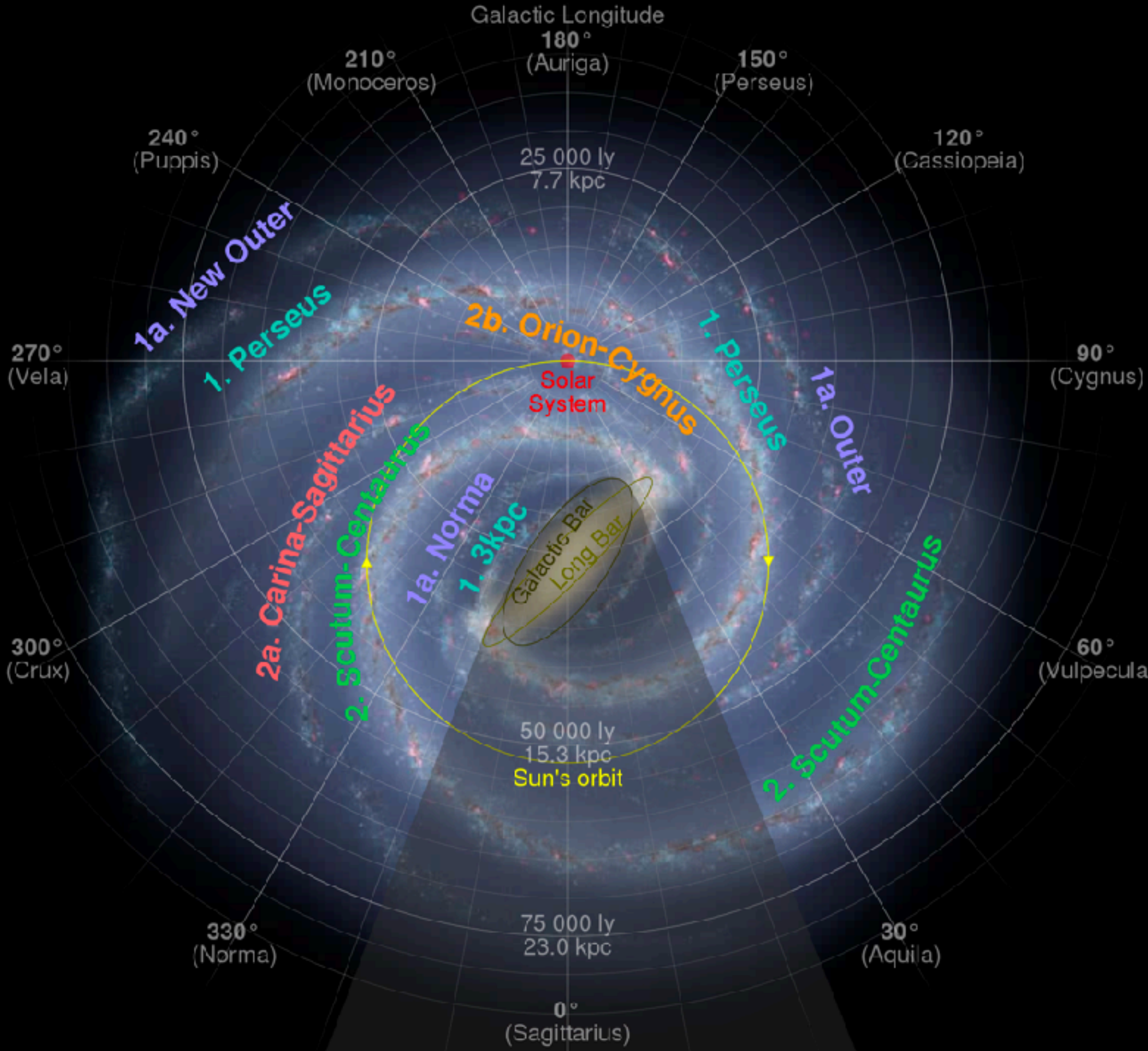
Lecture 8:

"Diffuse and dense interstellar medium”

Scheme of Milky Way

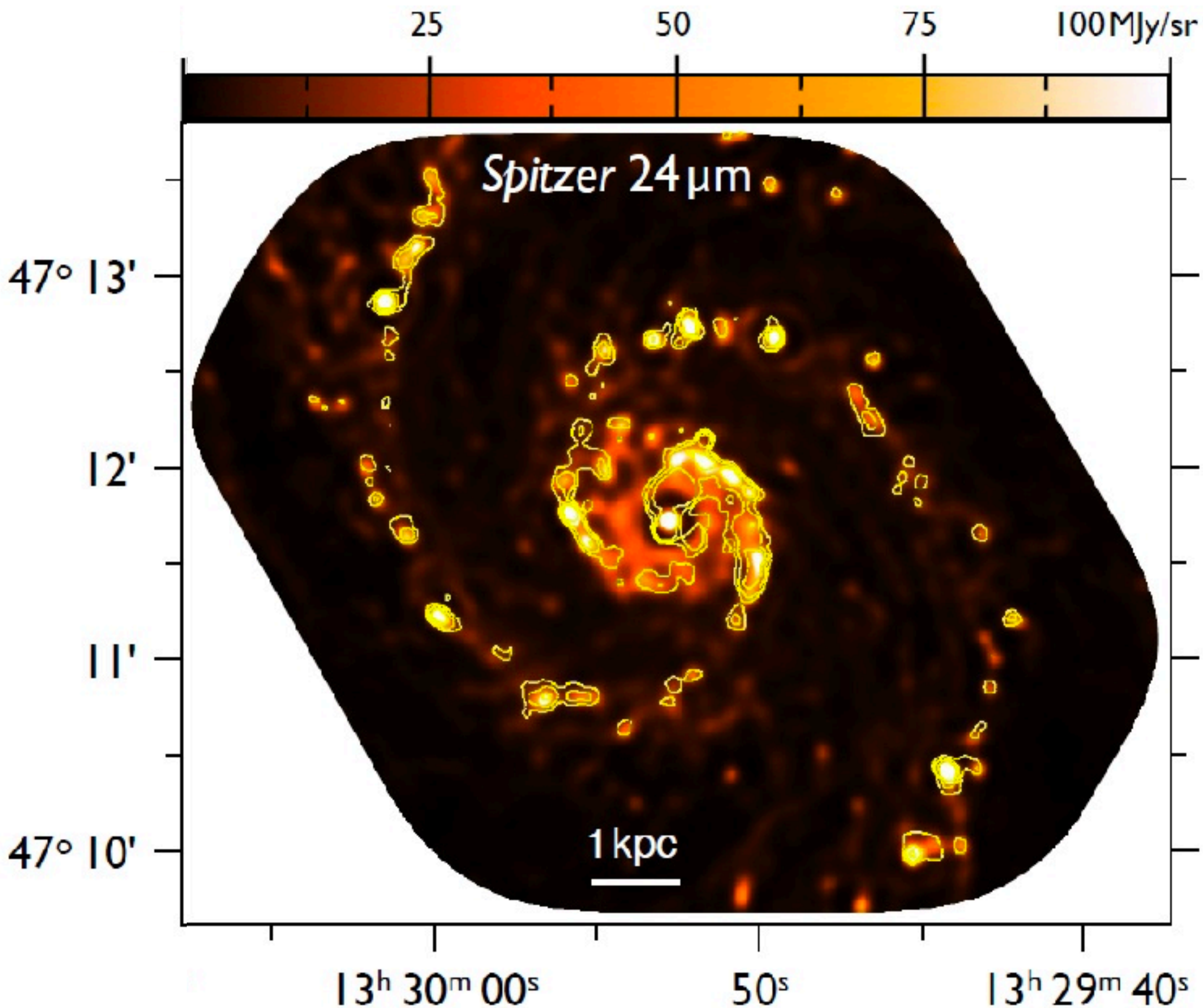


NASA

Galactic-scale picture: M51 (visible)

- Spiral arms: density waves, differential rotation, star formation
- Bright regions: excited diffuse gas, scattering of light by dust
- Dark regions: dense gas, absorption and reddening of light by dust

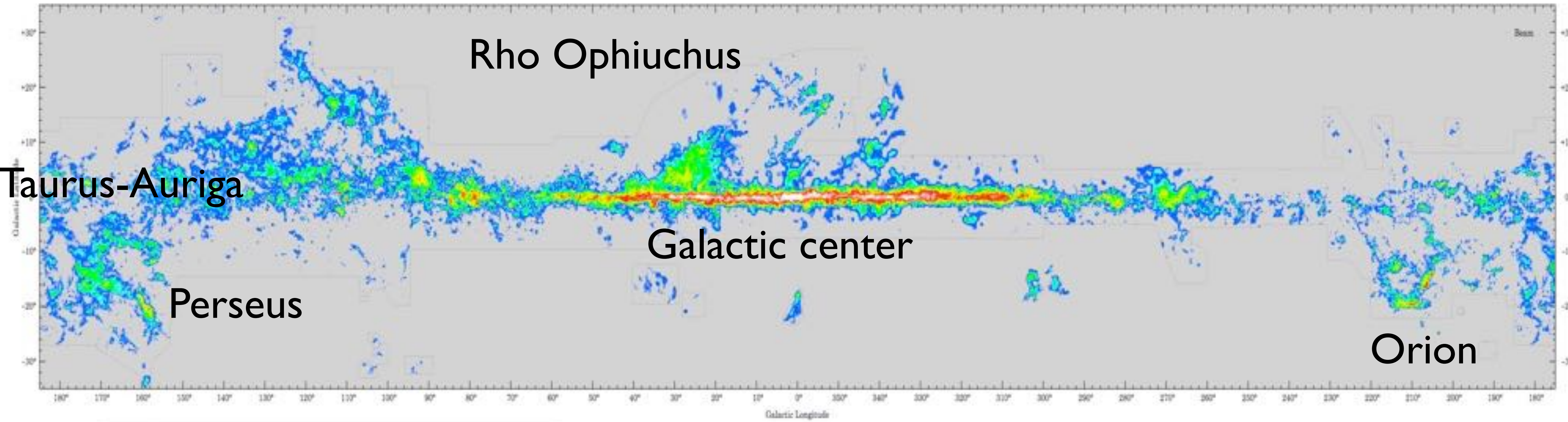
Galactic-scale picture: M51 (24μm)



Querejeta et al. (2019), A&A

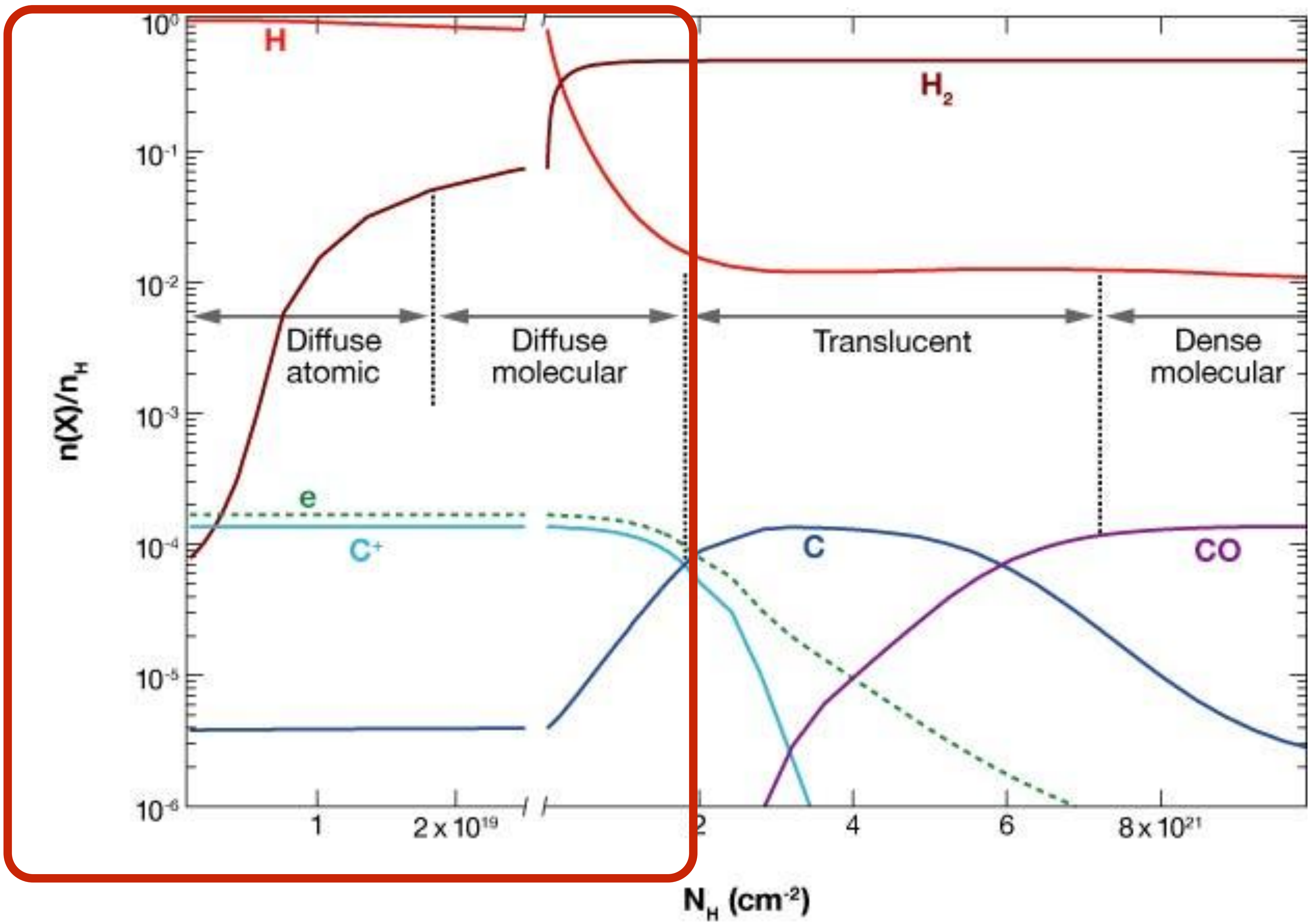
- Warm dust in spiral arms: tracer of star formation

Milky Way: CO (1-0) emission



- Giant Molecular Clouds: ~10^4 – 10^7 M_{sun}, ~10–200 pc
- Gravitationally bound, turbulent, filamentary
- Large-scale diffuse gas
- Small-scale dense clumps and cores

