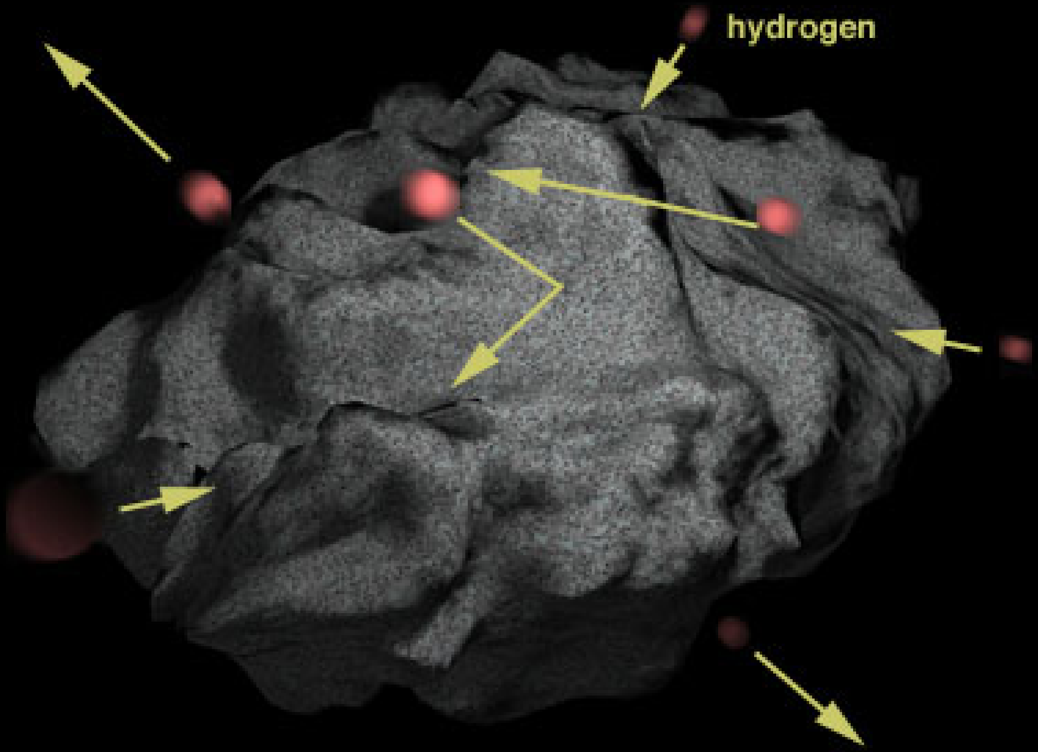

Gas-grain processes in the ISM

Paola Caselli

Outline

- ü The formation of H_2 and other surface processes
- ü Cosmic ray ionization of H_2
- ü The chemistry initiated by H_3^+
- ü Formation and destruction of CO
- ü Nitrogen chemistry
- ü PDR chemistry
- ü The freeze-out of molecules
- ü Action items

1. The formation of H_2

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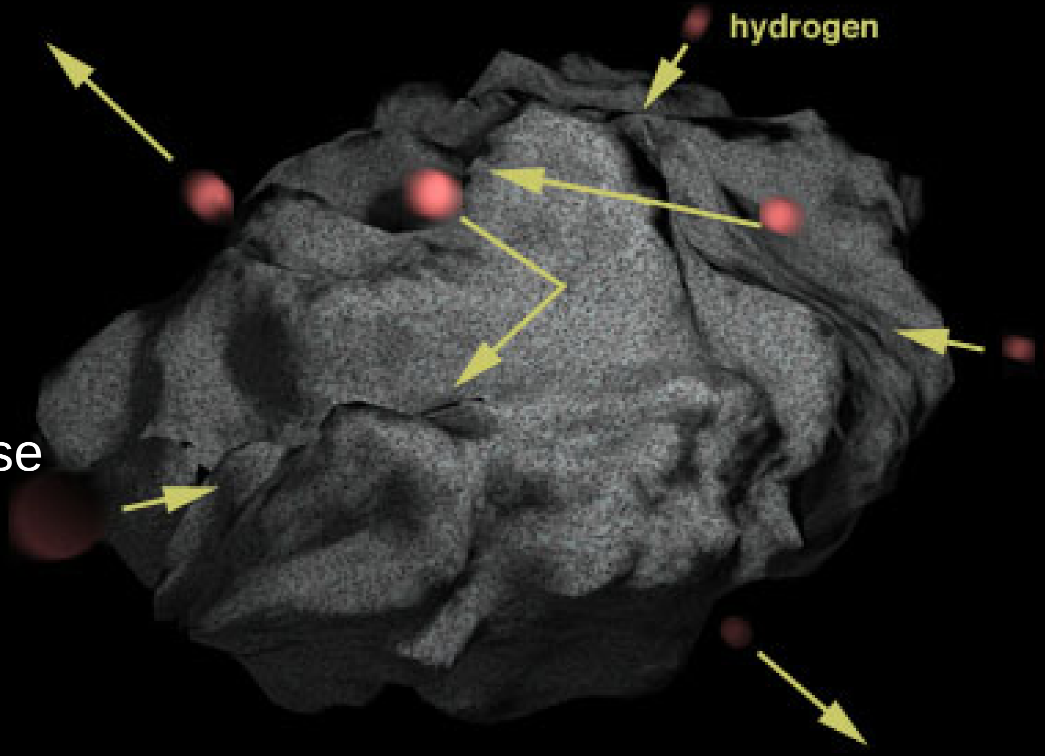
$H + H \rightarrow H_2$ on the surface of dust grains

(Gould & Salpeter 1963; Hollenbach & Salpeter 1970; Jura 1974; Pirronello et al. 1999; Cazaux & Tielens 2002; Habart et al. 2003; Bergin et al. 2004; Cuppen & Herbst 2005)



$n_H \equiv$ gas number density
$v_H \equiv$ H atoms speed in gas-phase
$A \equiv$ grain cross sectional area
$n_g \equiv$ dust grain number density
$S_H \equiv$ sticking probability
$\gamma \equiv$ surface reaction probability

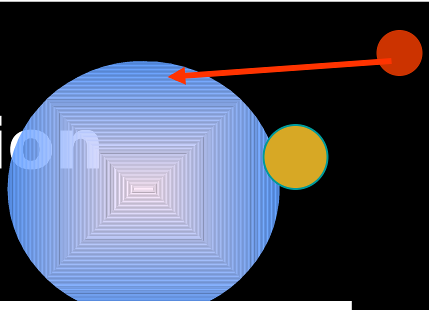
ther surface processes..

REACTANTS: MAINLY MOBILE ATOMS AND RADICALS

$A + B \rightarrow AB$ association

$H + H \rightarrow H_2$

$H + X \rightarrow XH$ (X = O, C, N, CO, etc.)



Accretion

$\propto 10/[T_k^{1/2}\ n(H_2)]$ days

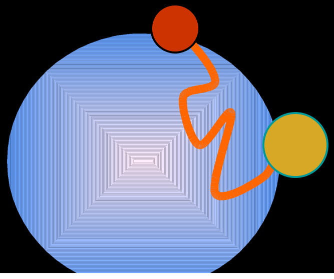
WHICH CONVERTS

$O \rightarrow OH \rightarrow H_2O$

$C \rightarrow CH \rightarrow CH_2 \rightarrow CH_3 \rightarrow CH_4$

$N \rightarrow NH \rightarrow NH_2 \rightarrow NH_3$

$CO \rightarrow HCO \rightarrow H_2CO \rightarrow H_3CO \rightarrow CH_3OH$



Diffusion+Reaction

$t_{qt}(H) \sim 10^{-5}$-10^{-3} s

RE: Watson & Salpeter 1972; Allen & Robinson 1977; Pickes & Williams 1977; d'Hendecourt et al. 1985; Hasegawa et al. 1992; Caselli et al. 1993

