The Effects of UV Continuum and Lyman $\alpha$ Radiation on the Chemical Equilibrium of T Tauri Disks

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ABSTRACT

We show in this Letter that the spectral details of the FUV radiation fields have a large impact on the chemistry of protoplanetary disks surrounding T Tauri stars. We show that the strength of a realistic stellar FUV field is significantly lower than typically assumed in chemical calculations and that the radiation field is dominated by strong line emission, most notably Lyman $\alpha$ radiation. The effects of the strong Lyman $\alpha$ emission on the chemical equilibrium in protoplanetary disks has previously been unrecognized. We discuss the impact of this radiation on molecular observations in the context of a radiative transfer model that includes both direct attenuation and scattering. In particular, Lyman $\alpha$ radiation will directly dissociate water vapor and may contribute to the observed enhancements of CN/HCN in disks.

Subject headings: accretion, accretion disks, astrobiology, astrochemistry — circumstellar matter — stars: pre-main sequence — ultraviolet:stars

1. Introduction

Over the past few years it has become evident that the protoplanetary disks surrounding newly formed stars contain a rich evolving chemistry, which is a vital ingredient in the overall structure and dynamics of the disk. Because the dominant molecule (H$_2$) is unexcited at the cold temperatures ($T \sim 10 \text{ – } 70$ K) characteristic of most of the disk mass, trace species provide cooling for upper layers that are unable to radiate via H$_2$ emission. Moreover, the most promising process for the required angular momentum transport is via

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the magnetorotational instability (Balbus & Hawley 1991). This process is critically tied to the abundance of charged particles that is set by the penetration of energetic radiation and chemical reactions (Gammie 1996, Stone et al. 2000).

At present, emission from CO has been detected in many systems (Dutrey et al. 1996; Koerner 1997), while emission from other less abundant and more complex molecular species has only been detected in a handful of sources (Kastner, Zuckerman, Weintraub, & Forveille 1997; Dutrey, Guilloteau, & Guelin 1997; Goldsmith, Langer, & Velusamy 1999; Qi 2001). Analysis of the observations reveals that the molecular emission is arising primarily from the disk surface and that chemistry controlled by energetic ultraviolet (UV) and X-ray radiation (which dissociates molecules and is active on surfaces) must contribute to the observed abundances (Aikawa & Herbst 1999; Willacy & Langer 2000; van Zadelhoff et al. 2001).

Chemical models of these systems have been developed to examine the impact of stellar and interstellar (ISRF) FUV radiation on the chemistry at the disk surface (Aikawa & Herbst 1999; Willacy & Langer 2000; Aikawa et al. 2002; van Zadelhoff et al. 2002). These models typically assume that the stellar FUV field has the same wavelength dependence as the ISRF, and it is $\sim 10^4$ stronger than the ISRF at 100 AU. However, in this paper we argue that the strength of the FUV radiation field from a typical accreting T Tauri star (TTS) is much weaker than previously assumed and show that the observed stellar spectra do not have the same wavelength dependence as the ISRF.

In addition, the presence of strong line radiation, especially Lyman $\alpha$, has yet to be recognized in chemical models and may have important effects. For instance, nearly all T Tauri disks detected so far appear to have large ratios of CN relative to HCN (Dutrey et al. 1997; Kastner et al. 1997; Qi 2001). These two species are linked to Lyman $\alpha$ radiation because the main dissociative photoabsorption channels for CN are shortward of 1150 Å (Nee & Lee 1985); in contrast, HCN will be subject to photodissociation by Lyman $\alpha$ photons near 1216 Å (Nuth & Glicker 1982). The high CN/HCN ratio has been attributed to the photodissociation by continuum FUV radiation from the star or the interstellar medium (Aikawa et al. 1999; Willacy & Langer 2000; van Zadelhoff et al. 2002). However, strong Lyman $\alpha$ fluxes may also contribute to elevate the CN/HCN ratio and to the preferential destruction of other species including water vapor.

