# PDR Theory: Overview

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Collaborators

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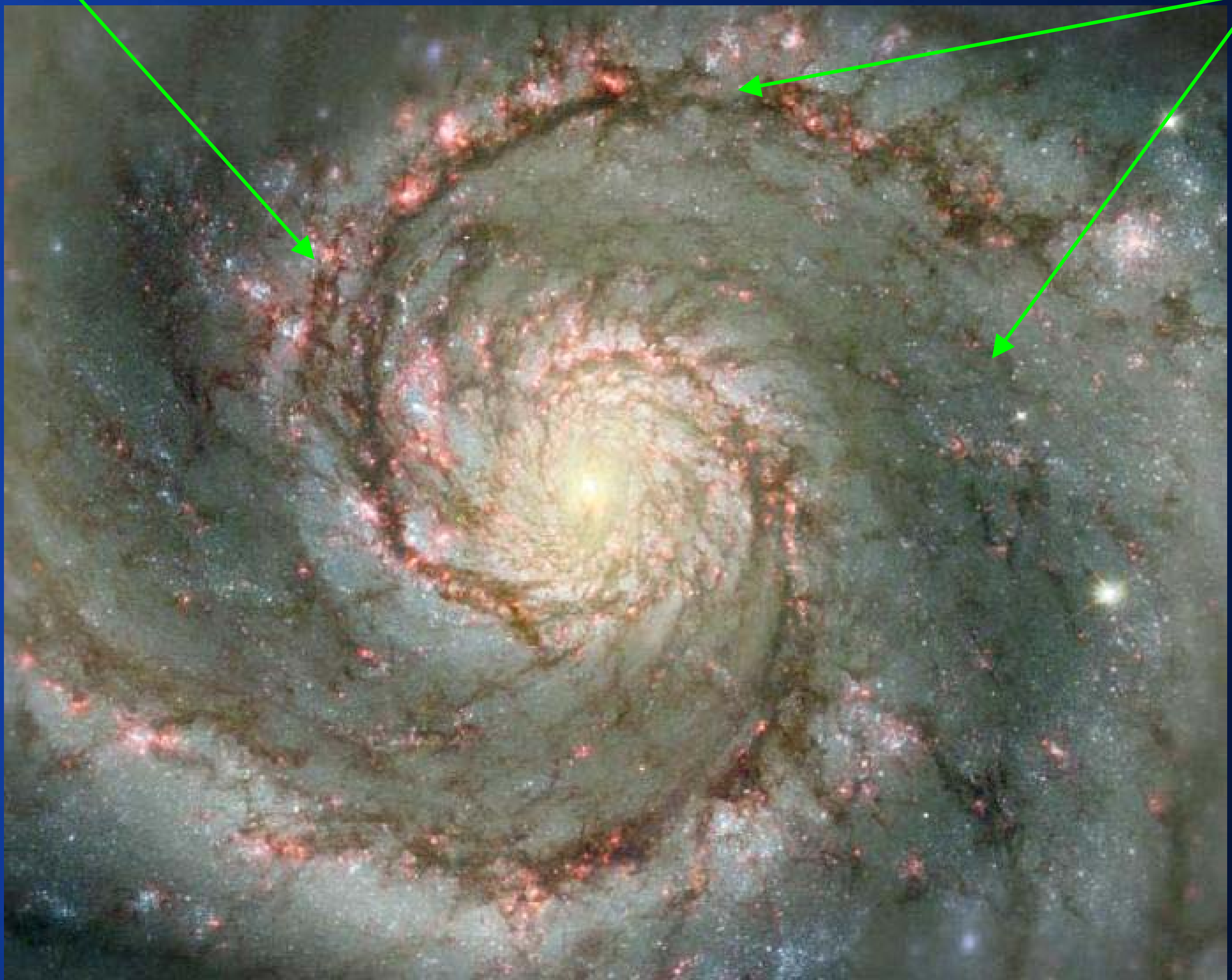
# Overhead View



# FIR Emission from the ISM

Dominated by PDRs → FUV controls heating/chemistry to $A_v \sim 5\text{-}10$ in neutral gas

- Neutral atomic diffuse/translucent clouds ($A_V \leq 1\text{-}2$)
- Surfaces of Molecular clouds
  H → $H_2$ transition ($A_v \sim 1$- few)
- Clumpy GMCs - FUV permeates clouds

"All the gas in a galaxy is in a PDR!"

