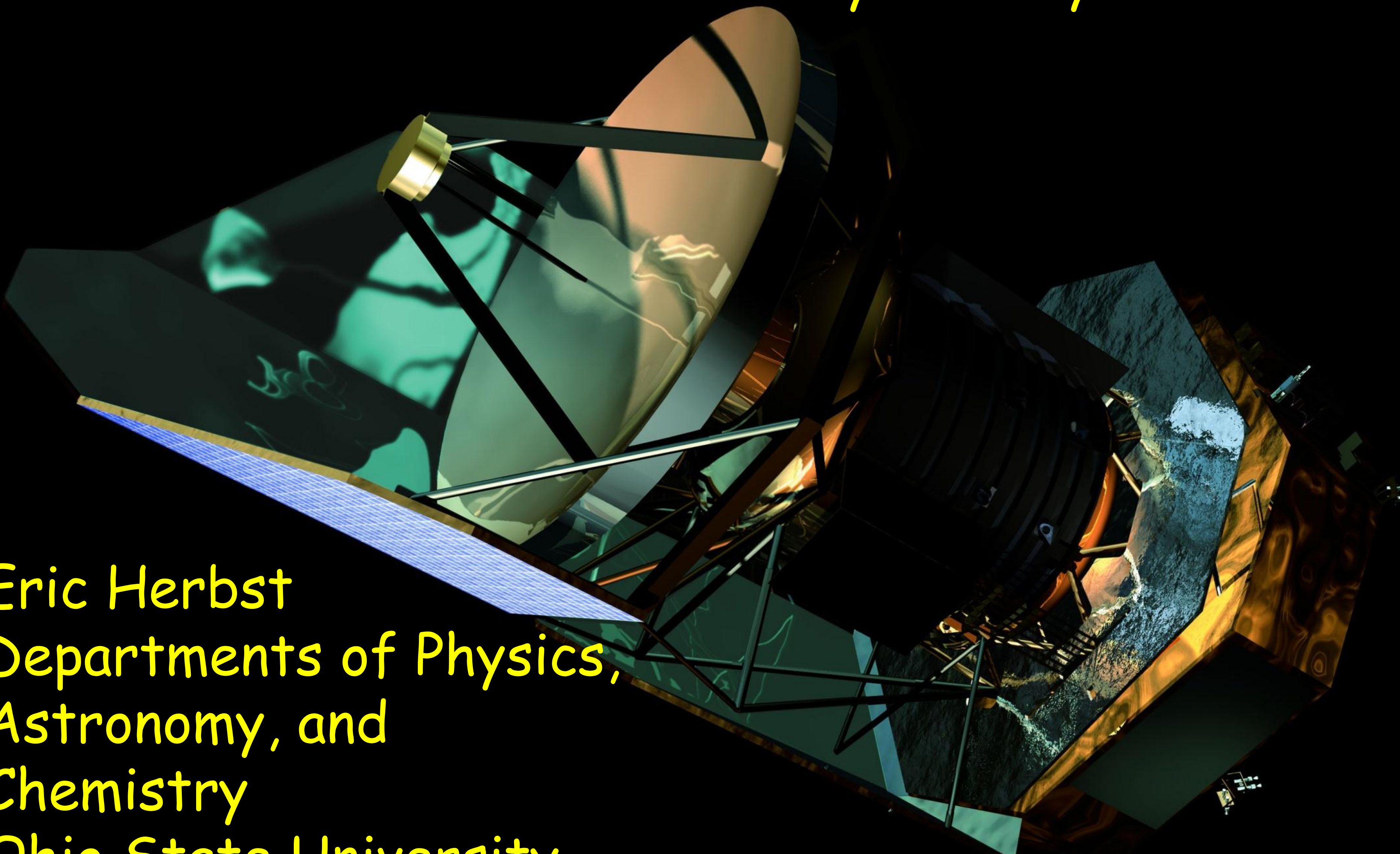
Cosmic-Ray Ionization and Chemistry: Theory



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In the gas phase of interstellar objects:

145 neutral molecules (2011)

21 molecular ions (main isotopes)

