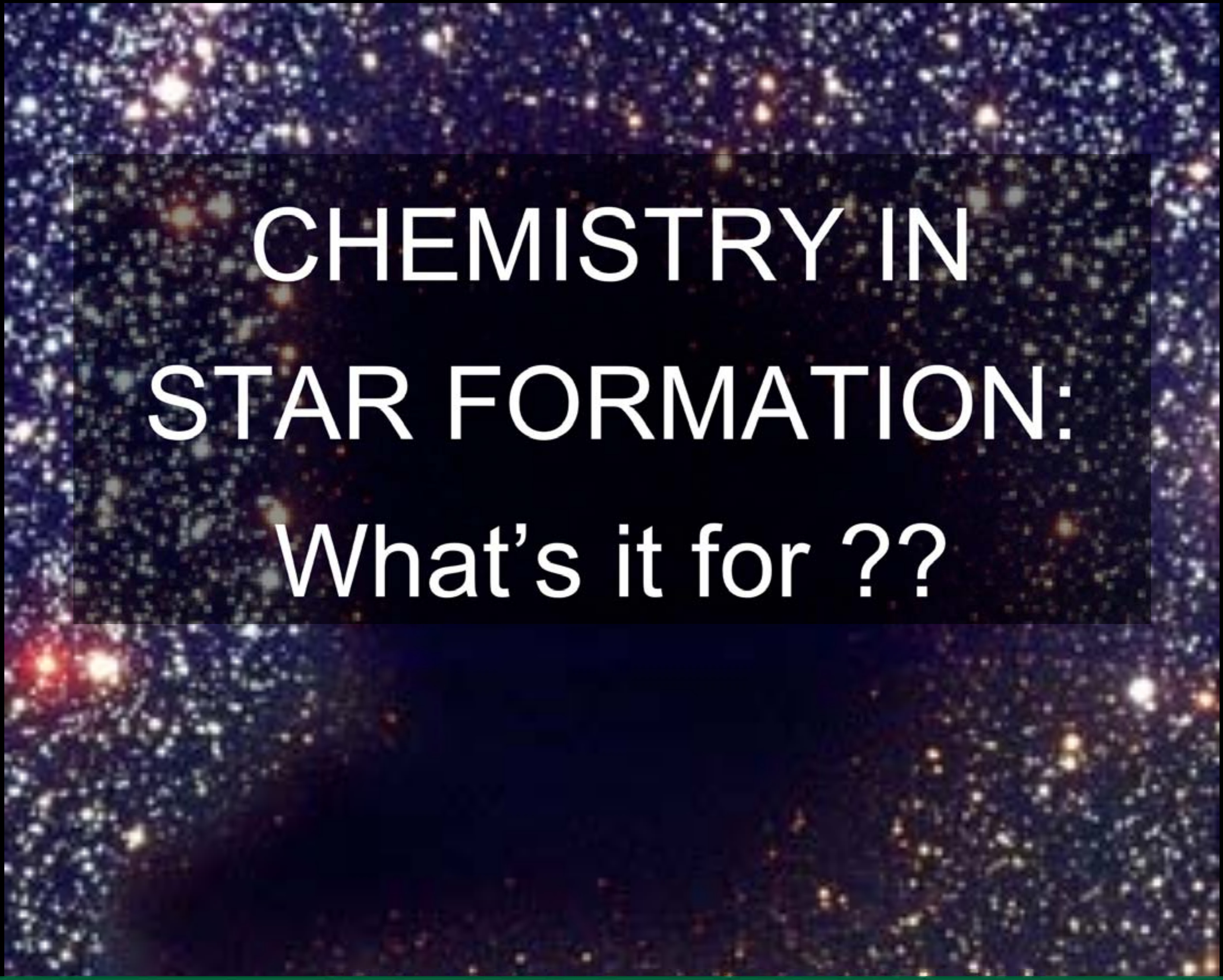

CHEMISTRY IN STAR FORMATION: What's it for ??

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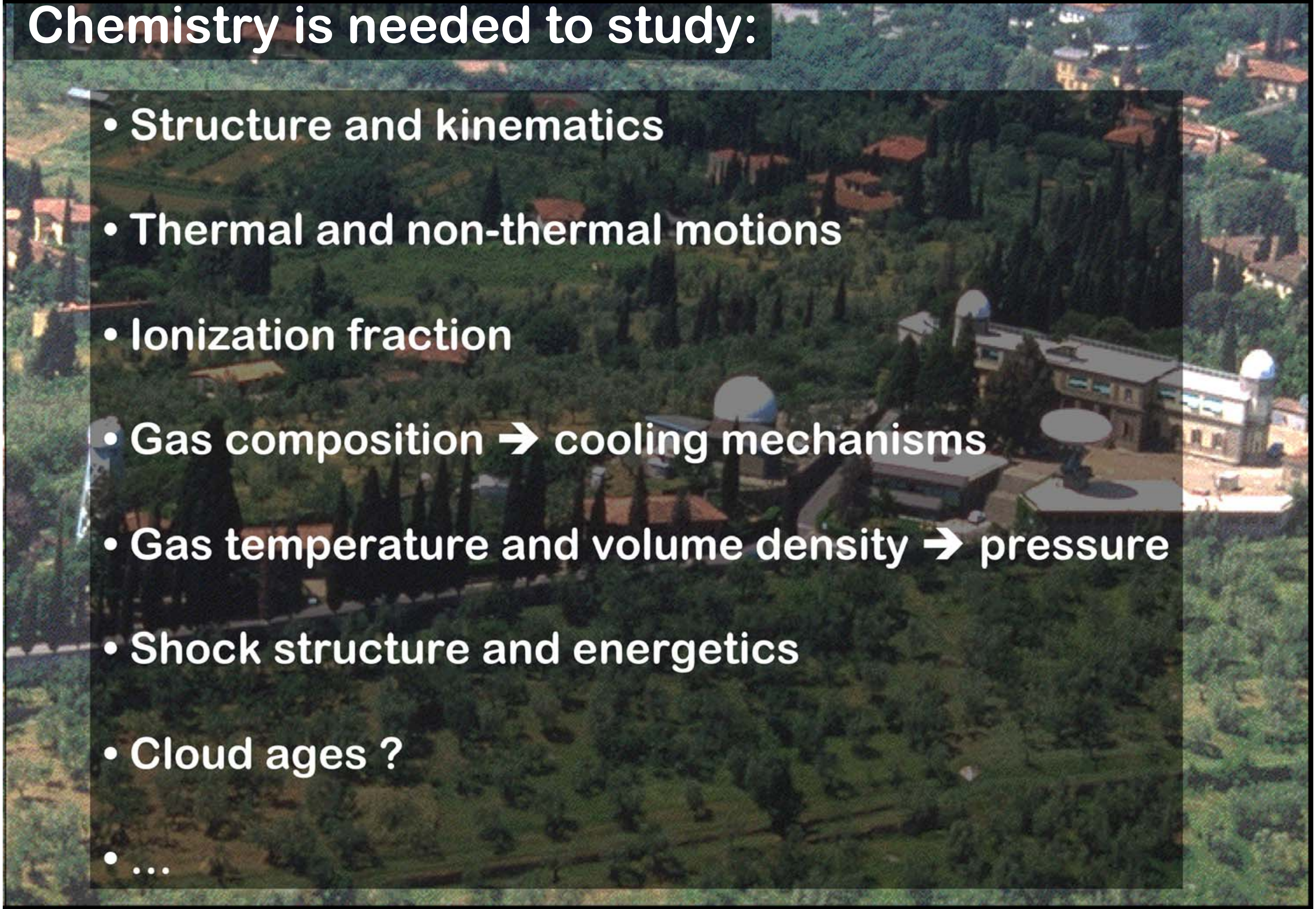
Chemistry is needed to study:



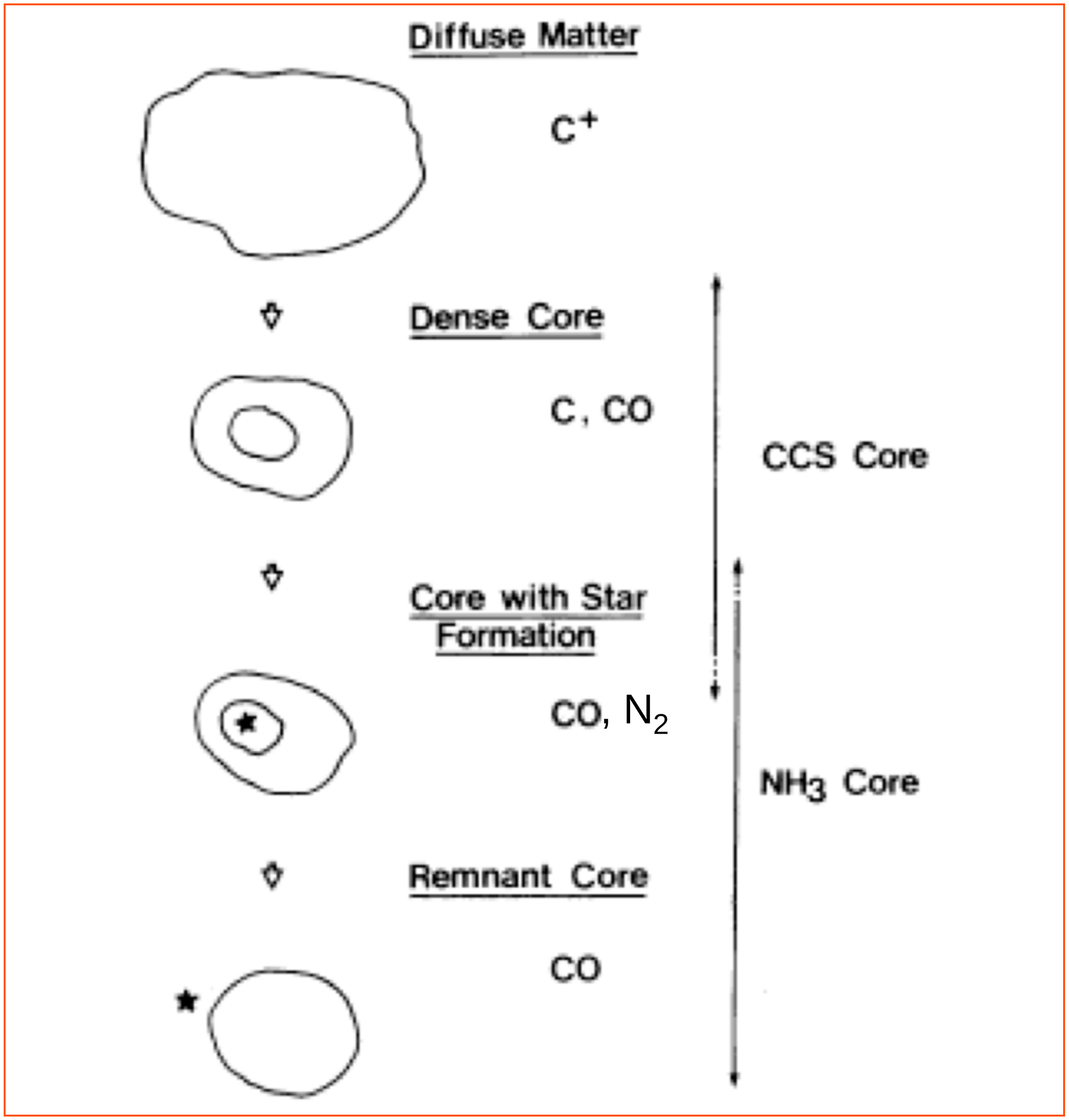
- Structure and kinematics
- Thermal and non-thermal motions
- Ionization fraction
- Gas composition → cooling mechanisms
- Gas temperature and volume density → pressure
- Shock structure and energetics
- Cloud ages ?
- …