# Model Inputs

Geometry

UV Field and Penetration

Chemistry

Grains/PAHs

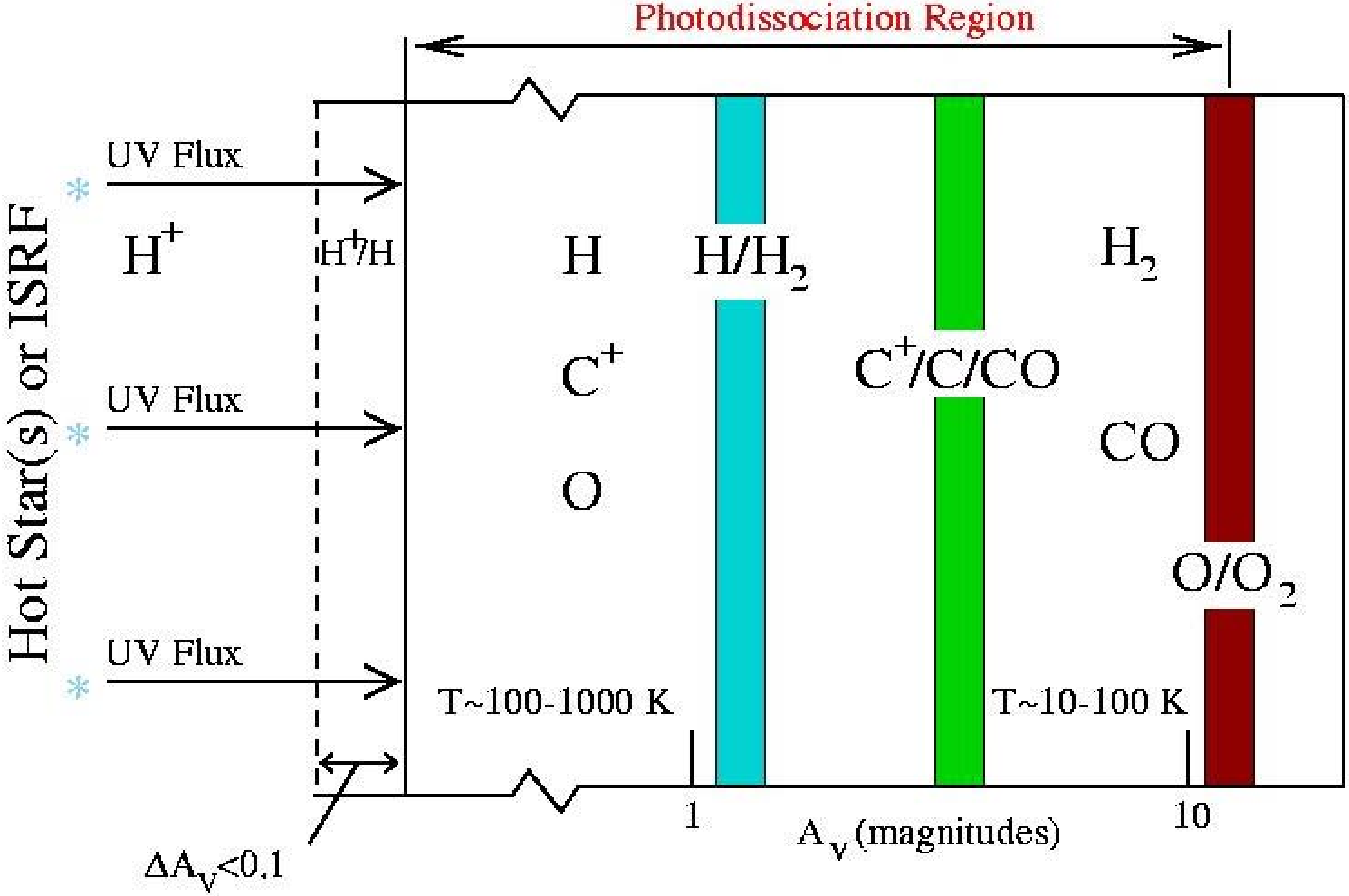
$H_2$ Formation

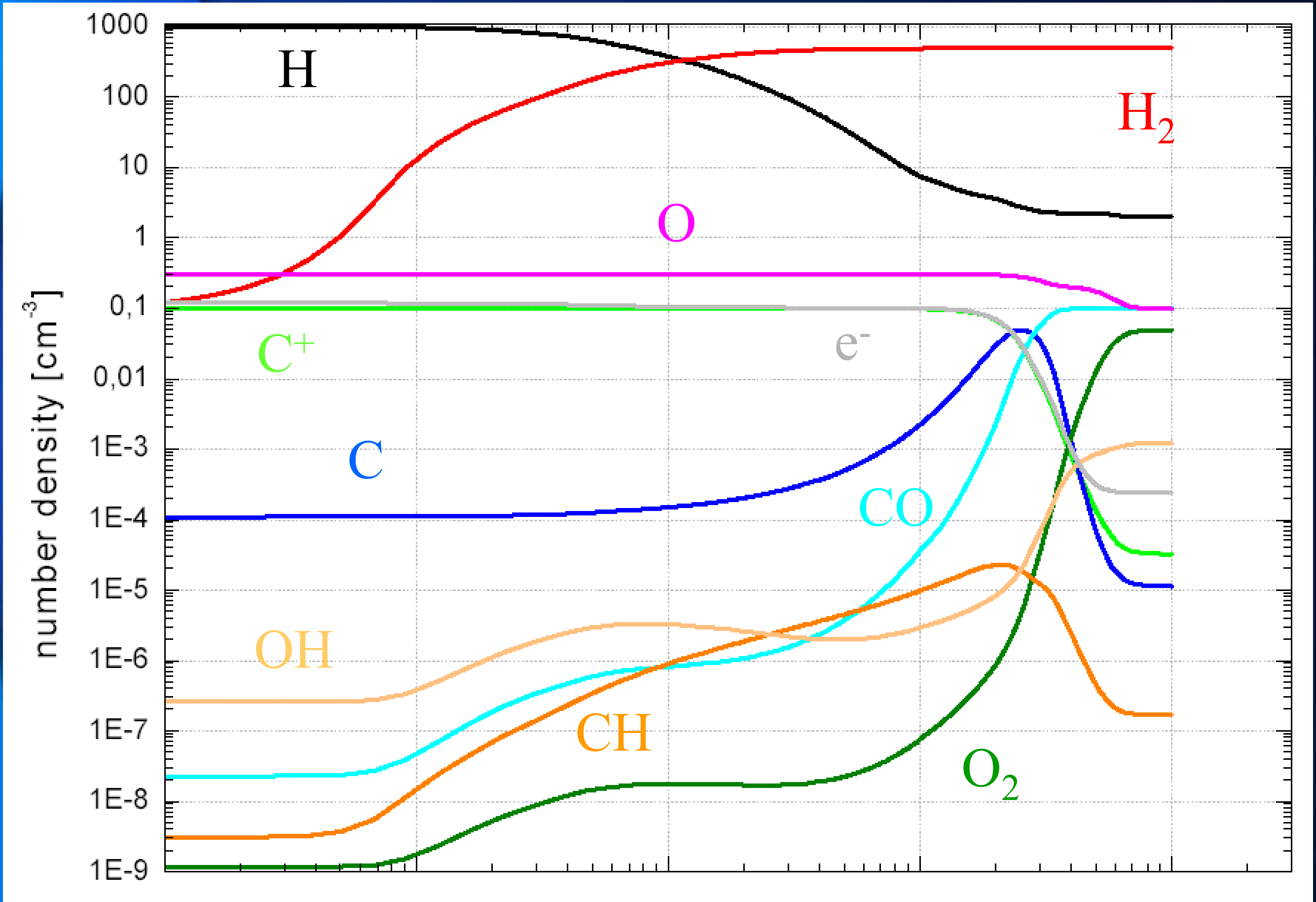
Line transfer/cooling

Photoelectric Heating

Cosmic Ray Ionization

# PDR Schematic





1000
100
10
1
0,1
0,01
1E-3
1E-4
1E-5
1E-6
1E-7
1E-8
1E-9
number density [cm-3]
H
H2
O
C+
e-
C
CO
OH
CH
O2

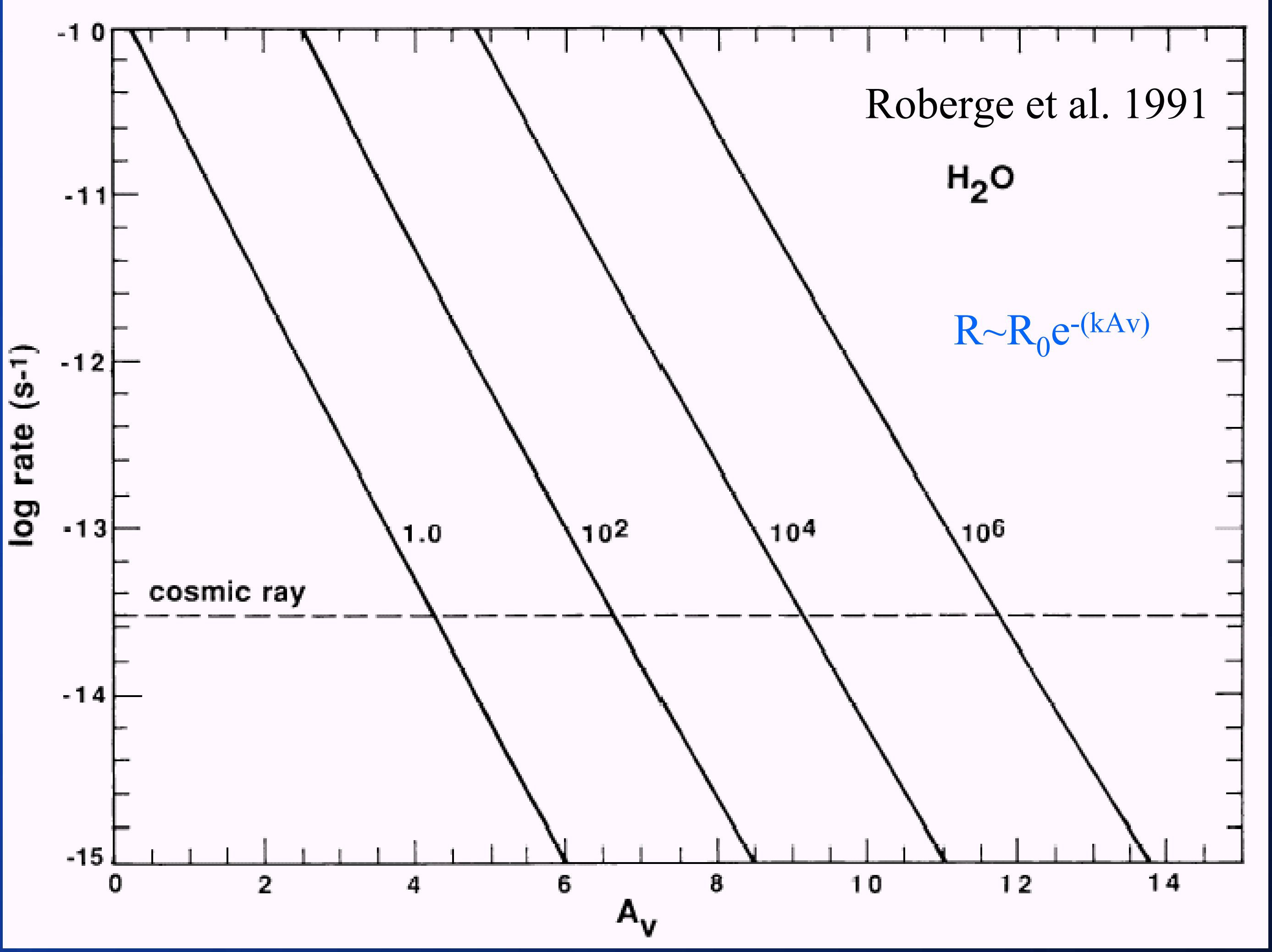
# Outline

- Radiative transfer
  - FUV
  - dust emission
- Role of Molecular Hydrogen
  - formation
  - detailed treatment of line emission
- Heating & Cooling
- Chemistry

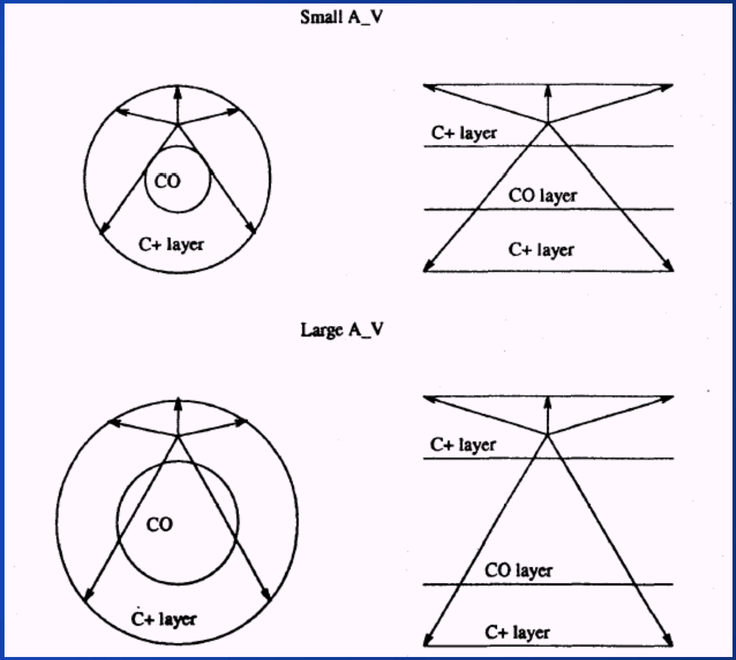
# FUV Penetration

- Continuum attenuated by dust
- Depends on absorption/scattering properties measured in diffuse clouds (e.g. Draine & Lee 84)
- Roberge et al. (1991) and van Dishoeck et al (1988) calculated unshielded photodissociation/photoionization rates in local ISRF, fit decrease in rates with increasing $A_V$… good for R=3.1! (N.B. Dense clouds have higher R values)

