Clouds and star forming regions

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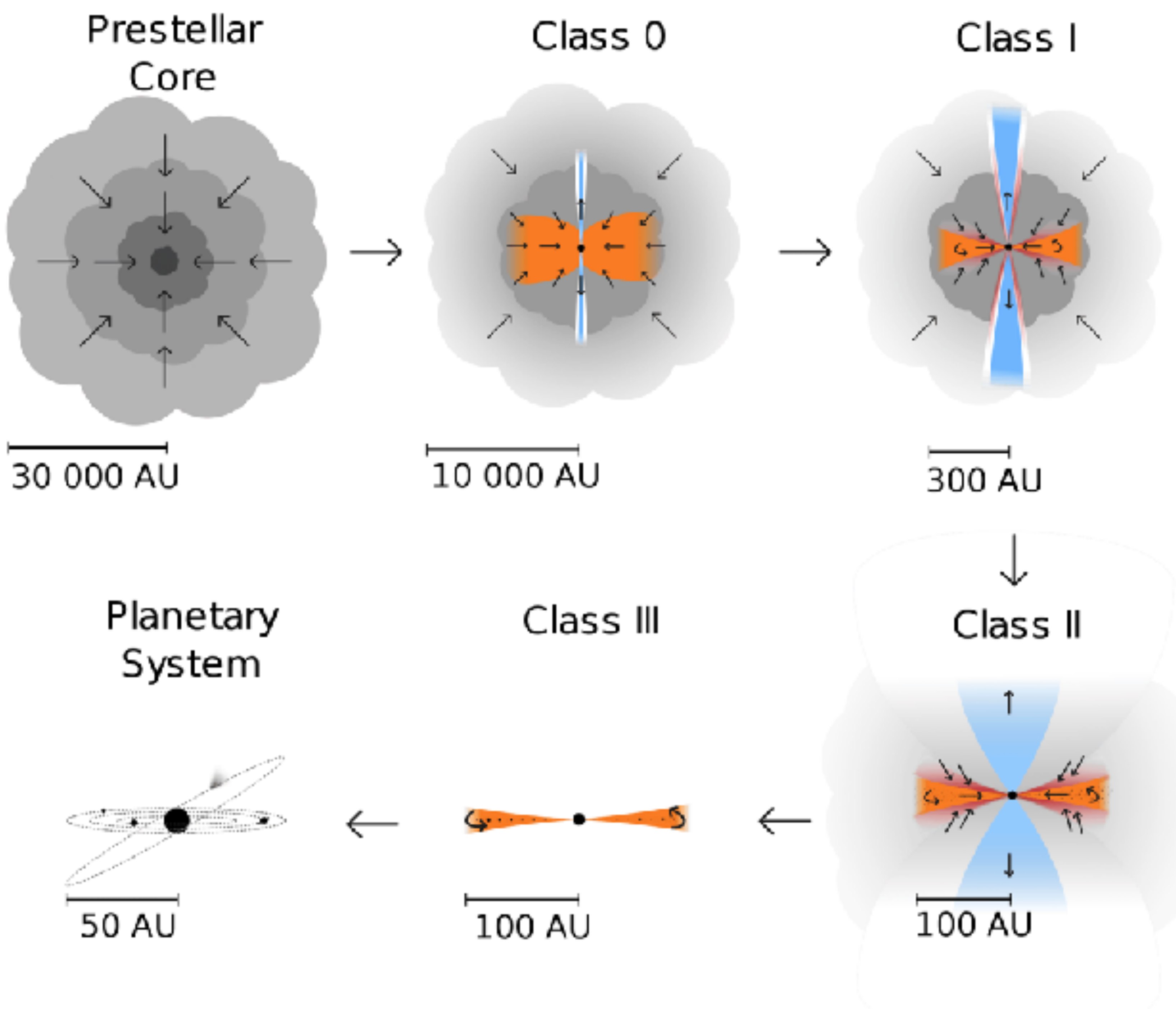
- Shocks

Star formation



Star formation

- **Starless cores (diffuse-dense clouds)**: $T \approx 10\text{-}20$ K, $n \approx 10^4$ cm^{-3}
  - Quiescent ion-molecule chemistry
  - Radicals and carbon chains
- **Pre-stellar cores and collapse**: $T \approx 10$ K, $n \approx 10^5\text{-}10^8$ cm^{-3}
  - Heavy freeze-out of molecules onto grains
  - Grain surface reactions produce new species:

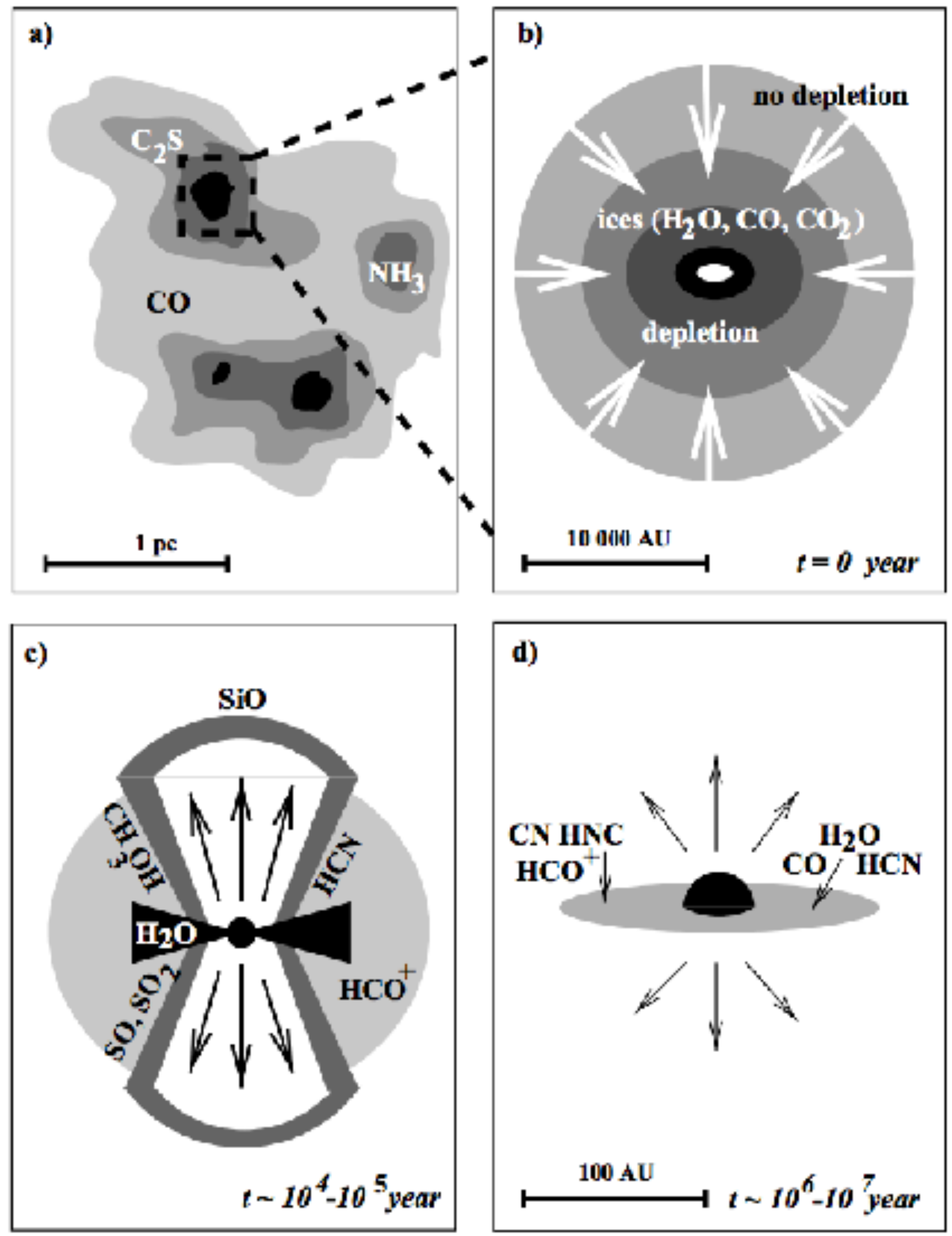
$$\mathrm{O, C, N, CO} \xrightarrow{\mathrm{H}} \mathrm{H_2O, CH_4, NH_3} \\ \mathrm{H_2CO, CH_3OH}$$

$$\mathrm{CO} \xrightarrow{\mathrm{O}} \mathrm{CO_2}$$

Star formation

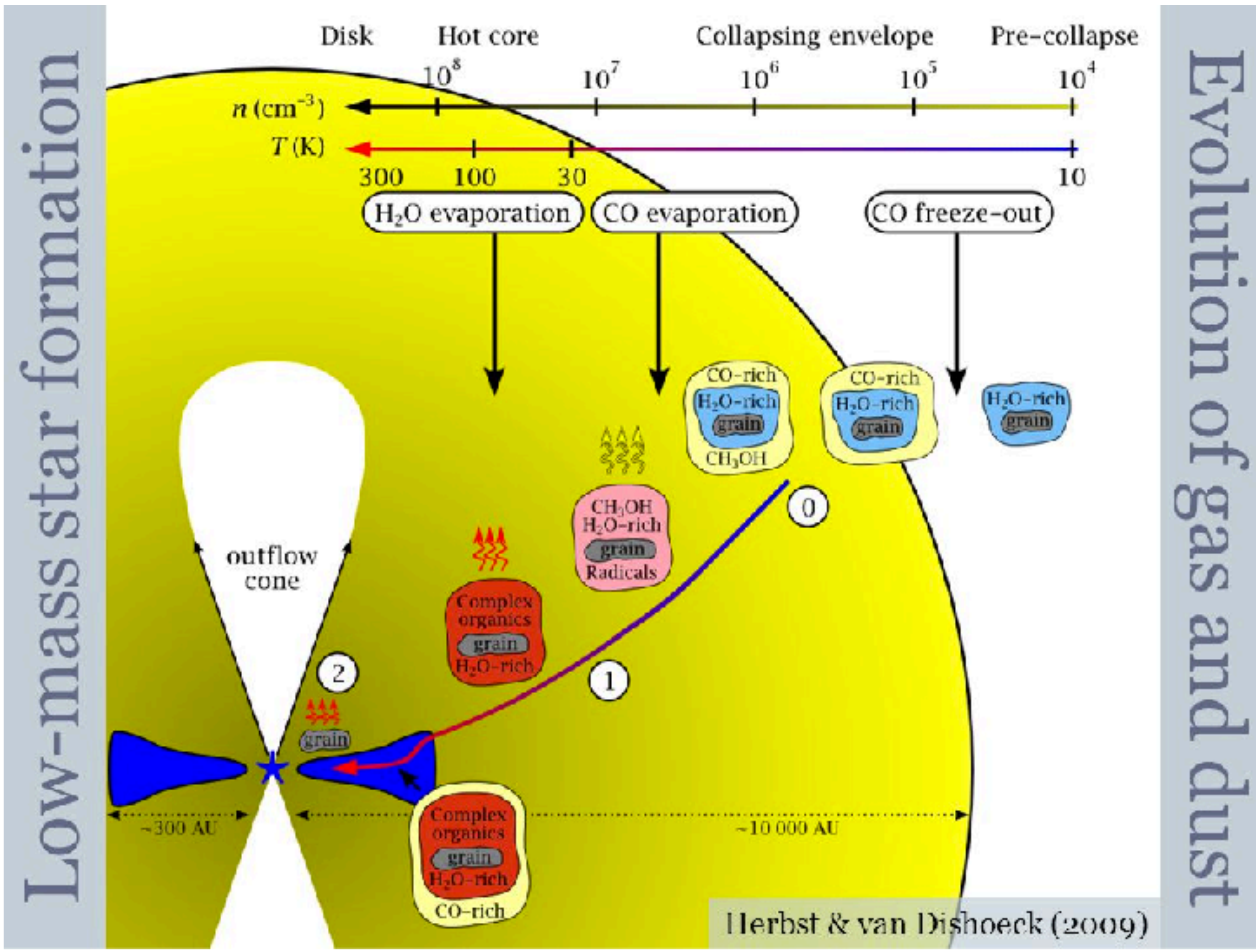
- **Embedded YSO phase**: T≈10-300 K, n≈10^5-10^9 cm^{-3}
  - Gas and dust heated by accretion luminosity, UV + X-rays
  - young star; production more complex organics
  - Evaporation of molecules from grains: H_2O, CH_3OH, CH_4, complex organics?....
  - Sequence according to evaporation temperatures
  - Hot core chemistry: complex organics, HCN, ...
- **Bipolar outflows**: T≈200-2000 K, n=10^5-10^7 cm^{-3}
  - Interaction outflow with envelope => shocks
  - High-T chemistry: H_2O, ...
  - Return icy mantles to gas: H_2O, CH_3OH, CH_4, ...
  - Destroy grain cores: SiO, ...

