The Atomic to Molecular Transition in the Interstellar Medium

Theoretical, Laboratory, and Observational Perspectives

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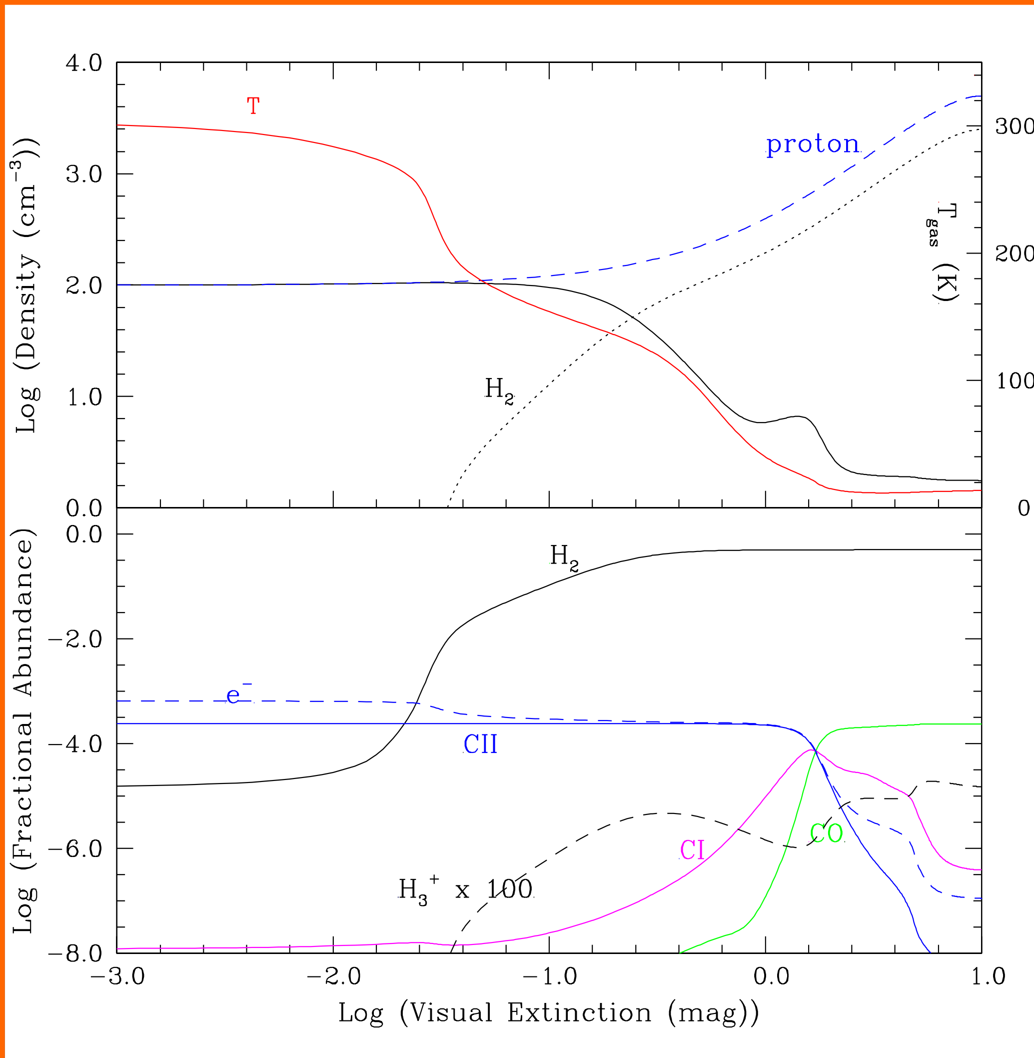
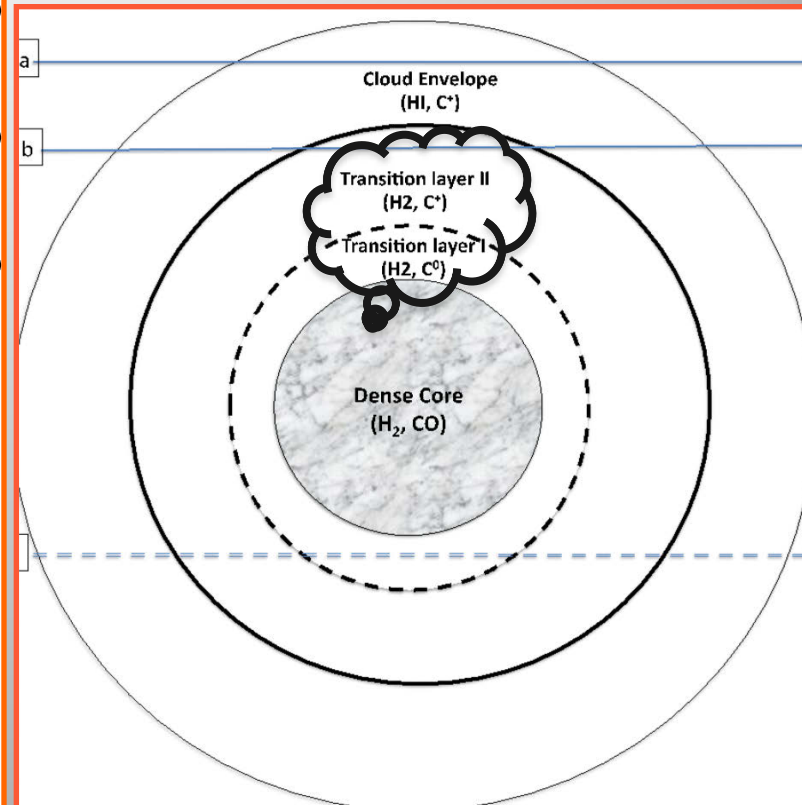
Definitions of a "Molecular Cloud"

- The logical definition of a molecular cloud is a region in space in which molecules are the predominant form of matter
  - This is equivalent to saying regions in which hydrogen is predominantly H_2
- The observational definition of a molecular cloud is the region in space defined by ^{12}CO emission

The availability of improved observational data on other key constituents and coolants (CI, CII) as well as HI, together with evolving theoretical models of cloud evolution suggest that reexamination of the atomic-to-molecular transition is timely

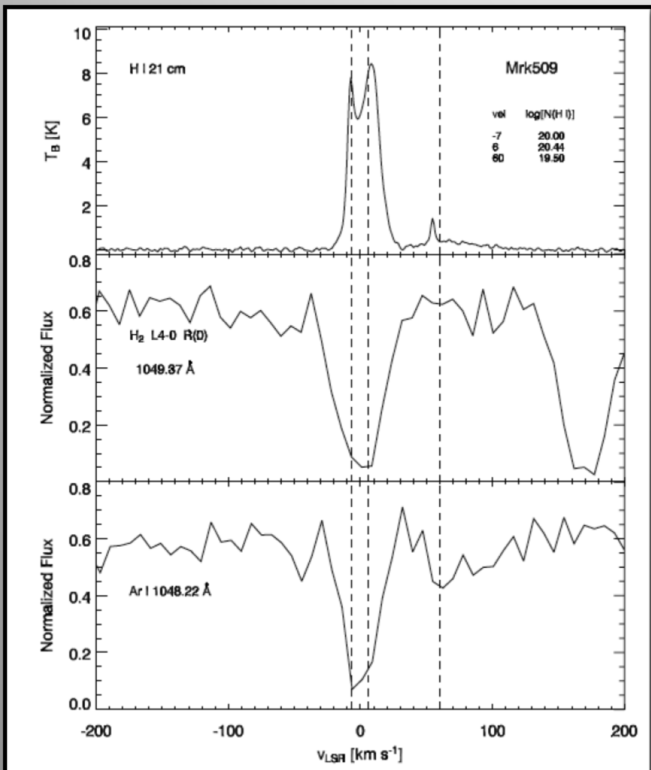
The Transition Phase

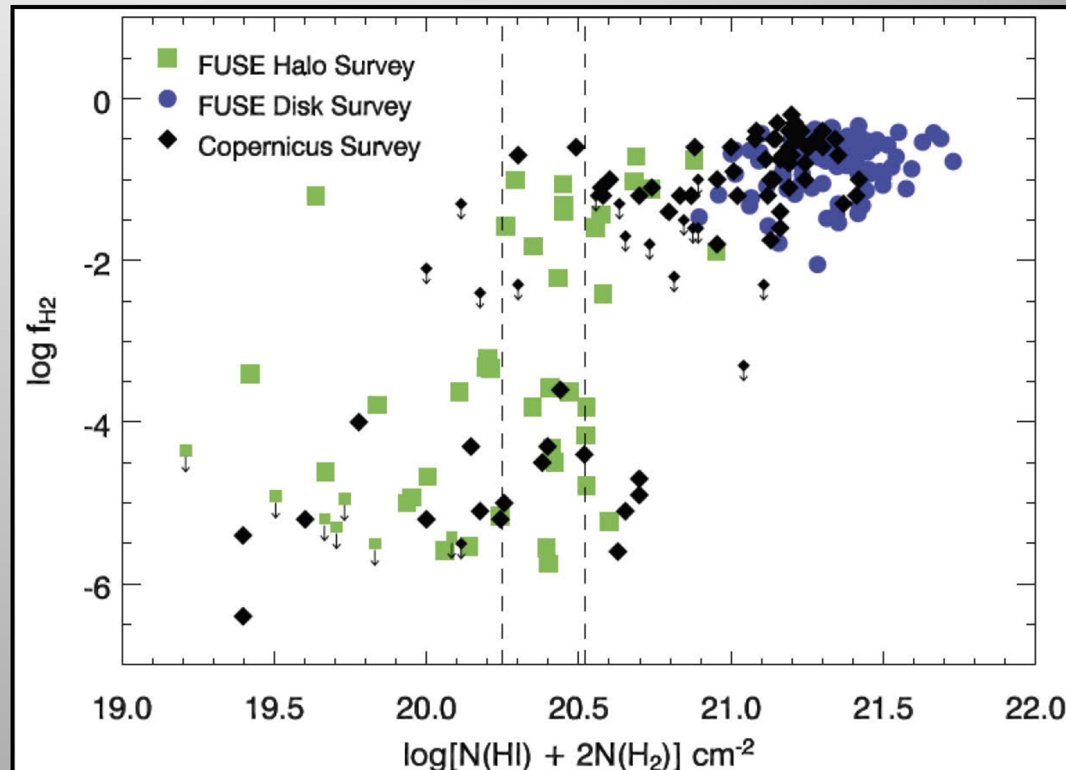




The HI-H_2 Transition Should be "Simple"

HI measured by 21cm emission; H_2 by UV absorption (towards stars and extragalactic sources) *Gillmon+ 2006*





H_2 photodissociation rate is large in unshielded regions. Self-shielding determines the "transition" at $20 \leq \log N/\mathrm{cm}^{-2} \leq 20.5$