Main Uncertainties

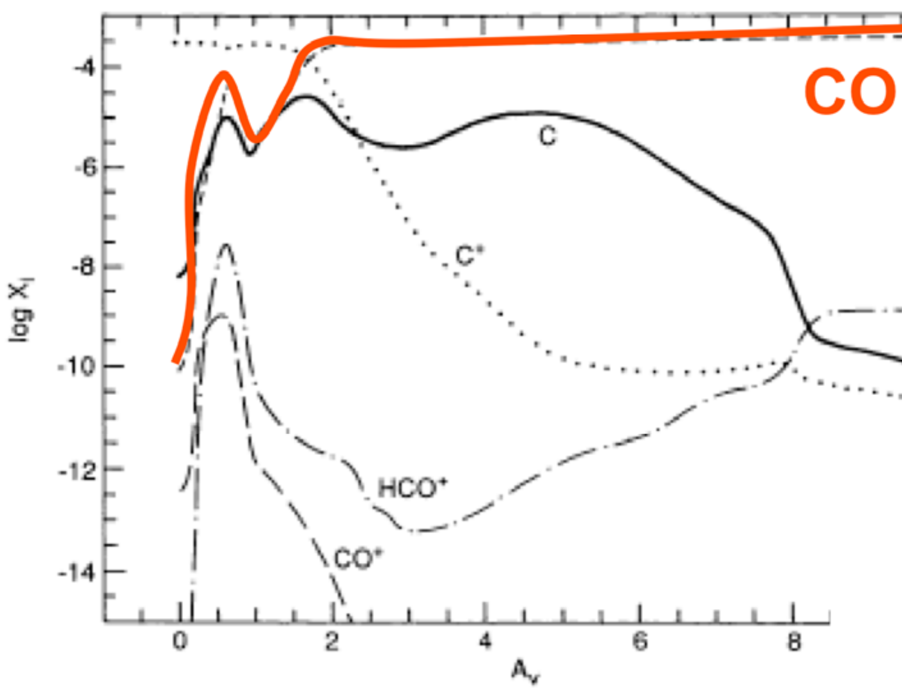
- **Cosmic-ray ionization rate**
- **Elemental abundance (e.g. metals)**
- **Oxygen chemistry**
- **PAHs abundance**
- **Surface chemistry**
- **H_2 ortho-to-para ratio**

Constant need of interaction with **real** chemists (theory + lab, gas-phase+solid state), who provide rate coefficients, collisional rates, transition frequencies…