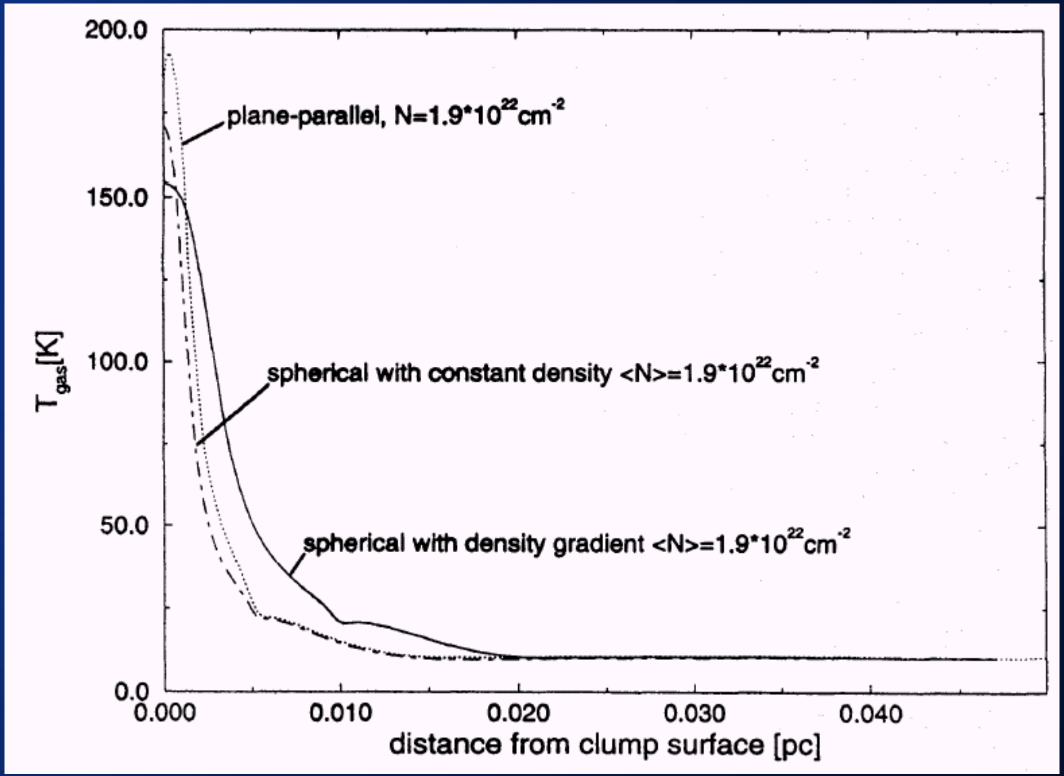
# Photodissociation of $H_2O$



# Spherical Geometry




Stoerzer et al. 1996



# Dust Emission

- Usually not the goal of PDR models ➔ very approximate treatments
- e.g.: calculate $T_d$ at surface and $\tau$ to reemitted surface IR at all other depths
- Observations (esp. extragalactic) would benefit from more accurate modeling ➔ get $G_0$ from the SED

# Molecular Hydrogen

- Key to structure of PDRs
  - Dominant species (once it forms)
  - Kicks off all molecular chemistry
  - Heats gas under certain conditions
  - Formation pumping can drive chemistry

    ==>Get it right!

# $H_2$ Formation

- Gould & Salpeter (1963) recognized inefficiency of gas-phase $H_2$ formation → suggested grains as catalytic sites
- Hollenbach & Salpeter (1971) : H must be chemisorbed to allow efficient formation at high grain temperature
- Numerous attempts at laboratory, theoretical, and observations constraints on formation rate ==> KEY to PDR structure

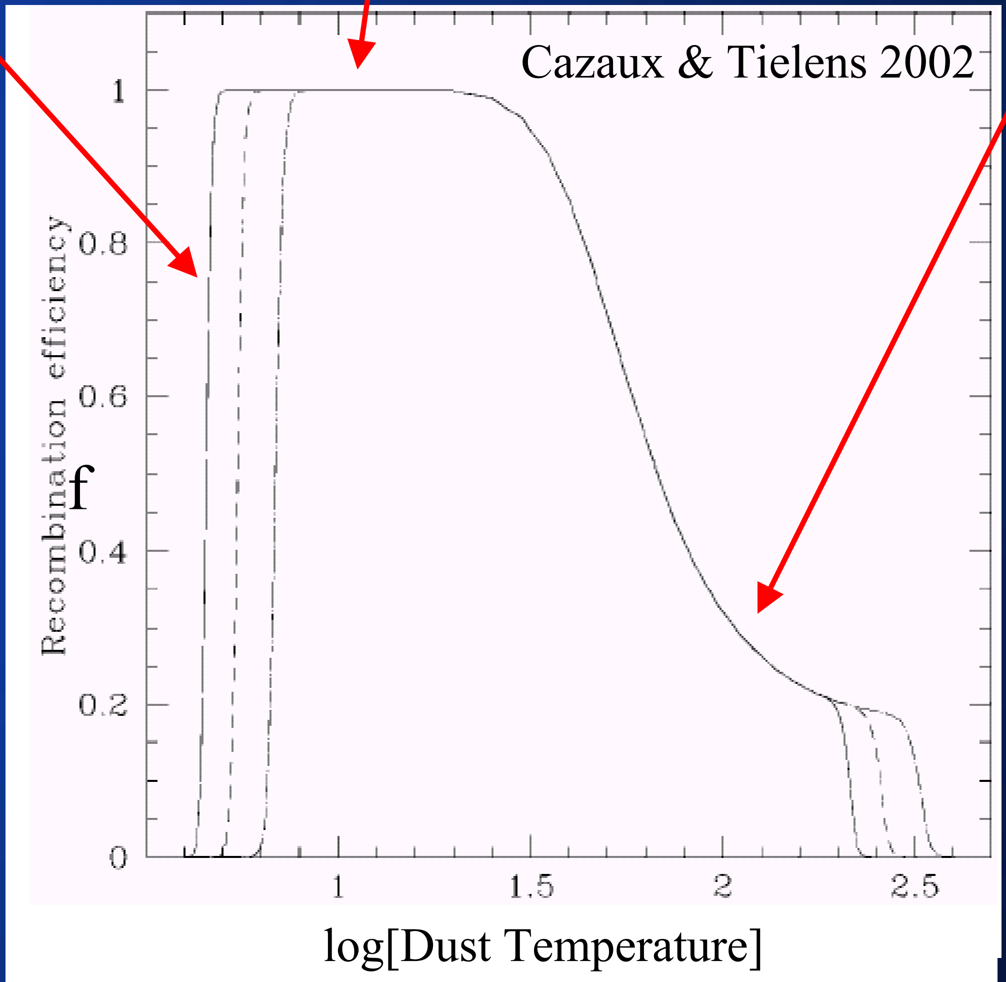
# Amongst the rates are….

- $R = 3 \times 10^{-18} f\, S\, T^{1/2}$ $cm^3\ s^{-1}$ where f =f $(T_d,E_b)$, $S=S(T,T_d)$ [Hollenbach & Salpeter 71, Sternberg & Dalgarno 95]
- Same, but with assumption that f,S=1
- $3 \times 10^{-17}$ $cm^3\ s^{-1}$ under assumption that $T_{gas} \sim$ 100 K in formation region and other properties are too poorly known anyway!

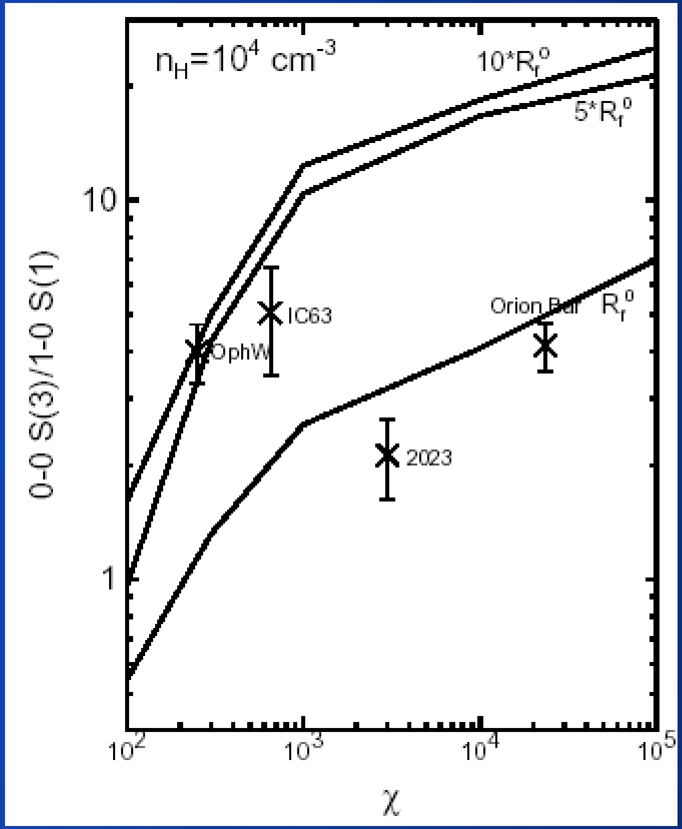
$H_2$ formed but grains too cold ==> sites blocked

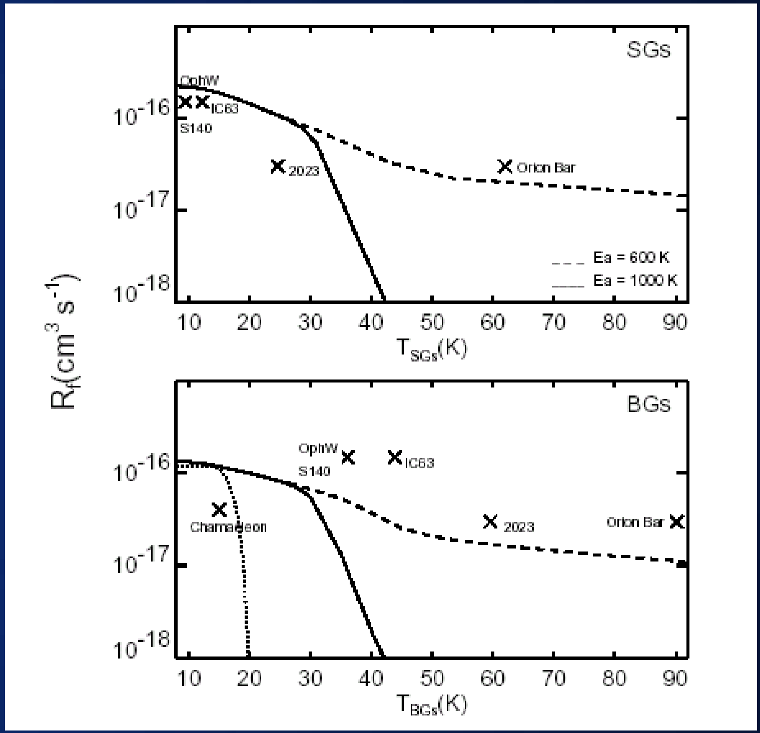
Thermal hopping allows H to find chemisorbed H

