GAS-PHASE WATER IN THE SURFACE LAYER OF PROTOPLANETARY DISKS

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ABSTRACT

Recent observations of the ground-state transition of HDO at 464 GHz toward the protoplanetary disk of DM Tau have detected the presence of water vapor in the regions just above the outer disk midplane (Ceccarelli et al.). In the absence of nonthermal desorption processes, water should be almost entirely frozen onto the grain mantles, and HDO undetectable. In this Letter we present a chemical model that explores the possibility that the icy mantles are photodesorbed by FUV (6 eV ≤ hν ≤ 13.6 eV) photons. We show that the average interstellar FUV field is enough to create a layer of water vapor above the disk midplane over the entire disk. Assuming a photodesorption yield of 10−3, the water abundance in this layer is predicted to be ~3 × 10−7, and the average H2O column density is ~1.6 × 1015 cm−2. The predictions are very weakly dependent on the details of the model, like the incident FUV radiation field, and on the gas density in the disk. Based on this model, we predict a gaseous HDO/H2O ratio in DM Tau of ~1%. In addition, we predict the ground-state transition of water at 557 GHz to be undetectable with Odin and/or with the Herschel Space Observatory Heterodyne Instrument for the Far Infrared (HIFI).

Subject headings: planetary systems: protoplanetary disks — stars: formation — stars: pre–main-sequence — ISM: molecules

1. INTRODUCTION

Water is a key ingredient in many astrophysical environments, including circumstellar disks. It is the main constituent of the icy mantles coating interstellar grains and can be one of the most abundant molecules in the gas phase. For these reasons, water may dominate both the chemistry (being a major oxygen reservoir) and the thermal balance (i.e., cooling) of the gas component of protostellar disks. In addition, water vapor and water ice in protoplanetary disks are the major reservoirs of water later to be found in planets, asteroids, and comets and therefore are of great relevance for understanding the origin of the solar system and the distribution of volatiles within it. Unfortunately, the observation of water molecules in interstellar space is nearly impossible from the ground because of the absorption by the terrestrial atmosphere. So far, just a handful of space-based instruments (ISO, SWAS, and Odin) have carried out observations of water vapor lines in interstellar molecular clouds, but these instruments did not have the sensitivity to observe water protoplanetary disks. However, the upcoming ESA/NASA mission Herschel will provide a sensitive instrument, HIFI, for these studies (Dominik & Ceccarelli 2005). Also, SOFIA has potential for water observations.

Meanwhile, HDO, as the most important isotope of water, is currently the best ground-based probe of the presence of water in astrophysical environments. Recently, Ceccarelli et al. (2005) reported the first discovery of HDO (and therefore also the first discovery of water) in a protoplanetary disk, namely, DM Tau. The observations show an absorption line of gas-phase HDO with a line-to-continuum ratio of 0.9 that translates into an average column density through the disk of ~1.6 × 1015 cm−2. In the region where HDO is located, its fractional abundance is estimated to be about 3 × 10−7. If the abundance of gaseous H2O is similar to the value observed in molecular clouds and protostars, ~10−7, the HDO/H2O ratio is 0.01. The fact that the line is a deep absorption line immediately indicates that HDO must be present above the midplane (from where the submillimeter continuum is emitted). It must also be present in the outer radial regions (≥ 2600 AU) of the disk since the continuum originates from an extended region. The presence of a large column of HDO in this location was a surprise since the grain temperatures in this region are below 25 K and since H2O and HDO should be almost entirely frozen out onto grains. Chemical models, including the thermal desorption of water ice and the gas-phase formation of H2O (Aikawa et al. 2002; van Zadelhoff et al. 2003), predict an H2O column of 1014 cm−2 at about 400 AU, only a factor of 5 larger than the observed HDO column. Willacy & Langer (2000) included photodesorption by a strong stellar UV field and found H2O column densities of about 5 × 1015 cm−2 at 700 AU. An extended component of HDO (and consequentially water) therefore indicates a desorption agent from grain surfaces. Important possibilities are X-rays originating from the star, and penetrating throughout the entire outer disk, and UV photons, either from the star or simply due to the interstellar radiation field.