15 positive, 6 negative

H

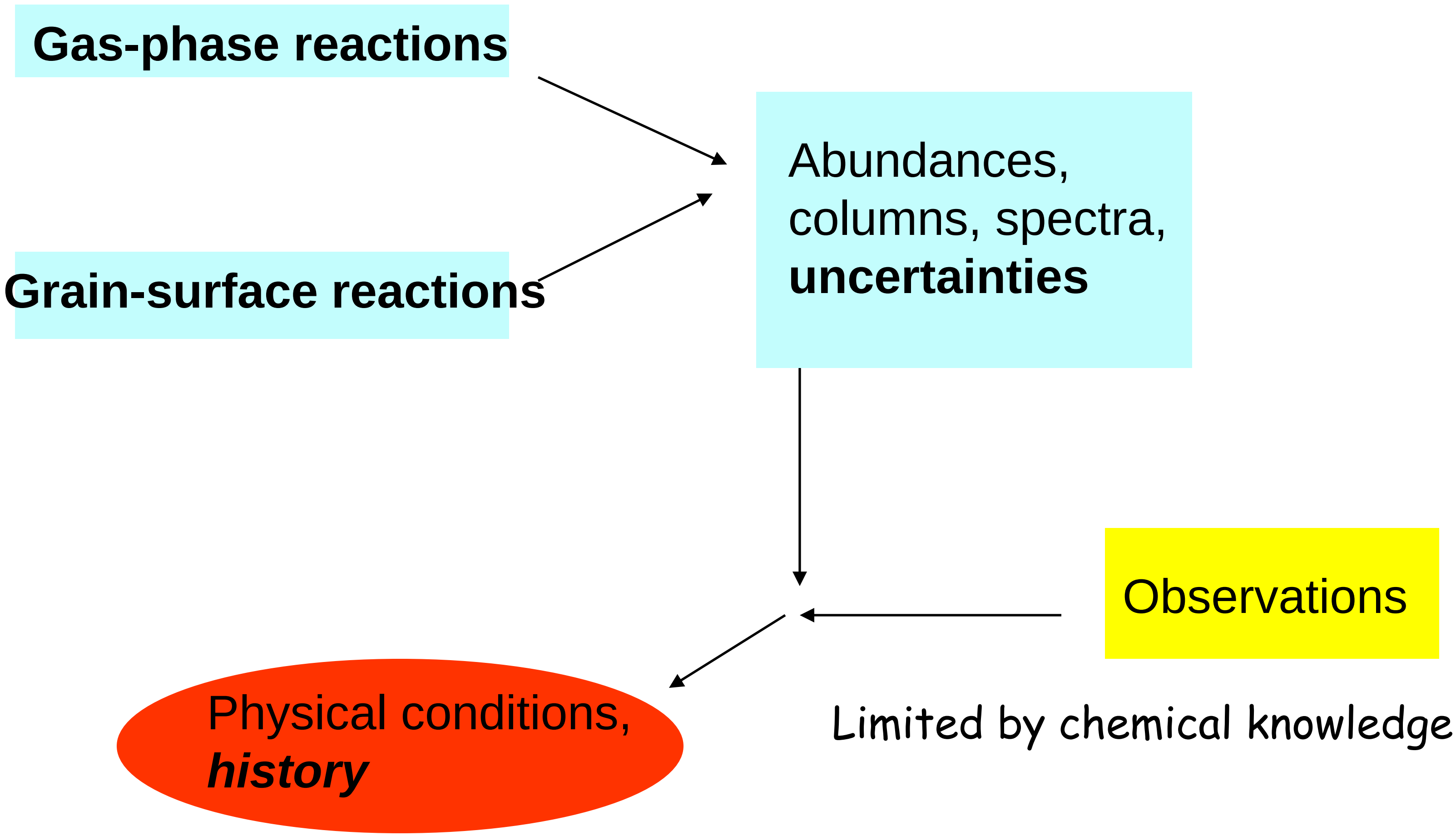
C, N, O

Radicals, isomers, overwhelmingly organic,

Up to 13 atoms in size

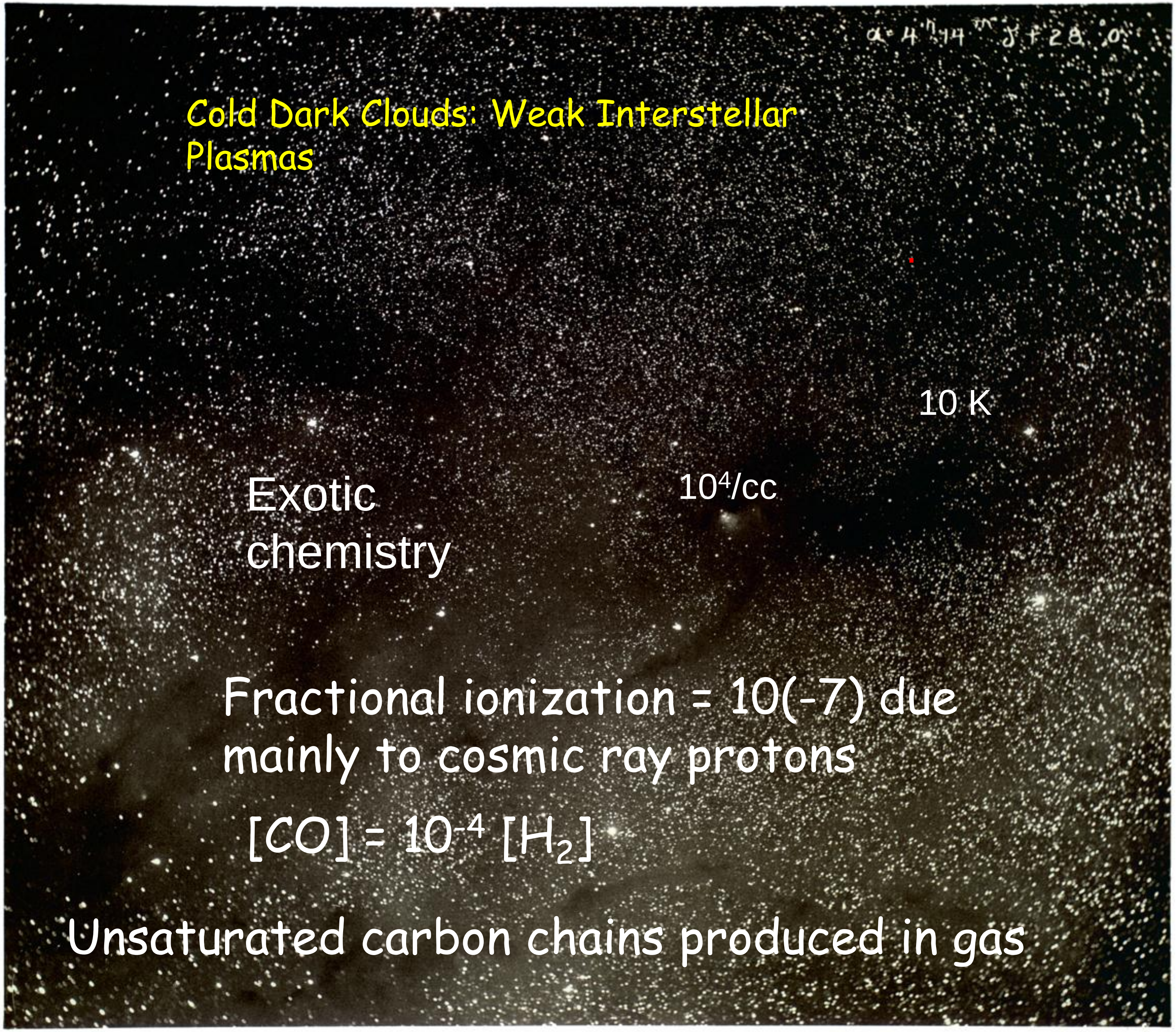
In the ice phase, dominant molecules are water, CO, CO2, and methanol.

Chemical Models



Cool and relatively diffuse clouds in spiral arms can absorb continuua from warmer distant objects in the THz region

$T = 50\text{-}100$ K;
$n = 10\text{-}10^3\ cm^{-3}$
$H \geq H_2$



Cold Dark Clouds: Weak Interstellar Plasmas

10 K

Exotic chemistry

10^4/cc

Fractional ionization = 10(-7) due mainly to cosmic ray protons

$[CO] = 10^{-4} [H_2]$

Unsaturated carbon chains produced in gas

Gas-phase Chemical Networks

Two major public networks:
udfa.net, osu (10 K – 800 K)

Cosmic ray ionization
Photoionization/dissociation
Ion-molecule reactions
Radical-neutral reactions
Dissociative recombination
Radiative association
Electron attachment
+ ion - - ion neutralization
Dissociative attachment

H + CRP → H+ + e-
Normally treated with a first-order rate coefficient $\zeta(s^{-1})$

Roles of ζ

- Ionization of atomic hydrogen ζ_H (s^{-1})
- Ionization of molecular hydrogen
- Secondary ionization and excitation by electrons
- H2 fluorescence followed by indirect photodissociation of many species in clouds with high extinction: rate coefficient $A\zeta$
- Sputtering of species off dust; dissociation of species on dust.

