Key Ingredients

- For completeness:
  - shocks --> what about the accretion shock onto the disk
  - high temperature chemistry --> 1 big effect that should be stated

- Radiation -- provides source of ionization to power chemistry and warms grains to release frozen molecules
  - Cosmic Rays
  - UV
  - X-rays
  - Extinct Radionuclides

The Accretion Shock

- During the initial stages of infall and the formation of the disk material will rain on central star and on inner disk -- providing a accretion shock
- As the infall proceeds the centrifugal radius, r_c, (the inner radius within which infall occurs) grows: $r_c \propto t^3$ (see Tereby, Shu, and Cassen 1984; Hartmann 1998)
- When shock speeds exceed ~15-20 km/s the mantle can be sputtered off the grain surface (Caselli et al. 1997; Schilke et al. 1997)
  - Lunine et al. 1991 used this idea to suggest all ices sublimate and recondense with the effects greatest in the inner (< 30 AU) disk

The Accretion Shock

- Neufeld and Hollenbach 1994:

$$v_s = \sqrt{\frac{GM}{3r_c}} = 17.2 \left[\frac{M(t)}{M_\odot}\right]^{1/2} \left[\frac{r_c(t)}{1AU}\right]^{-1/2} \quad km\ s^{-1}$$

- Should lead to copious water creation (sputtering of infalling water coated grains) in early stages for the inner disk.
- Less important for outer disk and at later evolutionary stages.
- Means most material should arrive on disk unaltered from ISM initial state.

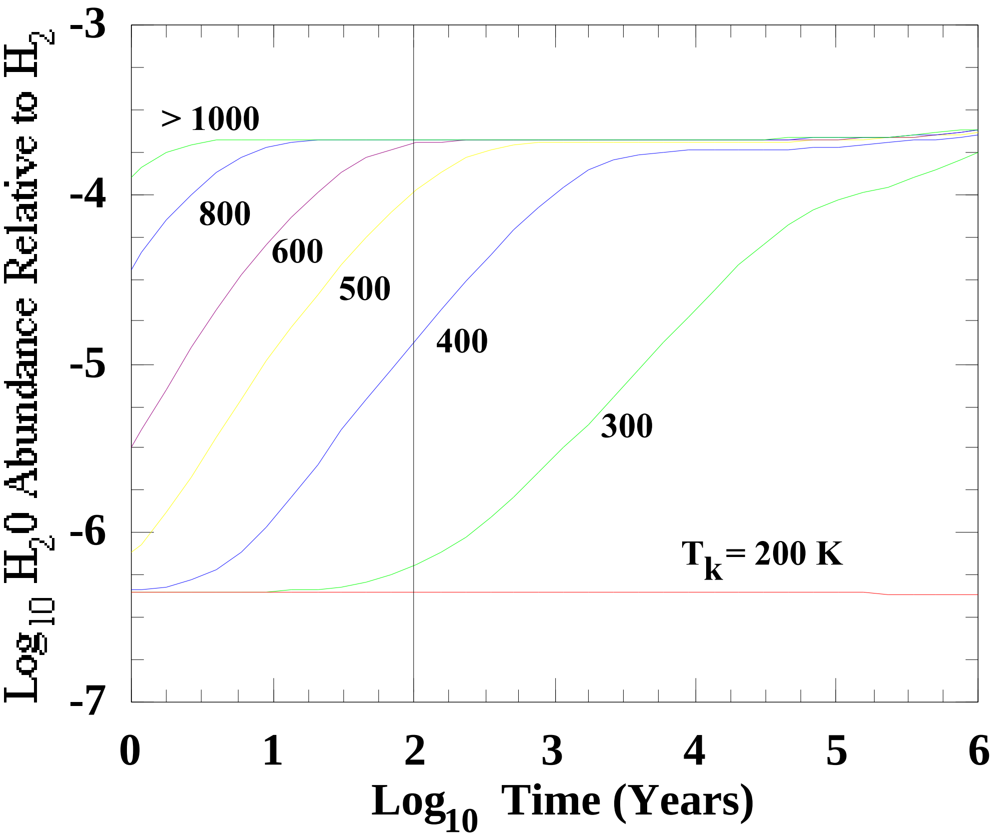
High Temperature Chemistry

- When gas temperatures exceed > 300 K a series of well studied reactions lead to all atomic oxygen going into water.

$O + H_2 \rightarrow OH + H$

$OH + H_2 \rightarrow H_2O + H$

-- inner nebula must have been rich in water vapor



Bergin et al. 1998

Cosmic Rays

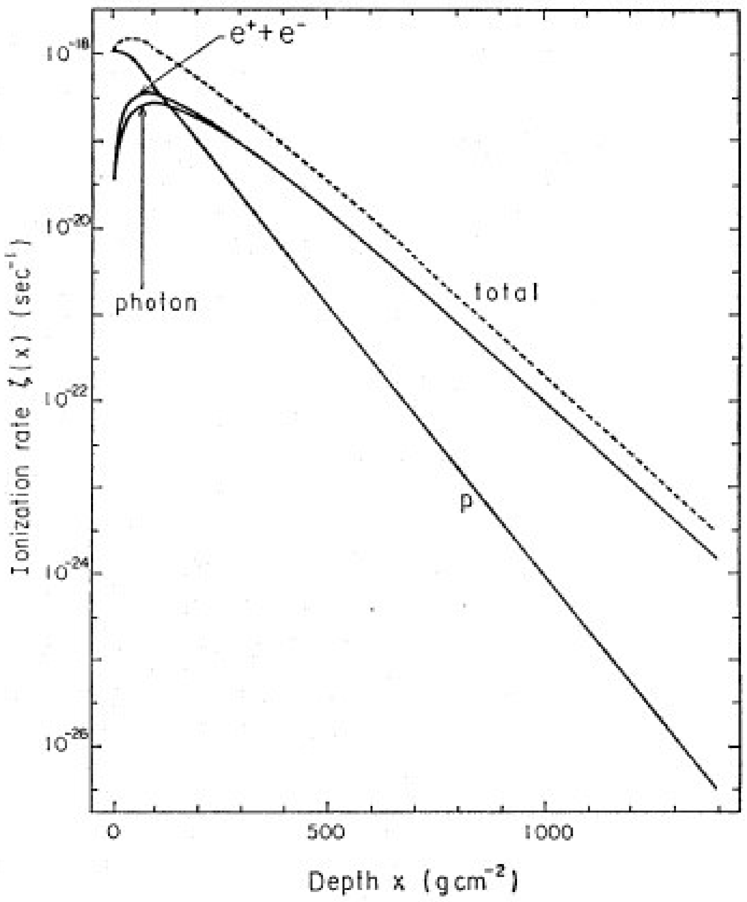
- Cosmic ray ionization rate estimated from ISM observations and Voyager data.

$$\zeta_{cr,0} = 1.3 \times 10^{-17}\ \mathrm{s}^{-1}$$

  - Webber 1998
  - van der Tak and van Dishoeck 2000
- Umebayashi and Nakano (1981) examined penetration depth of cosmic rays –find:

$$\Sigma_{cr} = 96\ \mathrm{g\ cm}^{-2}$$

- Rate goes as (Σ_1 = gas column from above and Σ_2 = gas column



$$\zeta_{cr} = \frac{\zeta_{cr,0}}{2}\left[\exp\left(-\frac{\Sigma_1}{\Sigma_{cr}}\right) + \exp\left(-\frac{\Sigma_2}{\Sigma_{cr}}\right)\right]$$

Cosmic Rays

- Caveat:
  - Cosmic rays in our solar system are scattered by the solar magnetic field
  - Only high energy C.R. penetrate -- not the ones responsible for ionization
  - Cosmic rays represent the best mechanism to ionize the midplane where most mass resides
  - The detection of ions and comparison with models suggest that some mechanism is active at large radii
  - Cosmic rays are likely available for the outer disk ($r > 100$ AU)
  - Confirming inner disk will require ALMA

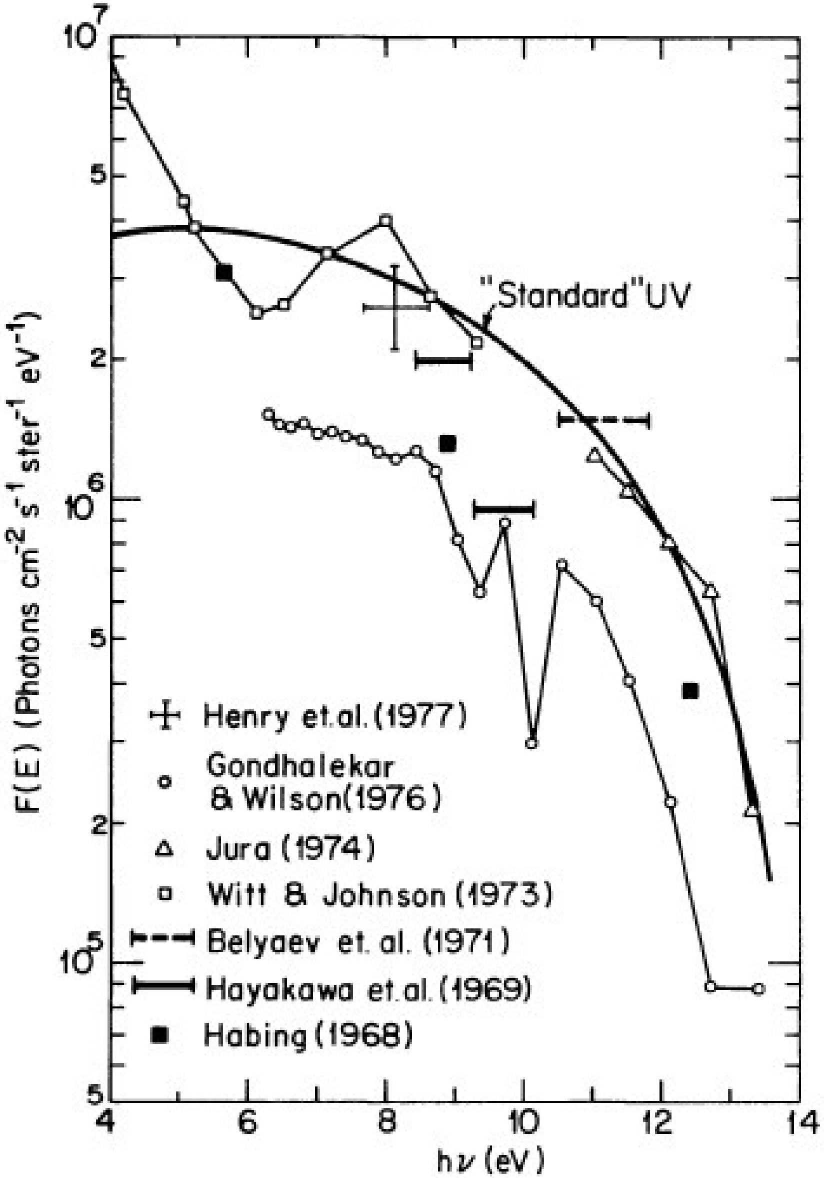
Ultraviolet Radiation

- T Tauri stars have excess UV flux much higher than their effective temperature ~ 3000 K
  - From accretion shock and potential contributions from active chromosphere (Calvet and Gullbring 1998; Alexander et al. 2005)
- Observations suggest it plays a key role in observed molecular emission.
- Willacy and Langer (2000) and Aikawa et al. (2001) first noted importance of photoprocessing in terms of chemistry.
  - Observed effects such as CN/HCN ratio and its similarity to enhancements seen in ISM noted earlier.
- 2 fields to consider --
  - Stellar radiation field
  - Interstellar radiation field: especially if star born within a cluster (this area has not yet fully been examined)

Stellar Radiation Field

- Initial studies placed field in context of interstellar radiation field.
  - Habing (1968): $G_0 = 1$ defined as equivalent to 1.6×10^{-3} erg cm^{-2} s^{-1}
  - Draine (1978): $\chi = 1$

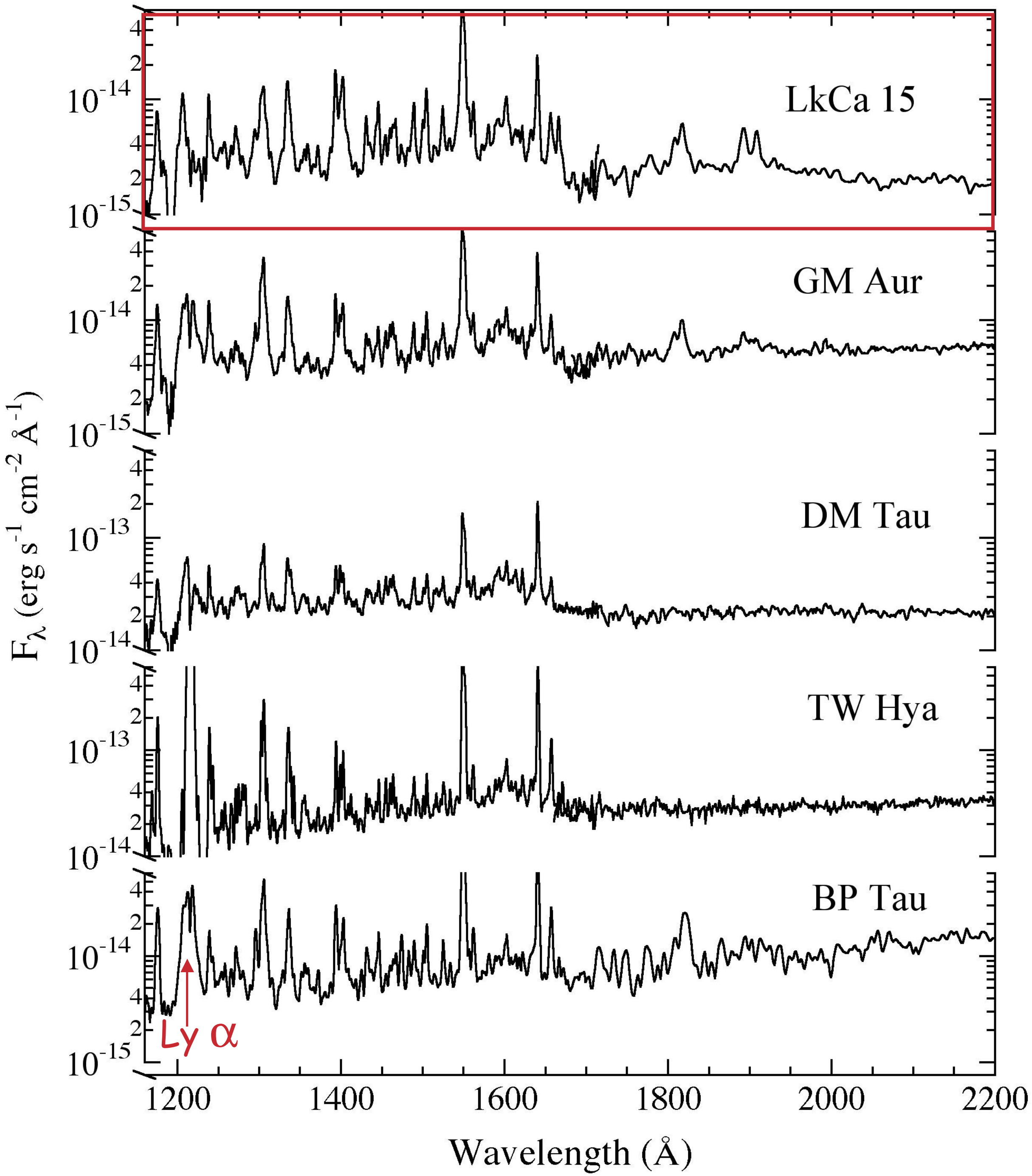
  $\chi = G_0 \times 1.7$
- Enables use of ISM chemical networks developed using models of interstellar grain absorption and scattering.
  - Roberge et al. 1981
  - Roberge et al. 1991
  - Cecchi-Pestellini et al. 1995
  - Nice summary in van Dishoeck (1988), *Rate Coefficients in Astrochemistry*



Draine 1978

Stellar Radiation Field

- Stellar UV generated at least in part by accretion (may be an active chromospheric component: Calvet, Clarke)
- First pass: using IUE obesrvations of T Tau and RU Lup
- FUV below 2000 Å:
  - $F_\lambda = 3 \times 10^{-13}$ erg cm^{-2} s^{-1} Å^{-1}
  - Scaled to 100 AU and integrated over 1000 Å (Lyman limit to 2000 Å): 23.5 erg cm^{-2} s^{-1}
  - $G_0 = 1.5 \times 10^4$ at 100 AU
  - Will scale as $1/r^2$ with radius
- BUT: not all T Tauri stars are the same -- T Tau and RU Lup are strong accretors with $dM/dt \sim 10^{-7}\ M_\odot\ \mathrm{yr}^{-1}$
- Typical TTS has $dM/dt \sim 10^{-8}\ M_\odot\ \mathrm{yr}^{-1}$