In this Letter we use FUV data of TTS to construct a FUV radiation field which is representative of low mass T Tauri stars with average accretion properties. Using this field, we examine its effect on the chemical equilibrium on the proto-planetary disk surface.
2. The FUV spectrum of Classical T Tauri stars

In most calculations of chemical equilibrium in TTS disk to date it has been assumed that the stellar FUV flux is $10^4$ times higher than the ISRF at $R = 100$ AU (Willacy & Langer 2000; Aikawa et al. 2001). This value is taken from Herbig & Goodrich (1986) IUE observations of T Tau and RY Tau. The FUV spectra below $\sim 2000$ Å of these two stars is similar with $F_\lambda \sim 3 \times 10^{-13}$ erg cm$^{-2}$ s$^{-1}$ Å$^{-1}$, yielding a flux at $R = 100$ AU integrated over 1000 Å of $23.5 \times 10^4$ Habing (1 Habing $= 1.6 \times 10^{-3}$ erg cm$^{-2}$ s$^{-1}$; Tielens & Hollenbach 1985). However, there are reasons to expect that these spectra do not represent the typical FUV flux of TTS. For one thing, T Tau and RY Tau have larger masses and radii than typical TTS, and thus are not representative of the class (Kenyon & Hartmann 1995). In addition, the mass accretion rate in their disks is $\dot{M} \sim 10^{-7}$ M$_\odot$ yr$^{-1}$ (Calvet et al. 2003, in preparation), higher than the mean TTS mass accretion rate, $\sim 10^{-8}$ M$_\odot$ yr$^{-1}$ (Hartmann et al. 1998). This is important, because the luminosity in the FUV scales with accretion luminosity (Calvet et al. 2003).

We now have a much better knowledge of the FUV fields characteristic to TTS. Figure 1 shows the FUV spectrum of BP Tau, a TTS with mass, radius, $\dot{M}$, and age (0.5 M$_\odot$, 2 R$_\odot$, $3 \times 10^{-8}$ M$_\odot$ yr$^{-1}$, and $\sim 2$ Myr; Gullbring et al. 1998) typical of the class. The observations were obtained in HST program GO9081 and are reported elsewhere (Calvet et al. 2003b, in preparation). The low resolution (G140L) spectrum has been scaled to 100 AU, using 140 pc as the distance of Taurus (Kenyon, Dobrzycka, & Hartmann 1994), and corrected for reddening using the interstellar law and $A_V = 0.5$ (Gullbring et al. 1998).

We also show in Figure 1 the spectrum of the 10 Myr old star TW Hya, from Herczeg et al. (2002). This star has a mass of 0.8 M$_\odot$, a radius of 1 R$_\odot$ (Webb et al. 1999) and a mass accretion rate $\sim 10^{-9}$ M$_\odot$ yr$^{-1} - 10^{-8}$ M$_\odot$ yr$^{-1}$ (Alencar & Batalha 2002). The flux from TW Hya suffers little or no reddening, but has been scaled by $\sim 3.5$ to match the continuum of BP Tau. Comparison between the spectra of BP Tau and TW Hya indicates that the shape of the continuum is roughly similar. More differences can be seen in the strength of the emission lines which permeate the spectra. These are lines of highly ionized metals, He, and Hydrogen Lyman series (Valenti, Johns-Krull, & Linsky 2000; Ardila et al. 2002). The largest difference can be seen in Lyman $\alpha$, shown in the right inset in Figure 1. The core of the line is lost to absorption in the line of sight to BP Tau. We also show the Lyman $\alpha$ profile of CY Tau, a star with similar parameters to BP Tau (Gullbring et al. 1998), but a lower reddening, $A_V = 0.3$, so more of the Lyman $\alpha$ core can be seen. Still, the flux in

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4 This is consistent with the ratio of their mass accretion rates, allowing for intrinsic variability and uncertainties of the mass accretion rate determination.
Lyman $\alpha$ is much lower than that of TW Hya. This comparison indicates variations of more than a factor of 10 are expected in the flux of the Lyman $\alpha$ line among T Tauri stars.

With this information, we have constructed a composite FUV spectrum that is representative of the low mass T Tauri stars, which constitute the largest fraction of the newly born young stars. The adopted spectrum is equal to that of BP Tau between 1150 and 2000 Å, and to the scaled TW Hya FUSE spectrum down to 950 Å. Below 950 Å, we assume a linear extension with the same slope as the continuum. For the chemical calculations in §5, we integrate the adopted spectrum in 10 Å bins.