Star formation



Hogerheijde 1998

Star formation



Cartoon by Ruud Visser

Star formation

- High mass (>8 Msol) vs low mass stars:
  distance (observable scales), time scales, radiation fields
- Angular sizes:
  - clouds and molecular outflows: ~arcminutes => single dish maps
  - cores, high mass, outflow walls ~ few arc seconds => interferometry
- Densities: 10^4 to 10^{13} cm^{-3}
- Temperatures: 10-10 000 K
- Changing radiation fields (UV, X-rays, cosmic rays) and densities:
  history of chemistry visible (ice/evaporation!)
- Molecular outflows: shocks
- Dynamical evolution

Observations

Linear Size	Angular	size
	Taurus 140 pc	Orion 450 pc
5 AU Inner disk	0.04”	0.01”
100 AU Outer disk	0.7”	0.2”
1000 AU YSO envelope	7”	2”
10000 AU=0.05 pc Cloud core	74”	23”

Observations

- **(Sub)millimeter emission (0.4-3 mm, 100-800 GHz)**
  - rotational lines and cold dust continuum
  - very high spectral resolution ($R \sim 10^6$, <0.1 km/s)
  - many gas-phase molecule abundances down to 10^{-13}
  - emission: maps
  - single dish: APEX, JCMT, IRAM: >10”
  - interferometry: ALMA, SMA, PdBI: <0.1”
- **Infrared emission (3-200 micron)**
  - gas rovibrational lines, ice vibrational lines
  - moderate spectral resolution ($R \sim 10^4$)
  - gases and solids with molecule abundances down to 10^{-8}
  - molecules without dipole moment (H_2, C_2H_2, CH_4, CO_2)
  - mostly absorption (pencil beam line-of-sight), some emission: pencil
  - single dish: VLT, Keck, UKIRT, IRTF, ISO, Spitzer, Herschel, JWST: ~arcseconds-arcminutes

Importance astrochemistry

- Densities
- Abundance ratios: formation/destruction history
- Gas-grain chemistry: H_2 and ices (freeze-out, chemistry and evaporation)
- Shocks: change in chemistry
- Ionization fraction:
  coupling to magnetic fields: ability to collapse and form stars

see also van Dishoeck & Blake 1998

Importance astrochemistry

- Coupling physics and chemistry in hydro simulations:
  - chemistry ~ cooling rates
  - dynamical time scales ~ chemical time scales
- Molecules as velocity tracers using the line profiles (e.g. infall, outflows):
  - optical depth
  - critical density
  - constant abundance throughout

Diffuse clouds

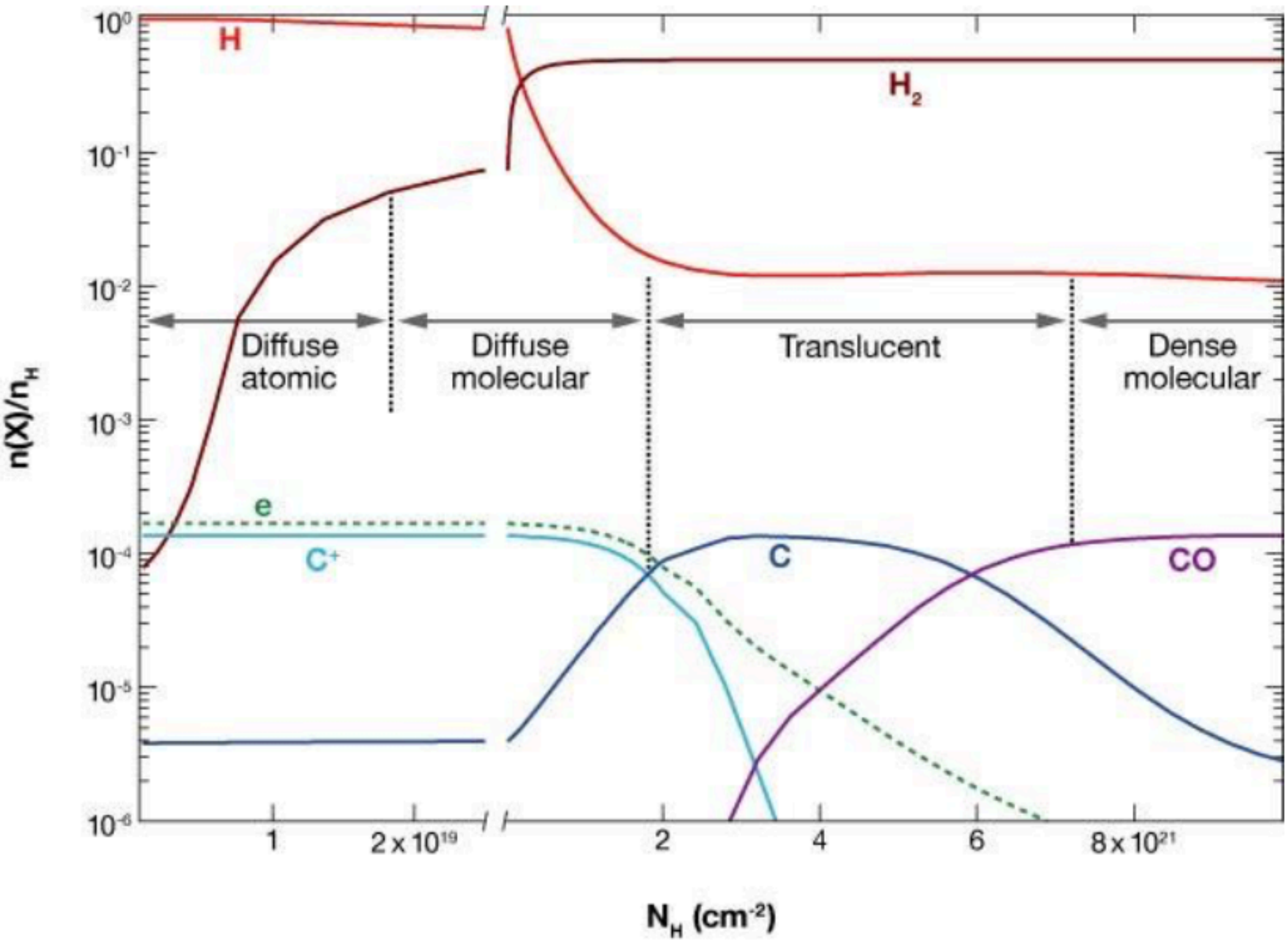
- Diffuse clouds: n~100-500 cm$^{-3,}$ T~25-100 K (edge-center), A_V ~ 1 mag
(before collapse or star formation!)
- Basic interstellar chemistry:
  - mostly simple diatomic molecules (e.g. H_2, HD, CH, CH^+, C_2, OH, OH^+, NH, CN, CS, HCl): gas-grain chemistry not so important and quick photodissociation by ISRF
  - optically thin: gas-phase abundances directly measured
  - UV-penetration: short timescales => chemical equilibrium

e.g. Kramers & ter Haar (1946)
Crawford & Williams 1997
Hogerheijde et al. 1995
Snow et al. 2000

Diffuse clouds

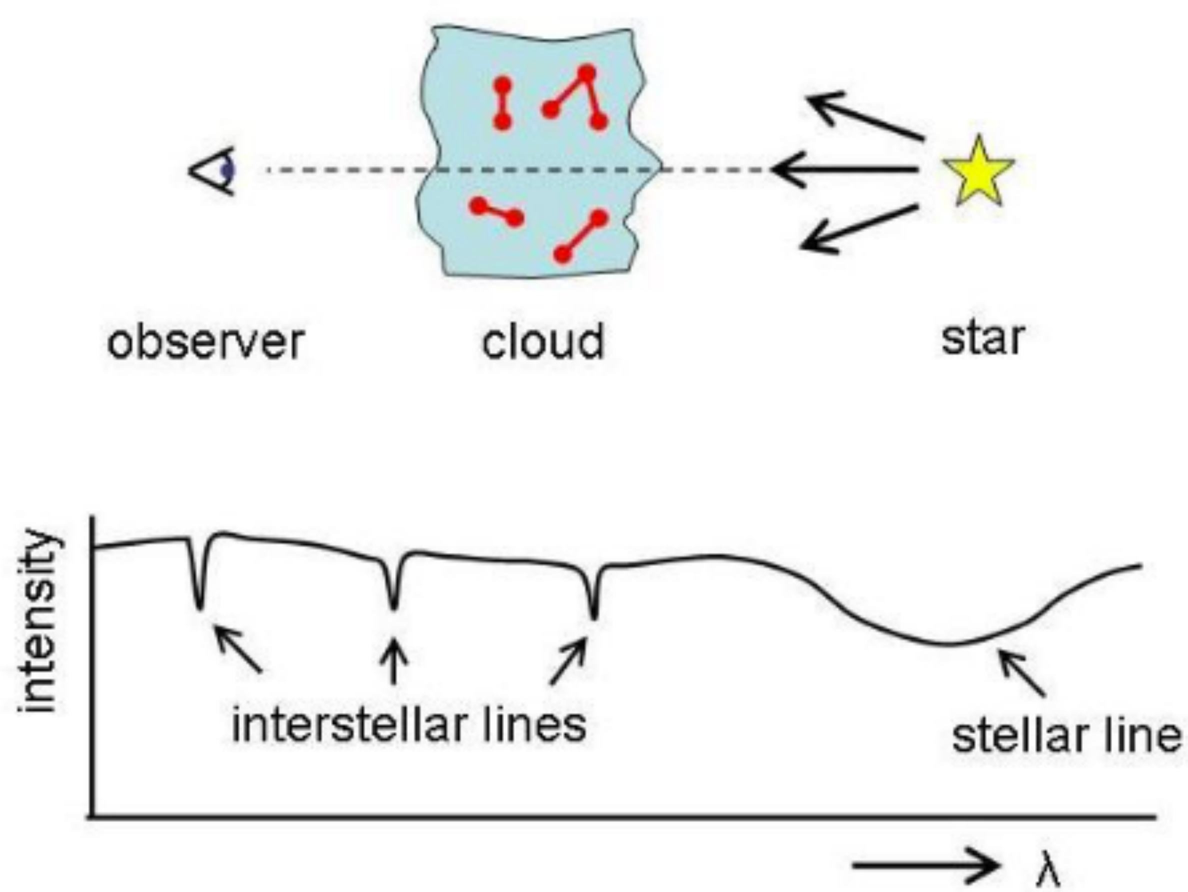
- Translucent clouds are ~10x denser and colder: ice chemistry starts to play a role
- Diffuse/translucent clouds are examples of PDRs: photon-dominated regions => UV photons control physical and chemical state of the cloud
  - strong atomic lines ([CII], [CI],[OI]) high-J sub-mm lines (CO 7-6, HCO^+ 4-3), NIR/MIR H_2
  - traditional PDR: dense clouds close to OB star: UV field 10^5xISRF (interstellar radiation field). Also PDR conditions in upper layers protoplanetary disks (Lecture 3)