G_0 at 100 AU

LkCa15: 240

GM Aur: 340

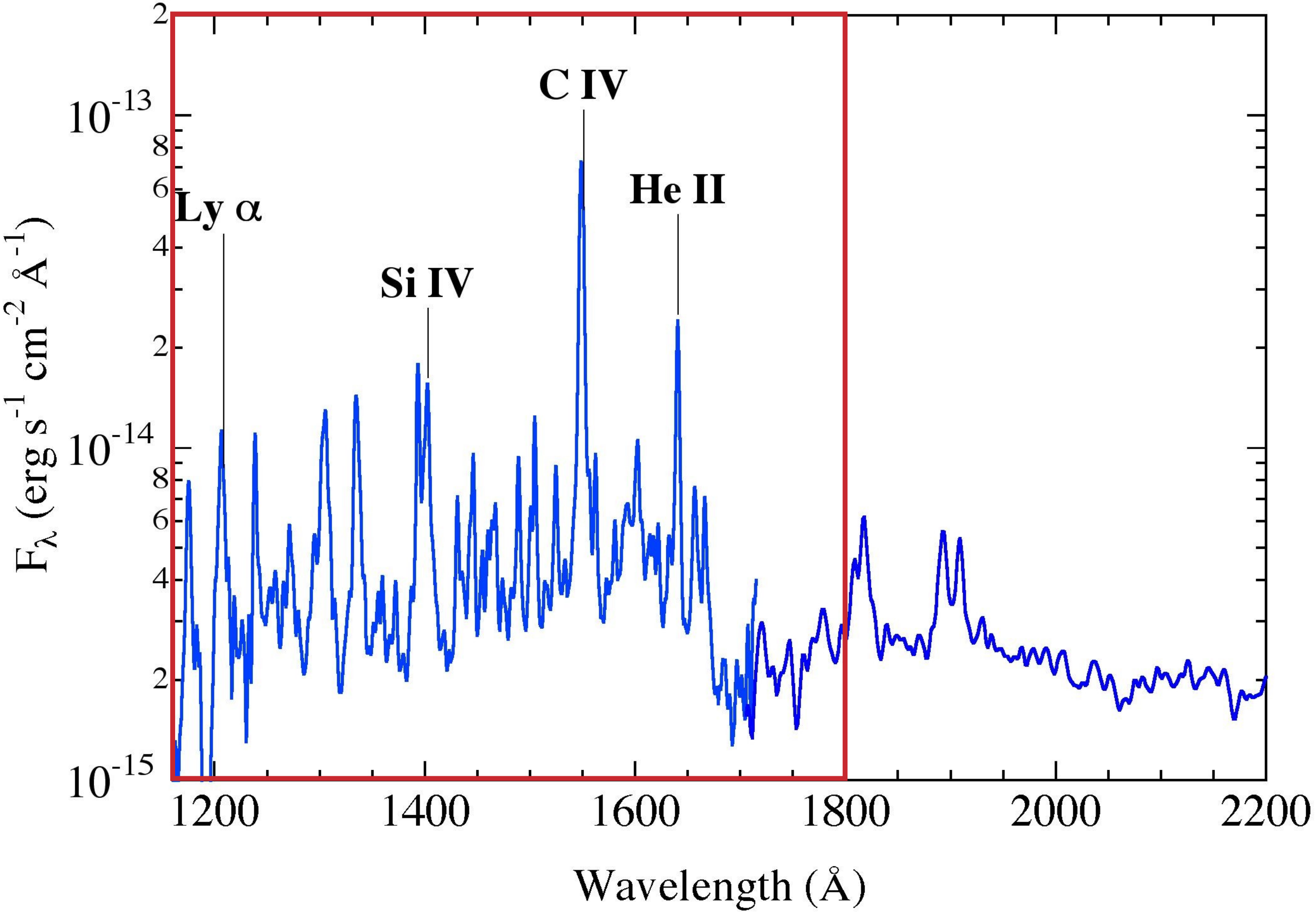
DM Tau: 1500

TW Hya: 3400

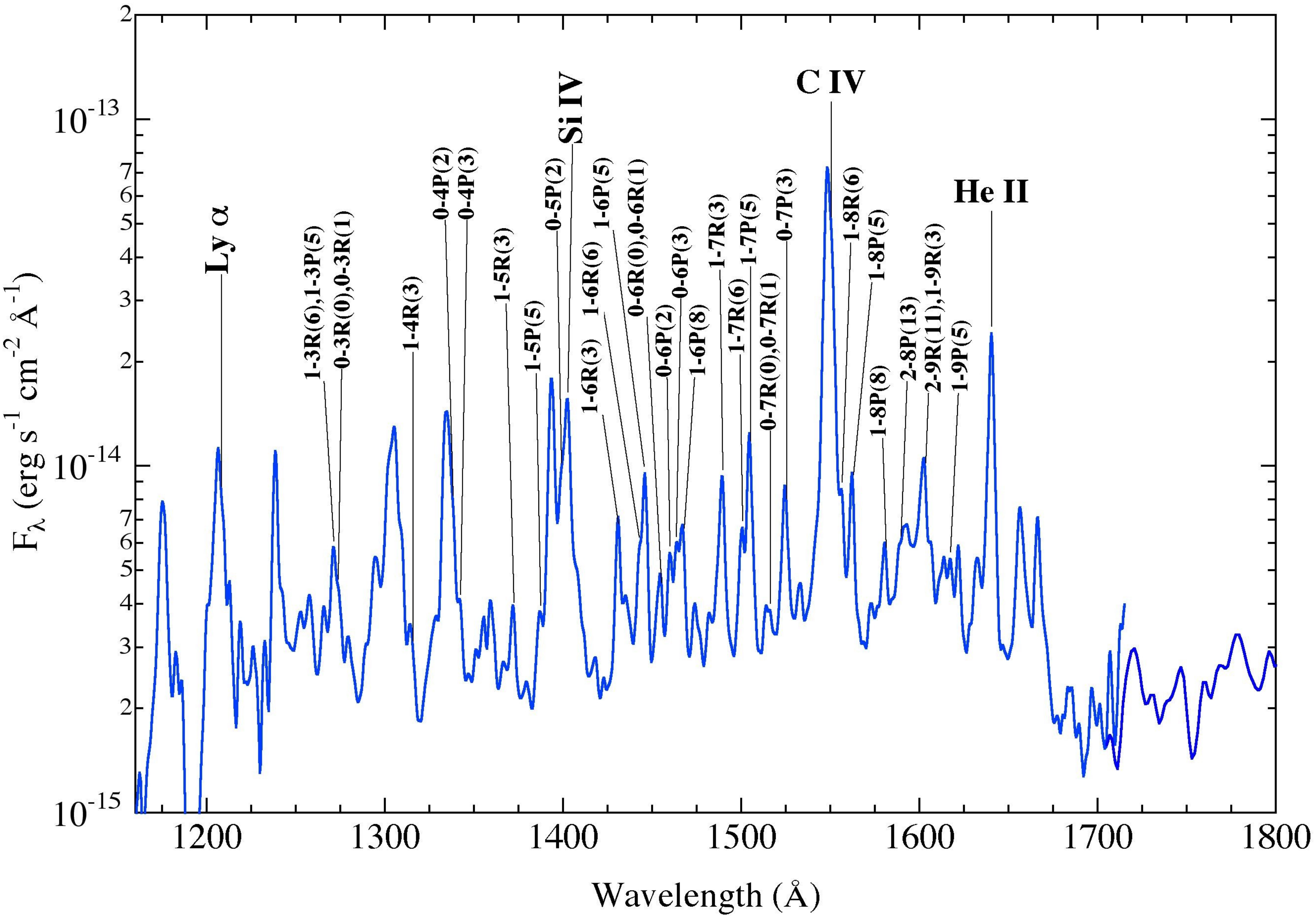
BP Tau: 350

Bergin et al. 2004

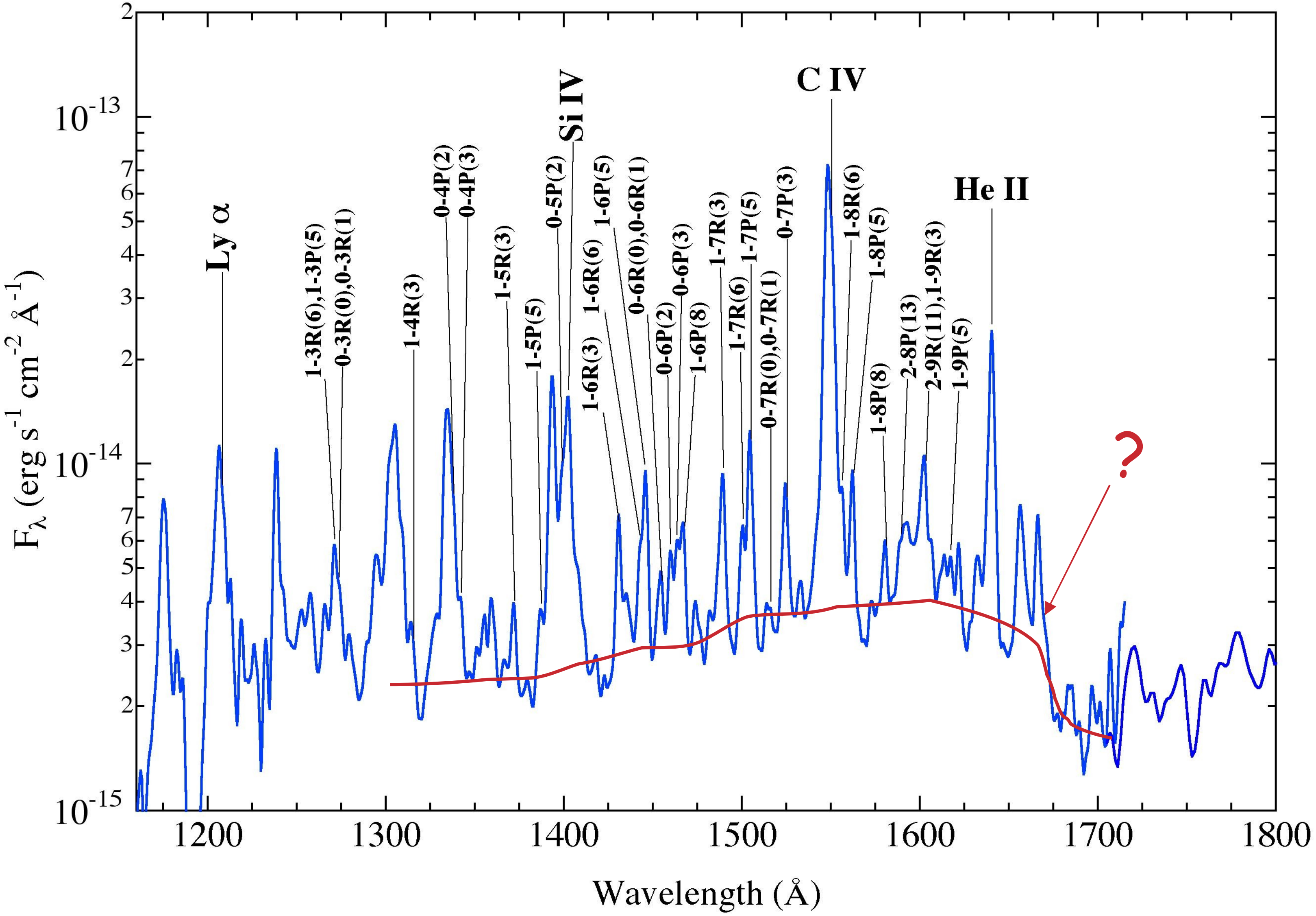
LkCa15 HST/STIS Spectrum

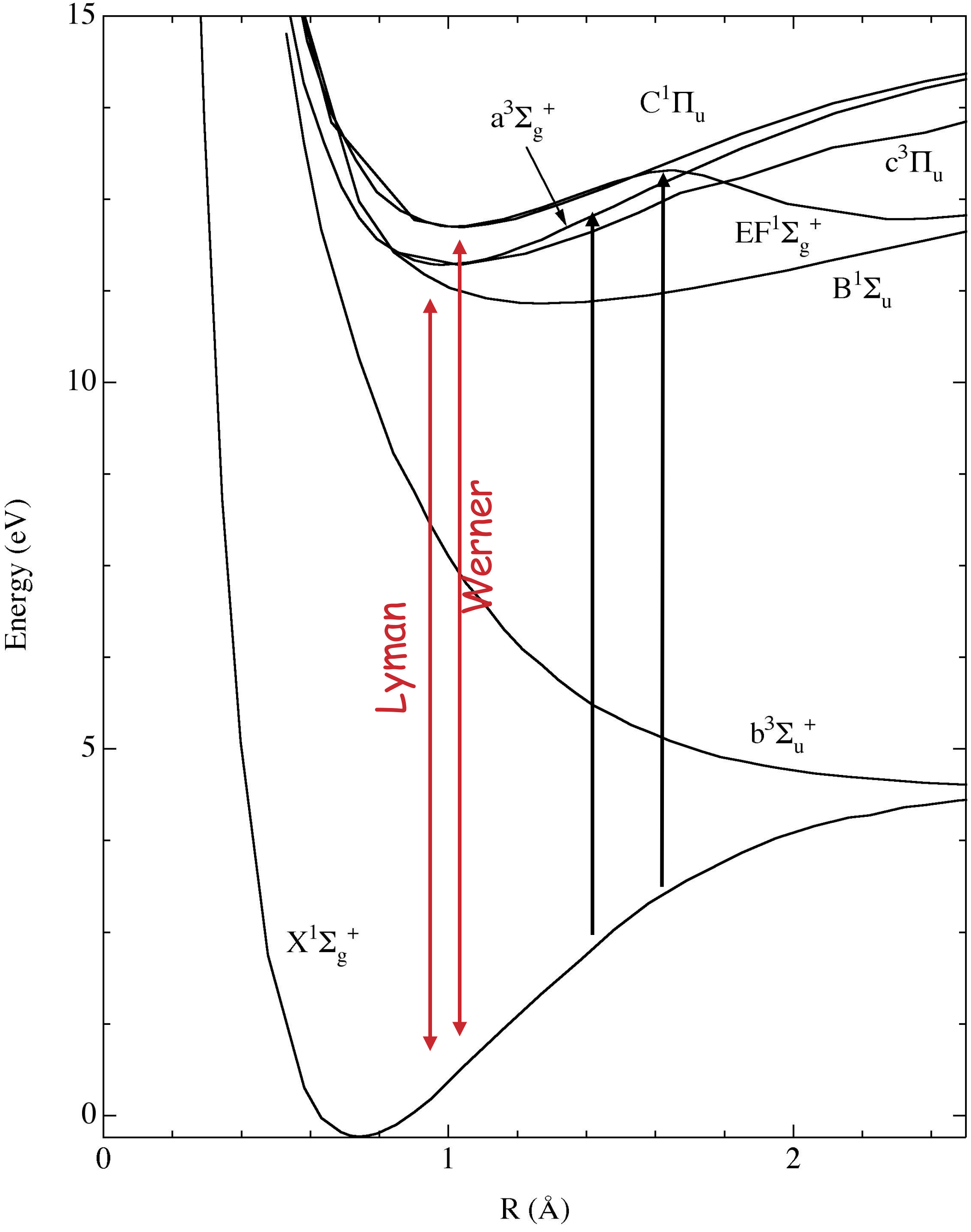


LkCa15 Ly α pumped H_2 Emission

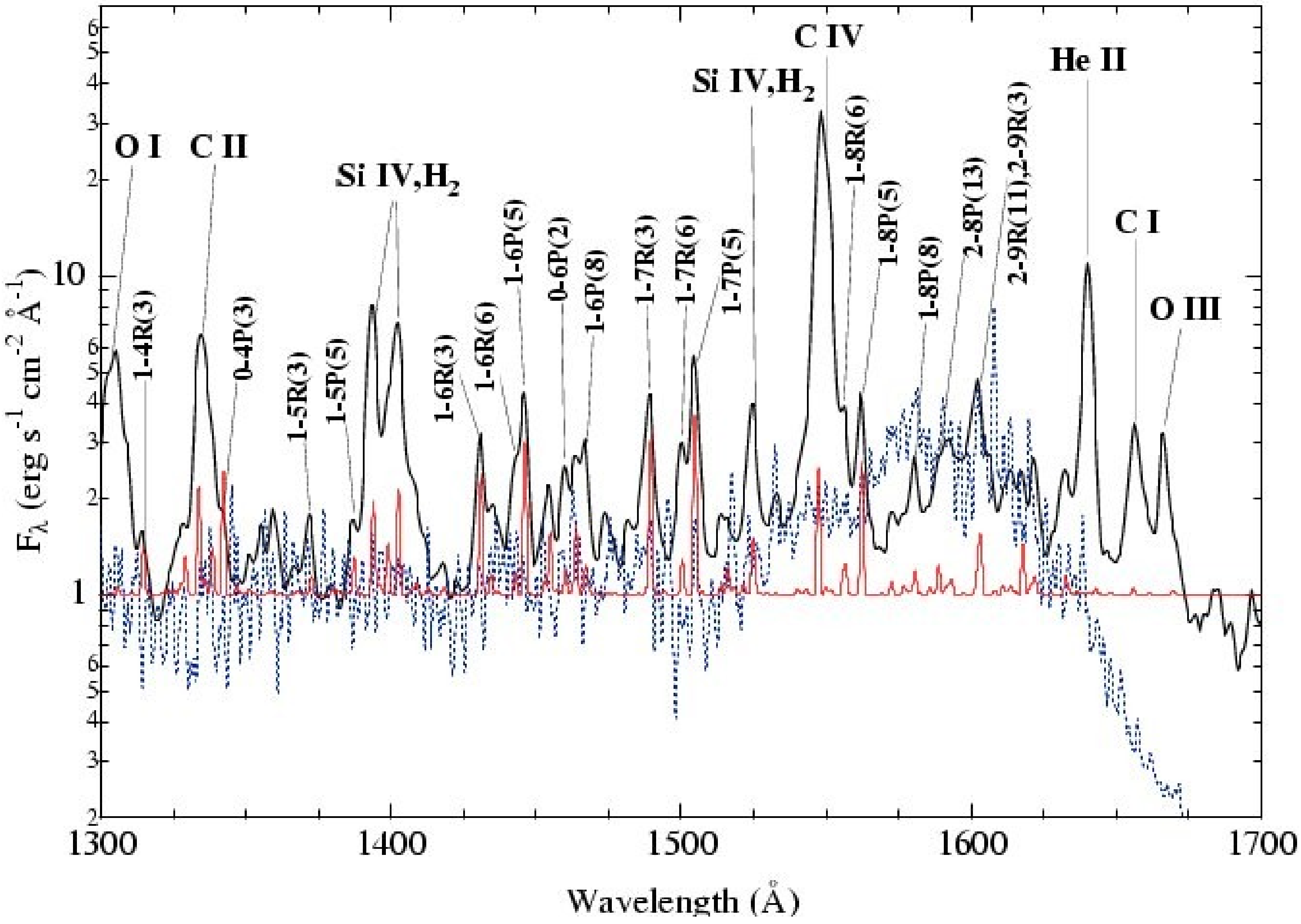


Electron Impact Excitation?