Warm grains evaporate H before recombination



# Observational Constraints on $H_2$ Formation




Habart et al. 2004

$R \sim 3x10^{-17}$ - $2x10^{-16}$ cm$^3$ s$^{-1}$

# Self-shielding

$R_{diss} = f_{shield\ x\ e}^{-\tau(1000)} R_{diss}(0)$

where

$f = 1 \quad N(H_2) < 10^{14}\ cm^{-2}$

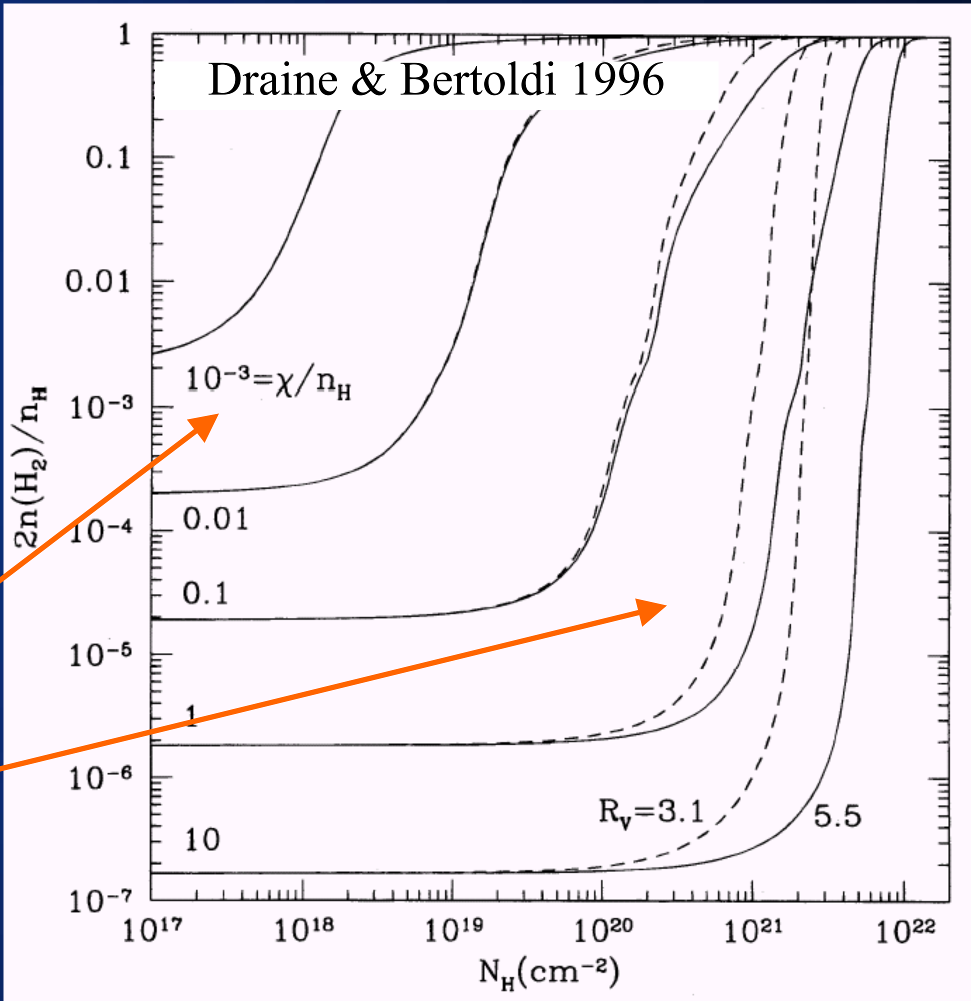
$f \sim (N(H_2)/10^{14}\ cm^{-2})^{-0.75}$

$N(H_2) > 10^{14}\ cm^{-2}$

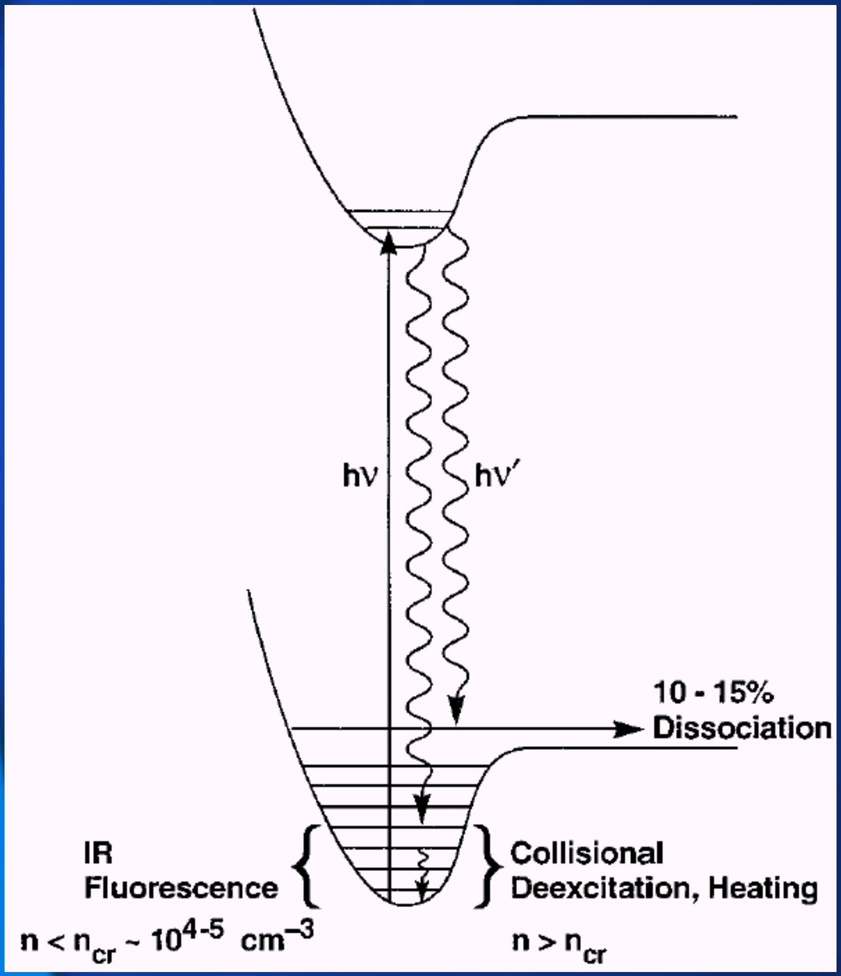
$\chi/n \leq 10^{-2}$ ==> self-shielding

$\chi/n \geq 10^{-2}$ ==> dust shielding

$n_H = 100\ cm^{-3}$, 28K lines!



# $H_2$ Pumping/dissociation/heating




•FUV pumping of $H_2$ in Lyman/Werner bands

(11.3-13.6 eV)

• ~90% fluoresce to to bound vibrational state with

~ 2eV ==> emitted in IR lines (low n)

**or** heat gas by collisional deexcitation (high n)

~ 10% fluoresce to vibrational continuum

==> dissociation

Very detailed treatment: Le Bourlot et al. 1993,

==> full accounting

Simplified : deexcitation into “pseudo-level”

