

The Atomic to Molecular Transition in the Interstellar Medium

*Theoretical and Observational
Perspectives*

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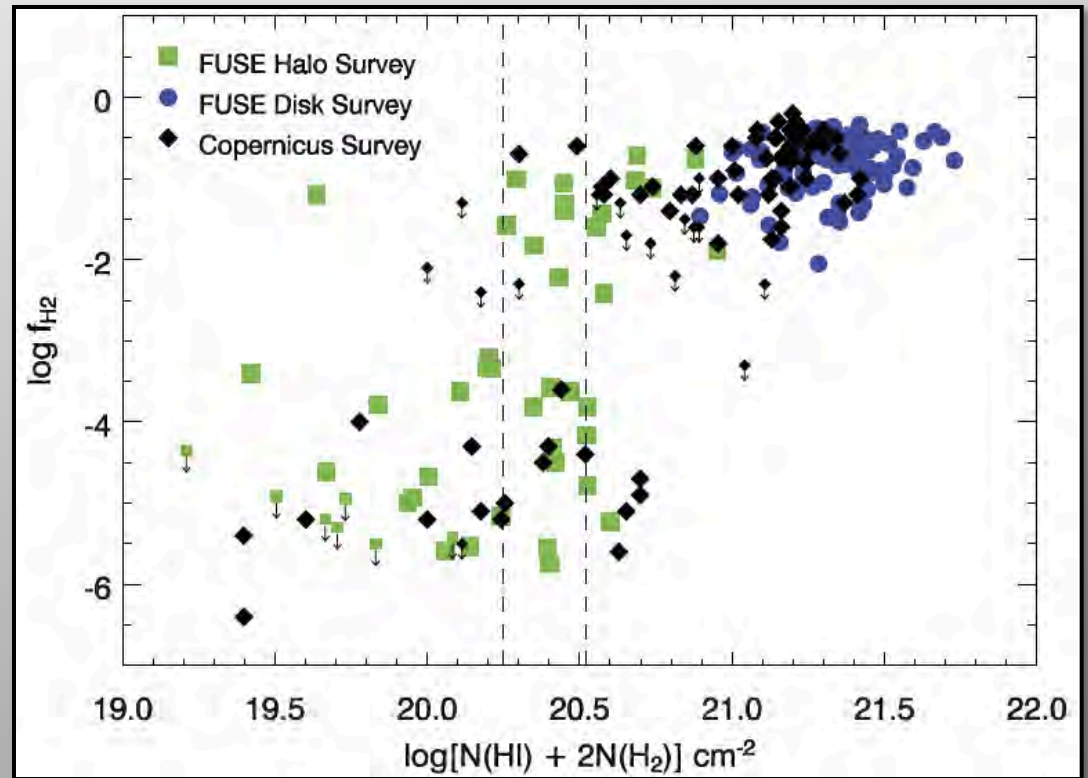
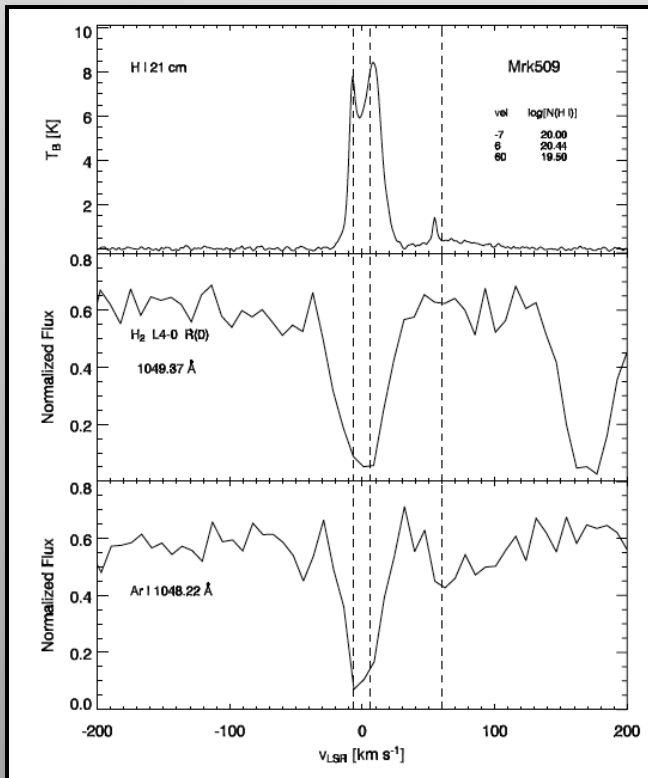
Definitions of a “Molecular Cloud”

- 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 H₂
- The observational definition of a molecular cloud is the region in space defined by ¹²CO 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 HI-H₂ Transition Should be “Simple”

HI measured by 21cm emission; H₂ by UV absorption (towards stars and extragalactic sources) Gillmon+ 2006



H₂ photodissociation rate is large in unshielded regions. Self-shielding determines the “transition” at $20 \leq \log N/\text{cm}^{-2} \leq 20.5$

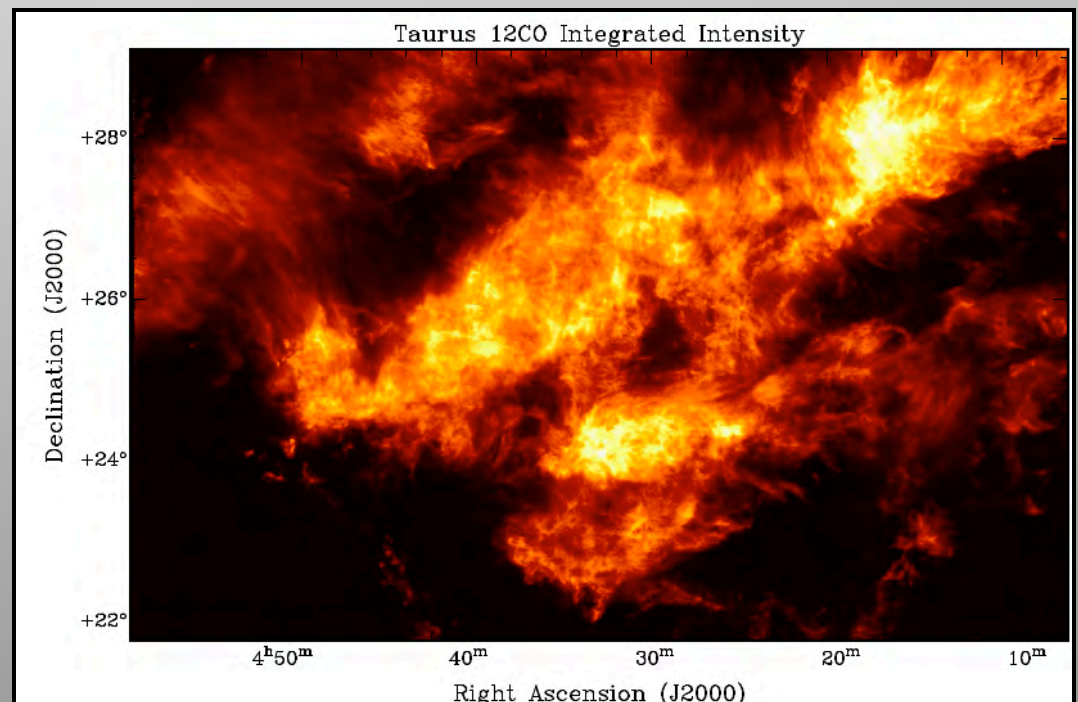
Tracing Molecular Clouds

- Molecular clouds are not readily mapped in H₂ absorption due to paucity of background sources and excessive opacity.
- The most important molecular gas tracers are the isotopologues of carbon monoxide. ¹³CO and C¹⁸O 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 ¹²CO, though very optically thick, shows surprising detail, especially of lower column density regions.

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

There are indications of material flows at cloud edges.

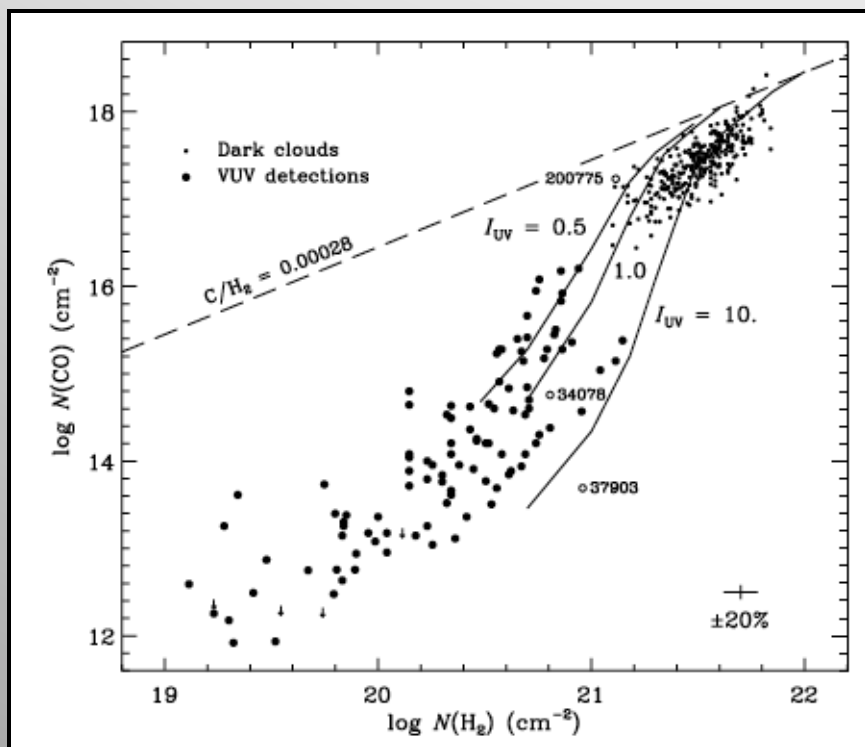


Column Density in Taurus

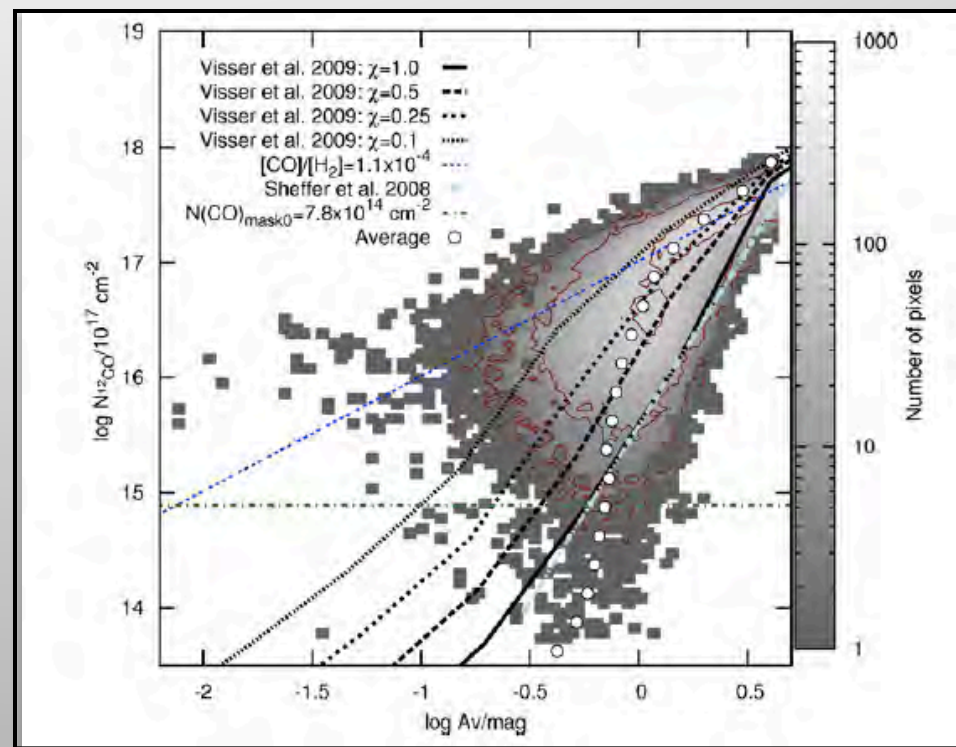


How do you define “molecular cloud”?