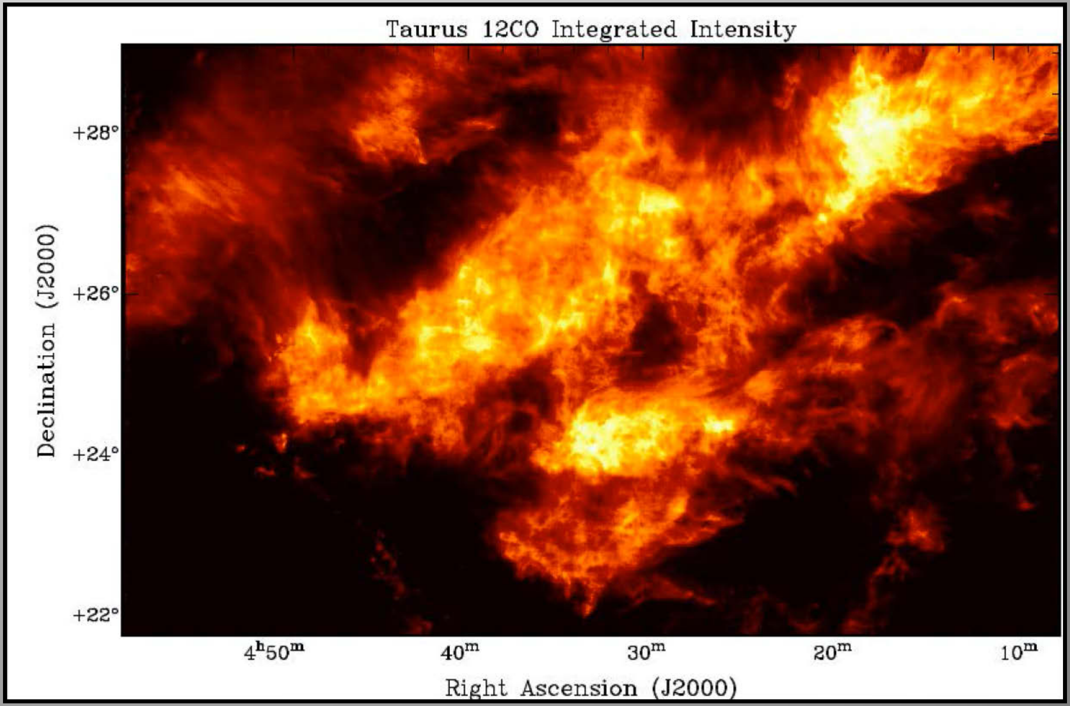
Tracing Molecular Clouds

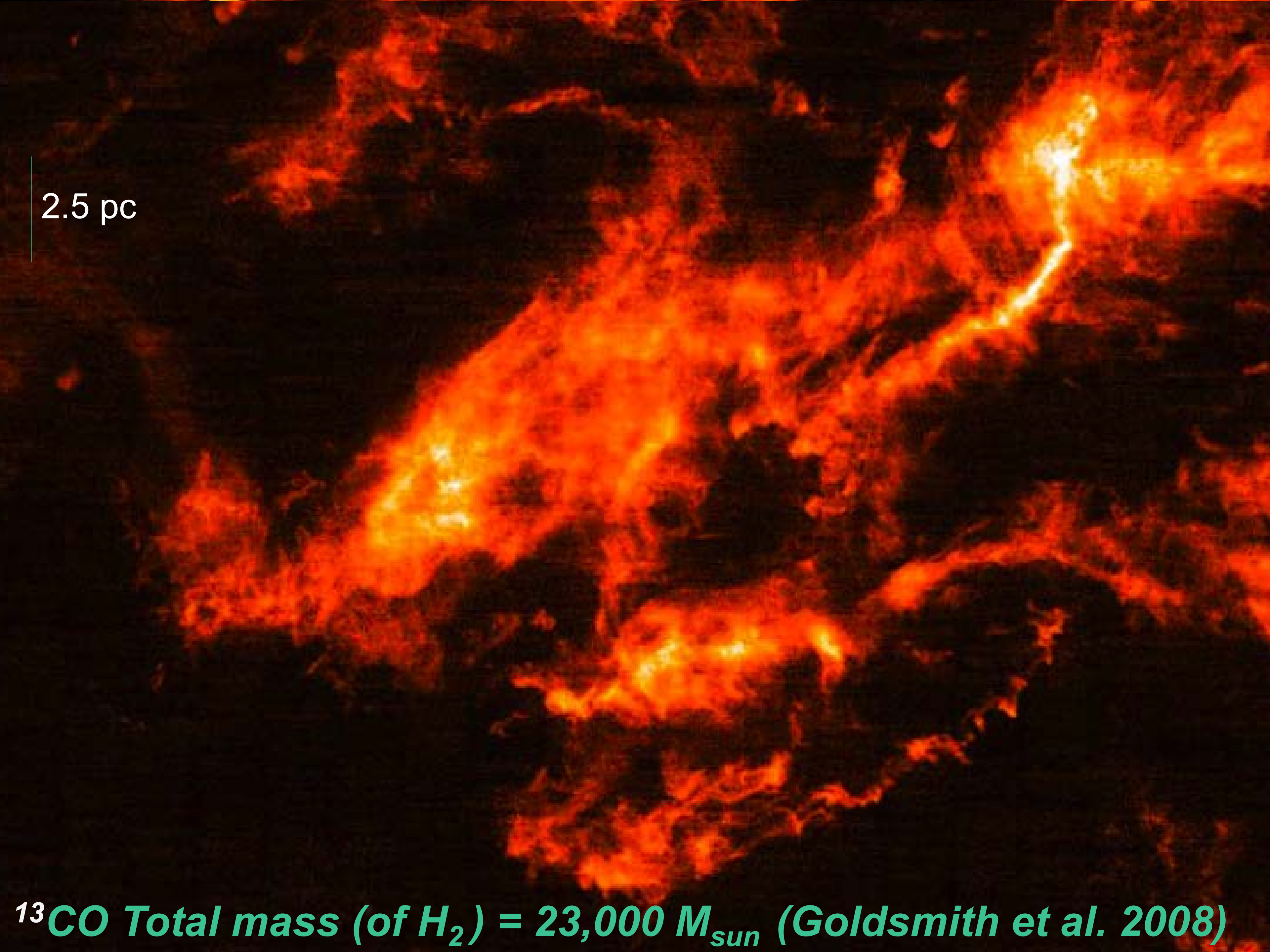
- Molecular clouds are not readily mapped in H_2 absorption due to paucity of background sources and excessive opacity.
- The most important molecular gas tracers are the isotopologues of carbon monoxide. ^{13}CO and $C^{18}O$ each have advantages and disadvantages in terms of abundance variations mitigated by chemical isotopic fractionation and depletion on to grain surfaces.
- Dust emission has great value, especially with availability of high sensitivity, high angular resolution observations, but it does not give any kinematic information.

Even ^{12}CO, though very optically thick, shows surprising detail, especially of lower column density regions.

In particular, ^{12}CO images suggest that boundaries of molecular clouds are highly structured.

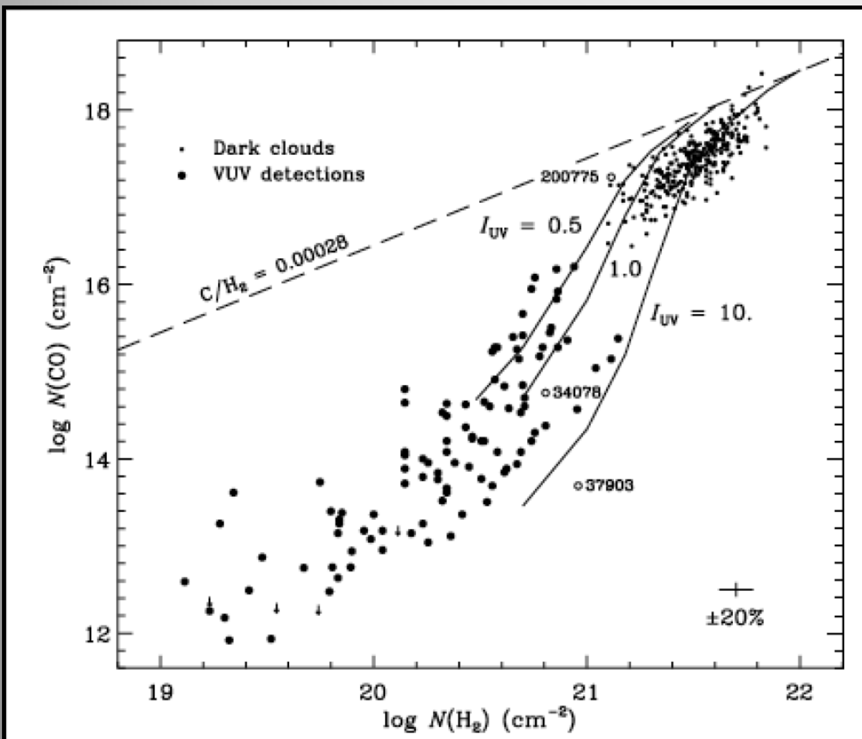
There are indications of material flows at cloud edges.

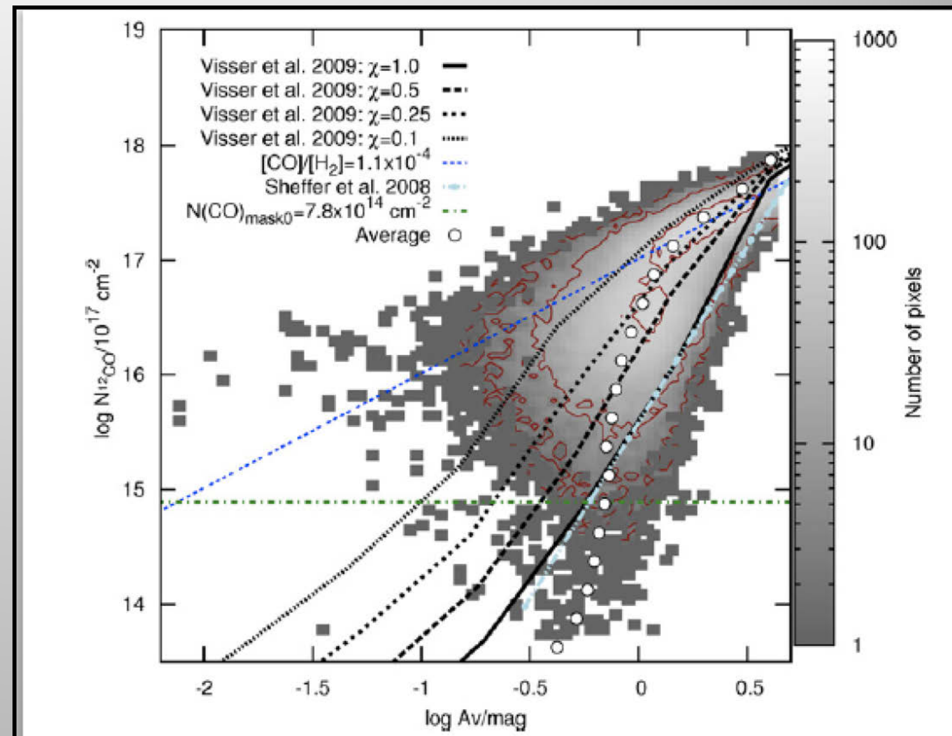




^{13}CO Total mass (of H_2) = 23,000 M_{sun} (Goldsmith et al. 2008)