Diffuse clouds



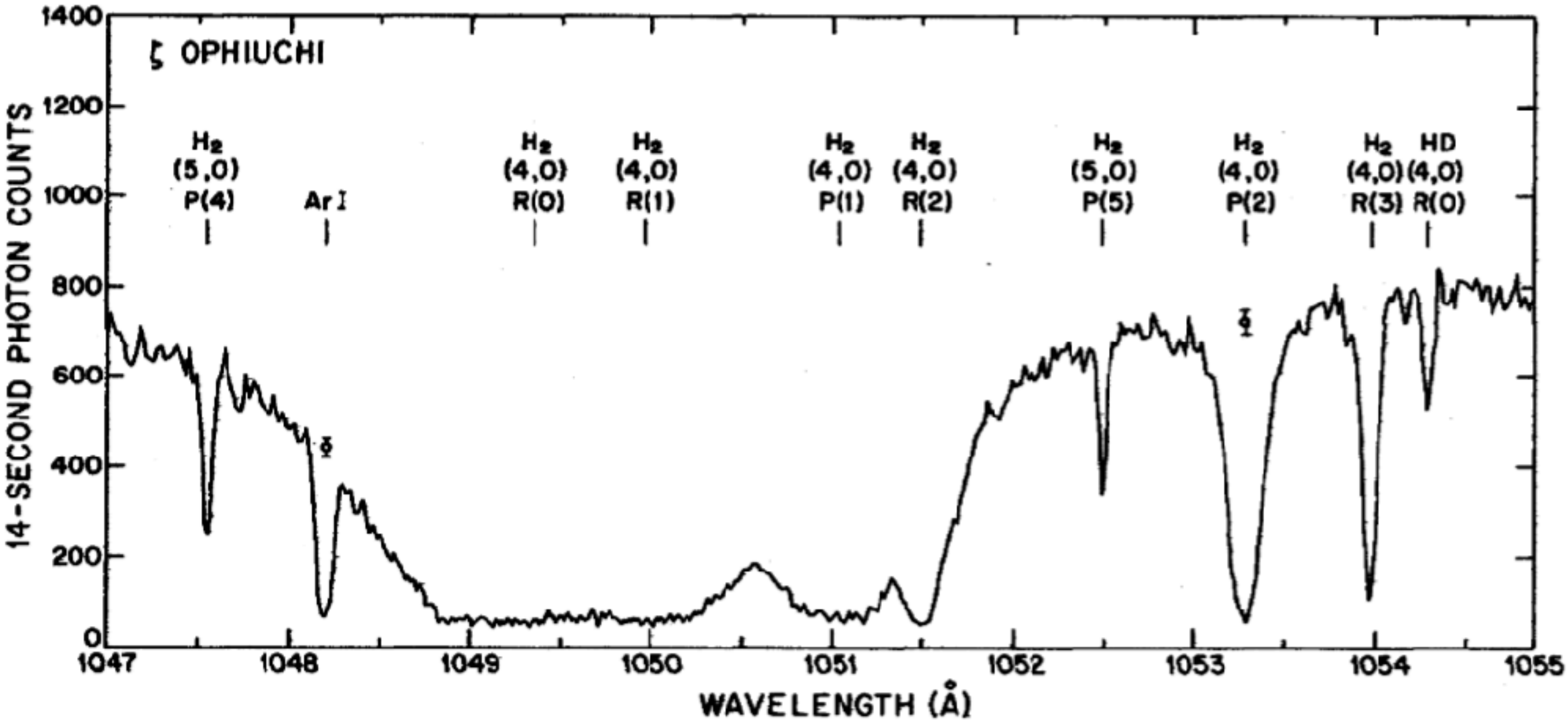
Diffuse clouds

- Observations primarily in absorption in visible/UV

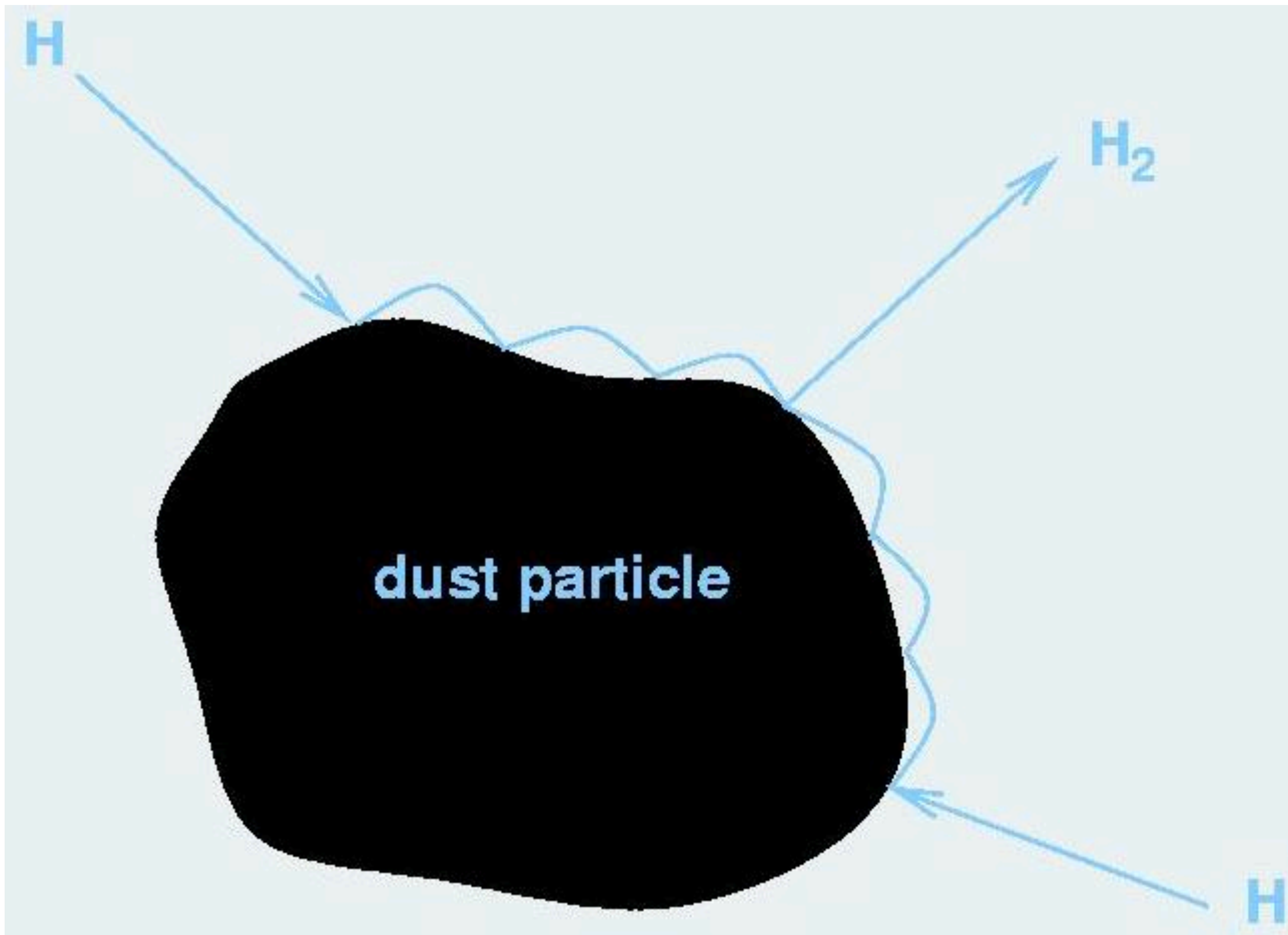


Diffuse clouds

- Example: observation H_2



H_2 formation



H_2 formation

- ***Diffusive mechanism*** (Langmuir-Hinshelwood)
  - $X + g{:}Y \rightarrow X{:}g{:}Y \rightarrow X\text{-}Y{:}g \rightarrow XY + g$

    sticking — diffusion + molecule formation — desorption

- ***Direct mechanism*** (Eley-Rideal)
  - $X + Y{:}g \rightarrow X\text{-}Y{:}g \rightarrow XY + g$

    direct reaction — desorption

H_2 formation (LH)

sticking	sticking	diffusion + molecule formation	desorption

- X+Y+g => X+g:Y => Y:g:X => X-Y:g => XY+g
- Several steps: **(no strong H_2-grain bonds)**
    - 1. H atom must collide with grain: H + g
    - 2. Colliding atom must stick to surface: H + g => H : g
    - 3. H atom must be retained until another atom gets absorbed: H:g => H:g:H
    - 4. H atoms must be mobile to find each other and form bond: H:g:H => H–H:g
    - 5. H_2 must be ejected from surface: H–H:g => H_2+g

H_2 formation (LH)

- Adsorption time t_a most important: first H-atom should stay around long enough for second H-atom to arrive:
  $t_a \sim \exp(-E_d/kT)$

- Physical adsorption: $E_d \sim 400$ K

  - $t_a \sim 10^5$ s at T~10 K

  - $t_a \sim 10^{-8}$ s at T~40 K => so need an alternative, e.g. chemical binding site at higher temperatures (such as diffuse clouds)

- Chemisorption: $E_d \sim 20\,000$ K => t_a becomes infinite

H_2 formation (ER)

- Eley-Rideal: direct reaction => no diffusion on surface
- If there are enough chemisorption sites so that the grain is saturated with H atoms, formation rate H_2 is controlled by arrival rate H atoms
- Important at high T

Self-shielding

- Photodissociation efficiently destroys H_2 and CO (second most abundant molecule: 10^{-4} w.r.t. H_2) in diffuse clouds. However, abundances are found to be large: why?
    - Photodissociation only through discrete absorption lines, so if the column is high enough it becomes optically thick to its own emission *=> self-shielding*
    - Dust shielding also prevents some photodissociation
    - What about deuterated hydrogen? (note $[D]/[H]=10^{-5}$)
      HD column too low for self-shielding => expect $HD/H_2 \sim 10^{-9}$
      => measured 10^{-6} => additional gas phase reactions:
        - $H^+ + D \Rightarrow H + D^+$
        - $D^+ + H_2 \Rightarrow H^+ + HD$

e.g. Draine & Bertoldi 1986
Bally & Langer 1982
van Dishoeck & Blake 1986,1988
Visser et al. 2009

Dark clouds and cores

- Dark clouds have A_V>5 mag, T≈10 K, $n_H \approx 10^4$-10^5 cm^{-3}: strongest lines at mm wavelengths (low-J)

- Ices are significant component!

