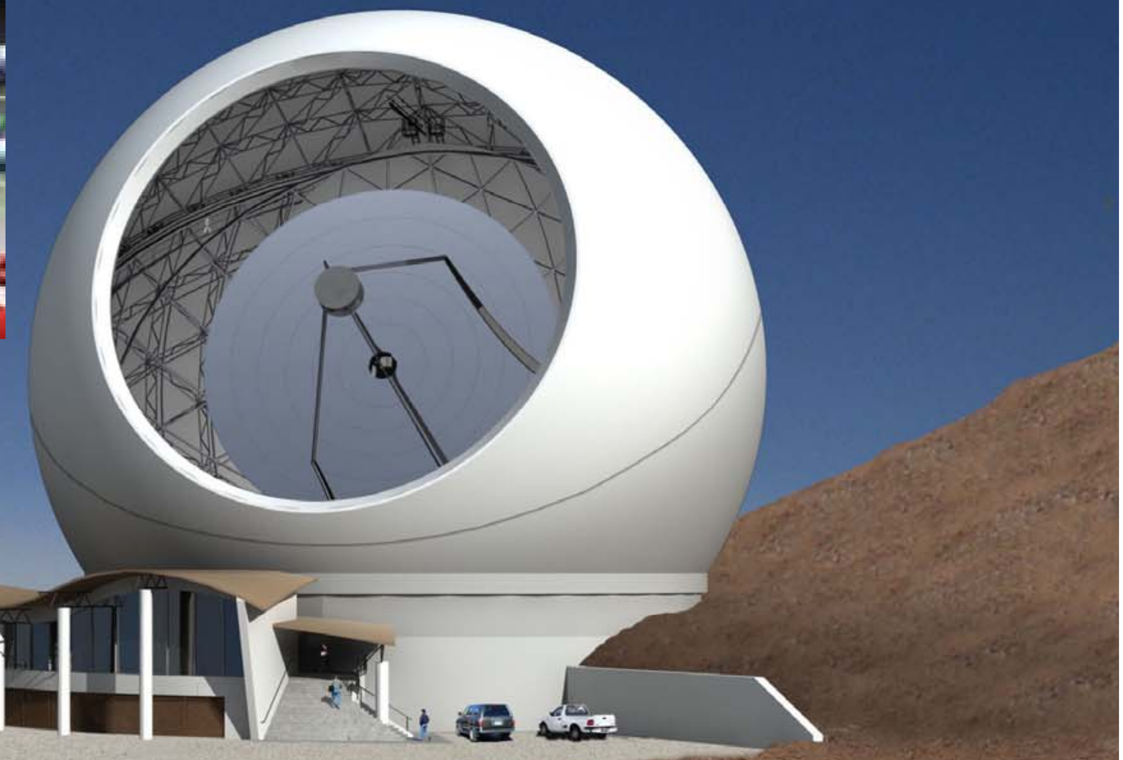
Astrochemistry with CCAT

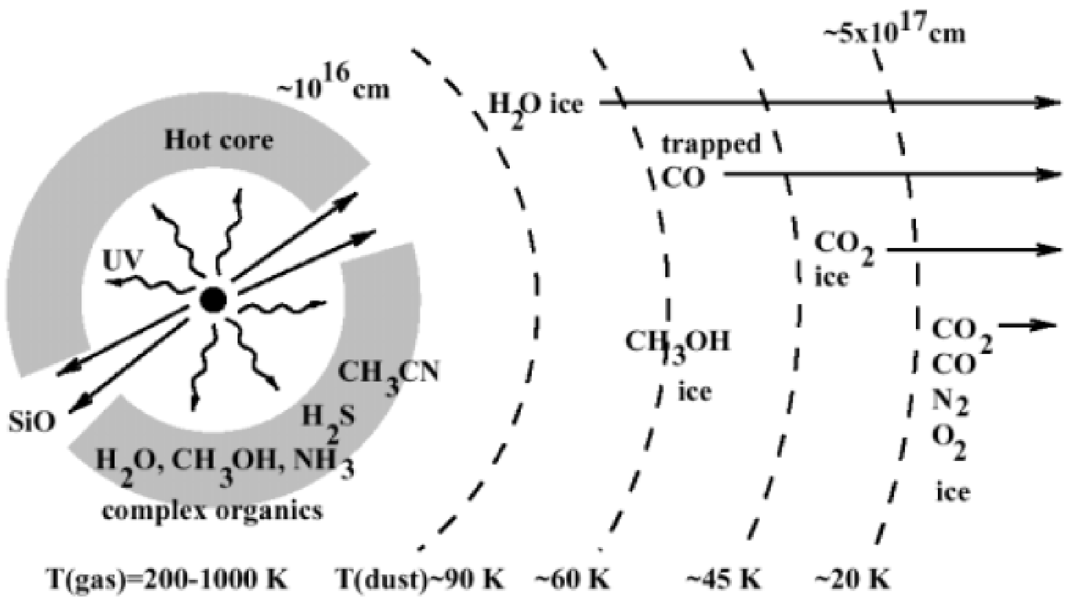


Darek Lis (Caltech)