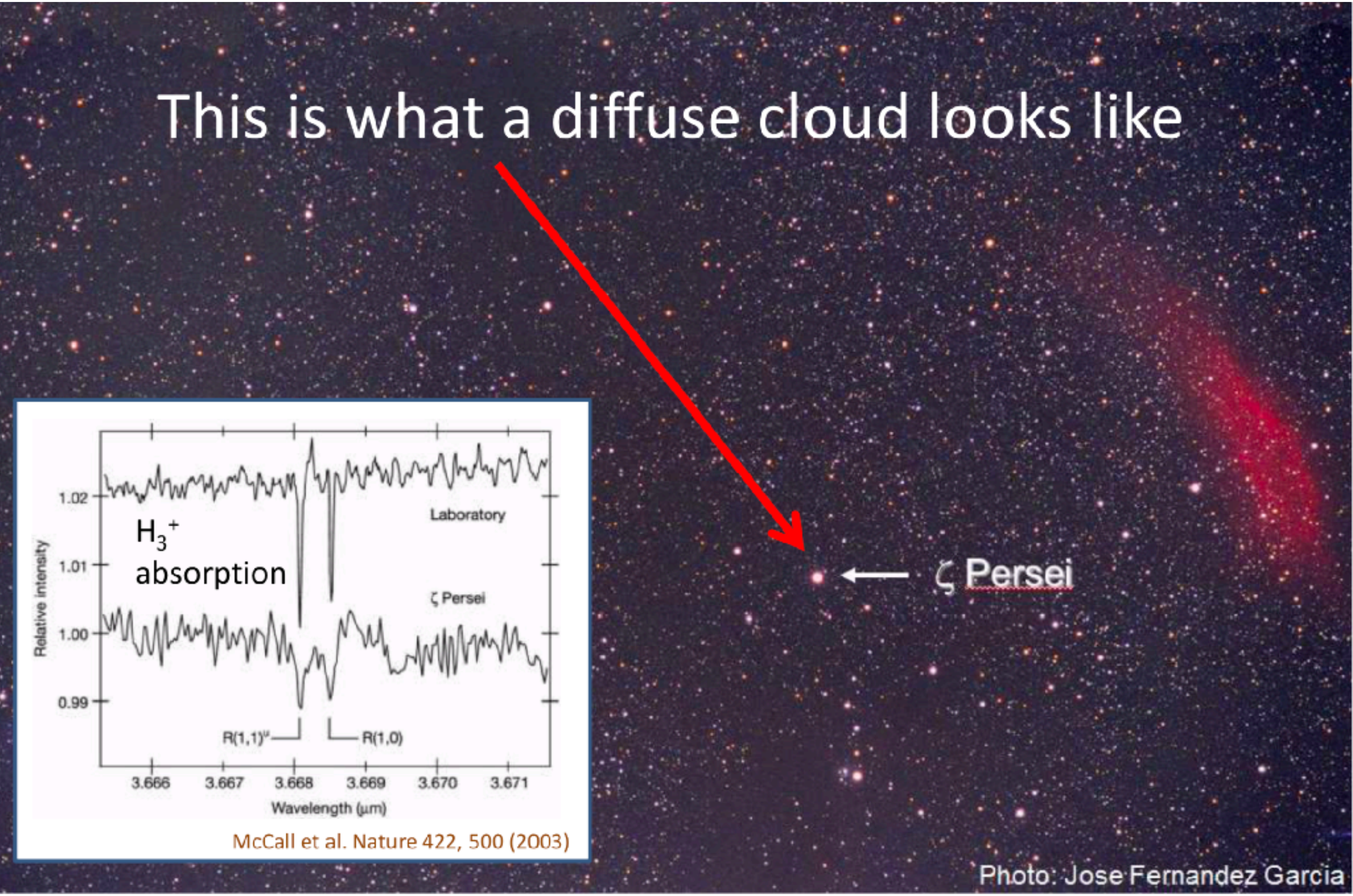
Diffuse clouds



- Diffuse clouds: T ~ 100 K, n_H < 100 cm^{-3}, A_V < 1 mag
- H/H_2 transition, n(e-) ~ n(C^+), a few radicals

Snow (2006)

This is what a diffuse cloud looks like



H_3^+ observations in diffuse ISM

H_2 + CRP ⇒ H_2^+ + e^-

H_2^+ + H_2 ⇒ H_3^+ + H

H_3^+ + e^- ⇒ H_2 + H or H + H + H

$$n(\mathrm{H}_3)_{\mathrm{diffuse}} \approx (\zeta / k_e)[n(\mathrm{H}_2)/n(\mathrm{e}^-)]$$

- $n(H_2)/n(e-) \sim 10^4$
- Dissociative recombination rate: $k_e \sim 10^{-7}$ cm^3 s^{-1}
- Cosmic ray ionization rate: $\zeta_{CRP} \sim 10^{-17}$ s^{-1}
- Result: $n(H_3^+) \sim 10^{-6}$ cm^{-3} ⇒ **must be non-observable!**
- What is wrong, k_e or ζ_{CRP}?

H_3^+ DR measurements

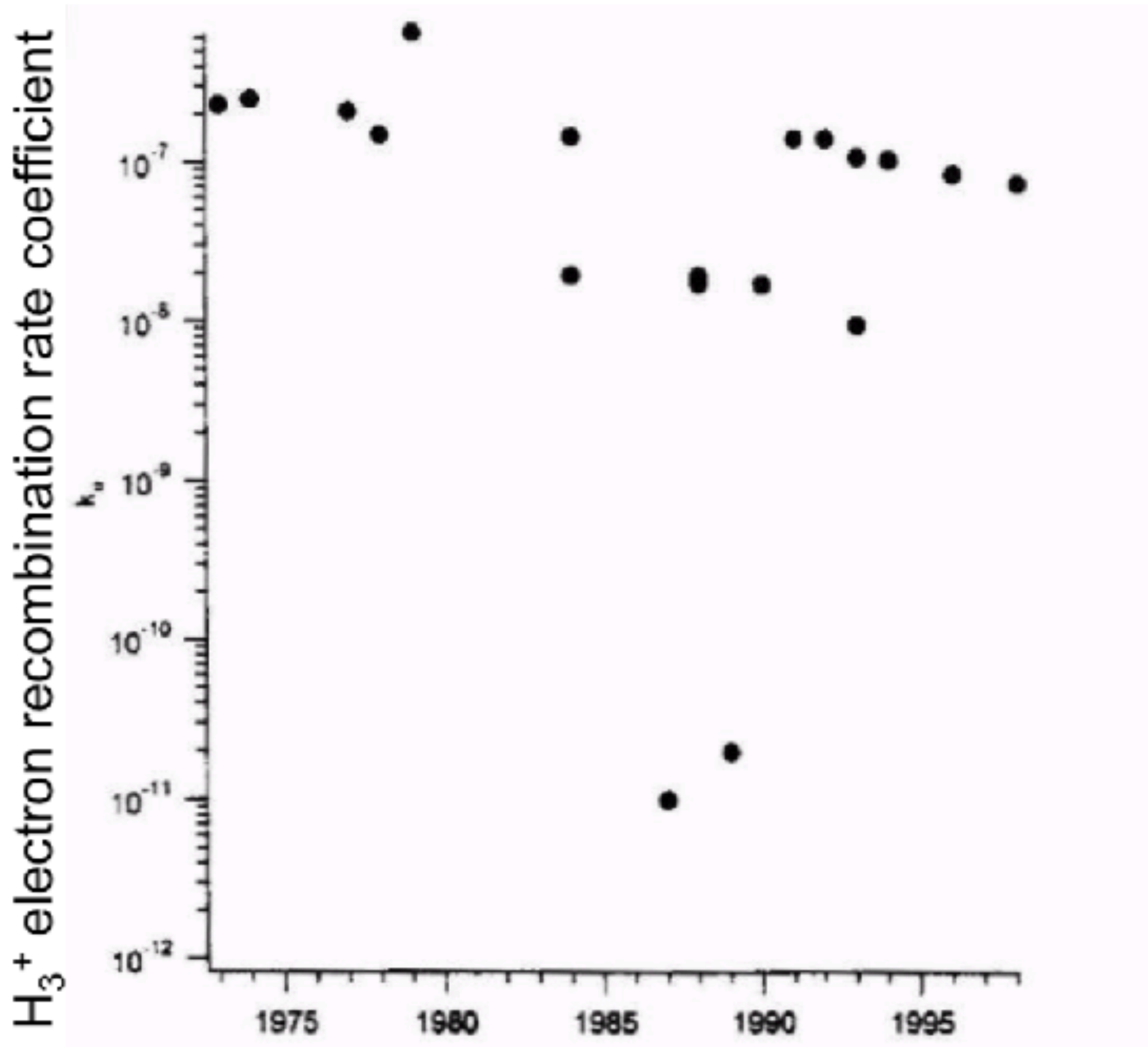


Fig. 5 Laboratory measurement of k_e over the years.

T. Oka, DR Conference Nässlingen (Stockholm), 1999

- A large scatter ⇒ temperature of H_3^+ in the experiment matters?

Accurate H_3^+ DR measurements

- CRYRING at Stockholm (Larsson ++ 2008)
- Test/Cold Storage Ring at MPIK (Kreckel ++ >2005)
- A good agreement for k_e $\Rightarrow$ higher CRP ionization: $\zeta \sim 10^{-15}$ s^{-1}

Effects of molecular rotation in low-energy electron collisions of

Andreas Wolf, H Kreckel, L Lammich, D Strasser, J Mikosch, J Glosík, R Plašil, S Altevogt, V Andrianarijaona, H Buhr, J Hoffmann, M Lestinsky, I Nevo, S Novotny, D.A Orlov, H.B Pedersen, A.S Terekhov, J Toker, R Wester, D Gerlich, D Schwalm and D Zajfman

Published: 25 September 2006 https://doi.org/10.1098/rsta.2006.1881

Abstract

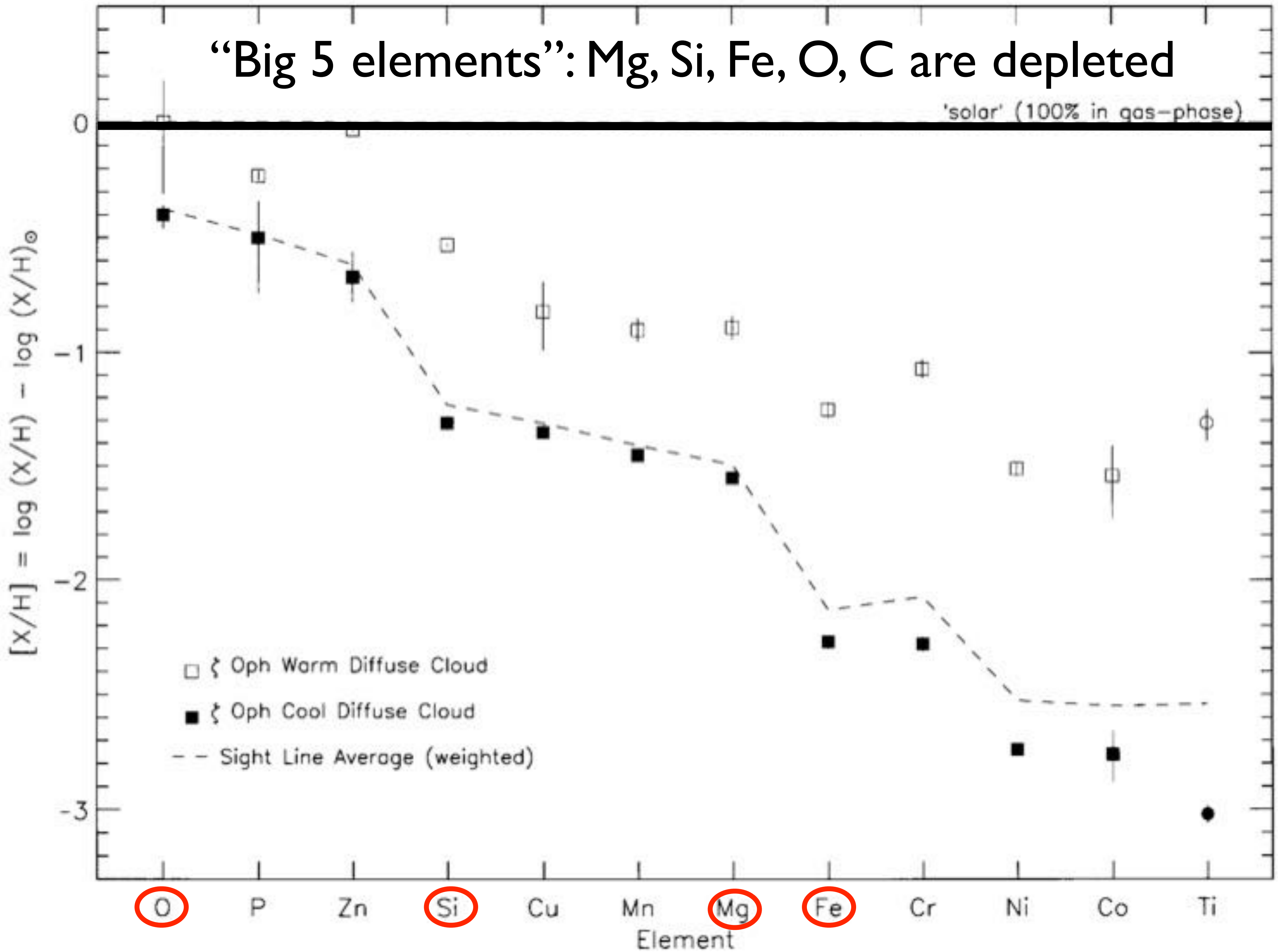
Measurements on the energetic structure of the dissociative recombination rate coefficient in the millielectronvolt range are described for H_3^+ ions produced in the lowest rotational levels by collisional cooling and stored as a fast beam in the magnetic storage ring TSR (Test Storage Ring). The observed resonant structure is consistent with that found previously at the storage ring facility CRYRING in Stockholm, Sweden; theoretical predictions yield good agreement on the overall size of the rate coefficient, but do not reproduce the detailed structure. First studies on the nuclear spin symmetry influencing the lowest level populations show a small effect different from the theoretical predictions. Heating processes in the residual gas and by collisions with energetic electrons, as well as cooling owing to interaction with cold electrons, were observed in long-time storage experiments, using the low-energy dissociative recombination rate coefficient as a probe, and their consistency with the recent cold H_3^+ measurements is discussed.

letters to nature

An enhanced cosmic-ray flux towards ζ Persei inferred from a laboratory study of the H_3^+–e^- recombination rate

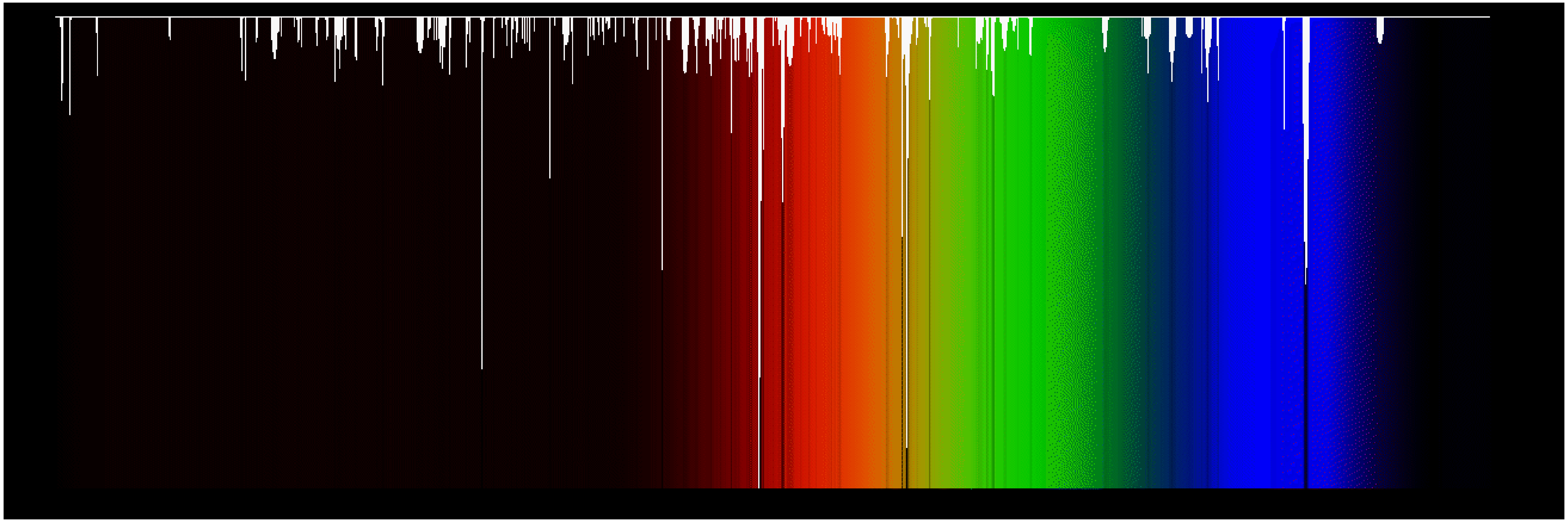
B. J. McCall*†, A. J. Huneycutt*, R. J. Saykally*, T. R. Geballe‡, N. Djuric§, G. H. Dunn§, J. Semaniak||, O. Novotny||¶, A. Al-Khalili#, A. Ehlerding#, F. Hellberg#, S. Kalhori#, A. Neau#, R. Thomas#, F. Österdahl☆ & M. Larsson#

Partition of elements between gas and dust phases

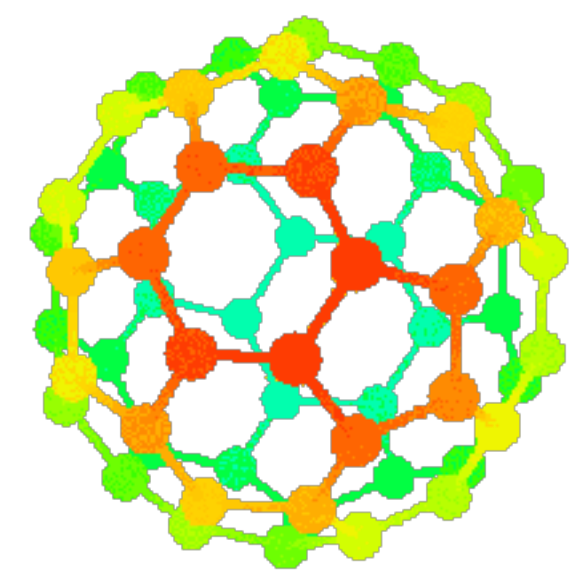


- Growth of dust grains in the ISM (silicates, C, S, P, etc.)