15
10
5
0
Energy (eV)
0
1
2
R (Å)
$a^3\Sigma_g^+$
$C^1\Pi_u$
$c^3\Pi_u$
$EF^1\Sigma_g^+$
$B^1\Sigma_u$
$b^3\Sigma_u^+$
$X^1\Sigma_g^+$
Lyman
Werner

Radiation Field: UV Emission from Molecules

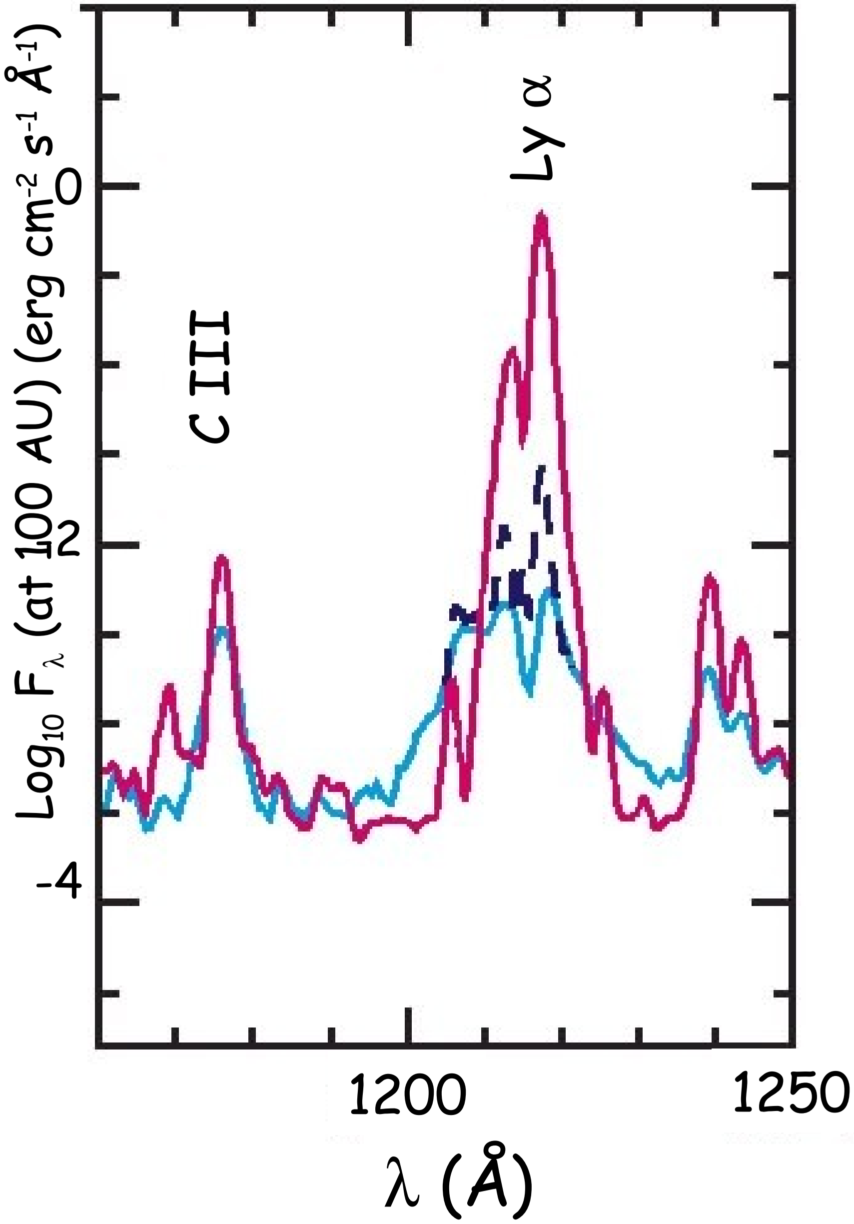


solid black line: observations
solid red line: model of H_2 Ly α fluorescence
dotted blue line: model of electron - H_2 collision emission
models of H. Abgrall and E. Roueff

Ly α Radiation

- Ly α radiation absent from ISRF

- Flux from TW Hya 2 orders of magnitude above BP Tau/CY Tau (no IS/local cloud absorption but is circumstellar absorption)

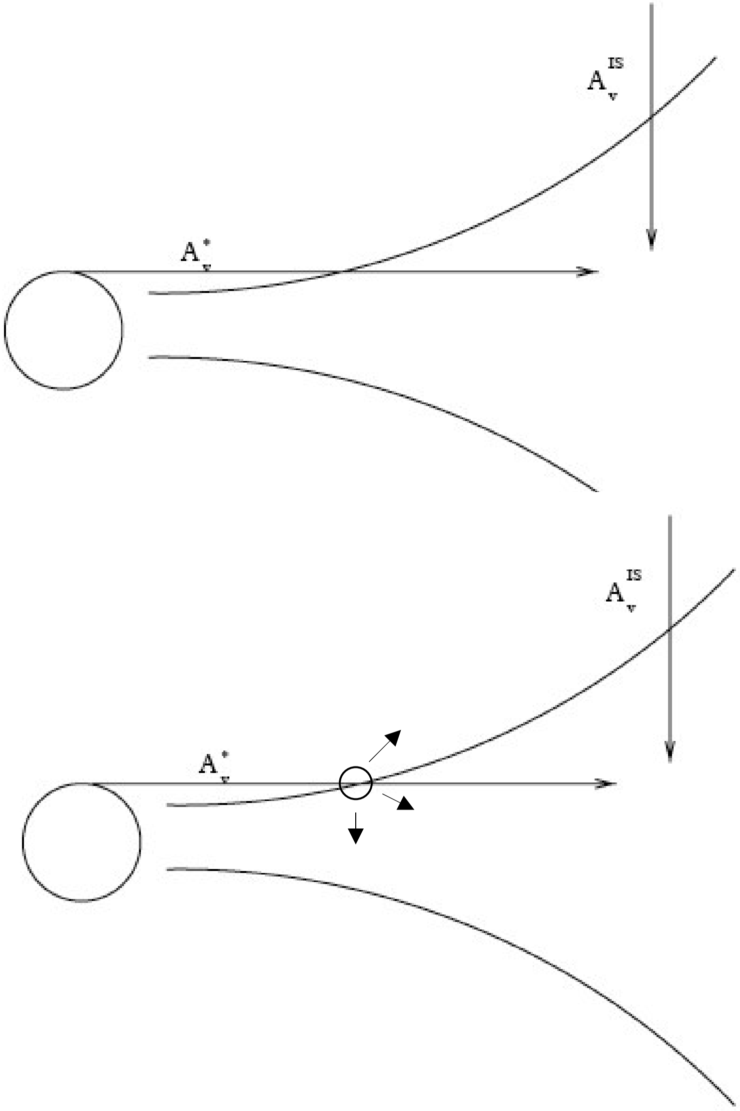


- Purple: TW Hya ($\dot{M} = 5 \times 10^{-9}$ M$_\odot$/yr)
- Light Blue: BP Tau ($\dot{M} = 3 \times 10^{-8}$ M$_\odot$/yr)
- Blue: CY Tau (~ BP Tau)

Bergin et al 2003

UV Radiation Transfer

- Stellar field has shallow angle of incidence on flared disk
- External/ISM field has normal angle of incidence
- van Zadelhoff et al. 2003: detailed model of UV radiation transfer.
  - showed that scattering aids the penetration of the stellar field
- Bergin et al. 2003: analytical solution



UV Radiation Transfer

- Define mean intensity: $J_\lambda = \frac{1}{4\pi}\int I_\lambda d\Omega$
- Mean intensity impinges on surface with angle θ_0; $\mu_0 \equiv cos\theta_0$
- J_λ decays by $e^{-\tau_\lambda/\mu_0}$; at R = 100 AU $\mu_0(1000\mathring{A}) = 0.07$
- solution of radiation transfer has 2 terms (use standard u, v forms in Mihalis 1978)

Direct attenuation of field

Scattered component

$$J_\lambda = \frac{I_*}{2} C_1 e^{-\tau_\lambda/\mu_0} + \sigma_\lambda I_* \mu_0 C_2 e^{\sqrt{3(1-\sigma_\lambda)}\tau_\lambda},$$

where

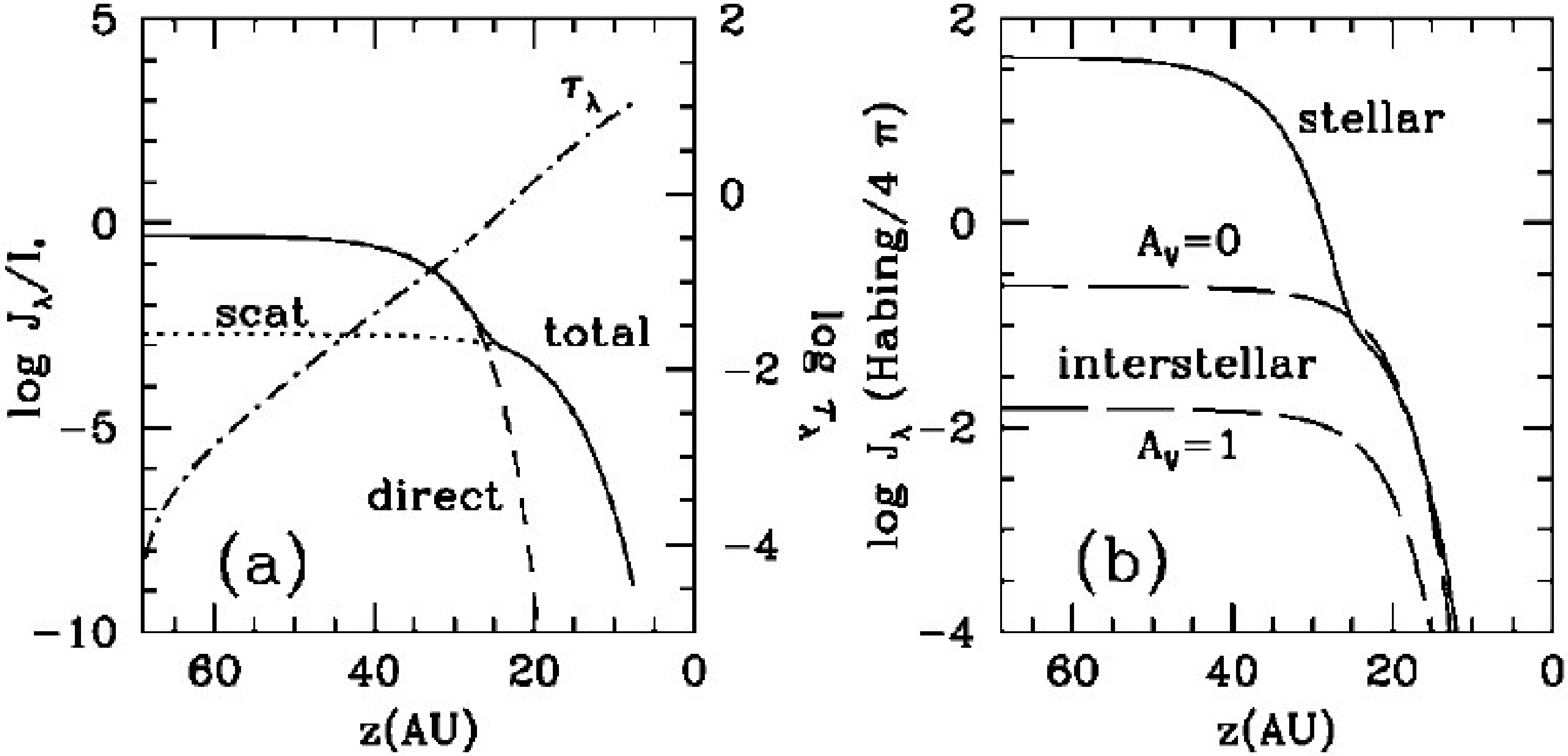
$$C_1 = 1 - 3\sigma_\lambda \mu_0^2,$$

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

Bergin et al. 2003

UV Radiation Transfer

Shown at 1500 Å and R = 100 AU



- Normal ISRF equivalent to stellar at 100 AU -- stellar field will dominate for r < 100 AU

- If IRSF field attenuated by 1 mag then stellar field dominates -- but ISRF can be enhanced locally if O or B star present.

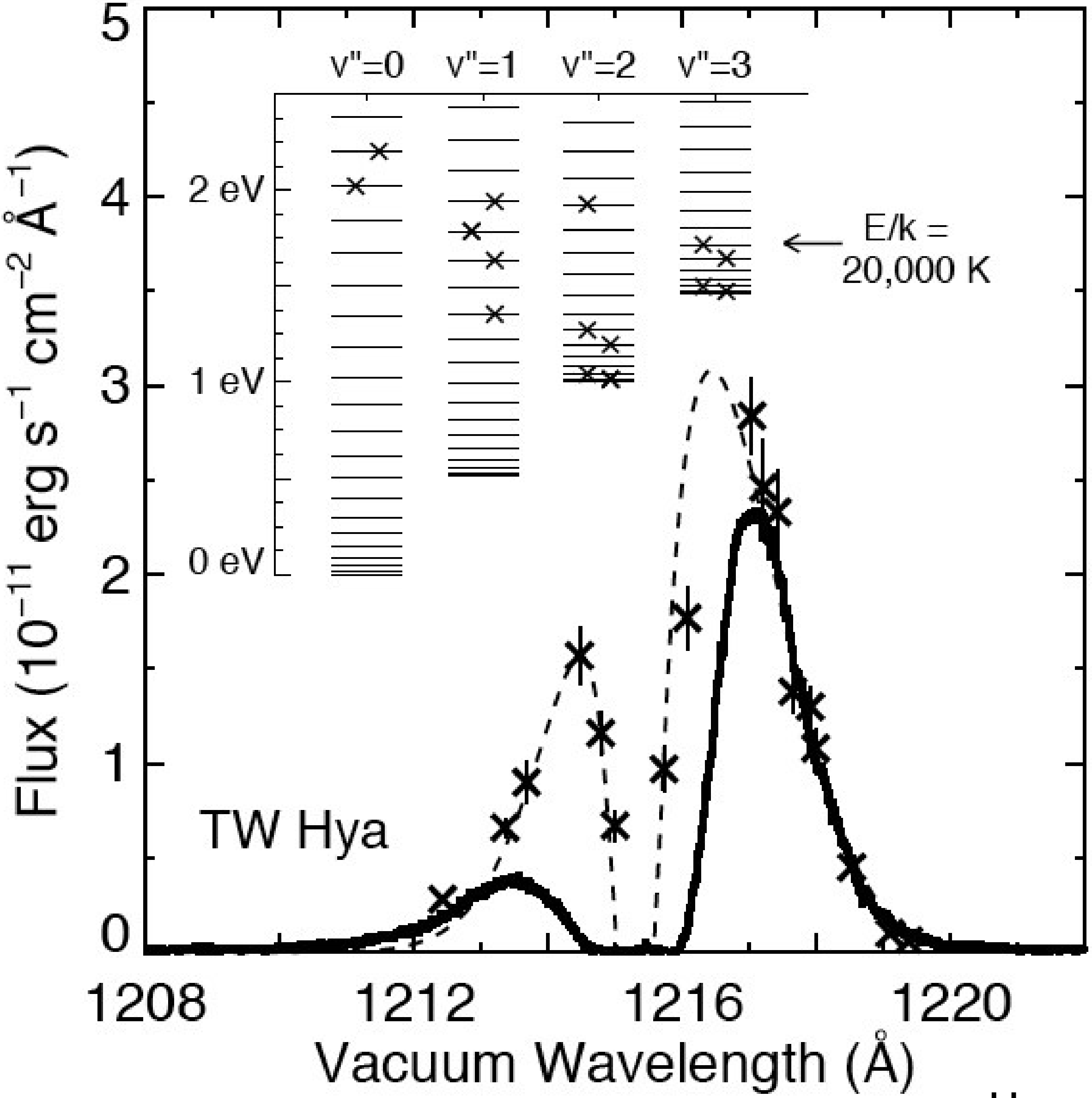
Penetration depth: $\Sigma_{uv} \sim 1.3$ x 10^{-3} g cm^{-}

Importance of Ly α Radiation?

- Dominates UV radiation field -- in TW Hya carries 85% of FUV flux (Herczeg et al 2004)
- H_2 emission is evident – reaching molecular layer
- Important for chemistry: HCN and H_2O (and other species) will be dissociated by Ly α photons -- CN is not (Bergin et al 2003).

- To include in chemistry need to answer some questions:
  - what is true line profile? TW Hya has circumstellar absorption, other sources have both circumstellar and interstellar absorption
  - radiation is clearly reaching molecular layer, but H I layer on surface will scatter photons (mostly out!)

Reconstructed Line Profile

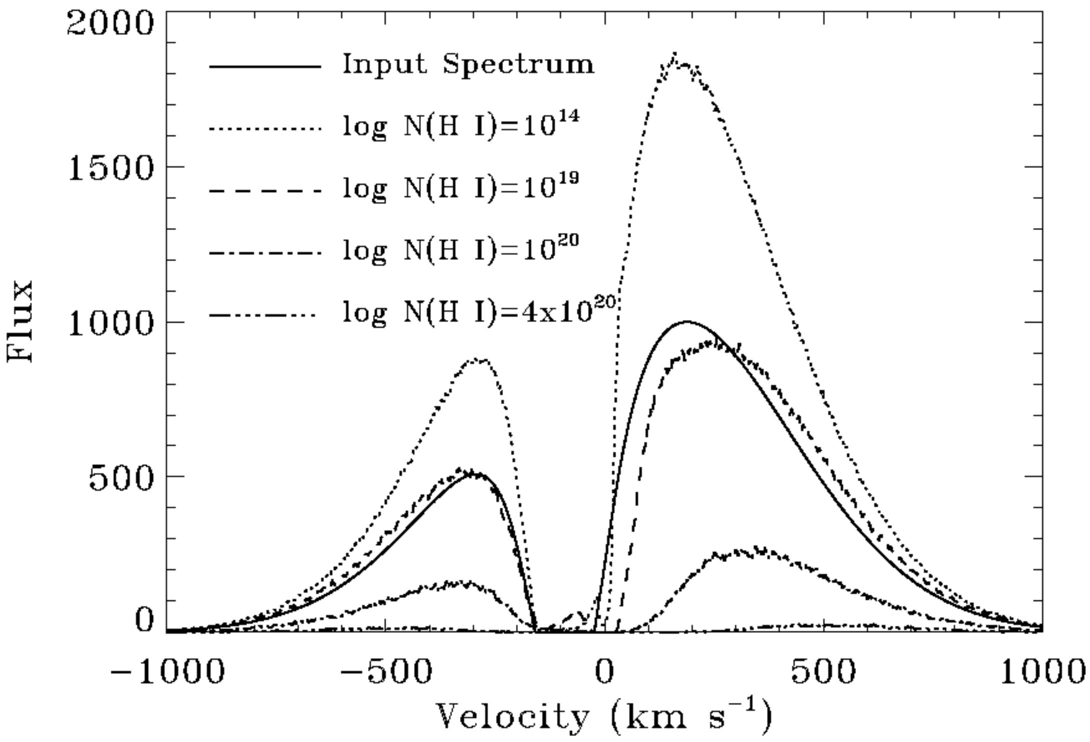


Herczeg et al. 2004

Radiative Transfer

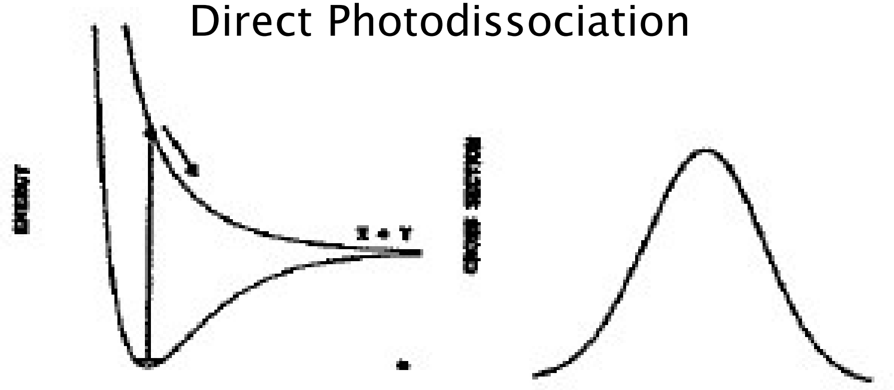
- two ways to be "destroyed"
  - H atom scattering out of surface
  - grain absorption
- photons in the wings need to be destroyed by grains
- at 100 AU about 10% of flux reaches molecular layer (A_V ~ 1) -- provided no additional absorption beyond PDR on disk surface (i.e. wind..)