CO Fractional Abundance Requires $A_V = 2 - 5$ mag. to Approach Saturated Value



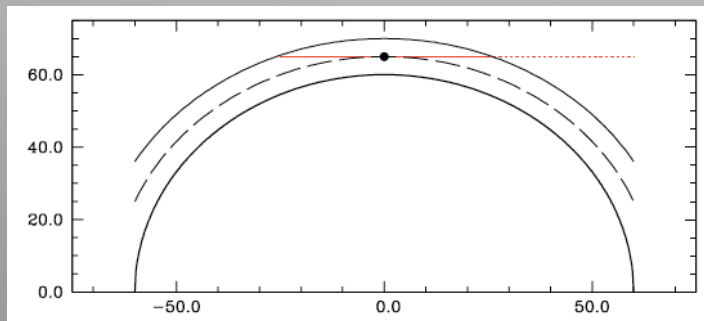
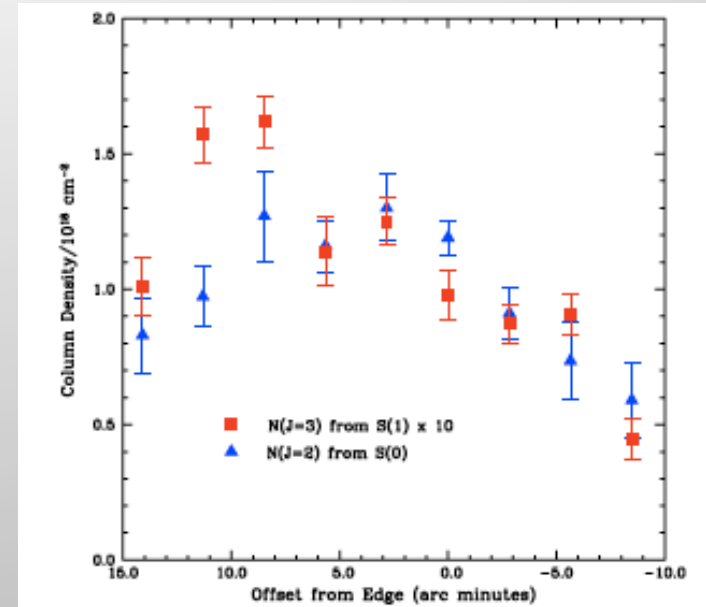
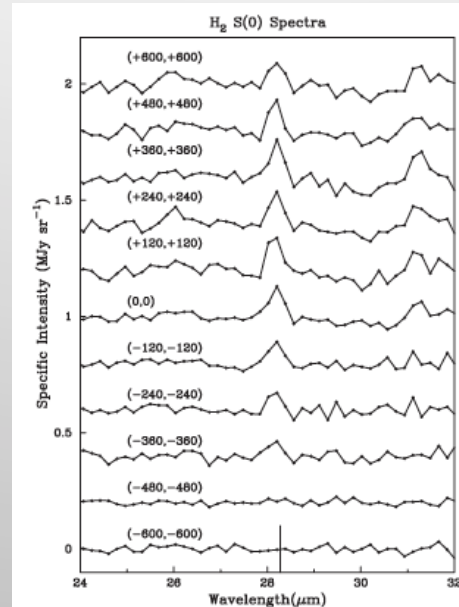
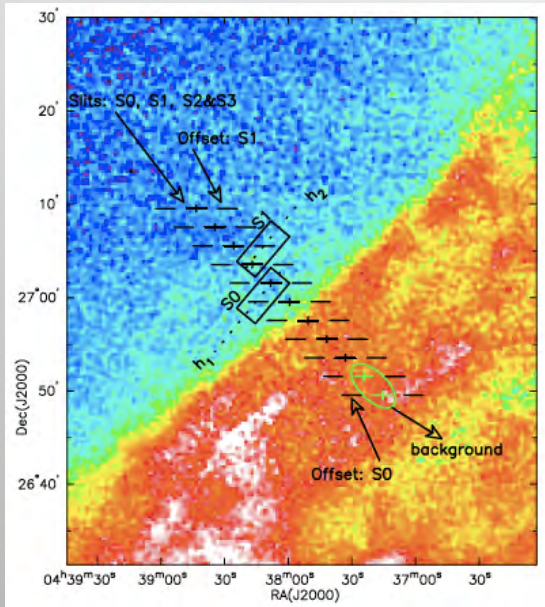
Sheffer+ 2008; UV absorption
Variety of UV radiation fields



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

Good, comprehensive models are needed to analyze cloud edges using carbon monoxide

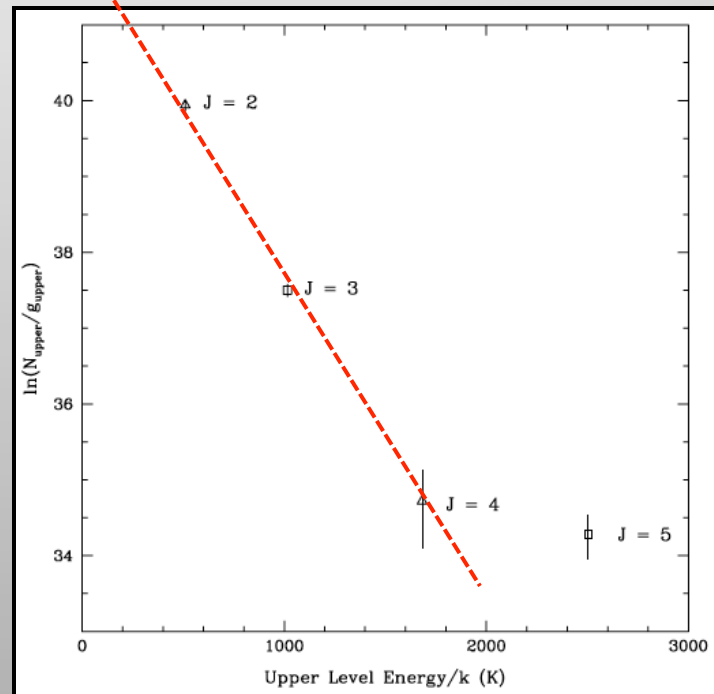
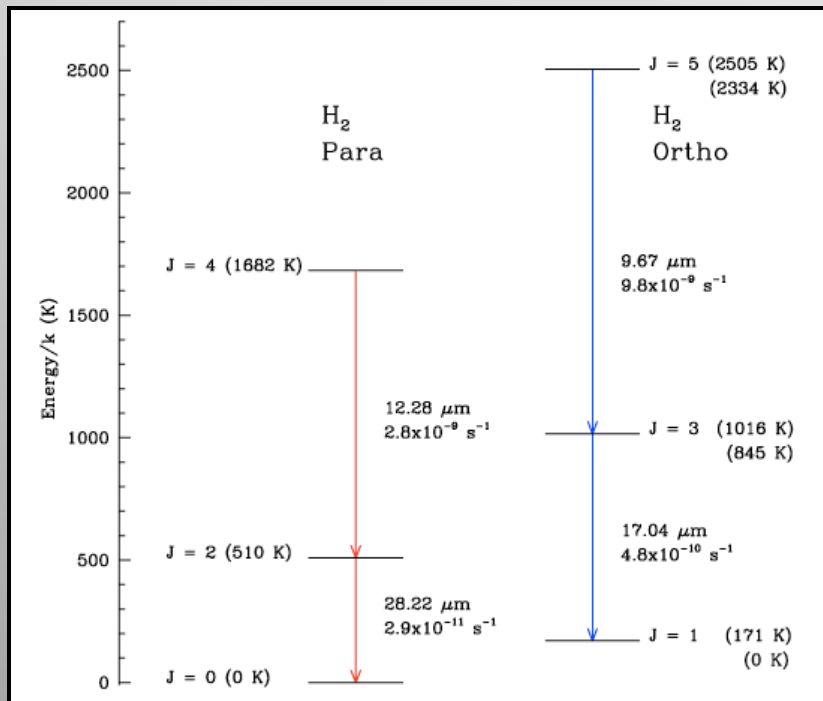
H₂ Pure Rotational Transition Emission From Edge of Taurus Molecular Cloud



Due to the local geometry, we are seeing “limb brightening” of the warm H₂ layer that surrounds the cloud defined by CO emission

The Observed H₂ is WARM T_{ex} ≥ 200K

N(H₂) in “warm layer” ~ 10¹⁸ cm⁻²



Average of “outside” positions

The observed H₂ is likely only a small fraction of total present in this layer, but there is still more “warm H₂” than can be explained by PDR models

H₂ 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
 $k = 1.5 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$