Boulder, May 14, 2008

Astrochemistry = Line Surveys

- Complete census of molecules in CNM; in regions with high line confusion essential for identification
- Submm λs give access to high-energy transitions, excited only in the immediate vicinity of the newly formed stars
- High-T chemistry driven by molecules evaporated from grain mantles (e.g., methanol)

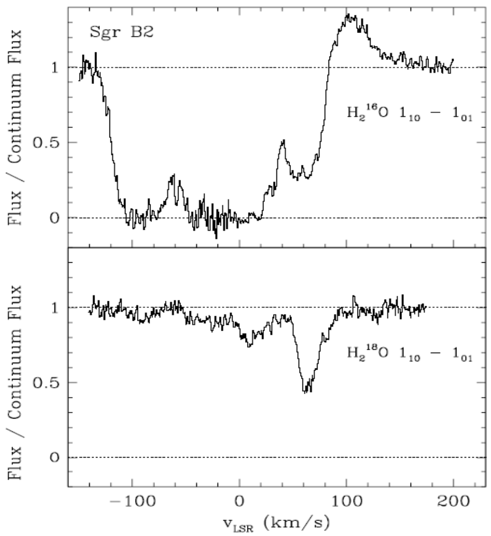


van Dishoeck 1998

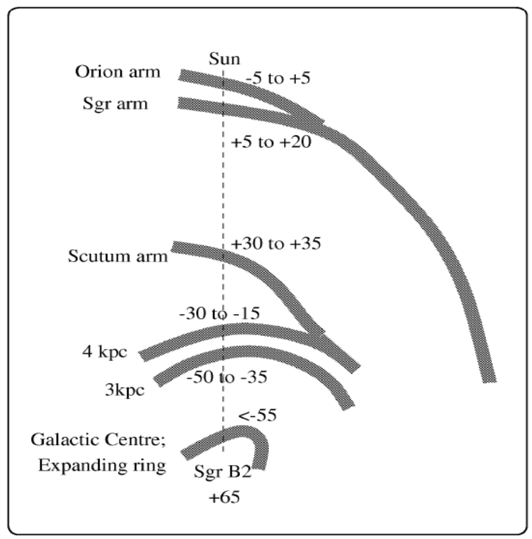
Fundamental questions:

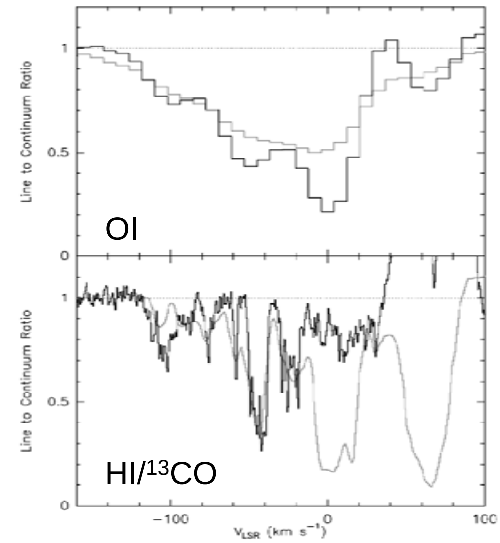
- Grain-surface vs. gas-phase processes
- Formation of large organic molecules → small grains (PAHs)
- Time scales
- Dependence on mass, luminosity etc.