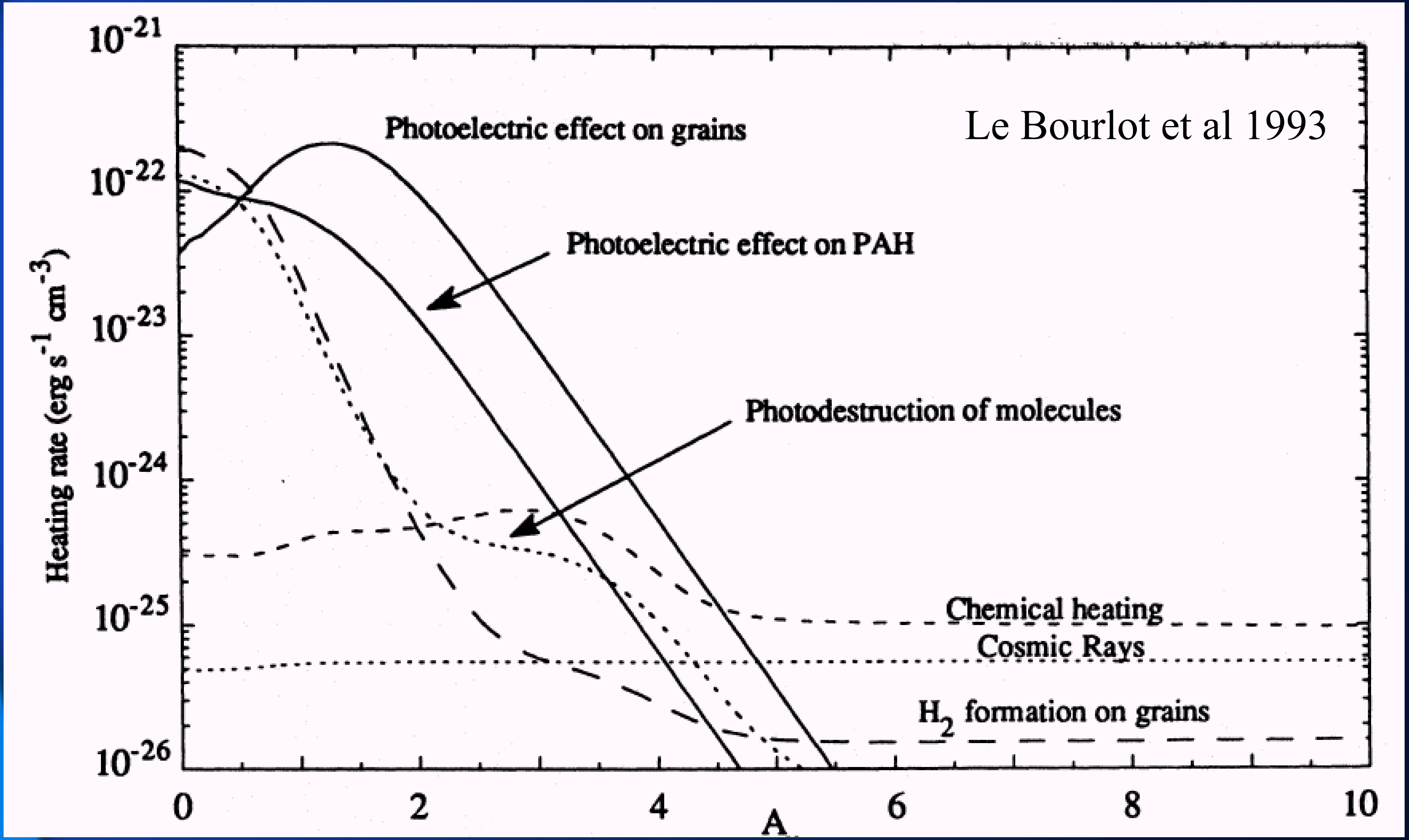
==>OK for approximate heating,

bad for specific line strengths

# Gas Heating & Cooling

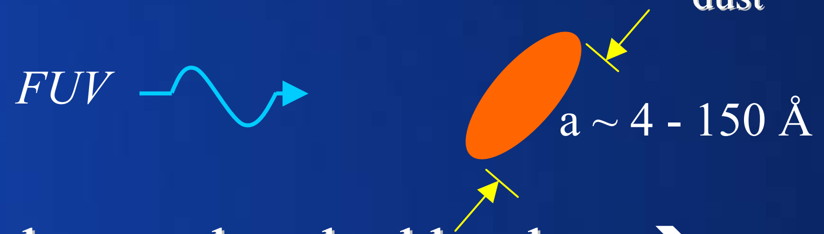
- Heating
  - Grain photoelectric
  - $H_2$ formation
  - cosmic rays
  - grain drift
- Cooling
  - line emission

# Heating Processes

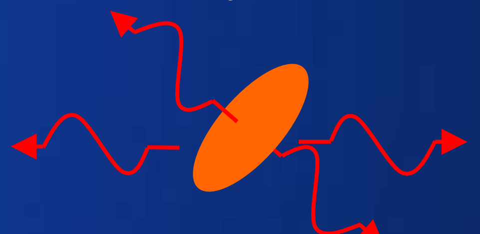


# Photoelectric Heating

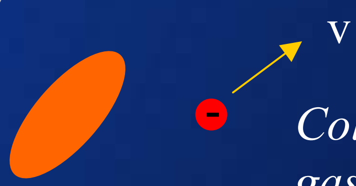
Dust absorbs most of the FUV: $\sigma_{dust} >> \sigma_{gas}$