G. Herczeg

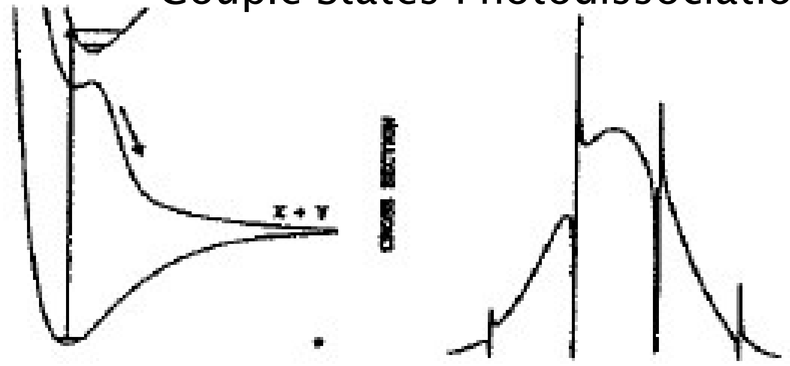


Photodissociation

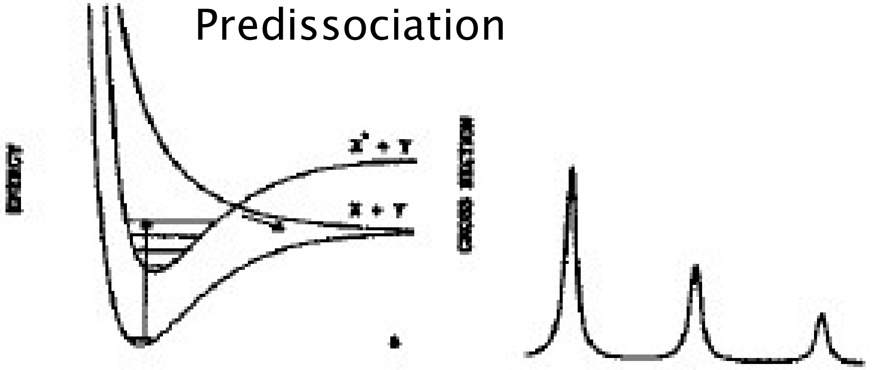
Direct Photodissociation



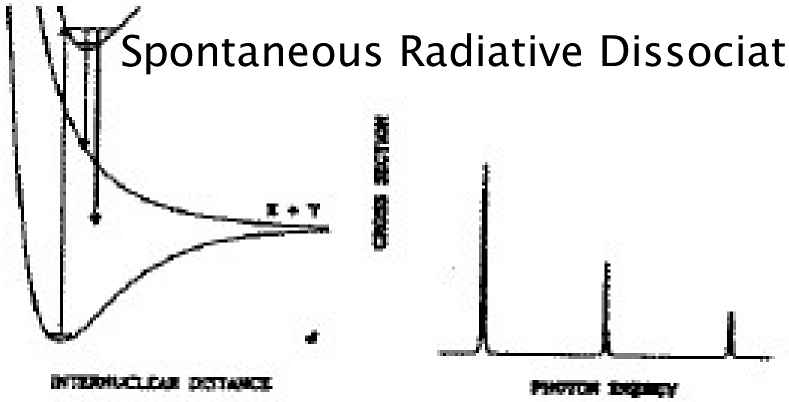
Couple States Photodissociation



Predissociation



Spontaneous Radiative Dissociation



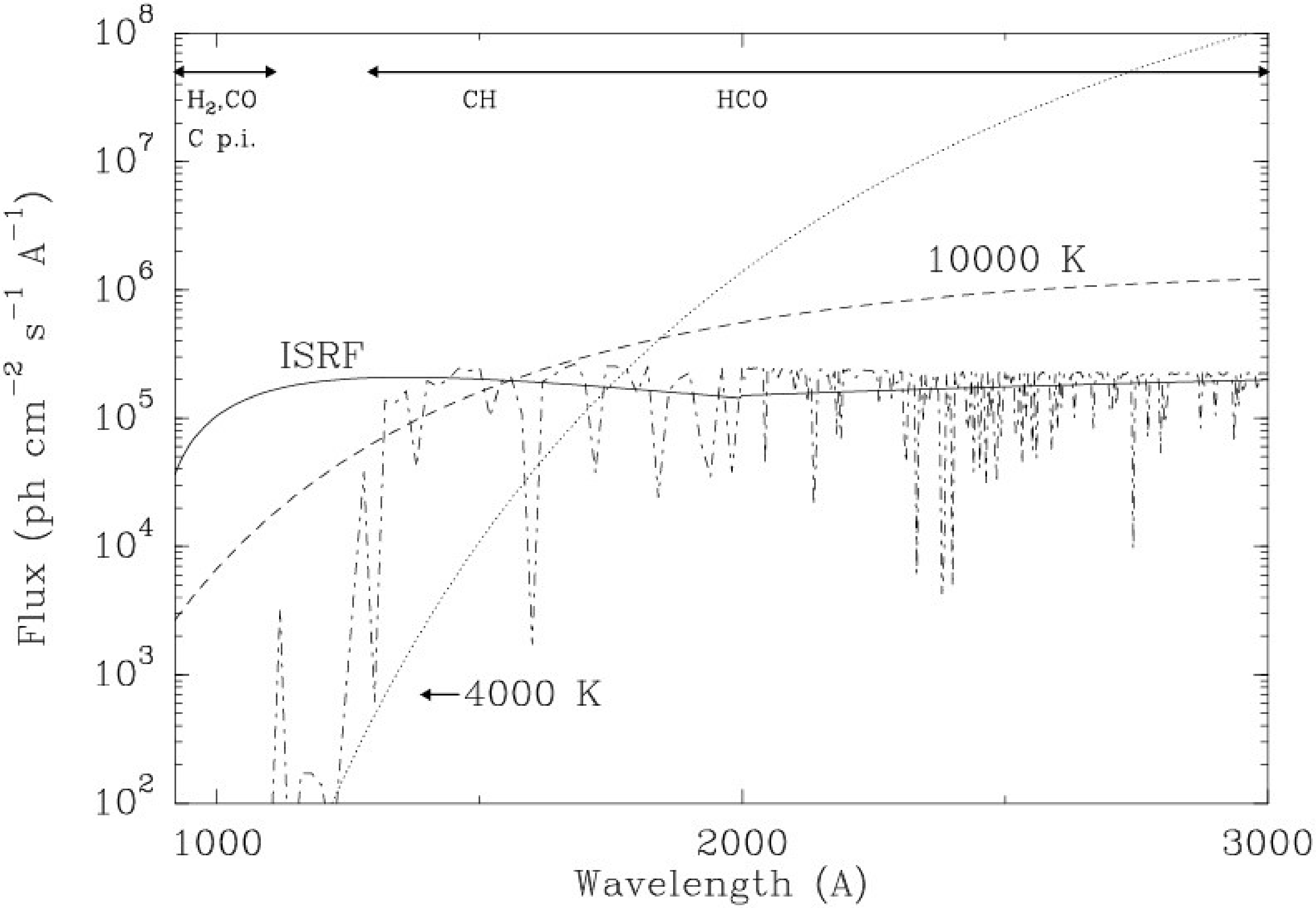
For CO primary dissociation bands < 1000 Å
For H_2 lines < 1300 Å
For H_2O dissociation x-section up to 2000 Å

Molecular Photodissociation

- If UV field parameterized as function of ISM field then can use previously calculated rates.
  - Includes only direct attenuation of the field – ignores scattering
  - General form: $k_{pd}(s^{-1}) = k_0 \exp(-\gamma A_v)$
  - Does not account for shape of the field
  - New: van Dishoeck (2006) present rates calculated for 4,000 K and 10,000 K blackbodies. (NEXT 2 SLIDES)
- If directly calculating field then must calculate the photorate using molecular photodissociation (and ionization) cross-sections
  - $k_{pd}(s^{-1}) = \int (4\pi\lambda/hc)\sigma(\lambda)J_\lambda d\lambda$

  $\sigma(\lambda)$ from literature – no good repository see previous calculations and follow reference trail

van Dishoeck 2006: Faraday Discussion



van Dishoeck 2006: Faraday Discussion

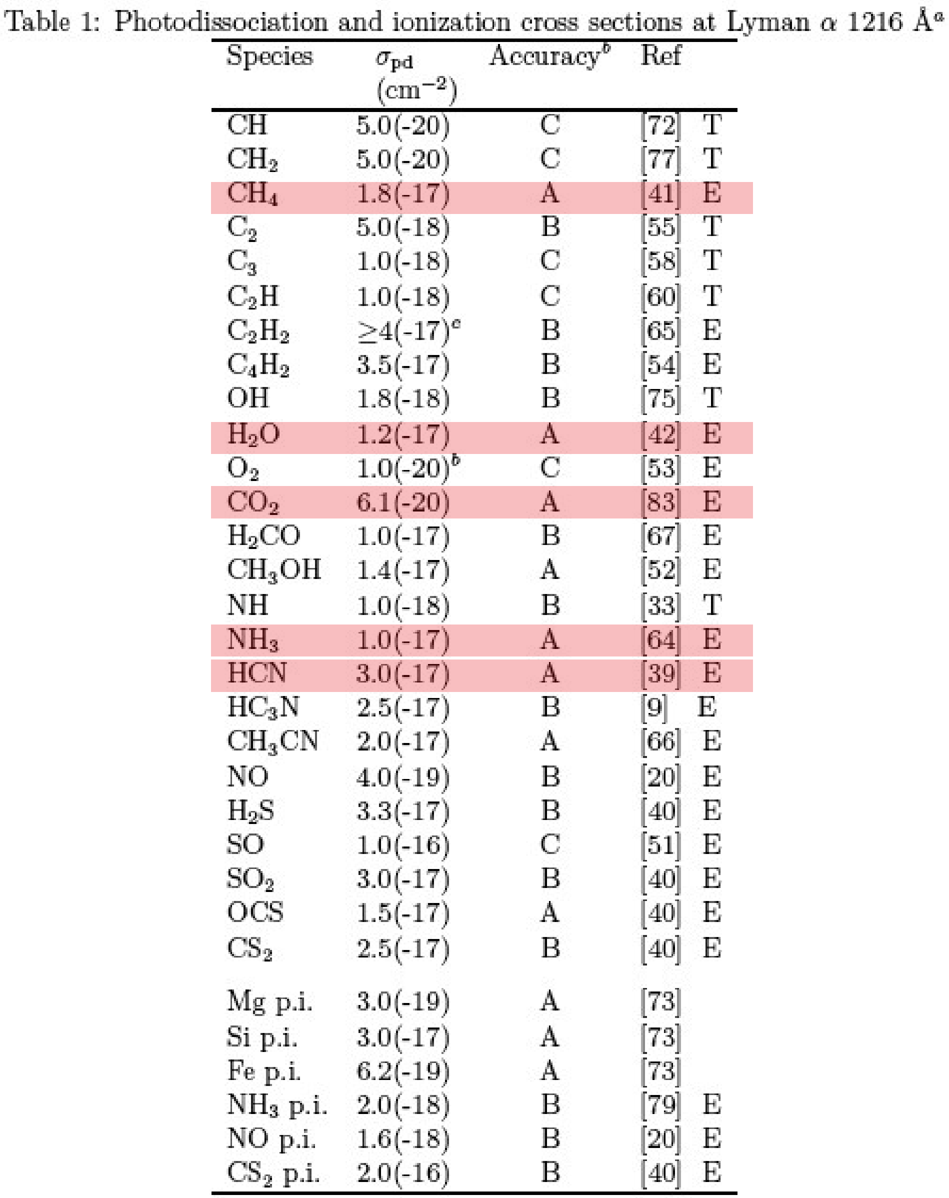


Table 1: Photodissociation and ionization cross sections at Lyman α 1216 Å^a

Species	σ_{pd} (cm^{-2})	Accuracy^b	Ref	
CH	5.0(-20)	C	[72]	T
CH_2	5.0(-20)	C	[77]	T
CH_4	1.8(-17)	A	[41]	E
C_2	5.0(-18)	B	[55]	T
C_3	1.0(-18)	C	[58]	T
C_2H	1.0(-18)	C	[60]	T
C_2H_2	$\geq$4(-17)^c	B	[65]	E
C_4H_2	3.5(-17)	B	[54]	E
OH	1.8(-18)	B	[75]	T
H_2O	1.2(-17)	A	[42]	E
O_2	1.0(-20)^b	C	[53]	E
CO_2	6.1(-20)	A	[83]	E
H_2CO	1.0(-17)	B	[67]	E
CH_3OH	1.4(-17)	A	[52]	E
NH	1.0(-18)	B	[33]	T
NH_3	1.0(-17)	A	[64]	E
HCN	3.0(-17)	A	[39]	E
HC_3N	2.5(-17)	B	[9]	E
CH_3CN	2.0(-17)	A	[66]	E
NO	4.0(-19)	B	[20]	E
H_2S	3.3(-17)	B	[40]	E
SO	1.0(-16)	C	[51]	E
SO_2	3.0(-17)	B	[40]	E
OCS	1.5(-17)	A	[40]	E
CS_2	2.5(-17)	B	[40]	E
Mg p.i.	3.0(-19)	A	[73]	
Si p.i.	3.0(-17)	A	[73]	
Fe p.i.	6.2(-19)	A	[73]	
NH_3 p.i.	2.0(-18)	B	[79]	E
NO p.i.	1.6(-18)	B	[20]	E
CS_2 p.i.	2.0(-16)	B	[40]	E

van Dishoeck 2006: Faraday Discussion

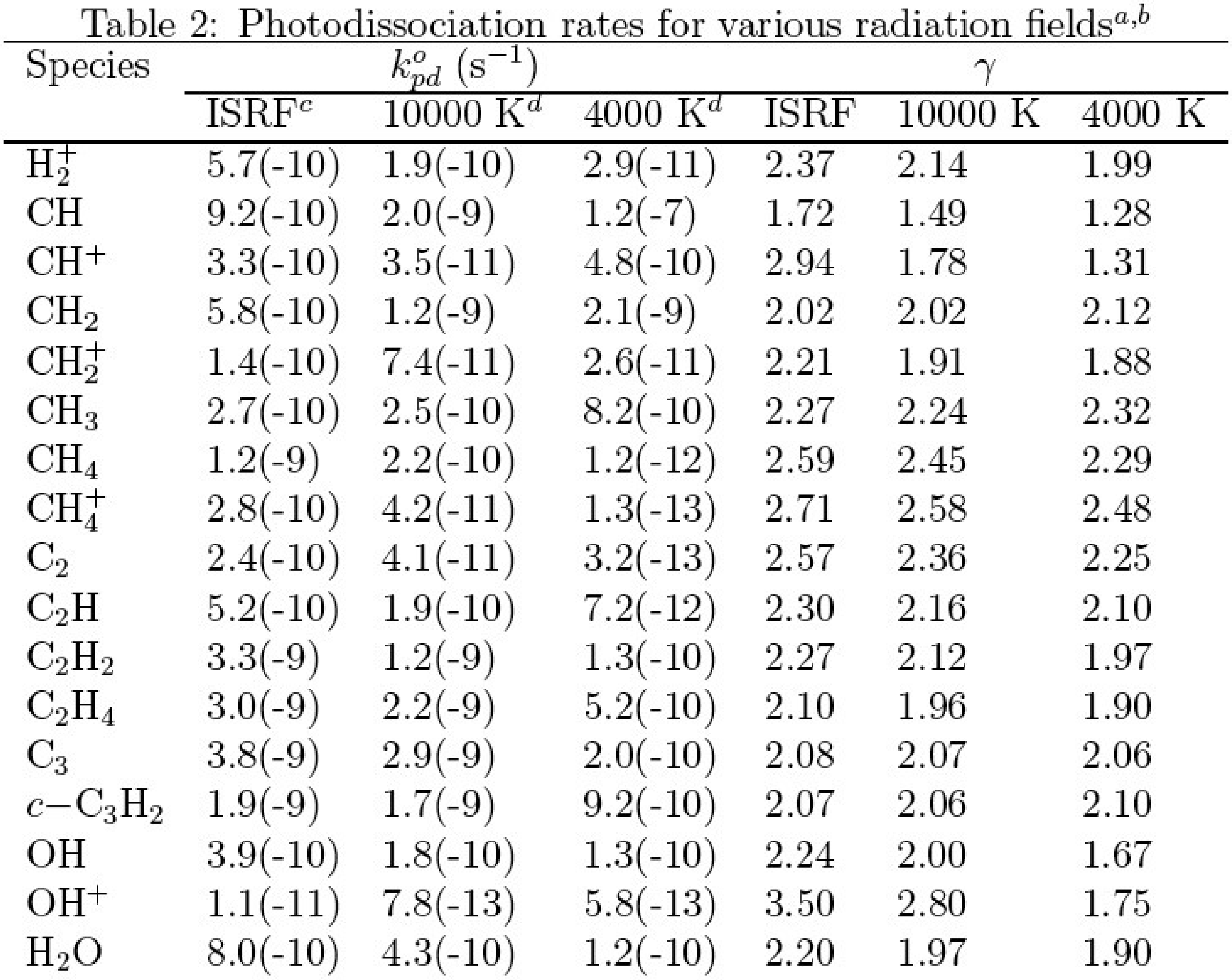


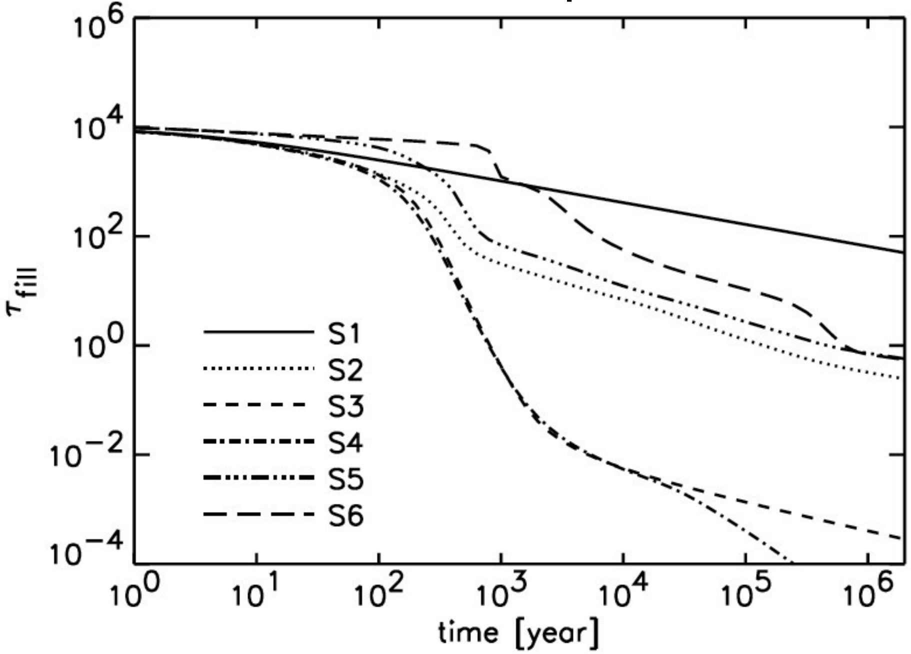
Table 2: Photodissociation rates for various radiation fields[a,b]

Species	k^o_{pd} (s^{-1})			γ		
	ISRF[c]	10000 K[d]	4000 K[d]	ISRF	10000 K	4000 K
H_2^+	5.7(-10)	1.9(-10)	2.9(-11)	2.37	2.14	1.99
CH	9.2(-10)	2.0(-9)	1.2(-7)	1.72	1.49	1.28
CH^+	3.3(-10)	3.5(-11)	4.8(-10)	2.94	1.78	1.31
CH_2	5.8(-10)	1.2(-9)	2.1(-9)	2.02	2.02	2.12
CH_2^+	1.4(-10)	7.4(-11)	2.6(-11)	2.21	1.91	1.88
CH_3	2.7(-10)	2.5(-10)	8.2(-10)	2.27	2.24	2.32
CH_4	1.2(-9)	2.2(-10)	1.2(-12)	2.59	2.45	2.29
CH_4^+	2.8(-10)	4.2(-11)	1.3(-13)	2.71	2.58	2.48
C_2	2.4(-10)	4.1(-11)	3.2(-13)	2.57	2.36	2.25
C_2H	5.2(-10)	1.9(-10)	7.2(-12)	2.30	2.16	2.10
C_2H_2	3.3(-9)	1.2(-9)	1.3(-10)	2.27	2.12	1.97
C_2H_4	3.0(-9)	2.2(-9)	5.2(-10)	2.10	1.96	1.90
C_3	3.8(-9)	2.9(-9)	2.0(-10)	2.08	2.07	2.06
$c-C_3H_2$	1.9(-9)	1.7(-9)	9.2(-10)	2.07	2.06	2.10
OH	3.9(-10)	1.8(-10)	1.3(-10)	2.24	2.00	1.67
OH^+	1.1(-11)	7.8(-13)	5.8(-13)	3.50	2.80	1.75
H_2O	8.0(-10)	4.3(-10)	1.2(-10)	2.20	1.97	1.90