  - In quiescent dark starless clouds, ices contain ~10- 50% of heavy elements

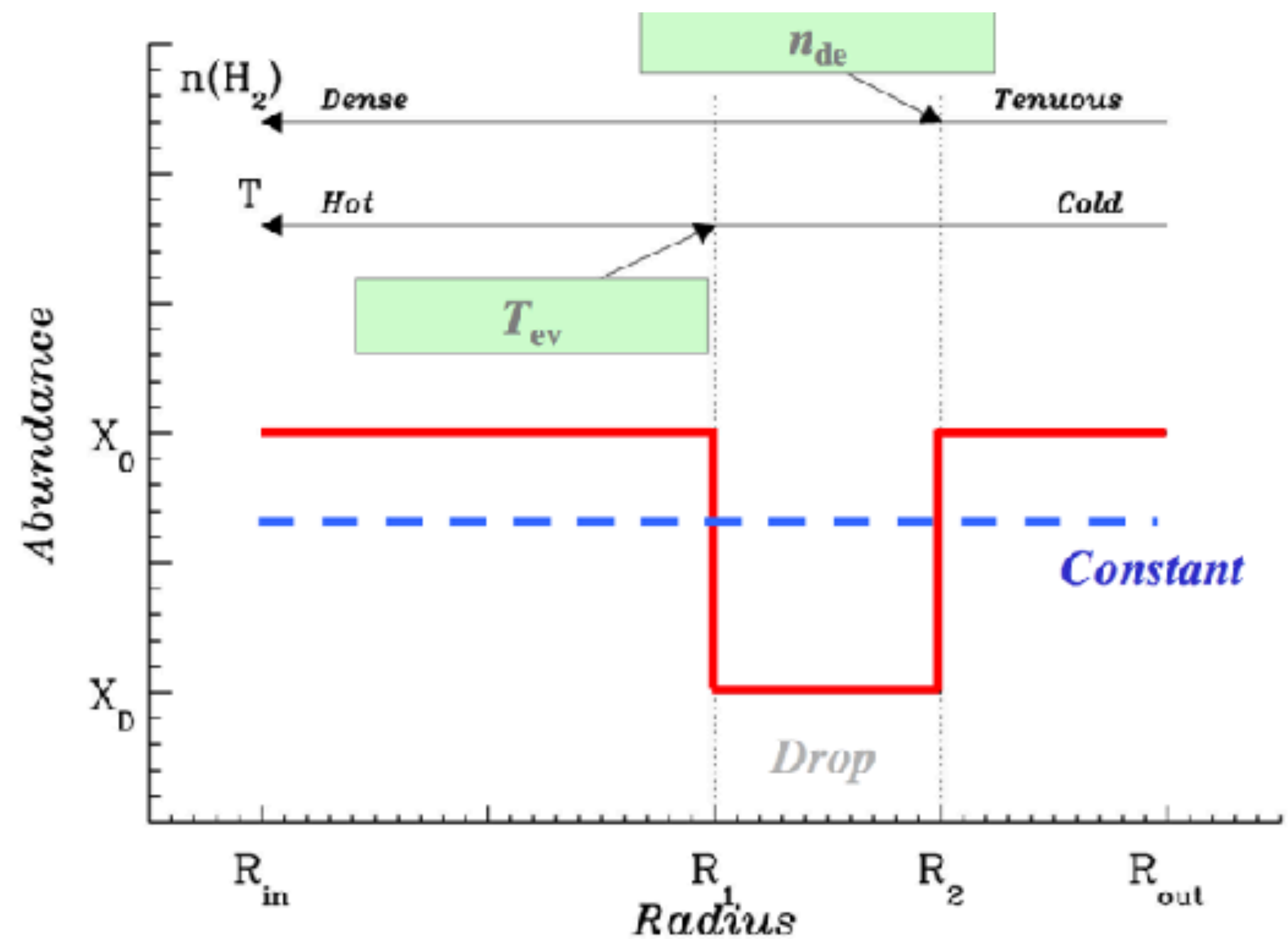
  - In the centers of pre-stellar cores with a central density concentration, up to 99% of the heavy elements may be frozen out

  - Gas-grain collisions (and chemistry) from $n > 10^4$ cm^{-3}

Dark clouds and cores

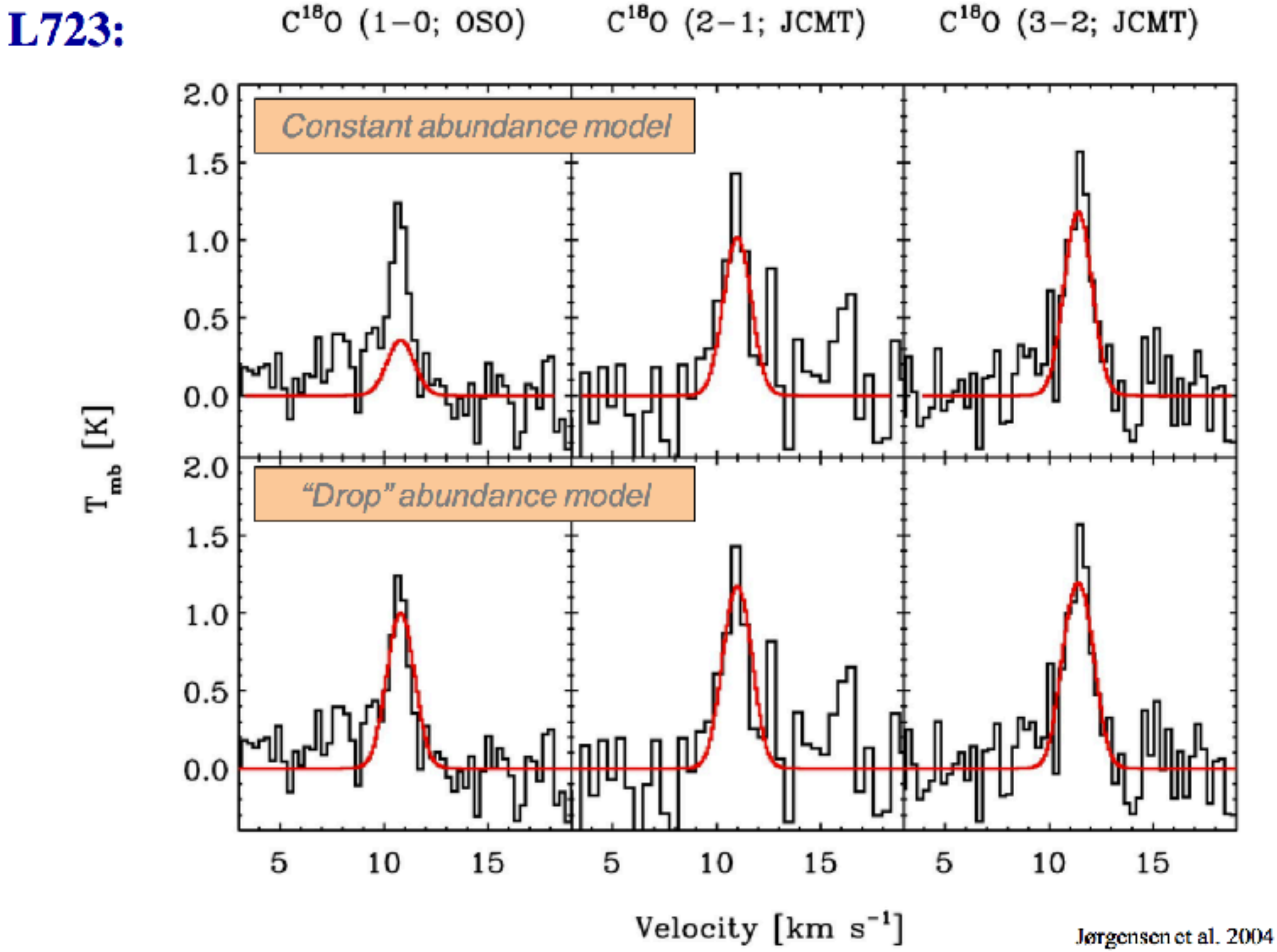
- Single dish observations of clouds often contain multiple components of a range of densities and temperatures

- Typical approach: derive abundances using a simple abundance profile and a radiative transfer code (e.g. constant or drop model)



Jorgensen et al. 2004

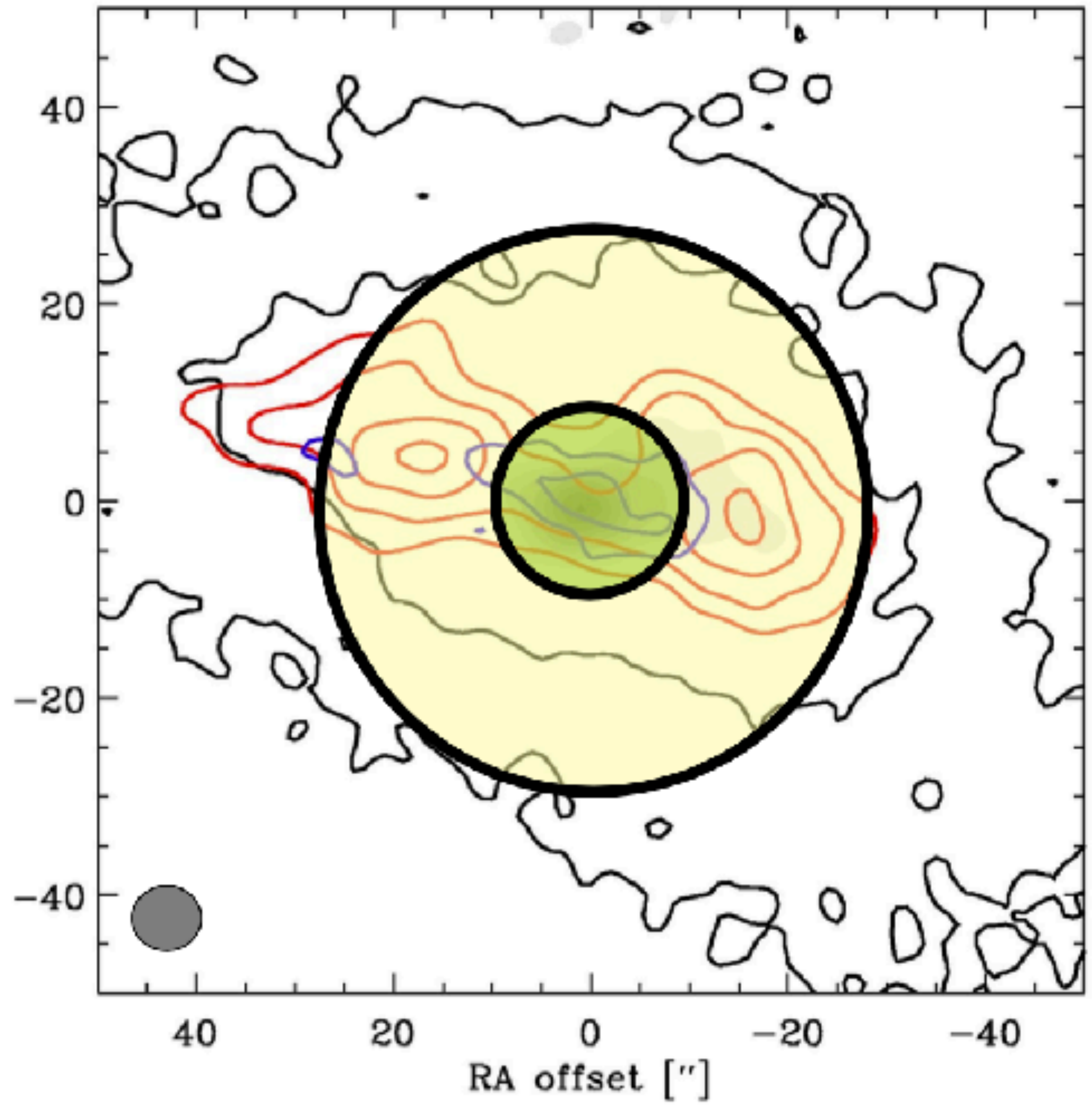
Dark clouds and cores



Jorgensen et al. 2004

Dark clouds and cores

- This particular structure was later confirmed by interferometry:
- **N_2H^+**
- **$C^{18}O$**