Suzuki et al. 1992

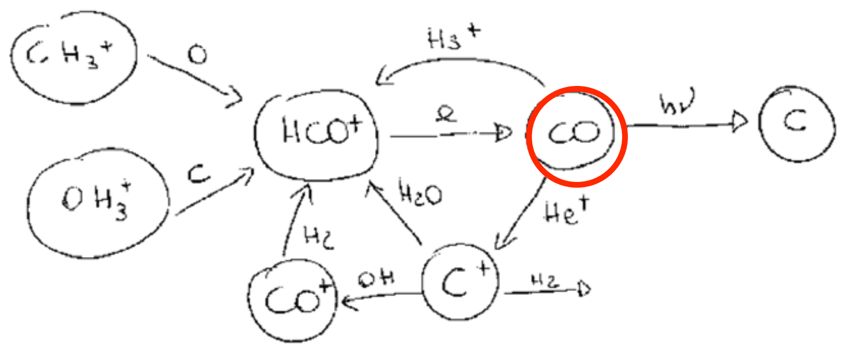


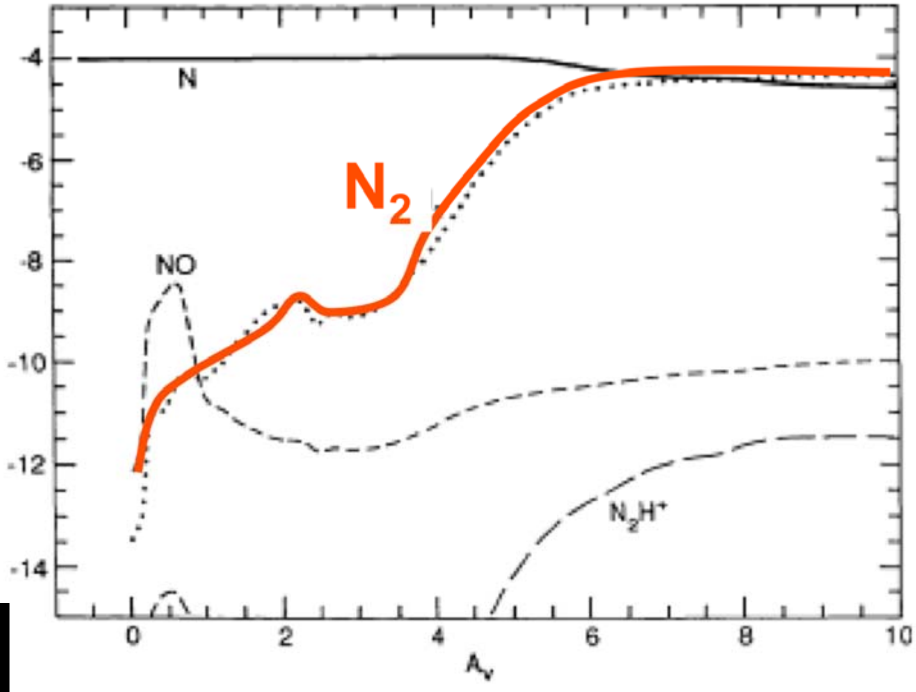
Sternberg & Dalgarno 1995



$t_{CO} \sim n_C/[\zeta n(H2)] \sim 10^5$yr

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





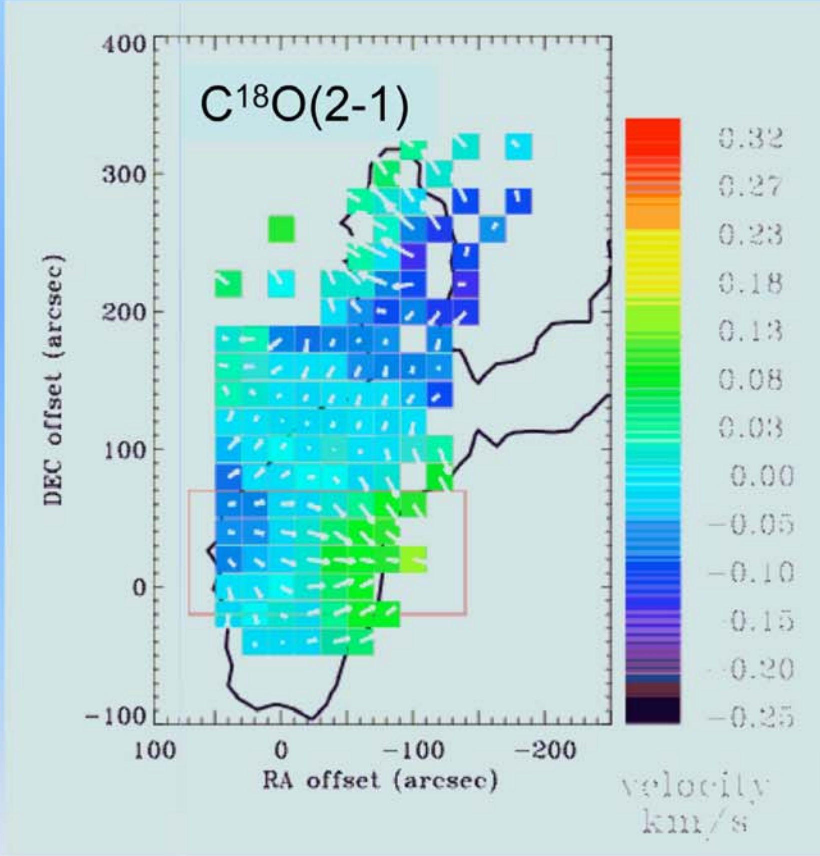
$N + H_3^+ \not\rightarrow NH^+ + H_2$

$N + OH \rightarrow NO + H$

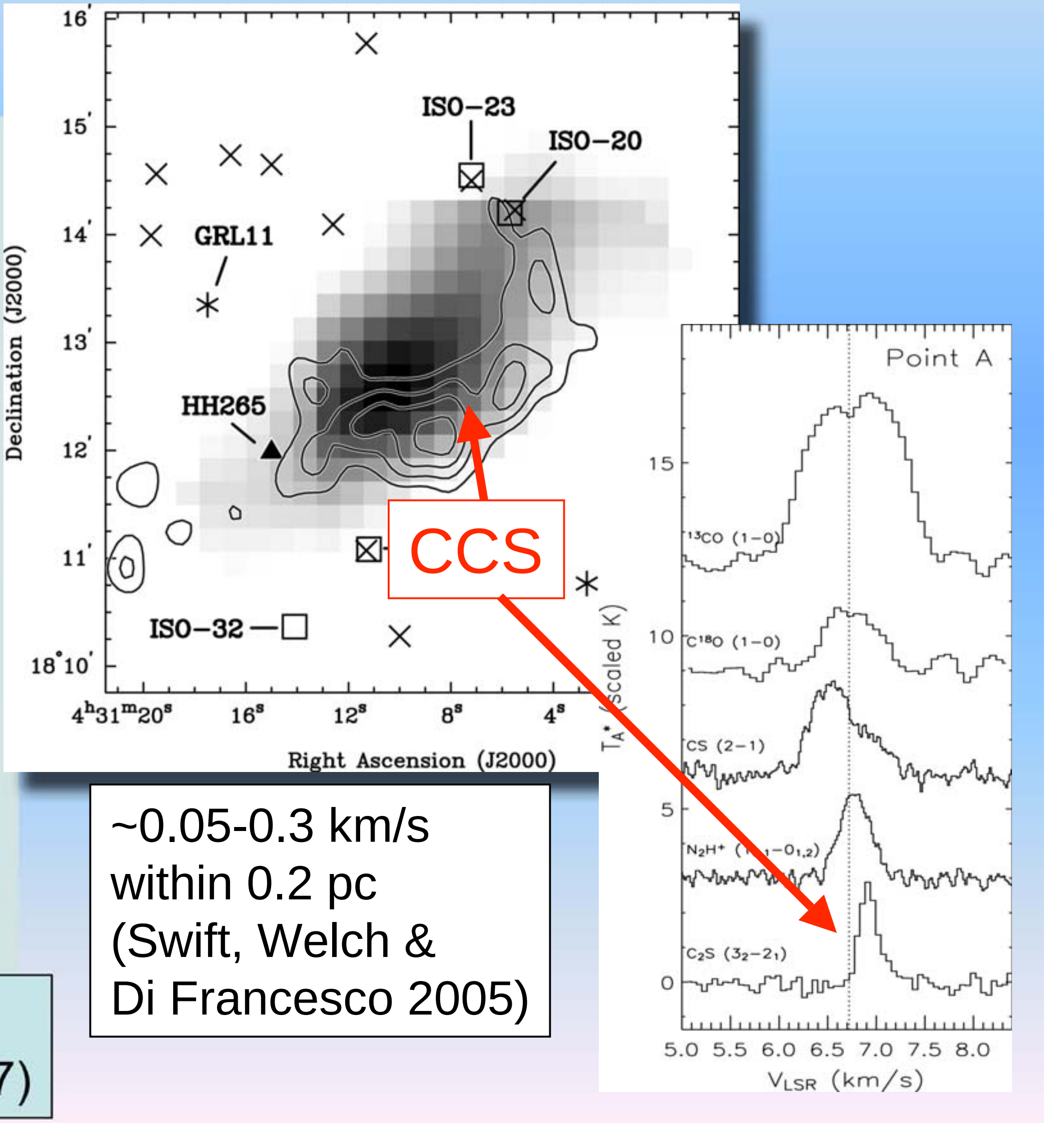
$NO + N \rightarrow N_2 + O$

$t_{N2} \sim 10^6$ yr in UV-shielded clouds

The majority of the cores are embedded in molecular clouds ➔ “chemically young” material may continue to flow in during core contraction and collapse !

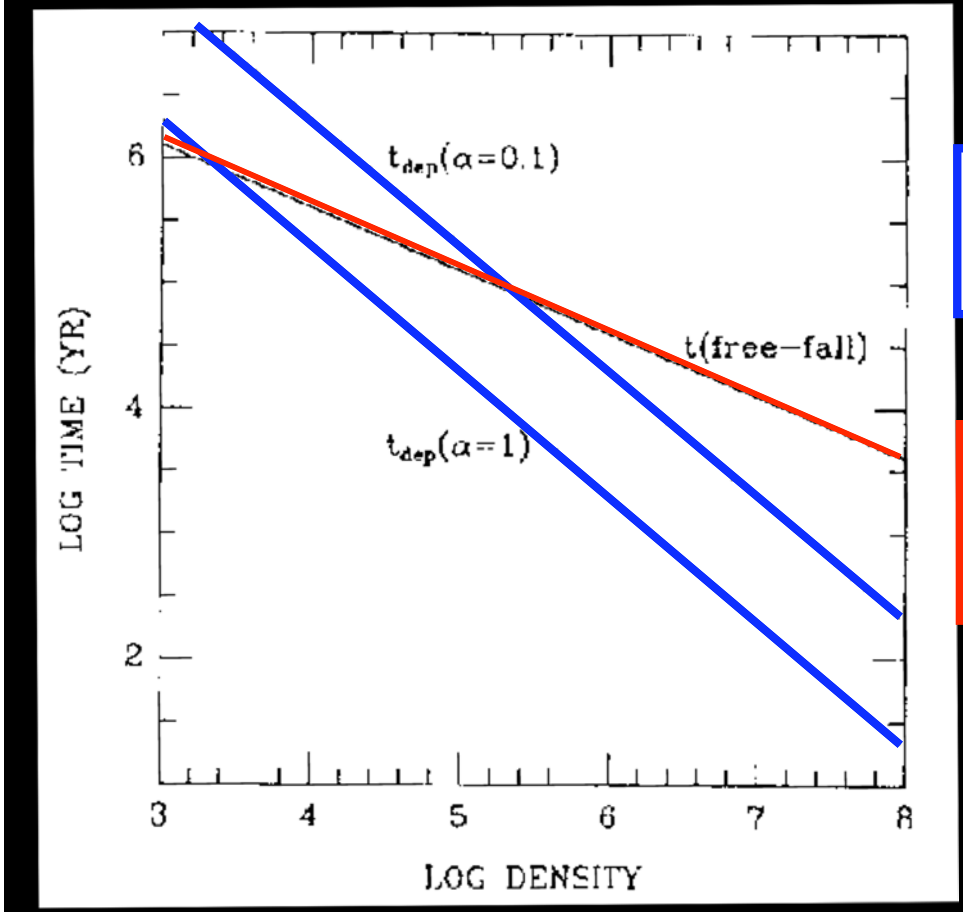


~0.05-0.3 km/s within 0.3 pc
(Schnee, Caselli, Goodman et al. 2007)



~0.05-0.3 km/s
within 0.2 pc
(Swift, Welch &
Di Francesco 2005)

Freeze-out vs. Free-fall



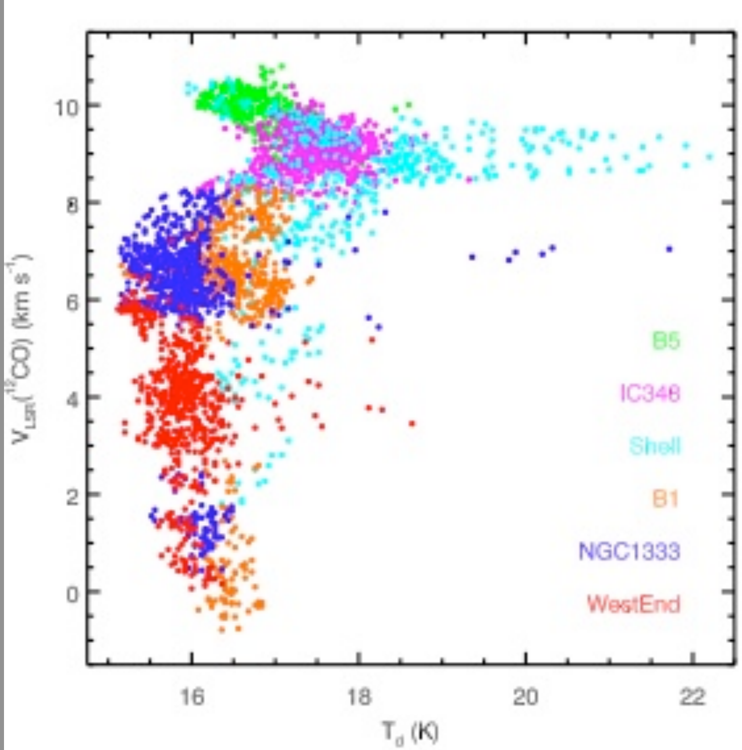
$$t_{dep} = \frac{1}{\alpha n_d \pi a_d^2 v_t} \approx 10^9 \sqrt{m_X / T}\,(n_H \alpha)^{-1}\ \mathrm{yr}$$