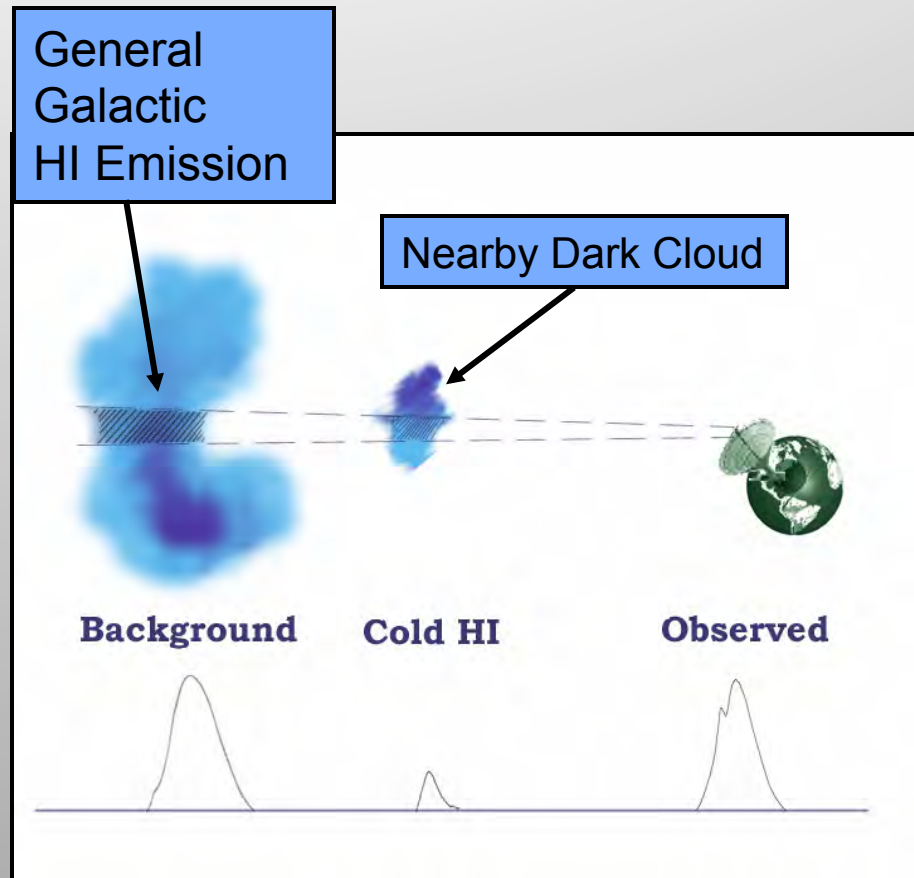
H₂ Observations: 2 Possibilities in Next Decade

- 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 $\sim 1.8''$ @ 17 μm
- MIRI Instrument on JWST
 - 12.3 μm S(2) and 17 μm S(1) lines will be covered at $R \sim 3000$
 - 28.2 μm S(0) line situation is not so clear
 - 0.2" to 0.3" pixel size on sky

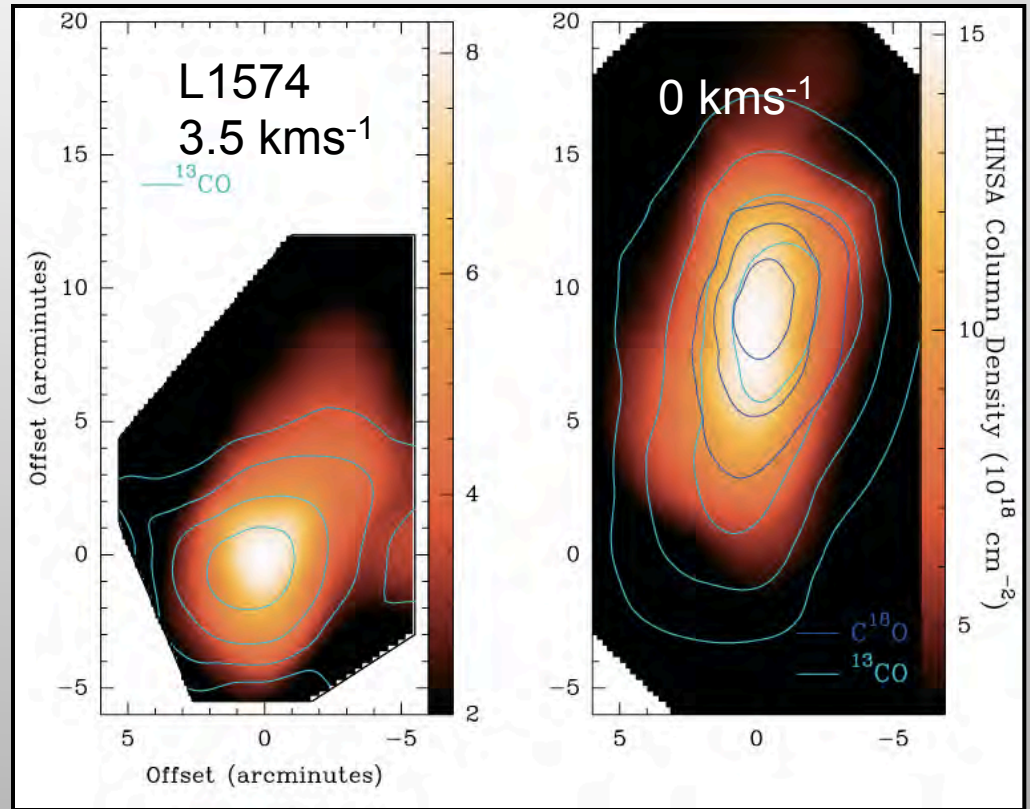
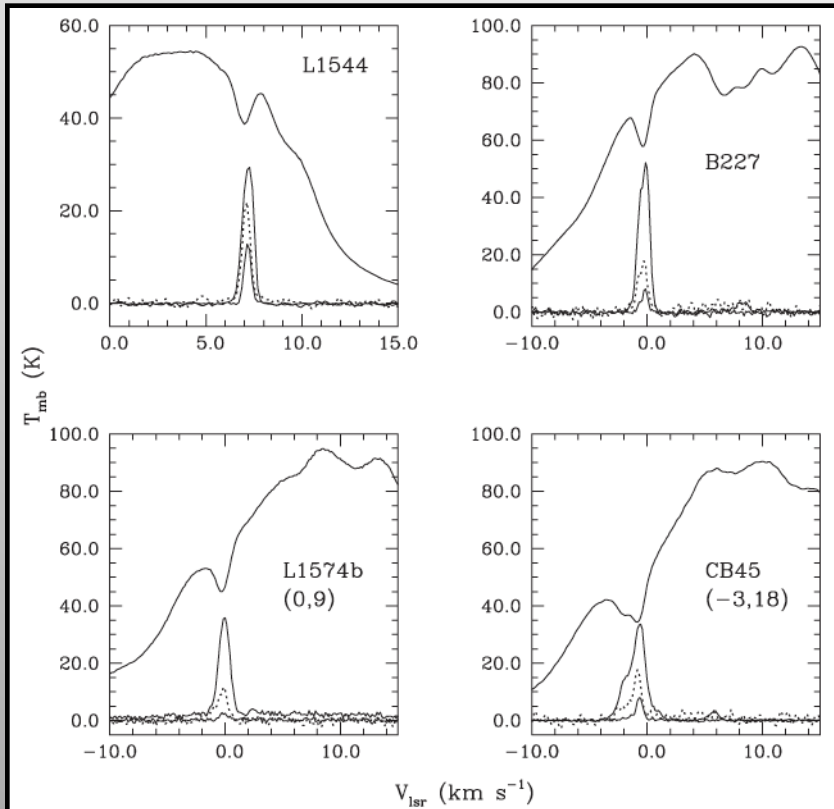
EXAMPLE: S(1) emission from Taurus equivalent to flux of $6 \times 10^{-20} \text{ Wm}^{-2}$. MIRI sensitivity $\sim 5 \times 10^{-20} \text{ Wm}^{-2}$ (10σ in 10^4 s) So this is feasible, if not easy. Higher G sources should be straightforward.

The Atomic Hydrogen Component of Molecular Clouds

HINSA: Narrow absorption features against background of HI emission profiles. HINSA profiles agree in velocity with OH, ^{13}CO and C^{18}O emission. Nonthermal HI line width \approx molecular line width. Correlates well spatially with molecules



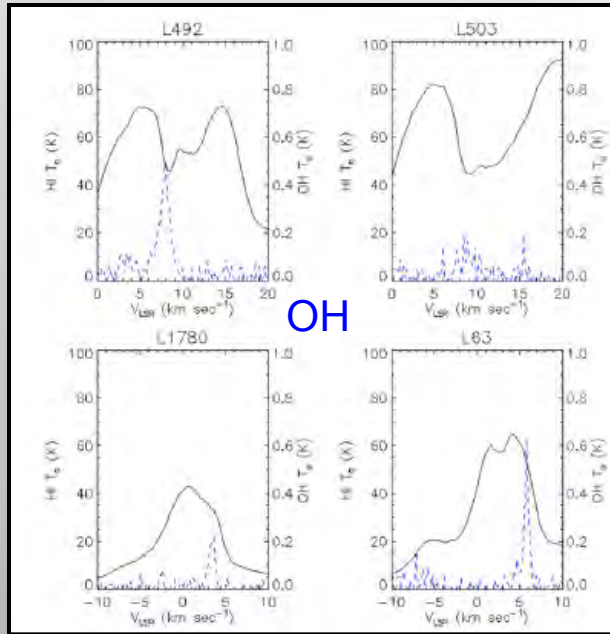
HI Narrow Self Absorption (HINSA)



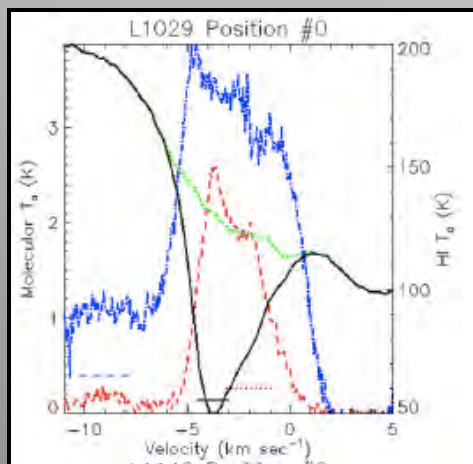
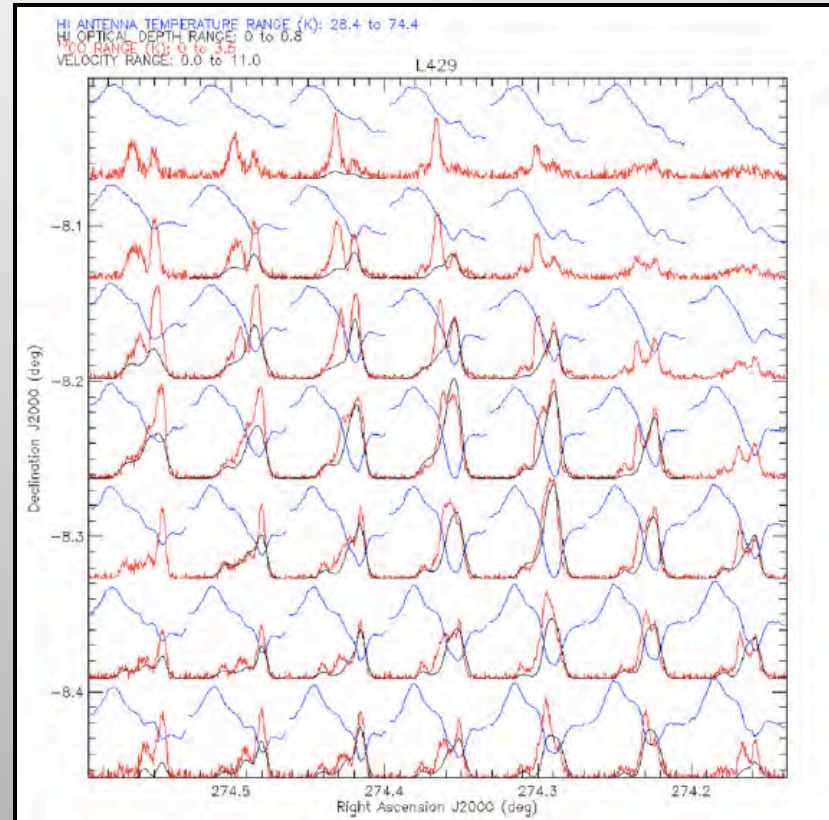
HI background is the Galactic HI emission. HINSA features are sometimes obvious, but broader "HISA" features are also common and confuse the situation.