Jorgensen et al. 2004b

Dark clouds and cores

- Anticorrelation CO and N_2H^+: modeling
- N_2H^+ can only survive when the CO is frozen out
- Formation:

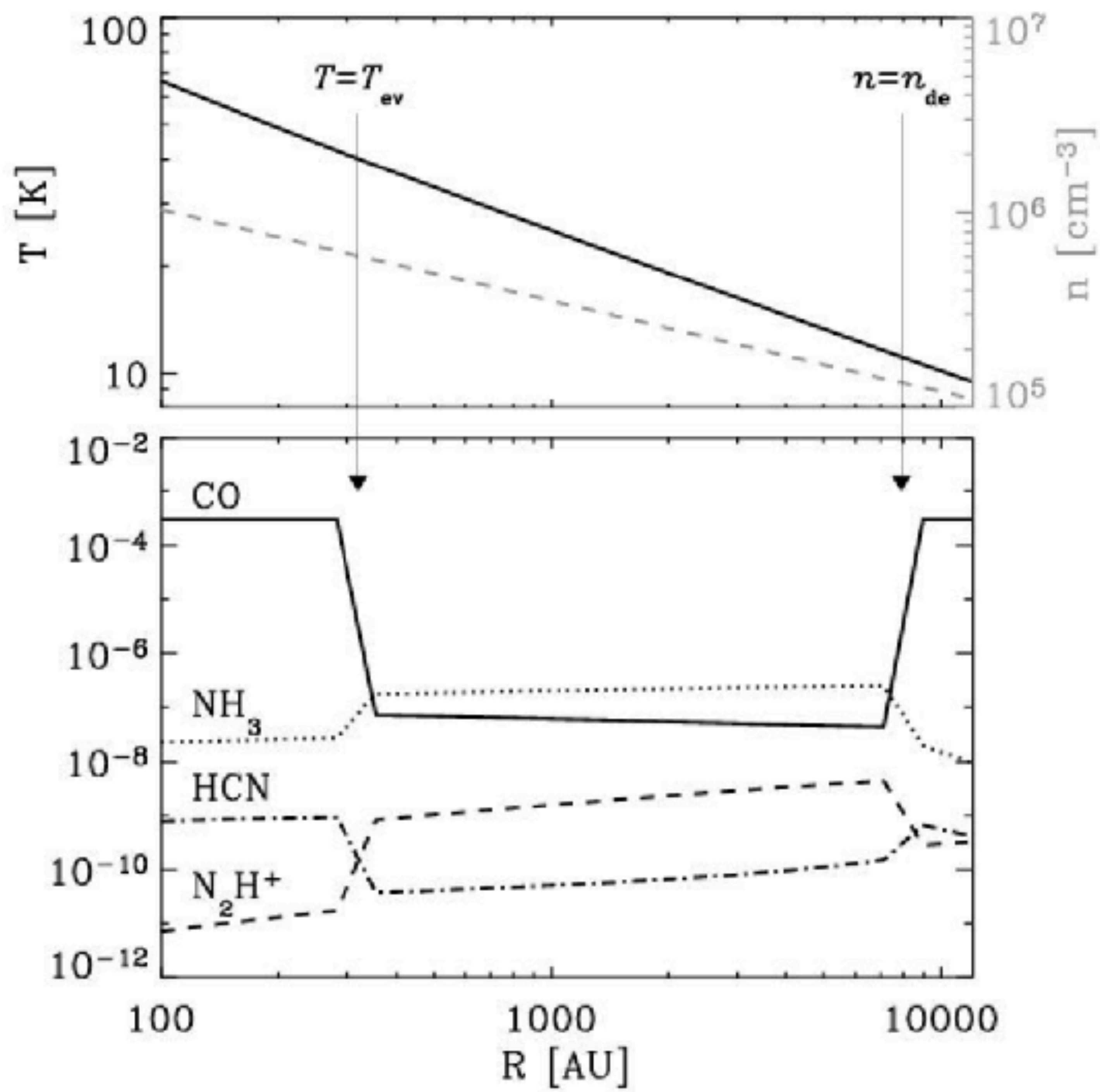
$$N_2 + H_3^+ \rightarrow N_2H^+ + H_2$$

- But

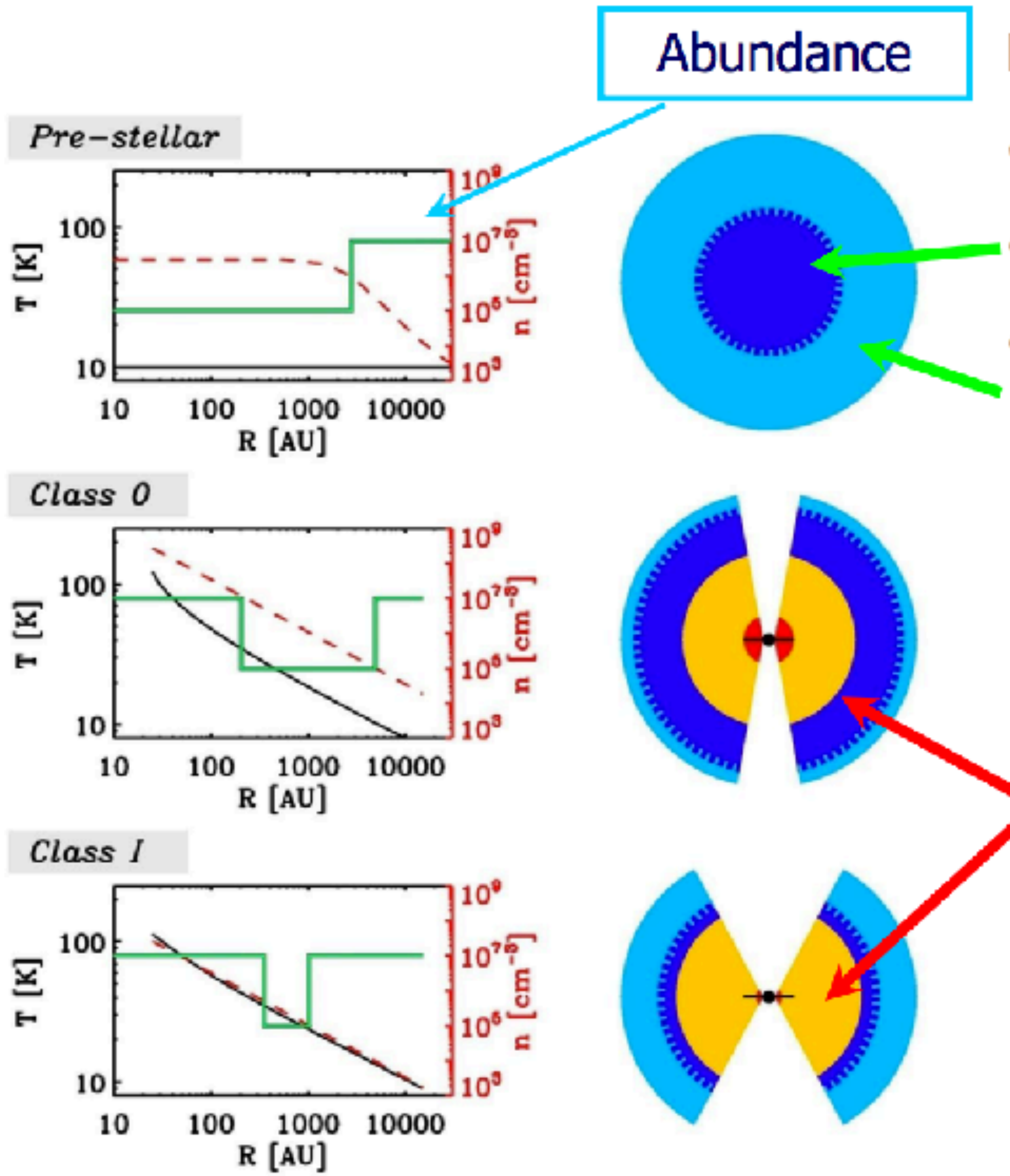
$$CO + H_3^+ \rightarrow HCO^+ + H_2$$

- and

$$N_2H^+ + CO \rightarrow HCO^+ + N_2$$



Dark clouds and cores



Pre-stellar core:

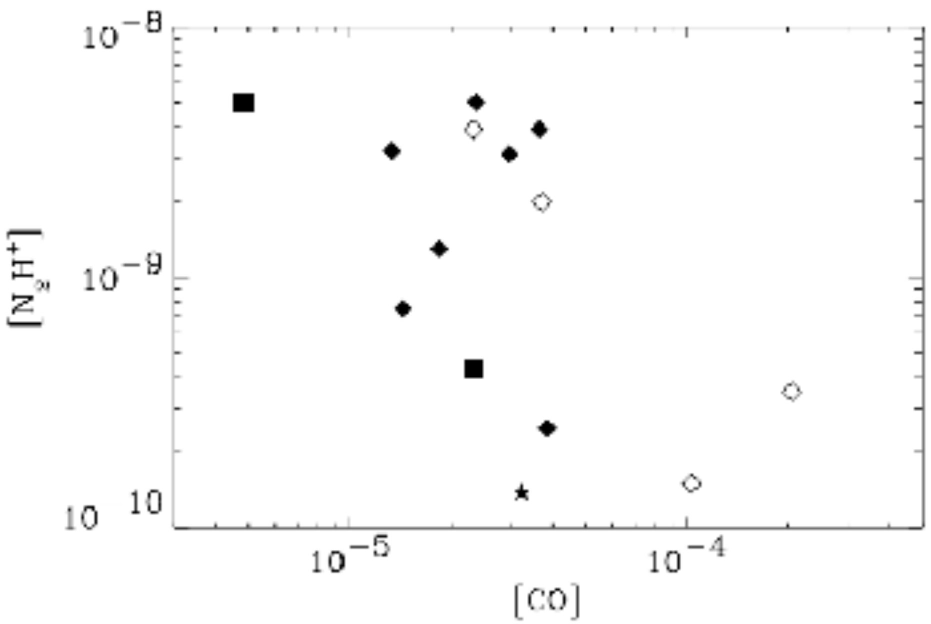
- Low temperature
- Depletion toward center
- …but not edge

Protostellar core:

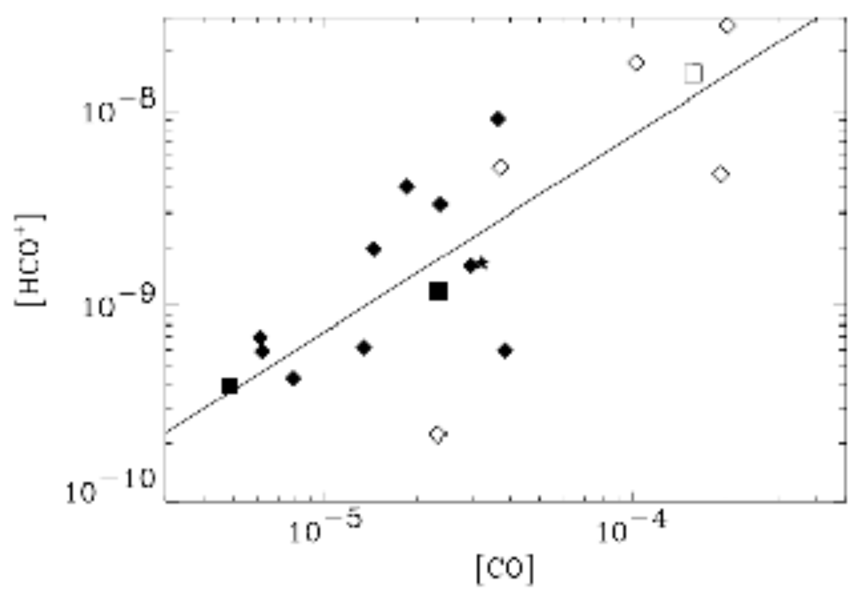
- Central heating ~ temperature gradient
- Thermal desorption toward center
- …outside (low T): depletion/no depletion regions as in pre-stellar stages