High-energy photons can, in principle, act to remove H2O molecules from the ice layers on dust grains. X-rays are energetic enough to remove a number of molecules, if sufficient energy can be concentrated close to the surface of the ice mantle on a grain. This idea has been explored by Najita et al. (2001), who considered X-ray heating of small grains or spot heating of larger grains. Small grains or small thermally insulated spots on a large grain can be heated strongly enough by a single X-ray photon to lead to thermal evaporation of part of the ice mantle.

An alternative mechanism is desorption by FUV photons (Willacy & Langer 2000). An FUV photon absorbed in the surface layer of an ice mantle can lead to the release of a molecule into the gas. In this Letter we explore the effect of just the interstellar FUV radiation field irradiating the disk surface of DM Tau. We show that such a scenario leads to a layer of water vapor in the disk surface with an FUV optical depth around unity. The column densities reached in steady...
state appear to be a viable explanation for the HDO absorption line seen in DM Tau. To show this, we developed a simple model of the chemistry leading to the presence of water vapor in irradiated gas containing grains covered by layers of water ice. A much more detailed discussion in the context of a full photodissociation region model, as well as analytical formulas to estimate H$_2$O column densities under such conditions, will be given by D. Hollenbach et al (2005, in preparation). Here we report the application of this model to the case of DM Tau.

A forthcoming paper will present the results of a larger parameter space study, which will explore the dependence of the model predictions on the characteristics of the grains (C. Ceccarelli et al. 2005, in preparation).

## 2. MODEL DESCRIPTION

The model computes the H$_2$O abundance across a protoplanetary disk, as a function of the radius and height. For the physical structure, we used the dust density and temperature profile that fits the spectral energy distribution (SED) of DM Tau (Ceccarelli et al. 2005) and that is shown in Figure 1. The gas is assumed to be fully coupled with the dust in terms of density distribution and temperature.

Due to the low temperature, the dust grains are covered with an ice layer. In our model, UV photons entering the disk surface are absorbed by dust grains and cause photodesorption of water molecules from the ice. Only UV photons absorbed directly at the surface of the ice mantle can desorb a molecule, so that only a small fraction of absorbed photons will cause the ejection of H$_2$O. Laboratory experiments at Ly$\alpha$ wavelengths have shown that the involved yields are typically between $10^{-3}$ and $10^{-2}$ molecules per photon (Westley et al. 1995b). The yield increases to some extent depending on the UV dose in the experiment, apparently because radical formation on the ice surface aids the desorption process (Westley et al. 1995a).

It is unclear how important this effect is in astrophysical environments, and we adopt a conservative value for the yield of $10^{-3}$ molecules per incident FUV (6 eV $\leq h\nu \leq$13.6 eV) photon. The yield probably introduces a factor of a few uncertainty into the computations (see below).

The desorption process at a given location will also depend on the attenuated FUV flux, and the rate per unit volume can be written as

$$k_{\text{des}} = G_o f_\nu Y \exp \left[-N(H_2)/N_{\text{eq}}\right] \sigma_{\text{gr}} n_{\text{gr}},$$

where $G_o$ is the FUV field in Habing (1968) units, $f_\nu = 10^8$ photons cm$^{-2}$ s$^{-1}$ is the FUV flux for the standard Habing interstellar field ($G_o = 1$), $Y$ is the photodesorption yield, $N_{\text{eq}}$ is the H$_2$ column density that gives $\tau_{\text{eq}} = 1$ between 6 and 13.6 eV (we adopted a value equal to $1.8 \times 10^{21}$ cm$^{-2}$; Tielens & Hollenbach 1985), $\sigma_{\text{gr}}$ is the grain geometrical cross section (equal to $\pi a_{\text{gr}}^2$, where we assume an average grain size of 0.1 $\mu$m), $n_{\text{gr}}$ is the grain number density, and the product $\sigma_{\text{gr}} n_{\text{gr}}$ is approximatively $10^{-21}$ cm$^{-2}$ times the gas density $n_{\text{H}_2}$, obtained by assuming a gas-to-dust ratio of 100. After being released into the gas phase, water either freezes out back onto a grain or is photodissociated by the FUV photons at the rates