CO Fractional Abundance Requires A_v = 2 – 5 mag. to Approach Saturated Value



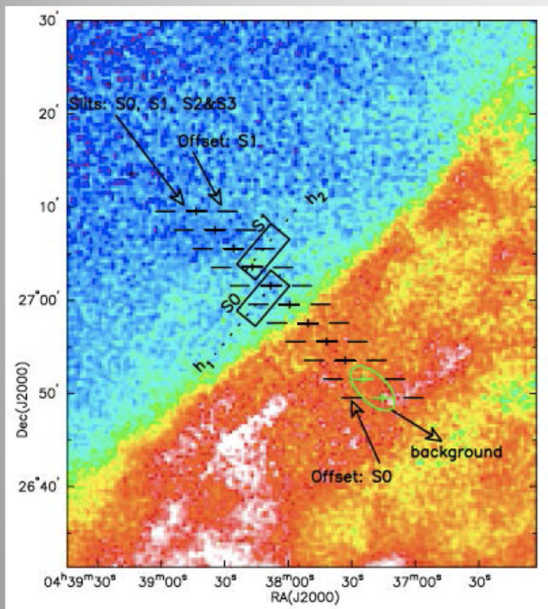


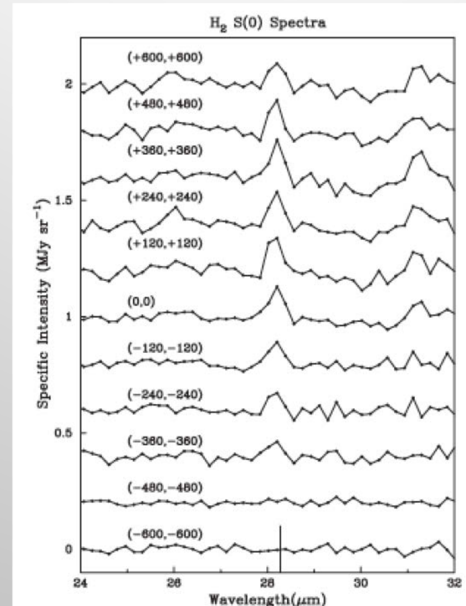
Sheffer+ 2008; UV absorption
Variety of UV radiation fields

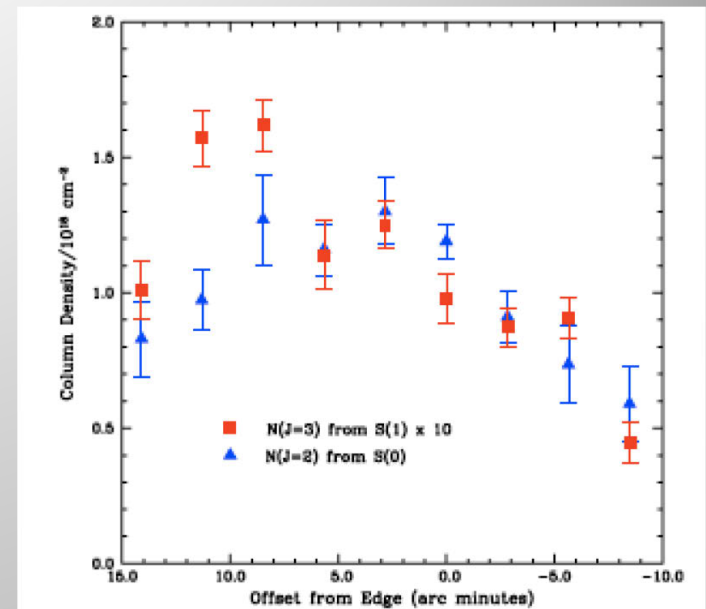
Pineda+ 2010; J=1-0 emission
Boundaries of Taurus Molecular Cloud with modest ISRF

Good, comprehensive models are needed to analyze cloud edges using CO

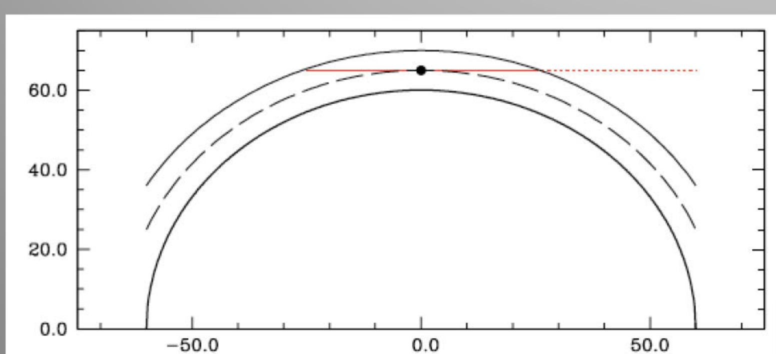
H_2 Pure Rotational Transition Emission From Edge of Taurus Molecular Cloud





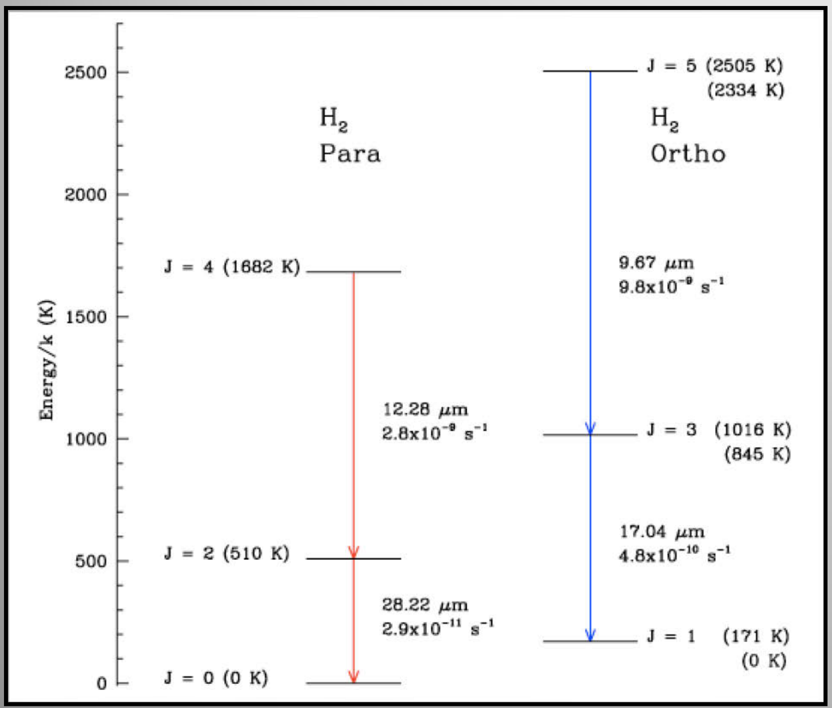


(Goldsmith, Velusamy, Li & Langer 2010)

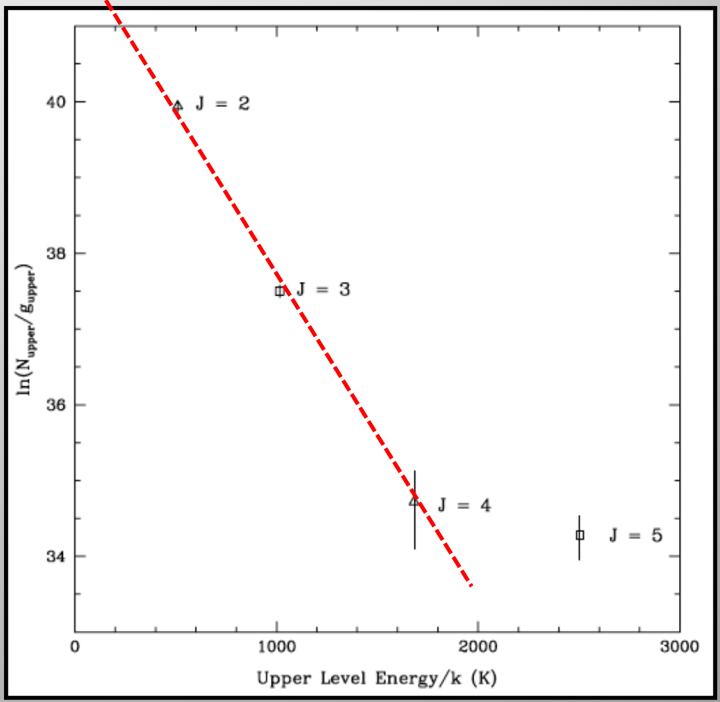


Due to the local geometry, we are seeing “limb brightening” of the warm H_2 layer that surrouds the cloud defined by CO emission

The Observed H_2 is WARM $T_{ex} \geq 200K$



N(H_2) in "warm layer" ~ 10^{18} cm^{-2}



Average of "outside" positions

The observed H_2 is likely only a small fraction of total present in this layer, but there is still more "warm H_2" than can be explained by PDR models

H_2 Emission Studied by *Habart+ A&A2011*

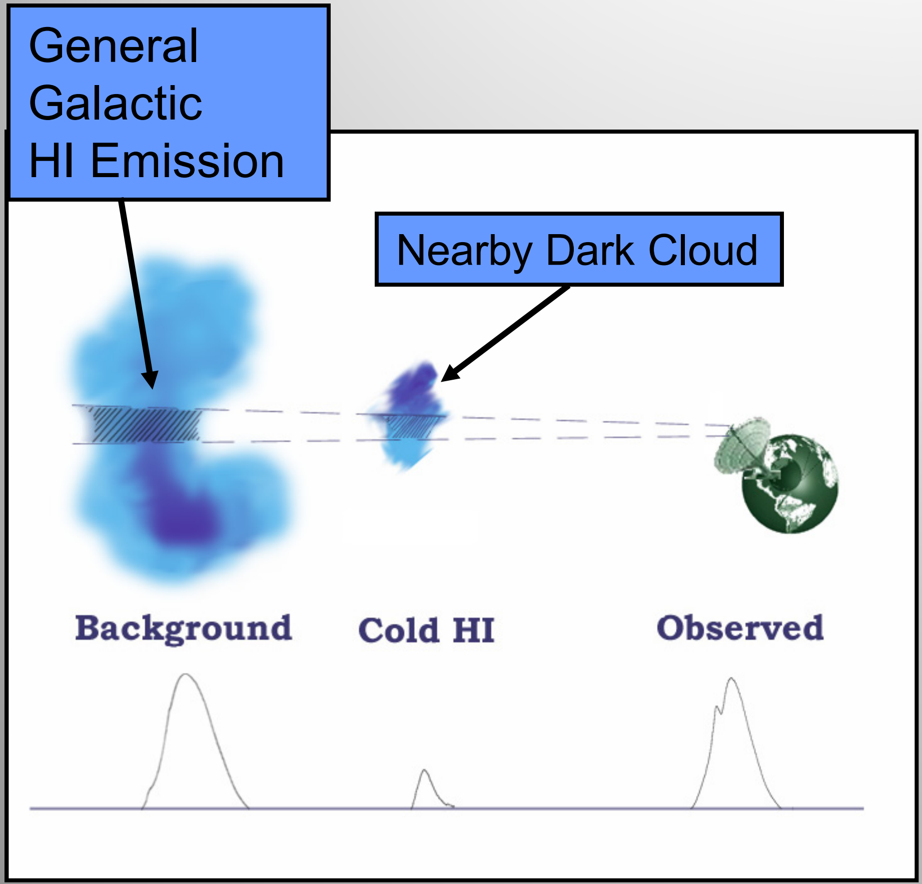
- 5 PDRs with radiation field enhancements in range 5 to 500
- With Spitzer, IRS measure pure rotational lines $2 \leq J \leq 7$ in $v = 0$ and $J = 3$ in $v = 1$
- Find a range of excitation temperatures from 200 K to 500 K, increasing with increasing J
- Excitation dominated by UV pumping, rather than collisions
- Enhanced formation rate, by factor ~ 5 required to give reasonable agreement with PDR model $k = 1.5 \times 10^{-16}\ cm^3 s^{-1}$

