bars for 10 x Ly$\alpha$ and at $5 \times 10^{-6}$ bars for the reconstructed Ly$\alpha$ flux.

The photolysis of H$_2$O affects the mixing ratios of other species in the atmosphere such as O, OH and H which increases with increasing H$_2$O photolysis. H$_2$O dissociation is followed by the destruction of H$_2$ because of a reaction with OH. As a consequence of these reactions, a large amount of H is created and H$_2$ is destroyed with increasing Ly$\alpha$ flux. H replaces H$_2$ as the most abundant gas in the atmosphere at pressures P < $5 \times 10^{-5}$ bars in all cases. OH increases with the Ly$\alpha$ flux because of the H$_2$O photolysis at $\sim 10^{-5}$ bars.

Note that CO photolysis is not considered because its photolysis is driven by EUV radiation which is not included in the model. Atomic O is produced from H$_2$O photolysis. At $10^{-5}$ bars, its mixing ratio is $10^{-7}$ for 1000 x Ly$\alpha$ and $10^{-10}$ for 1 x Ly$\alpha$ flux.

CO and CO$_2$ show different behaviors compared to their chemistry in hot Jupiters’ atmospheres, because CO is the dominant carbon compound in hot exoplanet atmospheres, whereas CH$_4$ is dominant in cooler planets. Self-shielding by CH$_4$ and other effects lead to differences in the chemistry and pressure where self-shielding occurs (Line et al. 2011). The CO-mixing ratio increases because of photochemistry at $\sim 0.01$ bars, increasing up to 2 orders of magnitude at $\sim 10^{-5}$ bars. CO$_2$ is formed after H$_2$O photolysis, with a local maximum at $\sim 10^{-4}$ bars for 1000 x Ly$\alpha$, at $5 \times 10^{-5}$ bars for 100 x Ly$\alpha$, at $8 \times 10^{-6}$ bars for 10 x Ly$\alpha$ and at $10^{-6}$ bars for 1 x Ly$\alpha$.

Our results for the dominant carbon and oxygen species in GJ 436b for 1 x Ly$\alpha$ flux are in good agreement with previous results by Line et al. (2011) and Moses et al. (2013), with small differences due to differences in the UV fluxes used, cross sections adopted, chemical schemes and thermal profiles.

3.1.2 Atmospheres with high metallicities

High metallicities are expected in some mini-Neptune atmospheres because of the enrichment inferred from interior modeling (Baraffe et al. 2008; Figueira et al. 2009; Fortney et al. 2013). As a test case, we compute simulations for the atmosphere of GJ 436b assuming 1000 x solar metallicity.

An atmosphere with 1000 x solar metallicity has lower hydrogen and helium and increased carbon and oxygen abundances (Moses et al. 2013). Fig. 4(c) shows the photolysis rates of CH$_4$ (blue), H$_2$O (black) and CO$_2$ (red) with the reconstructed Ly$\alpha$ flux of GJ 436 for a solar metallicity atmosphere (solid lines) and an atmosphere with 1000 x solar metallicity (dotted lines). H$_2$O shows the highest photolysis rates for both compositions. The CO$_2$ photolysis rate is smaller than CH$_4$ for solar composition, but it increases for the 1000 x solar model, becoming larger than H$_2$O at $P < 1 \times 10^{-6}$ bars. CH$_4$ has very low photolysis rates, especially for the case of an enriched atmosphere because it is shielded by H$_2$O and CO$_2$.

Figs. 5(c) - 5(d) show mixing ratios vs. pressure for H$_2$O, CO$_2$, CH$_4$ and for H, H$_2$ O, CO and OH, respectively, for an atmosphere of 1000 x solar metallicity and four scenarios: 1000 x Ly$\alpha$ (small dotted), 100 x Ly$\alpha$ (dot-
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Photolysis rates (left panels) and photodissociation coefficient (right panels) vs. pressure in the atmosphere of GJ 436 b for H$_2$O (black), CO$_2$ (red) and CH$_4$ (blue). Top panels: solar composition for four Ly$\alpha$ flux scenarios: 1000 x Ly$\alpha$ (small dots), 100 x Ly$\alpha$ (dotted), 10 x Ly$\alpha$ (dashes) and CH$_4$ flux (solid line). Bottom panels: comparison between solar composition (solid) and 1000 x solar metallicity atmosphere (dotted line) for the reconstructed Ly$\alpha$ flux. Note that solid lines in Figs. 4(c) – 4(d) are the same as in Figs. 4(a) – 4(b) respectively.