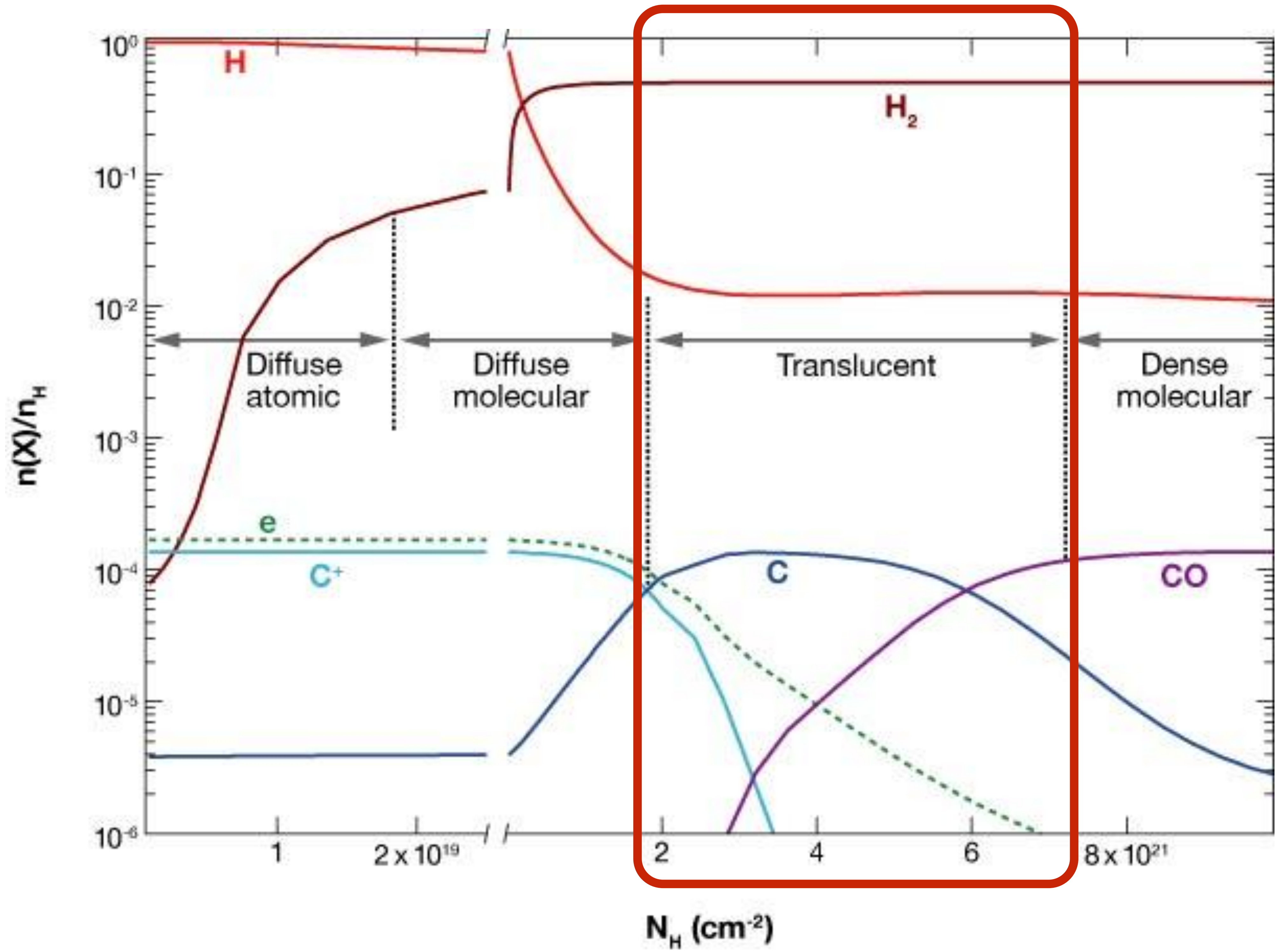
Diffuse Interstellar Bands (DIBs)



- Discovered by Heger (1922) and Merill (1934)
- ~ 500 DIBs in UV–near IR
- Very narrow lines, < 0.1 – 1Å
- Large PAHs and C-bearing species
- First laboratory identification of C_{60}^+ as a DIB carrier at 9,632.7 and 9,577.5Å (Campbell ++ 2015, *Nature*)



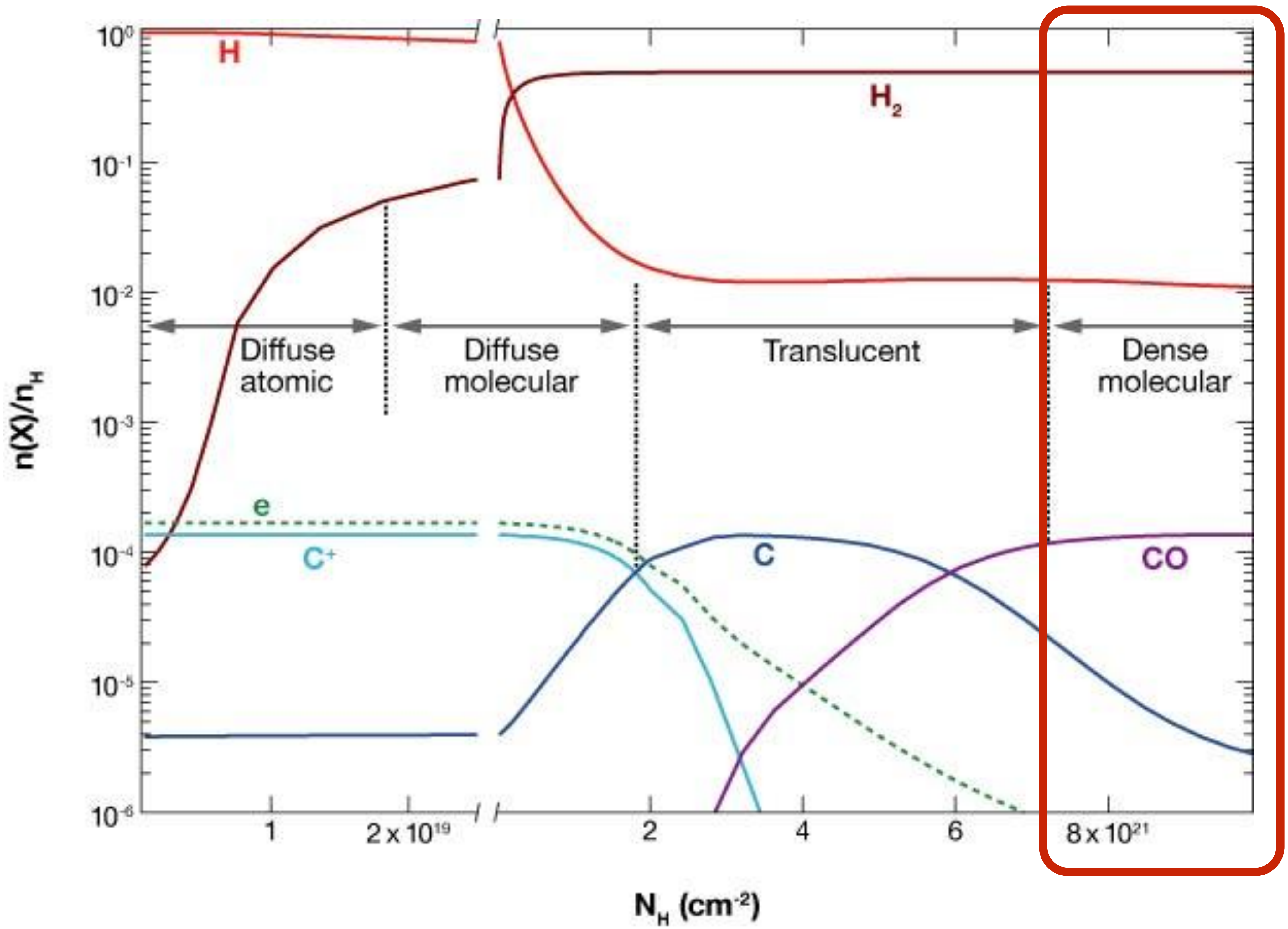
Translucent clouds



- Translucent: T = 50–100 K, $n_H = 10^2 – 10^3$ cm^{-3}, $A_V \sim 1 – 4$ mag
- Fully H_2, conversion of C^+ into C, more molecules

Snow (2006)

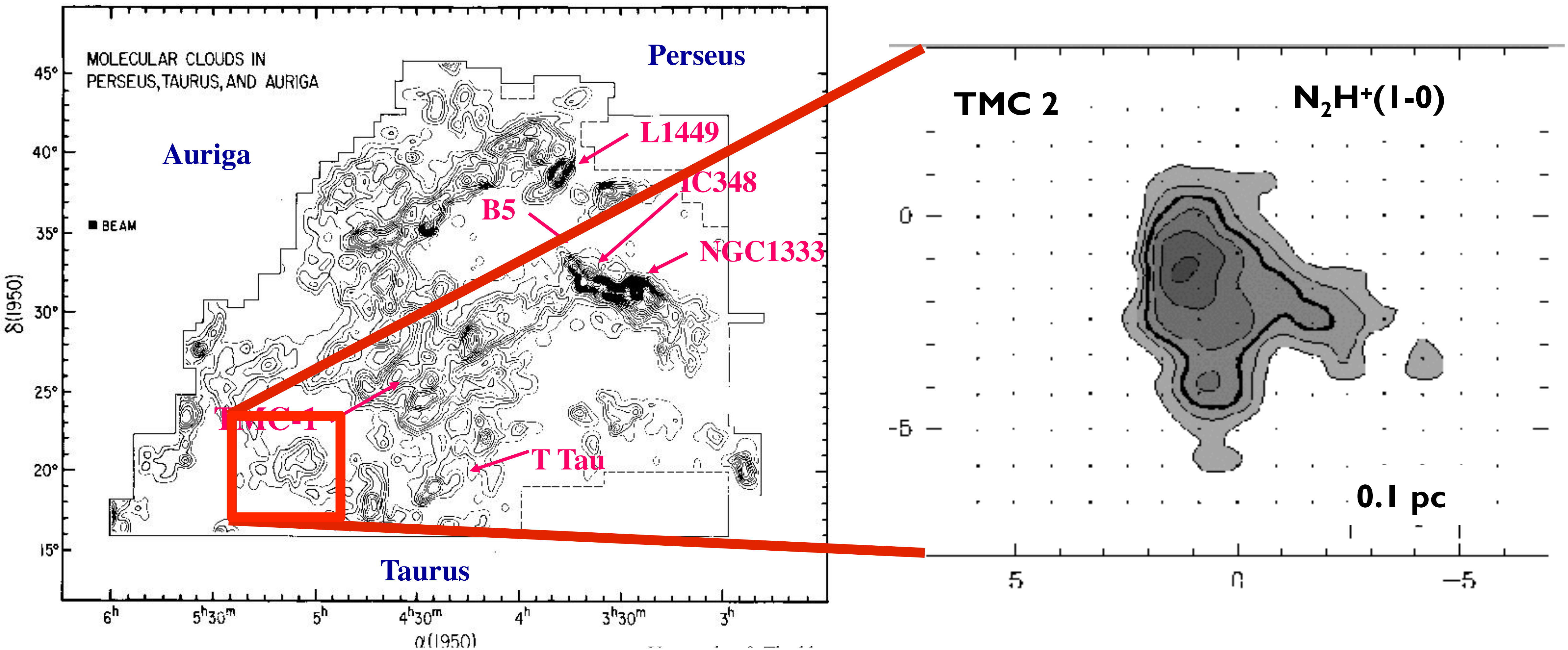
Dense clouds



- Dense clouds: T = 10 K, $n_H = 10^4 – 10^6$ cm^{-3}, $A_V > 5–10$ mag
- Complex molecules and ices

Snow (2006)

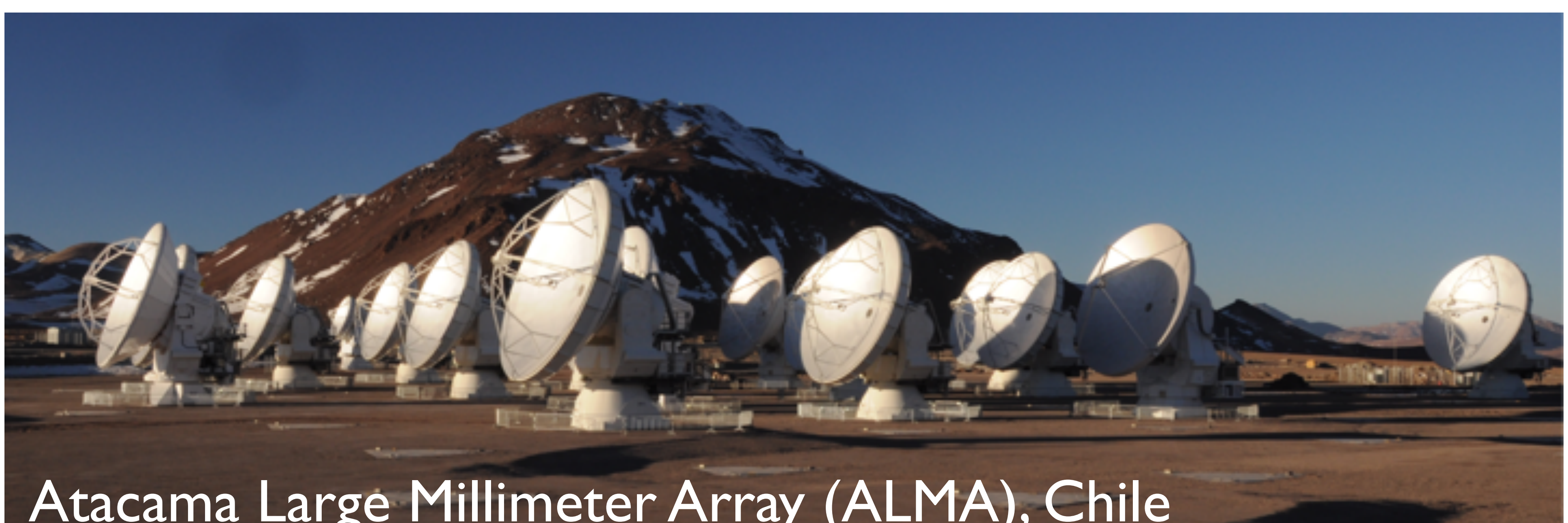
Dense cores (clouds)