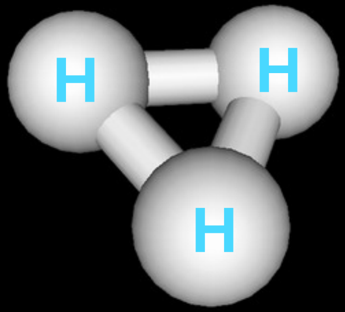
2. Cosmic-ray ionization of H_2

Cosmic rays ionize H_2 initiating fast routes towards the formation of complex molecules in dark clouds:

$$H_2 + \text{c.r.} \rightarrow H_2^+ + e^- + \text{c.r.}$$

Once H_2^+ is formed (in small percentages), it very quickly reacts with the abundant H_2 molecules to form H_3^+, the most important molecular ion in interstellar chemistry:

$$H_2^+ + H_2 \rightarrow H_3^+ + H$$



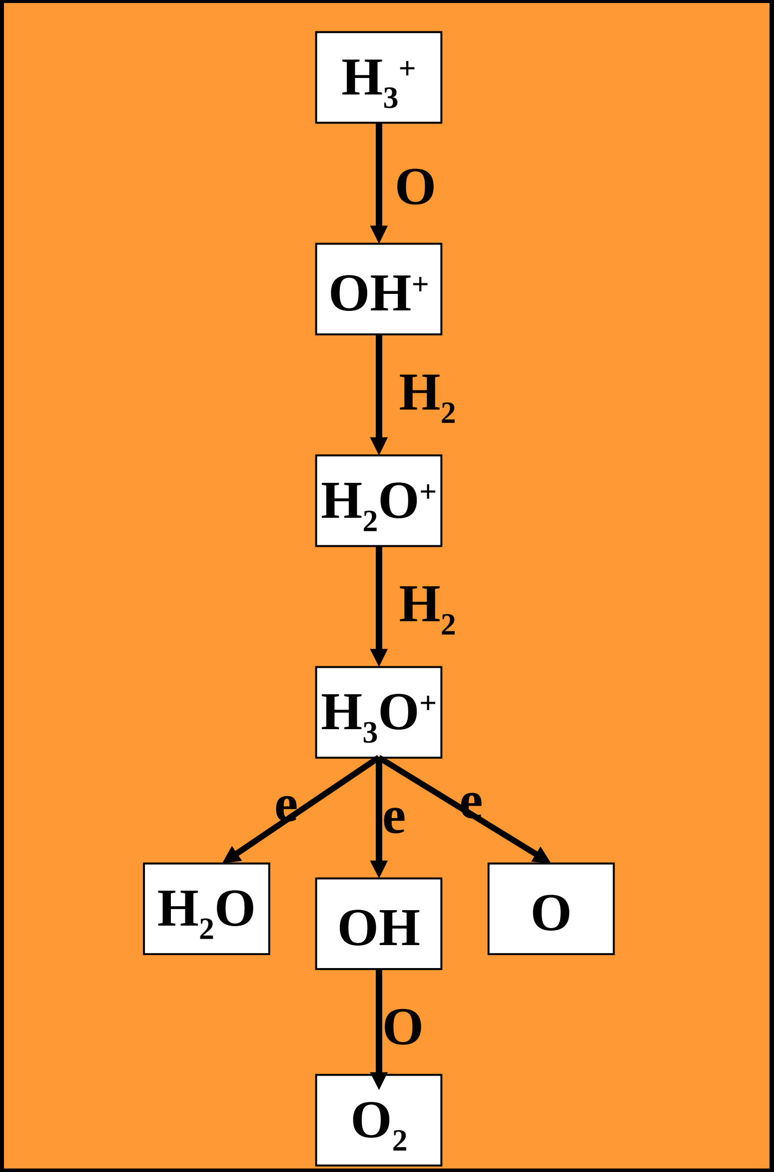
3. The chemistry initiated by H_3^+

Once H_3^+ is formed, a cascade of reactions greatly enhance the chemical complexity of the ISM.

In fact, H_3^+ can easily donate a proton and allow larger molecules to build.

Example →

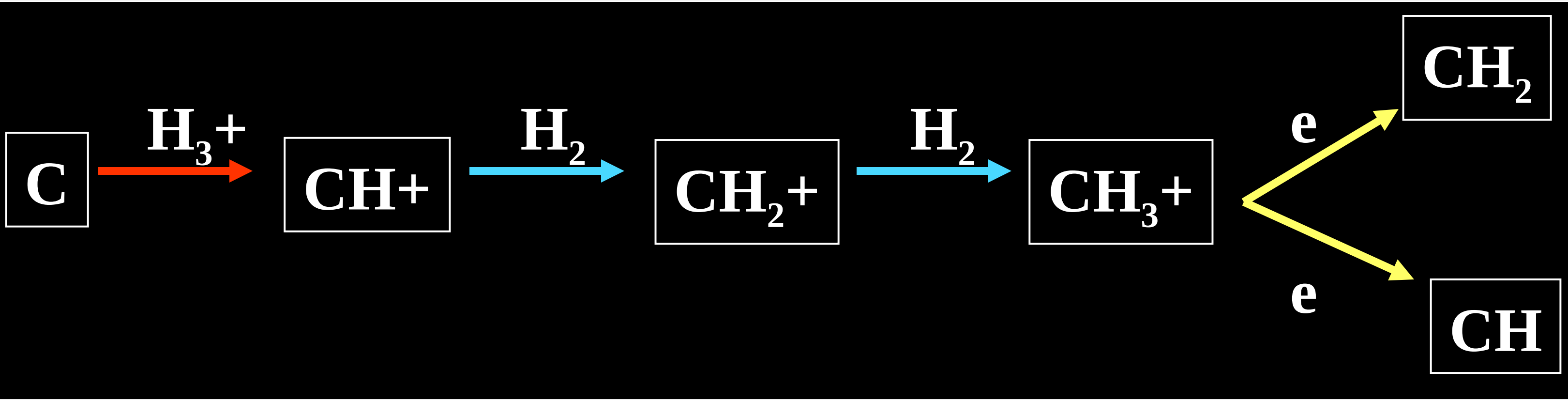
OXYGEN CHEMISTRY (the formation of water in the ISM)



Carbon chemistry

(the formation of hydrocarbons)

The formation of more complicated species from neutral atomic carbon begins with a sequence very similar to that which starts the oxygen chemistry:



$$C \xrightarrow{H_3+} CH+ \xrightarrow{H_2} CH_2+ \xrightarrow{H_2} CH_3+$$

$$CH_3+ \xrightarrow{e} CH_2 \qquad CH_3+ \xrightarrow{e} CH$$

A. Proton transfer from H_3^+ to a neutral atom;

B. Hydrogen abstraction reactions terminating in a molecular ion that does not react with H2;

C. Dissociative recombination with electrons.

4. Formation and destructio1n of CO

[a] $C + OH \rightarrow CO + H$

[b] $C + H_3O^+ \rightarrow HCO^+ + H_2$

[c] $O + CH_3^+ \rightarrow HCO^+ + H_2$

[d] $HCO^+ + e \rightarrow CO + H$ is the most important source of CO.

CO is very stable and difficult to remove. It reacts with H_3^+:

[e] $H_3^+ + CO \rightarrow HCO^+ + H_2$

but reaction [d] immediately reforms CO.

The main mechanisms for CO destruction are:

[f] $He^+ + CO \rightarrow He + C^+ + O$

[g] $h\nu + CO \rightarrow C + O$

Some of C^+ react with OH and H_2O (but not with H_2):

[h] $C^+ + OH \rightarrow CO^+ + H$

[i] $CO^+ + H_2 \rightarrow HCO^+ + H$

[j] $C^+ + H_2O \rightarrow HCO^+ + H$

5. Nitrogen Chemistry

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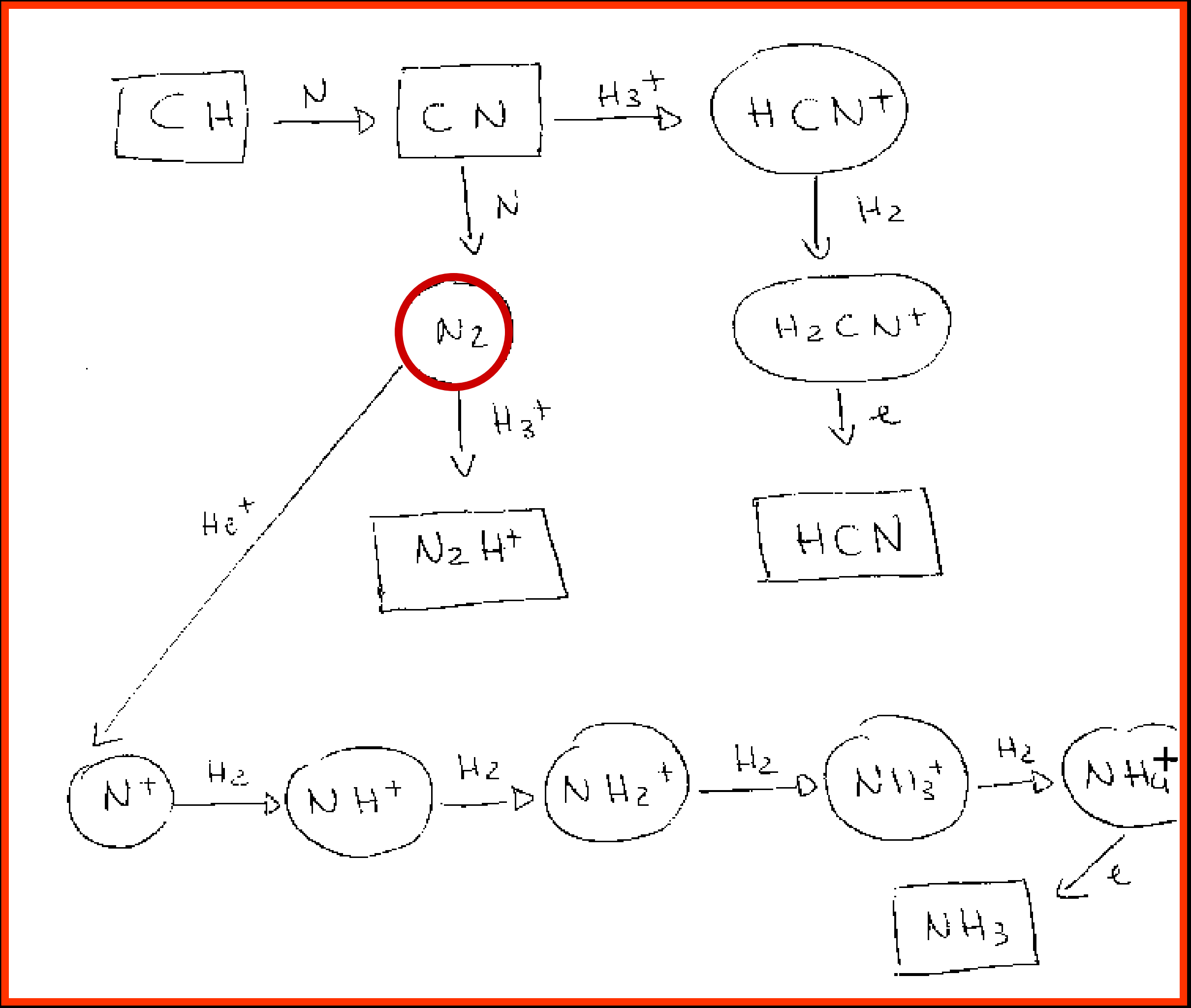
The nitrogen chemistry differs from that of oxygen and carbon:

$N + H_3^+ \not\rightarrow NH^+ + H_2$

The N-chemistry starts with a neutral-neutral reaction (e.g.):

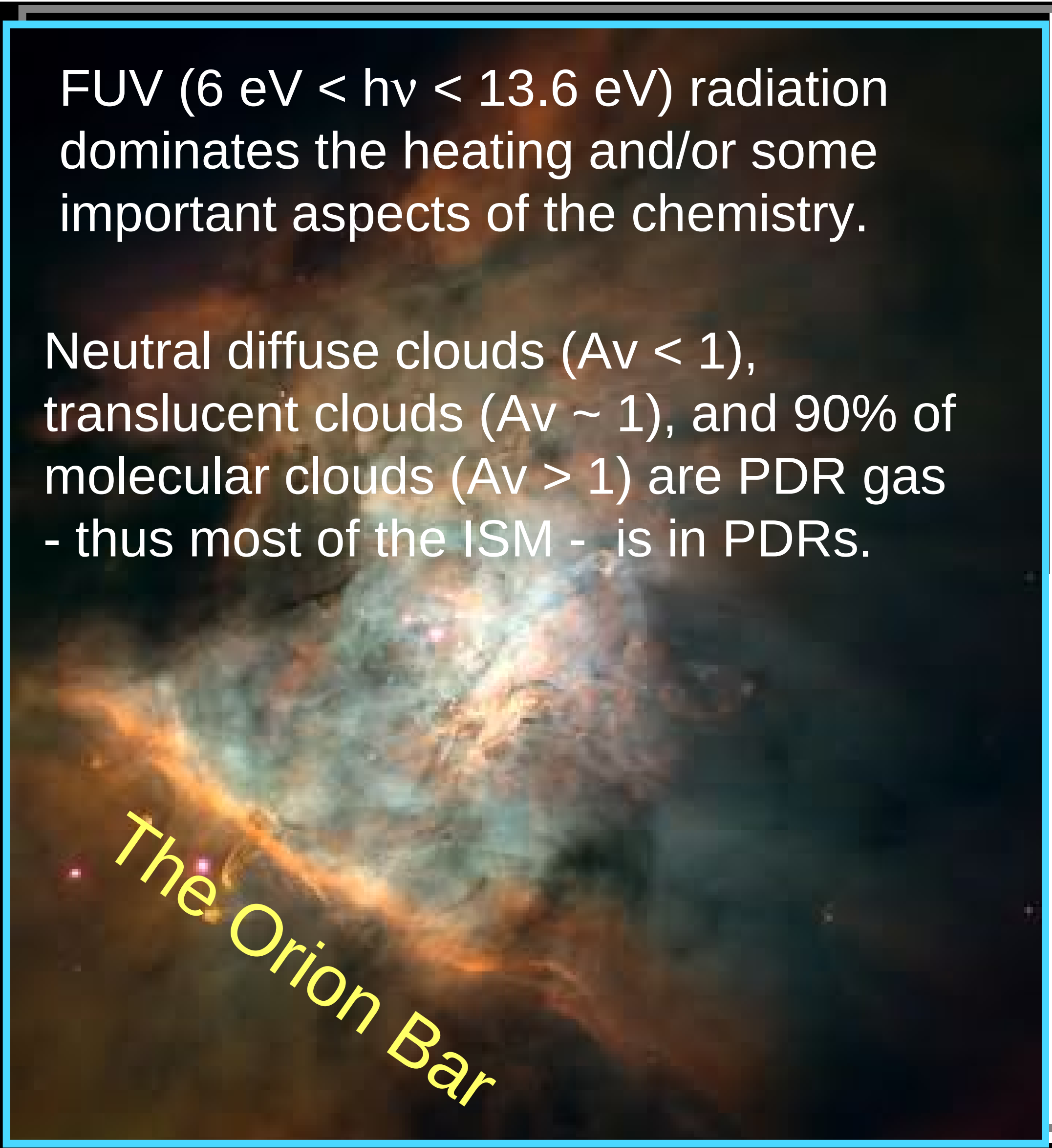
$CH + N \rightarrow CN + H$

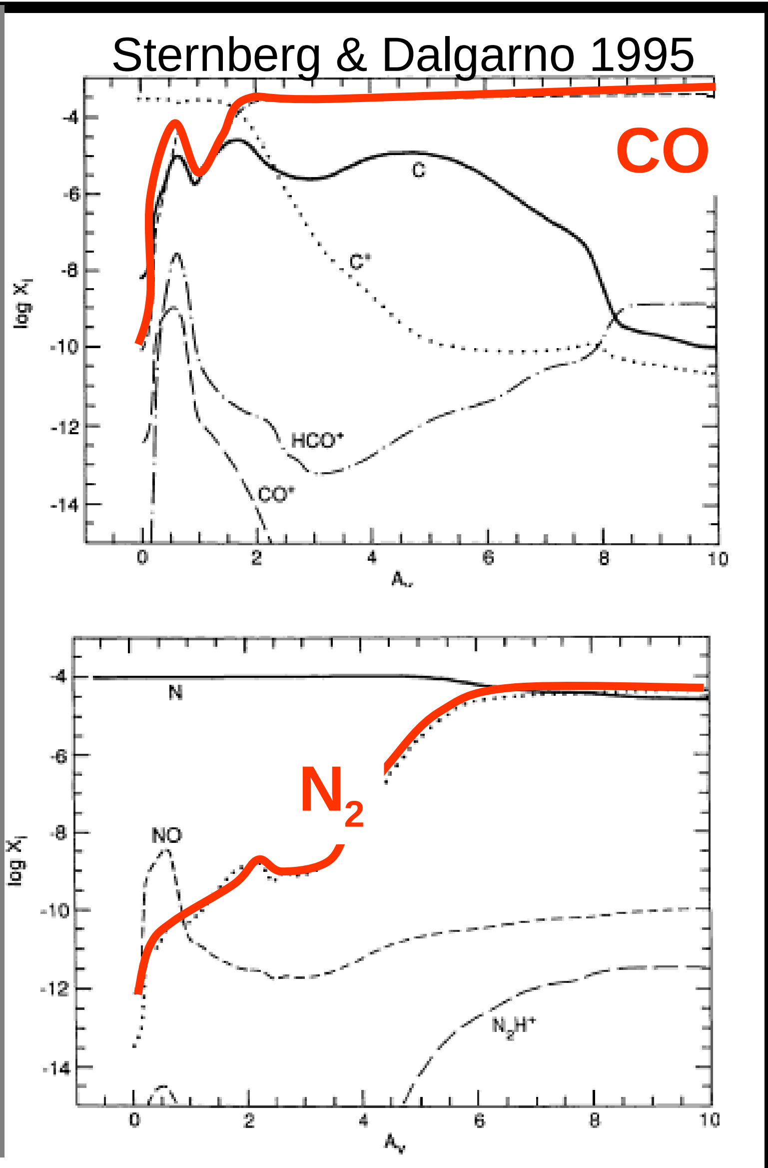


6. Photodissociation Regions (PDRs)

FUV (6 eV < hν < 13.6 eV) radiation dominates the heating and/or some important aspects of the chemistry.

Neutral diffuse clouds (Av < 1), translucent clouds (Av ~ 1), and 90% of molecular clouds (Av > 1) are PDR gas - thus most of the ISM - is in PDRs.

