Chemistry of a Protoplanetary Disk with Grain Settling and Lyman α Radiation

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Abstract

A critical component in calculating the correct chemistry of protoplanetary disks is the proper treatment of the incident UV field on these disks. We present results from a new model in which we directly calculate the changing propagation and penetration of the high energy radiation field as the dust grains evolve. We also have explored the effect of Lyman α photons on the disk chemistry, a component that has been left out of other disk chemistry models. In some T Tauri stars, Lyman α radiation has been shown to dominate the UV fields, carrying up to 75% of the UV flux. In addition, the dust grains' evolution plays a large role in determining how deep the UV radiation penetrates into the disk. Grain settling at the mid-plane leads to much smaller freeze-out regions and a correspondingly larger molecular layer, which leads to an increase in column density for molecular species such as CO, CN and SO in settled disks. The inclusion of Lyman α radiation impacts the disk chemistry through specific species that have large photodissociation cross sections at 1216 Å. These include HCN, NH_3 and CH_4, for which the column densities are decreased by an order of magnitude or more due to the presence of Lyman α radiation in the UV spectrum. A few species, such as CO_2 and SO, are enhanced slightly by the presence of Lyman α radiation, but rarely by more than a factor of a few.

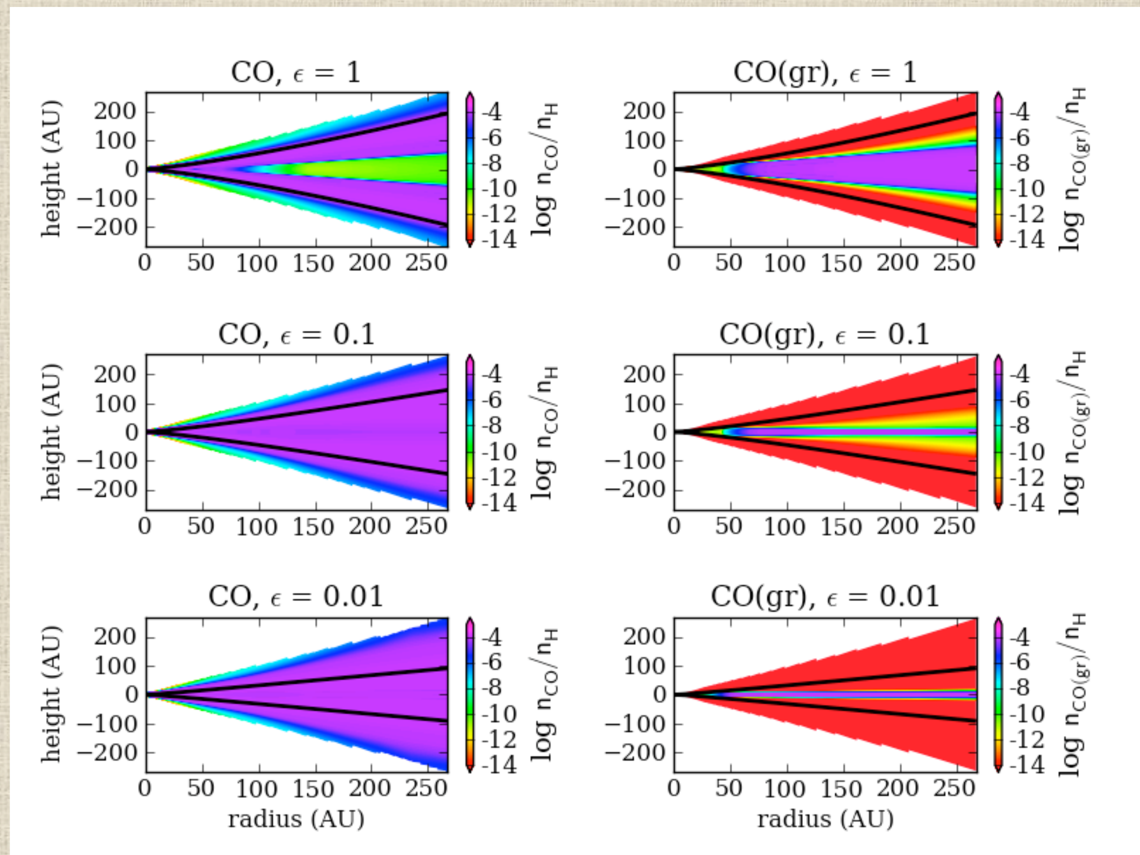
Introduction

•Disk chemistry models are highly dependent on the physical structure of the disk as well as the radiation field used in the model.