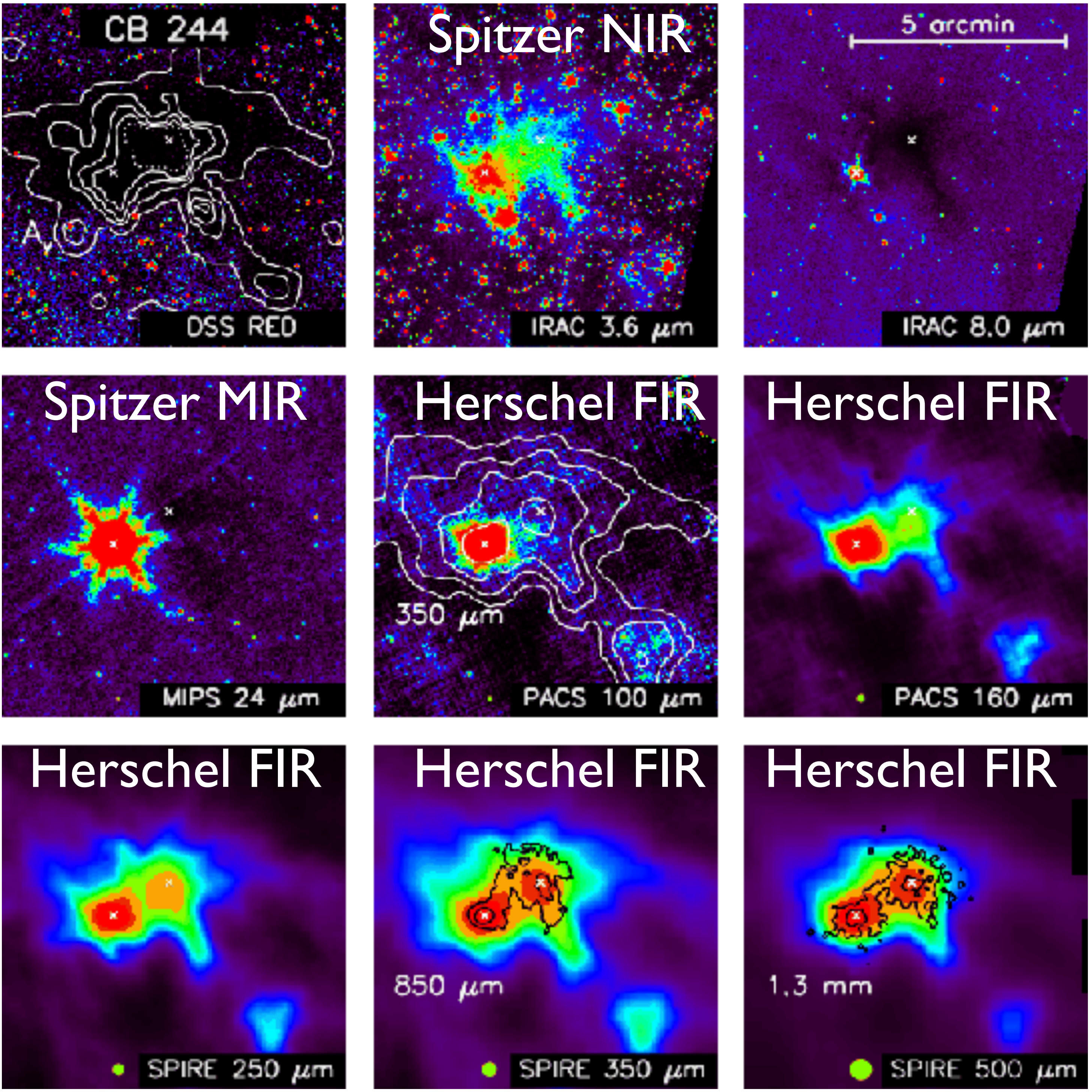
- Asymmetric structure, size ~ 0.1 – 1 pc
- Smooth gradients of density/temperature
- Central condensation(s) ⇒ protostar(s) in the future?

Observations of dense clouds

- "Classical" sources: TMC-1, L1544, B68
- Visual – IR: absorption and scattering by dust and PAHs
- (Sub-)millimeter: emission of dust and molecules
- Radio-telescopes: low spatial resolution, many clouds
- Radio-interferometers: high spatial resolution, only a few clouds


Atacama Large Millimeter Array (ALMA), Chile

Deriving cloud physics by observations

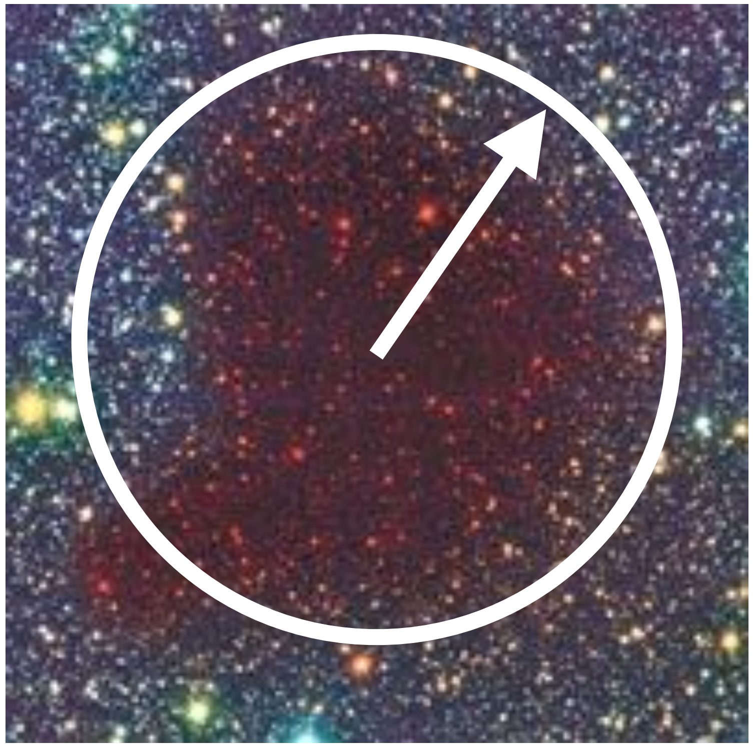


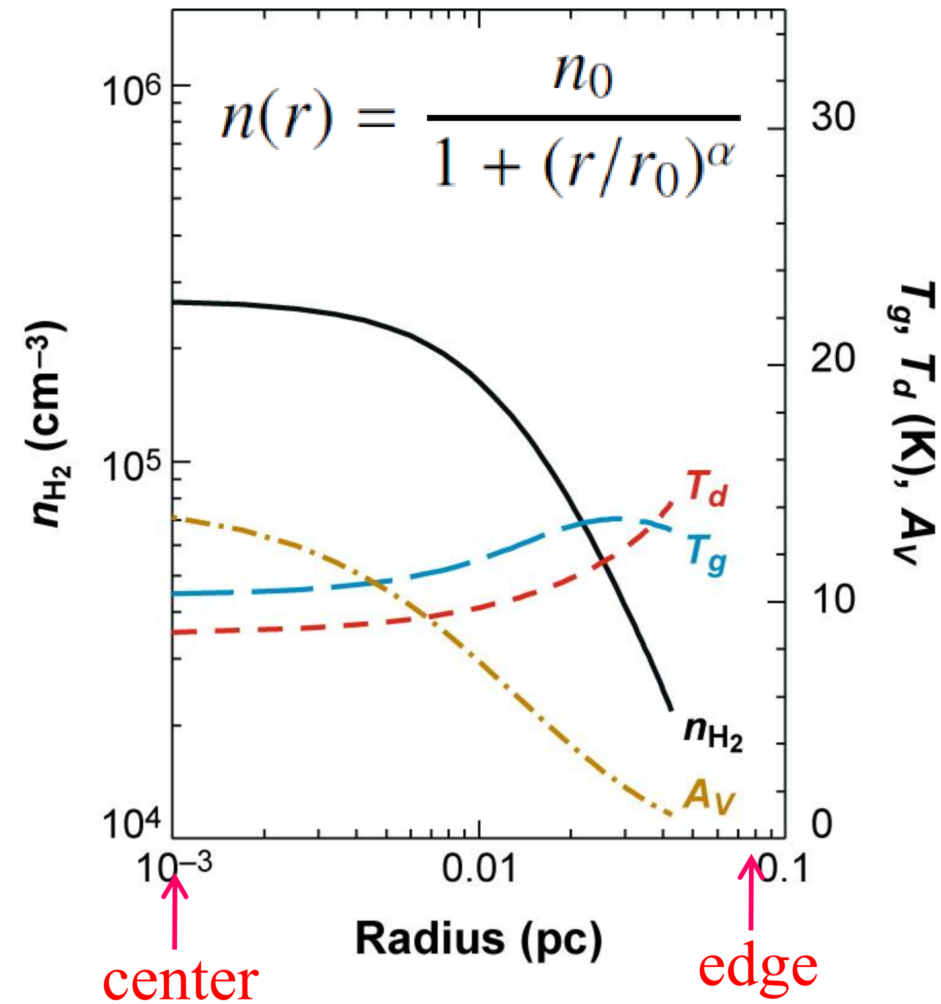
Stutz et al. 2013

- CB244: dense core and protostar
- Total mass: M ~ 15 +/- 5 M_{Sun}
- Dense core: M ~ 5 M_{Sun}, T~ 10 K
- Protostar: M ~ 1.5 M_{Sun}, T~ 18 K
- Density: n_H ~ 10^4 – 10^5 cm^{-3}

Typical physical structure (B68)

Projected 3D

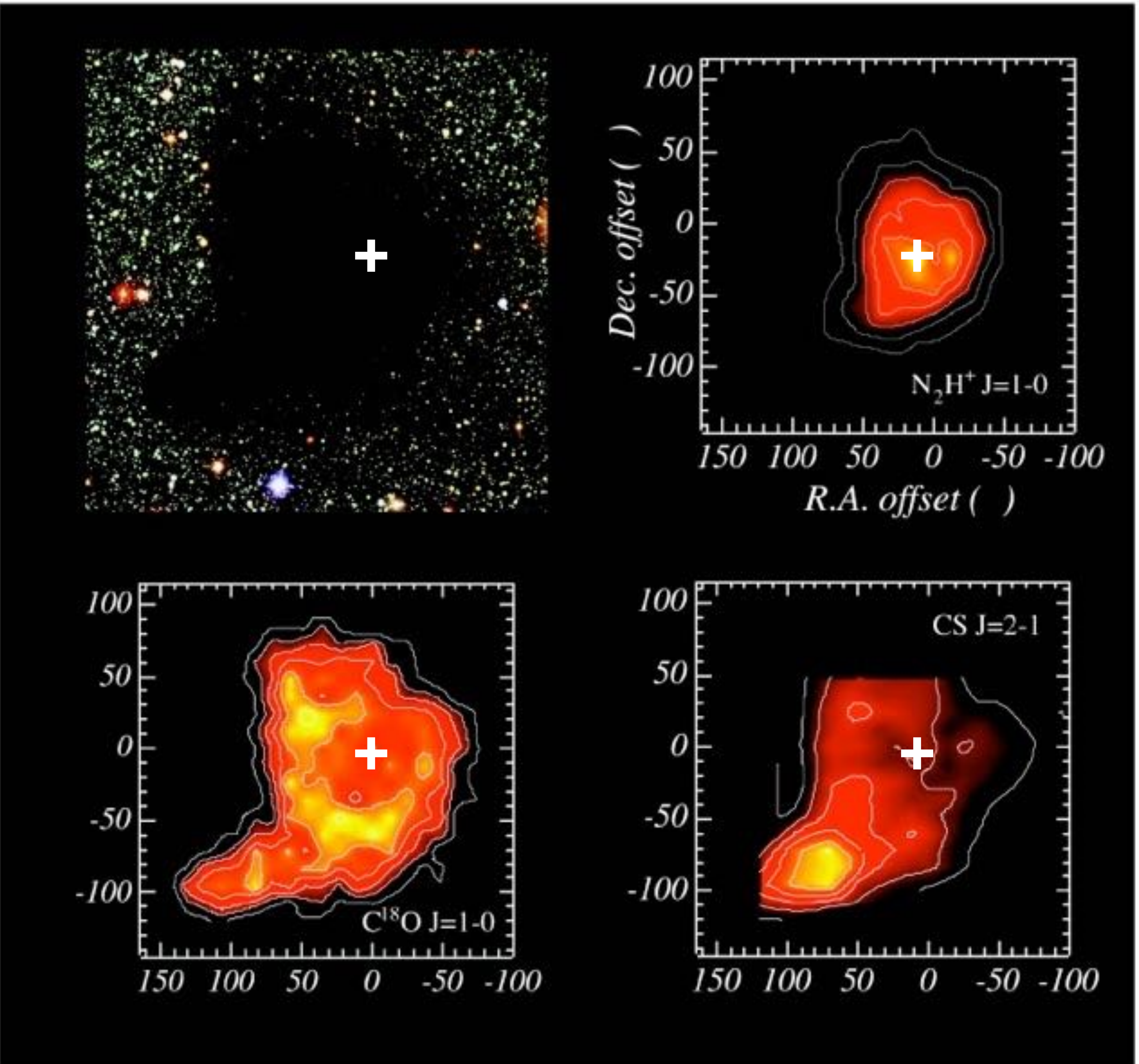




- Flat density profiles around the center $\Rightarrow$ hydrostatic equilibrium
- Heating: cosmic rays and UV
- Cooling: dust and molecular lines (C, C^+, O, CO, OH)
- Tdust ≠ Tgas, outward temperature gradient

Alves et al. 2001, Bergin & Tafalla 2007

Typical chemical structure (B68)

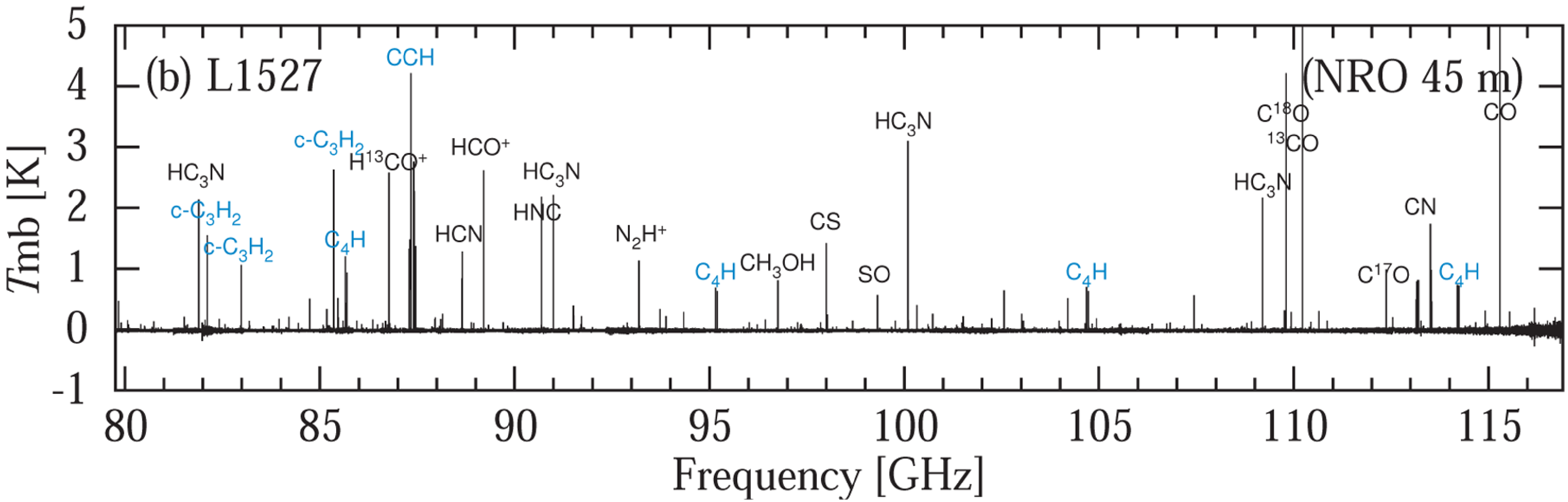


Alves et al. 2002

- CO is depleted in the center (+): freeze-out
- N_2H^+ peaks in the center:

  $N_2H^+ + CO \rightarrow N_2 + HCO^+$
- CS peaks in a smaller (younger?) core

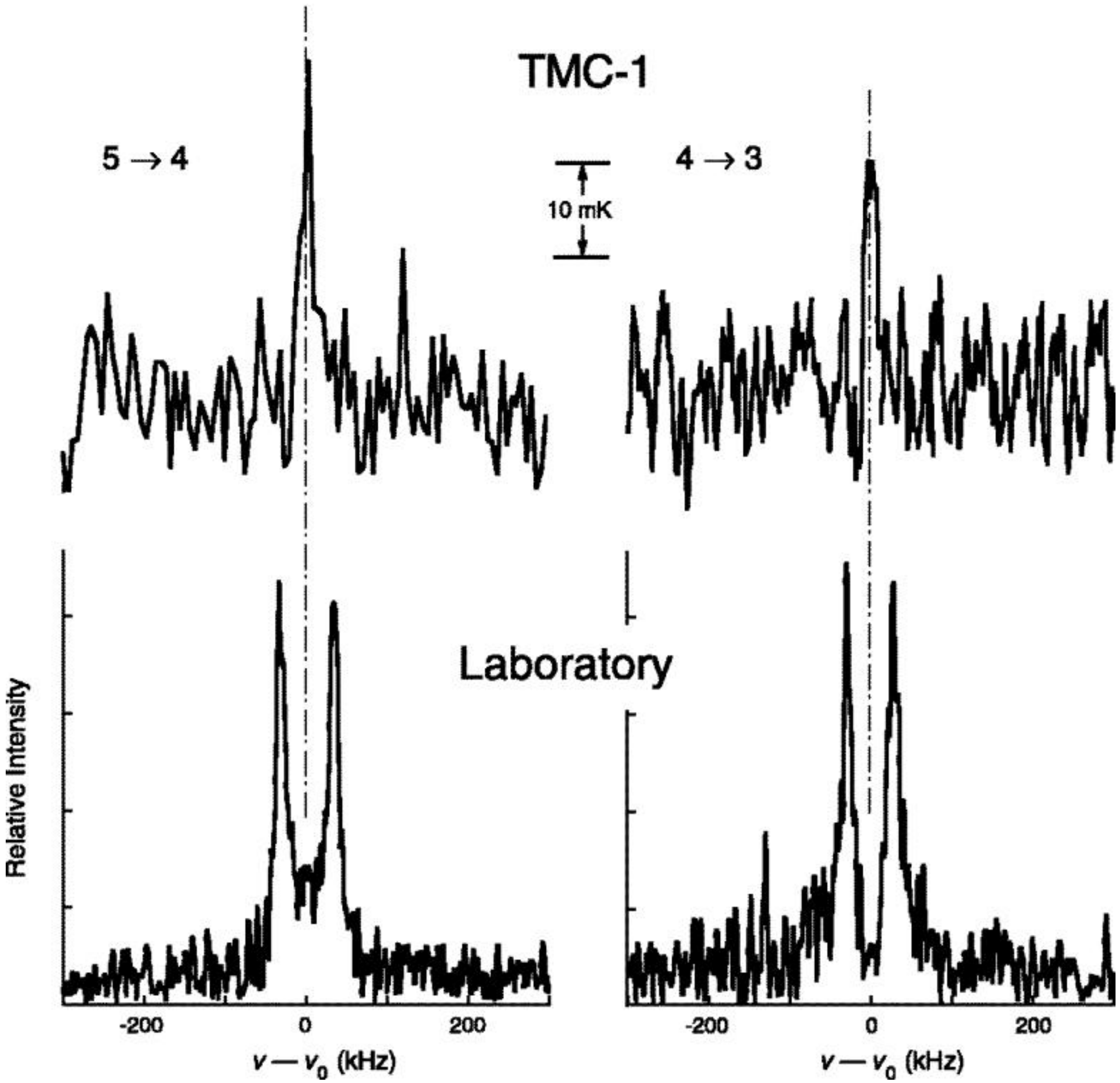
Molecules in dense clouds



- Major molecules: H_2, CO, N_2, H_2O
- Many hydrocarbons and C-chains: C_nH_m, HC_3N, CCS, …
- Several negative ions: C_6H^-,…
- Deuterated species: DCO^+,N_2D^+, o-H_2D^+…
- Organic molecules (ices): H_2CO, CH_3OH, CH_3OCH_3,…

Negative ions in TMC-1

$C_6H + e^- \Rightarrow C_6H^- + h\nu$



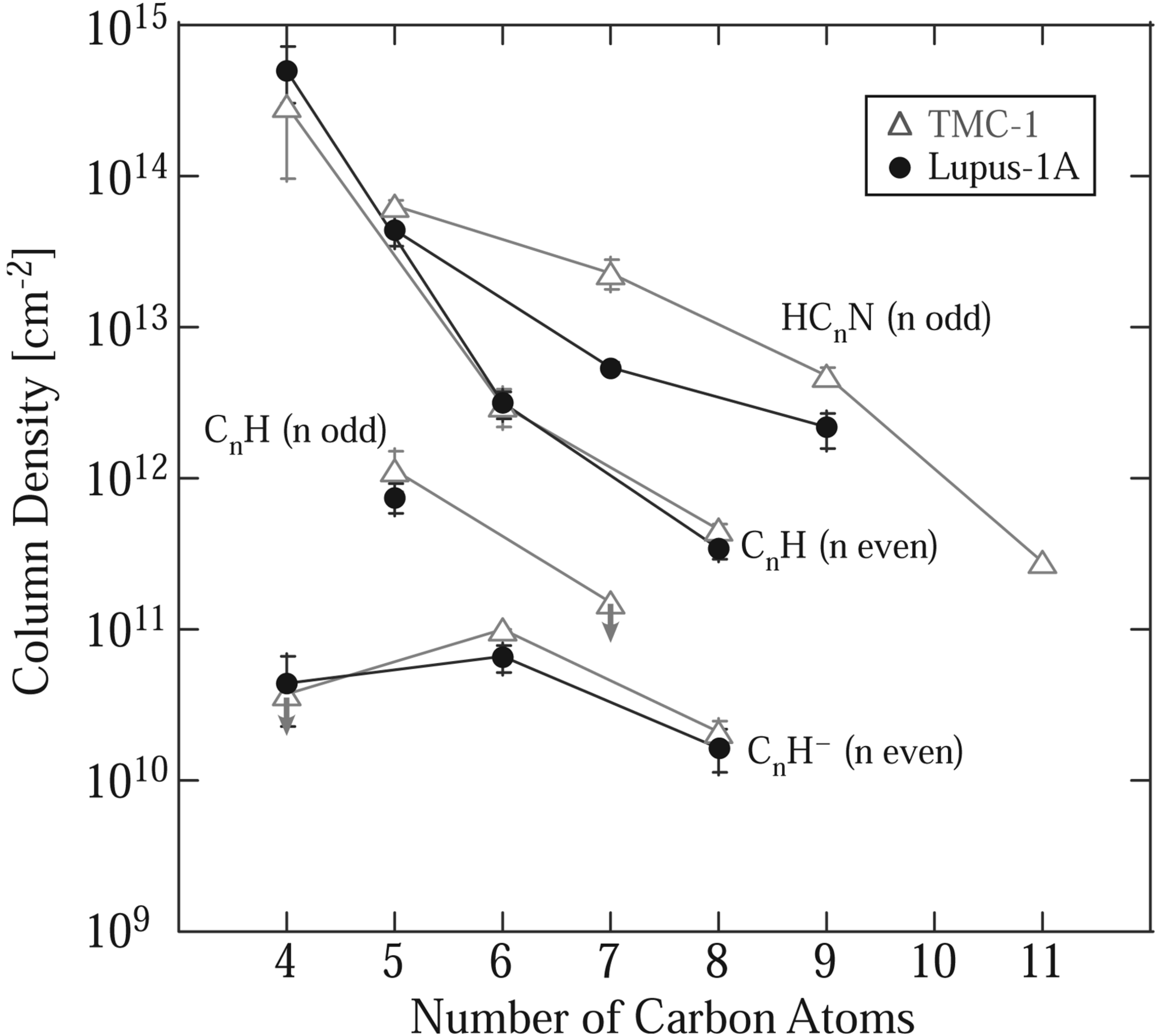
McCarthy et al. 2006

<10% of anion/neutral

(predicted by Herbst in 1981)

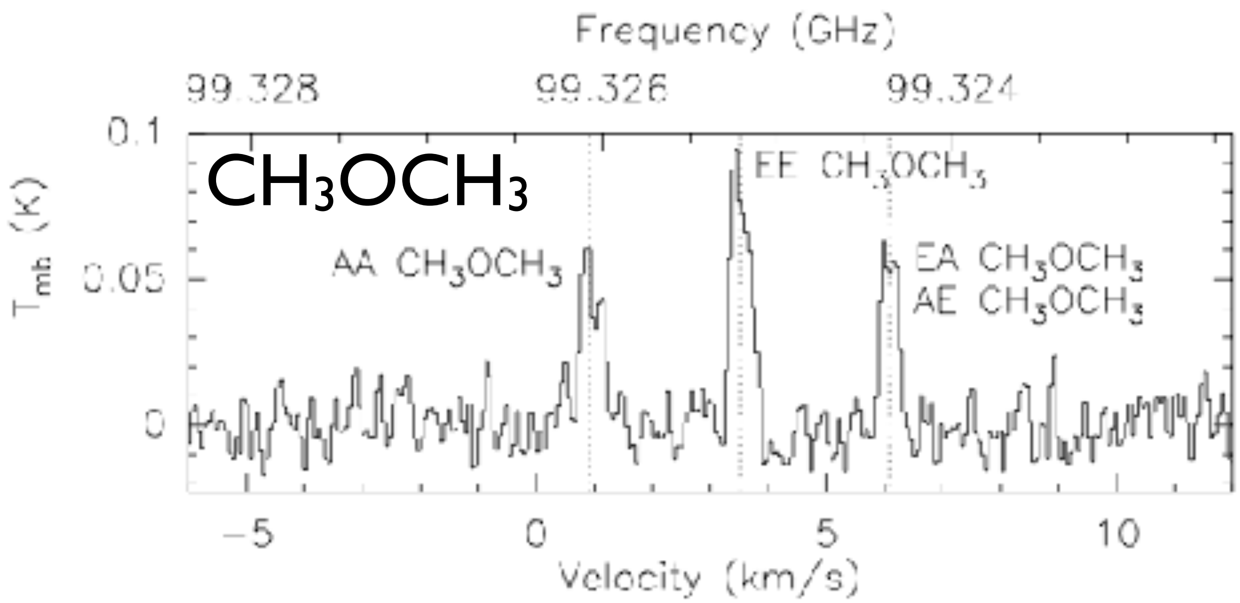
Discovered when laboratory spectra became available (McCarthy et al. 2006, Bruencken et al. 2007)