$$k_{\text{freeze}} = S_p \sigma_{\text{gr}}^2 n_{\text{gr}} n_{\text{H}_2,O} \langle v_{\text{th}} \rangle$$

and

$$k_{\text{phd}} = G_o I_\nu \exp \left[-N(H_2)/N_{\text{eq}}\right] n_{\text{H}_2,O},$$

where $S_p$ is the sticking coefficient, for which we use 1 (Burke & Hollenbach 1983), $\langle v_{\text{th}} \rangle$ is H$_2$O molecule thermal velocity, and $I_\nu = 5.1 \times 10^{-10}$ s$^{-1}$ (Le Teuff et al. 2000) is the rate of FUV dissociation in an unshielded $G_o = 1$ field.

Gaseous atomic oxygen can freeze out onto grains, where it is assumed to form water ice by reactions with hydrogen atoms on the grain surfaces. O atoms may also form water in the gas phase via the standard sequence of reactions started by the reaction between O and H$_2$. The gas-phase formation of water thus proceeds at a rate

$$k_{\text{gas}} = k_{\text{form}} n_O n_{\text{H}_2},$$

where $k_{\text{form}}$ is equal to $8 \times 10^{-10}$ s$^{-1}$ cm$^{-3}$ (the rate coefficient for the reaction O + H$_2$ $\rightarrow$ OH + H$_2$) times 0.33 (the last factor accounts for the fraction of H$_2$O$^+$ recombinations with electrons forming H$_2$O; Le Teuff et al. 2000). The atomic oxygen abundance is also computed by the steady state equilibrium between formation and destruction processes: photodissociation of gas-phase water (eq. [3]) for the formation, and formation of gaseous water via reaction with H$_3^+$ (eq. [4]) and freezing onto the grains for the destruction of O. We assume that these reactions are the dominating processes and that all the oxygen not contained in CO or silicates is contained in O, H$_2$O, and H$_2$O ice.

Finally, the H$_3^+$ abundance is computed as follows. H$_3^+$ is formed by the cosmic-ray ionization of H$_2$ to form H$_2^+$, followed by the reaction with H$_2$ to form H$_3^+$. In the regions where CO molecules are not frozen onto the grain mantles, H$_3^+$ is destroyed by the reaction with CO. Elsewhere, the H$_3^+$ abundance is computed following the model described in Ceccarelli & Dominik (2005), which takes into account all three deuterated forms of H$_3^+$ and solves the chemical composition by considering the reactions between H$^+$, e$^-$, grains, and H$_3^+$ isotopologues.

## 3. DISCUSSION

Figure 2 shows the H$_2$O abundance (with respect to H$_2$) across the disk, for a standard interstellar UV field ($G_o = 1$). Figure 3 shows a vertical cross section of the chemical species involved in water formation at a radius of 700 AU. Despite the relatively large densities in the disk, water vapor has an abundance of $\sim 3 \times 10^{-7}$ in a large fraction of the outer disk,
indeed be found with relatively high abundances. The column does rise slightly with radius. Density is remarkably constant over most of the disk, although density is distributed as a function of the radius. The column.

FUV field by a factor of 10 results in decreasing the H$_2$O larger by only factor of 1.5 or 2, respectively. Decreasing the photodesorption rate of the grain mantles only at analytical proof of the insensitivity to ). The fundamental reason for this insensitivity is that in higher fields, the increased photodesorption of the ice is balanced by the increased photodissociation of gas-phase H$_2$O.