•Beyond ~100 AU the chemical structure of the disk can be divided into three layers: the photon dominated layer, where atoms dominate, the warm molecular layer, where gaseous molecules dominate and the midplane, where ices dominate.

•Our model explores some new effects, including the transfer of Lyman α radiation, which has been shown to dominate the UV field. In tandem we explore the effects of dust settling, which is the initial step for planet formation.

Effects of the Initial Stage of Planet Formation: Dust Settling



This plot shows molecular CO and CO frozen onto grains, CO(gr), for three different cases of dust settling. The dust settling parameter ε is defined as the ratio of the dust-to-gas ratio in the upper disk to the standard value. As the amount of dust settling increases, the warm molecular layer shifts lower in the disk (left plots). Additionally, the freeze-out region shrinks significantly with increased dust settling since the temperature at the midplane is now much higher (right plots).

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Summary

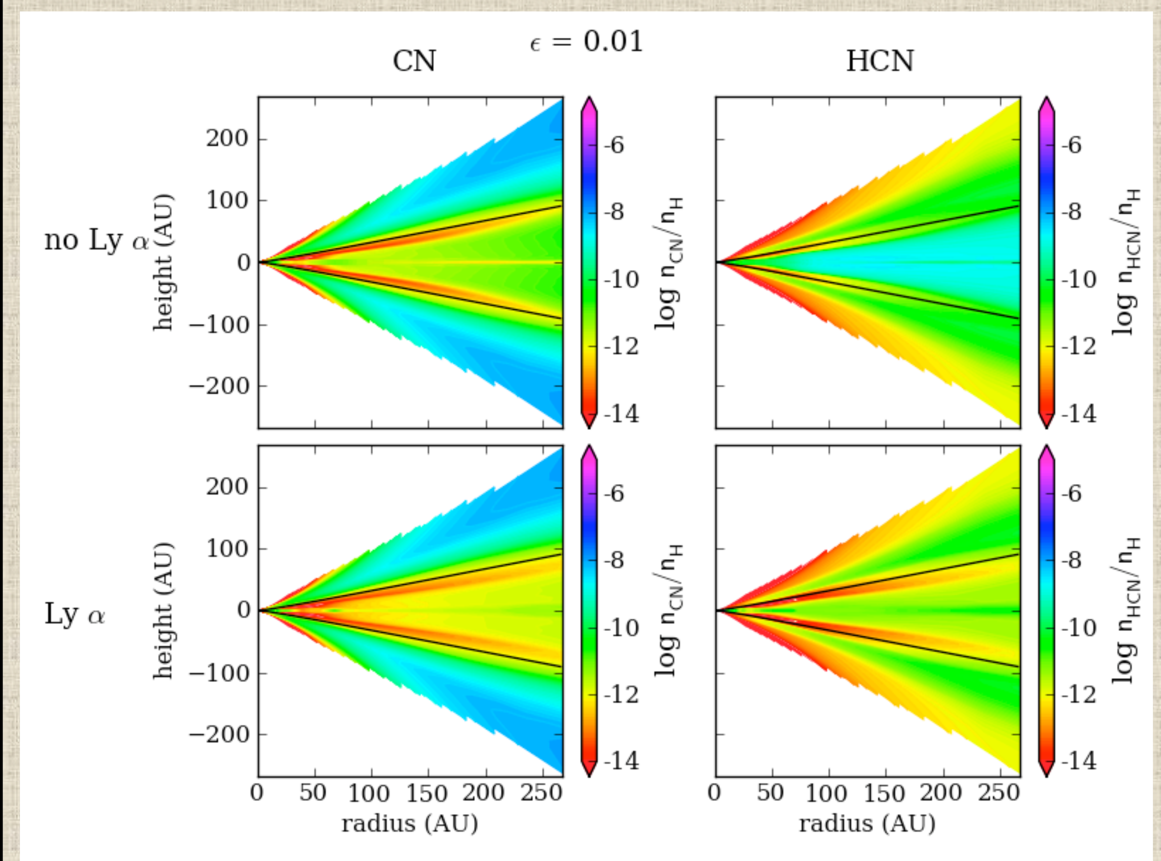
•Lyman α radiation and dust settling combined have a large effect on the chemistry of protoplanetary disks.