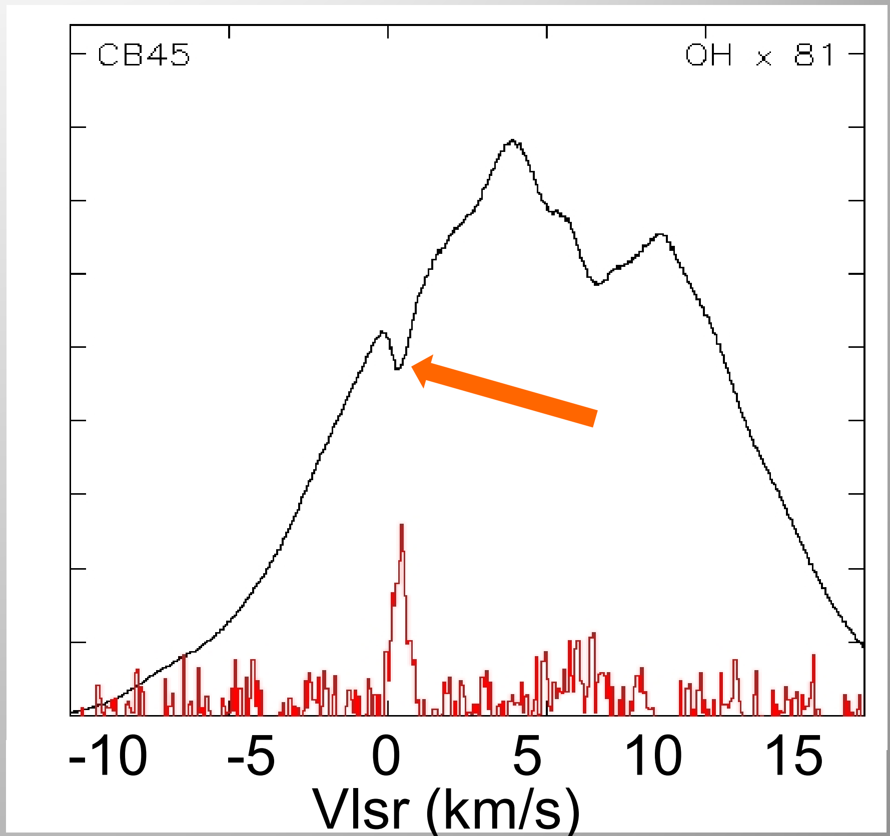
H_2 Observations: 2 Possibilities in Next Decade

- EXES – very high resolution grating spectrometer for SOFIA covering 5 µm to 28 µm
  - R = 3000, 10^4, 10^5
  - 1024 x 1024 Si:As BIB Detector array
  - Slit length = 11" at R = 10^5
  - angular resolution ~1.8" @ 17 µm
- MIRI Instrument on JWST
  - 12.3 µm S(2) and 17 µm S(1) lines will be covered at R ~ 3000
  - 28.2 µm S(0) line situation is not so clear
  - 0.2" to 0.3" pixel size on sky

EXAMPLE: S(1) emission from Taurus equivalent to flux of 6×10^{-20} Wm^{-2}. MIRI sensitivity ~ 5×10^{-20} Wm^{-2} (10σ in 10^4 s) So this is feasible, if not easy. Higher G sources should be straightforward.

The Atomic Hydrogen Component of Molecular Clouds

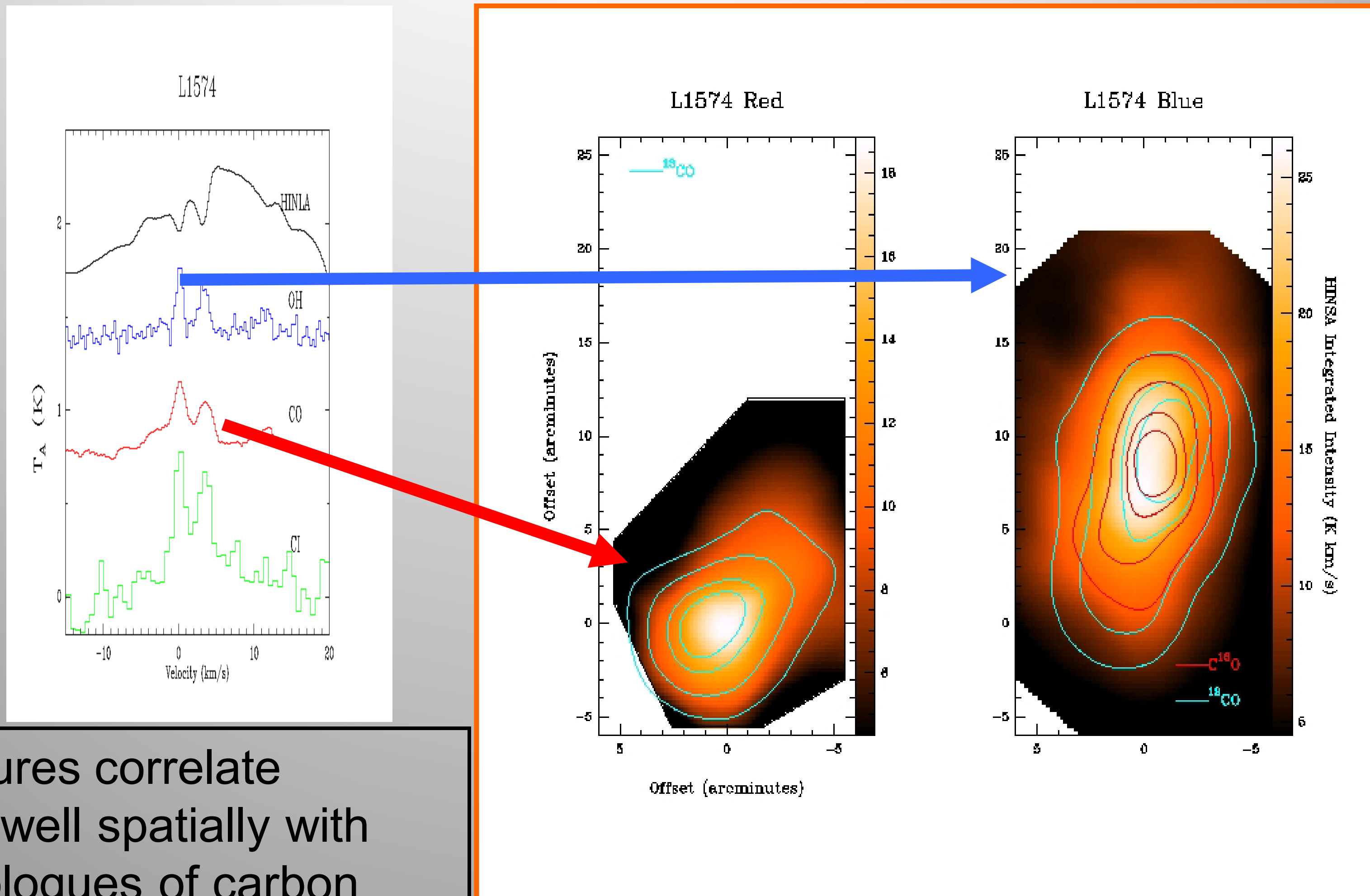




(Li & Goldsmith 2003)

HI Narrow Self Absorption (HINSA)

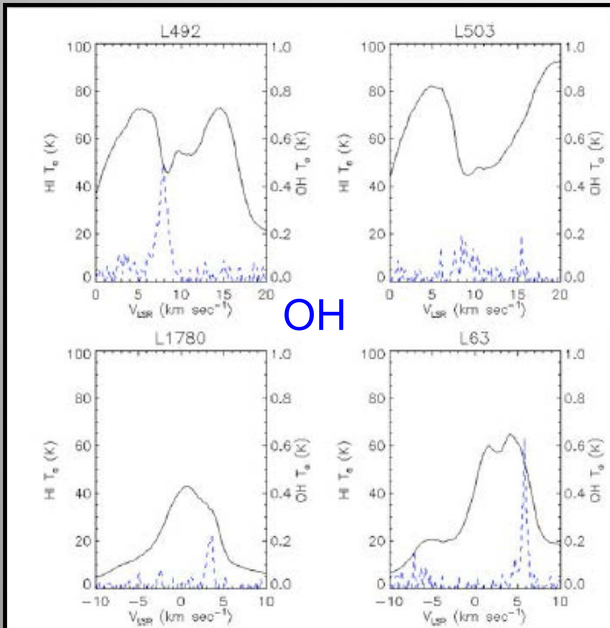
Correlation between HINSA and Molecules

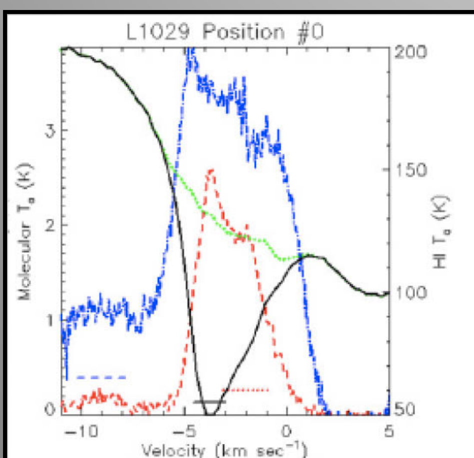


HINSA features correlate remarkably well spatially with rare isotopologues of carbon monoxide, even following details of distribution of different kinematic features.

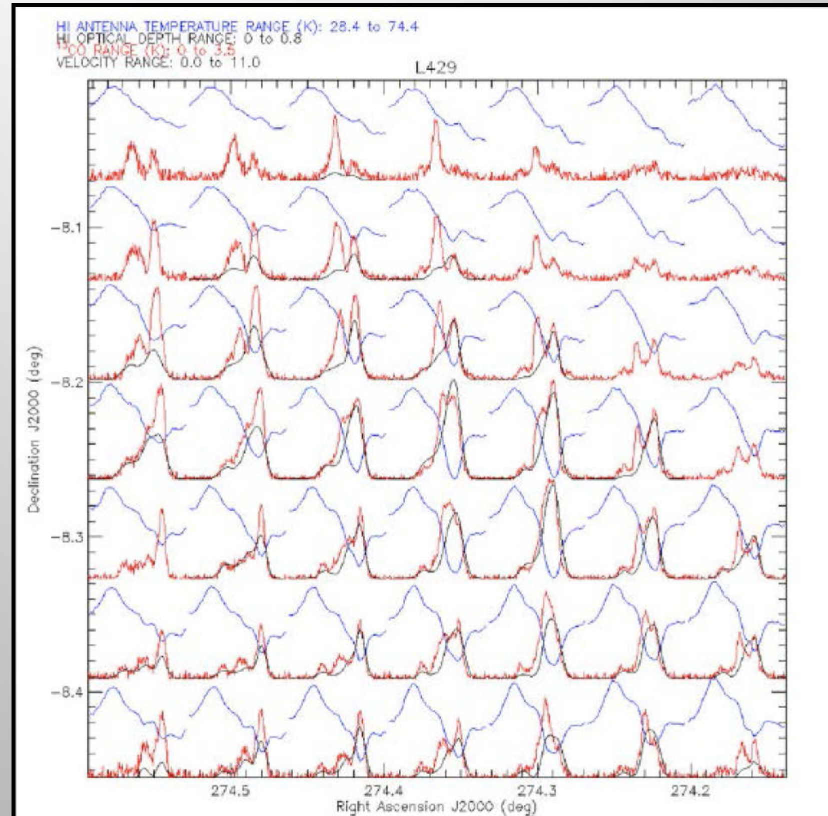
(Goldsmith & Li 2005)