As discussed above, the value of the photodesorption yield, $Y$, is only constrained within a factor of roughly 3–10 by laboratory experiments. This uncertainty causes an uncertainty in the predicted H$_2$O column density by the same factor. Another important, and poorly known, parameter that enters into these computations is the dust-to-gas ratio. In the standard case, we assumed the canonical mass dust-to-gas ratio equal to 1%. If this value is increased by a factor of 10 (which means decreasing by a factor of 10 the gas density in the plot of Fig. 1), the H$_2$O column density increases by a factor of $\sim$1.2. On the contrary, a decrease by a factor of 10 of the dust-to-gas ratio leads to a decrease by a factor of 1.2 of the H$_2$O column density. This is due to the fact that the UV optical depth is determined by the dust distribution only and independent of the gas density. As long as photodesorption, photodissociation, and freeze-out are the dominant processes, the derived densities and column densities (as opposed to the abundances) of H$_2$O are independent of the gas density. The small changes are due to regions in which the gas formation route of H$_2$O is important. Also, therefore, a

![Fig. 2.](image1.png)

**Fig. 2.**—The $n$(H$_2$O)/$n$(H$_2$) ratio as a function of position in the disk. The solid line shows where the UV optical depth measured vertically to the disk plane is unity: $\tau_{uv} = 1$ (see text). The dashed lines show isodensity contours: from the top to the bottom, they are $10^6$, $10^7$, and $10^8$ cm$^{-3}$. The white region was excluded from the calculation because of the low density there.

In the layers just above the midplane, where the $A_{\nu}$ to the disk surface is lower than $\sim$5 mag. By midplane here we mean the region where more than $\frac{1}{2}$ of CO molecules are frozen onto the grain mantles. This occurs at a height of about 230 AU at a radius of 700 AU, and 100 AU at a radius of 400 AU. Above this height, CO is desorbed thermally. The gas-phase water abundance peaks near the surface where the FUV desorbing flux is high and where the H$_2$O abundance is high. In practice, the freeze-out rate of the H$_2$O molecules is larger than the FUV photodesorption rate of the grain mantles only at densities larger than about $10^7$ cm$^{-3}$. At lower densities, assuming water is in the grain surfaces, water vapor is formed mostly through direct photodesorption from mantles and, to a lesser extent, by gas-phase reactions occurring among atomic oxygen (a product of H$_2$O photodissociation) and H$_2$. In the upper layers, atomic oxygen is predicted to be very abundant. The resulting average gas-phase H$_2$O column density of a face-on disk is $1.6 \times 10^{14}$ cm$^{-2}$. Figure 4 shows how the column density is distributed as a function of the radius. The column density is remarkably constant over most of the disk, although the column does rise slightly with radius.

The first conclusion of our study is that water vapor can indeed be found with relatively high abundances ($\sim 10^{-7}$ to $10^{-6}$) and column densities ($\sim 1.6 \times 10^{16}$ cm$^{-2}$) in the protoplanetary disks that surround low-luminosity protostars illuminated by the interstellar radiation field (ISRF), like in the case of DM Tau. This is caused by the photodesorption of the icy grain mantles by the average ISRF. Increasing the FUV field by a factor of 10 or 100 leads to H$_2$O column densities larger by only factor of 1.5 or 2, respectively. Decreasing the FUV field by a factor of 10 results in decreasing the H$_2$O column density by a factor a bit more than 2. Therefore, the H$_2$O column density is not sensitive to the addition of a possible FUV field from the central source or a nearby hot star (see D. Hollenbach et al. 2005, in preparation, for details and an analytical proof of the insensitivity to $G_0$). The fundamental reason for this insensitivity is that in higher fields, the increased photodesorption of the ice is balanced by the increased photodissociation of gas-phase H$_2$O.