FORMATION OF GASEOUS WATER AND HYDROXYL

H_2 + COSMIC RAYS → H_2^+ + e

Elemental abundances: C,O,N = 10(-4); C<O

H_2^+ + H_2 → H_3^+ + H

H_3^+ + O → OH^+ + H_2

OH_n^+ + H_2 → OH_{n+1}^+ + H

H_3O^+ + e → H_2O + H; **OH** + 2H, etc

+ longer pathways to unsaturated organic species……

Brief History of ζ_H (s^{-1}) in Models

- 1 x 10(-15)
- 1 x 10(-17)
- 1.5 x 10(-17) – 2.2 x 10(-17)
- 1 x 10(-16) – 1 x 10(-15)
- 2.5 x 10(-16)
- 1 x 10(-15)
- 6.0 x 10(-17) – 2.4 x 10(-16)
- 2 x 10(-14)

- Solomon & Werner (1971)
- Herbst & Klemperer (1973)
- Hartquist et al. (1978)
- McCall et al. (2002)
- Le Petit et al. (2004)
- Goto et al. (2008)
- Neufeld et al. (2010)
- Gupta et al. (2010)

- In general, dense clouds are fit better with the lower values of zeta and diffuse sources with the higher value, suggesting a column dependent zeta would be better.

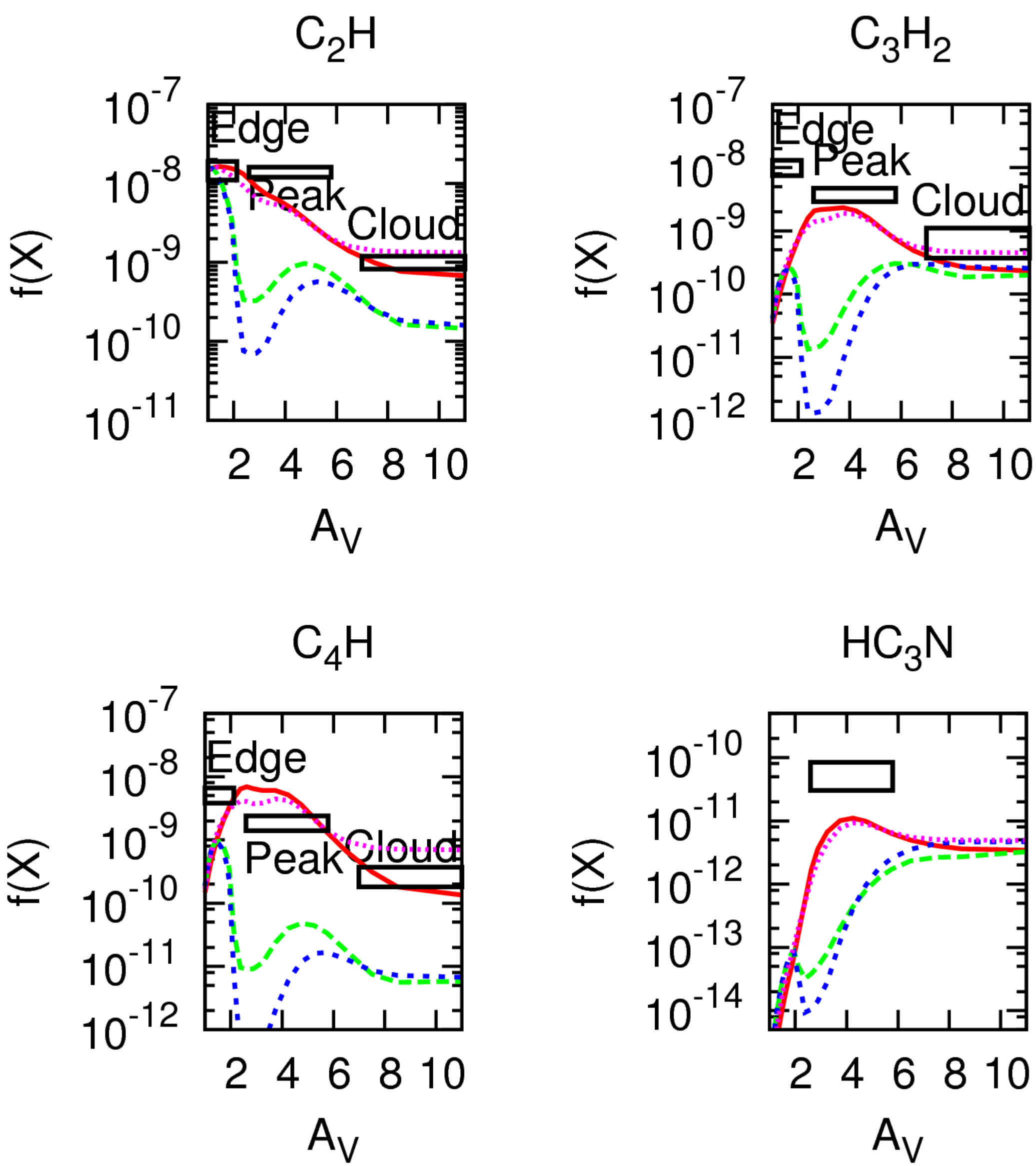
Column-dependent ζ

- Most reasonable way to distinguish between diffuse and dense cloud values of ζ.
- Recent calculations:
- Padovani et al. (2009); Padovani (2011)
- Rimmer et al. (2011a); includes magnetic effects. Used for PDR model of Horsehead Nebula.