99%: photon absorbed by dust ➔ warm dust



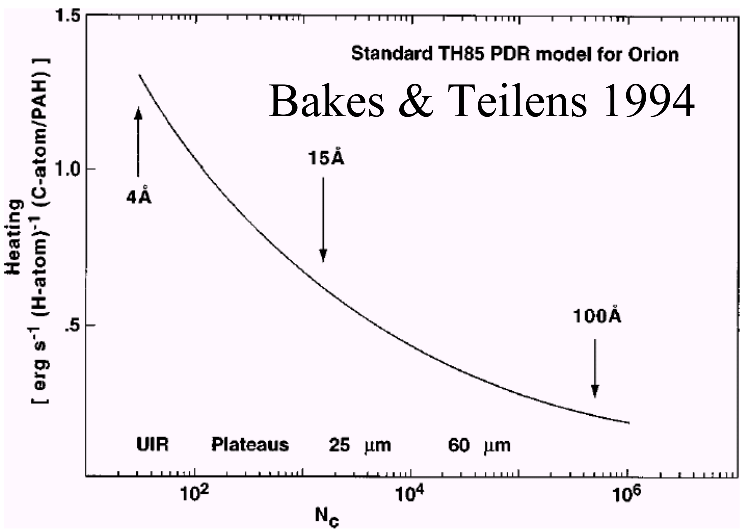

1% : "photoelectric ejection" ➔ warm gas

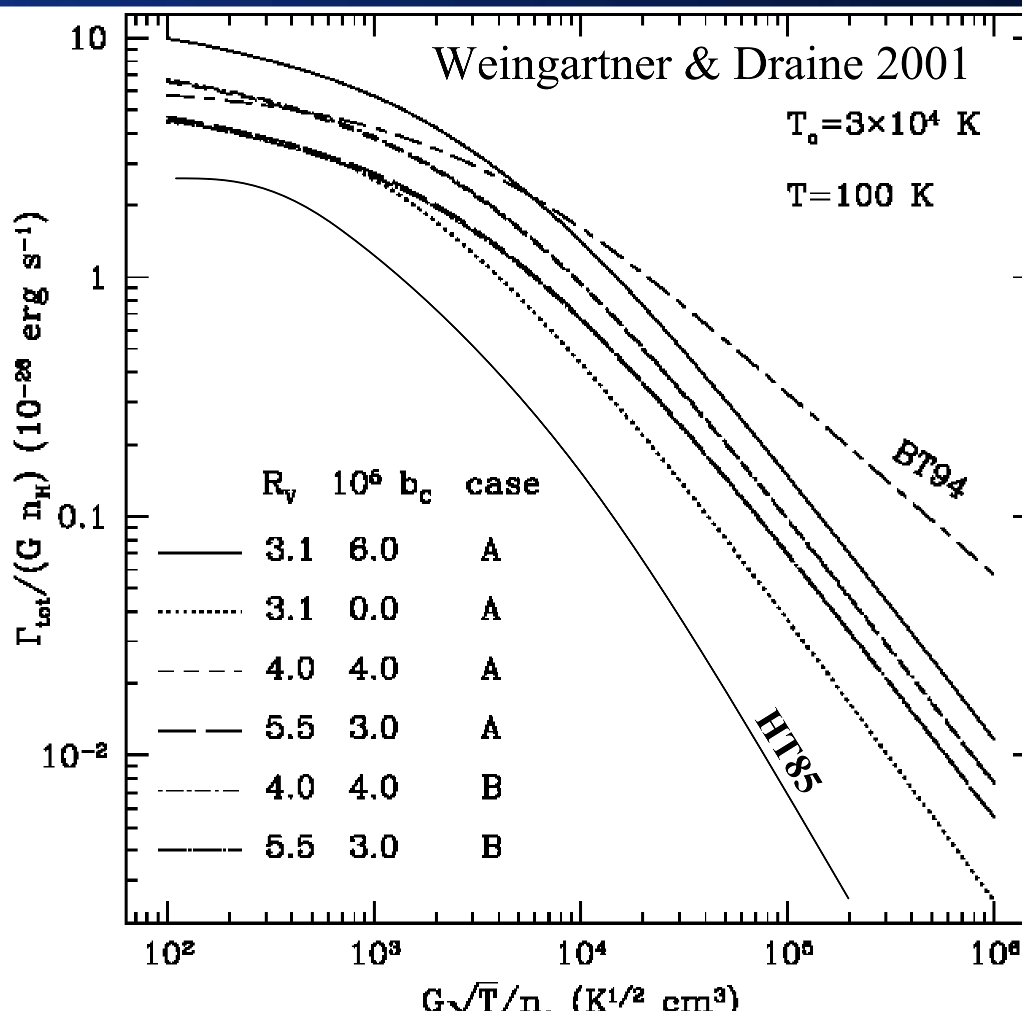



*Collides w/ gas →*
*gas heating → line cooling*

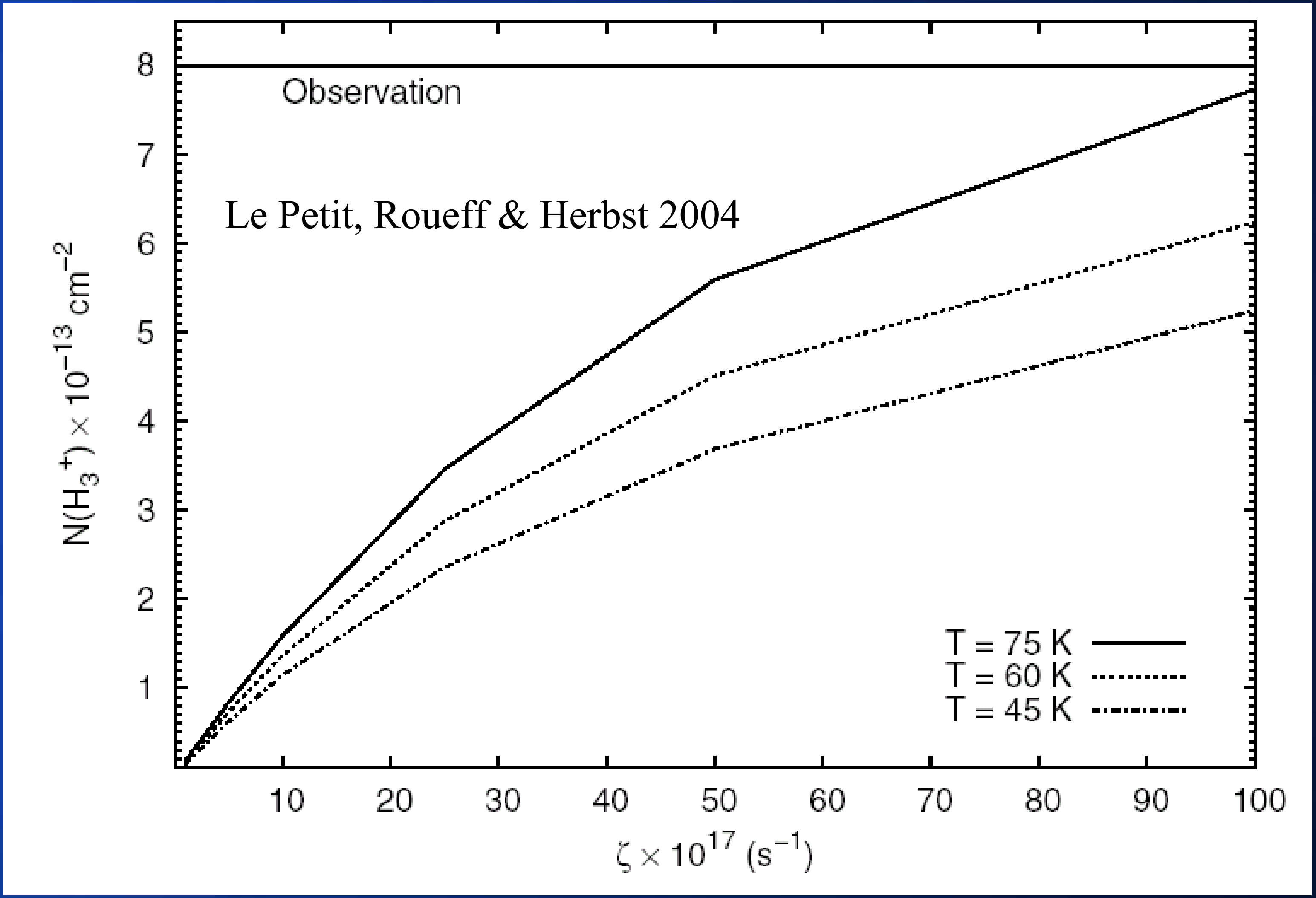
➔gas cooling/dust cooling = line/continuum ~ 1%

# Photoelectric Heating



# Cosmic Rays

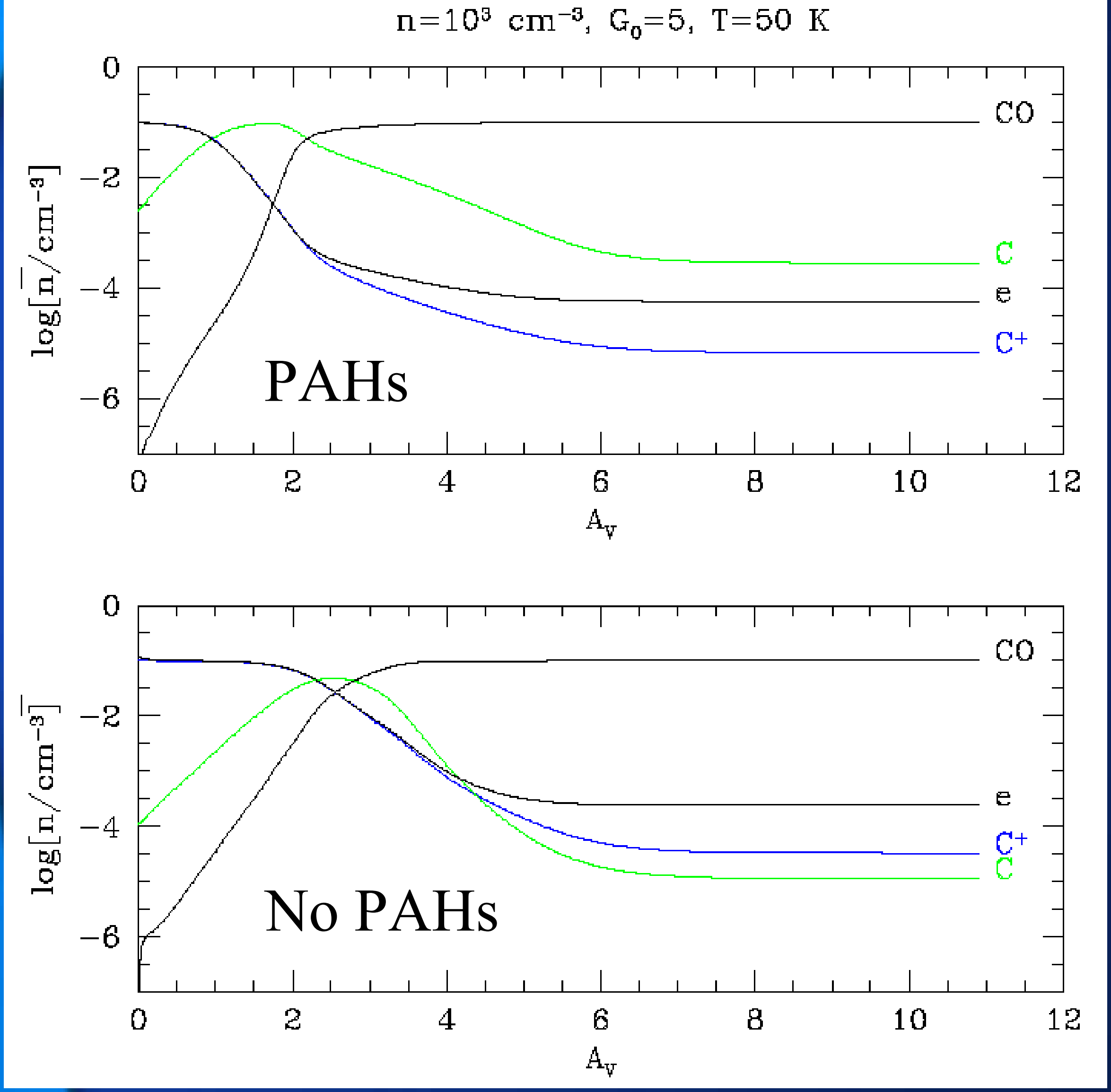


Observation
Le Petit, Roueff & Herbst 2004
$N(H_3^+) \times 10^{-13}$ cm$^{-2}$
$\zeta \times 10^{17}$ (s$^{-1}$)
T = 75 K
T = 60 K
T = 45 K
1
2
3
4
5
6
7
8
10
20
30
40
50
60
70
80
90
100

# Chemistry

- By definition, influenced by FUV photons (unlike dense cores where CR's dominate)
- Photo-reactions
- $H_2$ formation kicks off all other molecular species
- $C^+$ and O maintained to high depths
- Vibrationally-excited $H_2$

# The Chemical Effects of PAHs




$PAH + e \Longrightarrow PAH^-$

$PAH^- + C^+ \Longrightarrow PAH + C$

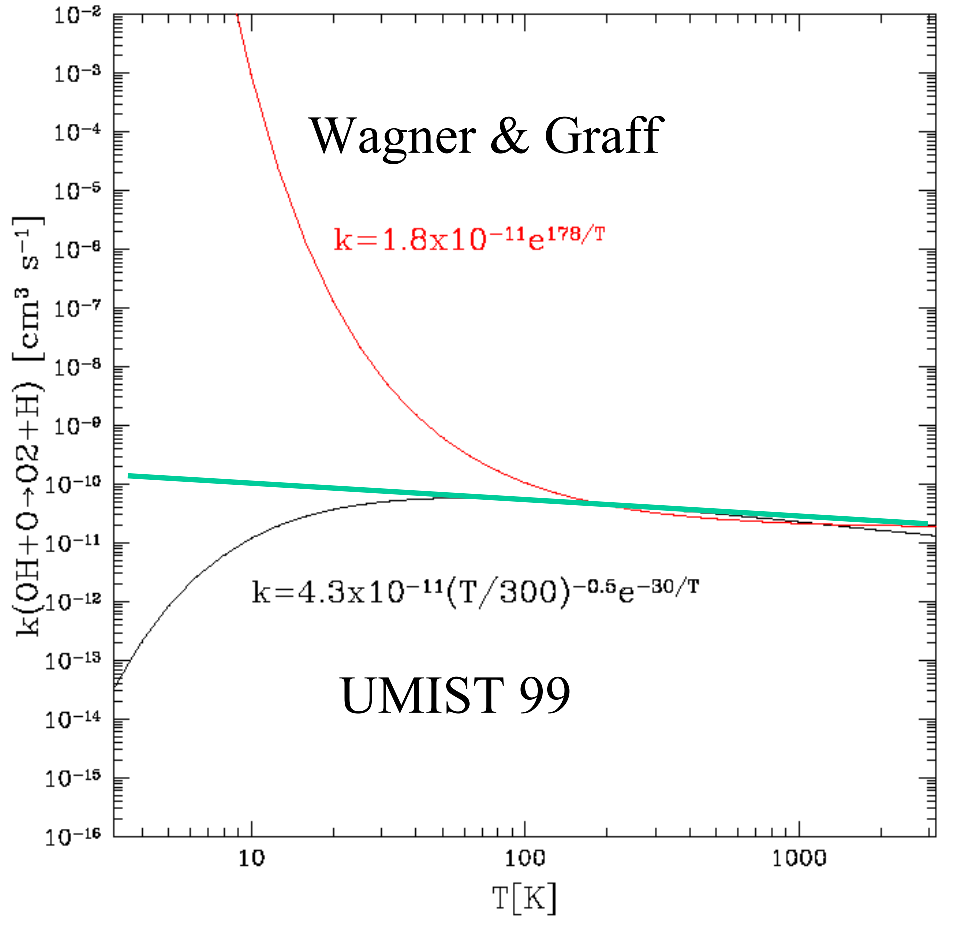
Result:

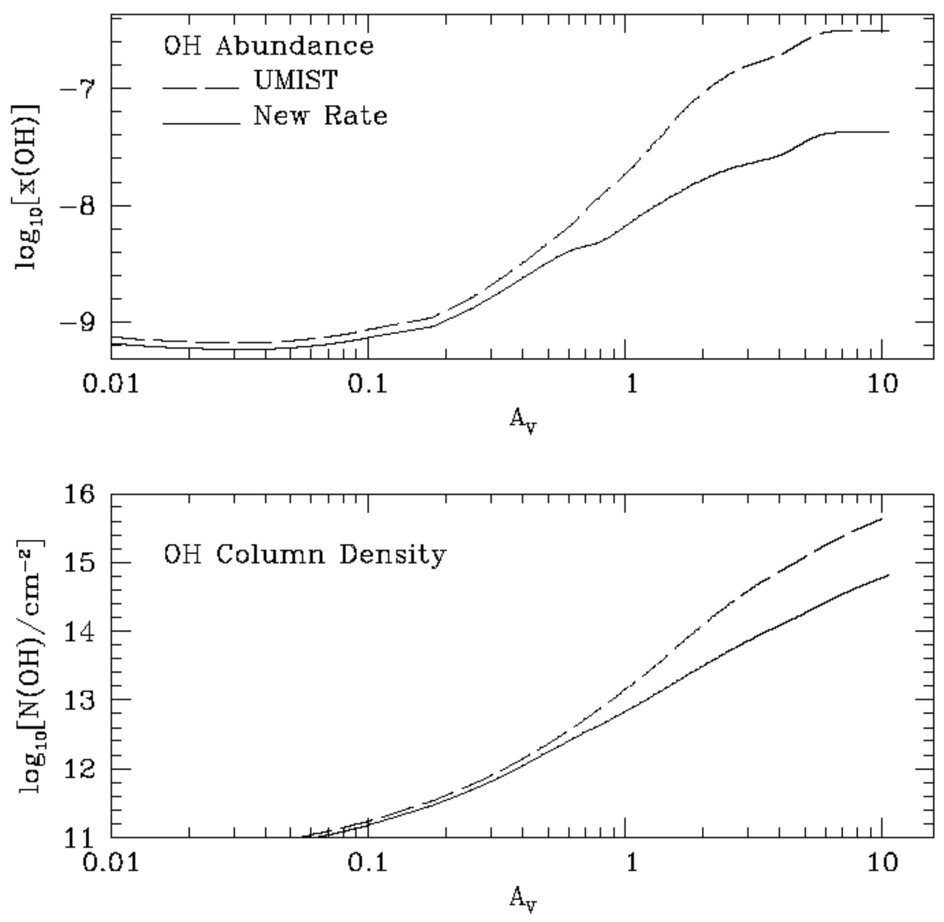
N(C) up by 2,

N($C^+$) down by 2

I(C)/I($C^+$) up by 4

# Example: Rates for OH + O



# Example: $H_2O$ in PDRs

- Formation:

$H_3O^+ + e^- \rightarrow H_2O + H$ (0.05 ***or*** 0.25)

$\rightarrow OH + 2H$ (0.65 ***or*** 0.75)

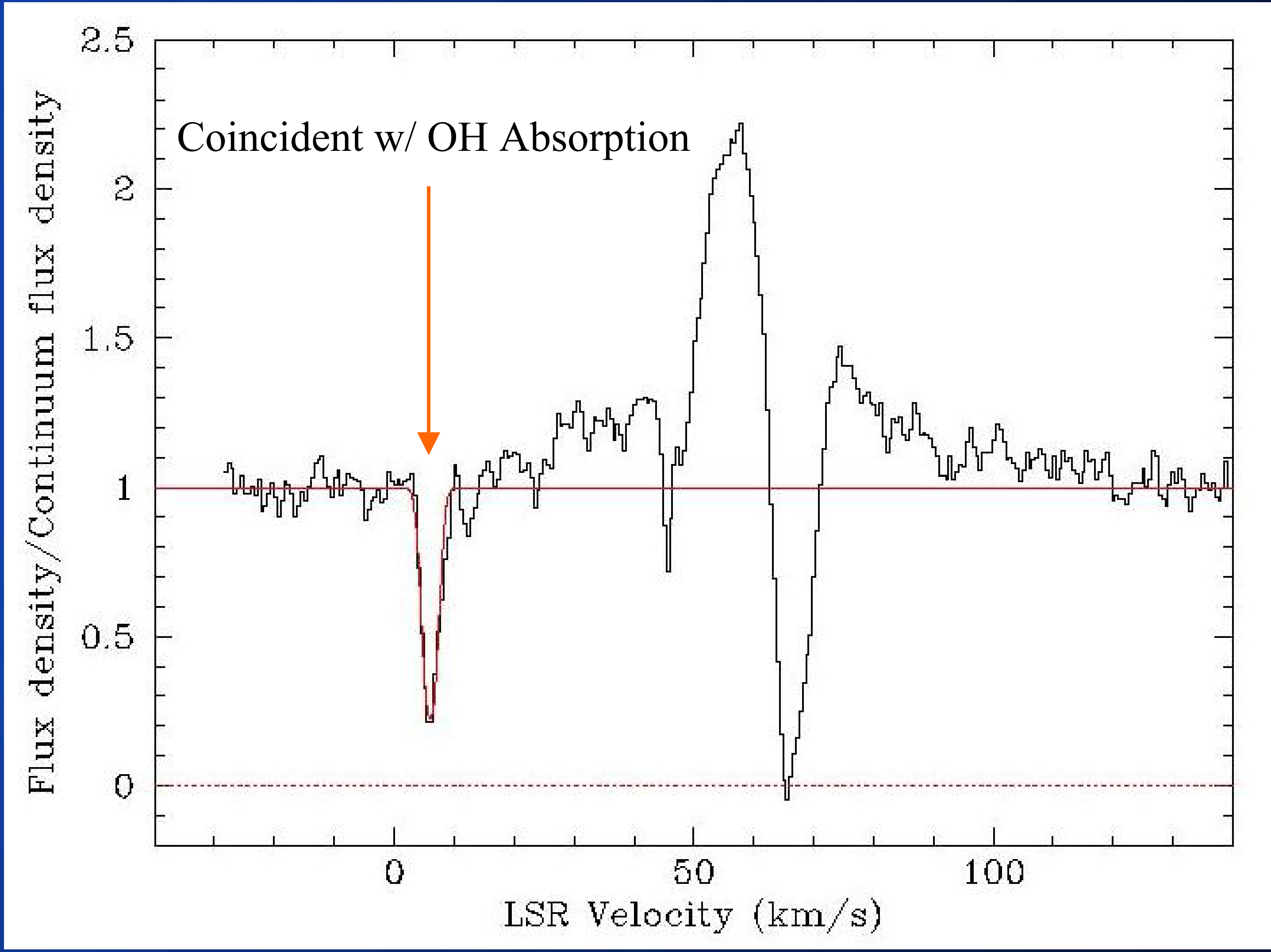
$\rightarrow O + H_2 + H$ (0.30 ***or*** 0.00)