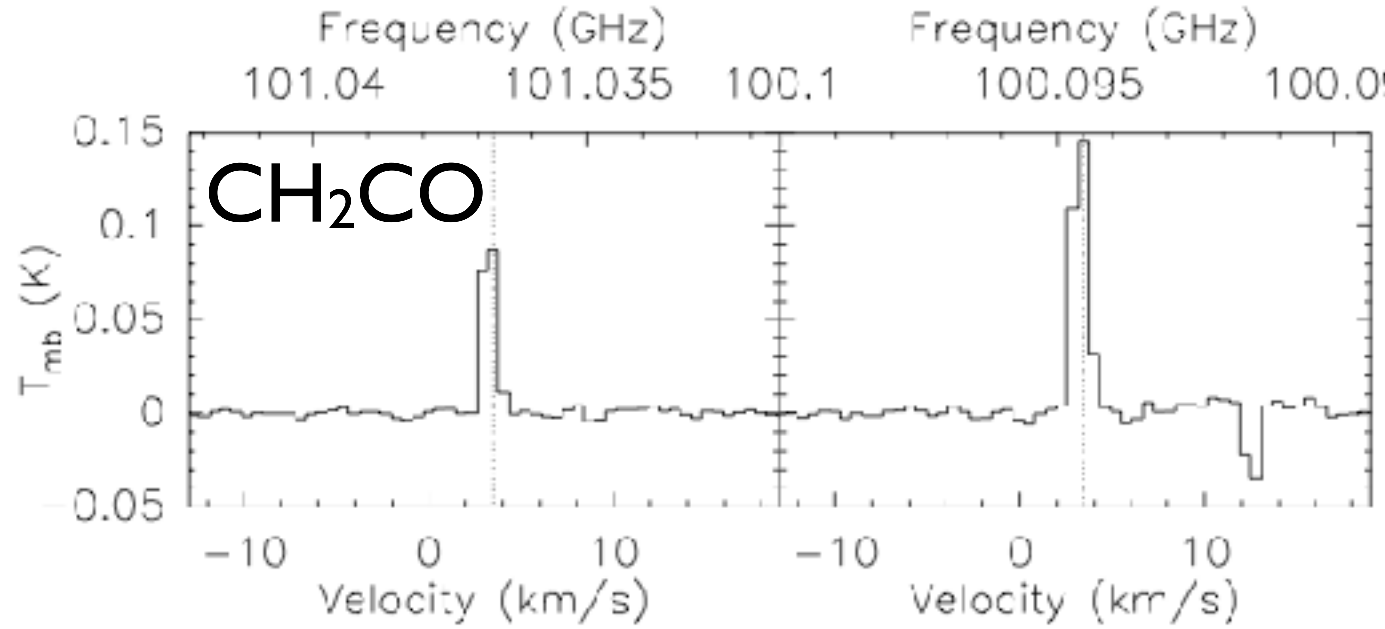
Long carbon chains and cyanopolyynes

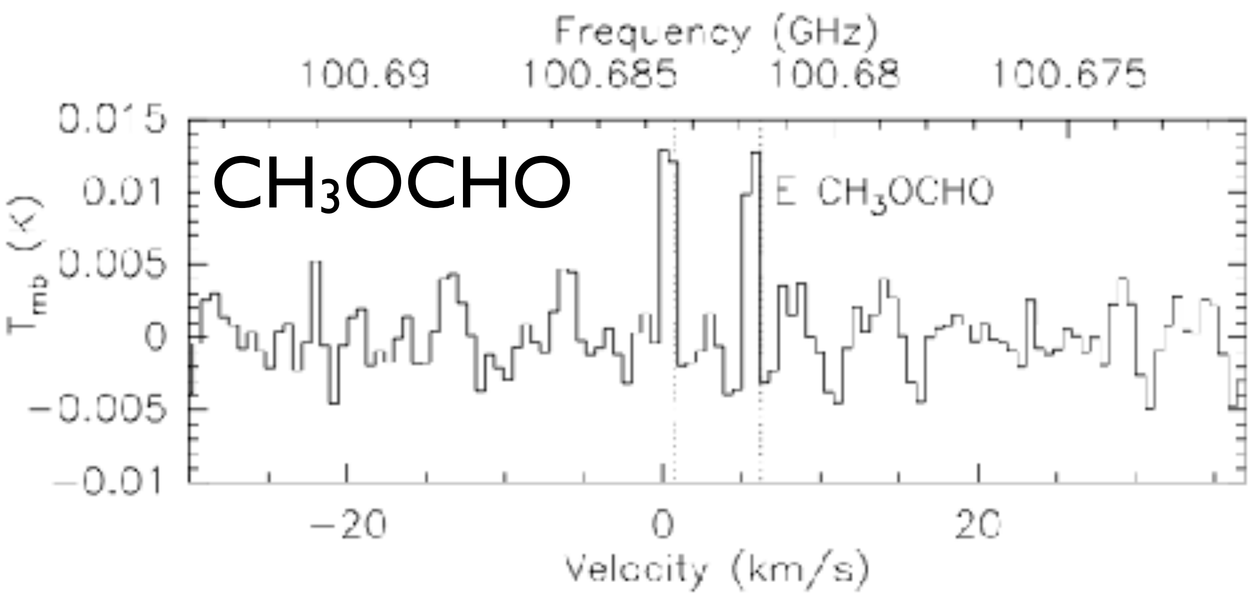


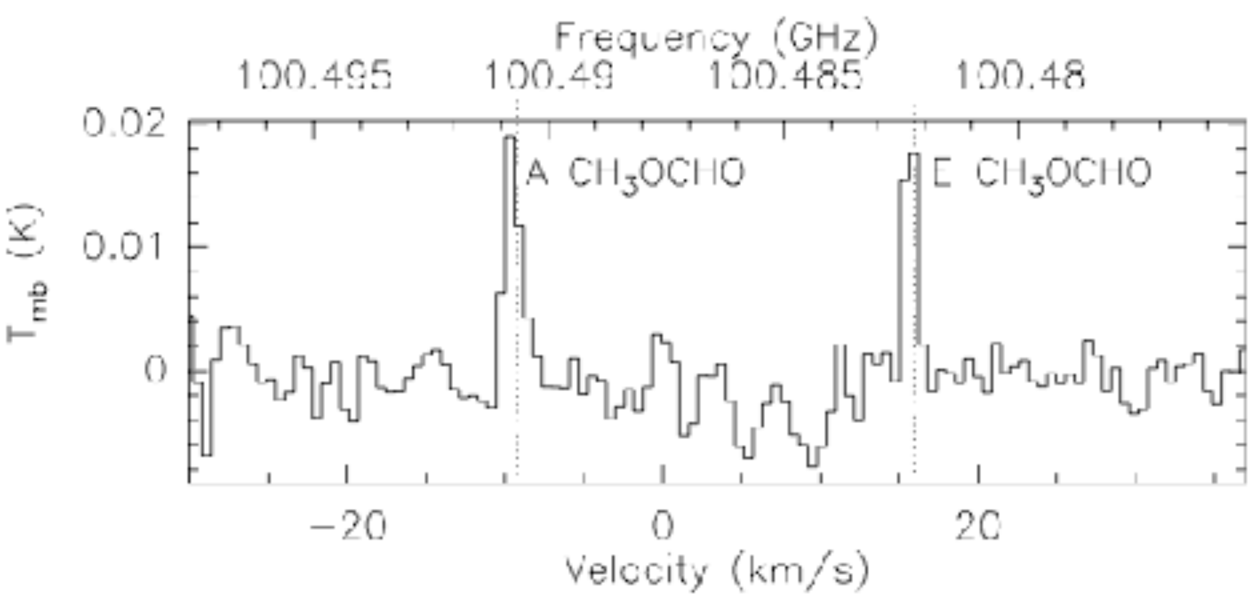
Sakai & Yamamoto 2013

Complex organic molecules





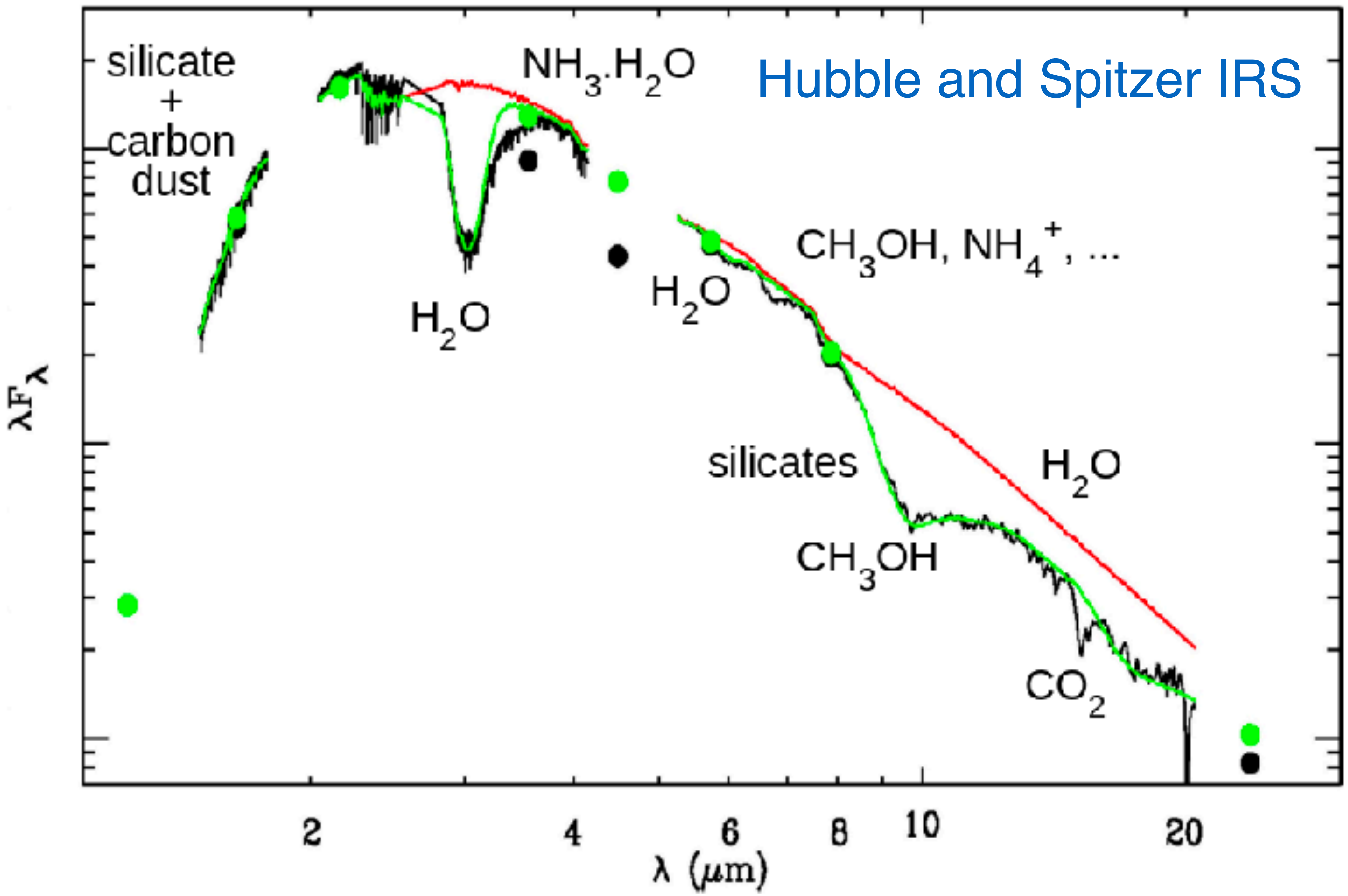




- Typical abundances in L1689:
  - CH_3OCH_3: 4 (-11)
  - CH_3CHO: 1 (-10)
  - CH_3OCHO: 2 (-10)
  - CH_2CO: 1 (-10)
- Mainly exist as ices

Bacmann et al. (2012)

Ices



- Observed in absorption against background stars
- Dominated by H_2O, CO_2, silicates
- Complex ices: HCOOH, CH_3OH,…
- ~10–50% of heavy elements are in ices

Oxygen chemistry

- I.P. of O > 13.6 eV ⇒ oxygen is mostly neutral
- Ionization provided by cosmic rays:

$H_2 \Rightarrow H^+, H_2^+, H_3^+$ (rapid)

$H^+ + O \rightarrow H + O^+$ (+227 K)

$O^+ + H_2 \rightarrow OH^+ + H$

$H_3^+ + O \rightarrow OH^+ + H_2$

Once OH^+ formed, rapid ion-molecule and dissociative recombination reactions produce OH, H_2O, and CO

Formation of water

$H_2 + CRP \Rightarrow H_2^+ + e^-$

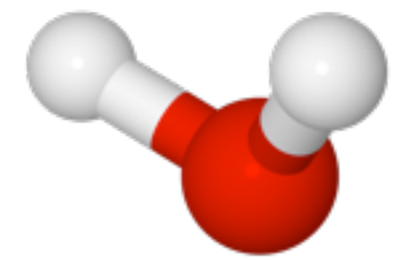
$H_2^+ + H_2 \Rightarrow H_3^+ + H$

$H_3^+ + O \Rightarrow OH^+ + H_2$

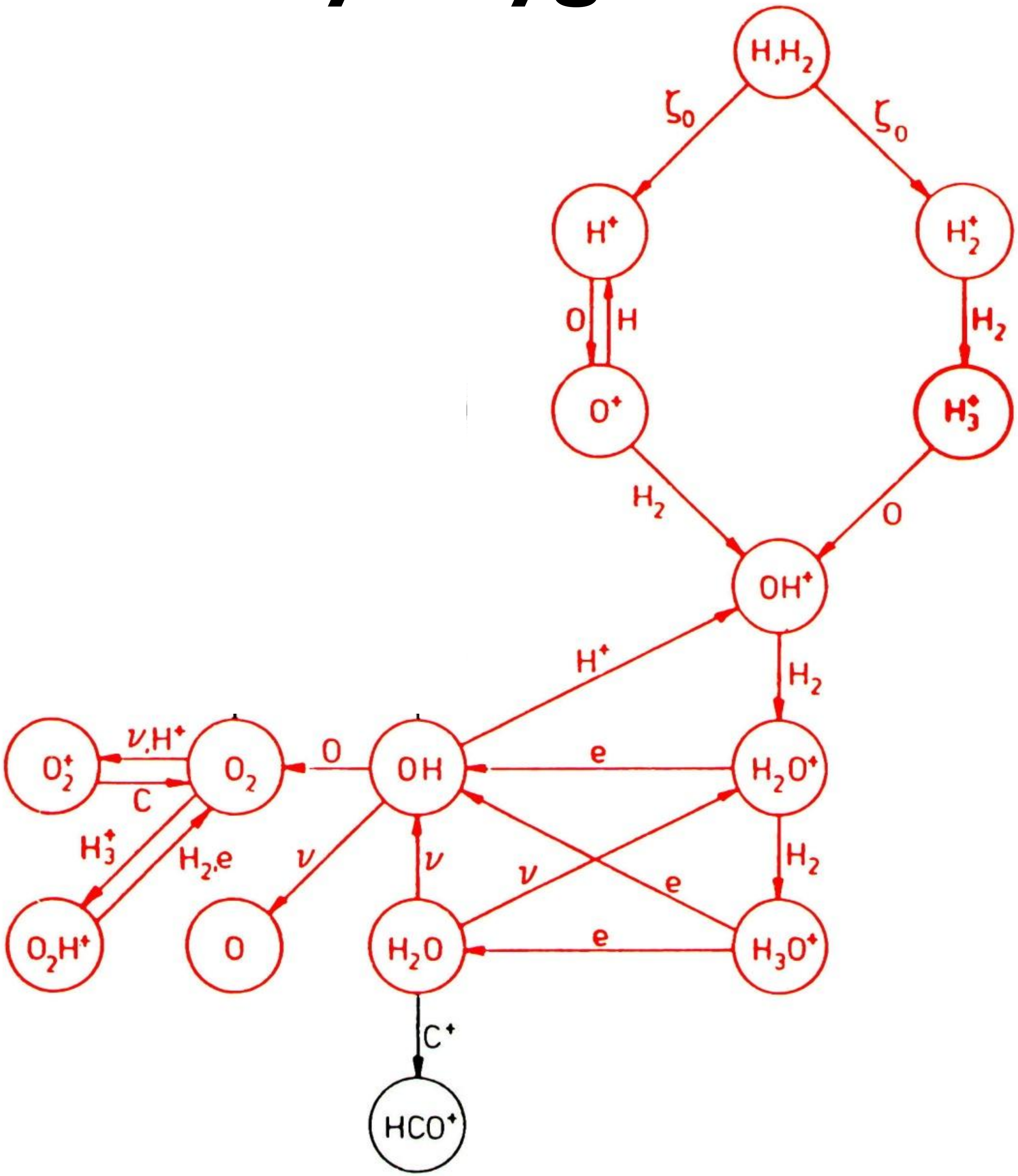
$OH^+ + H_2 \Rightarrow H_2O^+ + H$

$H_2O^+ + H_2 \Rightarrow H_3O^+ + H$

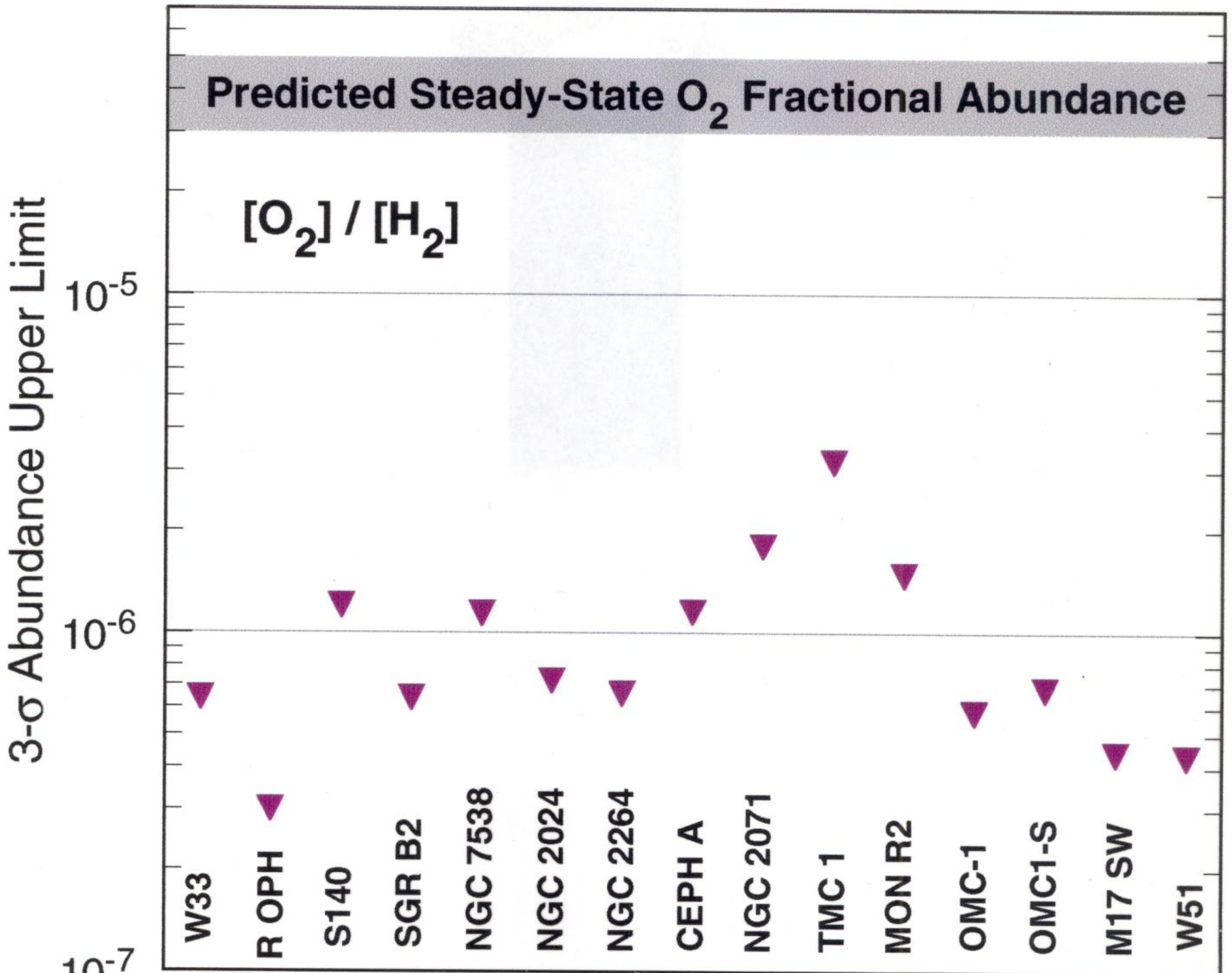
$H_3O^+ + e^- \Rightarrow H_2O + H$ or $OH + 2H$