Horsehead Nebula

Hubble Heritage

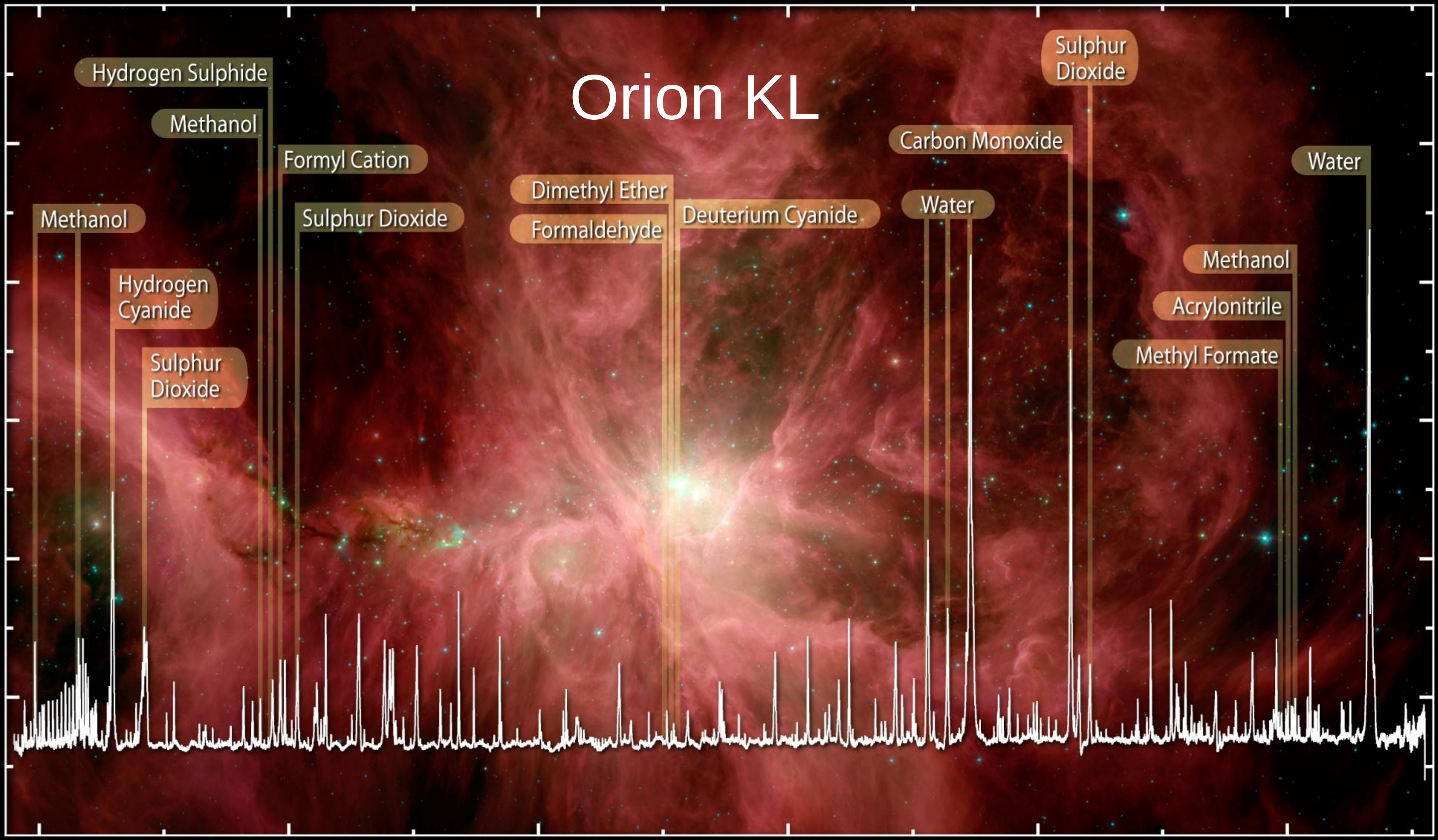
NASA, NOAO, ESA, and The Hubble Heritage Team (STScI/AURA) • Hubble Space Telescope WFPC2 • STScI-PRC01-12



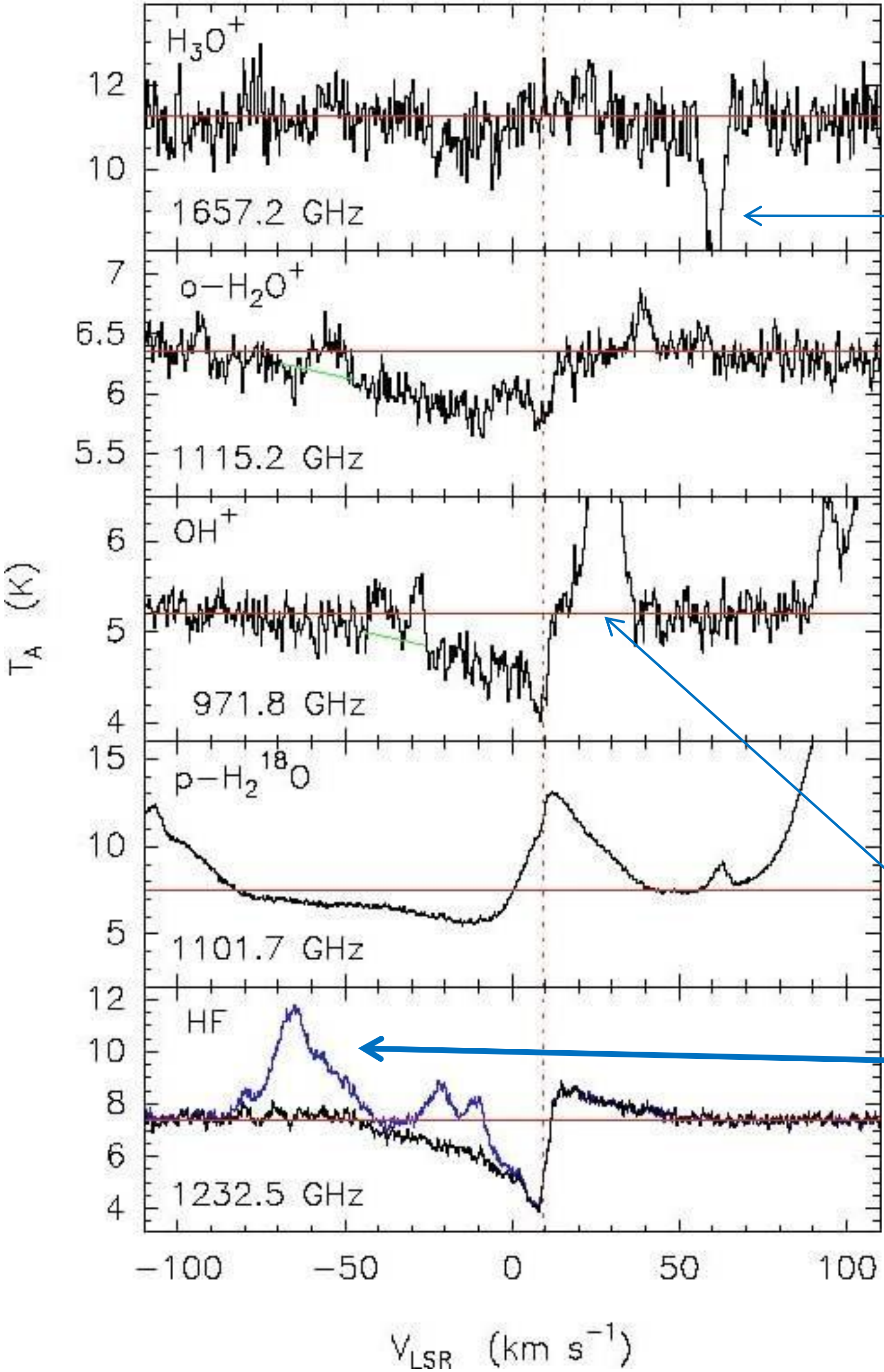
— column-dependent ζ with highest value at edge.