Dark clouds and cores

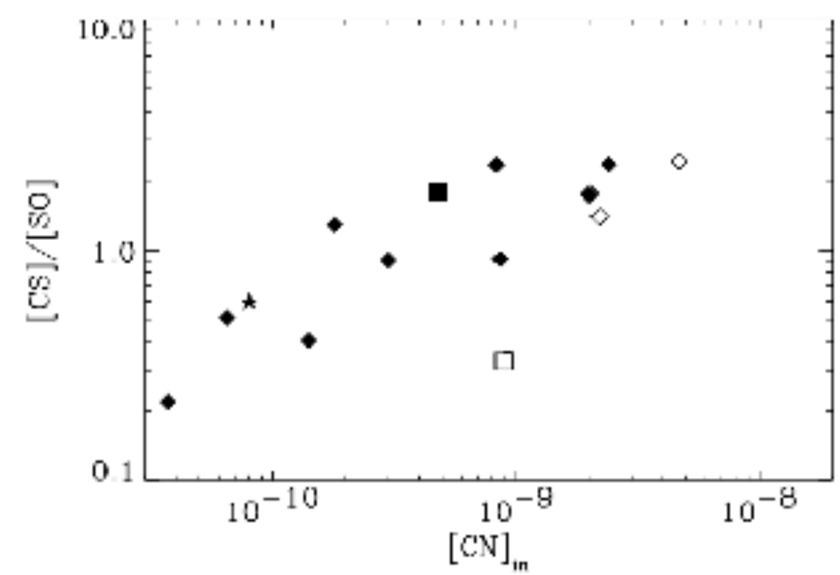
- Typical approach in understanding chemistry: search for correlations and find consistent reactions



anti correlation
CO and N_2H^+



correlation
CO and HCO^+

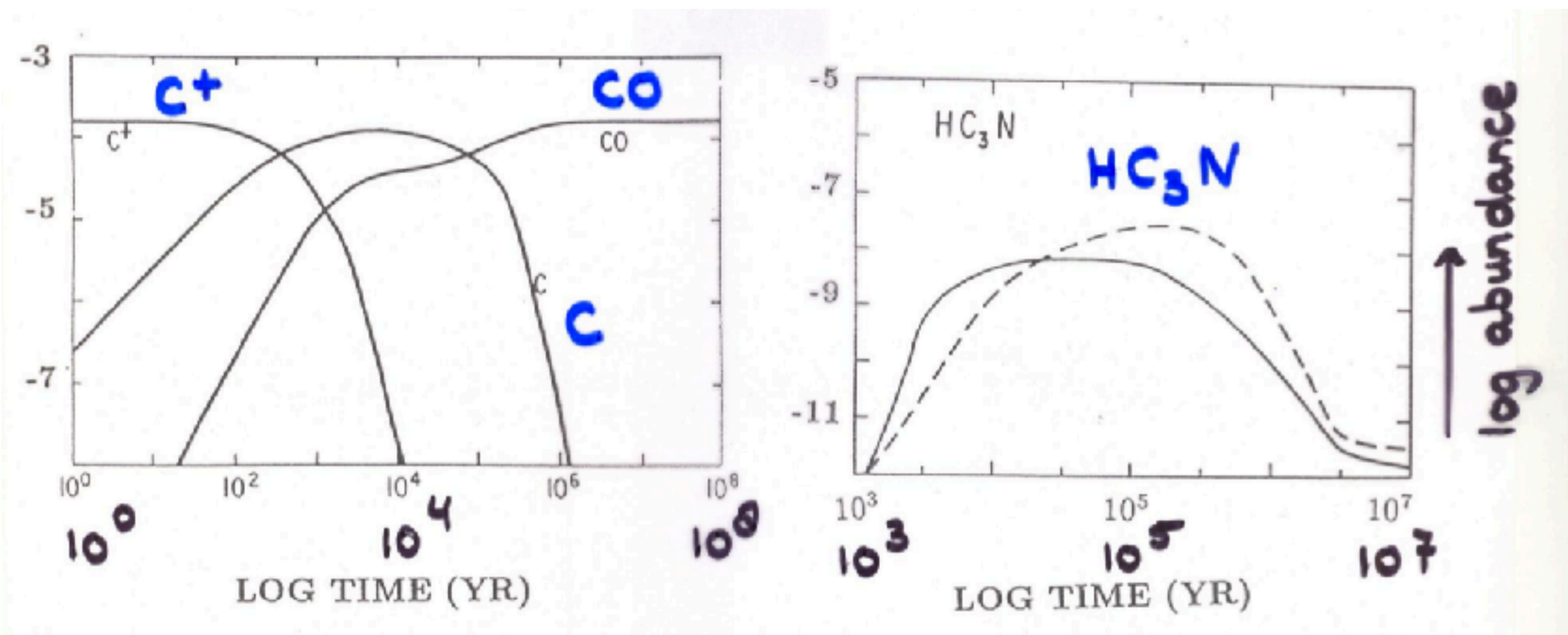


correlation
CS/SO and CN

Jorgensen et al. 2004

Dark clouds and cores

- Modeling approach:
  - Ignore depth dependence: solve chemical network for a given T and n at a single point with initial atomic abundances + H_2
  - pseudo-time-dependent: Solve chemical network as function of time for time-constant T and n at a single point

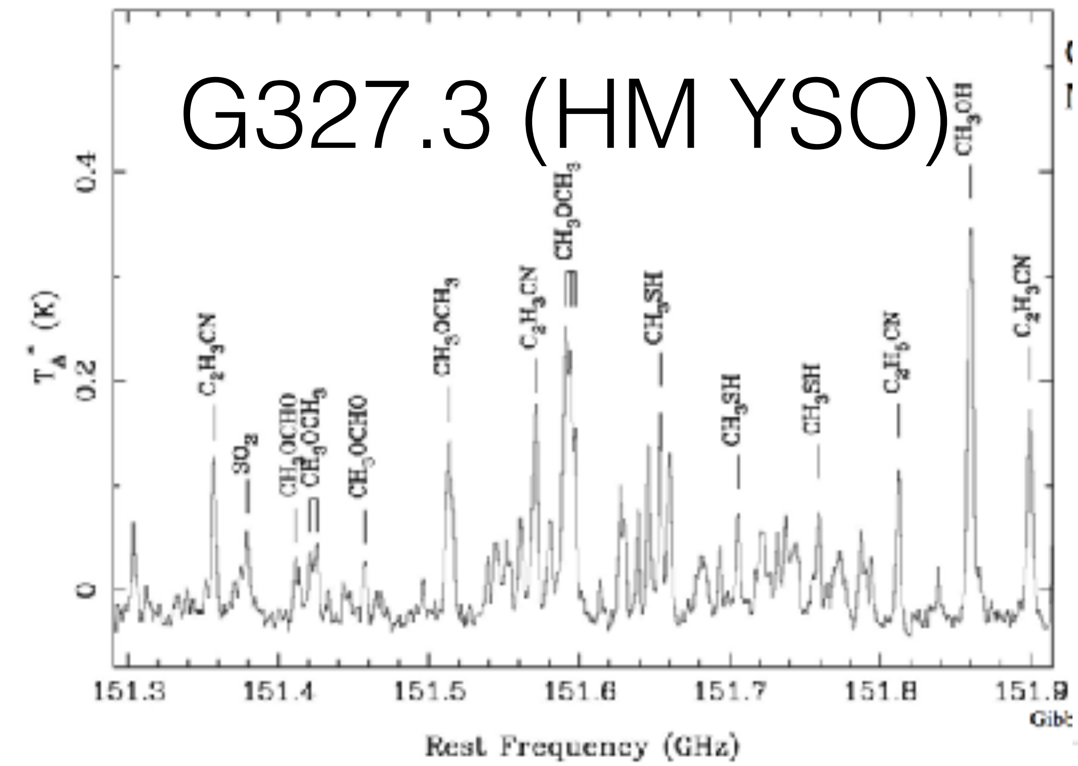


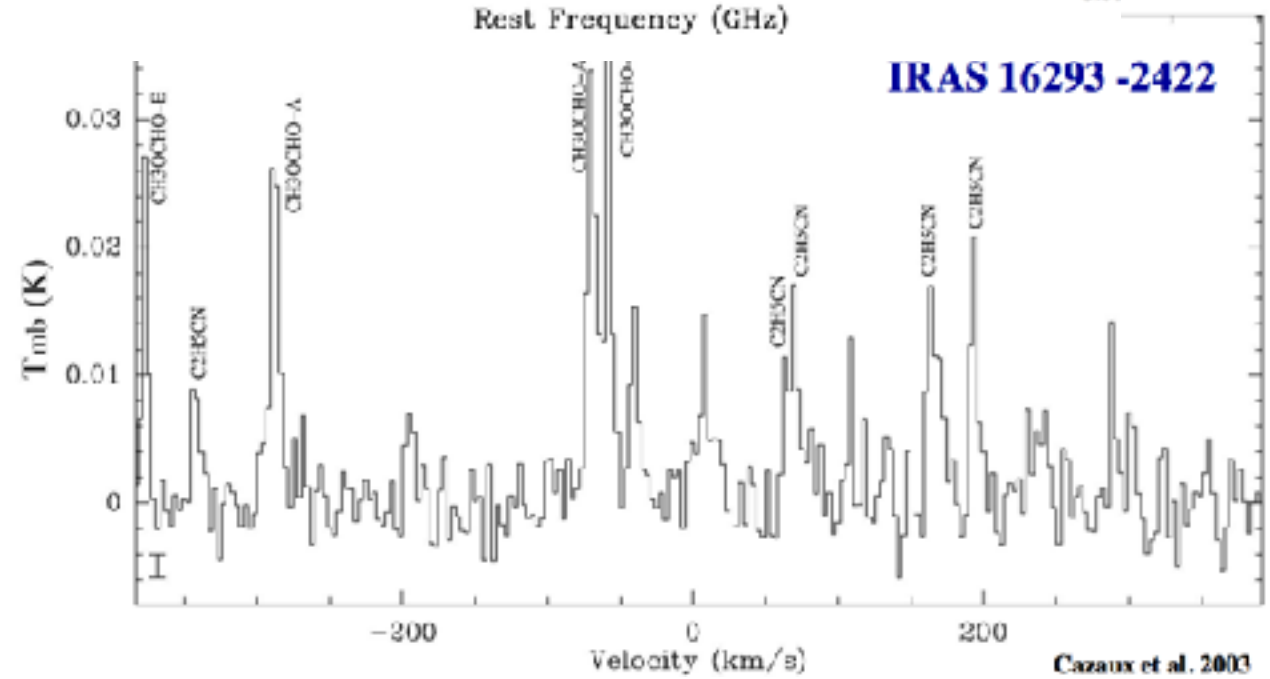
Dark clouds and core

- Adding more complexity (and computational time):
  - Dynamical models: n, T vary with time
    (collapse models)
    - Follow a parcel through evolution (e.g. Visser et al. 2009, Drozdovskaya et al. 2014)
  - Depth-dependent models: include e.g. photodissociation and shielding
  - Dynamical mixing models: parcels of gas cycle through dense and diffuse gas
  - Include gas-grain chemistry

Dark clouds and cores

- Hot cores show high abundances of COMs: T~100-200 K, n_H~10^7 cm^{-3}
- Historically for high mass YSOs (Orion, SgrB2, etc.), but in recent years also seen in low mass (sensitivity)
- Interpretation: evaporated molecules from processed ice mantles => ice provides possibilities for rich chemistry
- More in Lecture 4!