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

GBT Survey of HINSA by Krco & Goldsmith (2008, 2010)



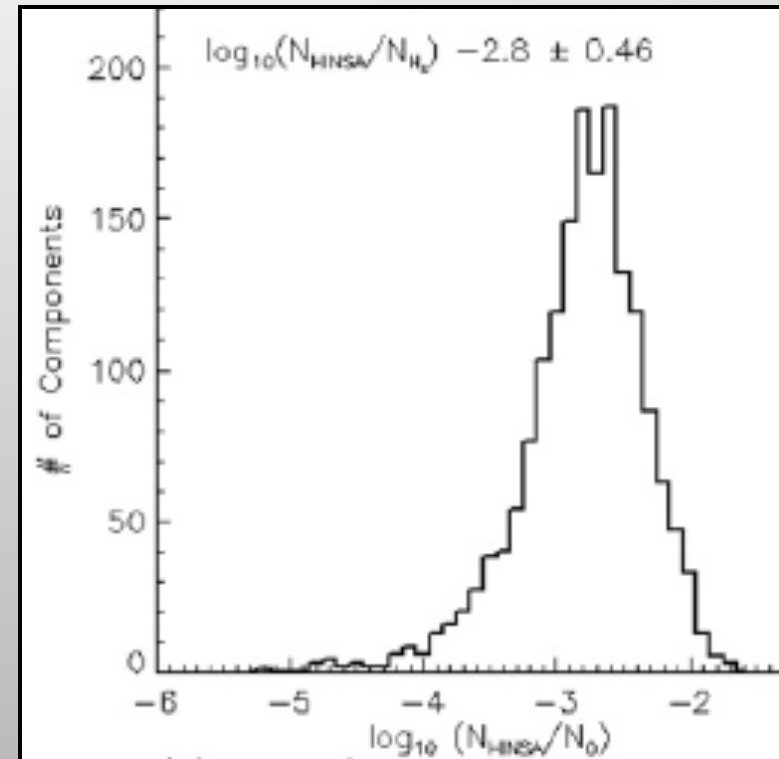
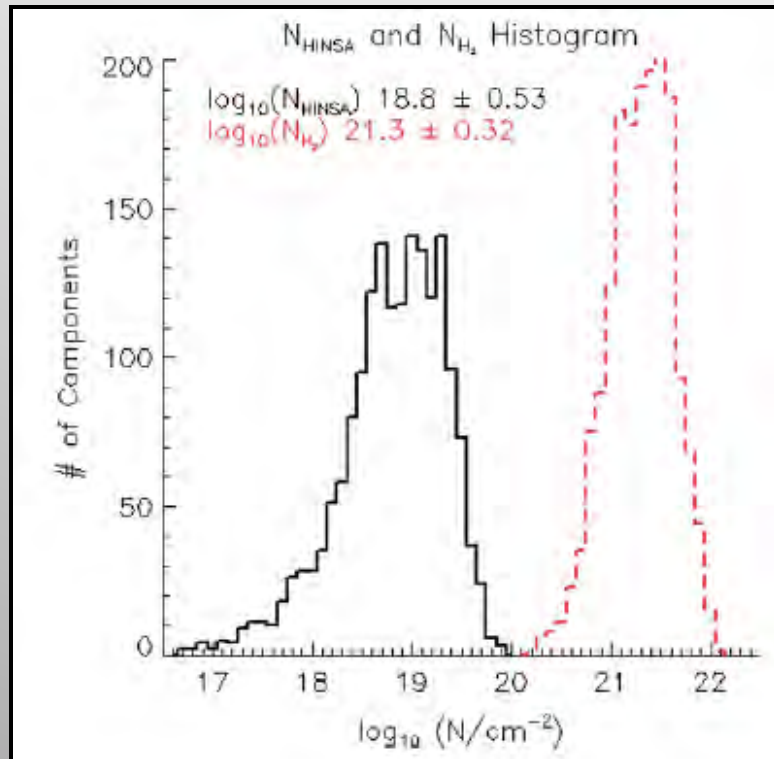
OH



¹²CO
¹³CO
 HI
 HI (rec)

HINSA features detected in 80% of clouds out to distance $D = 700$ pc without noticeable trend as function of distance.

Global Results of HINSA Survey

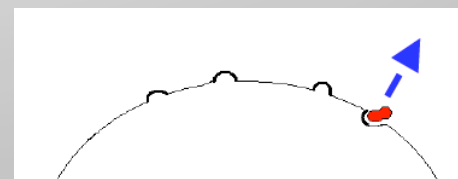
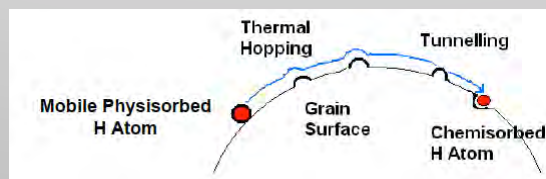


$$\langle N(\text{cold HI})/N(\text{H}_2) \rangle = 0.0016$$

Formation and Destruction of H₂

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 H₂ which has sufficient energy to desorb from grain surface



Destruction:

- (1) By cosmic rays with rate $\zeta \sim 5 \times 10^{-17} \text{ s}^{-1}$ 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.

H₂ Formation Rate and Rate Equation

$$R_{\text{H}_2} = \frac{1}{2} S_{\text{H}_1} \epsilon_{\text{H}_2} n_{\text{H}_1} \langle v_{\text{H}_1} \rangle \sigma_{\text{gr}} n_{\text{gr}}.$$

General H₂ formation rate

$$n_0 = n_{\text{H}_1} + 2n_{\text{H}_2},$$

Total proton density n_0

$$R_{\text{H}_2} = k'_{\text{H}_2} \text{MRN} n_{\text{H}_1} n_0,$$

H₂ formation rate in terms of n_0

$$k'_{\text{H}_2} = 3.5 \times 10^{-18} \left[\left(\frac{S_{\text{H}_1}}{0.3} \right) \left(\frac{\epsilon_{\text{H}_2}}{1.0} \right) \left(\frac{T}{10 \text{ K}} \right)^{0.5} \right] \left[\left(\frac{\rho_{\text{gr}}}{2 \text{ g cm}^{-3}} \right) \times \left(\frac{\text{GDR}}{100} \right) \left(\frac{a_s}{1.7 \times 10^{-5} \text{ cm}} \right) \right]^{-1} \frac{a_s}{\sqrt{a_{\text{max}} a_{\text{min}}}} \text{ cm}^3 \text{ s}^{-1}.$$

With MRN grain size Distribution

$$k' = 1.2 \times 10^{-17} \text{ cm}^3 \text{ s}^{-1}$$

$$\frac{dn_{\text{H}_2}}{dt} = k' n_{\text{H}_1} n_0 - \zeta_{\text{H}_2} n_{\text{H}_2}.$$

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

$$x_1(t) = 1 - \frac{2k'n_0}{2k'n_0 + \zeta_{H_2}} \left[1 - \exp\left(\frac{-t}{\tau_{H_1 \rightarrow H_2}}\right) \right].$$

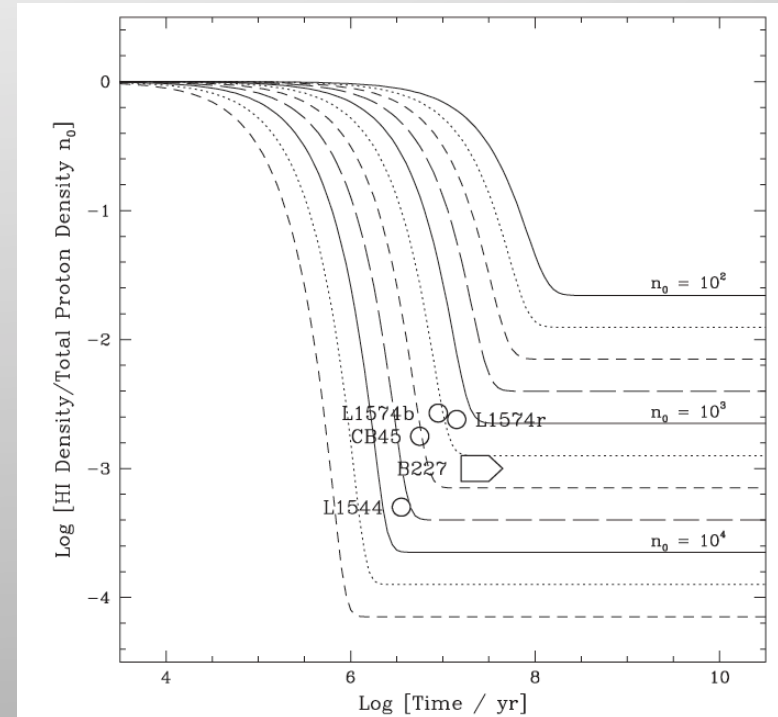
Characteristic Time Scale

$$\tau_{H_1 \rightarrow H_2} = \frac{1}{2k'n_0}, \quad T = 1.3 \times 10^9 \text{ yr}/n_0$$

Steady-State Abundance of HI

$$x_1 \rightarrow \frac{\zeta_{H_2}}{2k'n_0} \quad \text{or} \quad n_{H_1} \rightarrow \frac{\zeta_{H_2}}{2k'}$$

With $\zeta = 5 \times 10^{-17}$ and $k' = 1.2 \times 10^{-17}$
 n_{H_1} (steady state) = 2.5 cm^{-3}