--- high constant value of ζ

Edge, Peak, and Cloud sources from Pety et al. (2005), who suggested PAH fragmentation as the source of the high carbon chain abundances.



HIFI Spectrum of Water and Organics in the Orion Nebula



CH

Emission and absorption spectra from Orion KL region in terms of velocity

A violent place??

CH_3OH, SO_2

$OH^+ \approx 2 \times H_2O^+ \gg H_3O^+$

Gupta et al. (2010)

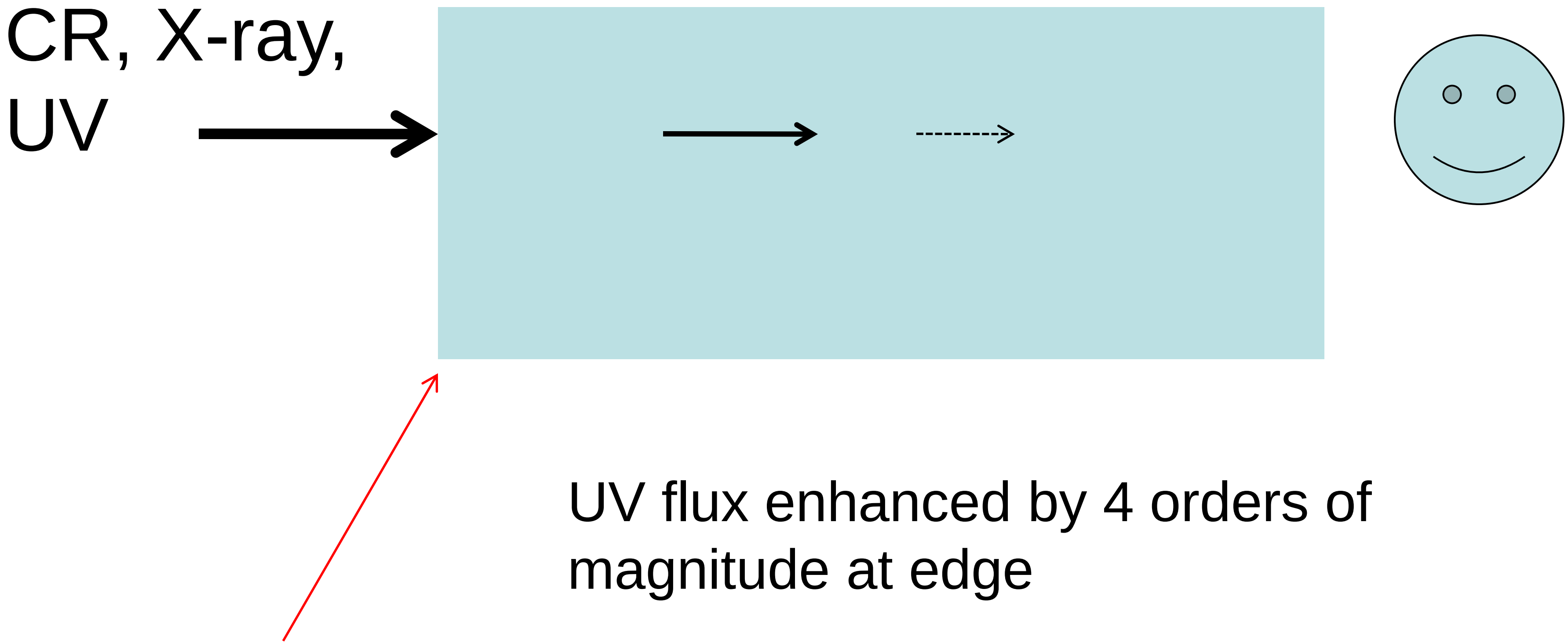
Extended Chemistry

- $O + H^+ \longrightarrow O^+ + H$
- $O^+ + H_2 \longrightarrow OH^+ + H$
- $O + H_3^+ \longrightarrow OH^+ + H_2$/ $H_2O^+ + H$
- $OH^+ + e \longrightarrow O + H$
- $OH^+ + H_2 \longrightarrow H_2O^+ + H$
- $H_2O^+ + e \longrightarrow OH + H$; $O + H_2$
- $H_2O^+ + e \longrightarrow O + H + H$
- $H_2O^+ + H_2 \longrightarrow H_3O^+ + H$
- $H_3O^+ + e \longrightarrow H_2O + H$; $OH + H_2$, $OH + 2H$
- $H_2O + h\nu \longrightarrow H_2O^+ + e$
- $OH + h\nu \longrightarrow OH^+ + e$
- $H_2 + CRP \longrightarrow H$ ....

Ultra-high Values of ζ?