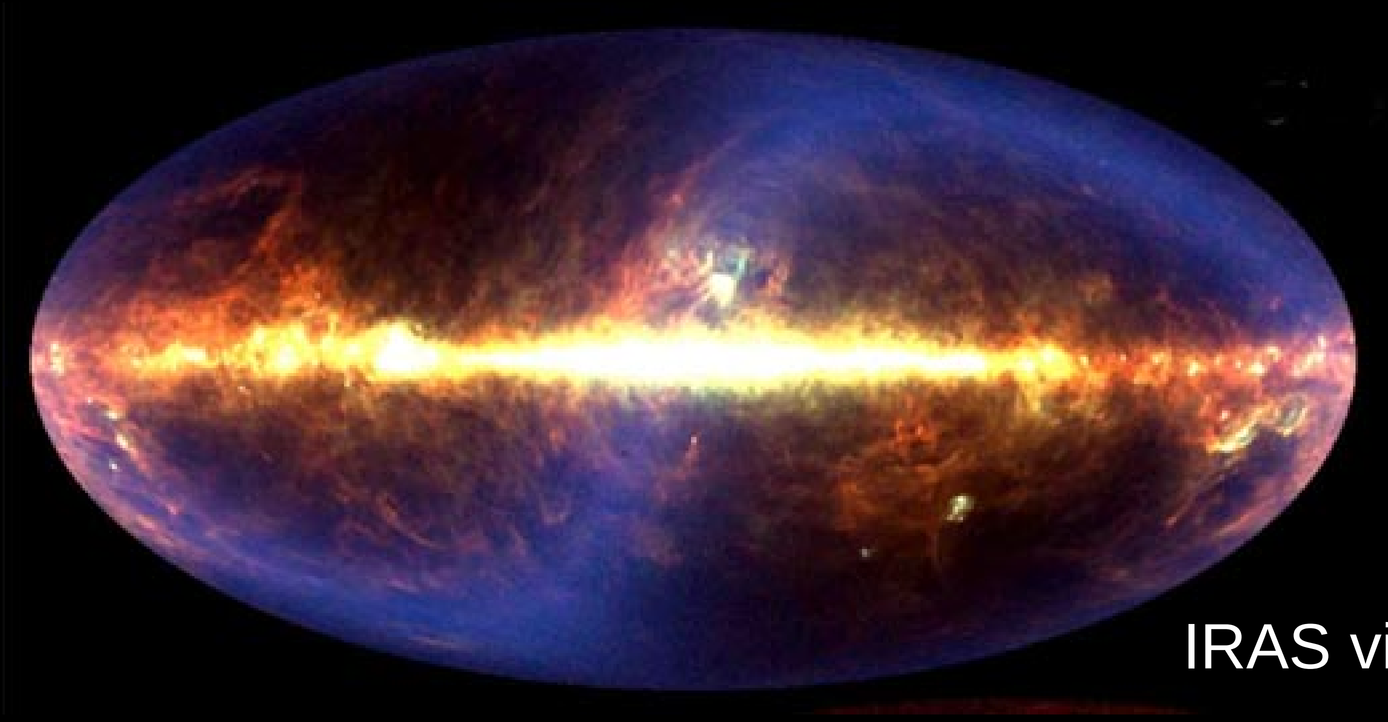



Sternberg & Dalgarno 1995

PDRs

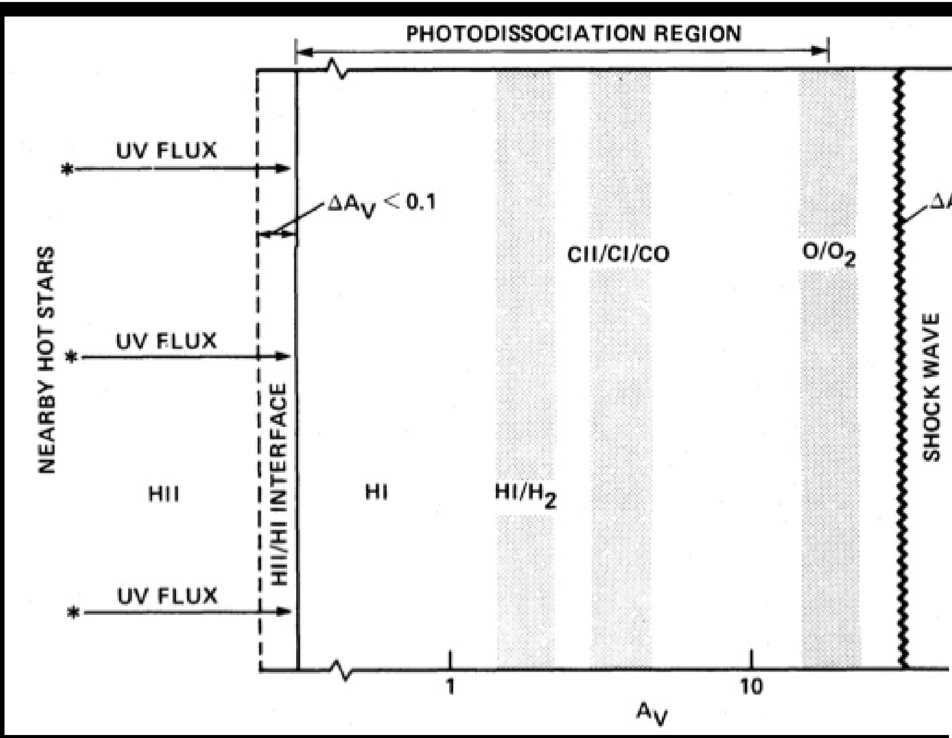
PDRs are the origin of much of the IR radiation from the ISM. The incident starlight is absorbed by dust grains and PAHs, and reradiated primarily as PAH IR features and IR continuum.

About 0.1-1% of the absorbed starlight is converted to gas heating via *photoelectric ejection of electrons from grains*.

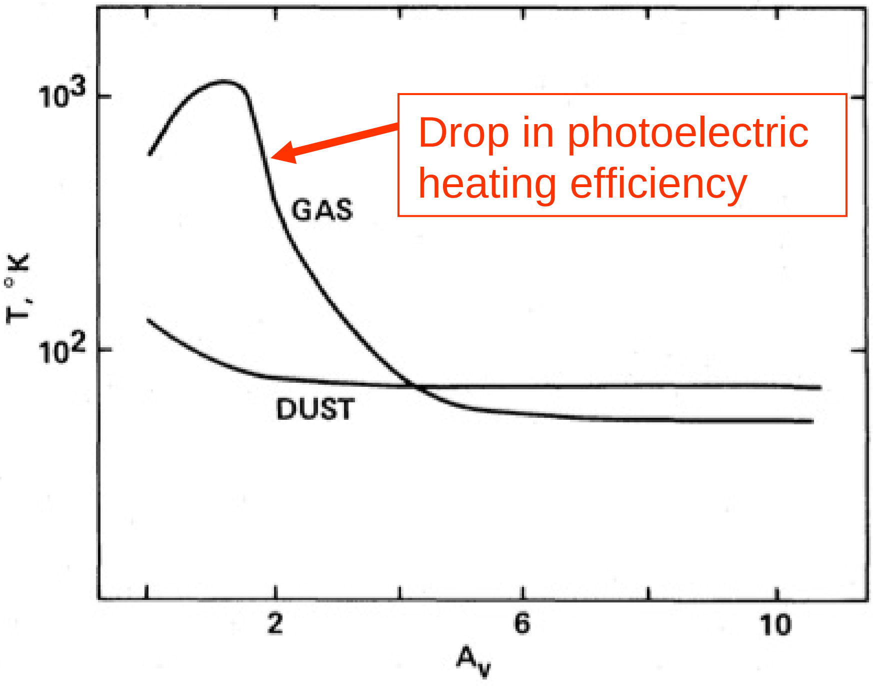


IRAS view

PDRs



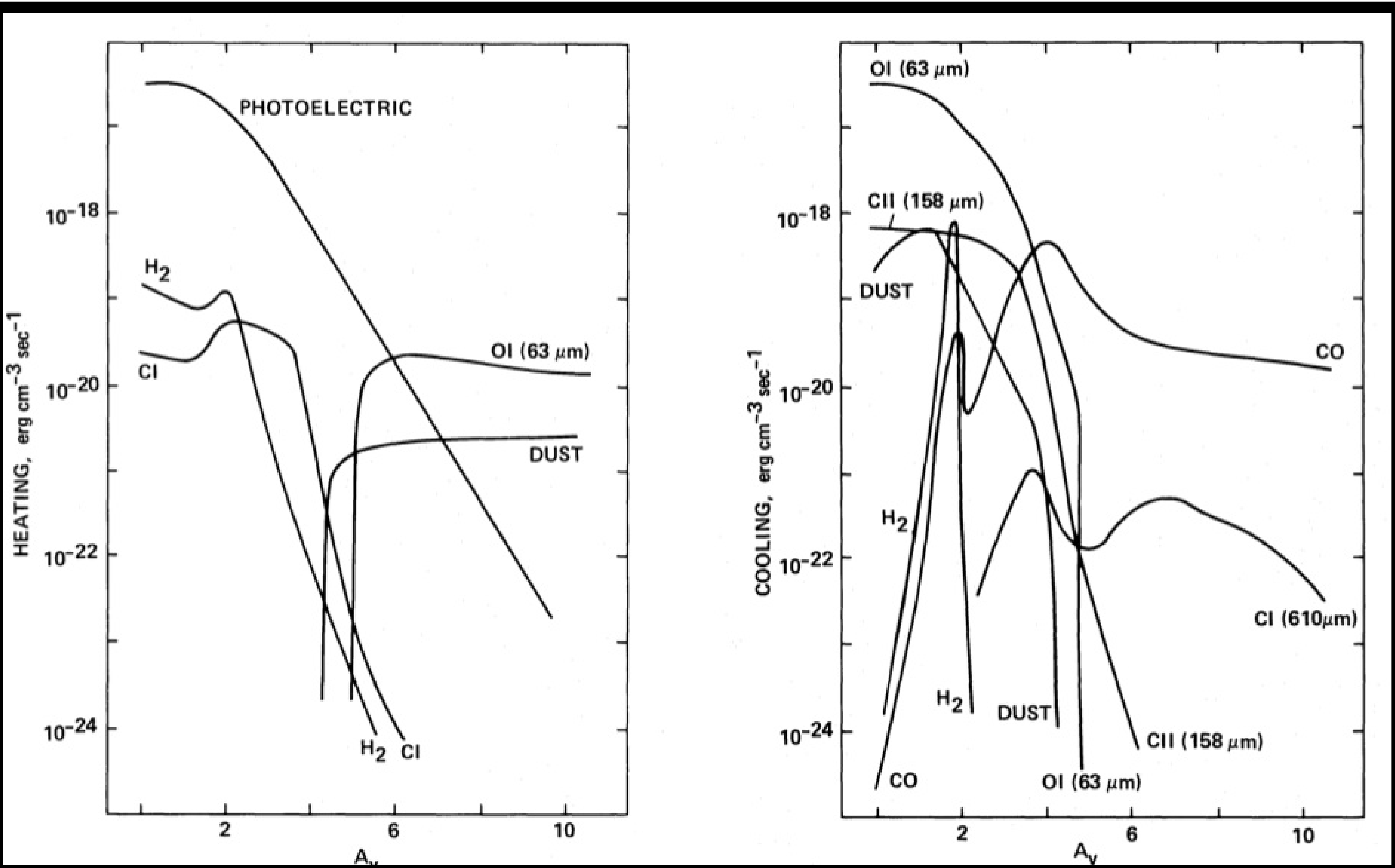
The Orion Bar:
$G_o \sim 10^5$ and $n_H \sim 10^5$ cm^{-3}