Summary: oxygen chemistry



A problem of observed low O_2



Goldsmith et al. 2000

- Factor of 100 discrepancy between observed and modeled O_2
- Solution: freeze-out of O ⇒ O converted to water ice rather than O_2 ice (Bergin et al. 2000)

Carbon chemistry

- I.P. of C < 13.6 eV ⇒ carbon is mostly ionized

- Ion-molecule reactions with H_2 and H_3^+:

  $C^+ + H_2 \rightarrow CH_2^+ + h\nu$ is possible at low T (initiating reaction)

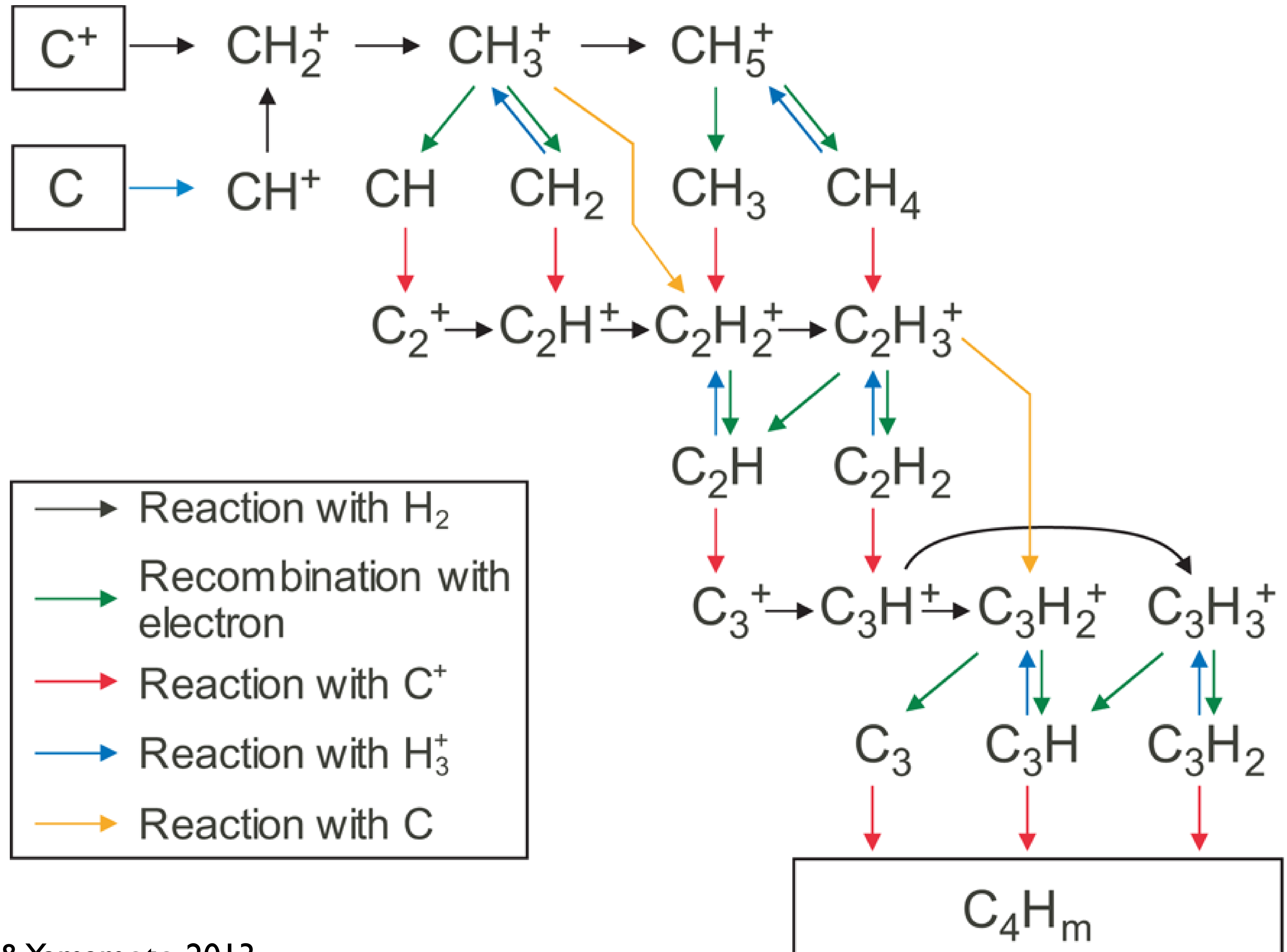
  $C^+ + H_2 \rightarrow CH^+ + H$:   endothermic by 0.4 eV

  $C + H_3^+ \rightarrow CH^+ + H_2$

  $CH_2^+ + H_2$ and carbon insertion ⇒ rapid ion-molecule

  reactions lead to CH, C_2, C_2H, C_2H_2, …

Carbon chemistry: hydrocarbons



Sakai & Yamamoto 2013

Carbon chemistry: formation of CO

- CO is formed after hydrocarbons:

C_2H / CH_2 + O $\Rightarrow$ CO + CH / H_2

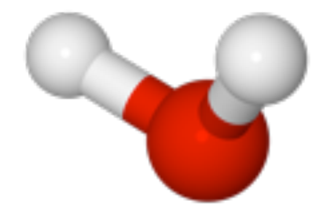
CH_3^+ + O $\Rightarrow$ HCO^+ + H_2

H_3O^+ + C $\Rightarrow$ HCO^+ + H_2

HCO^+ + e^- $\Rightarrow$ CO + H

- Key destruction reaction: CO + He^+ $\Rightarrow$ C^+ + O + He
- Timescale of CO formation: $<10^5$ years
- Freeze-out timescale: $\sim10^6$ years for $n_H \sim 10^4$ cm^{-3}

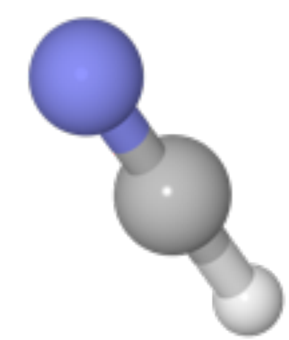
Gas-phase formation of organic molecules?



$C^+ + H_2 \Rightarrow CH_2^+$

$CH_2^+ + H_2 \Rightarrow CH_3^+ + H$

$CH_3^+ + H_2/O \Rightarrow CH_5^+/HCO^+ + H_2$



$CH_5^+ + e^- \Rightarrow CH_3 + H_2$

$CH_3 + O \Rightarrow H_2CO$

$CH_3^+ + H_2O \nRightarrow CH_3OH_2^+$ (too low rate, Luca et al. 2002)

$CH_3OH_2^+ + e^- \Rightarrow CH_3OH + H$ (3 ± 2%, Geppert et al. 2006)

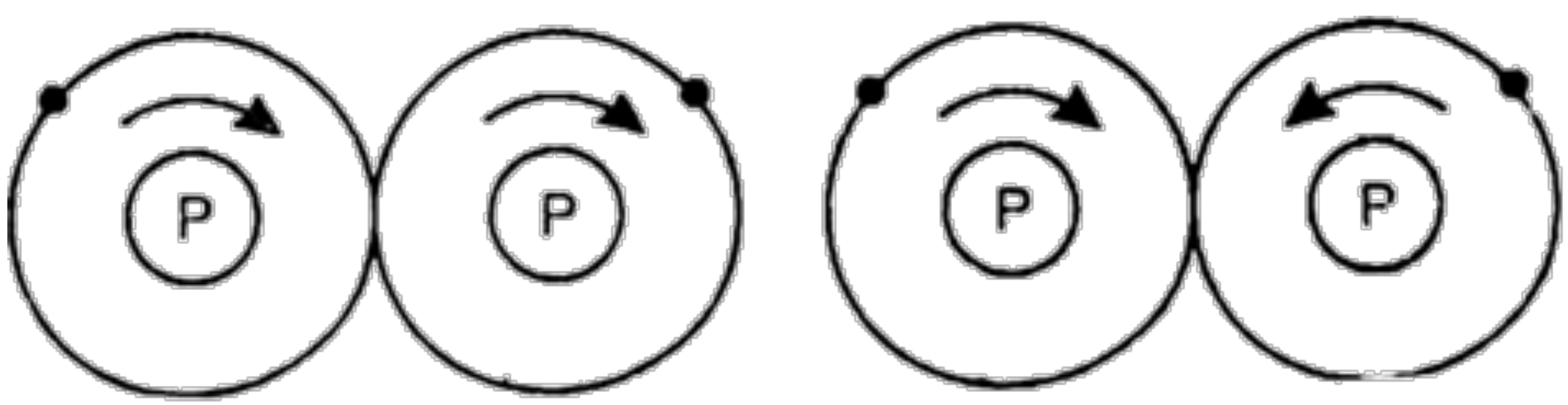
Nitrogen chemistry

- I.P. N > 13.6 eV $\Rightarrow$ nitrogen is mostly neutral
- The first steps via ion-molecule chemistry?:

$N + H_3^+ \rightarrow NH_2^+ + H$ (does not occur)

$N + H^+ \rightarrow N^+ + H$ (barrier of ~260 K)

$N^+ + H_2 \rightarrow NH^+ + H$ (barrier of ~100 K) $\Rightarrow$ works for ortho-H_2



ortho-hydrogen
(Parallel spins)

para-hydrogen
(Opposite spins)

Nitrogen chemistry

- However, in dense clouds H_2 is in the para state
- Initiating chemistry is hence neutral-neutral:

$CH + N \rightarrow CN + H$

$CH_2 + N \rightarrow HCN/HNC + H$

$CN + N \rightarrow N_2 + C$

$OH + N \rightarrow NO + H$

$NO + N \rightarrow N_2 + O$

- Timescale of N_2 formation: ~ 10^6 years $\Rightarrow$ N-species are „late“

Nitrogen chemistry

- After N_2 is formed, ion-molecule chemistry begins:

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

$N_2 + He^+ \rightarrow N^+ + N + He$

$N^+ + \text{ortho-}H_2 \rightarrow NH^+ + H$

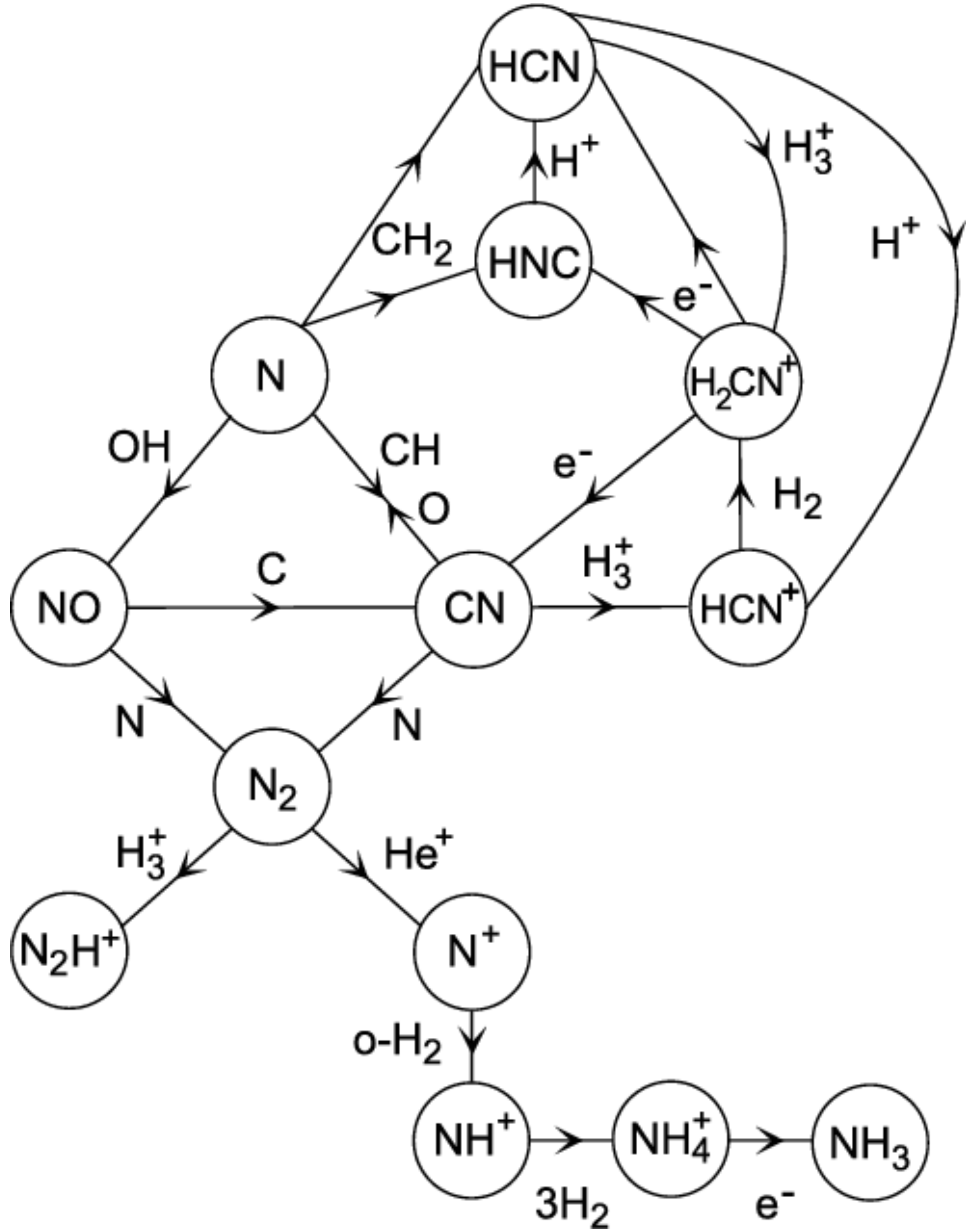
$NH^+ + H_2 \rightarrow NH_2^+ + H$

$NH_2^+ + H_2 \rightarrow NH_3^+ + H$

$NH_3^+ + H_2 \rightarrow NH_4^+ + H$

$NH_4^+ + e^- \rightarrow NH_3 + H$

Summary: nitrogen chemistry



Hily-Blant et al. (2010)

Early chemical models

- Gas-phase ion-molecule chemistry (Herbst & Klemperer 1973, Watson 1976, Dalgarno & Black 1977)
- Initially only H_2 formation on grains
- Later grain-surface chemistry included (Allen & Robinson 1978, Tielens & Hagen 1982, d'Hendecourt et al. 1985)