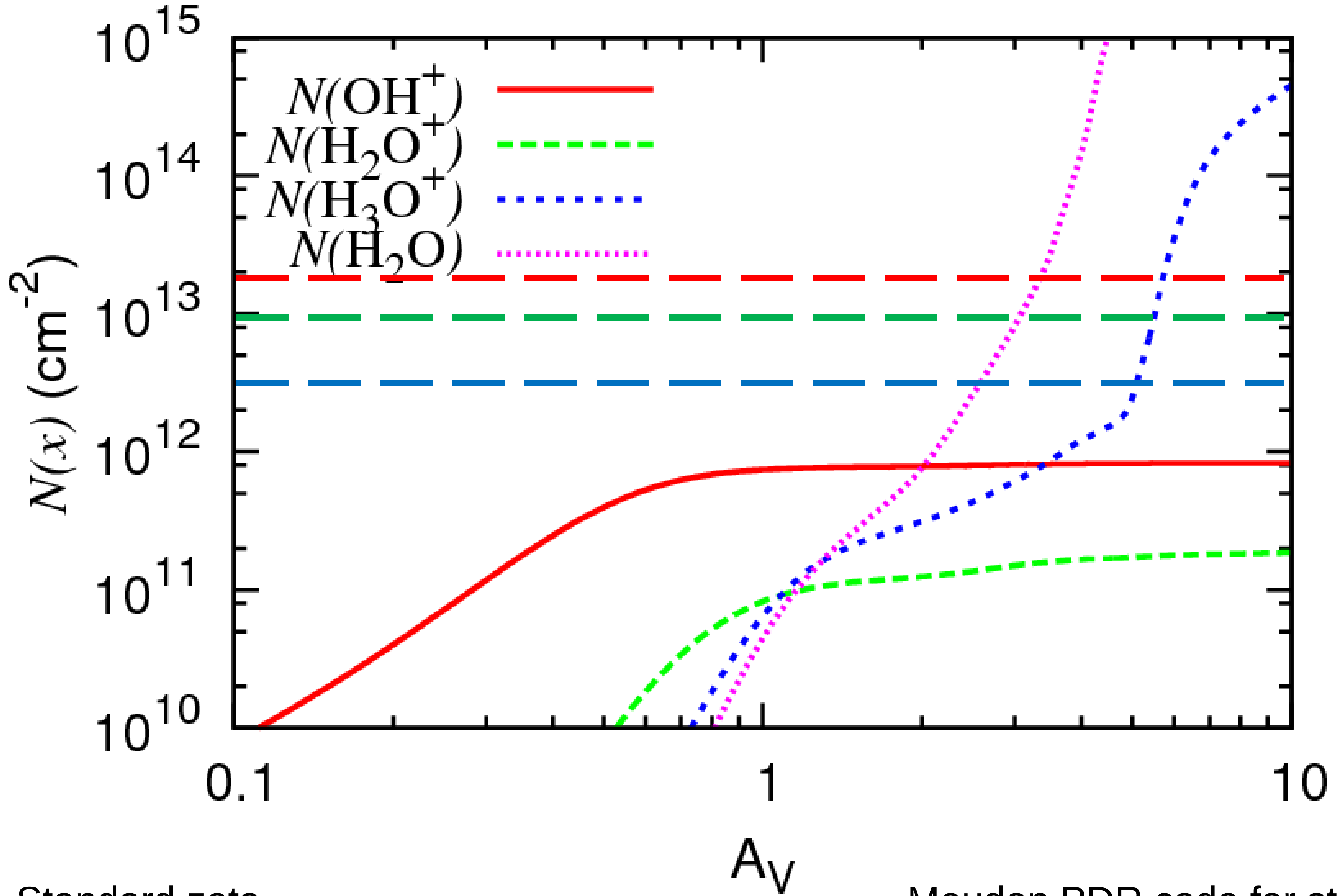
- The OH^+/H_2O^+ problem in the Orion Outflow (lots of UV radiation from OB stars): $OH^+ > H_2O^+ > H_3O^+$
- Model 1: Ultra-high ζ of 2×10^{-14} s^{-1} but too little water (under normal conditions, "essentially atomic" – Farquhar et al. (1994))
- **Model 2: water inflow allows lowering of ζ to a minimum of 10^{-15} s^{-1}; water accounted for.**
- Model 3: melting ice mantles supply the water; time dependent, gas-grain model