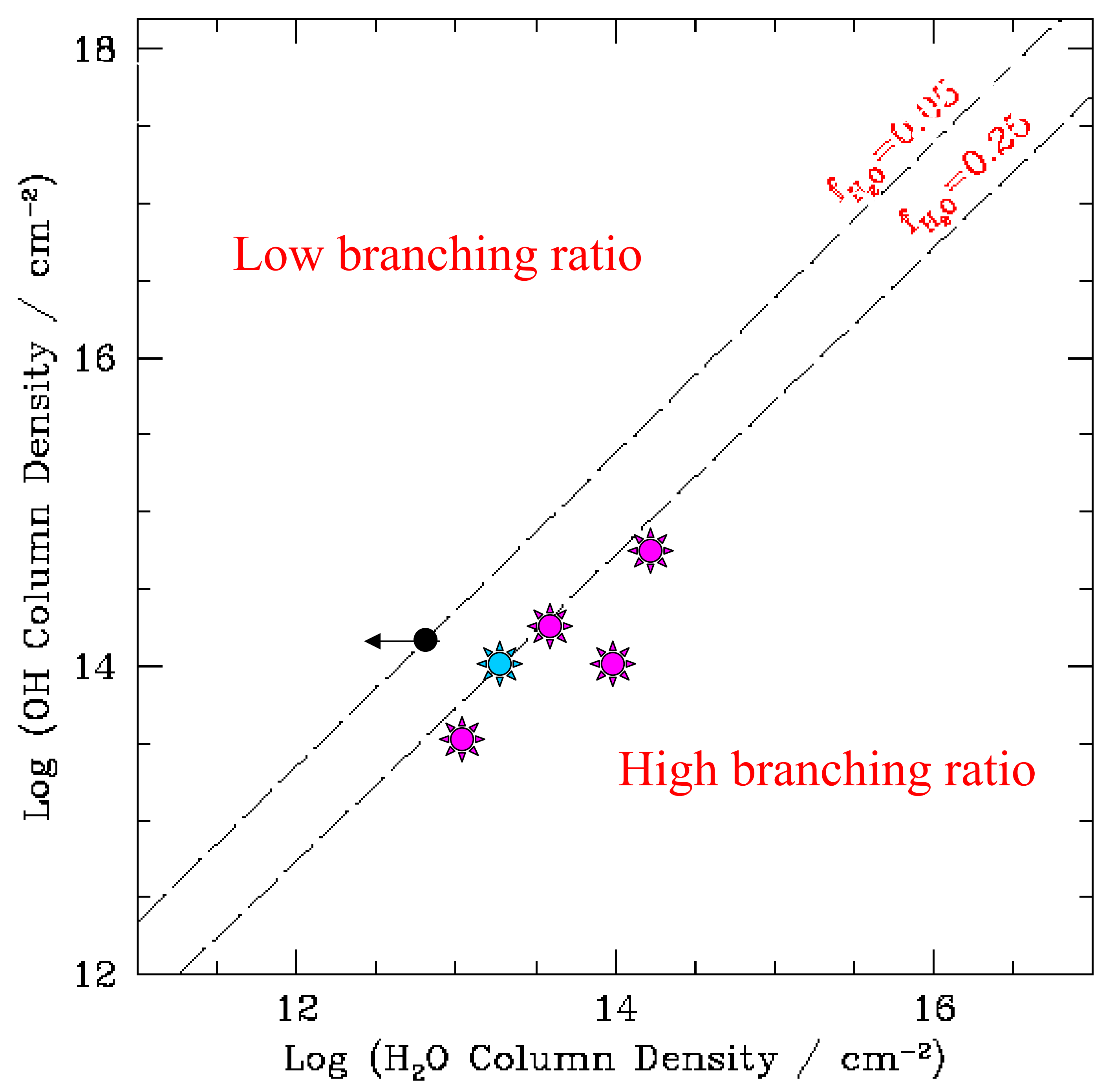
- Destruction

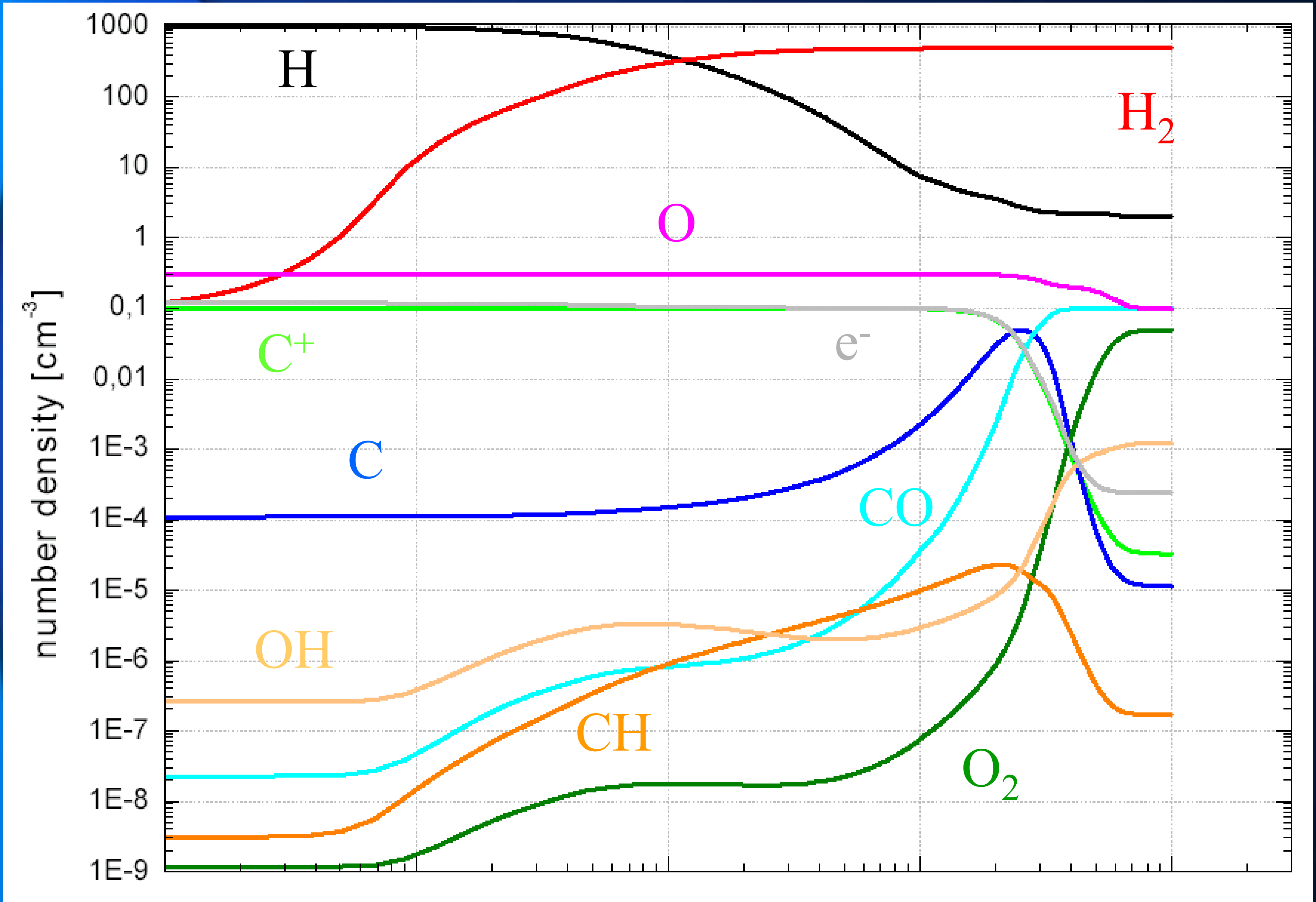
$H_2O$ + FUV photon $\rightarrow OH + H$

$C^+ + H_2O \rightarrow HCO^+ + H$

# W51 $H_2O$ Absorption: First Detection of $H_2O$ in Diffuse Gas

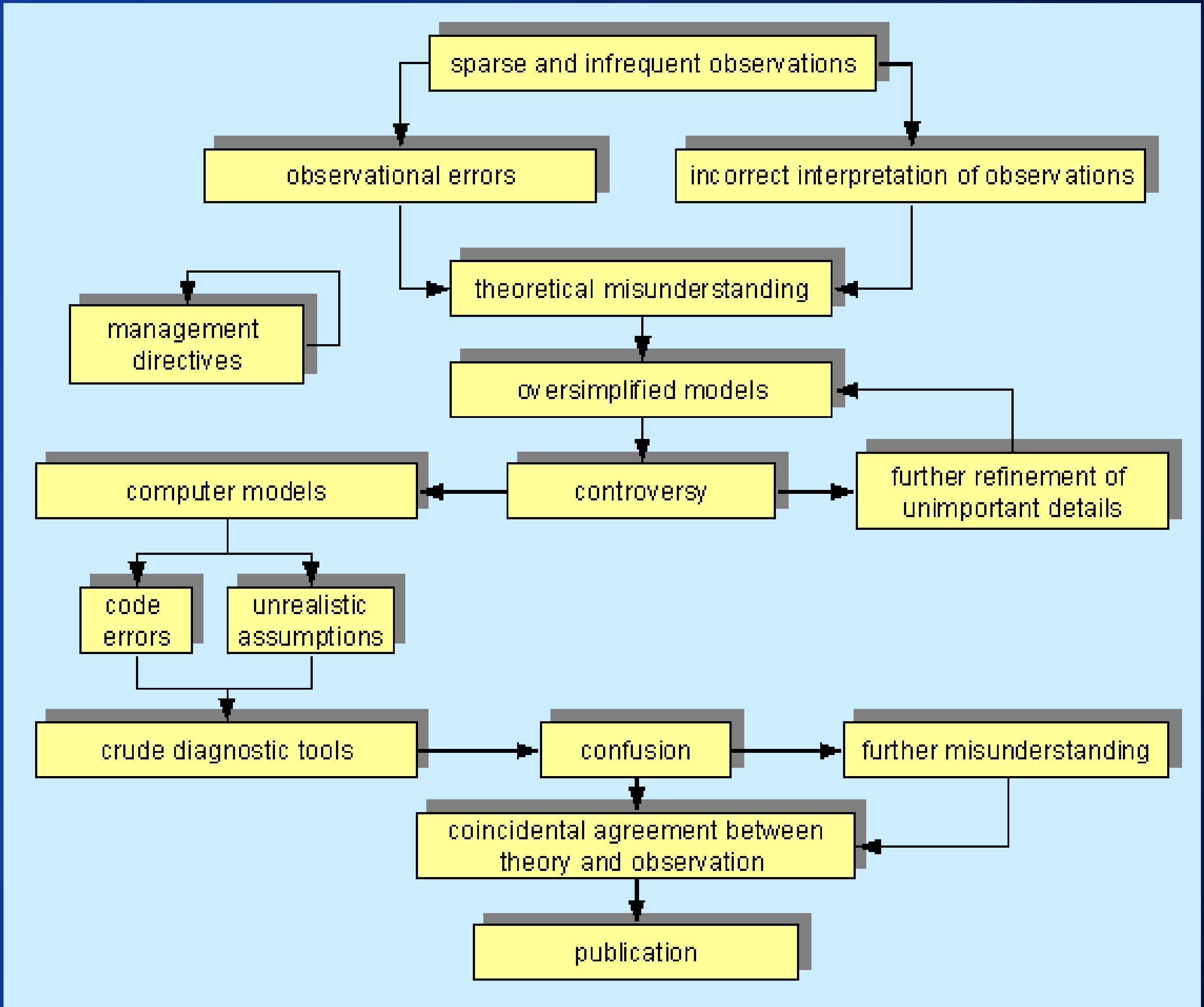



Low branching ratio
High branching ratio
f H2O=0.05
f H2O=0.25
18
16
14
12
12
14
16
Log (OH Column Density / cm-2)
Log (H2O Column Density / cm-2)



1000
100
10
1
0,1
0,01
1E-3
1E-4
1E-5
1E-6
1E-7
1E-8
1E-9
number density [cm-3]
H
$H_2$
O
$C^+$
$e^-$
C
CO
OH
CH
$O_2$

# Modeling



sparse and infrequent observations
observational errors
incorrect interpretation of observations
theoretical misunderstanding
management directives
oversimplified models
computer models
controversy
further refinement of unimportant details
code errors
unrealistic assumptions
crude diagnostic tools
confusion
further misunderstanding
coincidental agreement between theory and observation
publication