Drop in photoelectric heating efficiency

Tielens & Hollenbach 1985

PDRs



Tielens & Hollenbach 1985

PDRs

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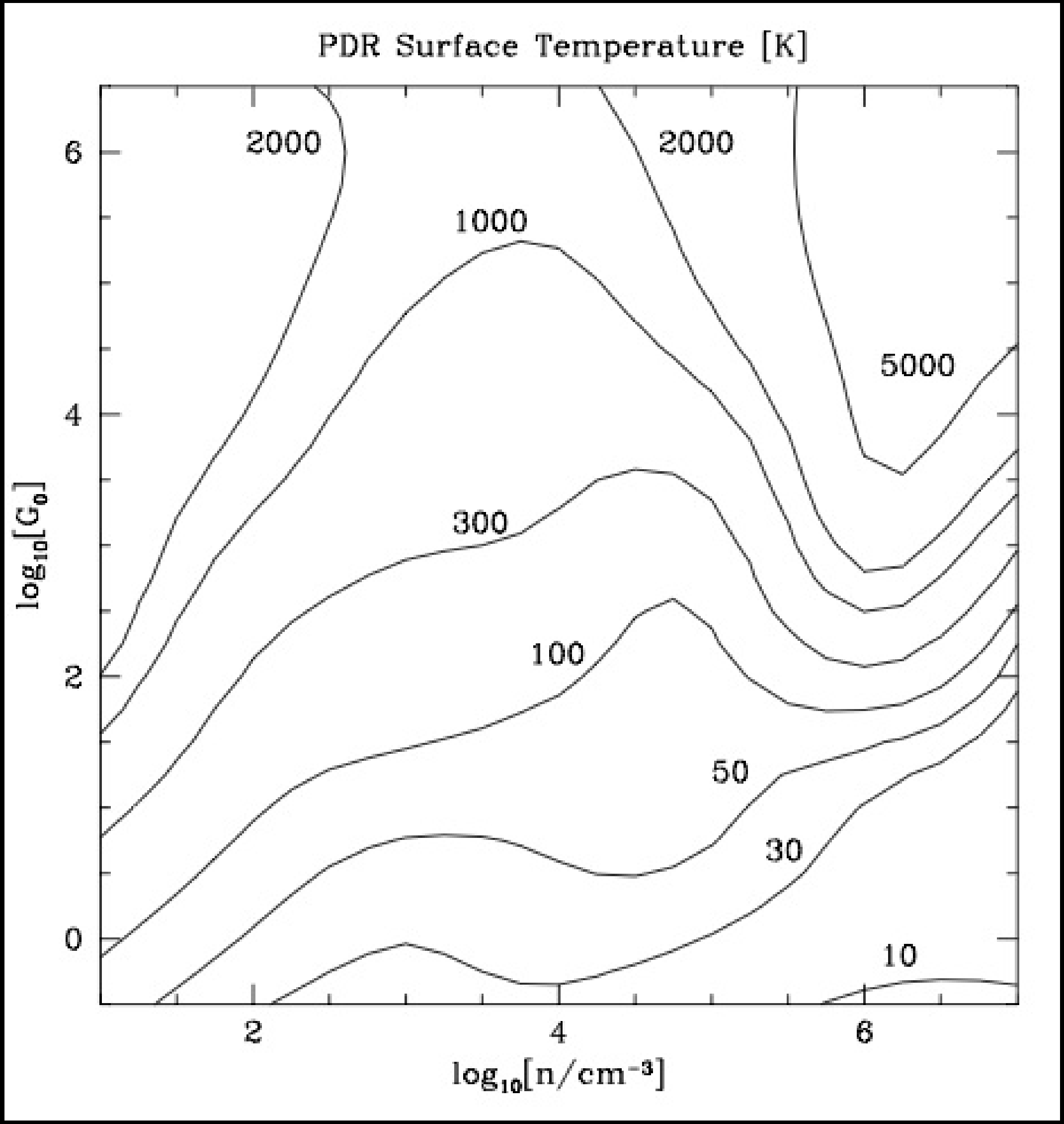
The PDR surface temperature typically increases with G_o.

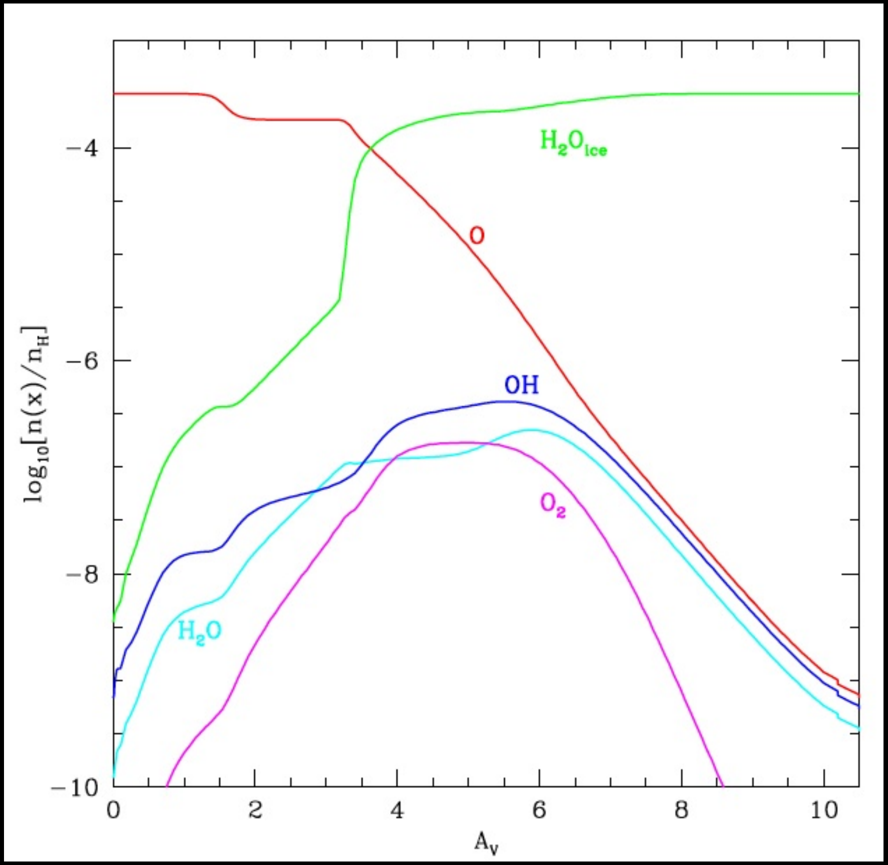
The effect of lowering the dust abundance is to increase the physical extent of a PDR model.