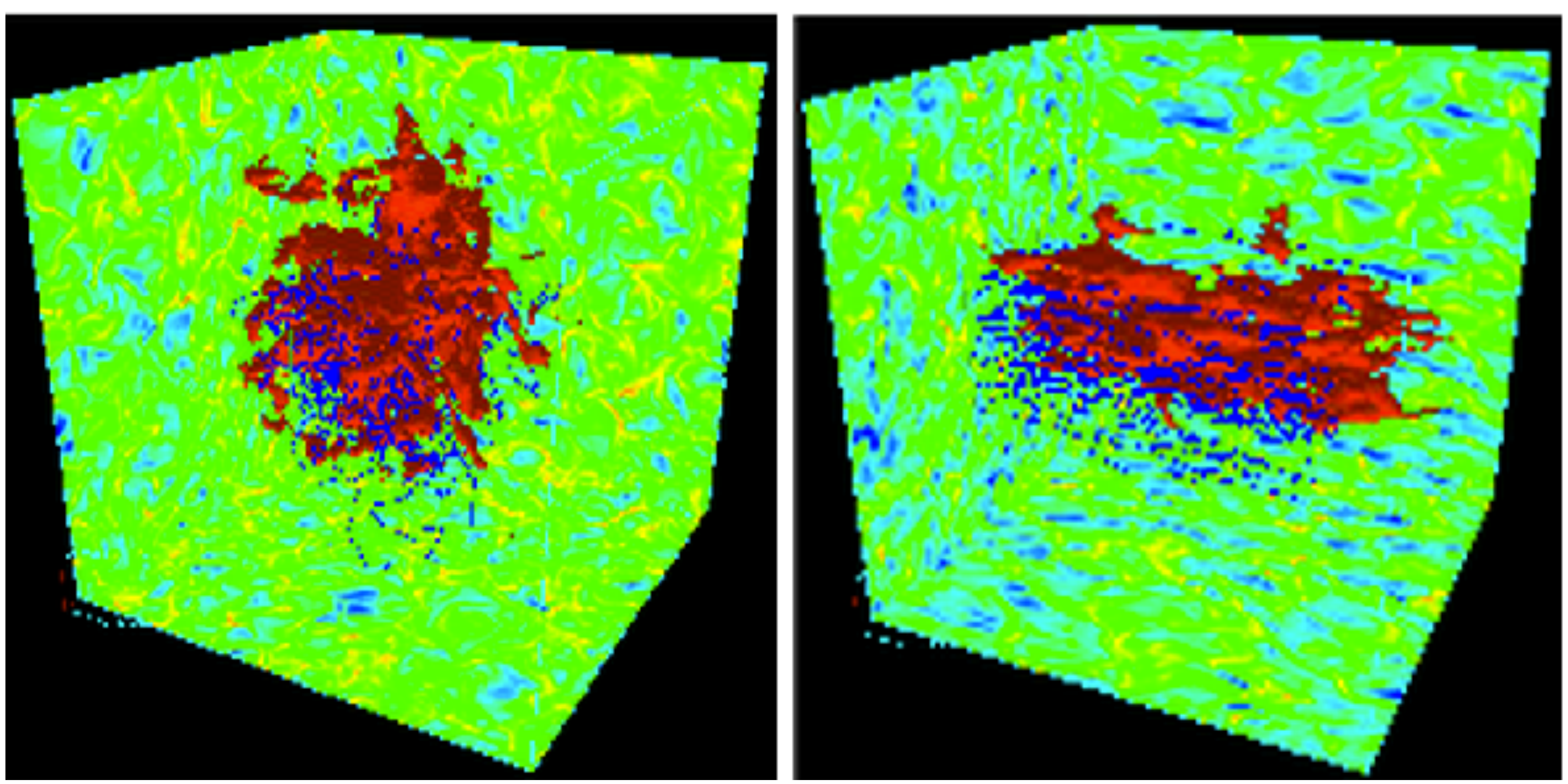
THE ASTROPHYSICAL JOURNAL, **185**: 505–533, 1973 October 15

THE FORMATION AND DEPLETION OF MOLECULES IN DENSE INTERSTELLAR CLOUDS*

ERIC HERBST† AND WILLIAM KLEMPERER
Department of Chemistry, Harvard University
Received 1973 April 9; revised 1973 May 24

More detailed chemical models

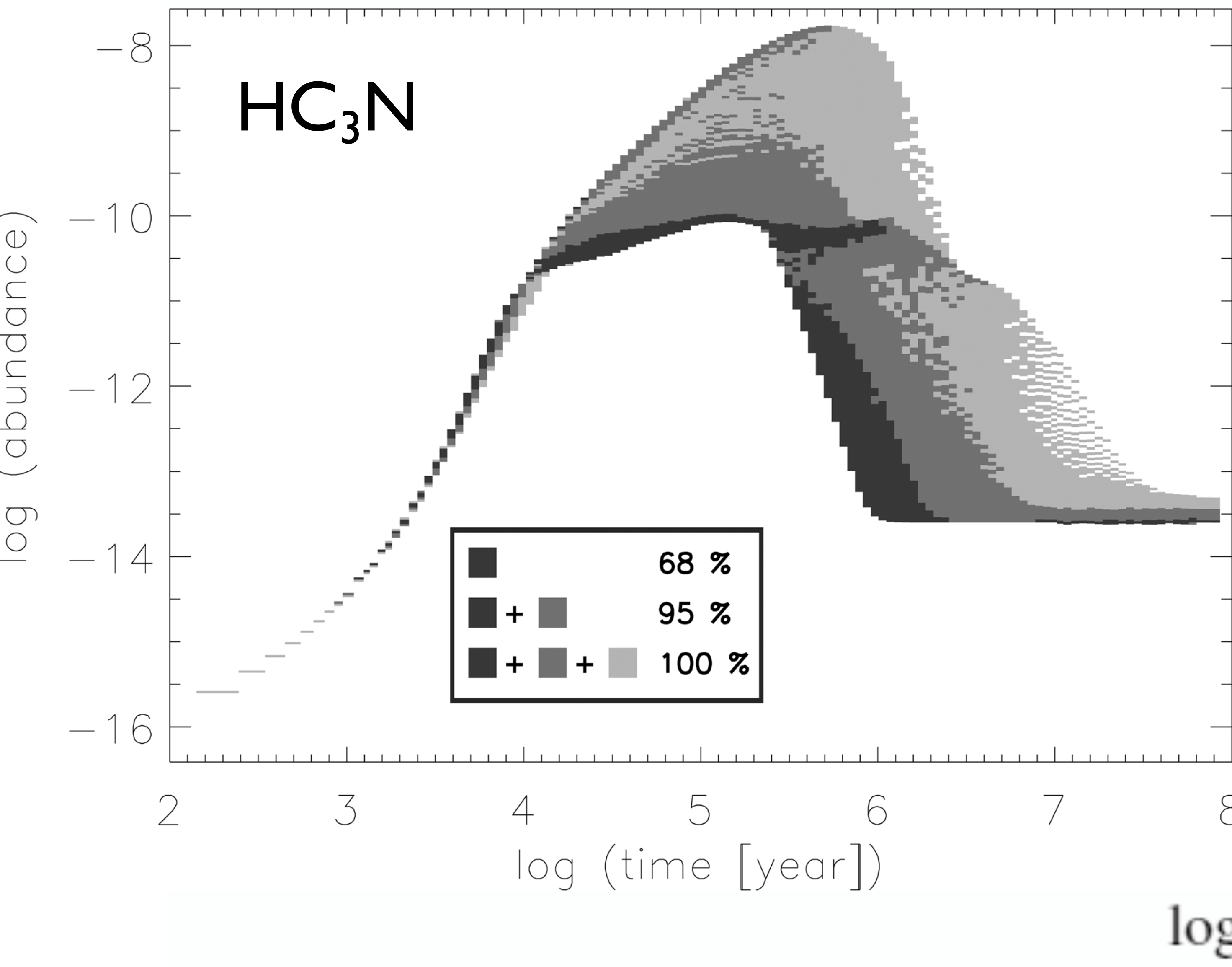
- 1–3D models with (magneto-)hydrodynamics and radiation (e.g., Aikawa et al. >1999; Commerson et al. >2012)
- Chemo-dynamical models: cycling of gas parcels from inner to outer to inner regions (e.g., Boland & de Jong 1982, Xie et al. 1995, Willacy et al. 2002, etc.)

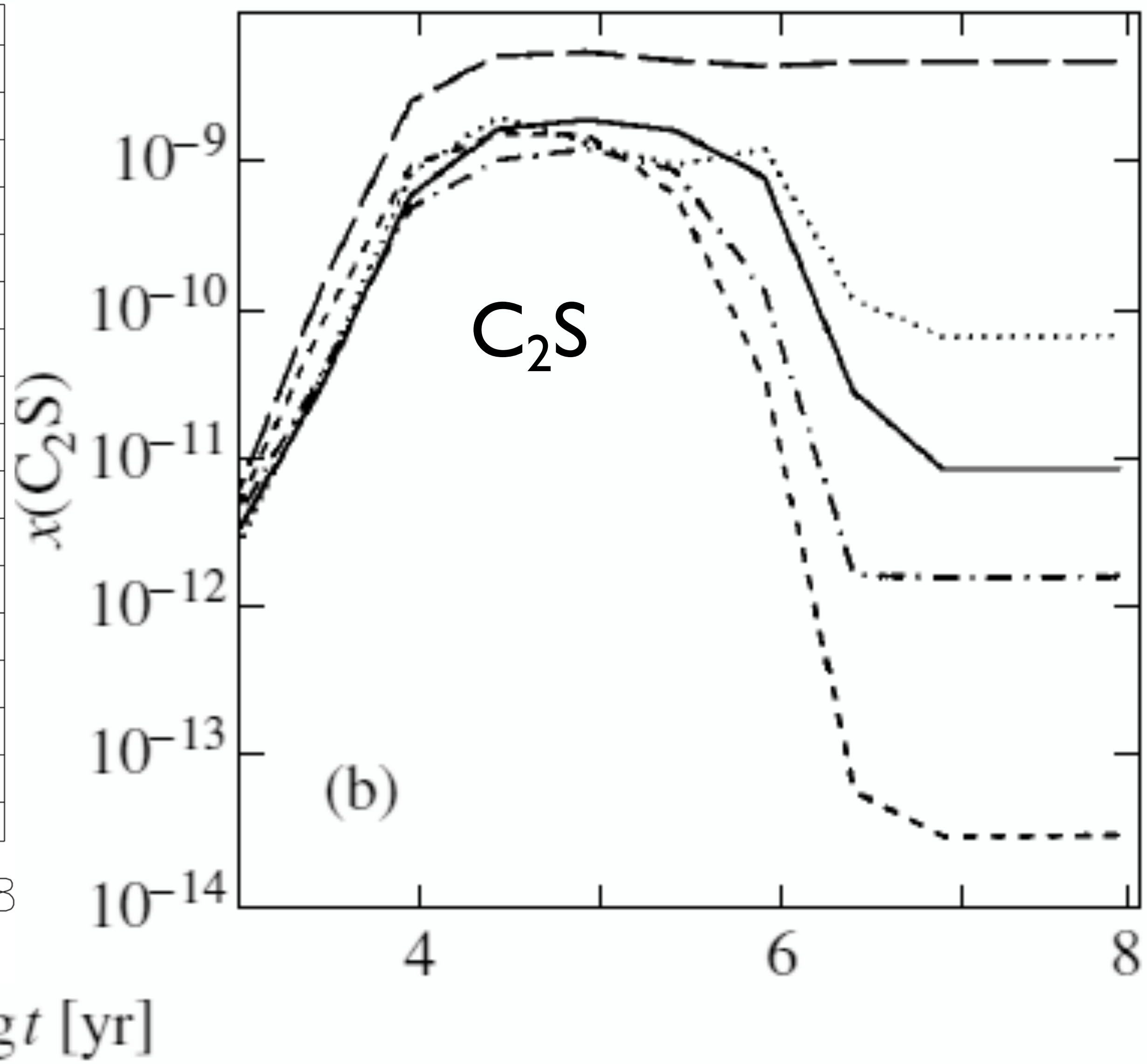


Problems of dense cloud models

- Is physics well known?
- How large is depletion of heavy elements?
- Initial abundances from an earlier diffuse phase?
- Are dust grains the same as in diffuse ISM?

Problems in dense cloud models: uncertain reaction rates



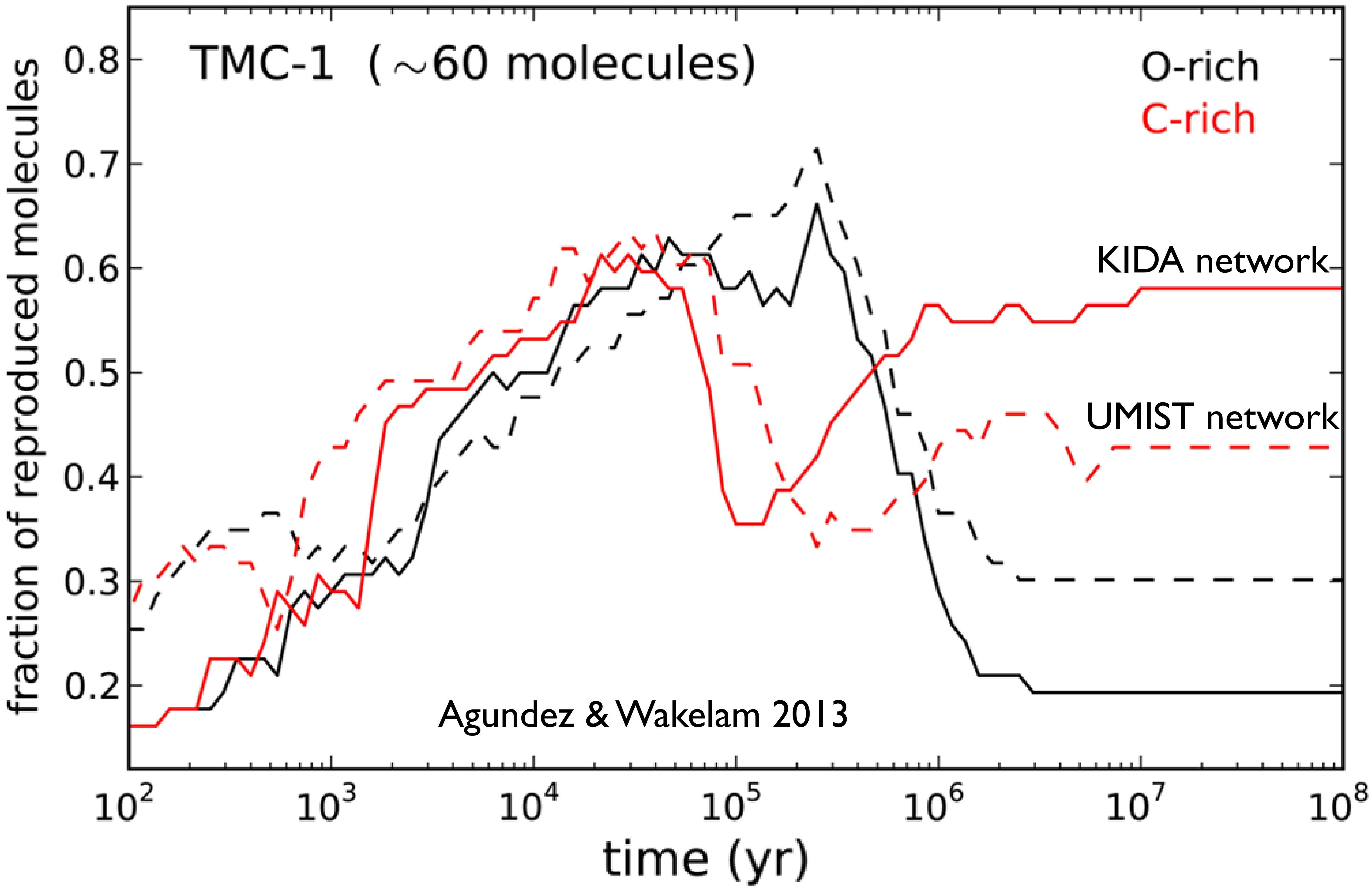


- Reaction rates are uncertain by factors of 1.25 – 10 ⇒

  Modeled abundances are uncertain by factors of >3

Vasyunin et al. (2004, 2007), Wakelam et al. (2005, 2006)

Feasibility of dense cloud models



- ~70% of 60 observed molecules are reproduced at 3 x 10^5 years
- Oxygen-rich initial abundances are preferred

Thank you!