PDR Models of Orion KL Outflow



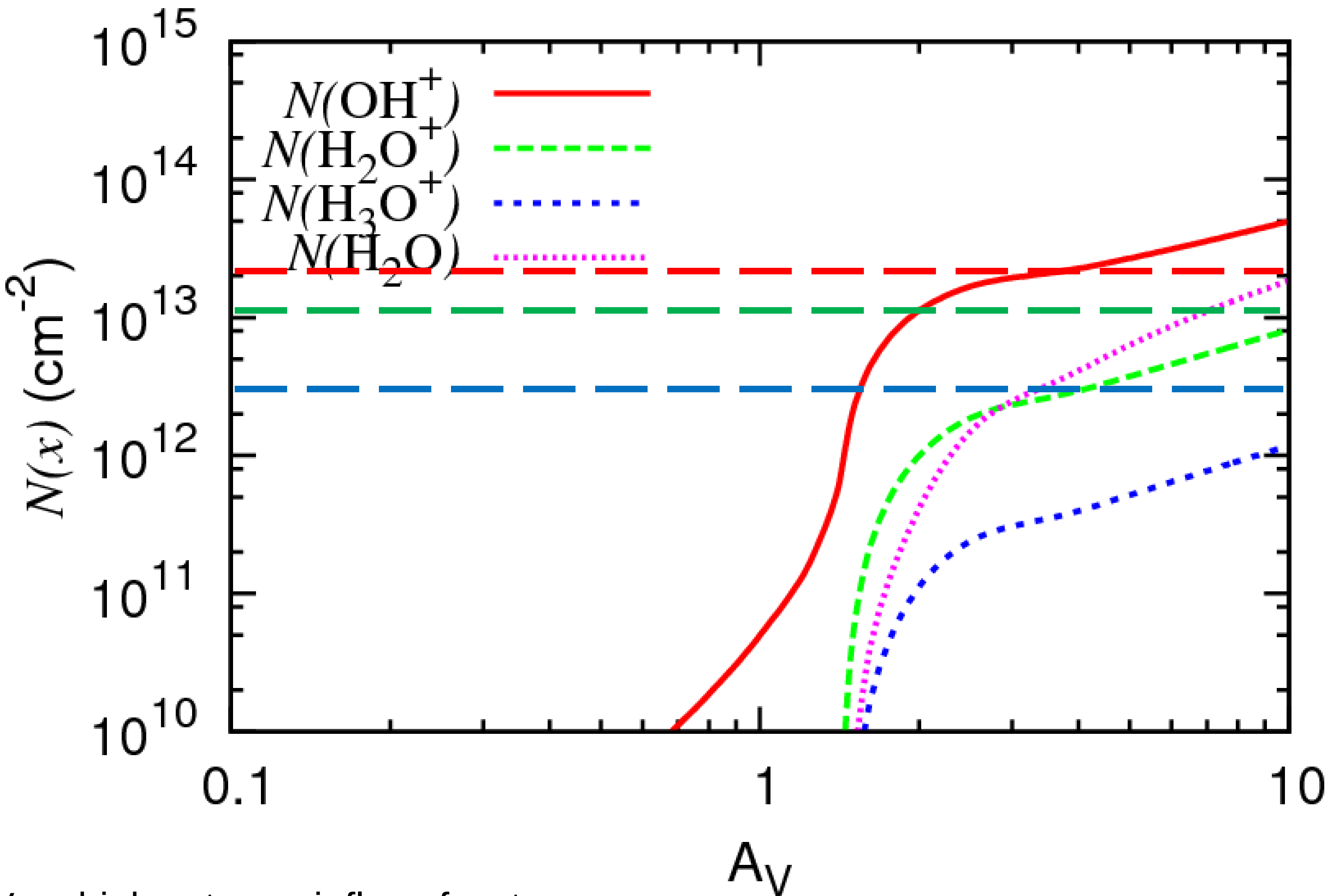
T = 400-500 K

Rimmer et al. 2011b



Standard zeta

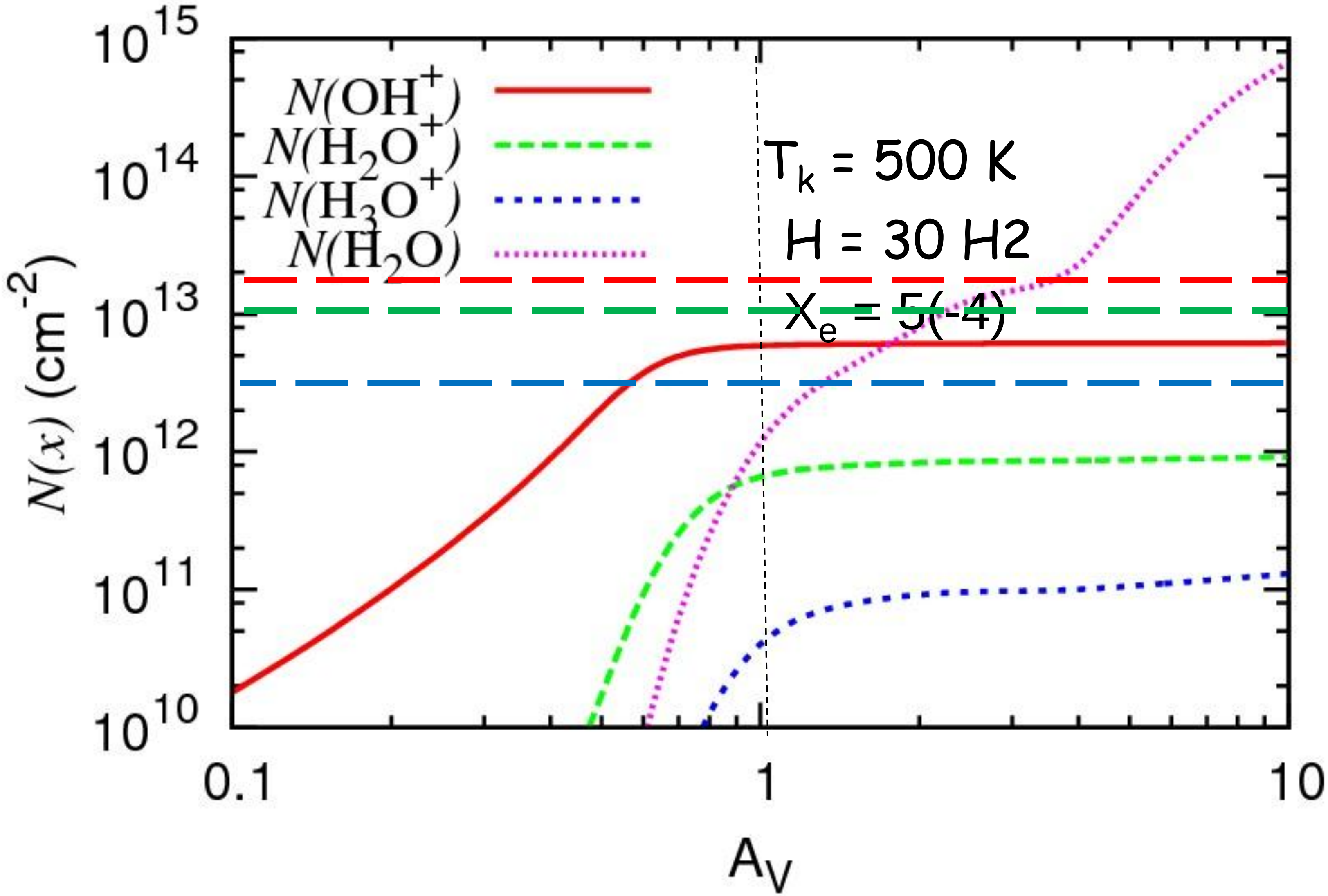
Meudon PDR code for steady-state studies.