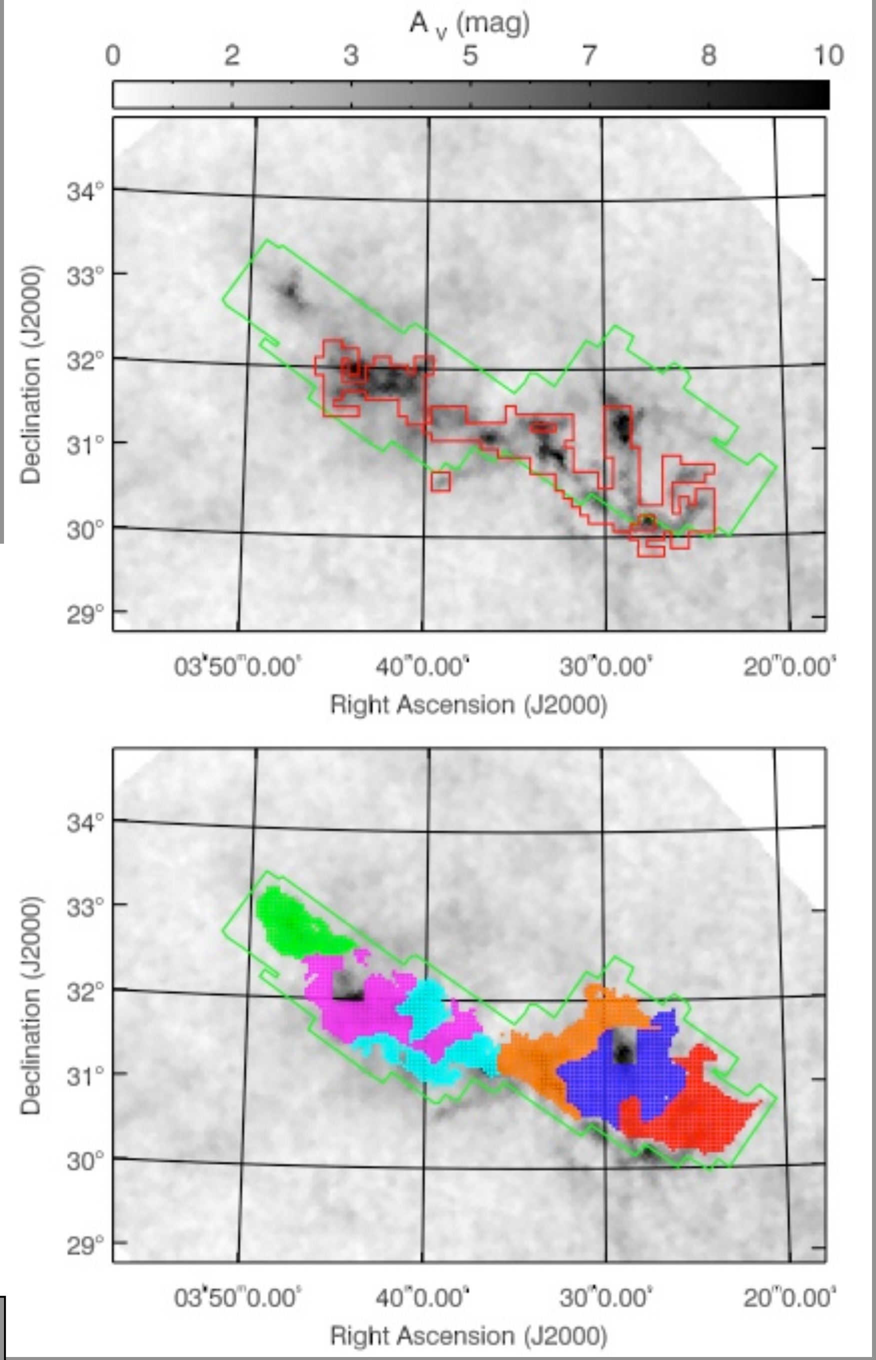
$$t_{ff} = \left(\frac{3\pi}{32G\rho}\right)^{-1/2} = 4 \times 10^7\ (n_H)^{-1/2}\ \mathrm{yr}$$

Walmsley 1991
van Dishoeck et al. 1993

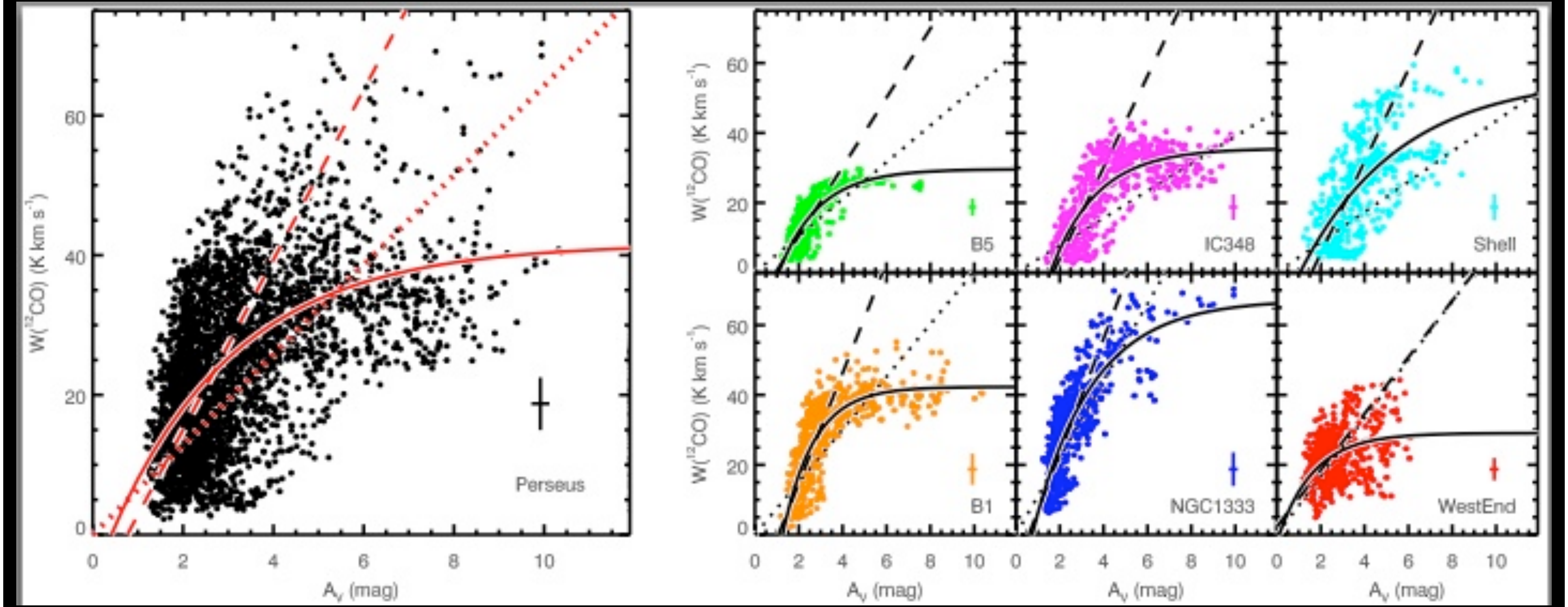
Pineda, Caselli & Goodman (2007)

CO isotopologues in Perseus: the X-factor and physical properties.





$X \sim 1\text{-}2 \times 10^{20}\ \mathrm{cm^{-2}\ K^{-1}\ km^{-1}\ s}$



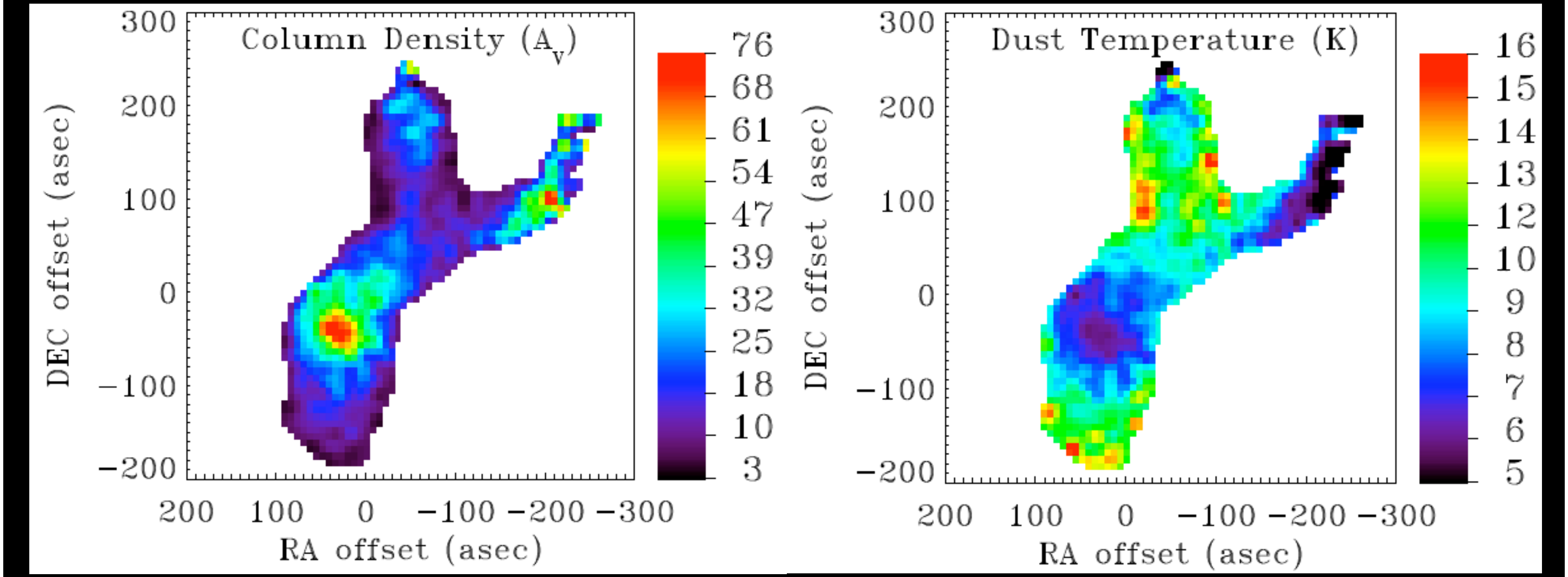
A_{Vth} ≤ 1 mag for ^{12}CO
~ 1-2 mag for ^{13}CO
~ 2-3 mag for $C^{18}O$

PDR codes: non-thermal motion and density changes can explain the obs. variation among the Perseus regions.