GBT Survey of HINSA



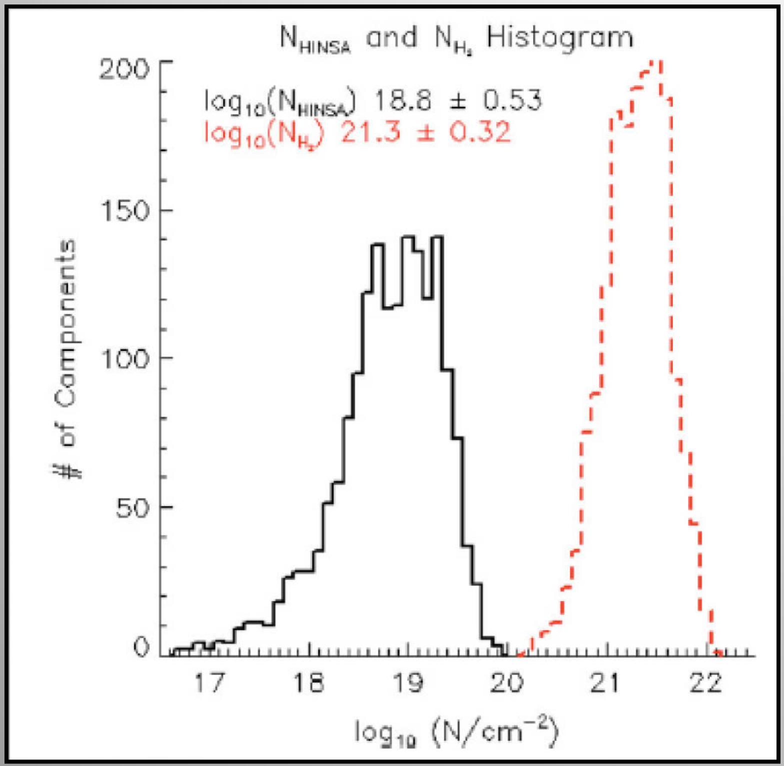


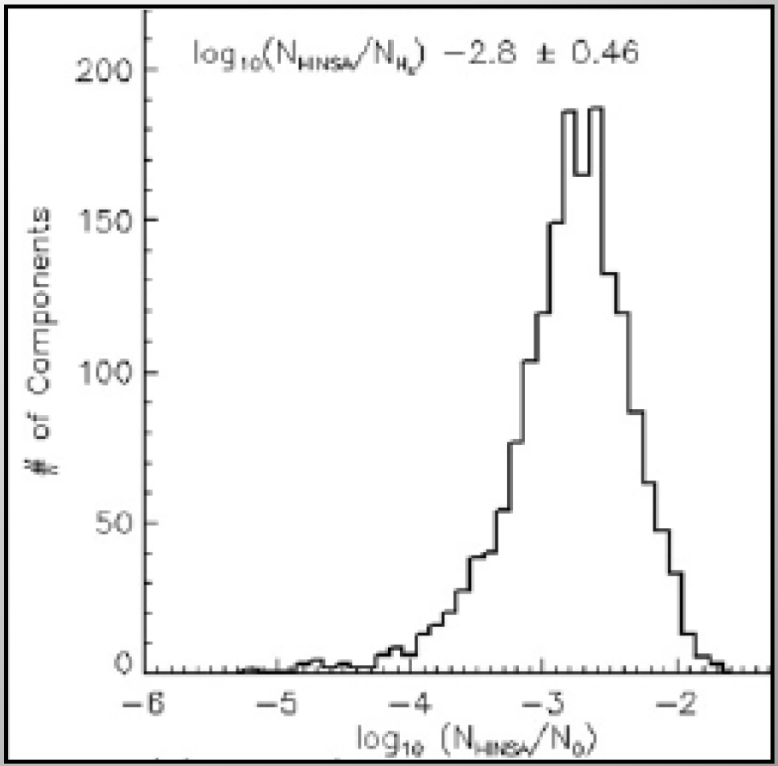
^{12}CO
^{13}CO
HI
HI (rec)



HINSA features detected in 80% of clouds out to distance D = 700 pc without noticeable trend as function of distance. (*Krco & Goldsmith 2008, 2010*)

Global Results of HINSA Survey





$<N(\text{cold HI})/N(H_2)> = 0.0016$

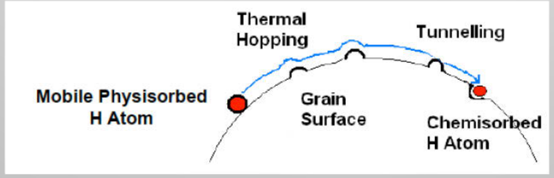
Formation and Destruction of H_2

Formation: on grains by one of various processes all of which depend on the grain surface area and the density of atomic H. Commonly envisioned scenario is

(1)An H atom hits and sticks to grain (2) Another H atom does the same

(3) H atoms hop or tunnel around grain surface until they "find" each other

(4) Two H atoms then form H_2 which has sufficient energy to desorb from grain surface



Destruction:

(1) By cosmic rays with rate $\zeta \sim 5\times10^{-17}\ s^{-1}$ within well-shielded regions, though may be greater at cloud edges/diffuse clouds

(2) By UV at cloud edges and in translucent/diffuse clouds. Critical parameters are the enhancement of UV field relative to standard ISRF and the total column density of hydrogen. The latter is critical due to significance of self-shielding.

H_2 Formation Rate and Rate Equation

$$R_{H_2} = \frac{1}{2} S_{H\,I} \epsilon_{H_2} n_{H\,I} \langle v_{H\,I} \rangle \sigma_{gr} n_{gr}.$$

General H_2 formation rate

$$n_0 = n_{H\,I} + 2n_{H_2},$$

Total proton density n_o

$$R_{H_2} = k'_{H_2\ MRN} n_{H\,I} n_0,$$

H_2 formation rate in terms of n_o

$$k'_{H_2} = 3.5 \times 10^{-18} \left[\left(\frac{S_{H\,I}}{0.3} \right) \left(\frac{\epsilon_{H_2}}{1.0} \right) \left(\frac{T}{10\ K} \right)^{0.5} \right] \left[\left(\frac{\rho_{gr}}{2\ g\ cm^{-3}} \right) \times \left(\frac{GDR}{100} \right) \left(\frac{a_s}{1.7 \times 10^{-5}\ cm} \right) \right]^{-1} \frac{a_s}{\sqrt{a_{max} a_{min}}}\ cm^3\ s^{-1}.$$

With MRN grain size Distribution
$k' = 1.2 \times 10^{-17}\ cm^3 s^{-1}$

$$\frac{dn_{H_2}}{dt} = k' n_{H\,I} n_0 - \zeta_{H_2} n_{H_2}.$$

ζ includes cosmic ray and UV dissociation
Only former is significant in cloud interior

Evolution of Model Cloud from Totally Atomic Phase at t = 0

Fractional Abundance of HI

$$x_1(t) = 1 - \frac{2k'n_0}{2k'n_0 + \zeta_{H_2}}\left[1 - \exp\left(\frac{-t}{\tau_{H\,I \to H_2}}\right)\right].$$

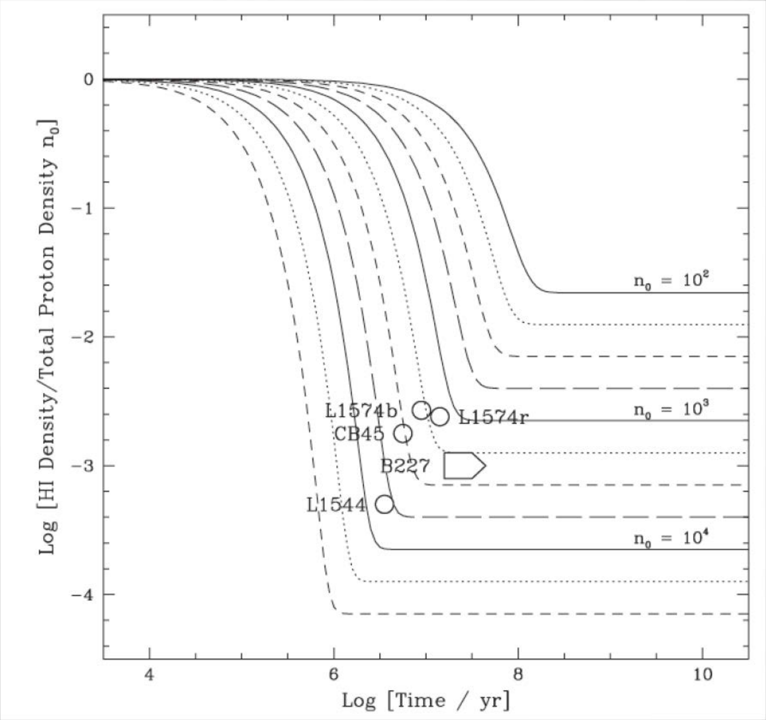
Characteristic Time Scale

$$\tau_{H\,I \to H_2} = \frac{1}{2k'n_0}.$$

T =1.3x10^9 yr/n_0

Steady-State Abundance of HI

$$x_1 \to \frac{\zeta_{H_2}}{2k'n_0} \quad \text{or} \quad n_{H\,I} \to \frac{\zeta_{H_2}}{2k'}.$$



(Goldsmith & Li 2005)