As discussed above, the value of the photodesorption yield, $Y$, is only constrained within a factor of roughly 3–10 by laboratory experiments. This uncertainty causes an uncertainty in the predicted H$_2$O column density by the same factor. Another

![Fig. 3.](image2.png)

**Fig. 3.**—Abundances and the visual extinction $A_V$ (from the disk surface) as a function of the height above midplane at 700 AU from the star. The solid and dashed lines show the abundance of H$_2$O and O, respectively. The dash-dotted and triple-dot-dashed lines show the abundance of CO and H$_3^+$, respectively. The dotted line indicates the $A_V$. The most important contribution to the H$_2$O column density is produced between $A_V \sim 1$ and $\sim$4 mag, and at a height between 100 and 250 AU. CO freezes out at a height of $\sim$230 AU. This causes a small increase of the H$_2^+$ abundance, since CO (along with O) is the main destroyer of H$_2^+$. The high abundance of CO at very low $A_V$ may be artificial because we have ignored CO photodissociation. The water ice abundance is not shown because it is almost constant $2 \times 10^{-4}$ throughout the plot.

![Fig. 4.](image3.png)

**Fig. 4.**—Gas-phase H$_2$O column density measured perpendicular to the disk midplane as a function of the radius. In the very inner regions, the H$_2$O column density decreases because the gas densities at $A_V \sim 1$ are higher, leading to a greater proportion of H$_2$O that is frozen out onto grains as opposed to photodesorbed. Once the grains are hotter than 100 K ($R \approx 30$ AU), water will not freeze out, and gas-phase abundances will rise again (not shown).

In our model, CO molecules are not photodesorbed from the mantles, although this is plausible, depending on the structure of the mantles and where on the grain the frozen CO is located. However, the gas-phase CO abundance has only a minor influence on the gas-phase H$_2$O abundance in our model.
drastic change in the dust-to-gas ratio does not cause much of a change in the H$_2$O vapor column density. Finally, the results will also depend on the grain size distribution. If much smaller grains than 0.1 $\mu$m dominate the grain surface area, the balance between the different formation and destruction rates will be shifted. This question will be discussed in a follow-up paper.

In conclusion, we predict an H$_2$O column density of a few times $10^{15}$ cm$^{-2}$ in protostellar disks similar to that surrounding DM Tau, which is rather insensitive to the external FUV field and/or the dust-to-gas ratio in the disk.

Ceccarelli et al. (2005) reported the detection of HDO in DM Tau, with an observed column density of $\sim 1.6 \times 10^{15}$ cm$^{-2}$. Based on the present theoretical model, the H$_2$O column density is predicted to be $\sim 2 \times 10^{15}$ cm$^{-2}$, within about a factor of a few, given the uncertainties in the yield, FUV field, and the dust-to-gas ratio. This implies an HDO/H$_2$O ratio equal to about 1%. This is consistent with estimates of the HDO/H$_2$O ratio in embedded low-mass protostars. Parise et al. (2005) measured an HDO/H$_2$O ratio equal to 3% in the sublimated ices surrounding bedded low-mass protostars. This is an excellent tool to measure the photodesorption yield $Y$. Because of the weak dependence on parameters, the measurement of the H$_2$O column density in protoplanetary disks is an excellent tool to measure the photodesorption yield $Y$.

The results reported in this Letter lead to the following important conclusions:

1. An external UV radiation field as weak as the average Habing field ($G_0 = 1$) can produce a layer of H$_2$O on top of a protoplanetary disk (like that surrounding DM Tau) with a column of a few times $10^{15}$cm$^{-2}$.

2. This column density is insensitive to external parameters like the strength of the radiation field: Variations in $G_0$ by 2 orders of magnitude only change $N$(H$_2$O) by a factor of 2.

3. Similarly, changing the dust-to-gas ratio (i.e., the gas density at a given dust density) has only a weak influence on the derived column densities.

4. Because of the weak dependence on parameters, the measurement of the H$_2$O column density in protoplanetary disks is an excellent tool to measure the photodesorption yield $Y$.

5. Combined with previous observations of HDO (Ceccarelli et al. 2005), we predict an HDO/H$_2$O ratio in the outer disk of DM Tau of 0.01, with an uncertainty of about a factor of a few.

6 We predict that the H$_2$O ground-state line at 557 GHz is undetectable in DM Tau with Odin and/or Herschel Space Observatory HIFI observations.

Finally, we remark that other molecules trapped in the water ices could also be released into the gas phase, keeping “alive” the gas chemistry in the layers above the midplane of the outer disk.

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