T_{ex} ~ 5 K at $A_V \leq 2$ mag
~ 13 K at $A_V \geq 4$ mag
$T_{ex} < T_{dust}$ ~ 16 K

➔

60% of the CO gas is subthermally excited, i.e. $n_H << 3000$ cm^{-3}



Multiwavelength study of TMC-1C:

- 850 and 450 μm (JCMT)
- 1.2mm (IRAM-30m)
- $C^{17}O$, $C^{18}O$, N_2H^+

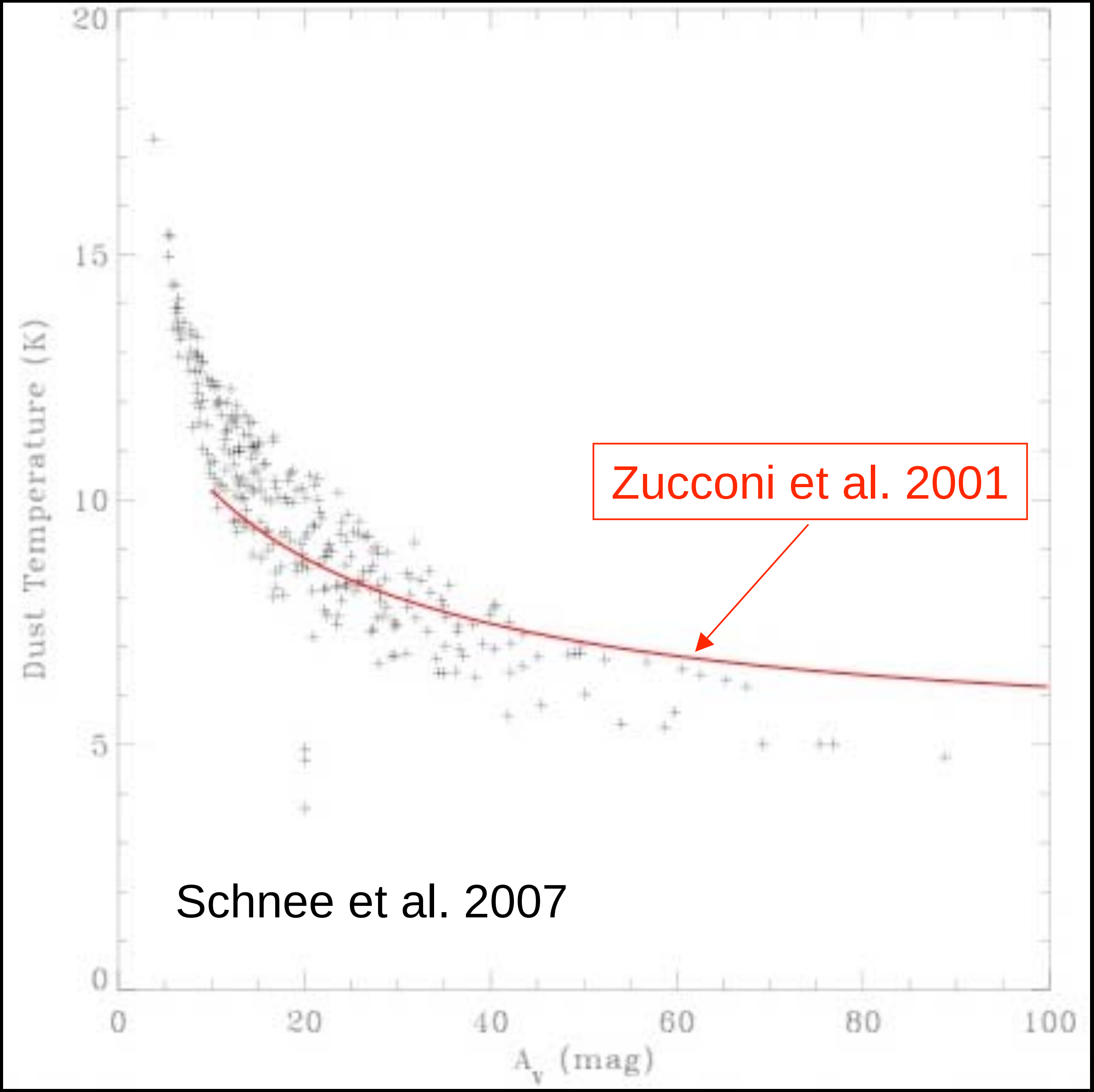
➔

At dust peak position:

- $T_{dust} \sim 6$ K, $n_c \sim 10^6$ cm^{-3}
- $T_{gas}(CO) \sim 12$ K (it drops outwards).

Schnee & Goodman 2005

Schnee, Caselli, Goodman et al. 2007

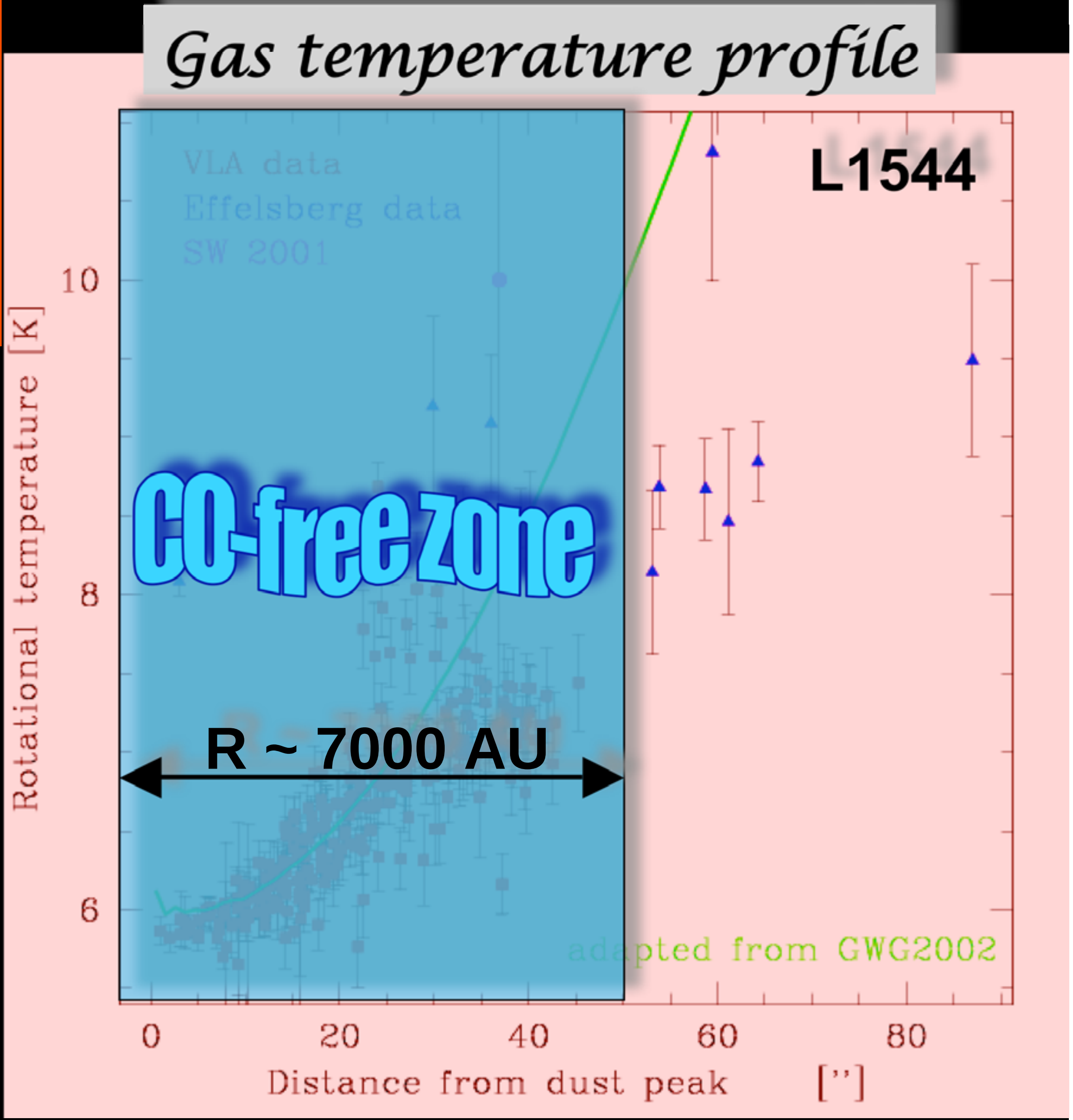


Zucconi et al. 2001

Schnee et al. 2007

Interferometric obs for L1544:
NH_3 @ VLA
NH_2D @ PdB

The gas temperature drops to 6 K in the central 1000 AU (2×10^6 cm^{-3}) !