With ζ = 5x10^{-17} and k' = 1.2x10^{-17}
n_{HI} (steady state) = 2.5 cm^{-3}

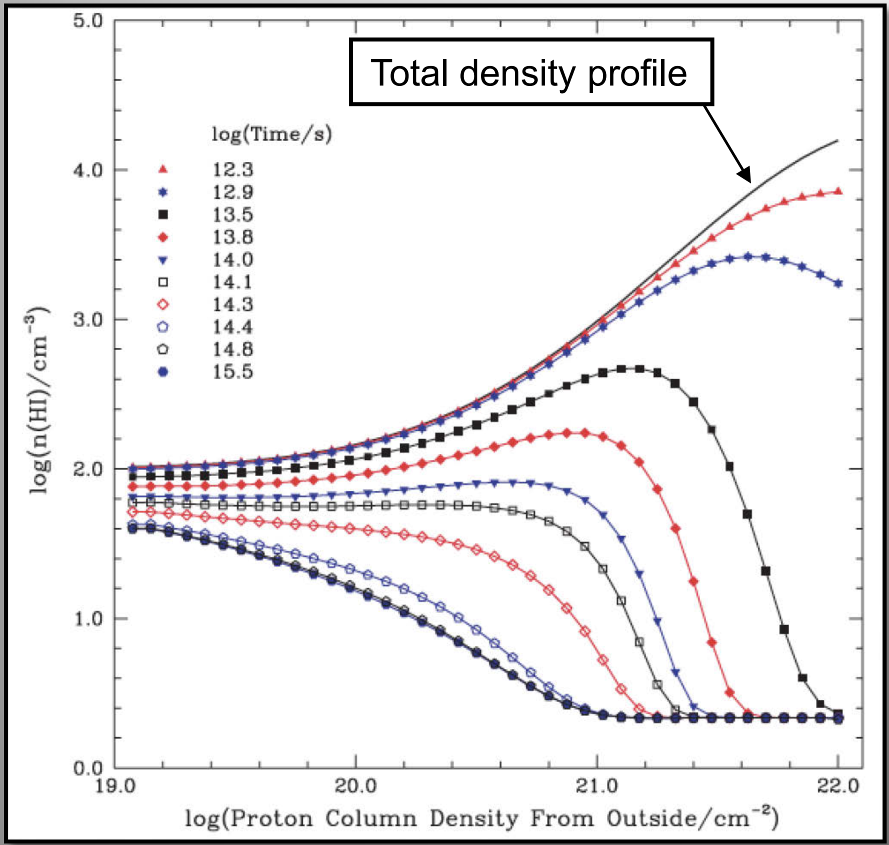
Some Conclusions from HI in Dark Clouds

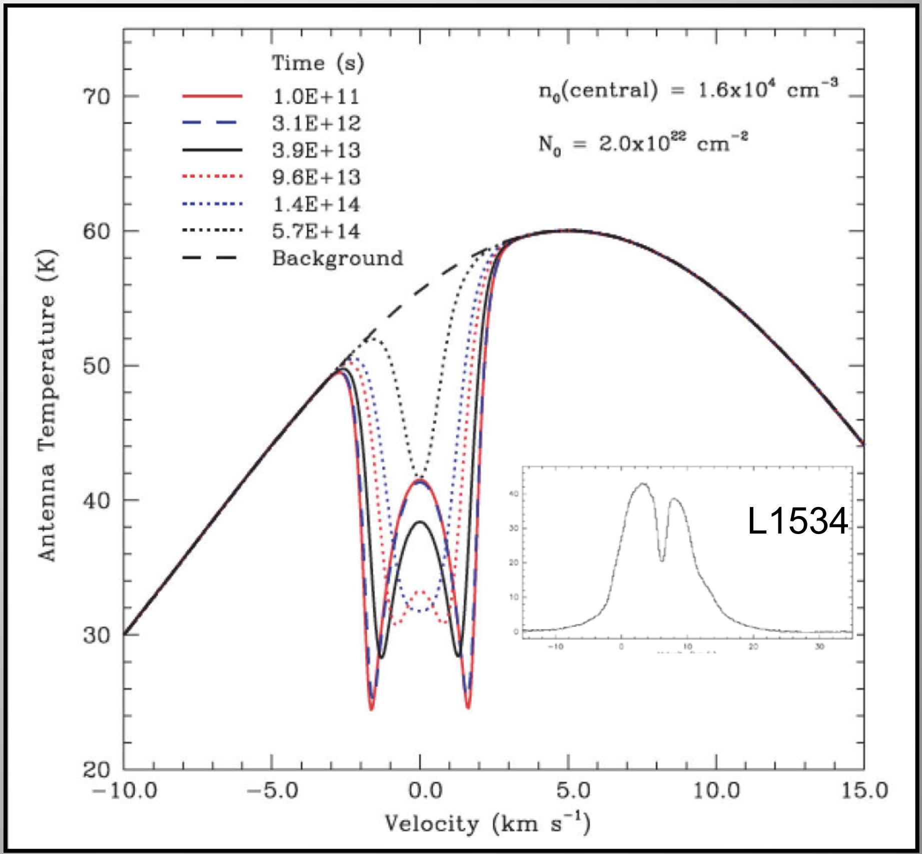
- Steady state fractional abundances of HI are $n(HI)/n(H_2) \sim 2x10^{-3}$ or $n(HI)/n_0 = 0.001$
- With central H_2 densities ~ 2000 cm^{-3}, n(HI) ~ 4 cm^{-3}. This is close to but slightly greater than steady-state value
- The implication is that these clouds have been evolving for 3 – 10 million years since "turnoff" of photodissociation. If the present density is larger than that in the past, the time elapsed is LONGER (see related discussion in *McKee & Ostriker 2007 in ARA&A*).

Evolution of Initially Centrally Condensed Atomic Cloud with N(HI) = 1×10^{22} cm^{-2} exposed to ISRF

H2 formation propagates like a wave from a centrally condensed cloud.

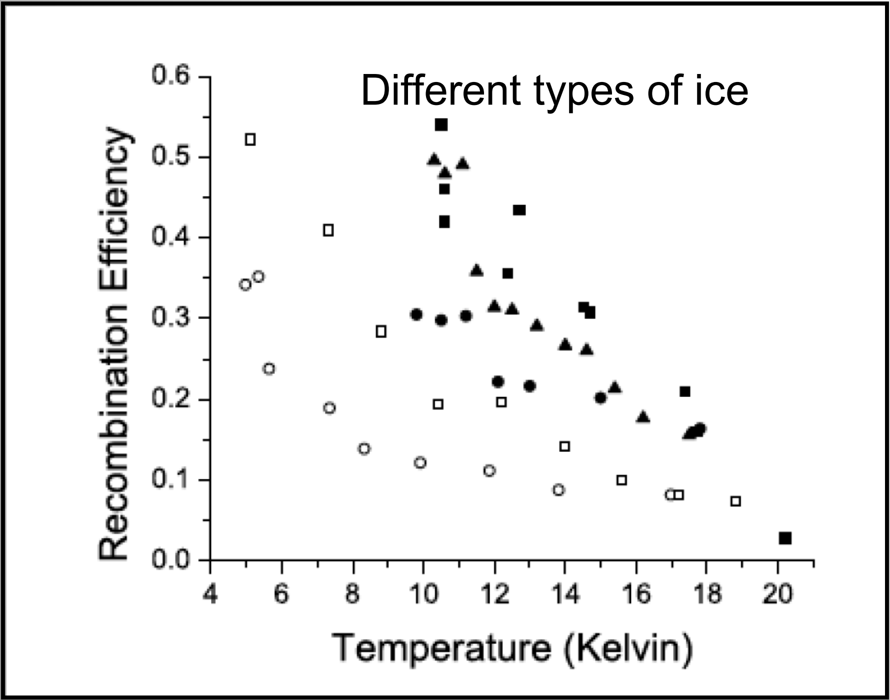
(Goldsmith, Li & Krco 2007)



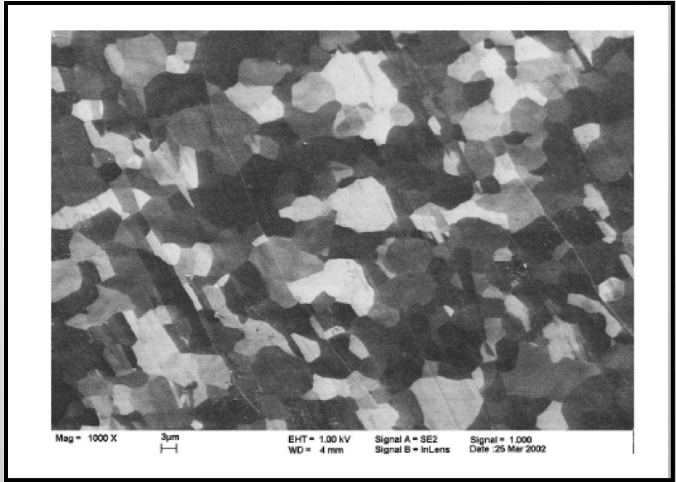


≥ 3×10^6 yr required to produce plausible line profiles and observed column densities of cold HI (≤ 10^{19} cm^{-2})

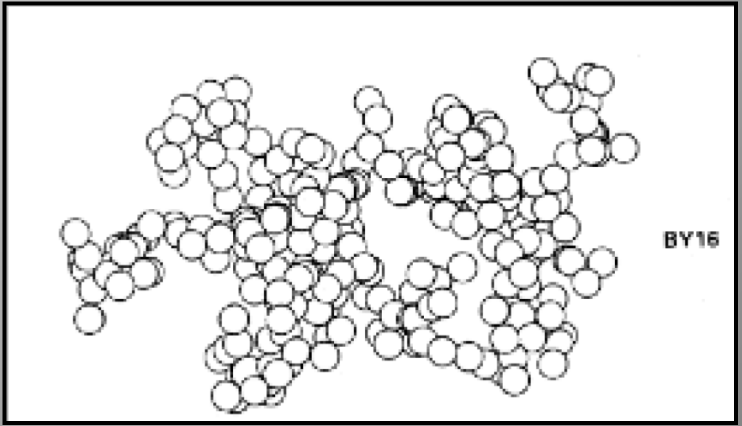
New Laboratory Measurements of H_2 Formation Efficiency Show Larger Temperature Range - but it is Still Small



Laboratory measurements of H_2 formation efficiency (Vidali et al. 2005)



Laboratory graphite surface (Zecho et al. 2002)



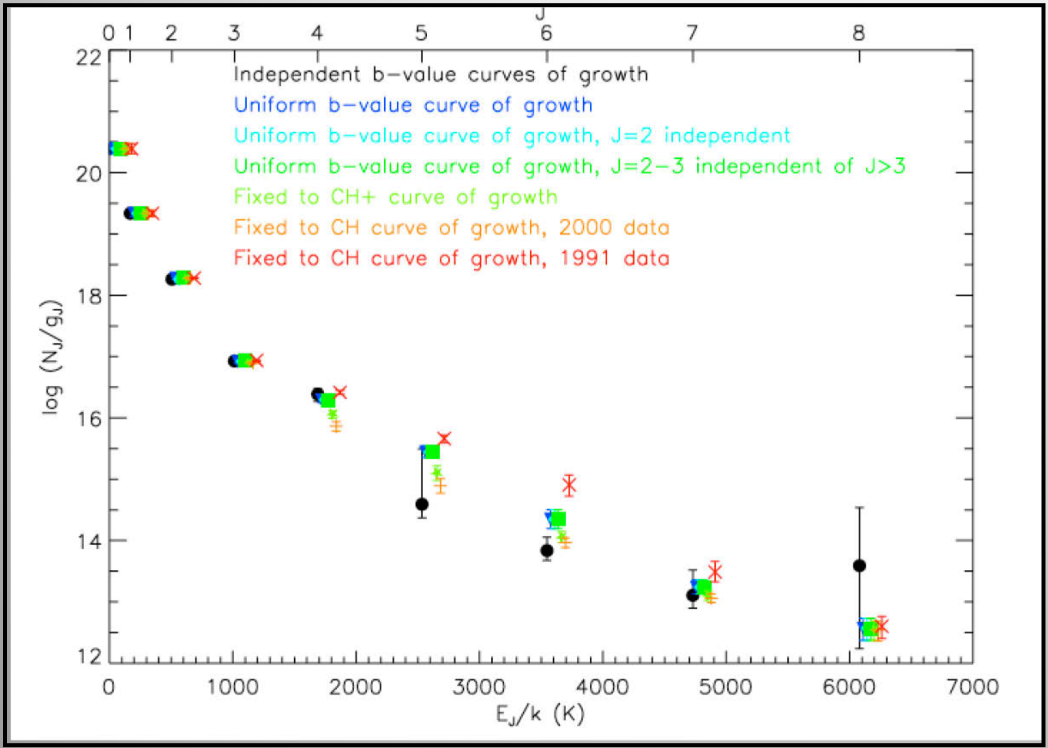
Model fractal grain (Wright 1987)

These spheres represent clusters of atoms

Effects of H_2 Formation

- Beyond the basic question of MAKING H_2, an important astrophysical input is the amount of energy with which a newly-formed molecule leaves the grain
- Historically, this has always been considered to be a large fraction of the 4.5 eV binding energy of H_2 molecule
- Recent measurements of H_2 formation on silicate surfaces suggest that H_2 molecules are thermalized with grain temperature and desorb with low kinetic energy – changes the energy flow in clouds and also initial level populations of newly-formed H_2. (Perets+ ApJ 2010)
- A related question is the ortho-to-para ratio (OPR) of H_2, which can affect collisional excitation of other molecules (e.g. Flower, Offer, & Schilke 1990)and also chemical reaction rates (e.g. deuteration; Flower+ A&A 2007.)

Excitation State and OPR of H_2



H_2 column densities in diffuse cloud towards HD38087 (*Jensen+ ApJ 2010*). Lower levels characterized by T_{ex} ~ 70 K, but higher levels ($J \geq 3$) have $T_{ex} \geq 450$ K. What is the origin of this high excitation?