•Lyman α should be included in the radiation field for all future models of disk chemistry.

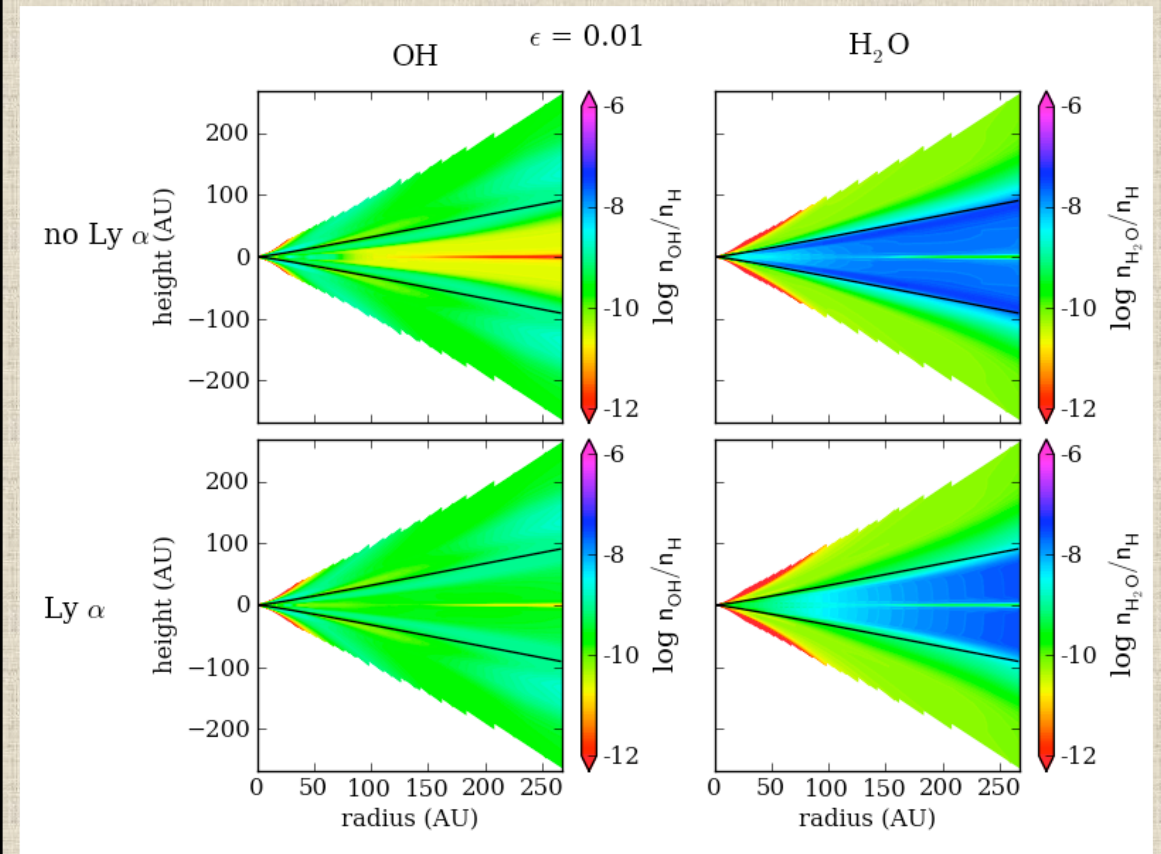
• The x-ray ionization rate can be significantly affected by dust settling

• The spectral type of the central star plays a large role in the chemistry of the protoplanetary disk.