UV Radiation: Grain Properties

- Grain absorption will vary with dust grain properties.
- As grains coagulate and settle to midplane the UV opacity will decrease
- Transition to optically thin disk
- Key question: presence of PAH's in the upper atmosphere -- will not settle. If present then UV radiation field will be reduced in disk (Jonkheid et al. 2004)

UV Opacity as a function of Dust Properties



Dullemond and Dominik 2005

X-ray Ionization

- X-rays are a key source of ionization and heating of protoplanetary disks.
- Typical X-ray luminosity (Orion): $L_x = 10^{28.5} - 10^{31}$ ergs s^{-1} with $T_{x} \sim$ 1-2 kev (Glassgold et al 2000, PPIV; Feigelson et al. 2005)
- Ionize the inner shells of heavy elements

Source: Glassgold et al 1997; Krolik and Kallman 1983

X–ray Ionization

- For atoms heavier than Li – inner shell ionization is followed by the Auger effect
  - Generates: $N_1 = 1 + A$ primary electrons with $E_{tot} = E_x - \text{I.P.}$ (I.P. = ionization potential)
    - $A = 1$ for $(3 < Z < 10)$
    - $A = 4.75$ for Fe
  - Each primary electron will produce secondary electrons by impact ionization of gas
  - Generates: $N_2 = E - \text{I.P.}/\Delta\varepsilon$ secondary electrons
    - ∀ $\Delta\varepsilon$ = mean energy to make an ion pair ≈ 37 eV (Shull and van Steenberg 1985)

Source: Glassgold et al 1997; Krolik and Kallman 1983

X-ray Ionization

- $N_2 >> N_1$ therefore for X-ray ionization rate, ζ_x:

$$\zeta_x = \zeta_1 + \zeta_2 = \zeta_2$$

- Therefore secondary electrons dominate (well known result -- as is the case for cosmic rays)
- In general there are ~ 30 atoms and molecules ionized per keV (Aikawa and Herbst 1999)

Source: Glassgold et al 1997; Krolik and Kallman 1983

X–ray Ionization

$$\zeta_x = N_2 \int_{1\ keV}^{30\ keV} \sigma(E) F(E) dE$$

where $\sigma(E)$ is the cross-section for direct ionization for all elements weighted by solar abundances and

$$F(E) = F_0 e^{-\tau(E)}$$

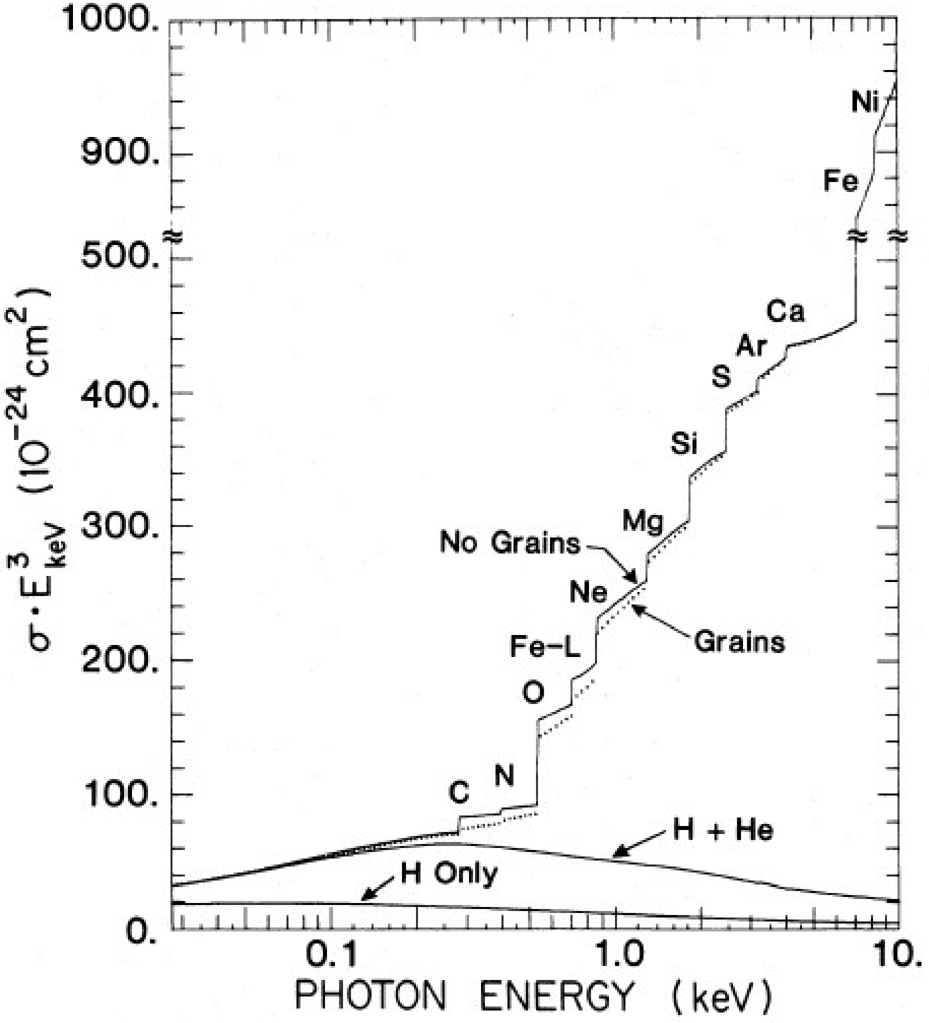
$$F_0 = f(T_x, L_x, E)$$

$-L_x$ is the X-ray luminosity and T_x the characteristic temperature of the X-ray spectrum.

Full expression in Glassgold et al. 1997

Source: Glassgold et al 1997; Krolik and Kallman 1983

X-ray Opacity and Cross-Section



Morrison and McCammon 1983

$\tau_x = N(H) \times \sigma_x(cm^2)$

Calculation of σ_x from Morrison and McCammon (1993)

- Assumed Solar abundances.

Opacity depends on atomic level absorption!!!!!

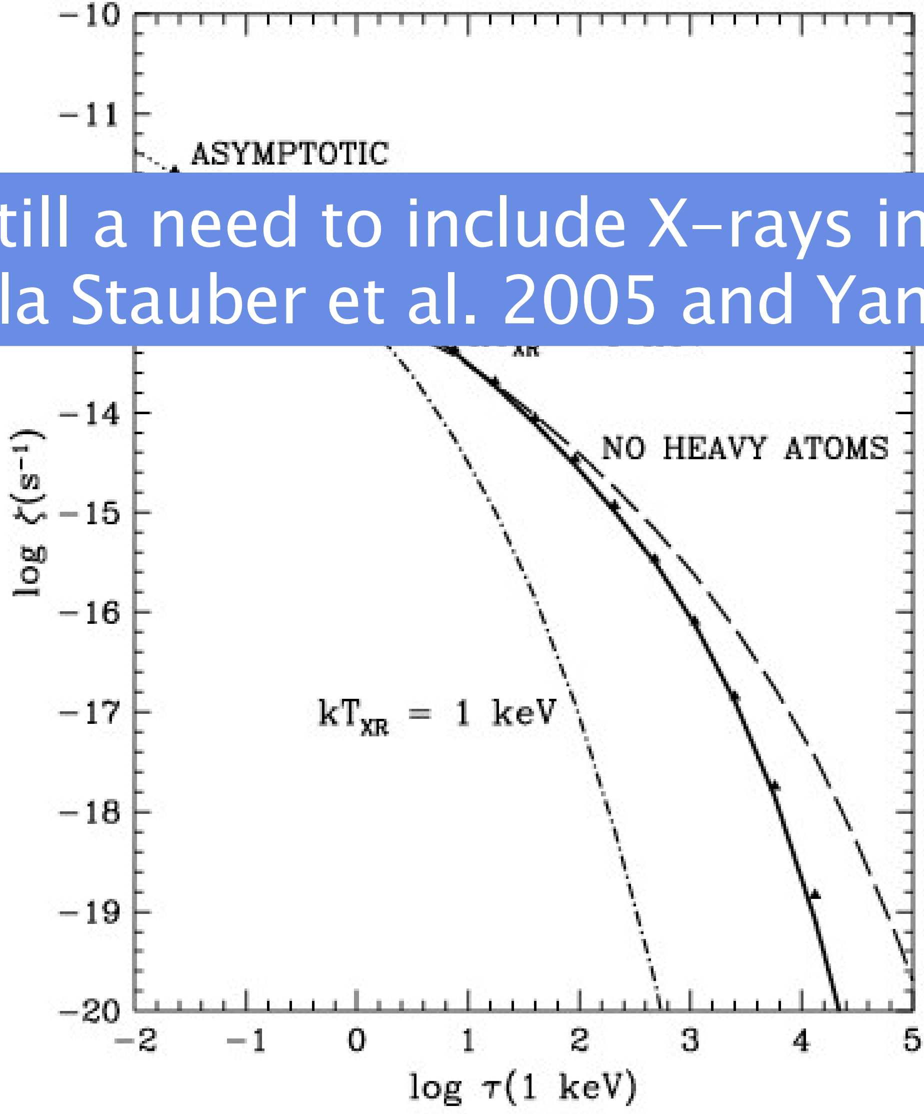
Will change if metals are depleted from the surface of the disk (via settling).

- Thus: $\sigma_x(r, z, t)$!

In this case need to calculate the absorption cross-sections directly using data Henke et al. 1993

X-ray Ionization

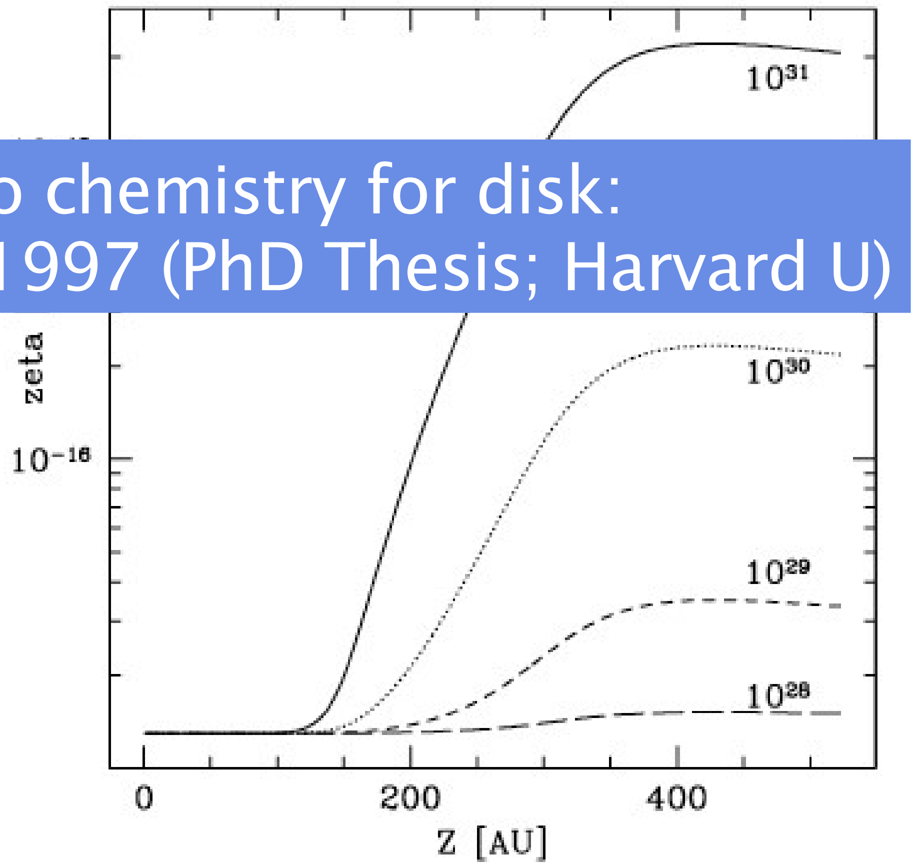
X-ray ionization Rate at 1 AU



Glassgold et al. 1997

Still a need to include X-rays into chemistry for disk:
ala Stauber et al. 2005 and Yan 1997 (PhD Thesis; Harvard U)

X-ray ionization Rate at 700 AU



Aikawa and Herbst 2001

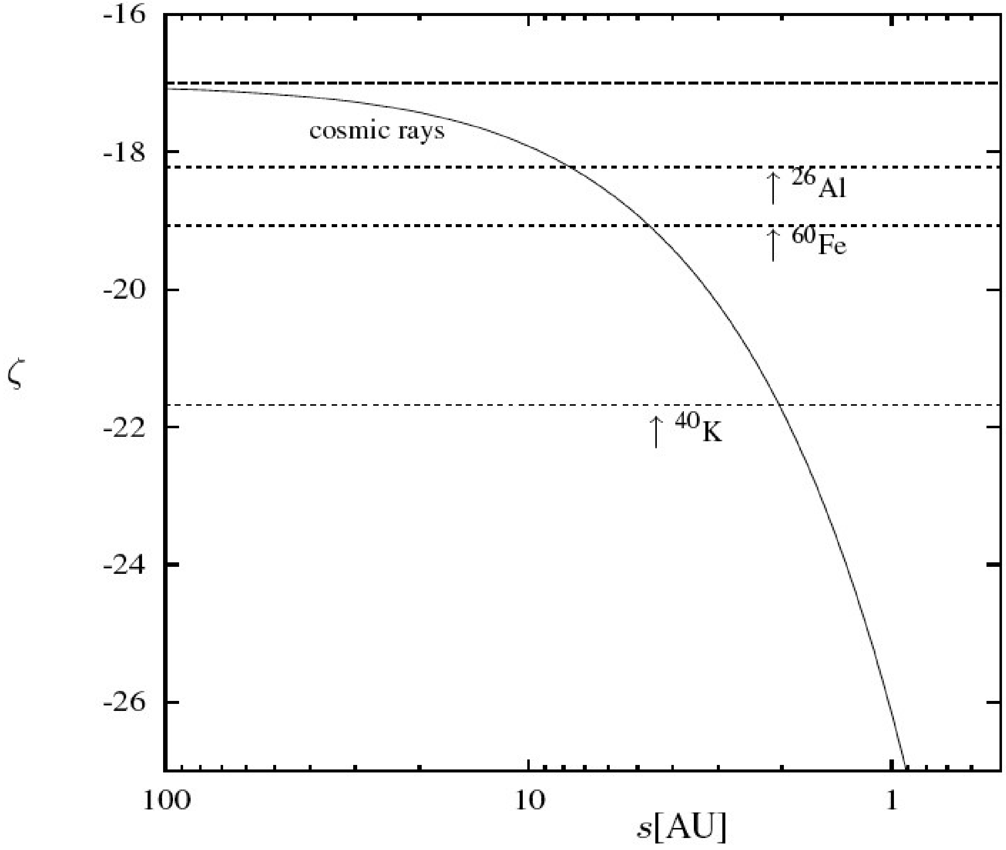
$\Sigma_{1\mathrm{keV}} = 0.008\ \mathrm{g\ cm^{-2}}$

$\Sigma_{10\mathrm{keV}} = 1.6\ \mathrm{g\ cm^{-2}}$

Extinct Radionuclides

- If cosmic-rays are excluded then radionuclides provide a baseline level of ionization.
- Question is what was present in our solar system

Ionization rate at midplane



Finocchi and Gail 1997

Kinetic Models

- Key Players (see papers)
  - Finnochi, Gail, … (dust destruction and formation, ionization)
  - Aikawa + (models of radial and vertical dependence)
  - Willacy + (models of radial and vertical dependence)
  - Kamp + (more evolved sources – debris disks and A/B stars)
  - Markwick + (inner disk)
  - Semenov + (Ion fraction/mixing/radial/vertical)
  - Ilgner + (turbulence/chemistry in inner disk)
  - Bergin + (UV/X-rays)
  - ……

Aikawa et al. (1996)
Bauer et al. (1997)
Finocchi & Gail (1997)
Willacy et al. (1998)
Aikawa & Herbst (1999)
Aikawa et al. (1999)
Aikawa & Herbst (1999b)
Willacy & Langer (2000)
Aikawa & Herbst (2001)
Aikawa et al. (2002)
Markwick et al. (2002)
van Zadelhoff et al. (2003)
Millar et al. (2003)
Ilgner et al. (2003)