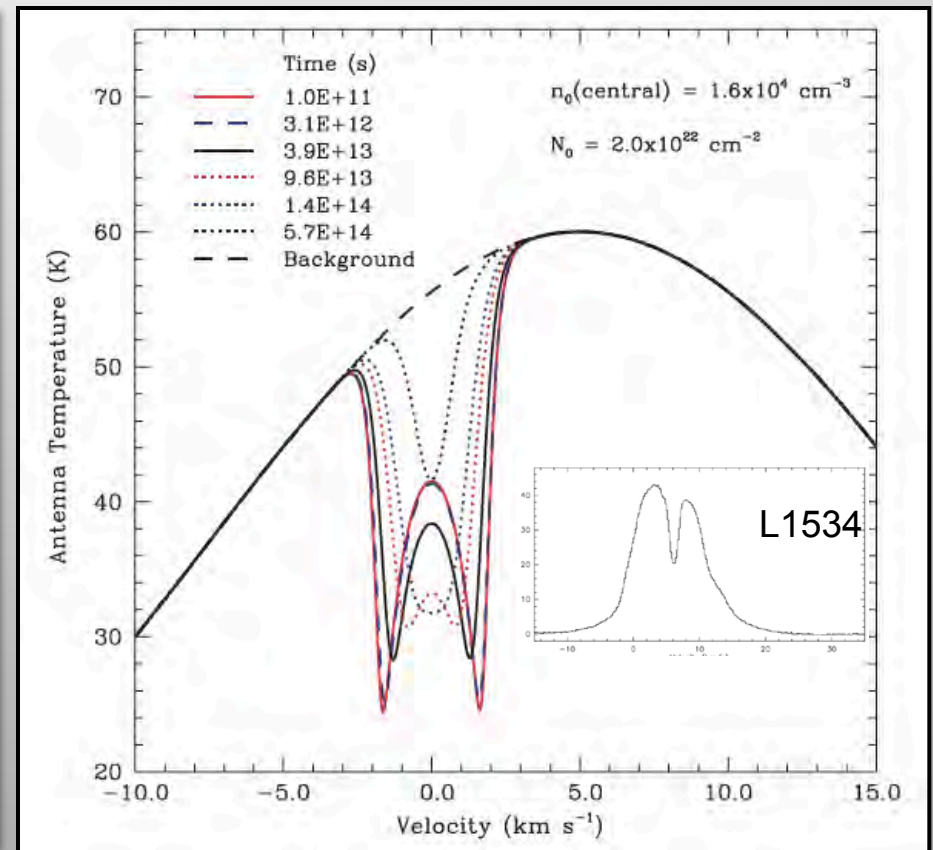
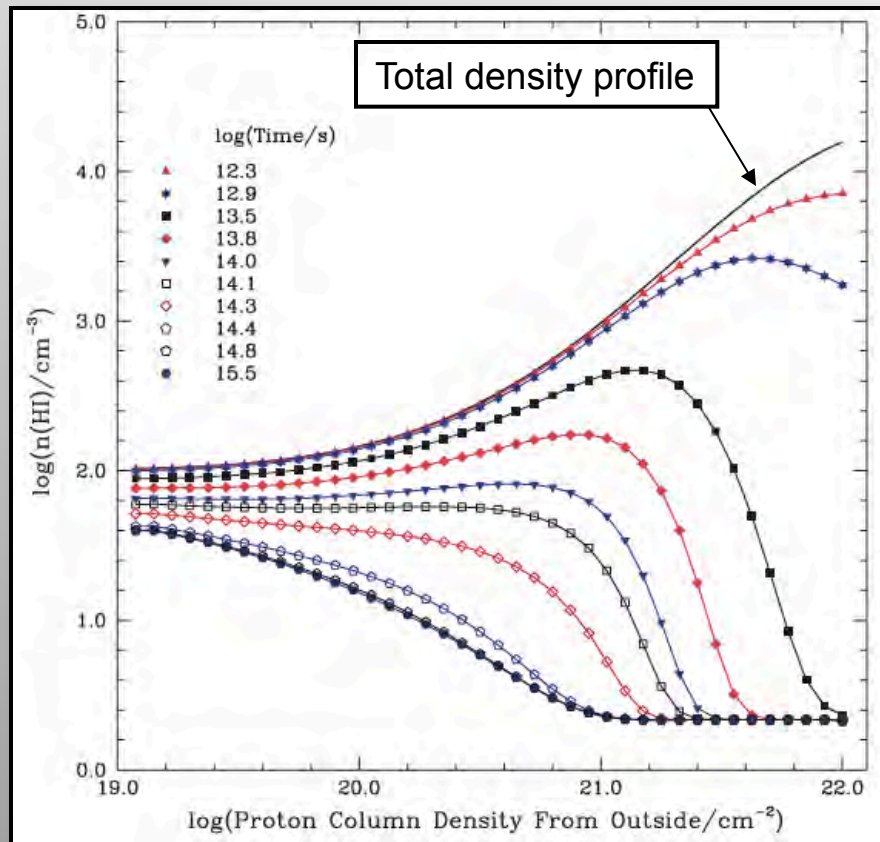


Some Conclusions from HI in Dark Clouds

- Steady state fractional abundances of HI are $n(\text{HI})/n(\text{H}_2) \sim 2 \times 10^{-3}$ or $n(\text{HI})/n_0 = 0.001$
- With central H_2 densities $\sim 2000 \text{ cm}^{-3}$, $n(\text{HI}) \sim 4 \text{ cm}^{-3}$. 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**

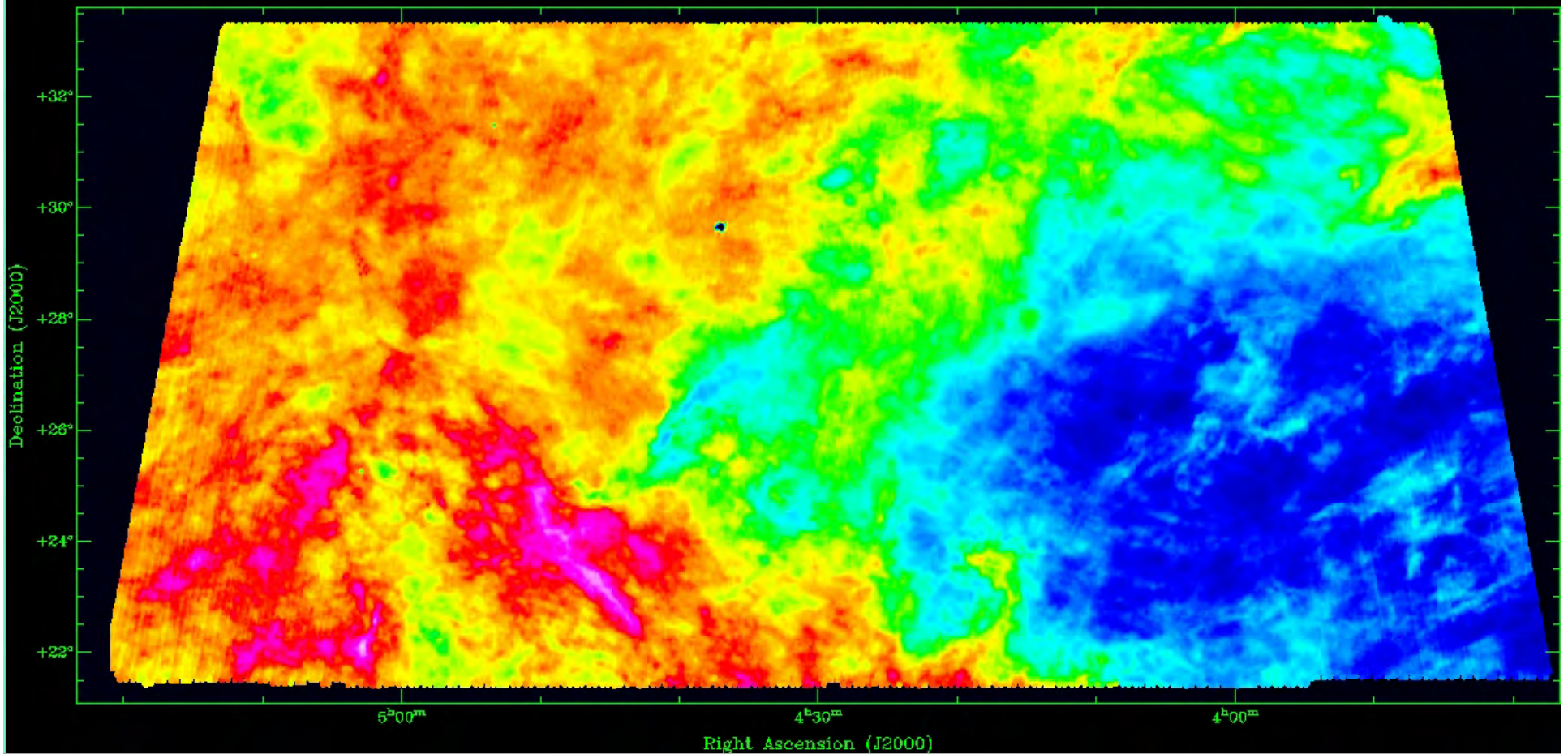
Evolution of Initially Centrally Condensed Atomic Cloud with $N(\text{HI}) = 1 \times 10^{22} \text{ cm}^{-2}$ exposed to ISRF

Higher density in center results in more rapid destruction of atomic hydrogen there – wave of destruction propagates outwards towards edge



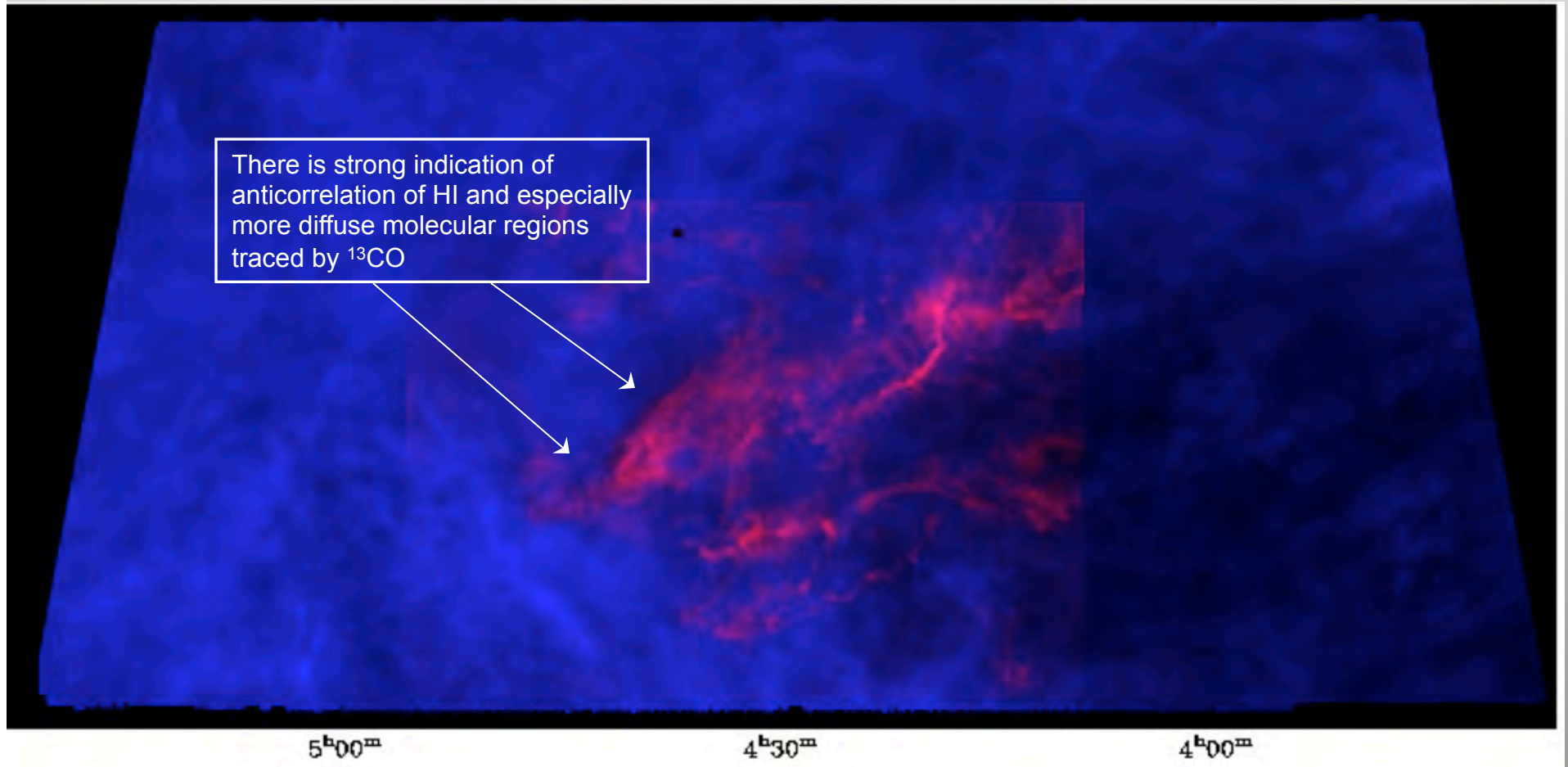
$\geq 3 \times 10^6$ yr required to produce plausible line profiles and observed column densities of cold HI ($\leq 10^{19} \text{ cm}^{-2}$)

Where Do Molecular Clouds Come From?