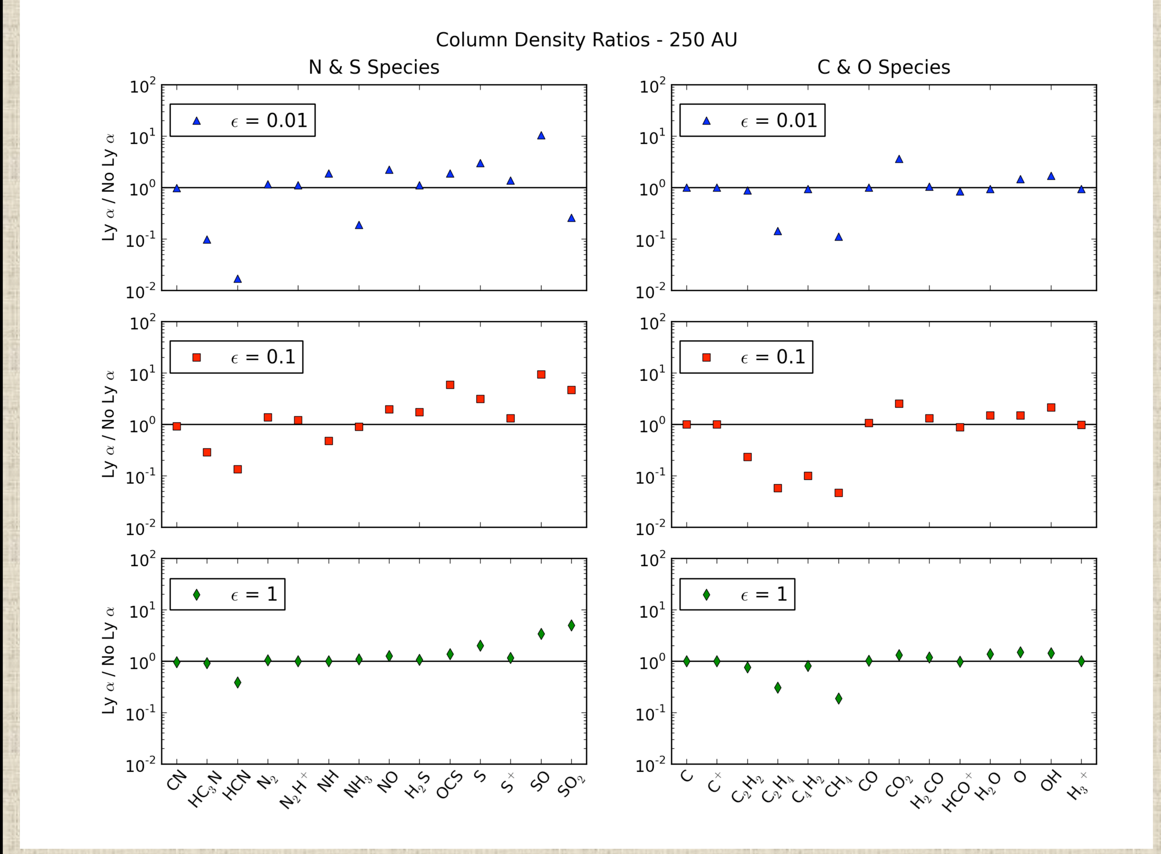
Lyman α Photons and Disk Chemistry



This 4-panel figure shows the abundances of CN and HCN with respect to H in the disk for models with and without Lyman α radiation included. The significant decrease in HCN abundance when Lyman α radiation is included is due to the fact that HCN has a large cross section at 1216 Å. This increases the photodissociation rate and lowers the abundance of HCN in the disk.