Kinetic Models: Time Dependence

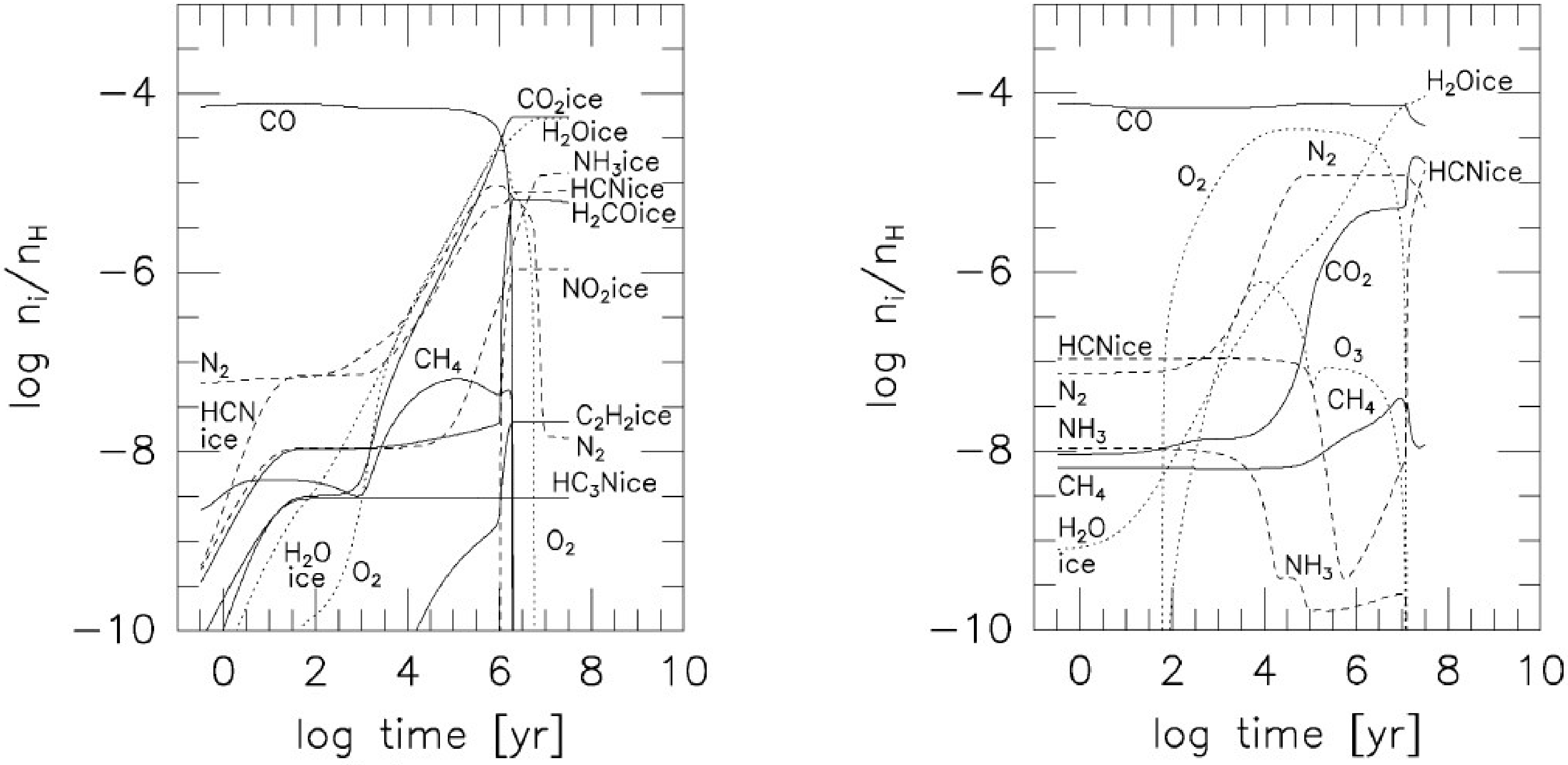


FIG. 1*a*

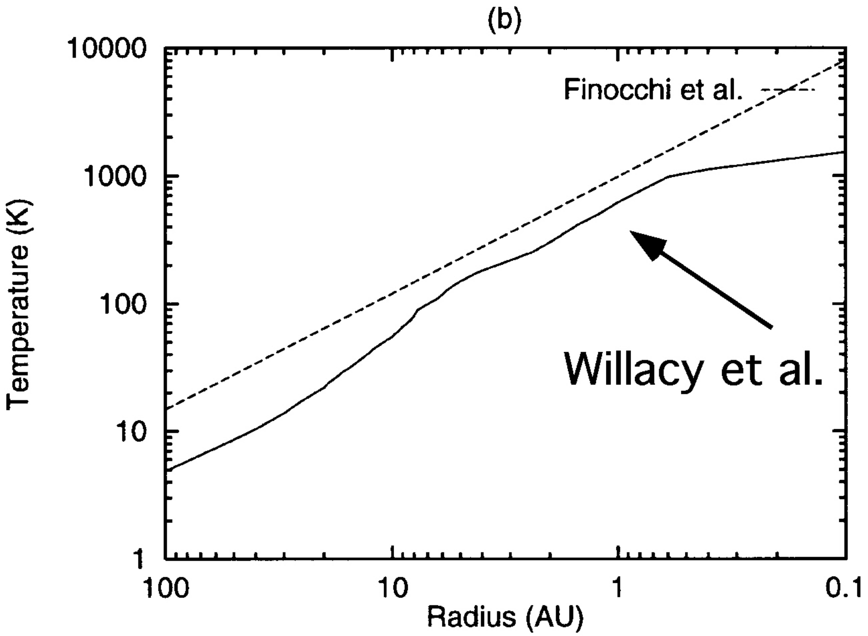
FIG. 1*b*

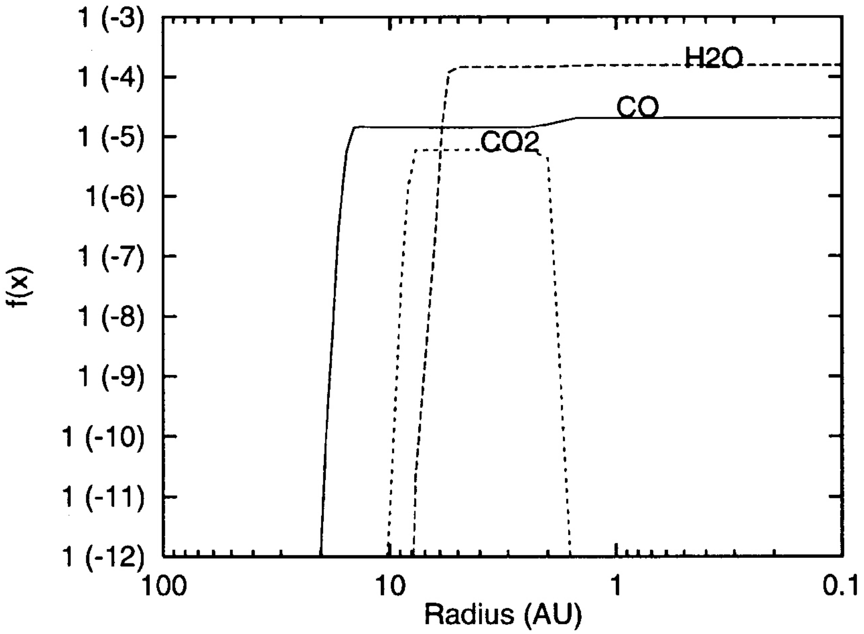
FIG. 1.—Evolution of the molecular abundance in two representative regions of the disk, (*a*) $R = 87$ AU ($n_H = 2.9 \times 10^9$ cm^{-3}, $T = 30$ K) and (*b*) $R = 9.7$ AU ($n_H = 1.2 \times 10^{12}$ cm^{-3}, $T = 90$ K). The initial molecular abundance was determined referring to the abundance in dark clouds. The solid, dotted, and dashed lines represent the abundance of carbon-, oxygen-, and nitrogen-bearing molecules, respectively, relative to hydrogen.

Aikawa et al. 1997

Disk Temperature Structure and Chemistry

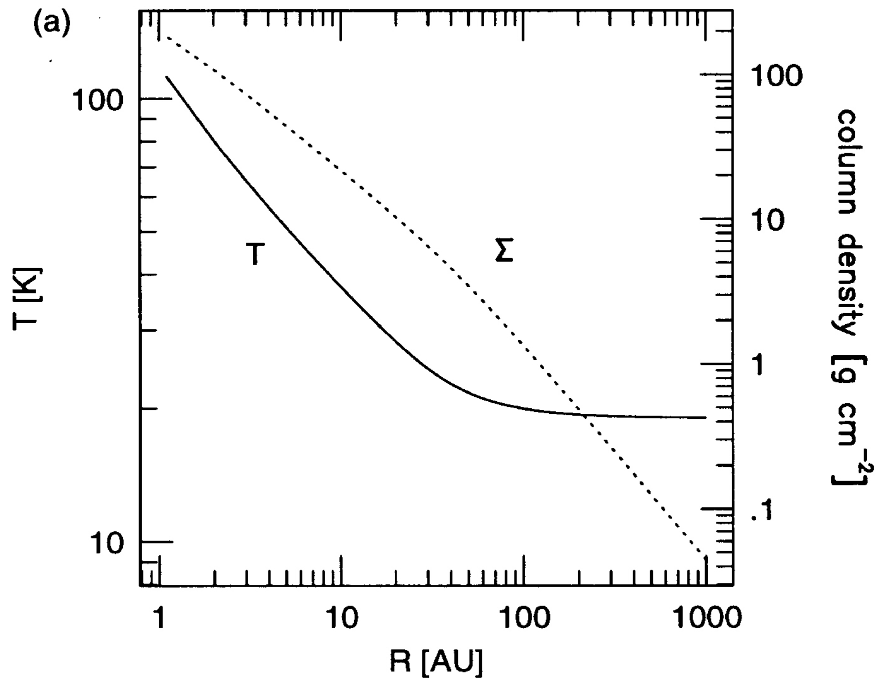
- Willacy et al. 1998: static model, radial dependence, midplane

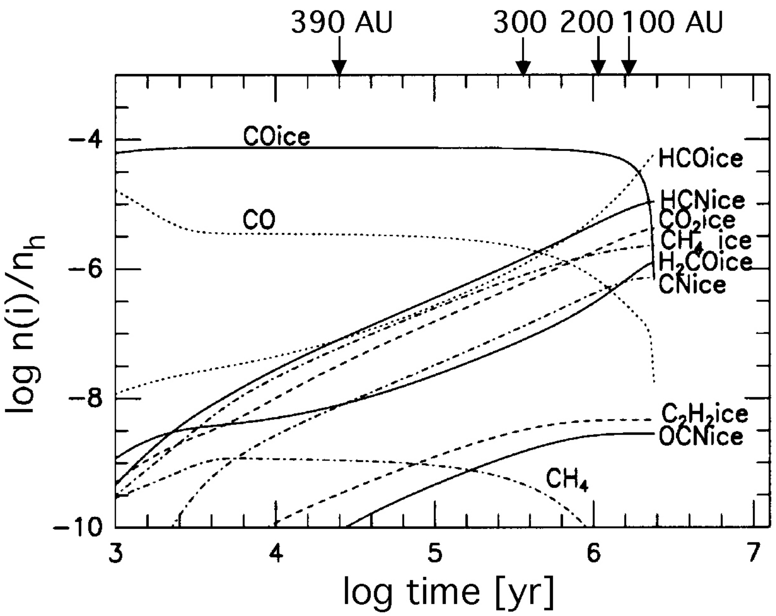




Disk Temperature Structure and Chemistry

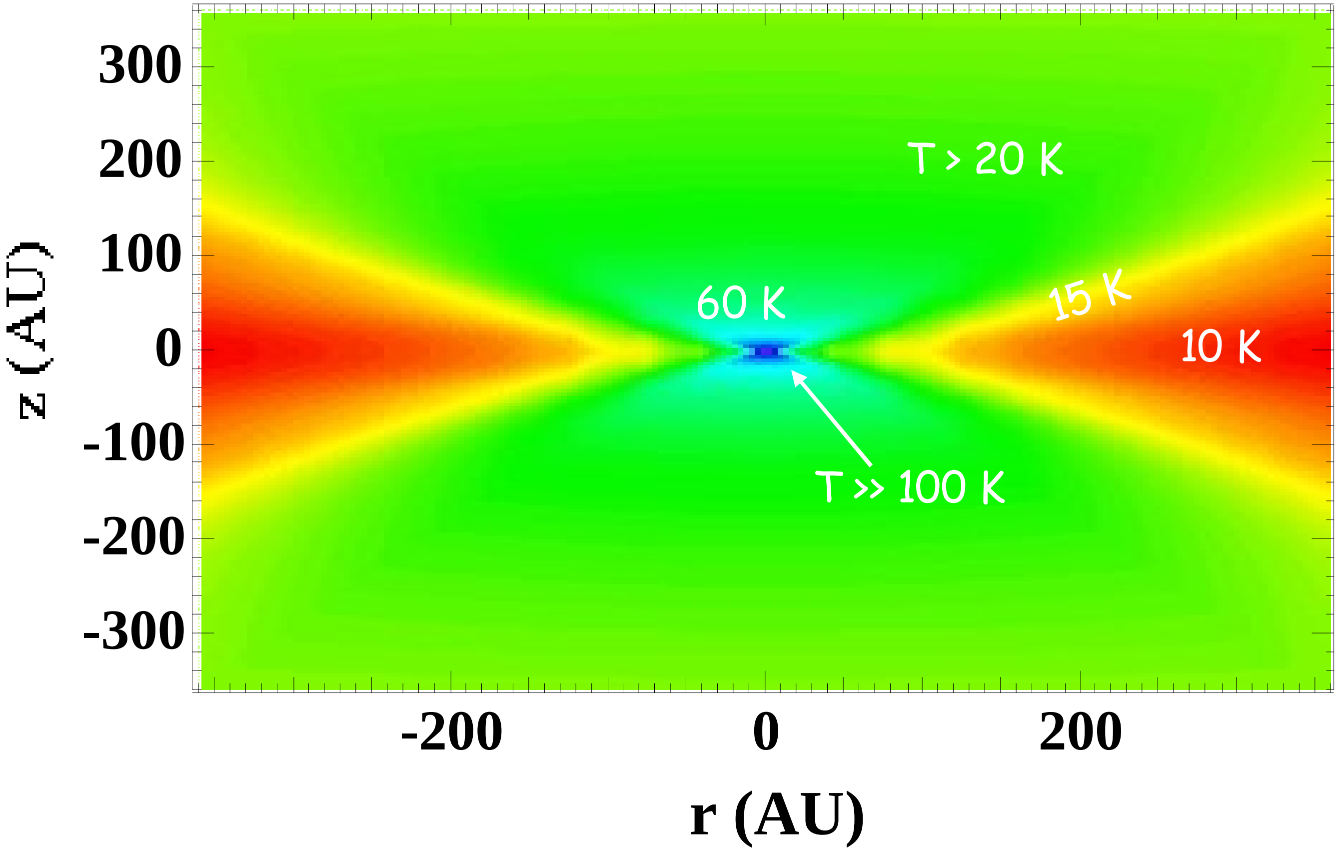
- Aikawa et al. 1999: accretion flow in radial direction





Warm Surface!

- > 2000, 2001 – models recognized the existence of hot surface -- allows for active gas phase chemistry
  - Models of D'Alessio, Calvet; Chiang, Goldreich which match dust Spectral Energy Distribution (SED) began to be used
  - provide a basis of n and T as a function of r,Z to model theory
  - greater role for photons to play in chemistry



Warm Molecular Layer

- Willacy and Langer (2000) noted the importance of the surface -- stressed photodesorption.
- Aikawa et al. 2002 -- formation of the "warm molecular layer"
  - Vertical layers where the grain temperature is high enough to sublimate molecules but UV reduced enough to allow molecular formation
- These works matched column densities and some variations seen in observations (e.g. CN/HCN)
- Generally accepted piece of disk chemistry.
- Results will strongly depend on adopted disk physical structure.

General Theoretical Picture

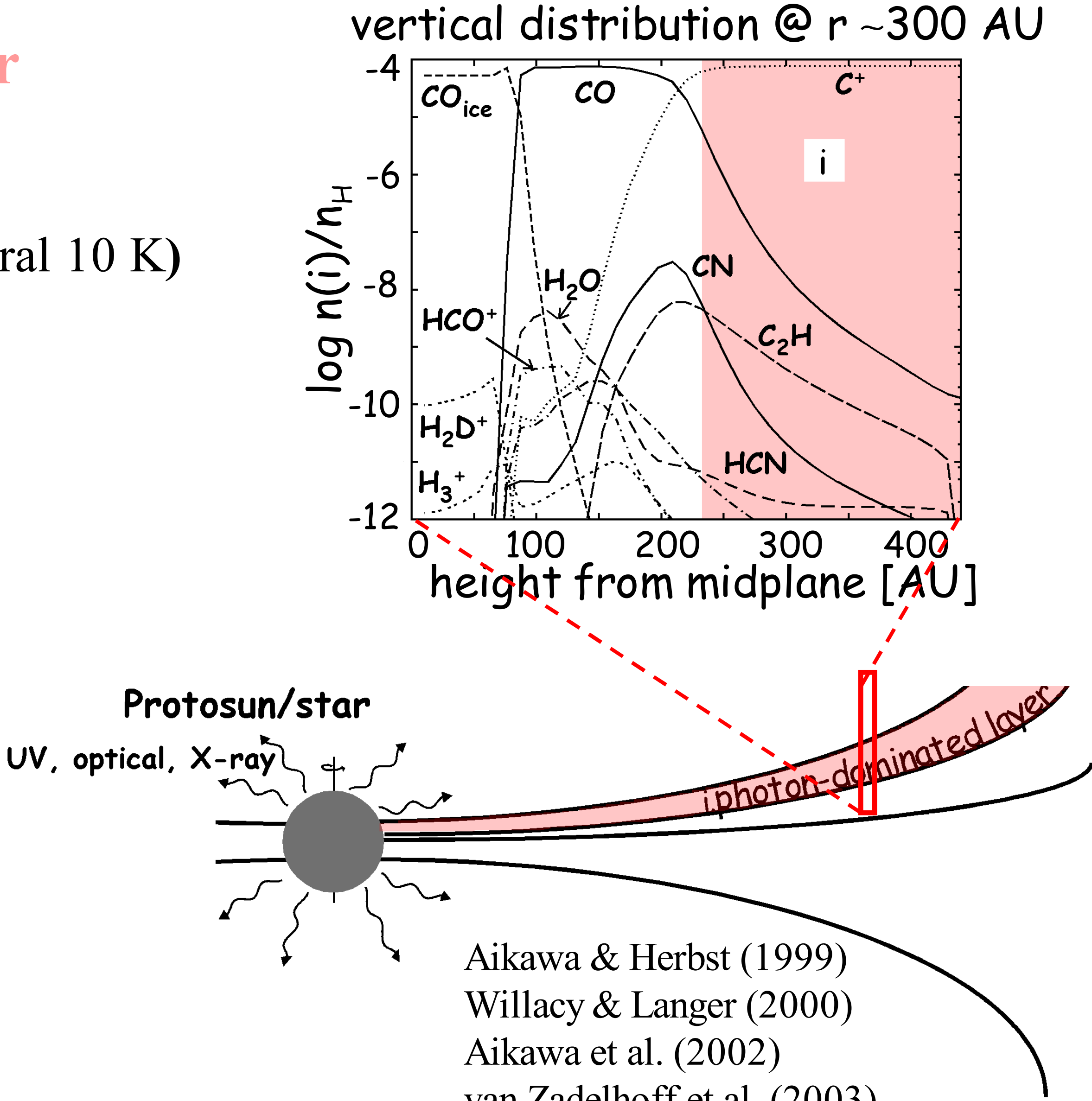
three-layer model

(i) photon-dominant layer

UV & X-ray irradiation

low density ($n_H < 10^5 cm^{-3}$)

high temperature (T > several 10 K)



Aikawa & Herbst (1999)
Willacy & Langer (2000)
Aikawa et al. (2002)
van Zadelhoff et al. (2003)

General Theoretical Picture

three-layer model

(i) photon-dominant layer

UV & X-ray irradiation

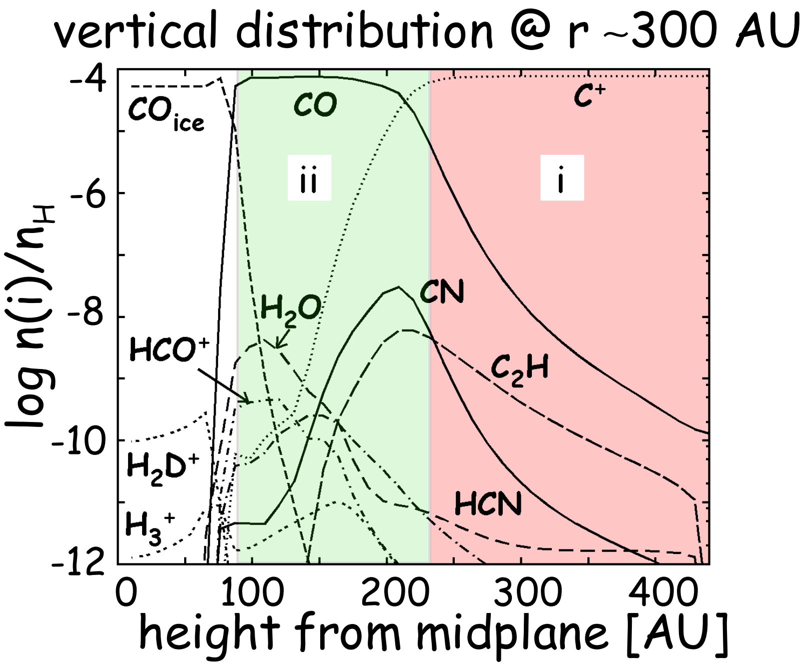
low density ($n_H < 10^5 \mathrm{cm}^{-3}$)