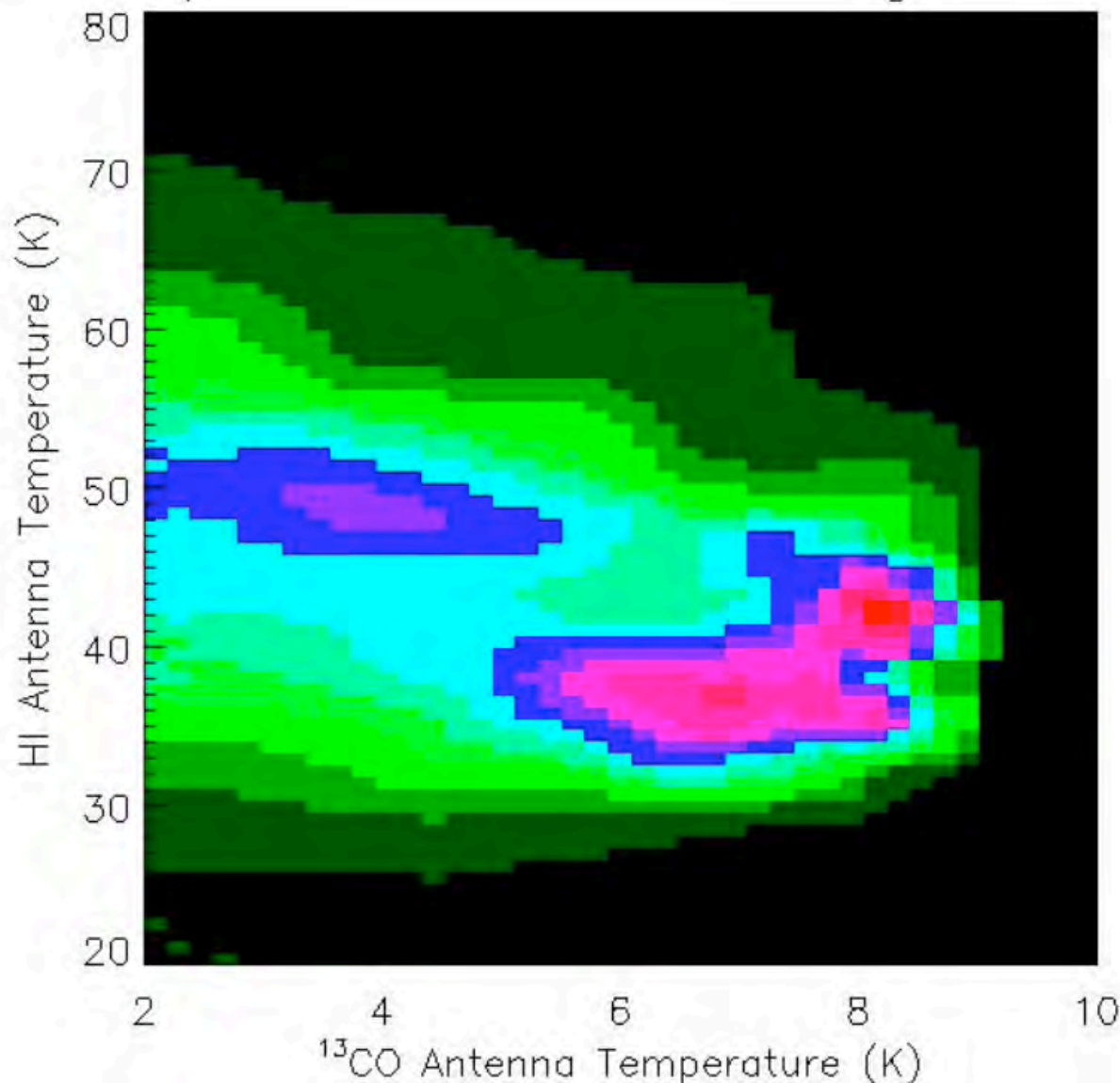


Large-scale HI Integrated Intensity map of Taurus Region
(Arecibo, 4' resolution, M. Krco PhD thesis, Cornell University)

HI with ^{13}CO Overlay (3 kms $^{-1}$ to 7 kms $^{-1}$)



HI-¹³CO Anticorrelation



Values from individual 1 kms⁻¹ velocity bins within Taurus map. The effect is clear, but not dramatic.

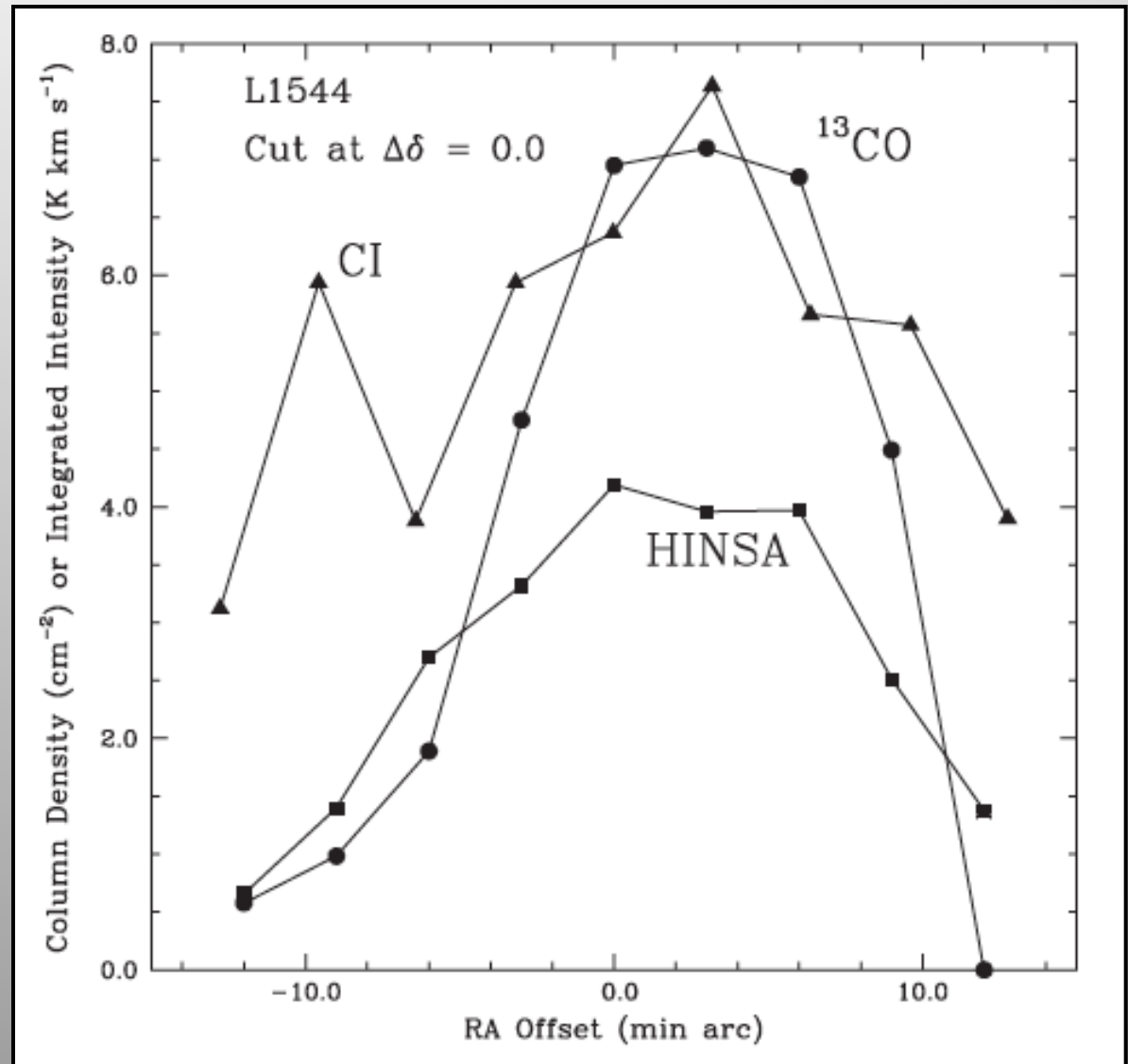
CI – Another Cloud Chronometer (?)

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 “Carbon Skin”

CI is formed by (1) recombination of C^+ [low A_V] and (2) photodissociation of CO [up to $A_V \sim \text{few}$]