Gas temperature profile

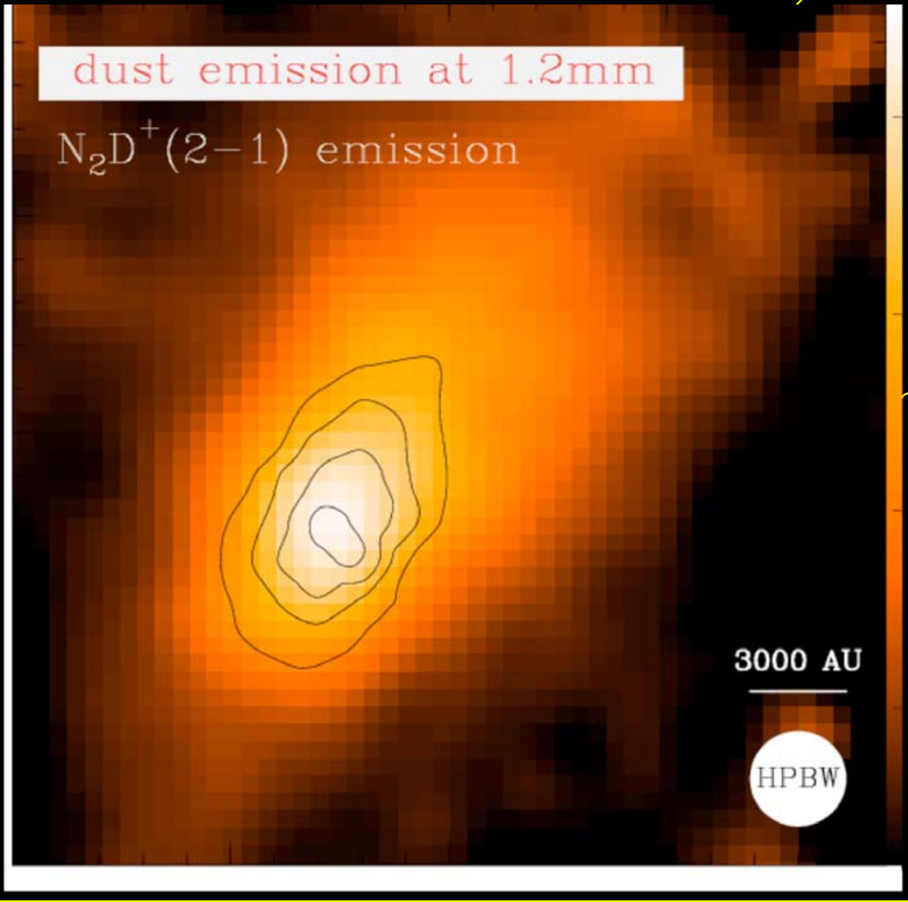
CO-free zone

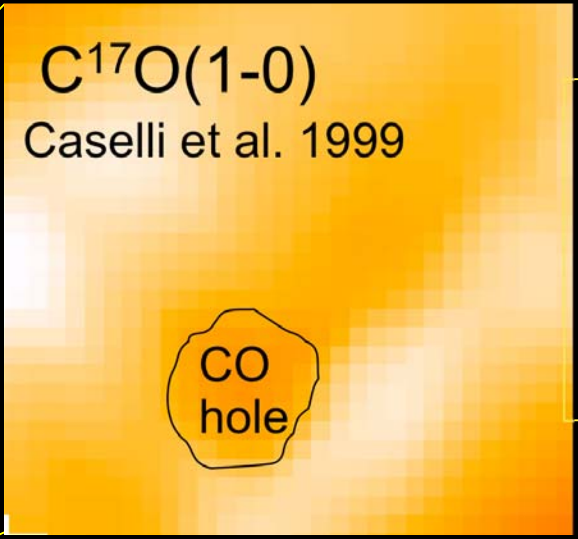
R ~ 7000 AU

adapted from GWG2002

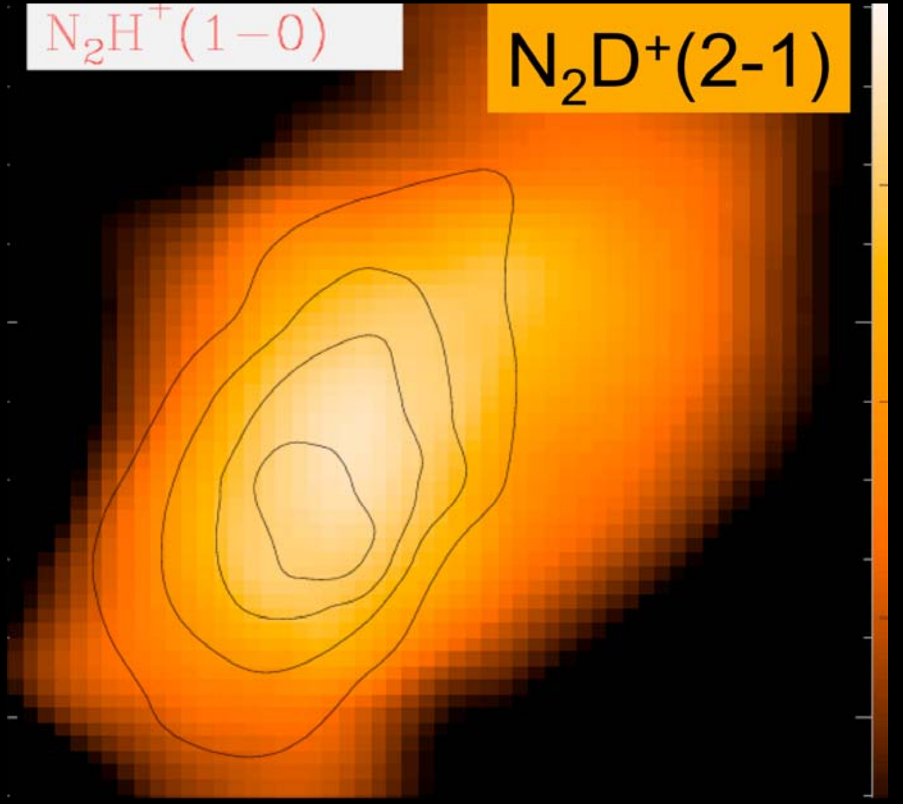
Crapsi, Caselli, Walmsley & Tafalla 2007

Chemical structure of L1544





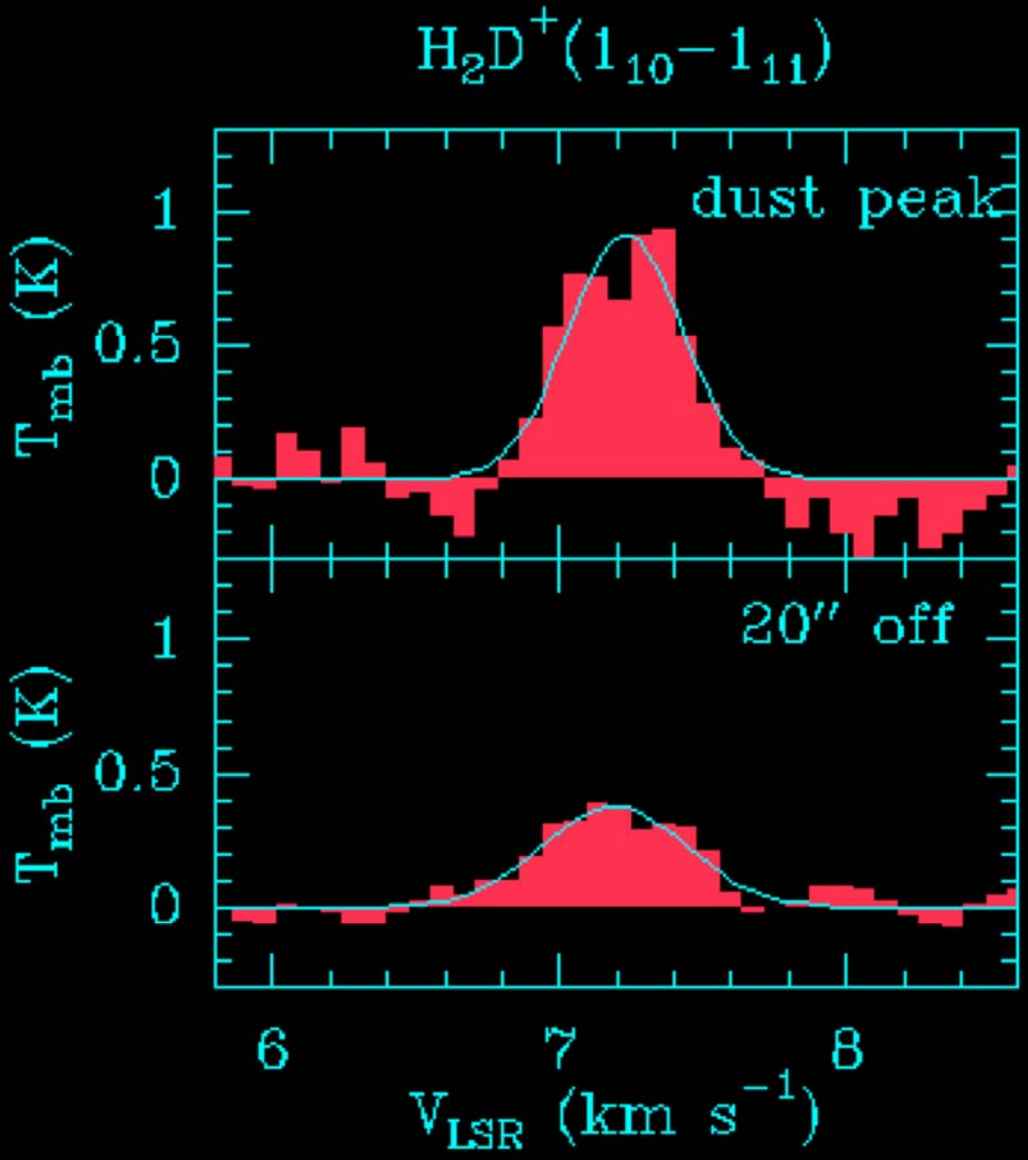
CO starts to disappear from gas phase at R< 7000 AU



N_2H^+ and N_2D^+ are good tracers of the core nucleus (Caselli et al. 2002b)

D-fractionation increases towards the core center (Caselli et al. 2002c)

The strong *ortho*-H_2D^+ emission:



$[H_2D^+]/[H_2]$ ~ 10^{-9} within R ~ 2500 AU

↓

CNO-bearing molecules are almost completely (≥ 98%) frozen within R

$[H_2D^+]$ ~ $[H_3^+]$

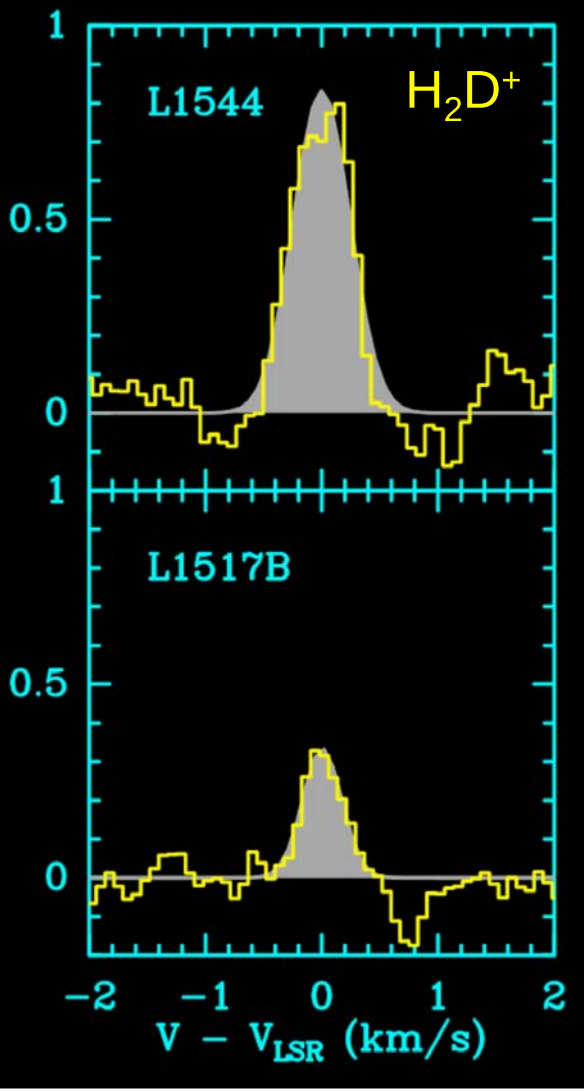
↓

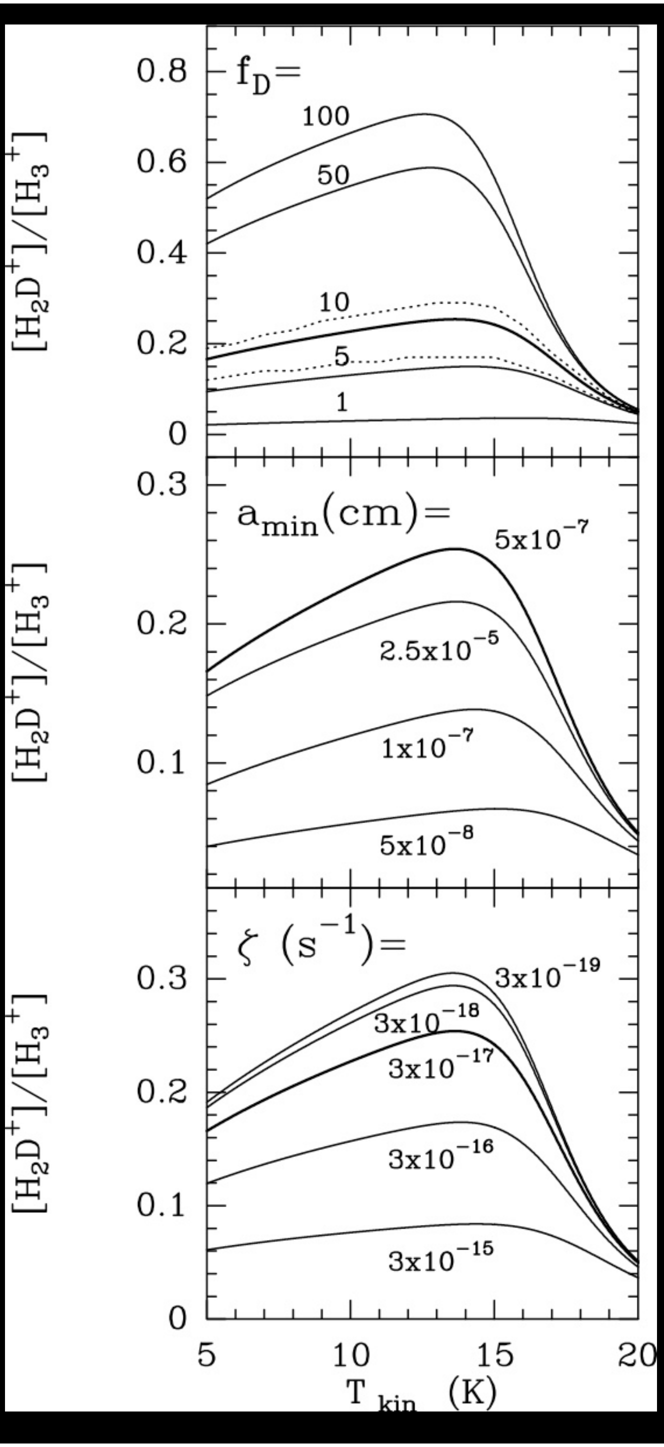
$[D_3^+]$~$[D_2H^+]$~$[H_2D^+]$

Caselli et al. 2003, A&A, 403, L37

Roberts et al. 2003, 2004
Walmsley et al. 2004
Hugo & Schlemmer, in prep.

Caselli et al., in prep.

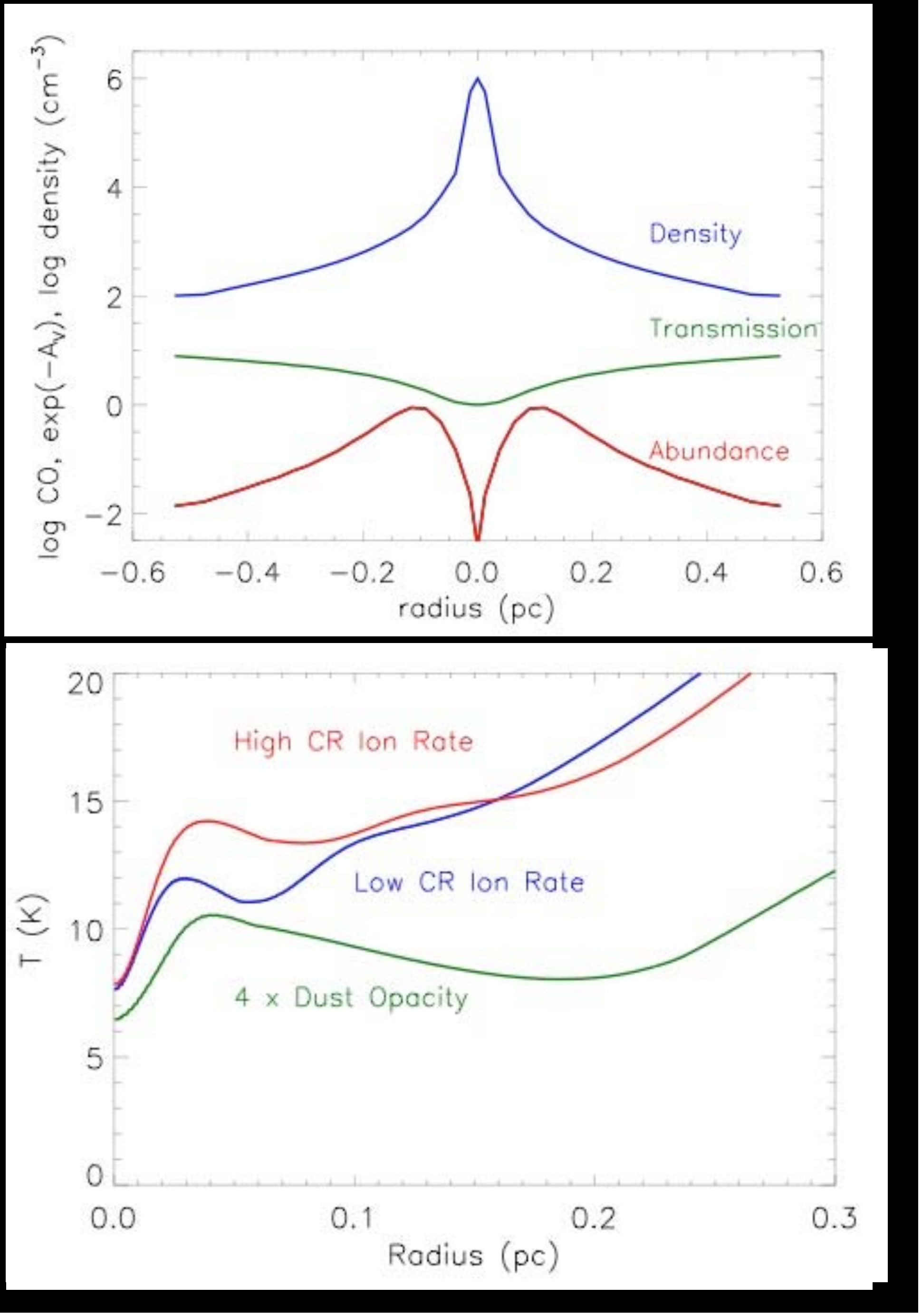




$$\frac{x(\mathrm{H_2D^+})}{x(\mathrm{H_3^+})} = \frac{k_1 x(\mathrm{HD})}{k_{-1} + k_{\mathrm{CO}}x(\mathrm{CO})/f_D + k_e x(\mathrm{e}) + k_{\mathrm{g}} x_g}$$

Keto & Caselli (in prep.)