We show in Figure 1 the ISRF scaled by 540 to match the total luminosity of the adopted spectrum between 900 and 1700 Å. The overall strength of the representative TTS FUV continuum spectrum at 100 AU is of the order of a few hundred Habing, significantly lower than generally assumed. In addition, Figure 1 shows that the representative FUV spectra differs from the interstellar field in several ways: (1) the shape of the continuum is different in the sense that the TTS spectra rises as wavelength increases; (2) the TTS spectra is dominated by emission lines, which carry at minimum $\sim 35\%$ of the flux.\(^6\)

### 3. Disk Model

For the calculations in this paper, we adopt a disk model which fits the median spectral energy distribution (SED) for classical (accreting) T Tauri stars (TTS) in the Taurus clouds (D’Alessio, Calvet, & Hartmann 2001). Typical stellar parameters are adopted, $M_* = 0.5\, M_\odot$, $R_* = 2\, R_\odot$ and $T_* = 4000\, \text{K}$ (Gullbring et al. 1998; Hartmann et al. 1998), and the mass accretion rate used, $\dot{M} = 3 \times 10^{-8}\, M_\odot\, \text{yr}^{-1}$, is near the average in Taurus (Hartmann et al. 1998). Dust grains were assumed to be segregate spheres of compounds with abundances as in Pollack et al. (1994), and with a size distribution given by $n(a)\, da \propto a^{-3.5}\, da$, where the grain radius $a$ varies between 0.005 µm and 1 mm. The disk outer radius is $R_d = 350\, \text{AU}$; with this, and $\alpha = 0.05$, the mass of the disk is $0.03\, M_\odot$.

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\(^5\)To make this comparison, we have used the expression for the interstellar field energy density $u_\lambda$ from Draine (1978) as given by Eq. (23) of Draine & Bertoldi (1996), with $J_\lambda = cu_\lambda/4\pi$. In addition we have adopted the scaling $\chi = 1$, which matches the interstellar field as estimated by Habing (1968). This field is lower by a factor of 1.71 than the one given by $hcI_\lambda/4\pi\lambda$, with $I_\lambda$ from van Dishoeck (1987). We have then used $F_\lambda = 4\pi J_\lambda = \int I_\lambda \, d\Omega$, with $\Omega$ the solid angle, to compare with the observed flux.

\(^6\)For BP Tau and TW Hya lines carry, respectively, at least 35% and 85% of the luminosity between 1100–1700 Å. These percentages are lower limits because of interstellar and wind absorption of Lyman $\alpha$ photons.
We self-consistently solve the complete set of vertical structure equations, including irradiation and viscous heating, resulting in detailed profiles of temperature and density with vertical height and disk radius. Figure 2 shows the vertical profiles of temperature and column density for the adopted disk model at a radius $R = 100$ AU, which will be used in the discussions of the following sections.

4. Transfer of FUV radiation

We follow the transport of FUV radiation through the disk using an analytical approximation that allows for the inclusion of scattering in addition to pure absorption (see also van Zadelhoff et al. 2002). We assume that stellar radiation at an ultraviolet wavelength $\lambda$ comes in a single beam which makes an angle $\theta_0(\lambda)$ to the local surface $z_s(\lambda)$, defined by the condition $\tau^\text{rad}_\lambda \sim 1$, where $\tau^\text{rad}_\lambda$ is the radial optical depth. We follow standard procedures for solving the transfer equations in the plane-parallel approximation\(^7\). We assume that there is no local emission at $\lambda$. Along the original beam, defined by $\mu_0 = \cos(\theta_0)$\(^8\), the mean intensity decreases as $\exp(-\tau_\lambda/\mu_0)$, where $\tau_\lambda$ is the vertical optical depth. A nearly isotropic diffuse field is created by photons scattered out of the beam. Following Mihalas (1978), we solve the transfer equations for symmetric and antisymmetric averages of the specific intensity $u$ and $v$, from which we can derive with usual boundary conditions the depth dependence of the mean intensity as

$$J_\lambda = \frac{I_*}{2}C_1e^{-\tau_\lambda/\mu_0} + \sigma_\lambda I_*\mu_0 C_2 e^{\sqrt{3(1-\sigma_\lambda)\tau_\lambda}}$$

where

$$C_1 = 1 - 3\sigma_\lambda \mu_0^2$$

$$C_2 = \frac{1+3/2\mu_0^2+3(1-\sigma_\lambda)\mu_0^2}{1+2\sqrt{(1-\sigma_\lambda)/3}}$$

and $\sigma_\lambda$ is the albedo. The first term in Eq. (1) corresponds to the direct incoming beam that is rapidly attenuated due to the oblique angle of incidence. The second term is the diffuse scattered radiation field which penetrates deeper than the direct radiation. The mean intensity $J_\lambda$ at $\lambda = 1500$ Å, normalized to the stellar intensity $I_*$ at the same wavelength, is shown in Figure 3a, where each contribution is shown separately. Similarly to the models of van Zadelhoff et al. (2002), the scattered field penetrates much closer to the midplane than the direct attenuated stellar component. This holds true to within a few hundred AU of the star.