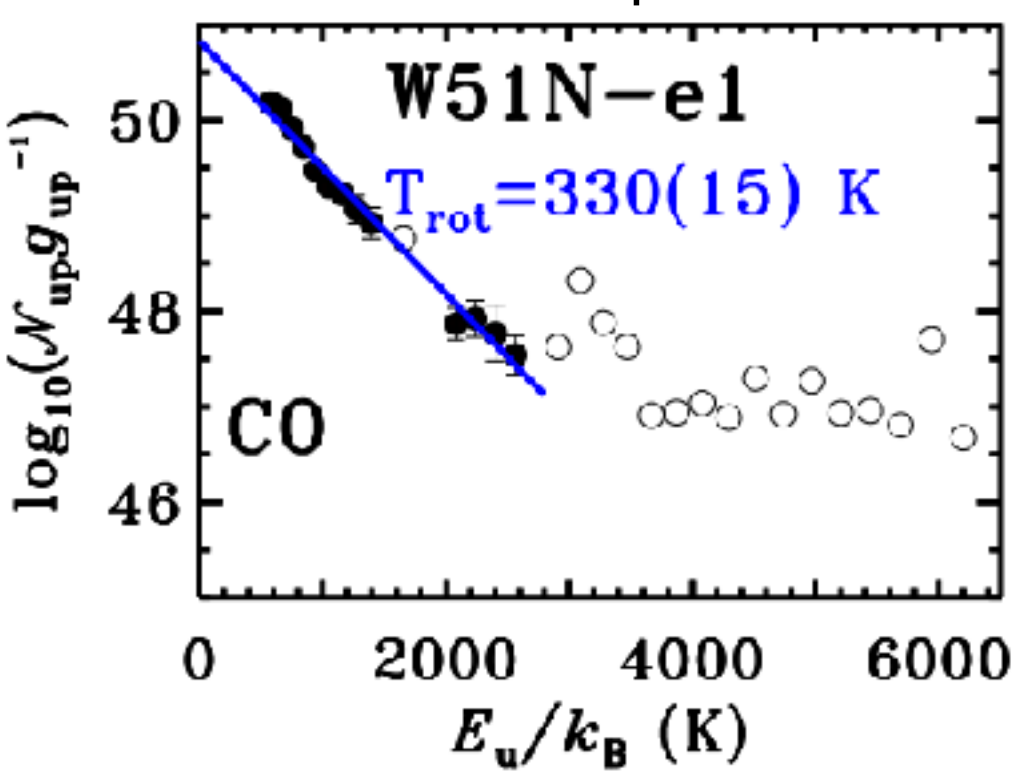


Gibb et al. 2000, Cazauz et al. 2003

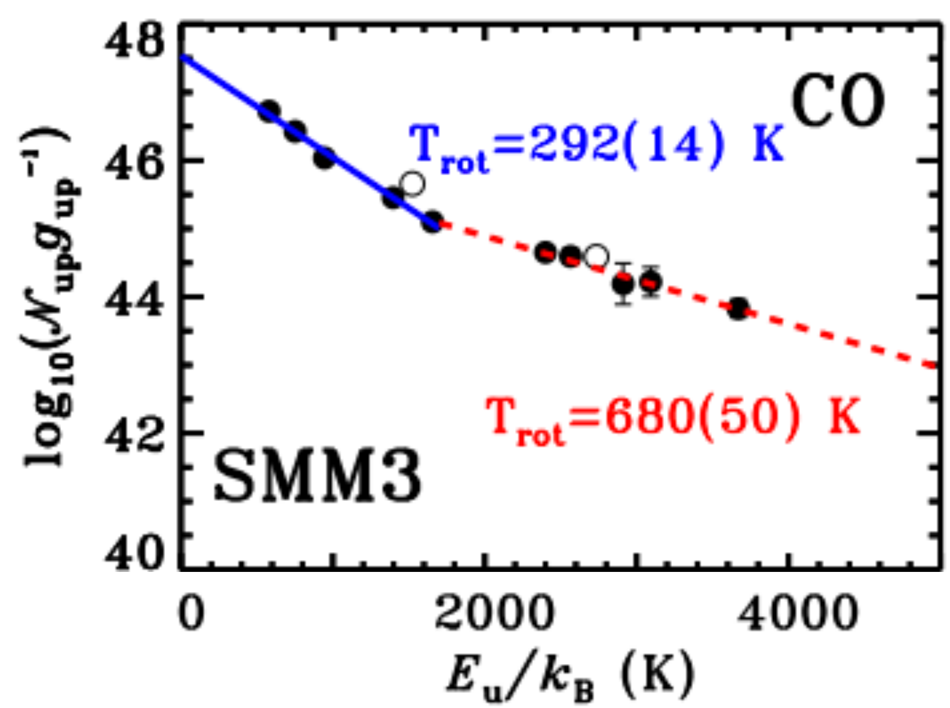
Dark clouds and cores

- Deriving column density and temperature for a gas-phase object (e.g. cloud or envelope)
  => rotational diagram

one component



two components:
warm and hot (shock?)



Karska et al. 2013, 2014

Dark clouds and cores

- Where does the linear relation originate?
  - In LTE: $N_u = \frac{N}{Q(T)} g_u \, e^{-E_u/kT}$

Q(T)=partition function

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N}{Q(T)}\right) - \frac{E_u}{kT} = -\frac{1}{T}\frac{E_u[\mathrm{erg}]}{k} + ln\left(\frac{N}{Q(T)}\right)$$

$$\underbrace{\ln\left(\frac{N_u}{g_u}\right)}_{y} = \underbrace{-\frac{1}{T}}_{a} \underbrace{E_u[\mathrm{K}]}_{x} + \underbrace{\ln\left(\frac{N}{Q(T)}\right)}_{b}$$

$$N_u = \frac{8\pi k \nu^2 \int T_{\mathrm{mb}} \mathrm{dv}}{hc^3 A_{ul}}$$

Dark clouds and cores

- Define antenna temperature T_A: $T_A(\nu) \equiv \frac{I_\nu}{2\nu^2 k c^{-2}} = \frac{I_\nu \lambda^2}{2k}$

  - In optically thin case and LTE, $I_\nu = B_\nu(T)\,\tau$

$$\Rightarrow T_A = \frac{\lambda^2 I_\nu}{2k} = \frac{\lambda^2}{2k} B_\nu \tau = \frac{\lambda^2}{2k} \frac{2h\nu^3/c^2}{e^{h\nu/kT}-1}\tau$$

$$\tau = \frac{N_u}{\Delta V}\frac{A_{ul}c^3}{8\pi\nu^3}\left(e^{h\nu/kT}-1\right) \rightarrow N_u = \frac{8\pi k\nu^2 \int T_{mb} dV}{hc^3 A_{ul}}$$

(optical depth gaussian line)

ΔV = FWHM of the line

$$\rightarrow \boxed{\frac{N_u}{g_u} = \beta \frac{(\nu[\mathrm{GHz}])^2 W\left[\mathrm{K\,km s^{-1}}\right]}{A_{ul} g_u}}$$

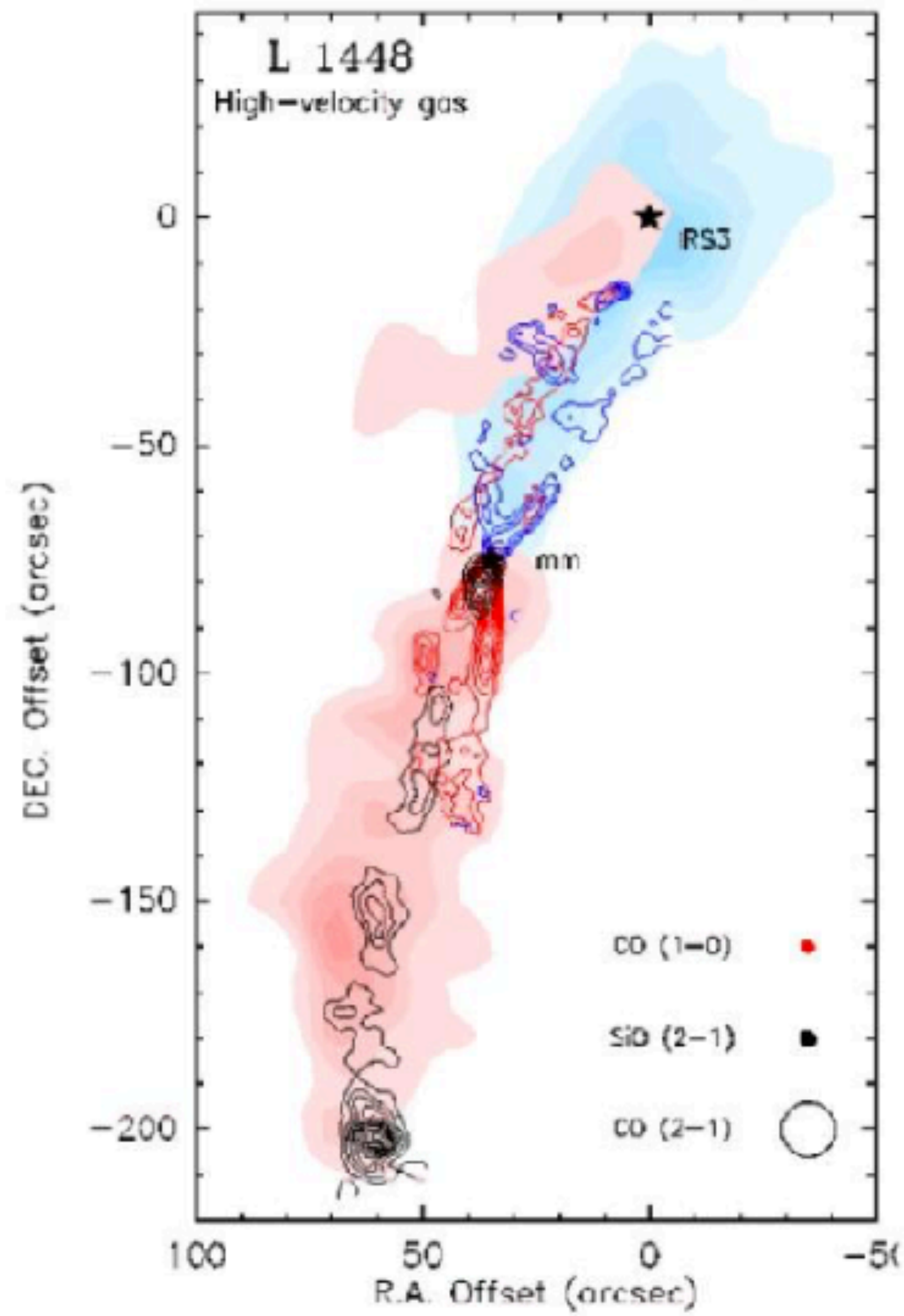
- $W = \int T_{mb} dv$ = integrated intensity
- β=constant~1937