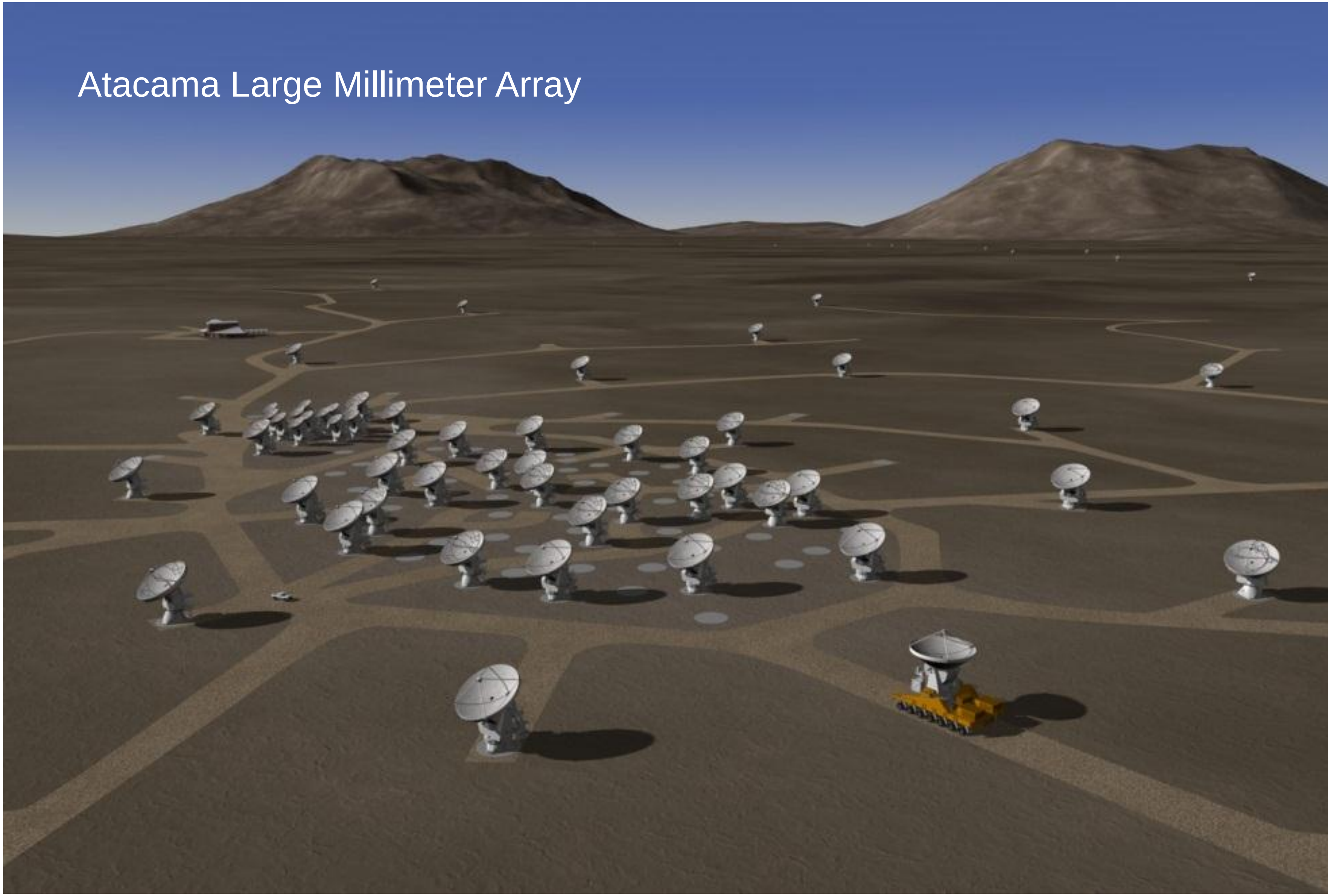
Very high zeta; no influx of water

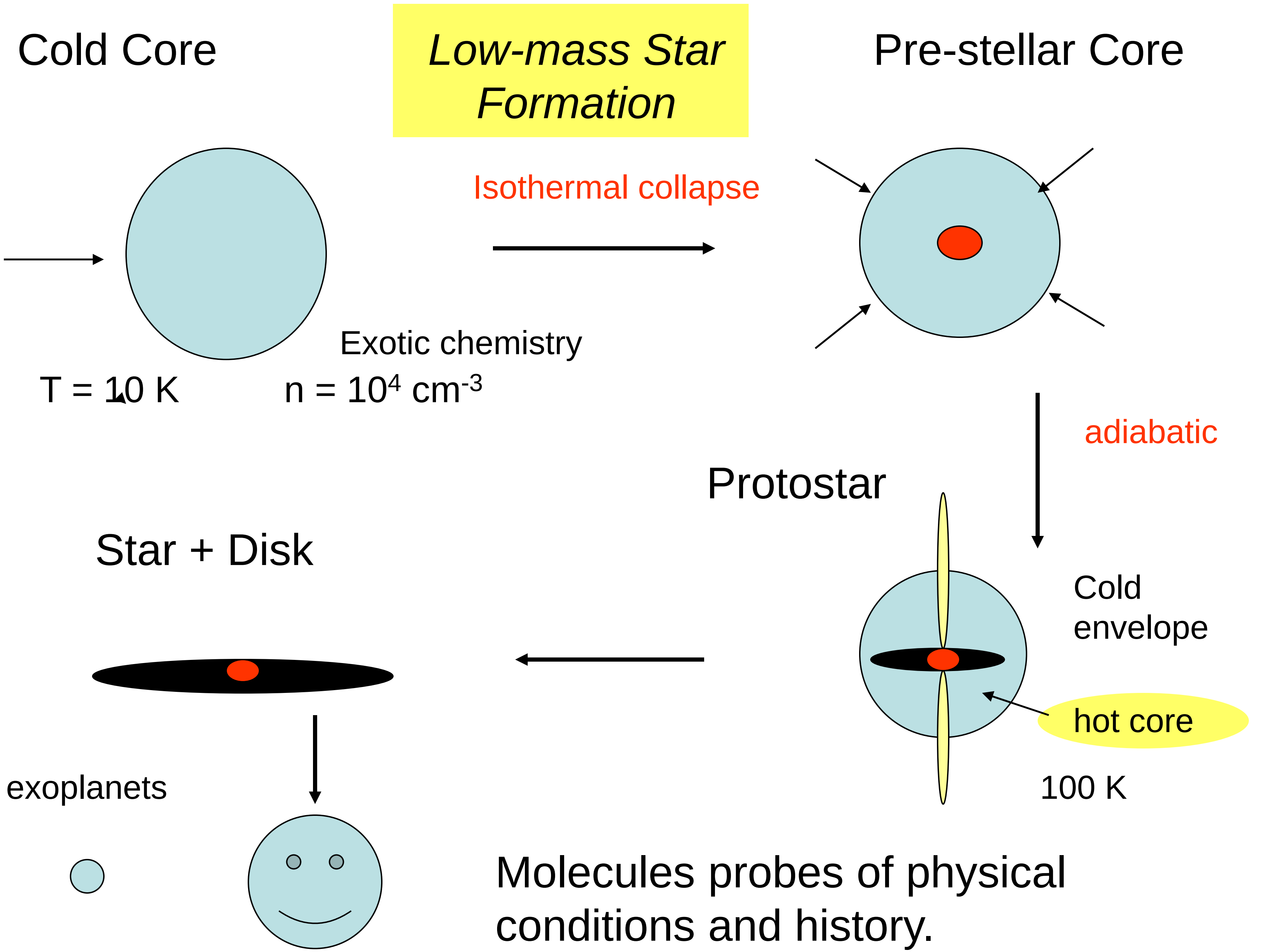
Model of Orion Low Vel. Outflow

Rimmer et al.



ζ= 5.0(-15) s-1; χ= 10(4); n = 1(03) cm-3


Atacama Large Millimeter Array


Low-mass Star Formation
Cold Core
Pre-stellar Core
Isothermal collapse
Exotic chemistry
T = 10 K
n = 10^4 cm^{-3}
adiabatic
Protostar
Star + Disk
Cold envelope
hot core
100 K
exoplanets
Molecules probes of physical conditions and history.

Chemical Processes in Cold Cores

- T=10 K, n = 10(4) – 10(6) cm-3

- cold gas-phase chemistry consisting of exothermic reactions without activation energy
- ion-molecule (unsaturated) chemistry plus some neutral reactions involving radicals.

- surface chemistry converts H into H_2 and builds up mantles of ices