\(^7\)This is justified because of the small geometrical thickness of the disk (cf. D'Alessio et al. 1999).

\(^8\)At $R = 100$ AU $\mu_0(1000\text{Å}) = 0.07$. 


The stellar specific intensity in Eq. (1) can be estimated assuming that the beam carries a flux equal to the observed flux \( F_\lambda \), so \( I_\star = F_\lambda / 2\pi \). Figure 3b shows the mean intensity \( J_\lambda \) at \( \lambda = 1500 \text{Å} \) and \( R = 100 \text{AU} \) from Figure 3a, scaled by \( I_\star \) calculated from the continuum flux at 1500 Å in Figure 1. We also plot for comparison the mean intensity corresponding to the ISRF (1 Habing) impinging on the disk surface with \( \mu_0 = 1 \) in Eq.(1). It can be seen that the stellar field dominates in the upper \( \sim 30 \text{AU} \) in the disk, while it becomes comparable or smaller than the interstellar field closer to the midplane (Willacy & Langer 2000; van Zadelhoff et al. 2002). However, TTS in Taurus have a mean extinction \( A_V \sim 1 \) along the line of sight (Kenyon & Hartmann 1995), which corresponds to an attenuation \( \sim 16 \) in the UV; the corresponding mean intensity is shown in Figure 3b. Moreover, radiation in the lines can be much higher than in the continuum (cf. Figure 1). Therefore, the stellar field is expected to be the dominant contributor to the FUV field illuminating the disk (see Aikawa & Herbst 2001).

5. Lyman \( \alpha \) and Molecular Photodissociation

Using the observed radiation field in Figure 1 we can examine the effects of Lyman \( \alpha \) on the photodissociation of CN, HCN, and H\(_2\)O. To calculate the photodissociation rate we use the following expression

\[
k_{pd}(s^{-1}) = \int \frac{4\pi \lambda}{hc} \sigma(\lambda) J_\lambda d\lambda.
\]

(3)

For the radiative transfer we use the procedure of §4 and the disk model in §3. In this calculation the Lyman \( \alpha \) flux is initially assumed to be a constant value between the peaks of the red and blue damping wings of the CY Tau profile (Figure 1 right, §2). As this is a lower limit, in one case we increase the flux of the Lyman \( \alpha \) feature between 1205 - 1230 Å by a factor of 10. This increases the total UV flux by a factor of three. For comparison we provide the corresponding photodissociation rate from a scaled interstellar FUV field that is attenuated only (i.e. without a scattered contribution, similar to Willacy & Langer 2000).

Our results are given in Figure 4. Two main factors are noticed in this plot. (1) For all species the inclusion of scattering allows for greater FUV penetration than in models which simply attenuate a parameterized ISRF (van Zadelhoff et al. 2002). (2) For HCN and H\(_2\)O the presence of an enhanced Lyman \( \alpha \) radiation field can increase photodissociation. Because of the difference in photodissociation channels, CN will exist over a larger range of vertical distances within the disk than either HCN or H\(_2\)O.
6. Discussion

While the primary photoabsorption bands for CO and H$_2$ lie short of 1100 Å numerous other molecules will be subject to photodissociation by Lyman α radiation (e.g. OH, CH$_4$, NH$_3$; Lepp & Dalgarno 1996). Thus, the presence of Lyman α photons can impact the chemistry on the disk surface beyond the CN/HCN ratio. Indeed FUV radiation will be of increasing importance in disk planet forming regions and Lyman α emission may be an important factor in limiting the abundance of water vapor. Young stars are also show evidence for significant emission from X-rays, which can ionize and dissociate H$_2$ molecules. This process results in the creation of an in situ Lyman α radiation field that can further alter the chemistry (Lepp & Dalgarno 1996).

Furthermore the FUV radiation field representative of low mass T Tauri stars with an average mass accretion rate is weaker than generally assumed in chemical calculations. The origin of the excess FUV flux is still under investigation, but in the study of a sample of HST/STIS spectra, the luminosity in the FUV is found to scale with the accretion luminosity (Calvet et al. 2003, in preparation). Since the mass accretion rates of the objects with the majority of molecular detections, DM Tau and LkCa15, are comparable and below that of BP Tau, respectively (Hartmann et al. 1998), this suggests that the FUV radiation field in these objects may be similar or weaker than BP Tau. With the stronger FUV field current models are capable of reproducing observed abundances of species such as CN and HCN in DM Tau (Aikawa et al. 2002); assuming a weaker FUV field may make it difficult to continue to match observations, but strong Lyman α radiation can provide an additional source of photodissociation to power the chemistry.