Shocks

- A shock wave is a pressure-driven compressive disturbance propagating faster than sound speed: material cannot dynamically respond -> shock compresses, heats and accelerates material => heated material cools through line emission and compresses further
- Shock waves produce an irreversible change in the state of a fluid
- Shocks are ubiquitous in the interstellar medium
  - Expanding H II regions
  - Supernova explosions
  - Stellar winds
  - Bipolar outflows
  - Accretion processes
  - Cloud-cloud collisions

Shocks

- Molecular outflows:
  Class 0, Class I objects
- Large scale high-velocity gas (e.g. CO) in double cone-shape in the envelope
- Result of bipolar jet from protostar: removing angular momentum from cloud
- Shocked gas along outflow walls



Bachiller & Tafalla 1999

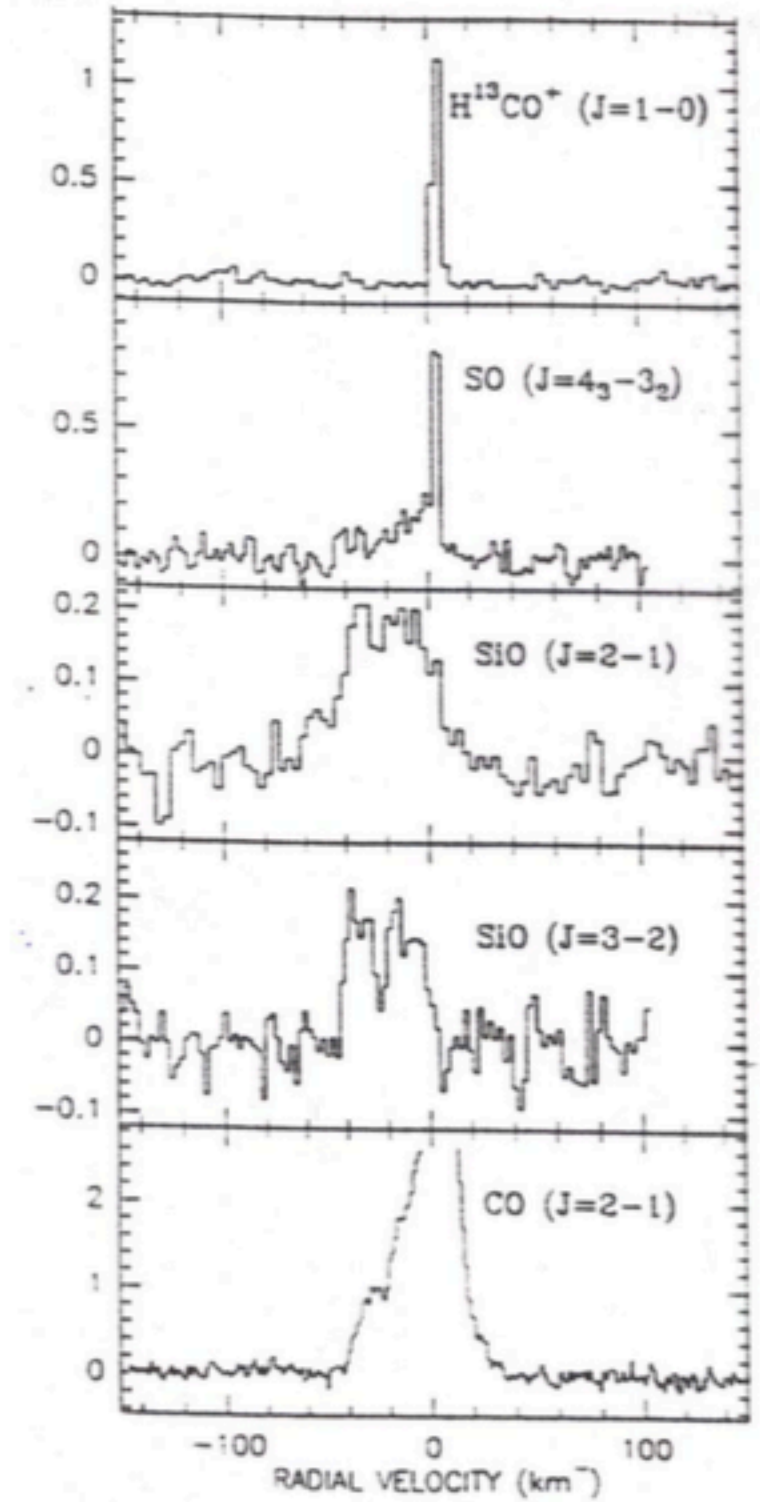
Shocks

- Two types:
- **J-type** (jump) shock: v>50 km/s
  - abrupt change
  - high temperature (T ~ 100 000 K)
  - molecular dissociation (followed by slow reformation)
  - production UV radiation: photodissociation molecules ahead of shock
  - thermal sputtering and destruction of grain cores: elementary Si and Fe
- **C-type** (continous) shock: v<50 km/s
  - continuous change of T, n
  - T ~ 2000-3000 K
  - too low for molecular dissociation, but increase in reactions with energy barriers (back reactions with H)
    - $O+H_2$ => OH => H_2O
    - $S+H_2$ => SH => H_2S
  - non-thermal sputtering of grain cores and ice mantles (but volatiles can survive for low speed)

Hollenbach et al. 1989

Shocks

SiO much broader than $H^{13}CO^+$

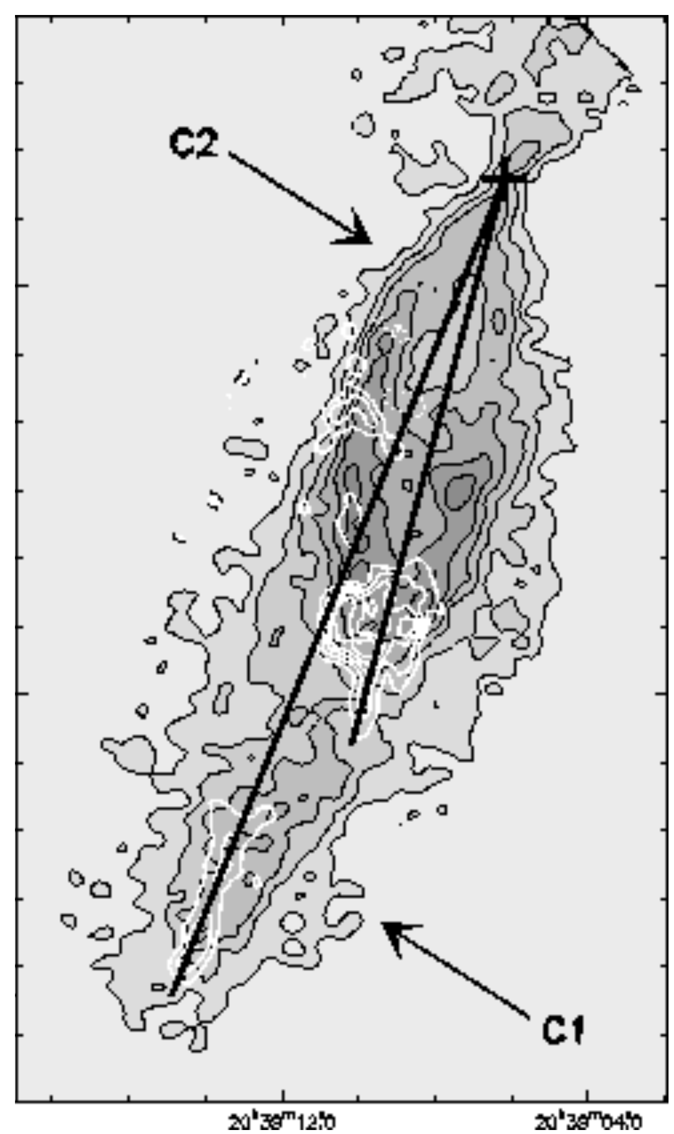


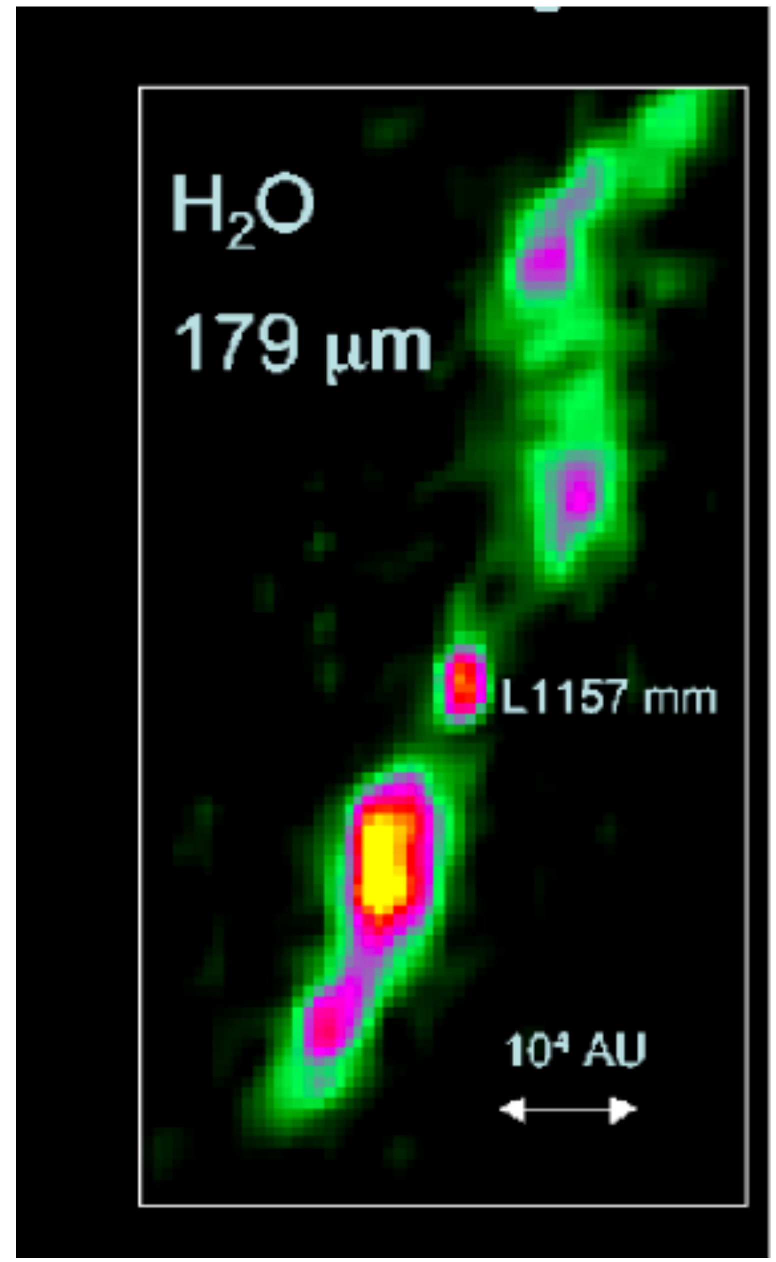
L1448

- Signatures of shocks:
  - SiO, Si, Fe
  - H_2O, OH
  - grain mantle products e.g. CH_3OH (C-type)

Shocks

L1157 outflow: *CO in grey, SiO in white contours*





Gueth et al. 1997
Nisini et al. 2010
Kristensen et al. 2010, 2011

Next week

- Protoplanetary disks
  - Disk structure
  - Disk processes
  - Inner disk vs outer disk
  - Observations
  - Modeling
  - Relation with comets