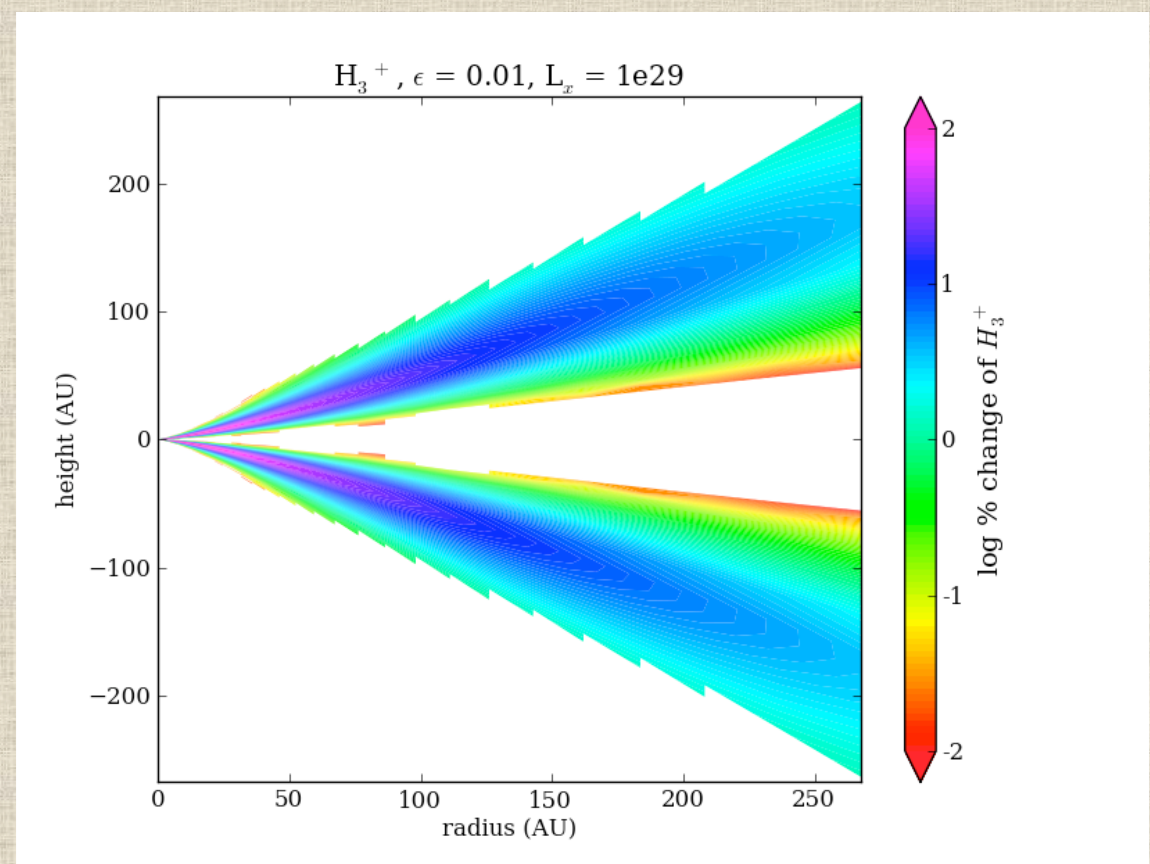
Unlike HCN, while H_2O has a large cross section at 1216 Å, it is not highly depleted when Lyman α radiation is included in the model. This is due to Lyman α photodesorption of H_2O(gr) replenishing the H_2O that is photodissociated. This effect can also be seen in the abundance of OH, which actually increases slightly due to the presence of Lyman α radiation due to the same photodesorption.



The figure above shows the effects of Lyman α radiation on the column density of molecules in the inner and outer regions of the disk for different dust settling parameters. The ratios are plotted as the column density for the model with Lyman α radiation divided by the column density for the same model, but with Lyman α radiation removed. A larger ratio means that the column density increased when Lyman α radiation was added to the model. Note the significant decrease in the column densities of both HCN and CH_4 for all of the models and the decreases in other molecules such as NH_3 and SO_2 in the cases where dust settling is significant.