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Several effects can moderate the importance of Lyman α radiation. The presence of a large column of hydrogen atoms will predominantly scatter Lyman α photons. This will result in the destruction of some photons through dust absorption. Using the calculations of Bonilha et al. (1979) we estimate that $N_H \sim 10^{21}$ cm$^{-2}$ is required to significantly attenuate the emission. In the inner disk, a water column of $\sim 10^{18}$ cm$^{-2}$ will be sufficient to extinguish the Lyman α line core radiation; larger columns are needed to absorb both line core and wing emission. This will not happen in the outer disk, where water is frozen on grains. Finally, H$_2$ atoms can also absorb Lyman α photons resulting in fluorescence emission.
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Fig. 1.— Left: FUV spectra of T Tauri stars. Heavy solid line: HST/STIS spectrum of BP Tau, obtained in program GO9081, with grating G140L. Light solid line: spectrum of TW Hya scaled by 3.5 to match the BP Tau continuum level. We have combined the HST/STIS E140M spectrum from program GO8041, above \( \lambda = 1150 \) Å, with the FUSE spectrum below (Herczeg et al. 2002). The STIS E140 M has been convolved to the G 140L resolution, while the FUSE spectrum has been smoothed by 10 Å. Identification of important emission lines is given. The extension below 960 Å adopted in the calculations for this work is shown as a dotted line (see §2). The interstellar field from Draine (1978) scaled by \( \sim 540 \) Habing to match the integrated flux of the adopted spectrum is shown in dashed lines. Right: region around the Lyman \( \alpha \) line. The echelle spectrum of CY Tau obtained with STIS and grating E140M in our program GO8206 (Saucedo et al. 2003), convolved to the resolution of G140L is shown with dashed lines. Other line styles are as in left panel. The reddening towards CY Tau is lower than towards BP Tau, and thus the central core of the line is more apparent. The dotted line shows one of the adopted approximations for the flux in the central core of the line (see §5).
Fig. 2.— Temperature and column density as a function of height $z$ at disk radius $R = 100$ AU for the disk model used in this work, which fits the median SED of Taurus stars (see §3).
Fig. 3.— (a) Normalized mean intensity at $\lambda = 1500$ Å and disk radius 100 AU as a function of disk height $z$. The total mean intensity (solid line) is separated into the direct stellar component (dashed line) and the diffuse scattered component (dotted line). The vertical optical depth is also shown for reference (dot-dashed line). The mean intensities are normalized to the incoming stellar specific intensity at the same wavelength. For the dust mixture considered in this work, the scattering coefficient $\sigma_{\lambda}$ goes from $\sim 0.4$ at 1000 - 1400 Å to $\sim 0.8$ at 2000 - 3000 Å. (b) Comparison between the mean intensities penetrating the disk at $\lambda = 1500$ Å and $R = 100$ AU: stellar field, with an incoming specific intensity $I_*$ corresponding to the continuum at 1500 Å in Figure 1; interstellar field (dashed lines), assuming $A_V = 0$ and 1 mag.
Fig. 4.— Photodissociation rate for CN, HCN, and H$_2$O calculated using FUV photoabsorption crosssections from Nuth & Glicker (1982), Lavendy, Gandara, & Robbe (1984), Nee & Lee (1985), Yoshino et al. (1996), and Chan et al. (1993). Three models are presented. (1) ISM att. only: using the ISM photodissociation rate taken from Millar, Farquhar, & Willacy (2000) scaled by $\sim 350$. This rate only includes attenuation within the disk model in §3 and no contribution from the diffuse scattered field. (2) $J_{\text{Ly}\alpha}$*1 using FUV radiative transfer as in §4, disk model from §3, and FUV field from Figure 1. The Lyman $\alpha$ flux is assumed to be a constant value between the red and blue damped wings shown in Figure 1. (3) $J_{\text{Ly}\alpha}$*10: same as (2) but the flux between 1205 - 1230 Å is increased by a factor of 10. Because there are no known CN photodissociation channel above 1150 Å this increase results in no change in the CN photodissociation rate, while the HCN and H$_2$O rates are drastically affected.