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

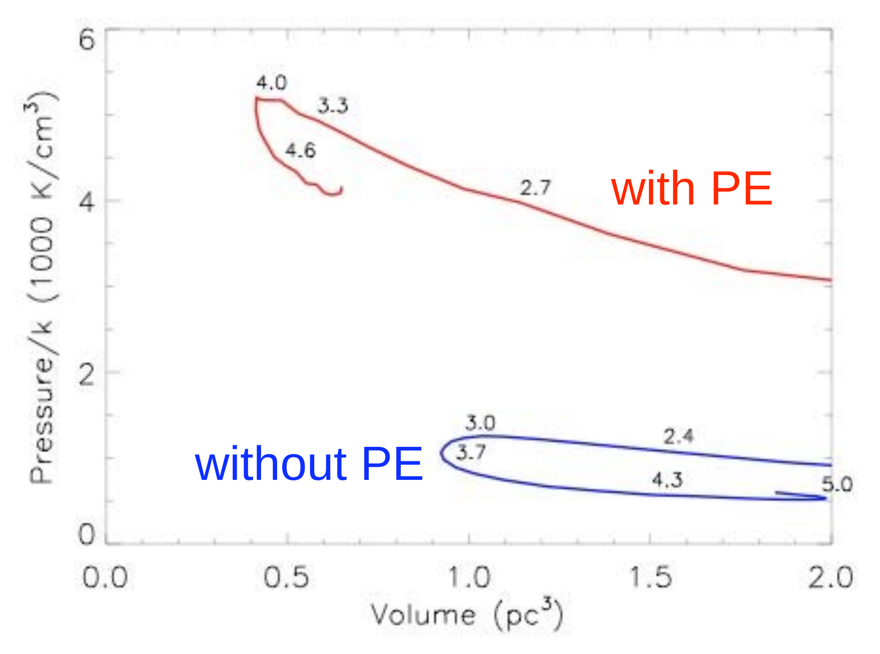


Photoelectric Heating (Bakes & Tielens 1994)

Heating rate: $\Gamma_{pe} = 10^{-24} \varepsilon G_{pe}(r) n(\mathrm{H}_2)\ \mathrm{erg\ cm^{-3}\ s^{-1}}$

Computing $G_{pe}(r)$, the intensity is averaged over frequency and angle, Ω, from point r to the surface:

$$G_{pe}(r) = \frac{\int \int_{6MeV}^{\infty} J_\nu \exp(-\tau_\nu(r,\omega))\, d\nu d\Omega}{\int \int_{6MeV}^{\infty} J_\nu\, d\nu d\Omega}$$



Conclusions

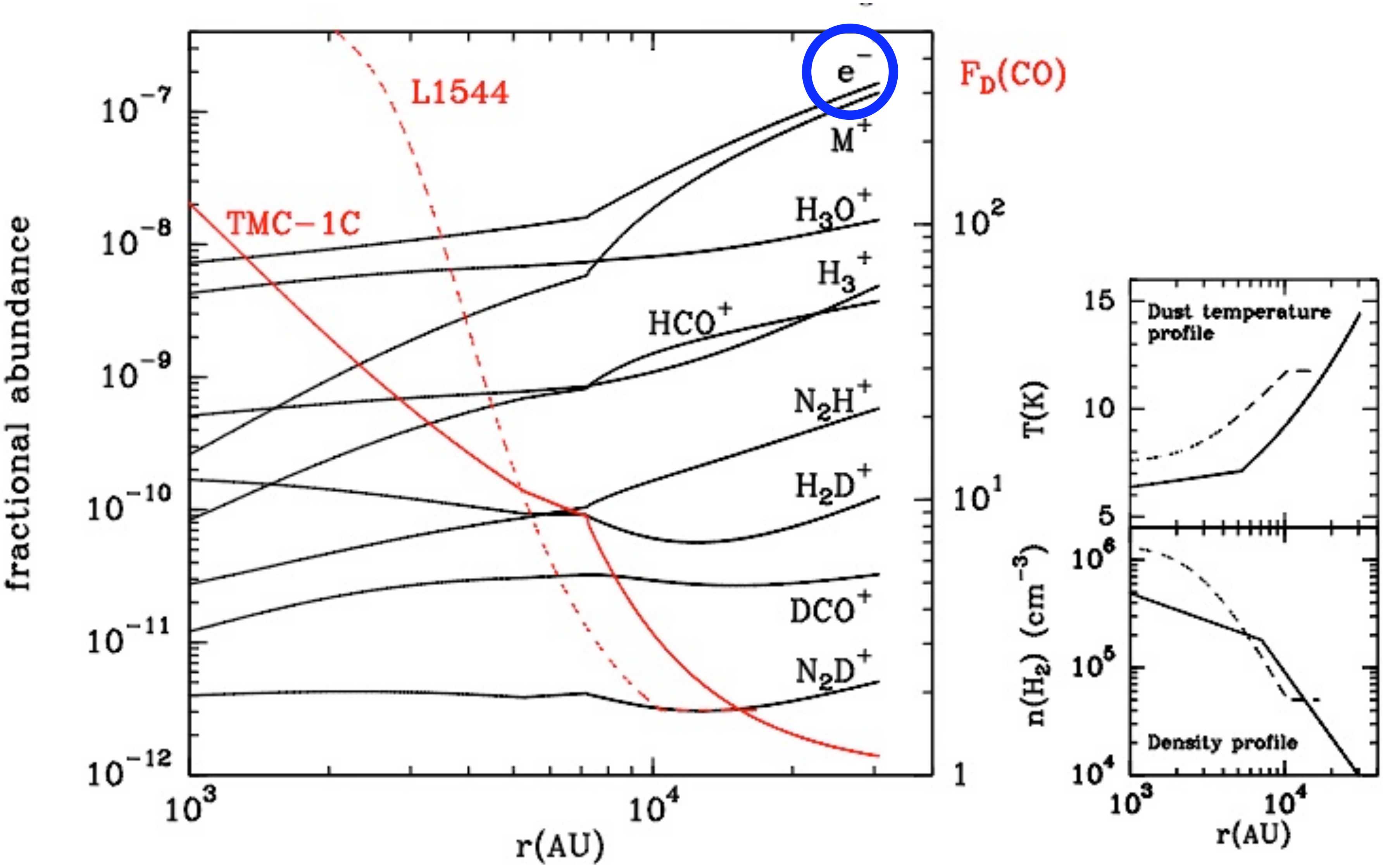
- Chemistry is needed to find the right tracers throughout interstellar clouds (and protoplanetary disks).

- In molecular clouds, CO is photodissociated at $A_V \leq$ 1mag, subthermally excited at $A_V \leq$ 4 mag and frozen-out at $n(H_2) \geq$ a few×$10^4 cm^{-3}$ (starless cores).

- Embedded dense cloud cores accrete material from the surroundings at velocities ~ 0.1..0.3 km s^{-1}.

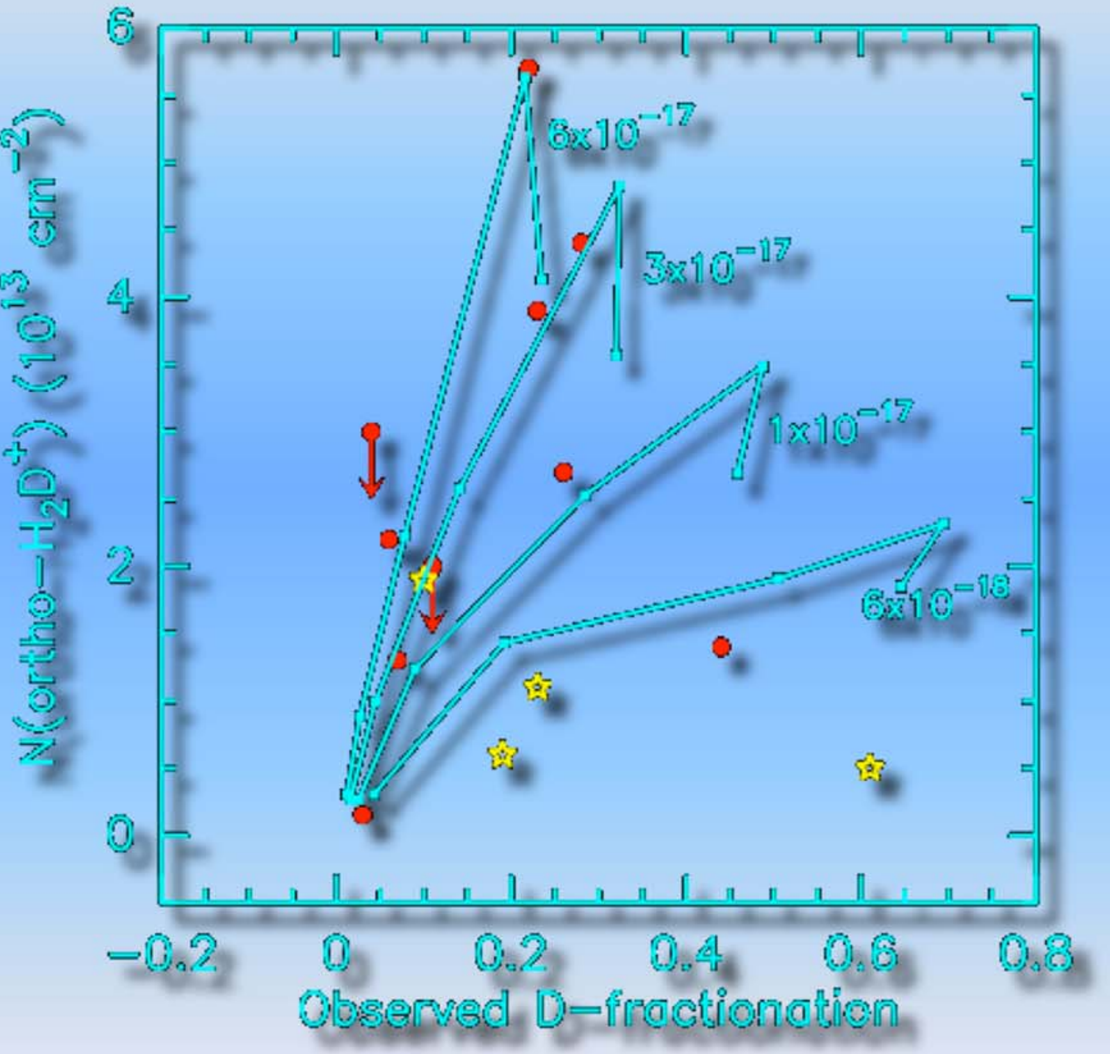
- In pre-stellar cores, the gas and dust temperature approach 6 K at $n(H_2) \sim 10^6$ cm^{-3}. Increase in dust opacity.

- H_2D^+ is a great tracer of kinematics and ion-fraction at $n(H_2) \geq 10^5$ cm^{-3}.



$\zeta = 1.3\text{x}10^{-17}$ s^{-1}

The cosmic-ray ionization rate (?)



see also Padoan & Scalo 2005