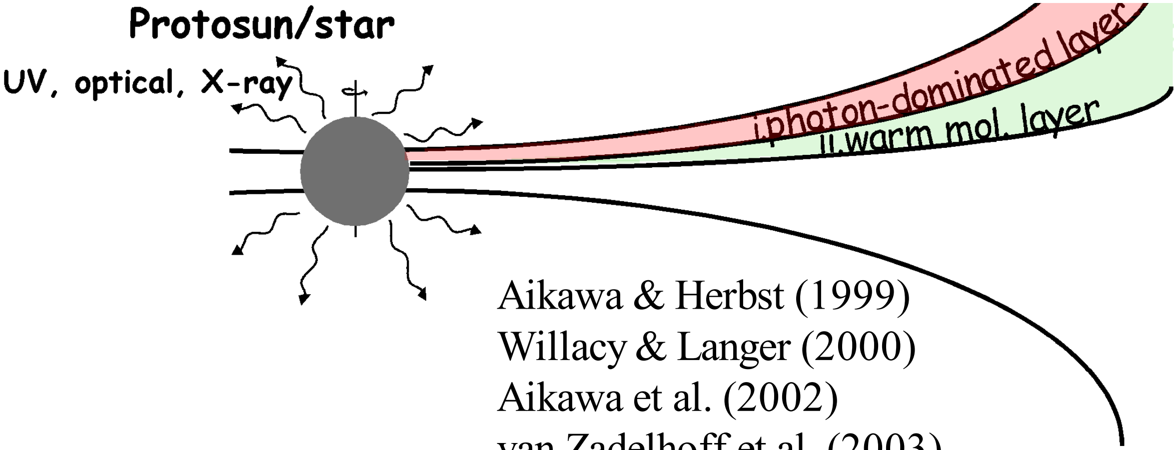
high temperature (T > several 10 K)

(ii) warm molecular layer

high density ($n_H > 10^5 \mathrm{cm}^{-3}$)

moderate temperature (T > 20 K)





Aikawa & Herbst (1999)
Willacy & Langer (2000)
Aikawa et al. (2002)
van Zadelhoff et al. (2003)

General Theoretical Picture

three-layer model

(i) photon-dominant layer

UV & X-ray irradiation

low density ($n_H < 10^5 cm^{-3}$)

high temperature (T > several 10 K)

(ii) warm molecular layer

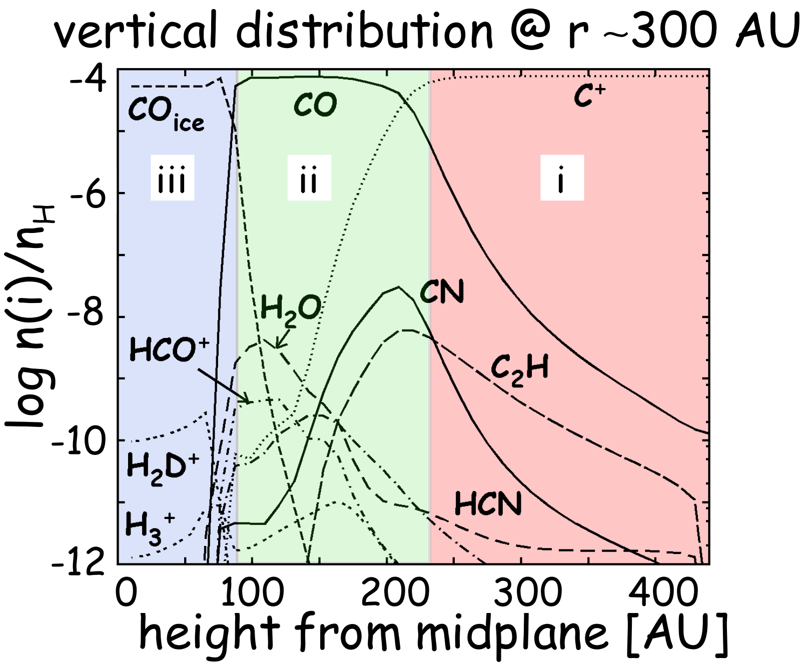
high density ($n_H > 10^5 cm^{-3}$)

moderate temperature (T > 20 K)

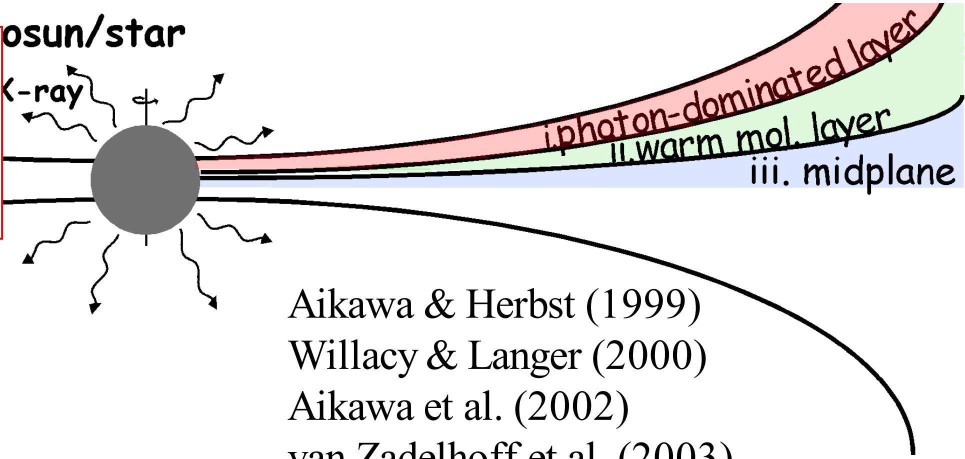
(iii) midplane freeze-out layer

very high density ($n_H > 10^7 cm^{-3}$)

low temperature (T < 20 K)



cf. Observation :
- **low abundance of gaseous molecules**
- **high CN/HCN ratio**



Aikawa & Herbst (1999)
Willacy & Langer (2000)
Aikawa et al. (2002)
van Zadelhoff et al. (2003)

General Theoretical Picture

three-layer model

(i) photon-dominant layer

UV & X-ray irradiation

low density ($n_H < 10^5 cm^{-3}$)

high temperature (T > several 10 K)

(ii) warm molecular layer

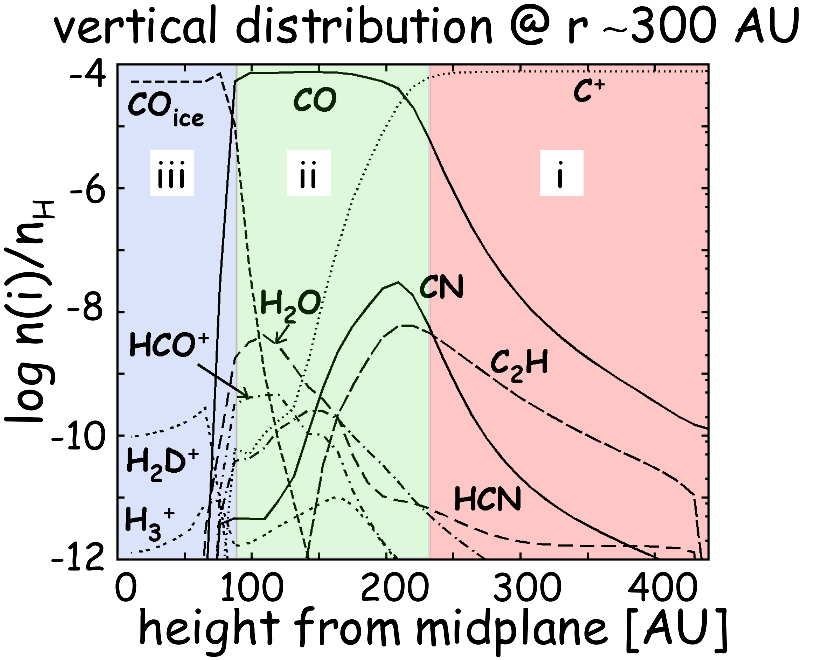
high density ($n_H > 10^5 cm^{-3}$)

moderate temperature (T > 20 K)

(iii) midplane freeze-out layer

very high density ($n_H > 10^7 cm^{-3}$)

low temperature (T < 20 K)

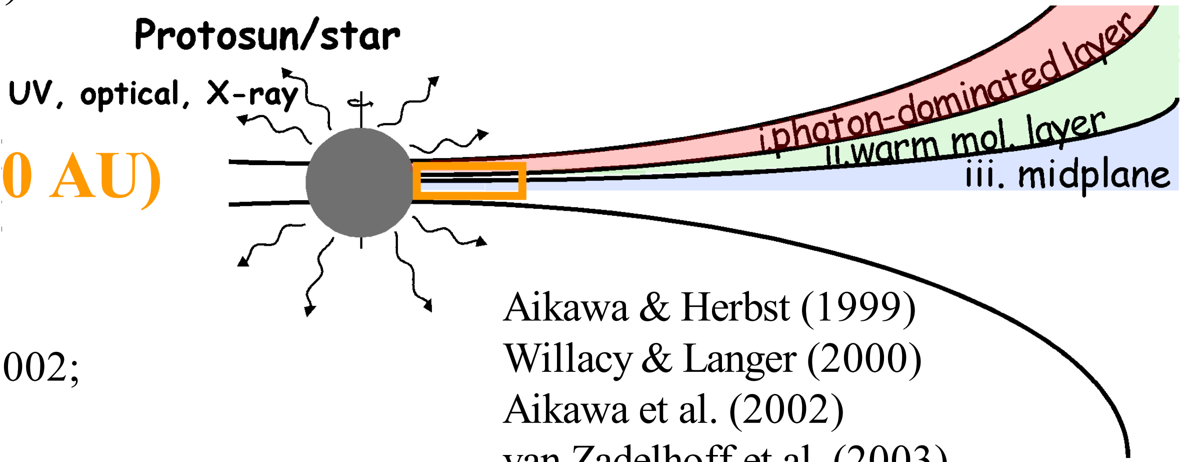


(iv) inside snow line (r < 10 AU)

thermal desorption

"hot core" like chemistry

(Najita et al. 2006/PPV, Markwick et al. 2002; Ilgner et al. 2004)



Aikawa & Herbst (1999)
Willacy & Langer (2000)
Aikawa et al. (2002)
van Zadelhoff et al. (2003)

Inner Disk Chemistry

- Effects of X-ray heating of upper atmosphere and resulting chemistry discussed in Glassgold et al. 2004

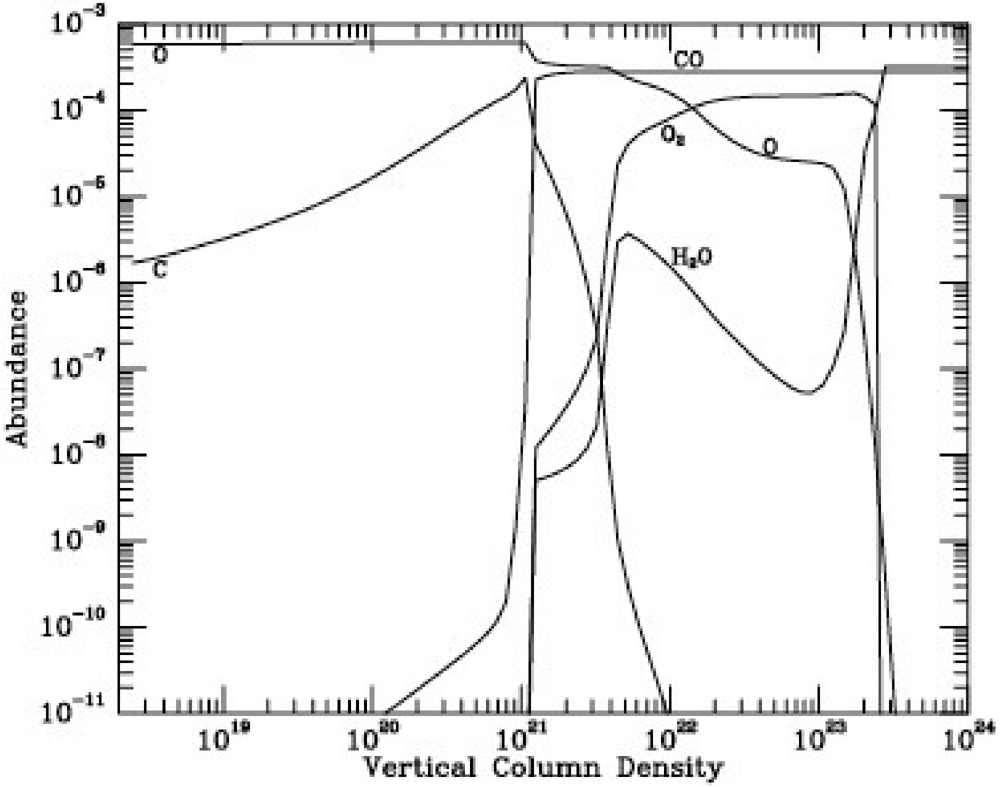
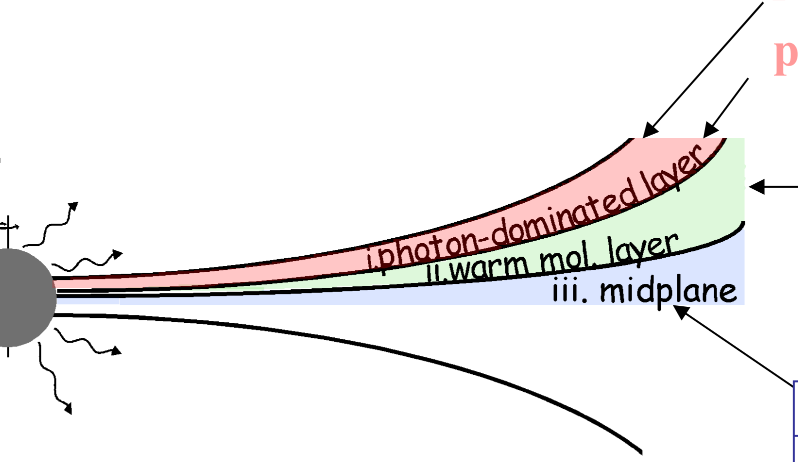


FIG. 5.—Abundances of the main oxygen species plotted vs. perpendicular column density at a radial distance of 1 AU for the case $\alpha_h = 1$.

Chemical-Physical Links: ion fraction

- **Ion fraction in models:**



(Sano et al. 2000; Semenov et al. 2004)

photoionization of H: $x_e > 10^{-4}$

photoionization of C: $x_e \sim 10^{-4}$

Cosmic-ray and X-ray ionization:

$x_e \sim 10^{-11}$ - 10^{-6}

HCO^+, H_3^+

Cosmic-ray and Radionucleide:

r < 3AU	3 AU < r < 60 AU	r > 60 AU
$x_e < 10^{-12}$ $Metal^+$ or grain	$x_e \sim 10^{-12}$ HCO^+ or grain	$x_e > 10^{-11}$ H_3^+ & D_3^+

- **Constraints from observation**

  - Dutrey et al. (1997):

    $x(HCO^+)=(1-7) \times 10^{-10}$

  - Qi et al. (2003)

    $x(e) > 10^{-8}$ at disk surface where $x(CO) \sim 10^{-5}$

    (from observation of HCO^+ and N_2H^+)

  - Ceccarelli et al. (2004)

    $(4-7) \times 10^{-10}$ from H_2D^+

So far, consistent with models…

Chemical Physical Links: Mixing

- Mixing -- long history
  - Presence of chondritic refractory inclusions in meteorites (MacPherson et al. 1998)
  - Crystalline silicates in comets (Bockelee-Morvan et al. 1998)
  - Gas mixing from warm planet forming nebula to outer cold nebula suggested to account for ammonia and methane in comets (Fegley and Prinn 1989)
- Classic references
  - Prinn 1990, 1993
  - Stevenson 1990

Chemical Physical Links: Mixing

To simplify the interaction between dynamics and chemistry - consider two timescales

- τ_{chem}: the chemical timescale
- τ_{dyn}: the dyanamical timescale

If $\tau_{chem} < \tau_{dyn}$ then chemistry can attain an equilbrium and is unaffected

If $\tau_{chem} > \tau_{dyn}$ then mixing alters the composition

Parameterize the transfer of angular momentum in terms of turbulent viscosity: $\nu = \alpha c_s H$

α is a dimensionless parameter (Shukura and Sunyaev 1973; Pringle 1981)
H is the scale height
c_s is the sound speed

The radial disk viscous timescale is $\tau_\nu = r^2/\nu$ or,

$$\tau_\nu \sim 10^4 \mathrm{yr} \left(\frac{\alpha}{10^{-2}}\right)^{-1} \left(\frac{T}{100\,\mathrm{K}}\right)^{-1} \left(\frac{r}{1\,\mathrm{AU}}\right)^{\frac{1}{2}} \left(\frac{M_*}{M_\odot}\right)^{\frac{1}{2}} .$$

Chemical Physical Links: Mixing

- The Diffusivity, *D*, is not the same as the viscosity, ν (Stevenson 1990)
  - Common to equate the two
- For MRI there may be a dead zone near the midplane where mixing will not occur -- may only be a surface effect.
- In the case of MRI the situation is unclear
  - Carballido et al. 2005 estimate $\nu/D \sim 11$ (turbulent mixing less efficient than angular momentum transport)
  - Turner et al. 2006 estimate $\nu/D \sim 1 - 2$
- Models grouped into 2 categories
  - Ones that include only advection (inward movement of material)
  - Models that include radial and/or vertical mixing

Chemical Physical Links: Mixing

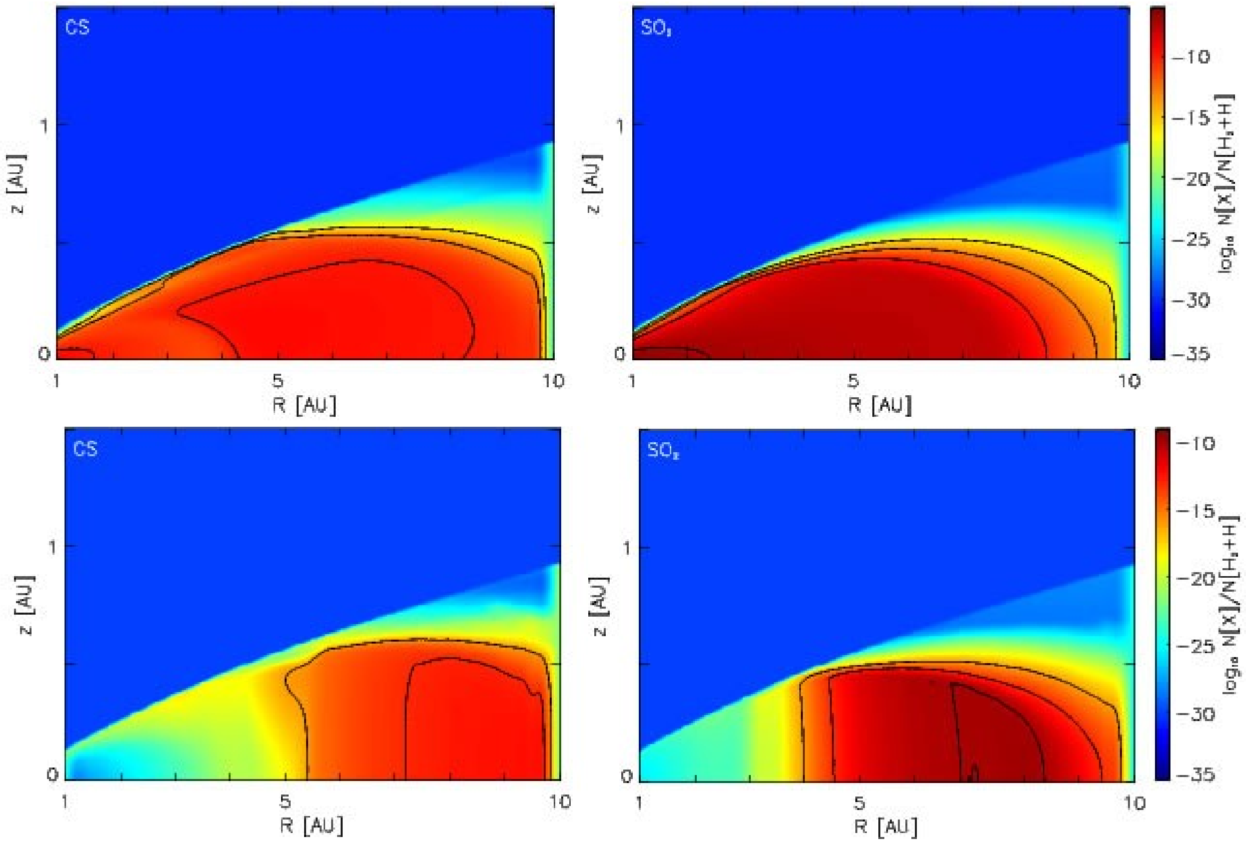
Advection

- Release of more volatile mantle material (e.g. CO, N_2) as material accretes inward
- Gas phase processing creating heavier molecules (e.g. HCN) which can freeze onto grains or remain in gas
- Chemistry should exhibit strong radial gradients – how to separate from other radial effects (increasing effects of radiation) is an area of interest.