Dust Dependent X-ray Ionization

X-ray ionization produces H_3^+, which is a major driver for chemistry in the disk. UV radiation, in comparison, creates C^+ through photodissociation. The x-ray ionization will therefore activate a different chemistry than the UV field does.



This figure shows the effect of including dust settling in the x-ray ionization rate calculation. The amount of H_3^+ can be enhanced by an order of magnitude or more, especially in the upper regions of the disk, as compared with a model that does not include dust settling in calculating the x-ray ionization rate

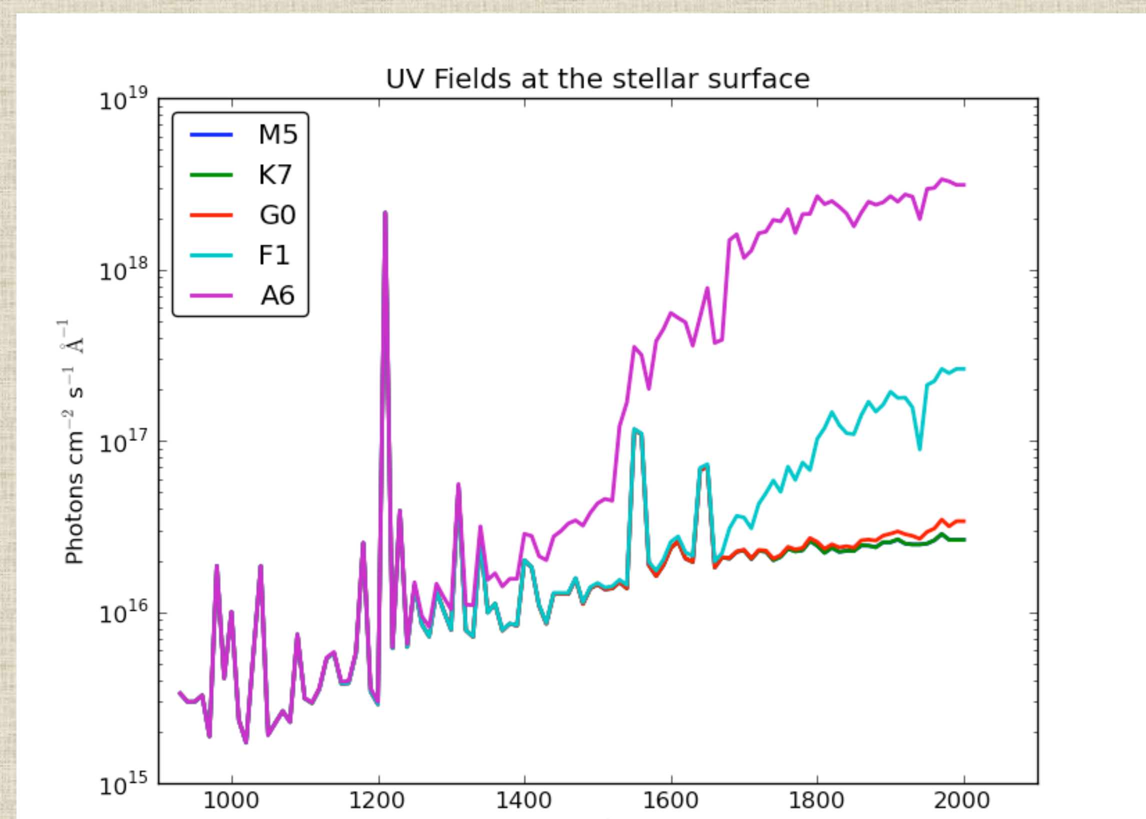
Effect of Central Star Spectral Type

• The central star determines the UV field incident on the disk

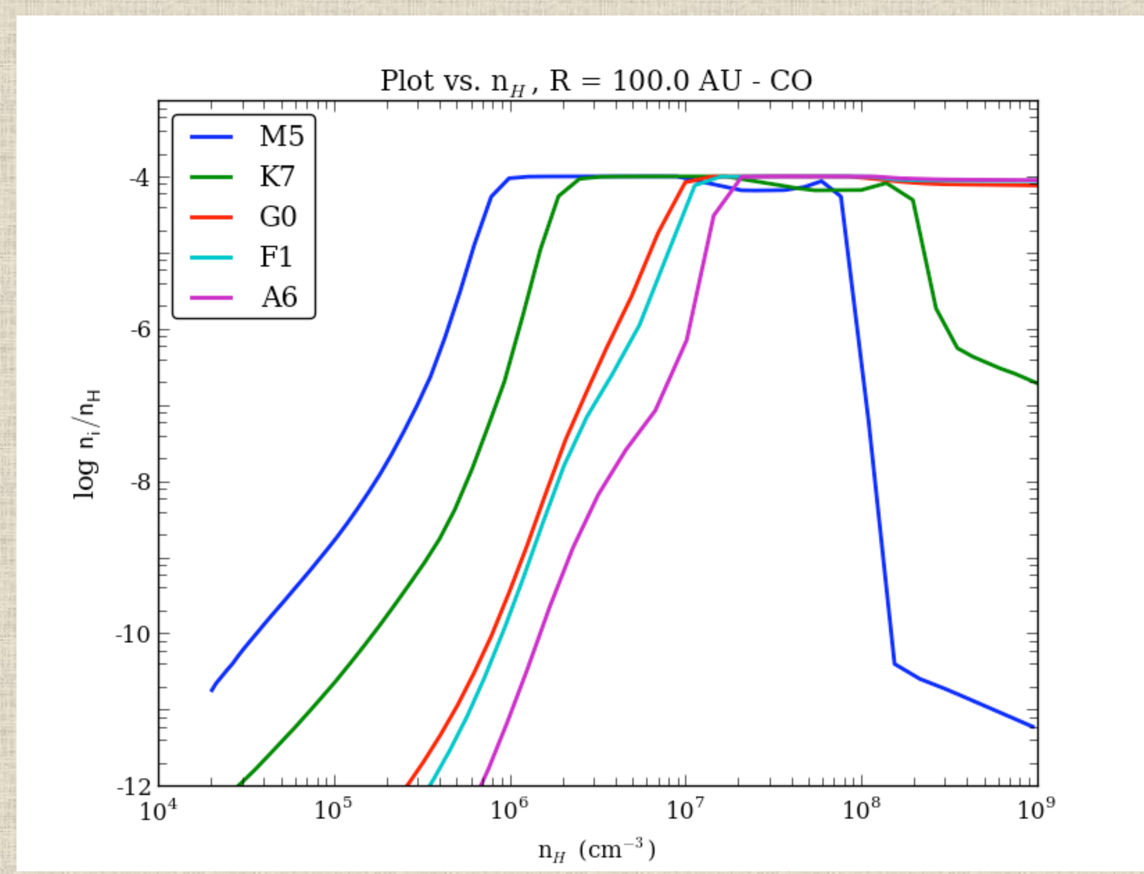
• Temperature structure of the disk is also dependent on the central star

• The chemistry is highly dependent both on the temperature of the disk and on photodissocation within the disk, so the central star plays a large role in determining the chemistry seen in these disks.

• The freeze-out region shrinks and the molecular region grows as the disk temperature is increased.



This figure demonstrates the importance of the central star's spectral type on the UV field incident on the protoplanetary disk. These fields were calculated by combining a Kurucz model for each type with the spectra of TW Hya.



The figure above shows a comparison of CO abundances at R = 100 AU for disks around different spectral type stars. The disks around the larger stars (G0, F1, A6) are warm enough that very little of the CO is frozen out onto grains at 100 AU. In comparison, there are clear molecular and freeze-out regions seen around the M5 and K7 stars.