3.2 Absorption of Ly$\alpha$ radiation in the extended H atmosphere

Some hot extrasolar planets have an extended atmosphere consisting primarily of atomic H which could efficiently absorb Ly$\alpha$ radiation, as shown by observations (Vidal-Madjar et al. 2003, Lecavelier des Etangs et al. 2011, Ehrenreich et al. 2012) and theoretical models (Koskinen et al. 2010, Lavvas et al. 2011). Some absorption of Ly$\alpha$ photons has even been detected in GJ 436b’s atmosphere (Kulow et al. 2014) which increases the importance of studying the absorption of Ly$\alpha$ radiation in an exoplanet’s atmosphere and the effects on photochemistry. The exoplanet thermosphere is characterized by an increase in temperature (Huitson et al. 2012) which may affect the resulting atmospheric composition. For those cases, thermochemical processes dominate the chemistry in the upper atmosphere, and the Ly$\alpha$ flux plays no role in defining the atmospheric composition (Lavvas et al. 2011). On the other hand, there are cooler planets, such as GJ 436b, for which the incident Ly$\alpha$ flux may be partially absorbed in the atmosphere, but the effects of this decreased flux on the resulting composition remain poorly understood. Lavvas et al. (2011) studied this problem and performed photochemical calculations taking into account the exoplanets’ thermosphere for three planets, including GJ 436b, where they found that Ly$\alpha$ flux plays a small role in the photochemistry. In the present work, we use the FUV flux taken from recent observations (France et al. 2013) which is at least one order of magnitude larger than the Ly$\alpha$ flux used in Lavvas et al. (2011). We assume that...
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In this paper, we use a simplified model in which a portion of the stellar Lyman α radiation is absorbed in the extended structure, photochemistry and thermosphere is beyond the scope of this paper. We consider the three possible absorption scenarios shown in Fig. 1(c): 0.1 x Lyα, 0.01 x Lyα, and 0.001 x the reconstructed Lyα flux.

In Fig. 5 we show the mixing ratios vs. pressures for GJ 436b for solar (top panels) and 1000 x solar metallicity (bottom panels) atmospheres. Left panels (Figs. 5(a) and 5(c)) show gas effects by Lyα flux: H2O (black), CH4 (blue), CO2 (red) and their concentrations for different Lyα flux conditions: 1000 x Lyα flux (small dotted), 100 x Lyα (dotted), 10 x Lyα (dots and dashes) and 1 x the reconstructed Lyα flux (solid line). Right panels (Figs. 5(b) and 5(d)) show the H, H2, O, CO and OH mixing ratios.

Figure 5. Mixing ratios vs. pressures for GJ 436b for solar (top panels) and 1000 x solar metallicity (bottom panels) atmospheres. Left panels (Figs. 5(a) and 5(c)) show gas effects by Lyα flux: H2O (black), CH4 (blue), CO2 (red) and their concentrations for different Lyα flux conditions: 1000 x Lyα flux (small dotted), 100 x Lyα (dotted), 10 x Lyα (dots and dashes) and 1 x the reconstructed Lyα flux (solid line). Right panels (Figs. 5(b) and 5(d)) show the H, H2, O, CO and OH mixing ratios.

For a solar composition atmosphere, the increase in the CO2-mixing ratio at 1 x 10^-5 bars is one order of magnitude. For solar composition and 1000 x solar metallicity atmospheres, the CO2-mixing ratio at lower pressures (P< 5 x 10^-6 bars) is dominated by its own dissociation, therefore the CO2-mixing ratio increases for higher Lyα flux absorption. The difference in the CO2-mixing ratios for the extreme cases (1 x Lyα and 0.001 x Lyα flux) is one order of magnitude. For solar composition and 1000 x solar metallicity atmospheres, the CO2-mixing ratio at lower pressures (P< 5 x 10^-6 bars) is dominated by its own dissociation, therefore the CO2-mixing ratio increases for higher Lyα flux absorption. The difference in the CO2-mixing ratios for the extreme cases (1 x Lyα and 0.001 x Lyα) at 1 x 10^-7 bars is one order of magnitude for a solar metallicity atmosphere and two orders of magnitude for a 1000 x solar metallicity atmosphere.

this Lyα radiation is not completely absorbed and therefore plays an important role in the photochemistry described in Section 3. It may be possible, nevertheless, that some Lyα radiation is absorbed. In this section, we explore the photochemistry effects of the absorption of Lyα flux in the atmosphere of GJ 436b. Since a self-consistent model of thermal structure, photochemistry and thermosphere is beyond the scope of this paper, we use a simplified model in which a portion of the stellar Lyα radiation is absorbed in the extended H atmosphere. We consider the three possible absorption scenarios shown in Fig. 1(c): 0.1 x Lyα, 0.01 x Lyα and 0.001 x the reconstructed Lyα flux.

In Fig. 6 we show the mixing ratios of H2O, CH4, CO2, O, OH, H, CO and H2 as a function of the pressure in GJ 436b’s atmosphere. We investigate the results of adopting solar composition (Fig. 6(a), 6(b)) as well as 1000 x solar metallicity in the atmosphere (Fig. 6(c), 6(d)) in the three explored scenarios (0.1 x Lyα, 0.01 x Lyα and 0.001 x Lyα). Since the atmosphere is exposed to reduced Lyα radiation, the photolysis rates are reduced in all cases compared to a deeper penetration of Lyα stellar flux (as adopted in Section 3). Decreased dissociation of H2O leads to an increase in its mixing ratio which is the highest in the case of extreme absorption (0.001 x Lyα). For the case of solar composition, the mixing ratio of H2O at 5 x 10^-6 bars is ∼ 2 x 10^-6 for 1 x Lyα and ∼ 2 x 10^-4 for 0.001 x Lyα (Fig. 6(a)), and for 1000 x solar composition, it is ∼ 1 x 10^-7 for 1 x Lyα and 0.05 for 0.001 x Lyα at the same pressure (Fig. 6(c)). These changes in the H2O-mixing ratios lead to changes in O, OH, H, CO and H2 (see Fig. 6(b), 6(d)).
CH$_4$ dissociation is caused mainly by radiation around 1300 Å (see Fig. 9). Since this molecule is also shielded by H$_2$O (solar composition) as well as by H$_2$O and CO$_2$ (1000 x solar metallicity), its mixing ratio does not change significantly with increasing absorption of Ly$_\alpha$.