Kaufman et al. (1999)

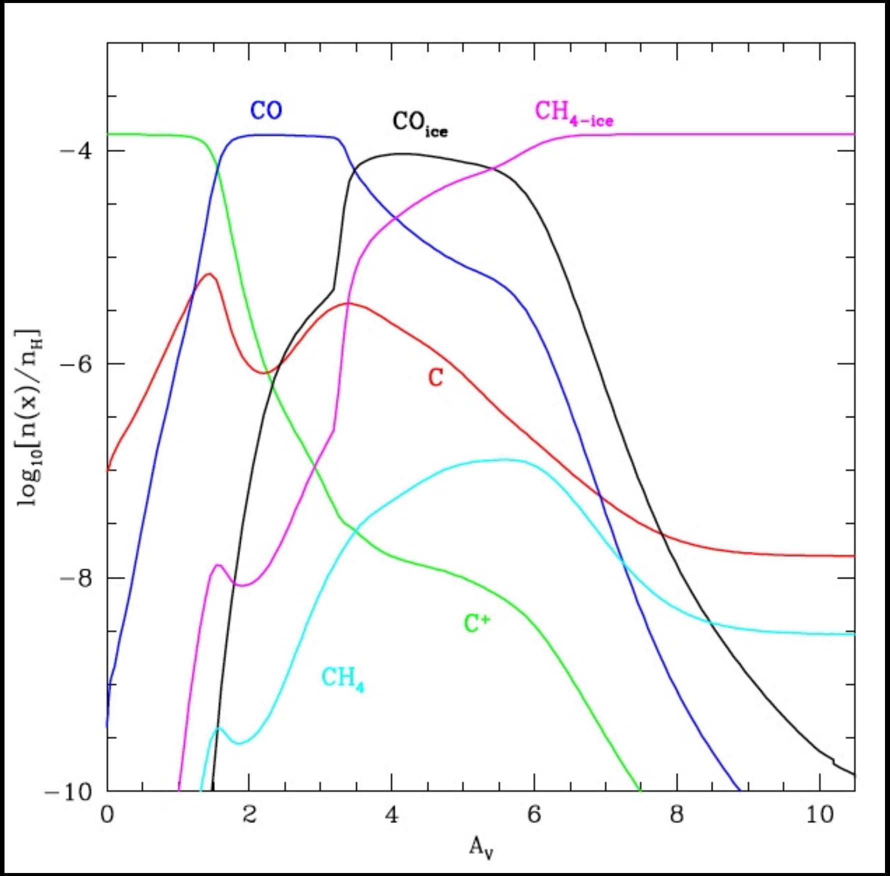


ome results (from Hollenbach et al. 2009

Oxygen Chemistry



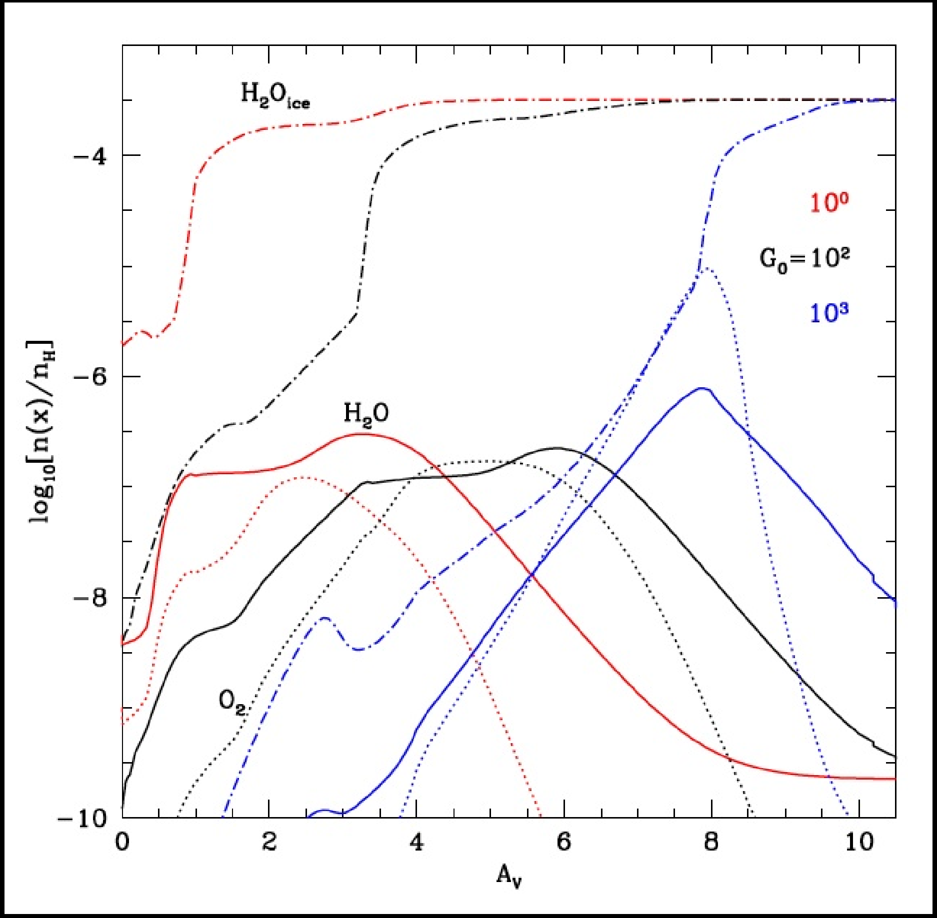
Carbon Chemistry



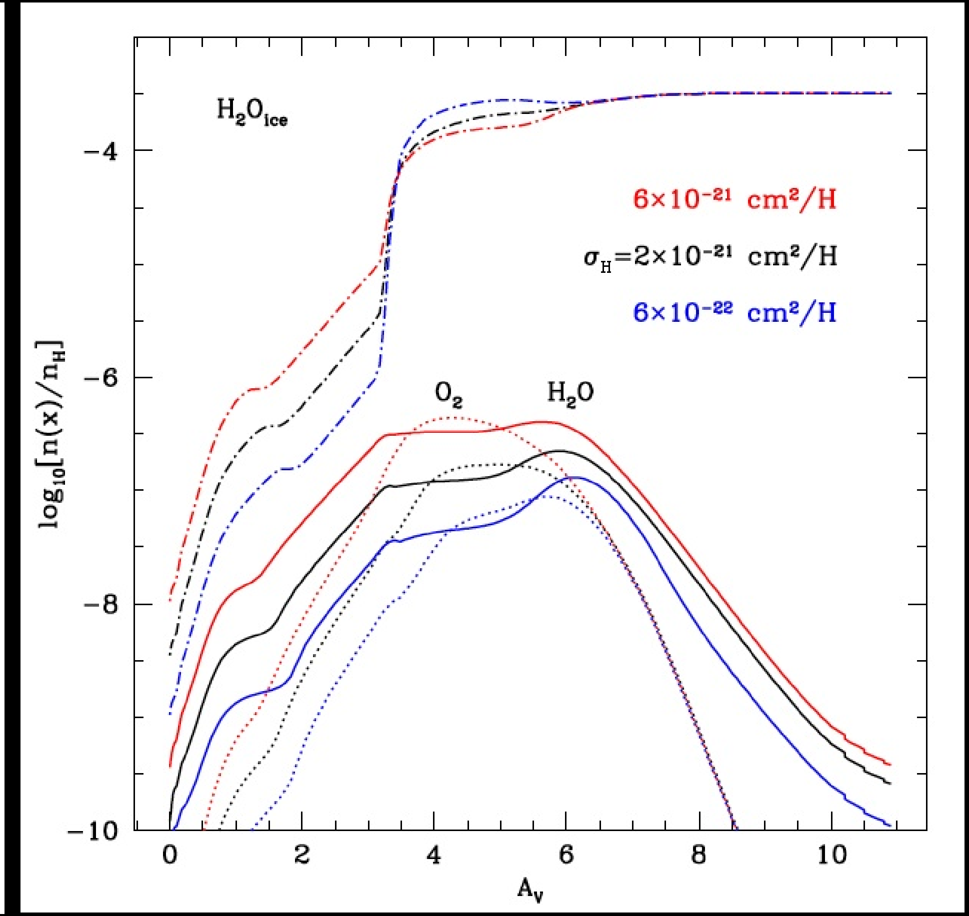
$n = 10^4$ cm^{-3}; $G_0 = 100$

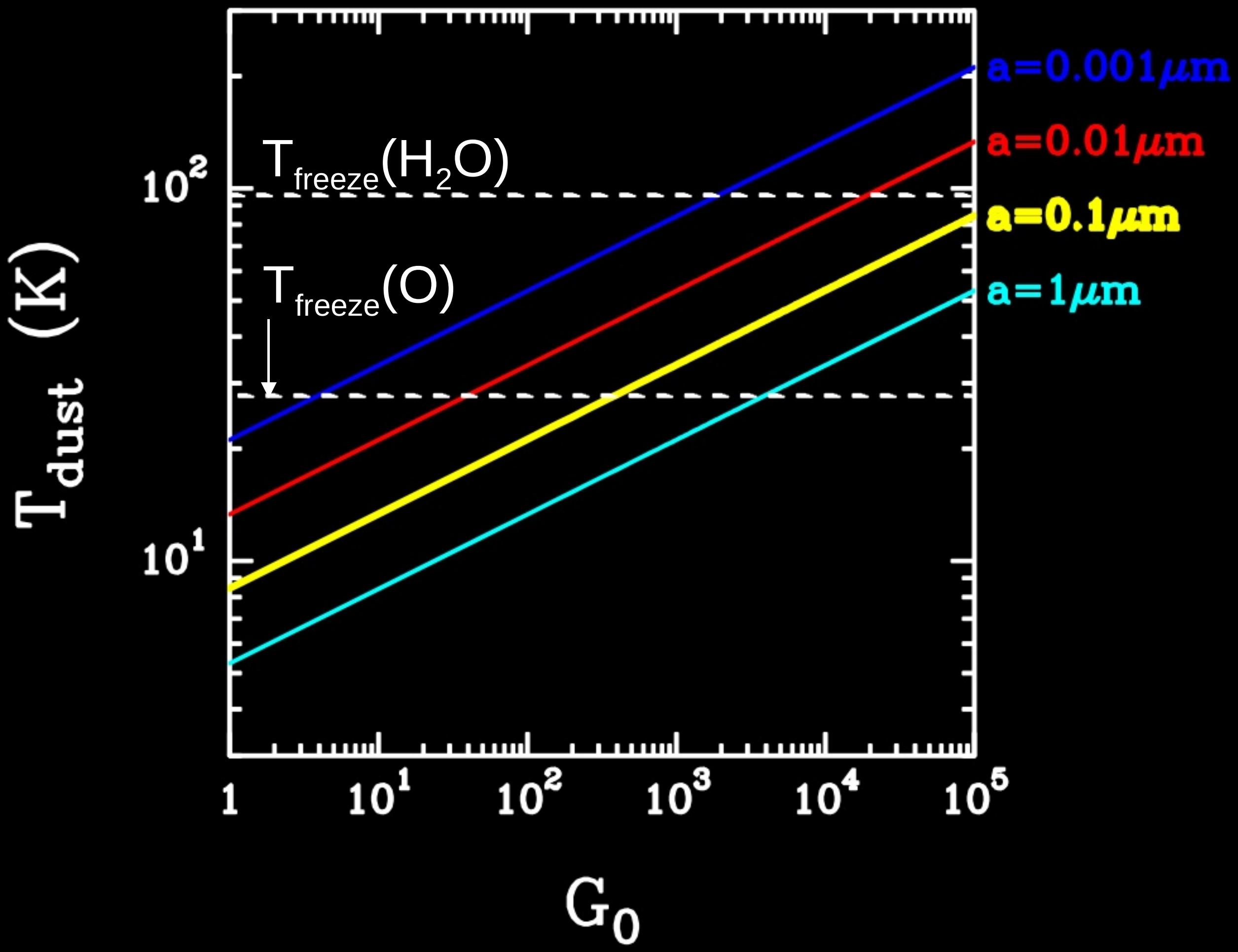
ome results (from Hollenbach et al. 2009

G_0 variations



Grain size variations




$T_{freeze}(H_2O)$
$T_{freeze}(O)$
a=0.001μm
a=0.01μm
a=0.1μm
a=1μm
10^2
10^1
T_{dust} (K)
1
10^1
10^2
10^3
10^4
10^5