For standard ISRF, the ‘CI-layer’ is located at $A_V \cong 1$

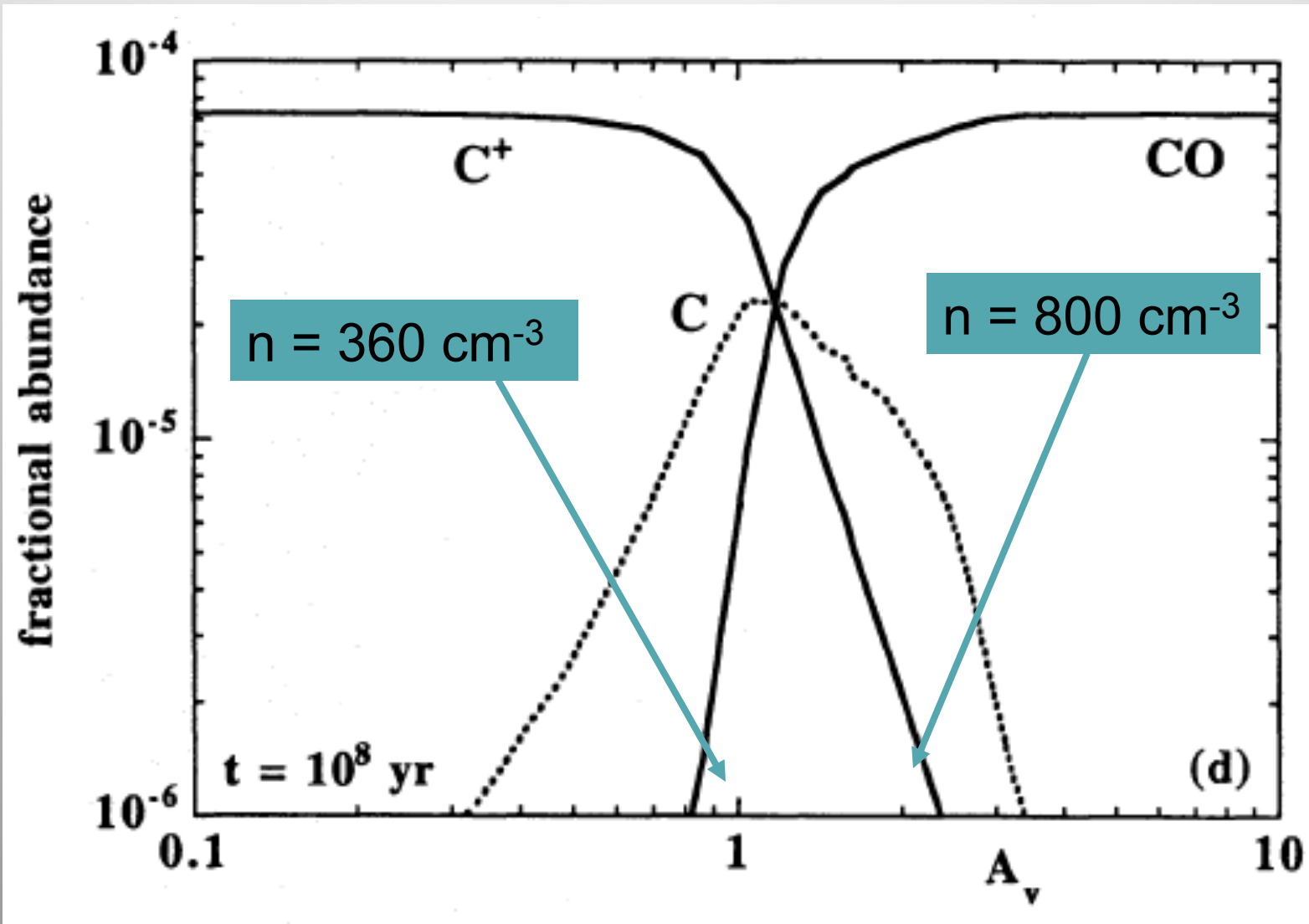
The density in this region is typically not large ($\sim 100 \text{ cm}^{-3}$) so that the timescale for the CI abundance to achieve its steady-state value is long.

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

$$n(A_V) = 10^2 [1 + 9(A_V/A_{V \text{ max}})]^2 \text{ cm}^{-3} \text{ for } 0 \leq A_V \leq A_{V \text{ max}} = 10$$

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

Cloud Composition as Function of A_v and Time

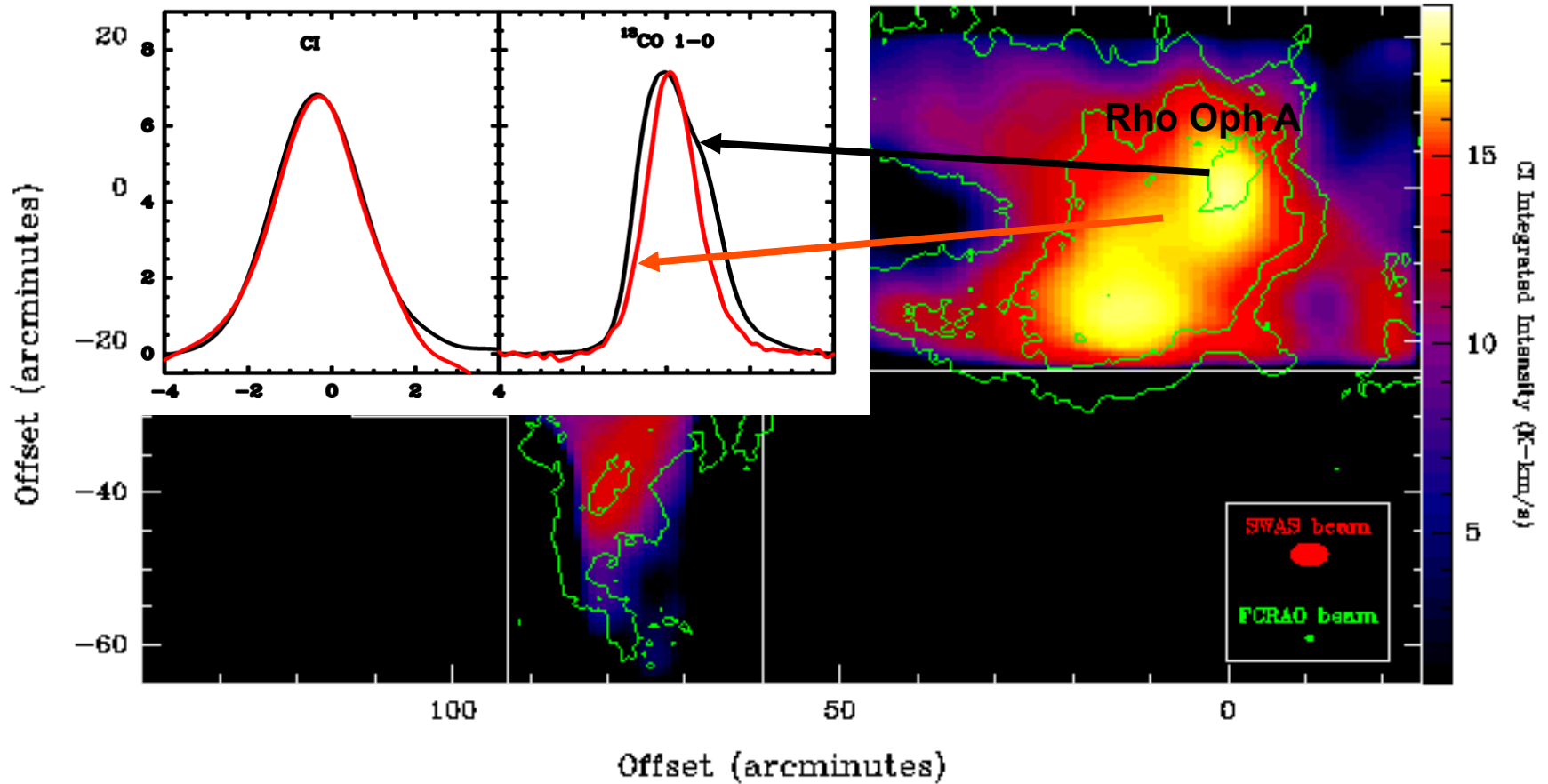


The Carbon Chronometer

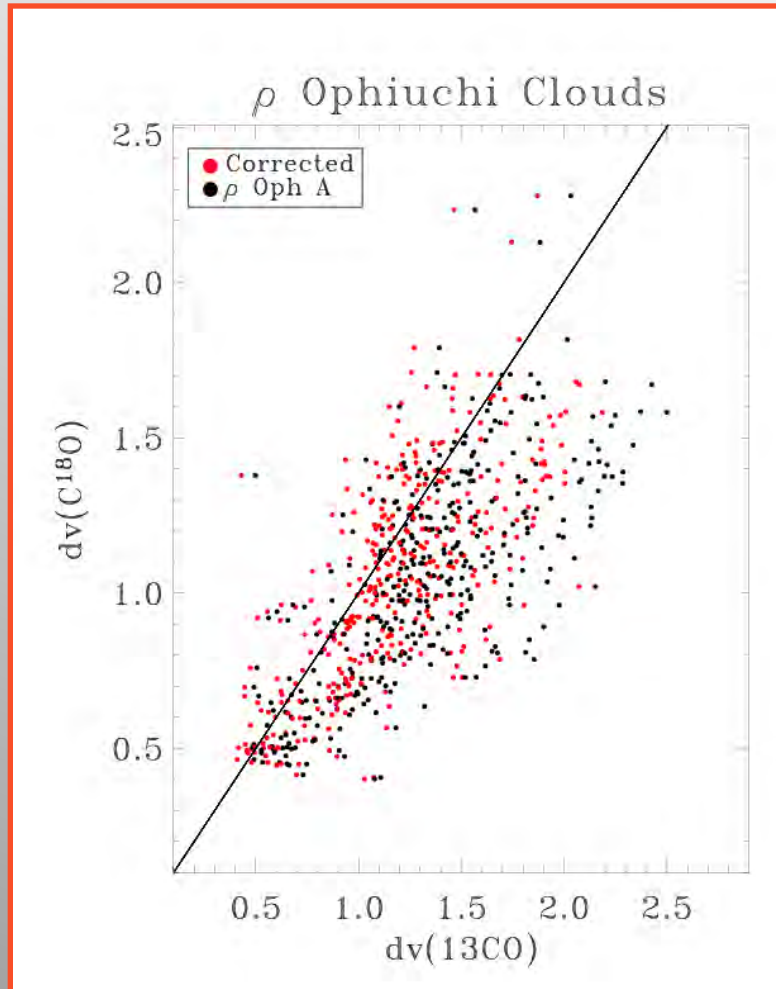
- The amplitude (column density) and thickness of the CI layer are sensitive probes of cloud evolution.
- We need good information on the volume density to analyze excitation conditions of CI as well as of CII and CO. Ideally having both CI lines (492 GHz and 809 GHz) will give the most accurate results, but both are challenging from the ground. Only modest angular resolution required ($L \sim 1$ pc) but very good sensitivity ($T_R = 1.6$ K for 492 GHz and 0.5 K for 809 GHz).
- The CI layer forms part of the **dark molecular gas** that is being probed by CII (Herschel OTKP “GOT-C+”), but it is very much more time-sensitive. The CI layer could thus be an powerful probe of cloud evolutionary state! The critical requirement is a good telescope on the right site.