Effects of Radial Diffusion

without

with



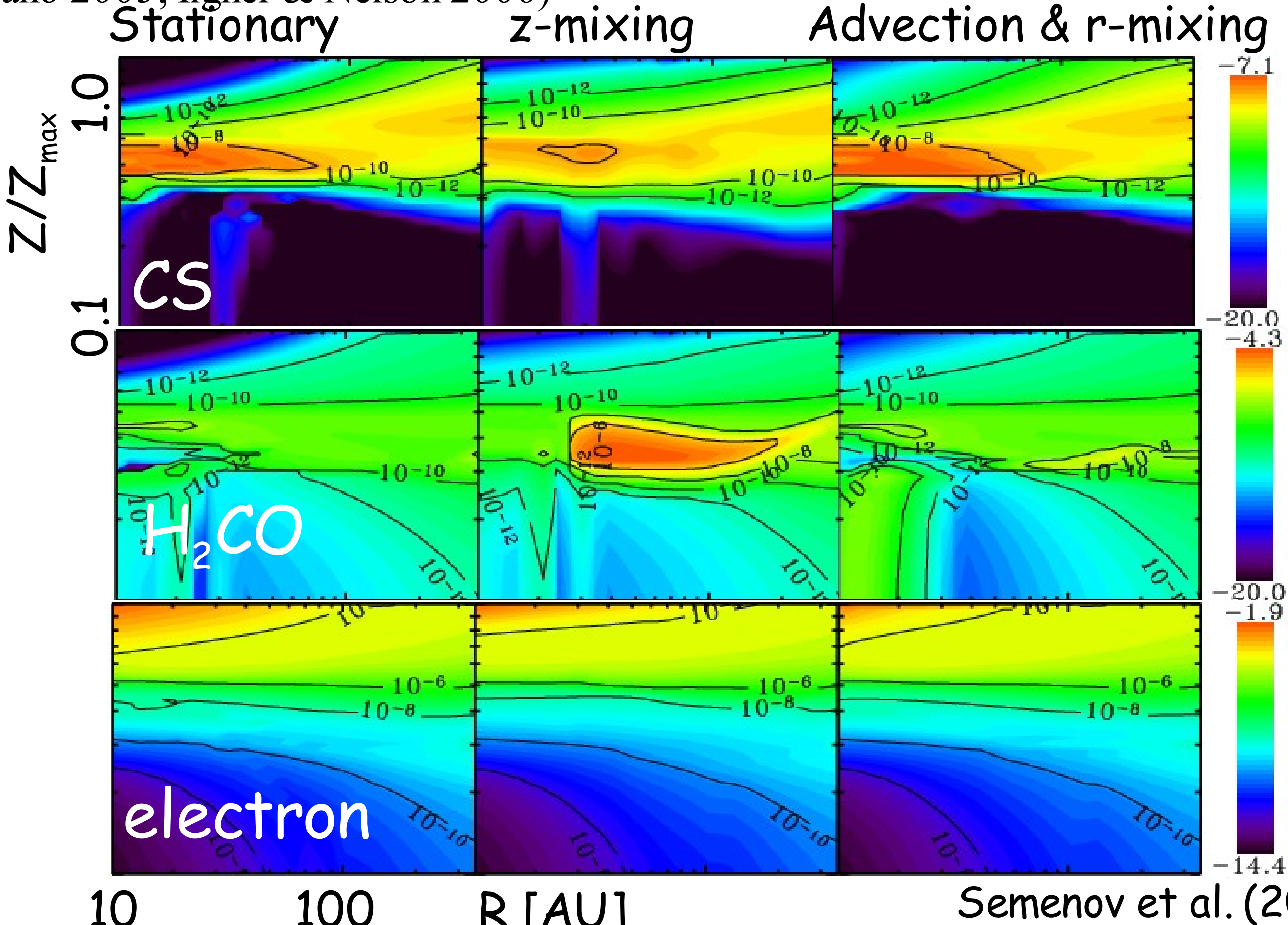
Ilgner et al. 2004

Chemical Physical Links: Mixing

Semenov et al. (2006) in prep

- Three-layer structure is preserved, because t_{chem} is small in the surface and midplane
- Species formed on grains (ex. H_2CO) are enhanced by vertical mixing
- Ionization fraction is not modified

➢Ionization can be enhanced by mixing if grains have grown or sedimented.
(Inutsuka & Sano 2005; Ilgner & Nelson 2006)



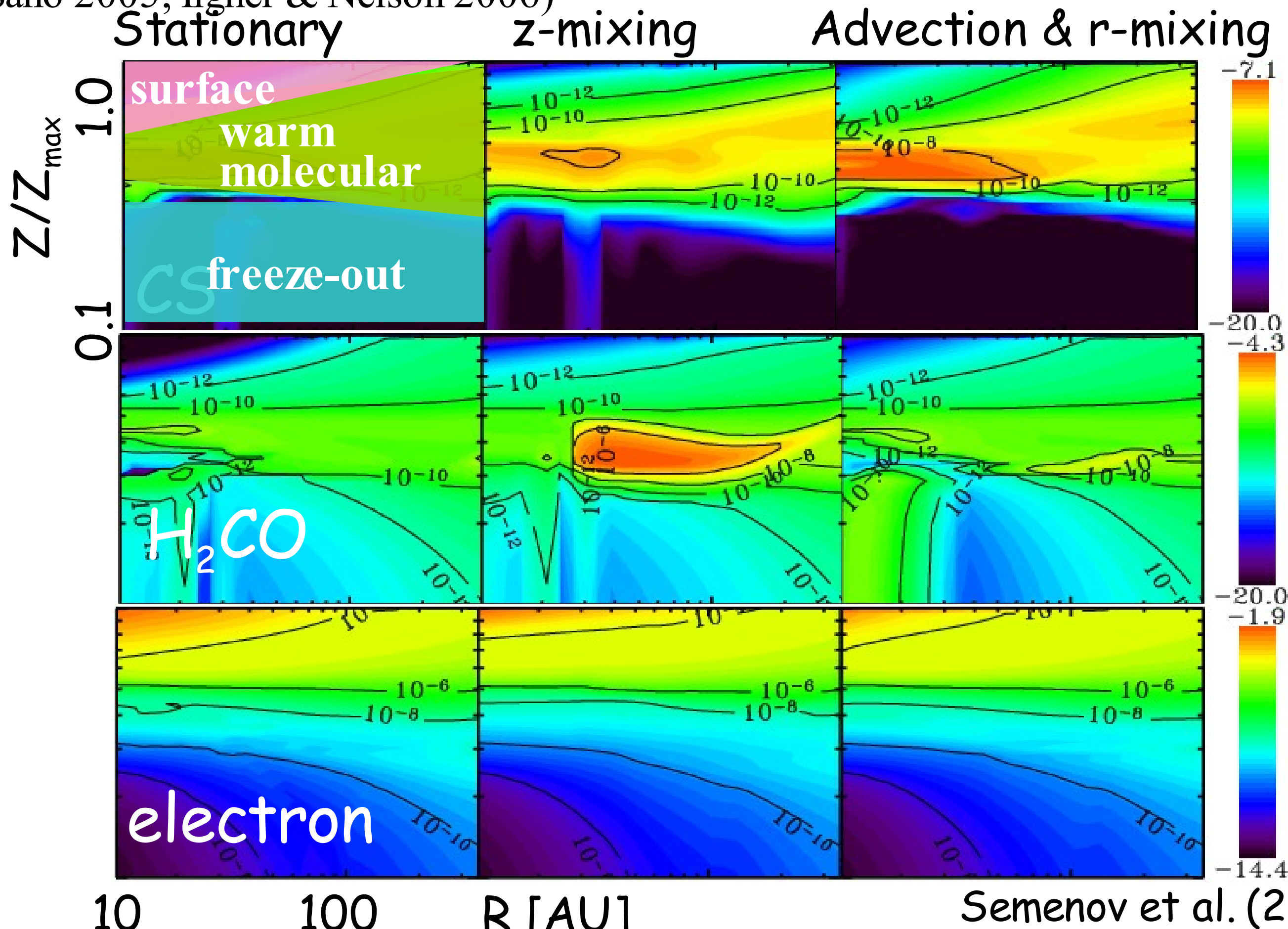
Semenov et al. (2006) in prep

Chemical Physical Links: Mixing

Semenov et al. (2006) in prep

- Three-layer structure is preserved, because t_{chem} is small in the surface and midplane
- Species formed on grains (ex. H_2CO) are enhanced by vertical mixing
- Ionization fraction is not modified

➢ Ionization can be enhanced by mixing if grains have grown or sedimented.
(Inutsuka & Sano 2005; Ilgner & Nelson 2006)



Semenov et al. (2006) in prep

Chemical Physical Links: Mixing

- Vertical structure is preserved but warm molecular layer is spread out in z direction: Willacy et al. 2006

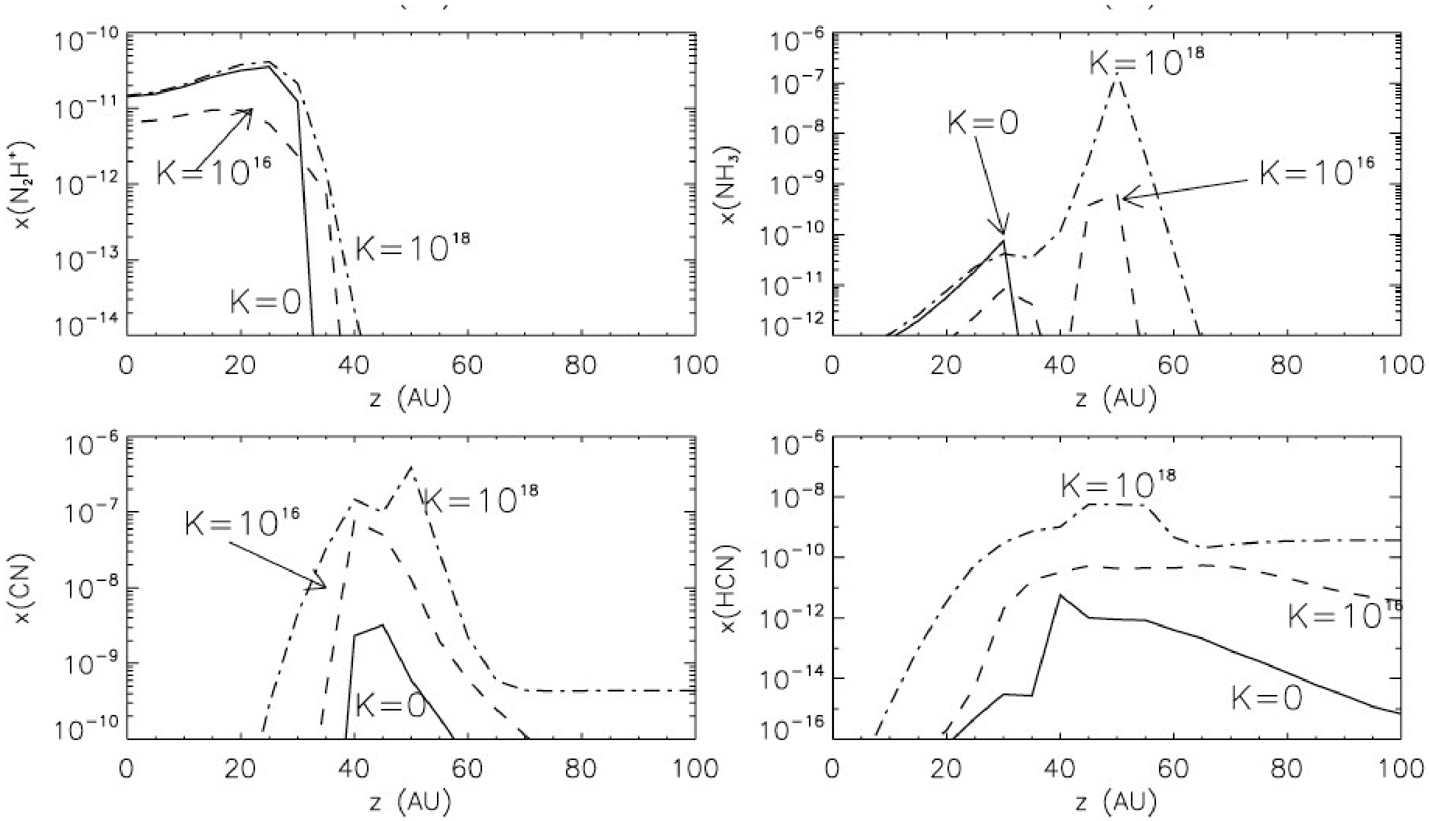


FIG. 4.—Fractional abundances with respect to H_2 as a function of height z above the midplane for $R = 100$ AU and a model time of 1 Myr. Lines are as in Fig. 3. Diffusion increases the peak abundance and the vertical extent of many molecules. At this radius, N_2H^+ traces the midplane, but NH_3 peaks in the molecular layer.

K = D = 10^{16} corresponds to $\alpha = 10^{-2}$ assuming $\nu = D$

Chemical Physical Links: Grain Evolution

Grains must coagulate & sediment to make planets

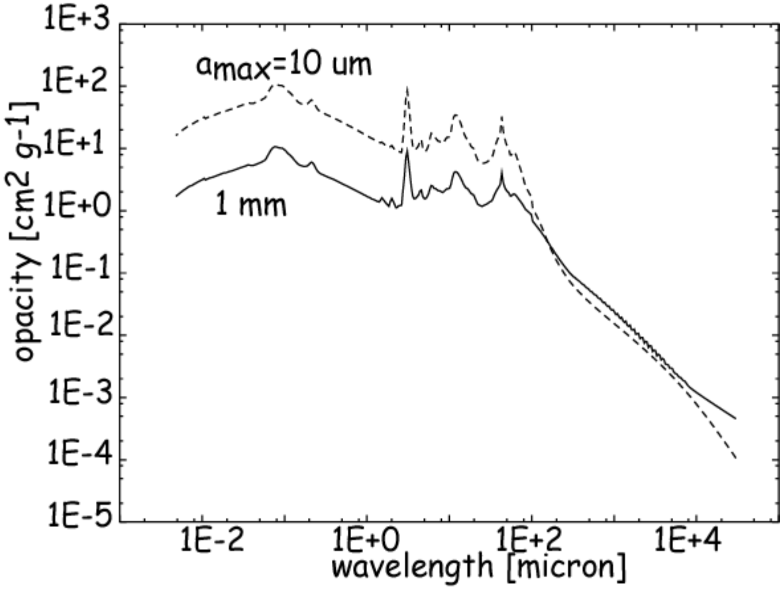
⇩

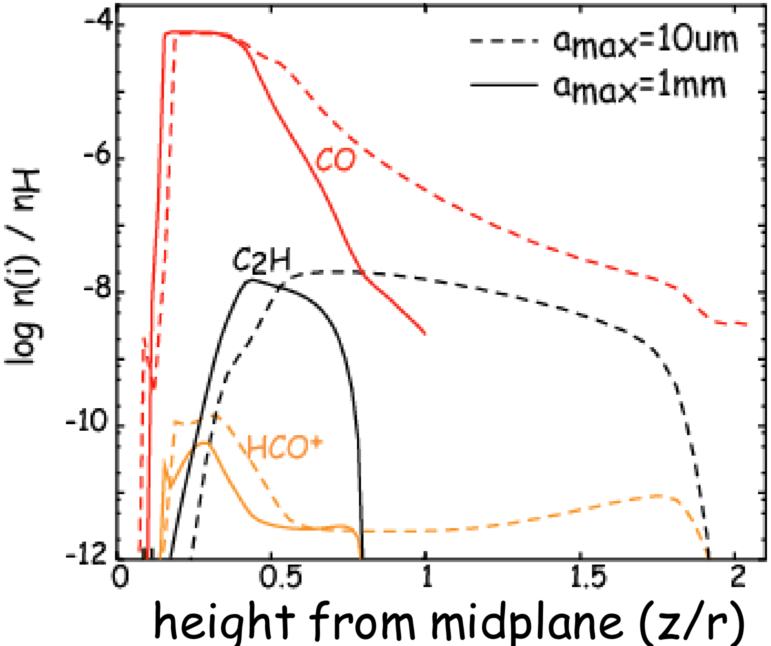
- **dust opacity decreases**

⇩

- **Molecular layer is pushed down to lower heights**
- **HCO^+, H_3^+, H_2D^+ are decreased**
- **Will have a radial dependence!**

Jonkheid et al. (2004); Aikawa & Nomura (2006)





Combined Chemical/Thermal Models

- Chemical composition influences the disk structure by mediating the abundances of coolants
- Disk gas heating
  - accretion (highly uncertain)
  - dust-gas coupling (full coupling expected for $n > 10^6$ cm^{-3}
  - UV radiation (will depend on presence/absence of PAHs)
    - H_2 fluorescence with collisional de-excitation
    - photoelectric effect
    - H_2 dissociation
    - Carbon ionization
  - X-rays
  - H_2 formation
  - Cosmic Rays
- Disk gas cooling
  - line emission
  - dust-gas coupling
- *Dust/gas are not thermally coupled in upper layers*

- Models:
  - Kamp et al. 2005 (IAU)
  - Jonkheid et al. 2004
  - Aikawa and Nomura 2006

see Hollenbach and Tielens RVMP 199