Ortho-Para Ratio (OPR)

Jensen+:

HD65056 0.885 ± 0.012
HD147888 0.209 ± 0.006

Gnacinski:

HD147888
v = 0 0.16
v ≥ 1 1.2

High energy H_2 with unexpected OPR could produce a variety of surprises

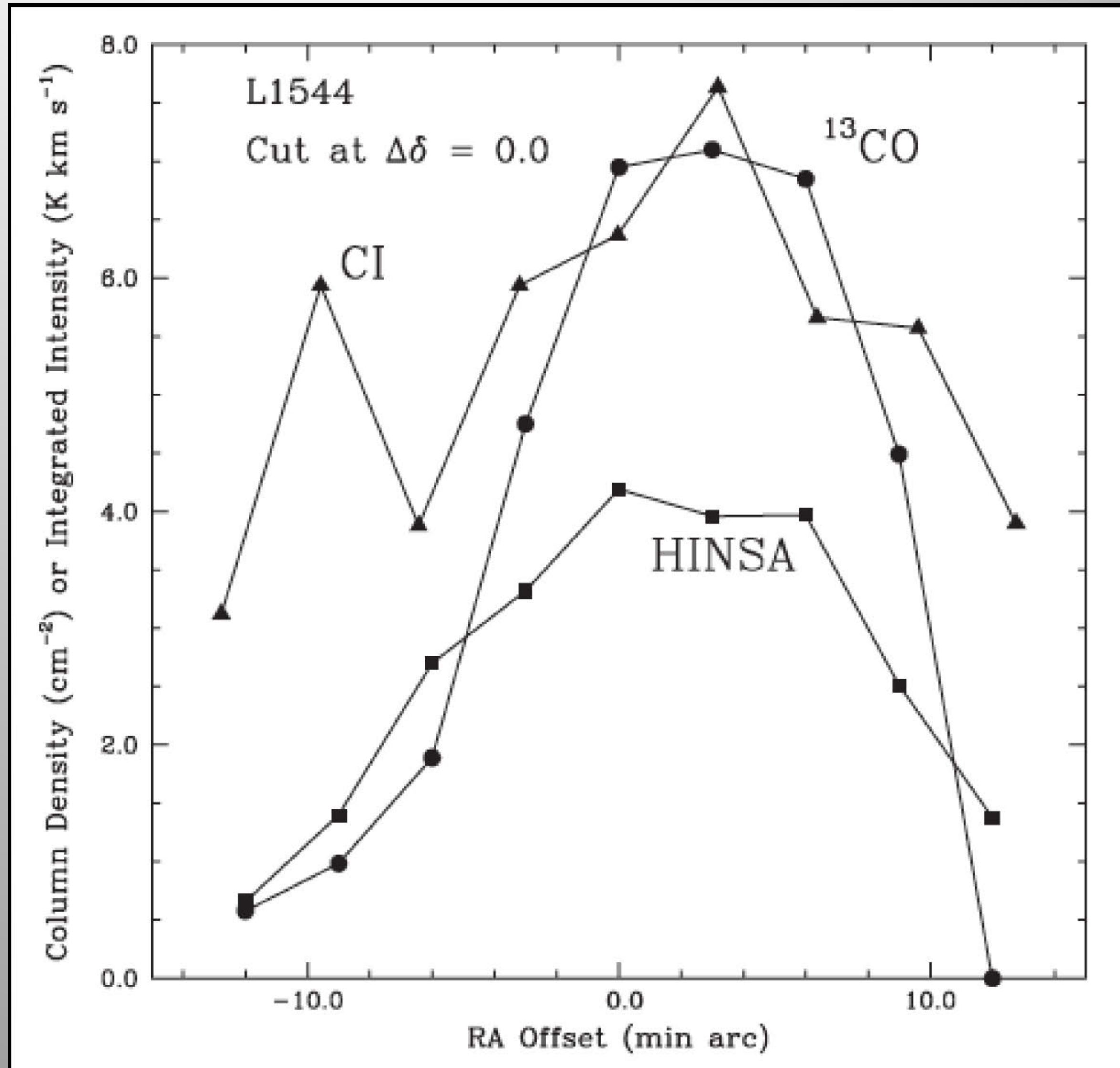
CI – Another Cloud Chronometer (?)

CI is rarely observed in dark clouds, but such observations can provide valuable information about cloud structure AND possibly of cloud evolutionary state.

High sensitivity required!

CI observations shown here obtained with SWAS satellite and long integrations (Goldsmith & LI 2005).

CI more spatially extended than ^{13}CO and even than ^{12}CO.



Explaining the CI "Onion Skin"

CI is formed by (1) recombination of C^+ [low A_v] and (2) photodissociation of CO [up to A_v ~ few]

For standard ISRF, the 'CI-layer' is located at $A_v \cong 1$

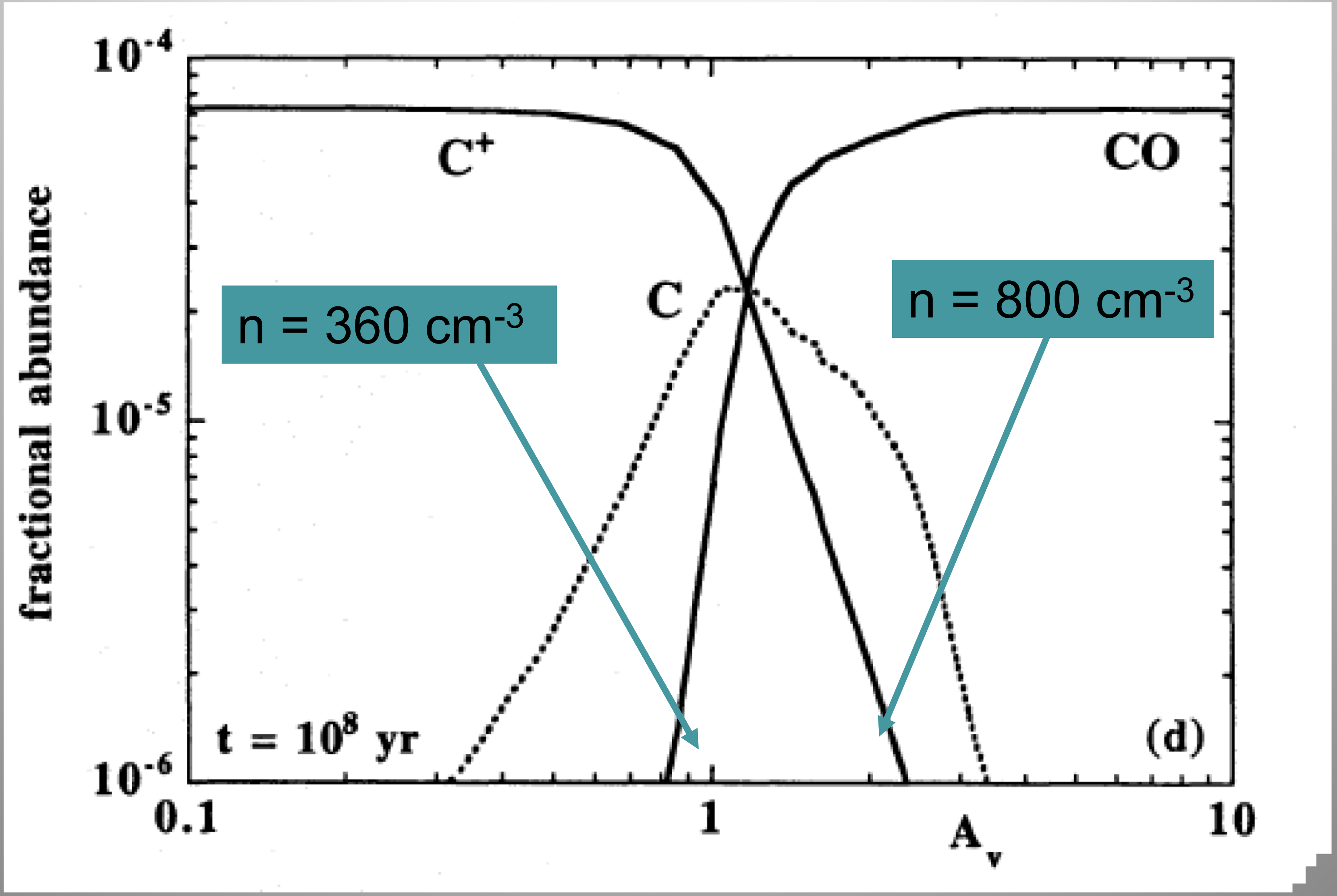
The density in this region is typically not large (~100 cm^{-3}) so that the timescale for the CI abundance to achieve its steady-state value is long.

Time-dependent model by Lee et al. (1996) treated a slab with uniform, time-independent temperature, but density profile

$n(A_v) = 10^2[1 + 9(A_v/A_{v\,max})]^2\ cm^{-3}$ for $0 \le A_v \le A_{v\,max} = 10$

External radiation field characterized by X = 1 incident from one side

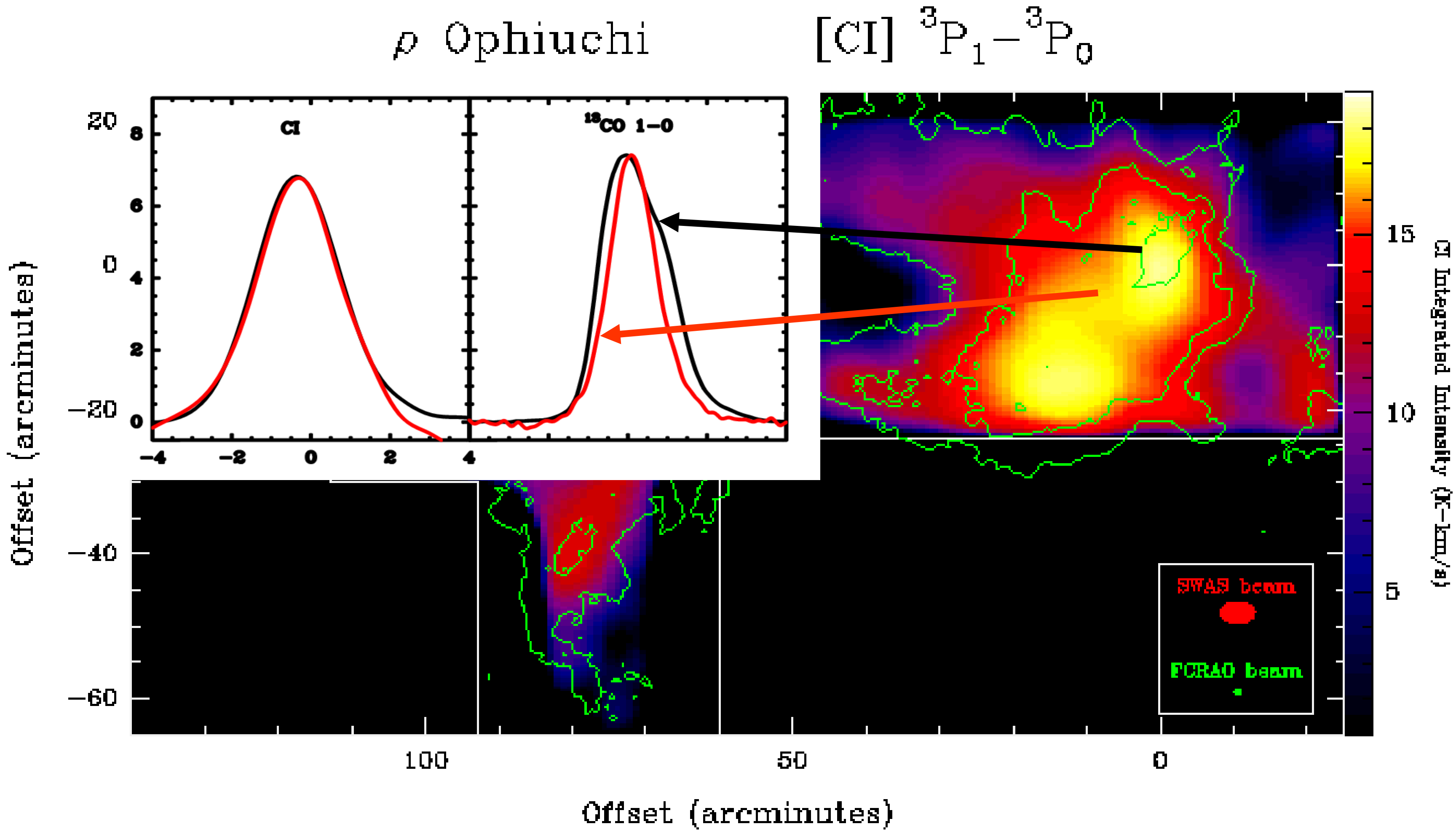
Cloud Composition as Function of A_v and Time