G_0

. The freeze out of molecules

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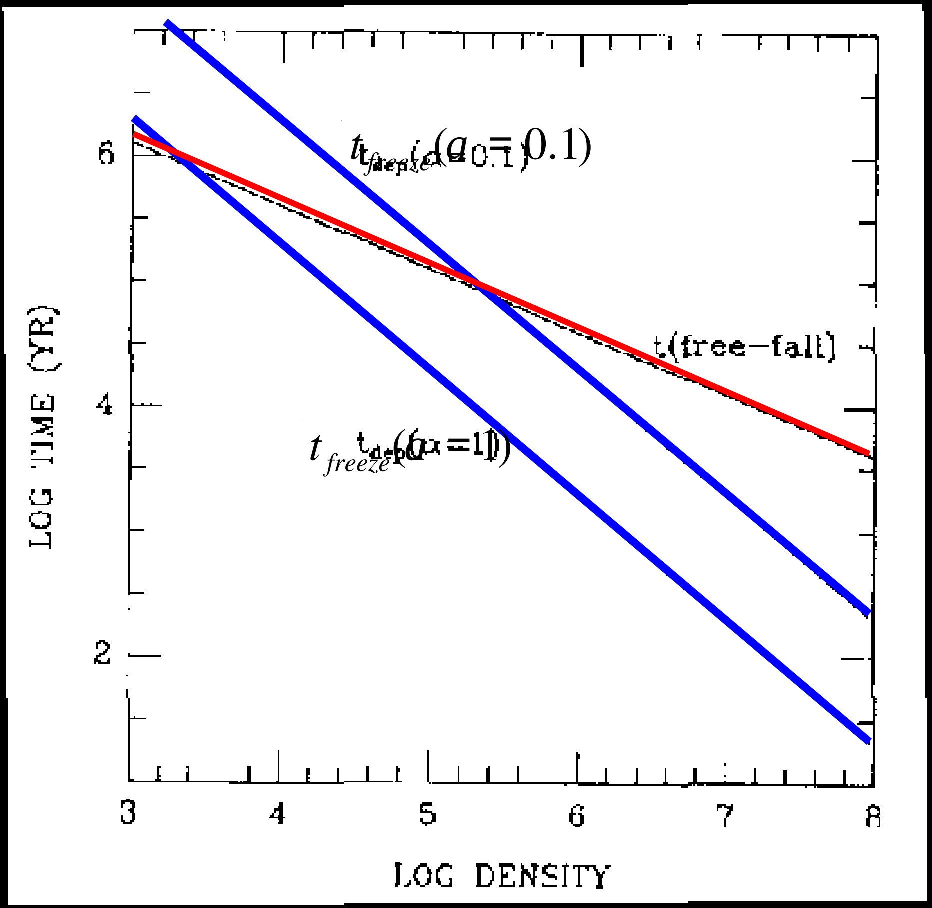
As long as the dust temperature is lower that the evaporation temperature, species will tend to stick onto dust grains…



Walmsley 1991
van Dishoeck et al. 1993

Evidence of freeze-out: the missing CO

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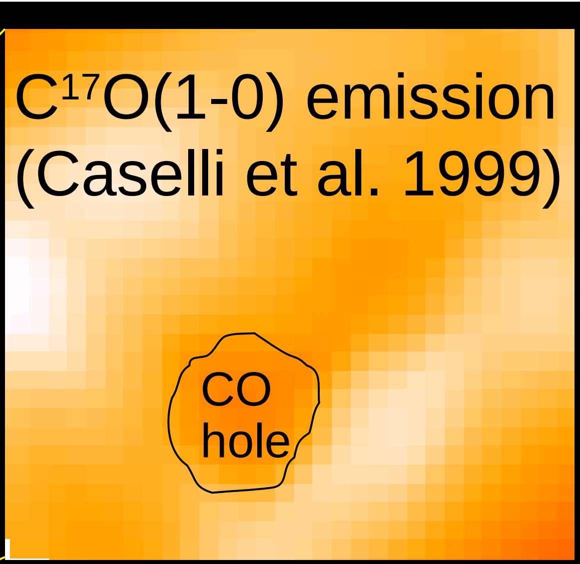
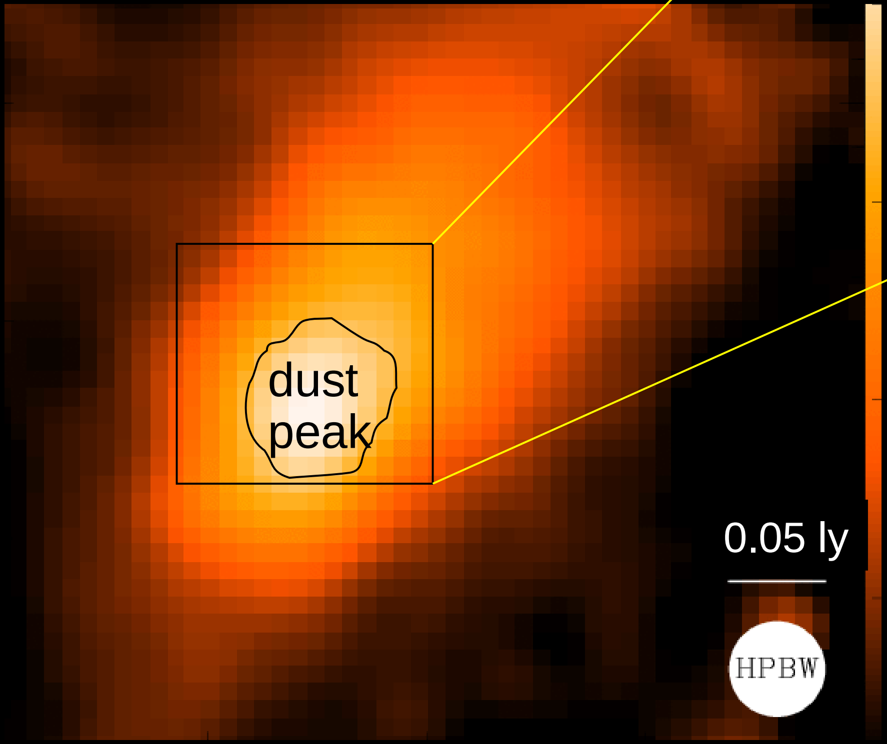
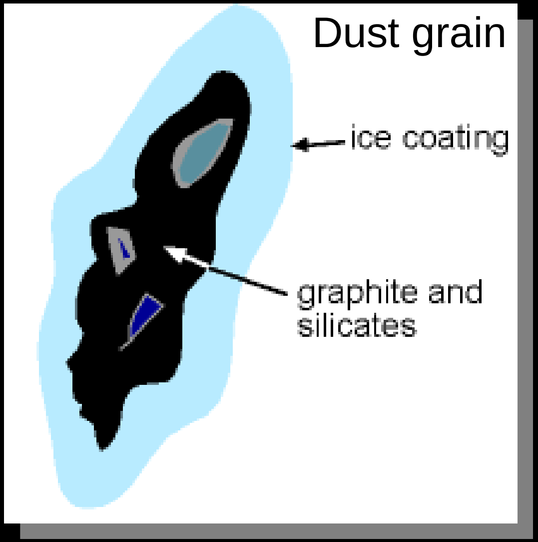