CI 3P_1 - 3P_0 in Rho Ophiuchi

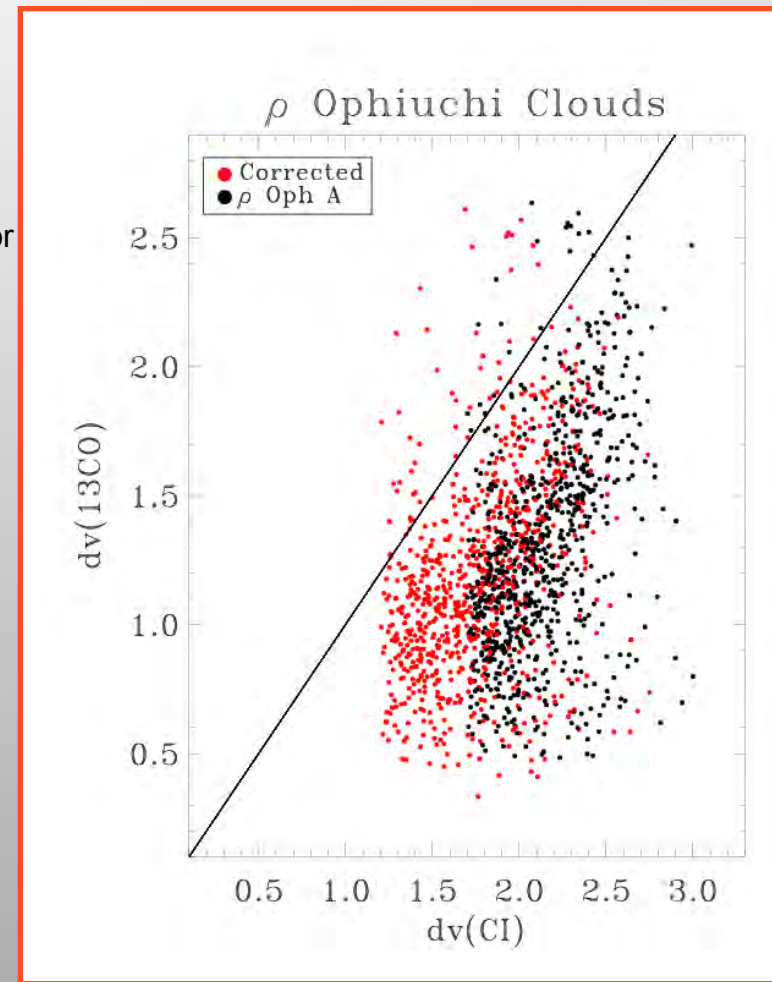
Max. Intensities Scaled to be Equal
CI line width is the same towards and away from cores
 ^{13}CO line narrows away from cores



Line Widths: CI is Broader

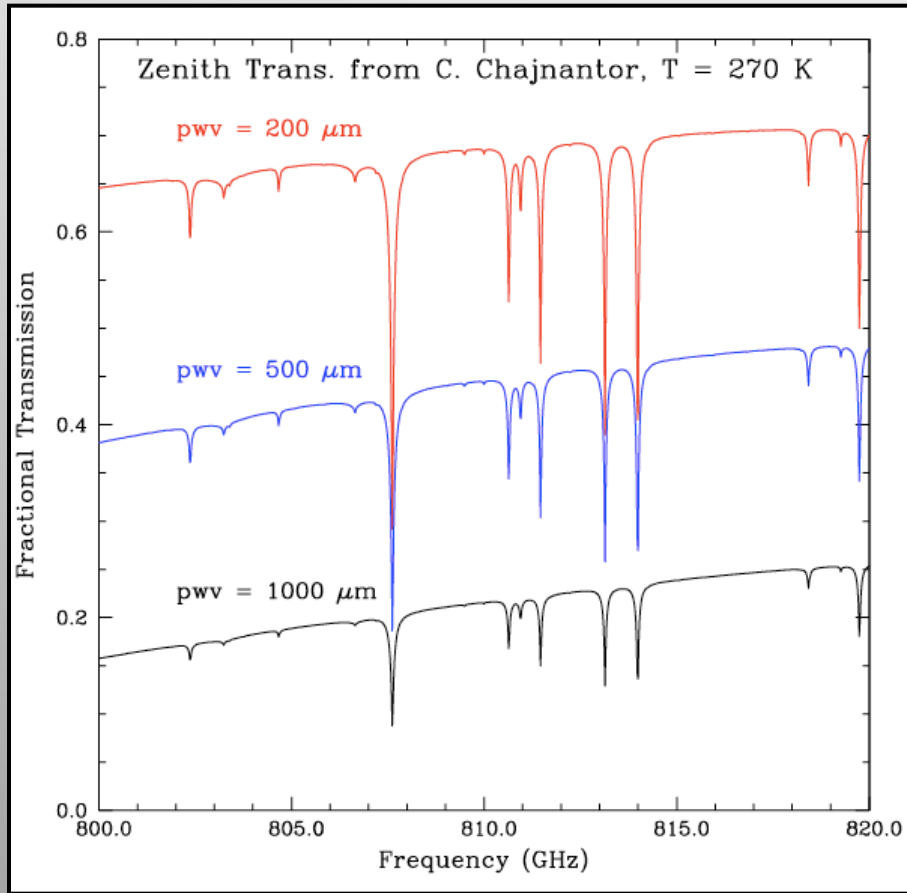


“Corrected” means corrected for thermal line width

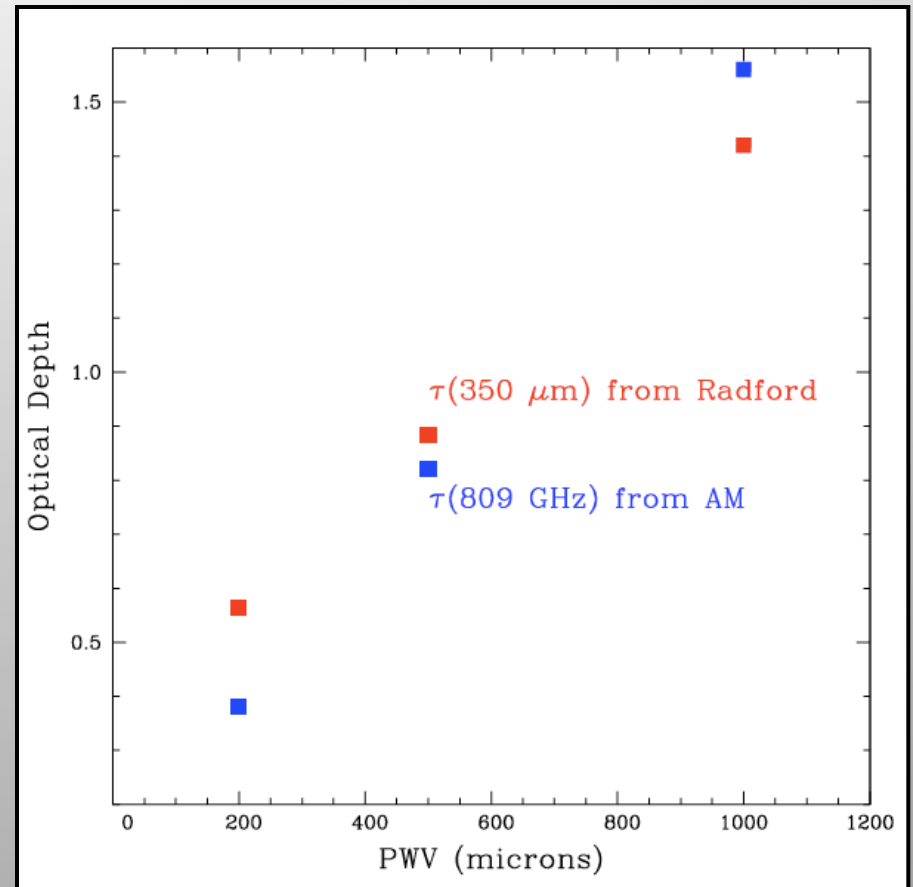


One Explanation is that $[CI]$ arises from an *Interclump Medium* that is present everywhere (in SWAS beam), while dense clumps are more localized. Possibly there is a distribution of clumps everywhere, each with its “carbon skin”, and it is the filling factor that changes.

Atmospheric Transmission in 800 GHz Range Above Mauna Kea & C. Chajnantor

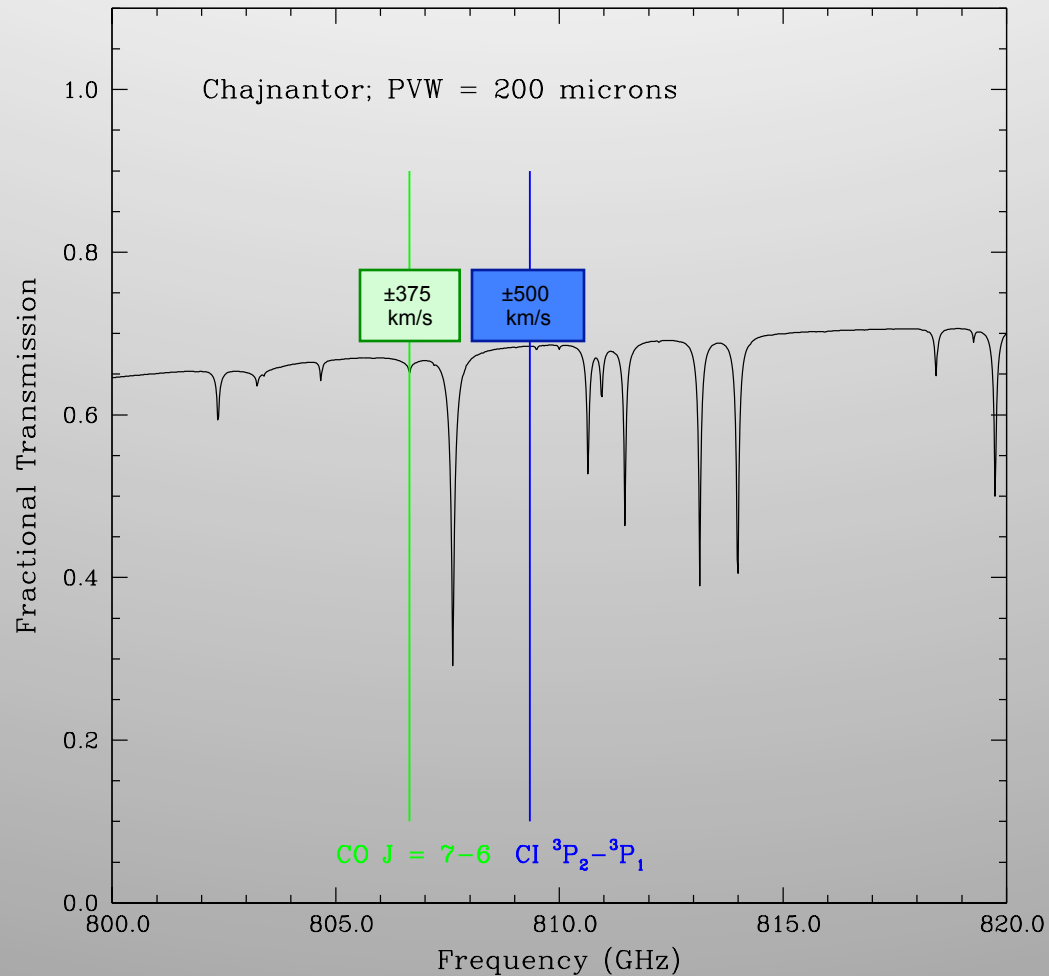


From AM Atmospheric Model
(S. Paine)



Narrowband vs. Broadband Optical
Depth Comparison

Atmospheric Transmission in Vicinity of $\text{Cl } ^3\text{P}_2-^3\text{P}_1$ and $\text{CO } J = 7-6$



CCAT on C. Chajnantor has potential for becoming THE definitive site for studying the C-Skin and exploiting the carbon chronometer for cloud evolution

Conclusions

- Study of H₂ in UV and IR continues to surprise us with complexity of H₂ excitation state, OPR, and its role in astrochemistry
- Atomic H in molecular clouds is a very powerful probe 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 H₂ 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.
- Exploiting the C-skin and the carbon chronometer are important areas on which CCAT can have a major impact.