The absorption of Ly$_\alpha$ radiation is important for the photochemistry in these exoplanet atmospheres. Different absorption scenarios lead to different mixing ratios and, therefore, it is necessary to know the amount of flux absorbed to know the effect on the photochemistry. Nevertheless, we notice that very strong absorption (0.001 x Ly$_\alpha$ flux) has only a small effect on the photochemistry (compared to the case of 0.01 x Ly$_\alpha$ flux) because the dissociation of molecules is mainly due to radiation at other wavelengths.

4 CONCLUSION

Ly$_\alpha$ radiation changes mini-Neptunes’ upper atmospheric chemistry significantly. We explore the effect of Ly$_\alpha$-driven photochemistry for atmospheres with different metallicities, comparing solar composition and a 1000 x solar composition. Focusing on GJ 436b as an example, we calculate the thermal structure and chemistry including equilibrium and disequilibrium chemistry (molecular diffusion, vertical mixing, and photochemistry). We use direct observations of the UV and the reconstructed Ly$_\alpha$ flux for the host star GJ 436 (France et al. 2013). We explore the effects on the planet’s atmosphere of increasing the incident Ly$_\alpha$ flux by factors of 10, 100 and 1000 as well as the case where the Ly$_\alpha$ flux is absorbed in the extended H atmosphere by factors of 0.1, 0.01 and 0.001.

For solar composition atmospheres, our results show that the mixing ratio of H$_2$O is most affected by Ly$_\alpha$ radiation as the H$_2$O photolysis rate strongly depends on the Ly$_\alpha$ flux even at pressures as large as ~ 0.08 bars. The H$_2$O-mixing ratios change by up to five orders of magnitude between the cases of 1000 x Ly$_\alpha$ and 0.001 x Ly$_\alpha$. The reconstructed Ly$_\alpha$ flux thereby significantly changes the upper atmospheric chemistry and the resulting observable spectral features. H$_2$O is one of the most abundant gases in the atmosphere, absorbing much of the Ly$_\alpha$ flux and shielding other species like CH$_4$. Changes in the H$_2$O photolysis rates also affect other molecules whose mixing ratios are largely affected by H$_2$O dissociation: for example, CO$_2$ changes by up to 3 orders of magnitude, OH by up to 5 orders of mag-

Figure 6. Photochemical mixing ratios vs. pressure for an atmosphere with solar composition (upper panels) and 1000 x solar metallicity (lower panels) for different Ly$_\alpha$ absorption scenarios: 1 x Ly$_\alpha$ (solid), 0.1 x Ly$_\alpha$ (dotted and dashes), 0.01 x Ly$_\alpha$ (dashed) and 0.001 x Ly$_\alpha$ flux (dotted line).
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Magnitude, $\mathrm{H}$ by up to 4 orders of magnitude, $\mathrm{O}$ by up to 6 orders of magnitude, $\mathrm{H}_2$ by 1 order of magnitude, and CO by less than 1 order of magnitude between the extreme cases of $1000 \times \mathrm{Ly} \alpha$ and $0.001 \times \mathrm{Ly} \alpha$ flux.

Because of the high abundance of $\mathrm{CO}_2$ in high metallicity atmospheres, $\mathrm{CO}_2$ competes with $\mathrm{H}_2\mathrm{O}$ for energetic FUV photons. The $\mathrm{CO}_2$ photolysis rate is largely affected by the Ly $\alpha$ flux, and therefore its mixing ratio changes by up to 4 orders of magnitude for the extreme irradiation scenarios we have explored. These two molecules absorb most of the Ly $\alpha$ radiation, thereby shielding $\mathrm{CH}_4$. The smaller effect on $\mathrm{H}_2\mathrm{O}$ also leads to smaller changes in the abundance of those other molecules for which mixing ratios in the upper atmosphere strongly depend on $\mathrm{H}_2\mathrm{O}$ photolysis.

Our models show that Ly $\alpha$ radiation from the host star affects mini-Neptune atmospheres significantly at low pressures and cannot be ignored in atmospheric modeling. Ly $\alpha$ radiation affects the photochemistry of important gases in the upper atmosphere and, therefore, also the resulting observable spectral features of mini-Neptunes. Observations of the UV flux from a wide range of stars as well as studies of the absorption of this radiation in the exoplanet thermospheres are essential for realistic interpretations of planetary spectra.

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