$C^{17}O(1-0)$ emission
(Caselli et al. 1999)



Dust emission in a pre-stellar core
(Ward-Thompson et al. 1999)

Molecules freeze out onto dust grains in the center of pre-stellar cores ➔



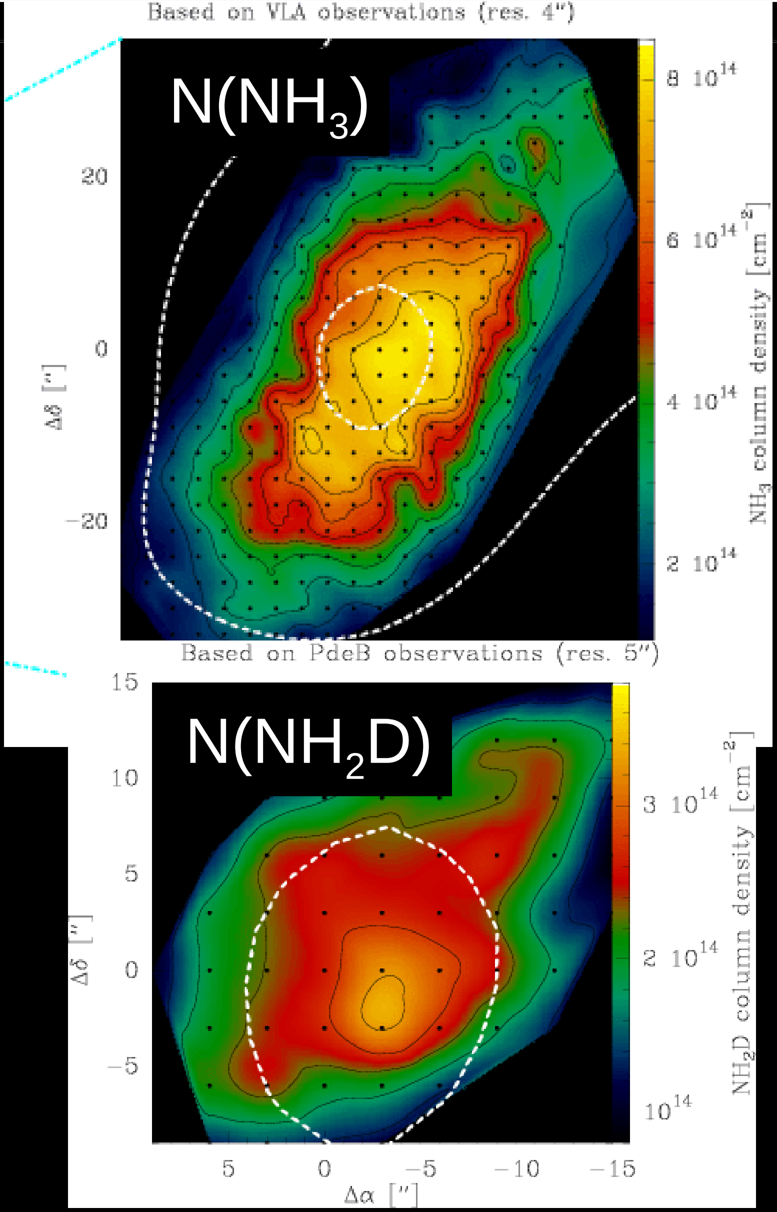
ut not all molecules freeze out…

$_3$ @ VLA + NH_2D @ PdBI

- On size scale of ▪ 800 AU: no evidences of NH_3 (and N_2) freeze-out (at $n(H_2) \sim 10^6$ cm^{-3})

- The gas temperature drops to ~6 K in the central 1000 AU

- The deuterium fractionation is ~0.4 in the central 3000 AU



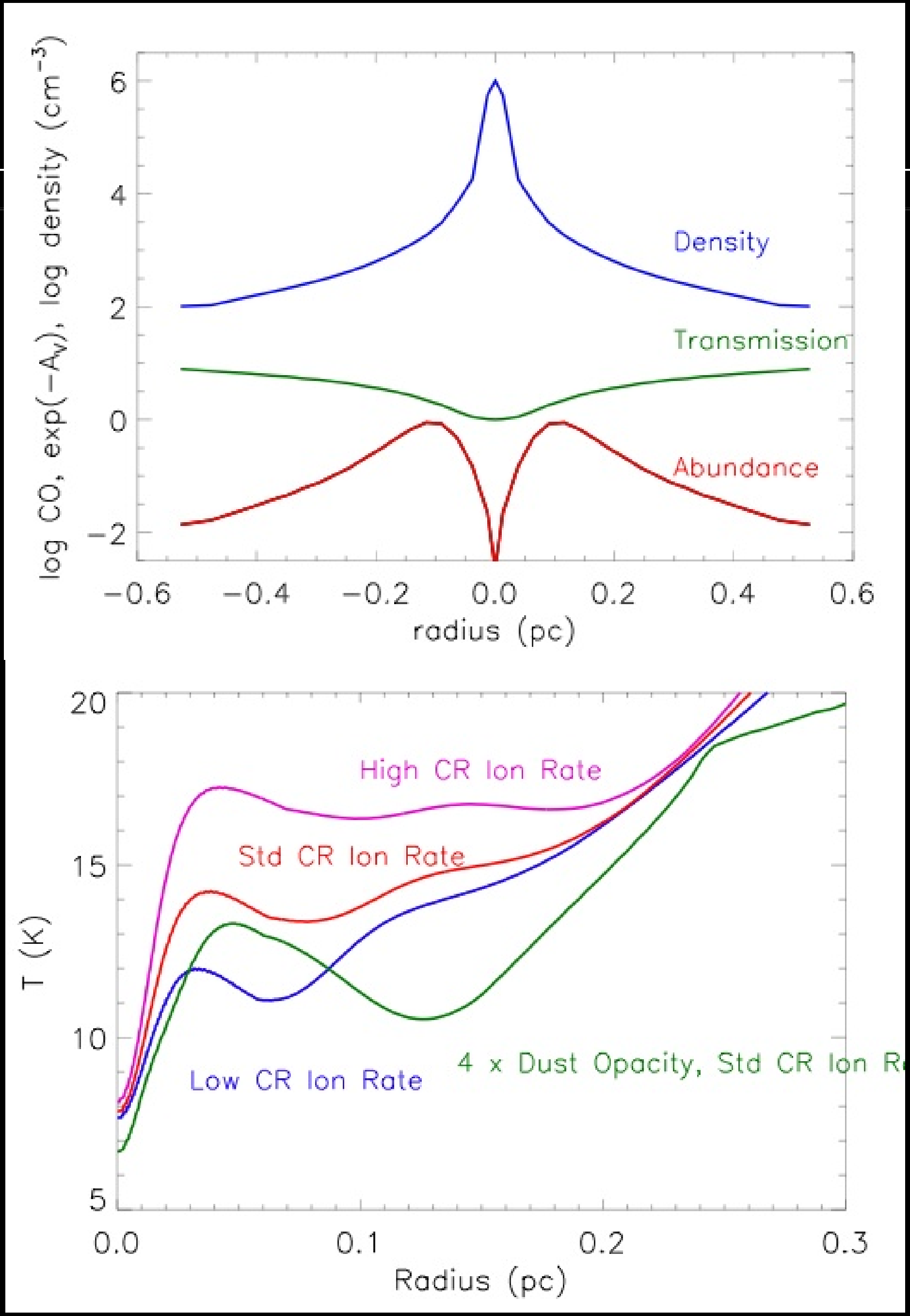
Crapsi, Caselli, Walmsley & Tafalla 2007

Radiative transfer Analysis: Static core

- Bonnor-Ebert sphere
- Simple CO chemistry (freeze-out + photodissociation)
- Radiative energy balance (+photoelectric heating)
- Radiative transfer

ζ ~ 1x10^{-17} s^{-1}, fluffy grains, n_H ~ 10^{7} cm^{-3} (r < 500AU)

Keto & Caselli 2008, 2010



8. Action items

THEORY:

- Update PDR models with (Stephanie’s) surface chemistry.
- Run PDR codes with different metallicities (taking into account changes in the grain size distribution).
- Study how abrupt drops in the photoelectric heating efficiency can drive thermal instabilities (--> SSC?)

OBSERVATIONS TOWARD LOW METALLICITY GALAXIES:

- Observe a group of molecular transitions predicted to be strong by PDR codes applied to low metallicity galaxies.
- Now: focus on possible Herschel proposals (OI, C, CII, high-J CO?).
- Fall: ask for PdBI (and SMA) time to resolve the compact/ high density molecular regions.