Absorption Spectroscopy of Hydrides and Deuterides



Neufeld 2000



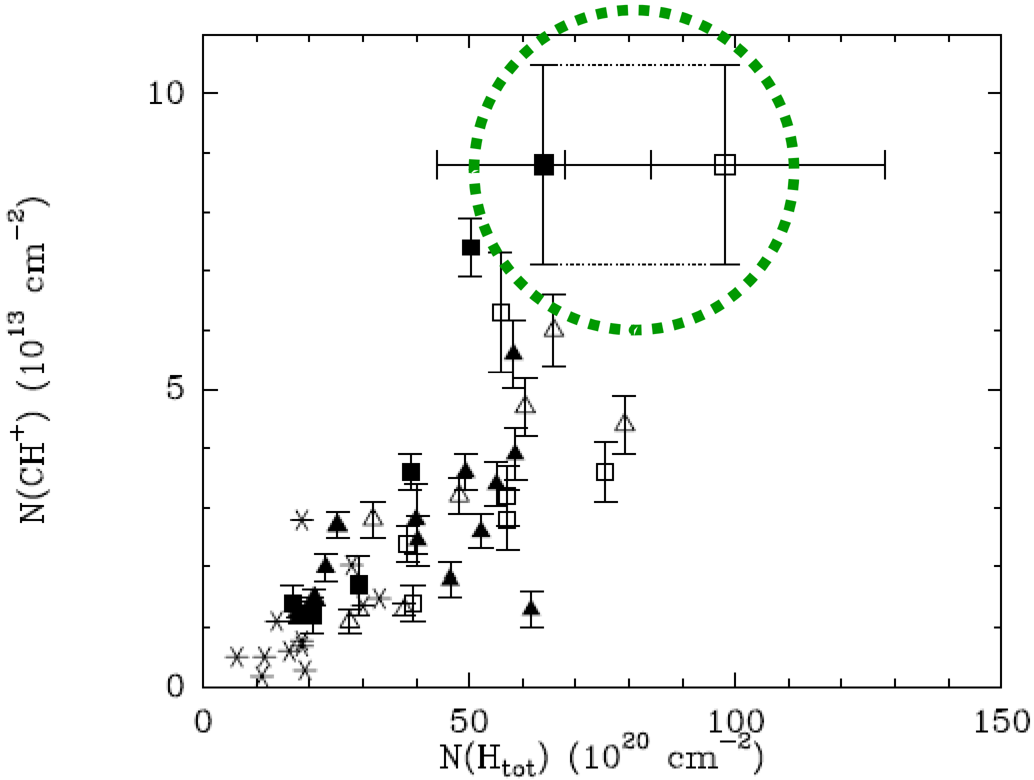


Lis 2001

- Detailed investigation of physics and chemistry of clouds with a *wide range of physical conditions*
- High-temperature chemistry of diffuse ISM (CH^+)
- Chlorine chemistry (HCl)
- Deuterium chemistry (H_2D^+, D_2H^+, HDO, also NH_2D)

CH^+ Chemistry

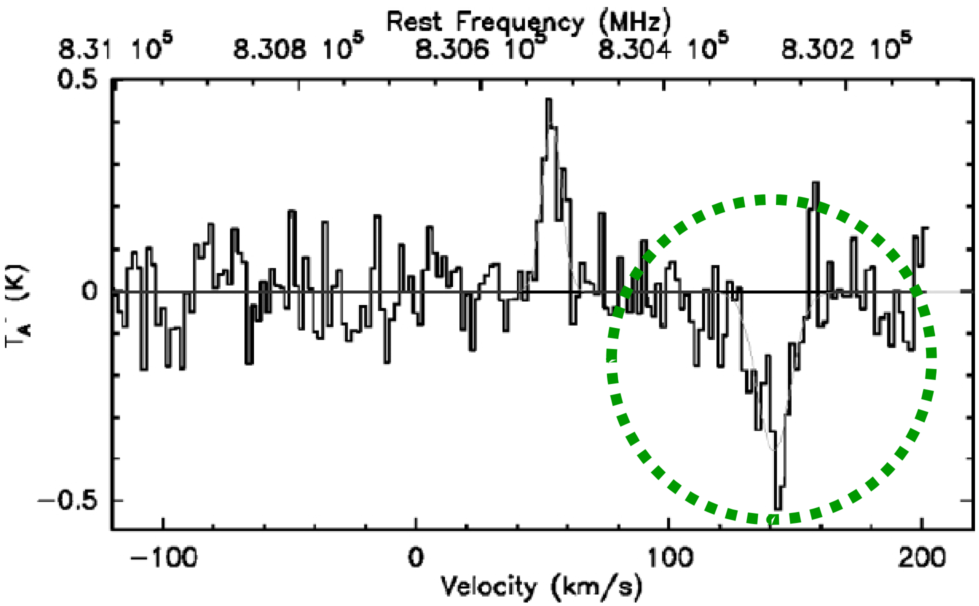
- CH^+, like other extremely reactive ions (e.g., H_2^+, CO^+, OH^+, H_2O^+) is particularly interesting as a diagnostic of interstellar processes
- Since it is destroyed rapidly (by collisions with H, H_2, and other neutrals) it may keep a memory of its formation process in its velocity distribution and rotational excitation (Flower & Pineau de Forêts 1998; Black 1998)
- The formation reaction ($C^+ + H_2 \rightarrow CH^+ + H$) is highly endothermic (4640 K), yet CH^+ is found associated with the CNM (based on line widths)
- A non-thermal energy source in diffuse cloud chemistry is needed to explain the high abundances of CH^+ (also OH and HCO^+; e.g., Liszt & Lucas 2000)



Observations

- Measured CH+ column densities (from visible and submm observations) are inconsistent with predictions of steady-state low-temperature chemistry (too high)
- The endothermic reaction between C^+ and H_2 is very slow at diffuse cloud temperatures of a few 10 K
- CH^+ is likely formed in very small, transient regions
- MHD shocks can explain observed CH^+ abundances and so can bursts of turbulent dissipation that locally heat gas to temperatures ~1000 K