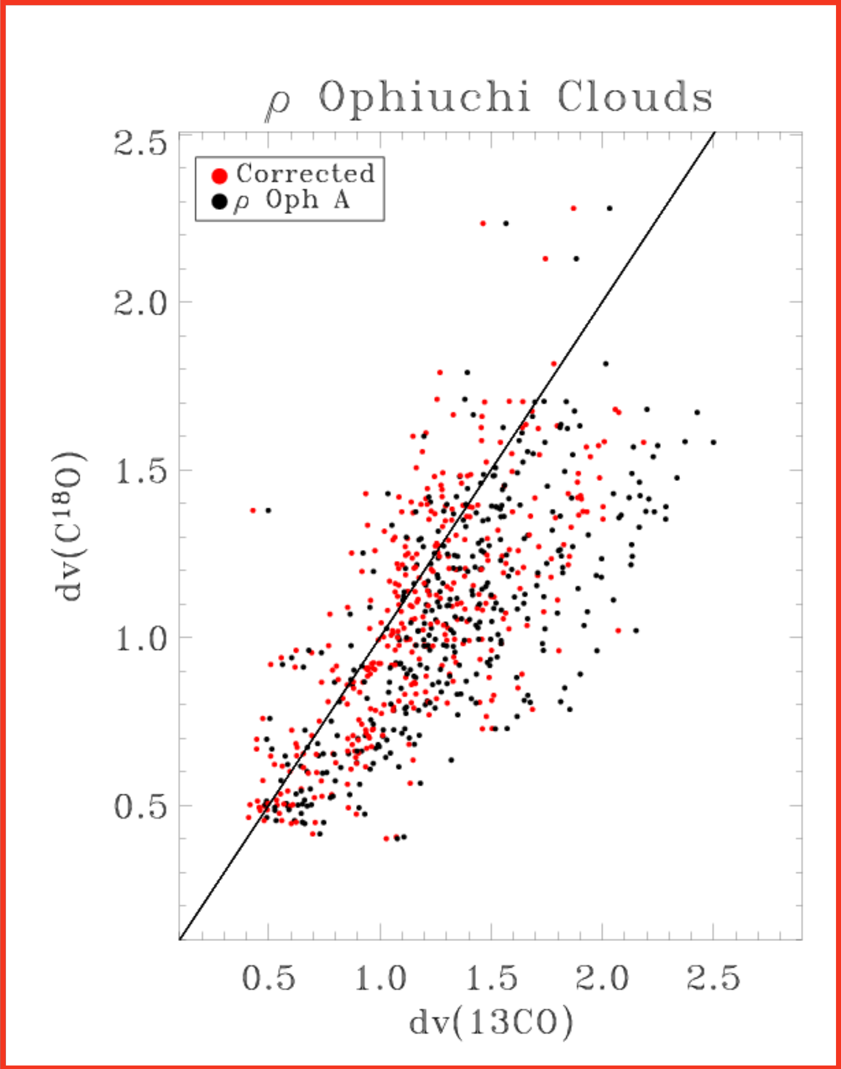
The Carbon Chronometer

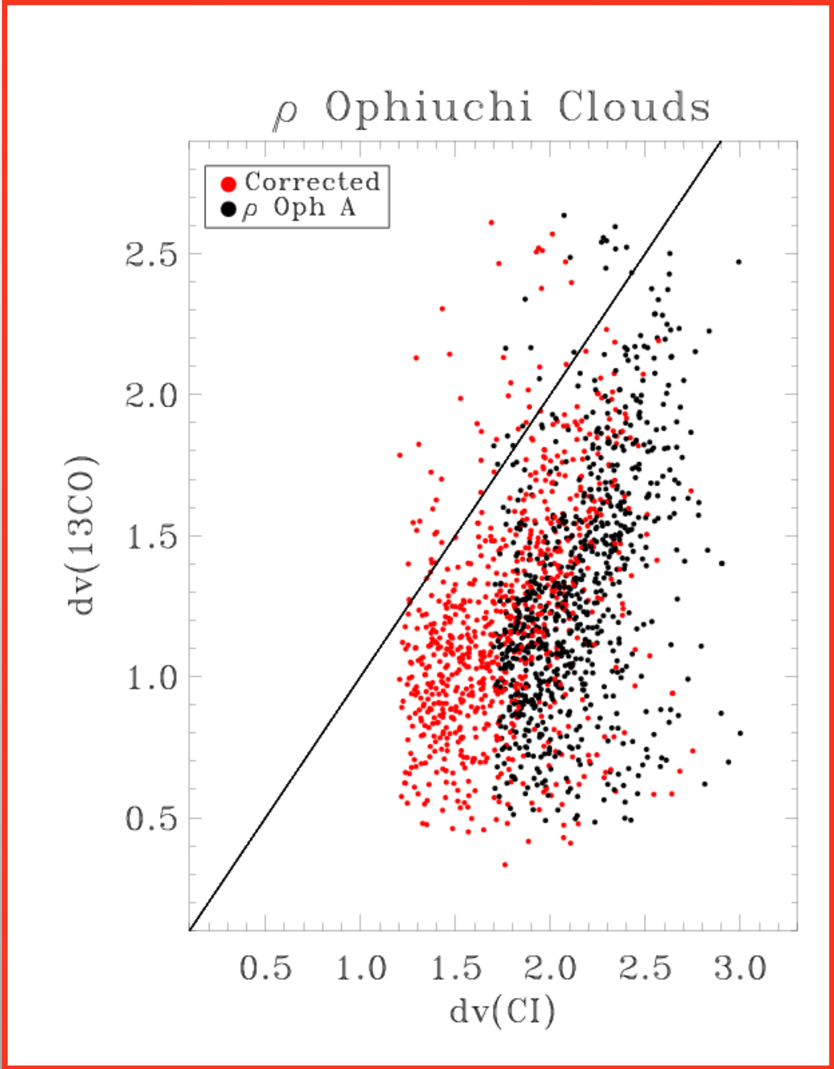
- The CII layer forms part of the **dark molecular gas** (talks by Pineda, Langer; poster 31 by Velusamy)
- The amplitude (column density) and thickness of the CI layer is a sensitive probe of cloud evolution and is time sensitive.
- Requires good information on density to analyze excitation conditions of CI as well as of CII and CO. Ideally having both CI lines (492 GHz and 809 GHz) will give the most accurate results, but both are challenging from the ground. Only modest angular resolution required (L ~ 1 pc) but very good sensitivity (T_R = 1.6K for 492 GHz and 0.5 K for 809 GHz).
- The carbon layers could be an powerful probe of cloud evolutionary state (poster 25 by Li et al.)!

Atomic Carbon in Rho Ophiuchi

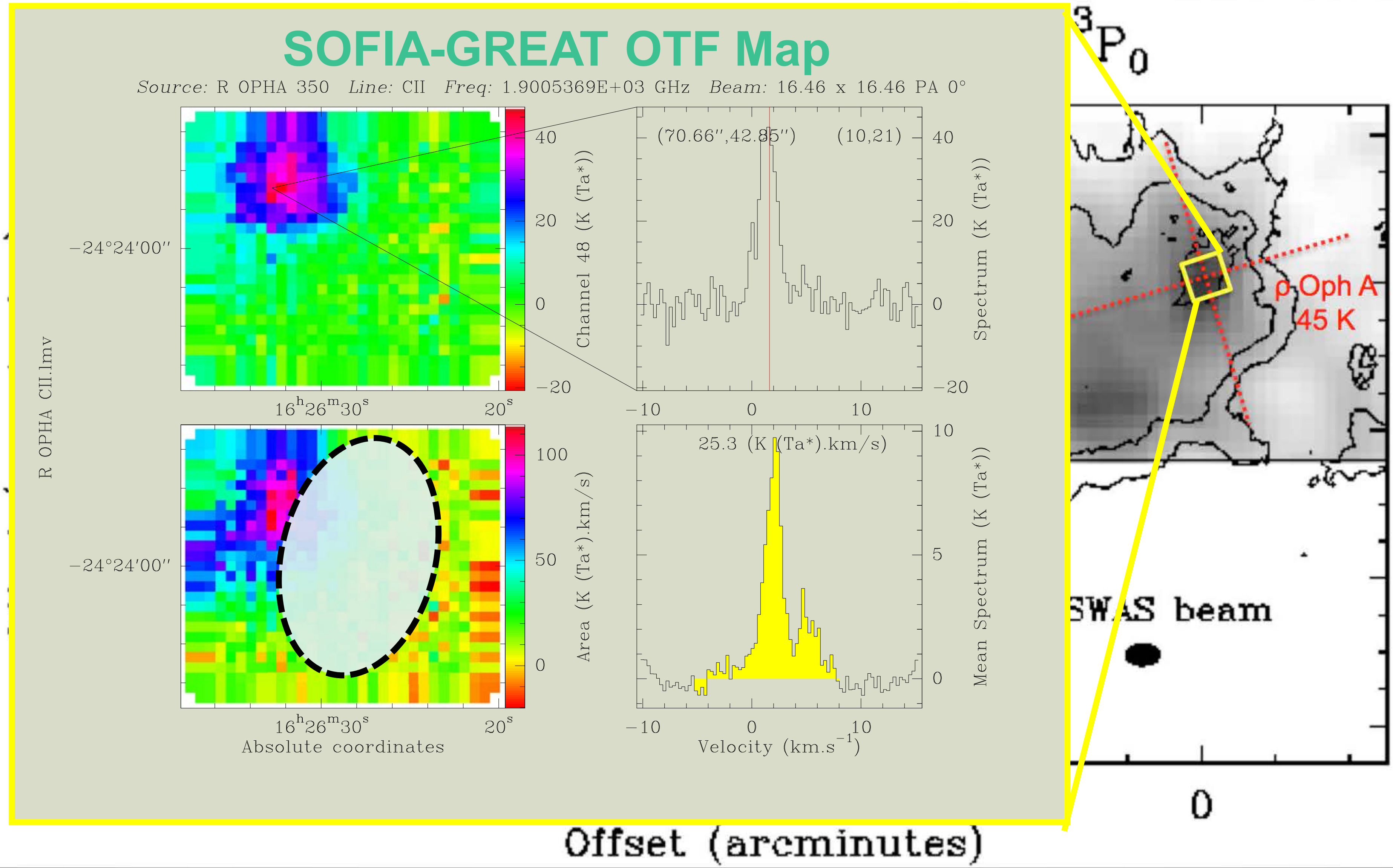


Turbulence Structure





Resolving the Transition Layers



Conclusions

- Study of H_2 in UV and IR continues to surprise us with complexity of excitation state, OPR, and role in astrochemistry
- Atomic H in molecular clouds is a very powerful tool suggesting that they are not "young" but that it takes millions of years to convert primarily atomic hydrogen clouds to 99.9% molecular form
- Laboratory data suggests that H_2 formation is efficient over broader range of temperatures than thought to be the case a few years ago, but range is still limited. Issues of complex grain morphology and surface structure make this a very difficult field in which to obtain definitively meaningful results
- Ongoing and future observations of CI and CII will improve our understanding of the structure of clouds, their total mass, and how they have evolved and will continue to do so