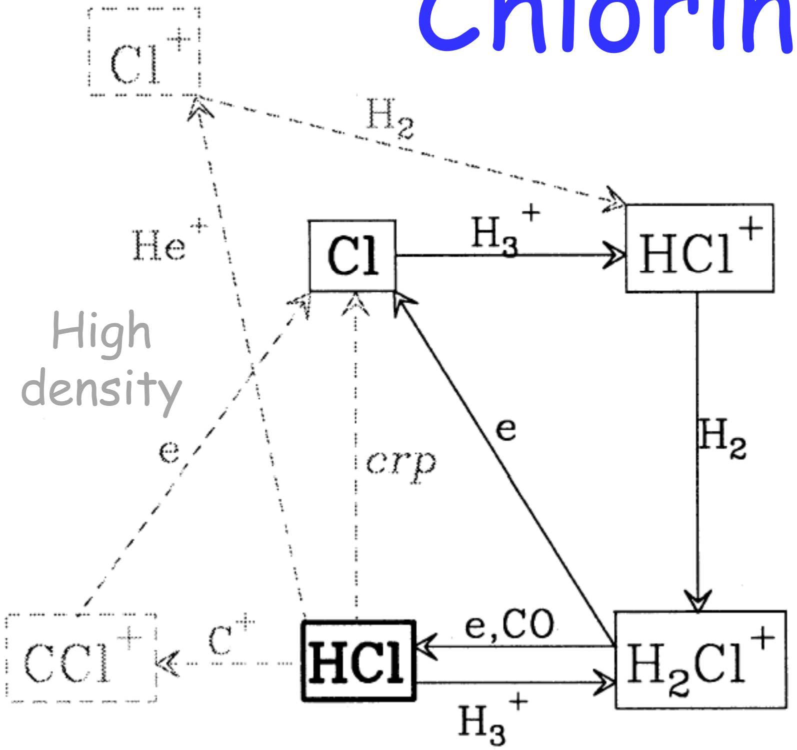
Detection of $^{13}CH^{+}$



Falgarone 2005

- CH^{+} can be observed in the optical (low-extinction regions)
- Not observable from the ground in the submm (atmosphere), but $^{13}CH^{+}$ 1—0 at 830 GHz has recently been detected in absorption toward G10.6 (Falgarone et al. 2005)
- New avenue for investigations of the high-temperature chemistry in *higher-extinction* regions

Chlorine Chemistry



$$\mathrm{Cl + H_3^+ \rightarrow HCl^+ + H_2}\,, \quad (1)$$

$$\mathrm{HCl^+ + H_2 \rightarrow H_2Cl^+ + H}\,, \quad (2)$$

$$\mathrm{H_2Cl^+} + e \rightarrow \begin{cases} \mathrm{HCl + H} & (10\%) \\ \mathrm{Cl + H_2} & (90\%)\,, \end{cases} \quad (3)$$

or

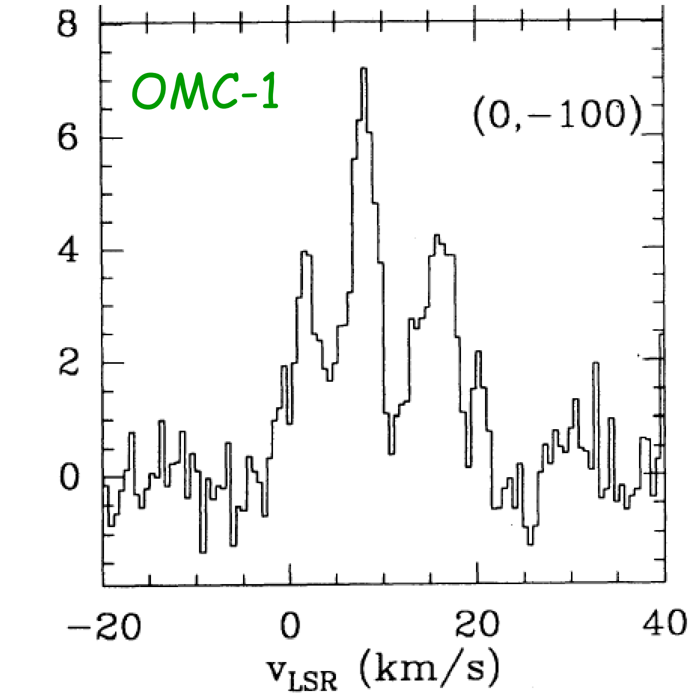
$$\mathrm{H_2Cl^+ + CO \rightarrow HCl + HCO^+}\,; \quad (4)$$

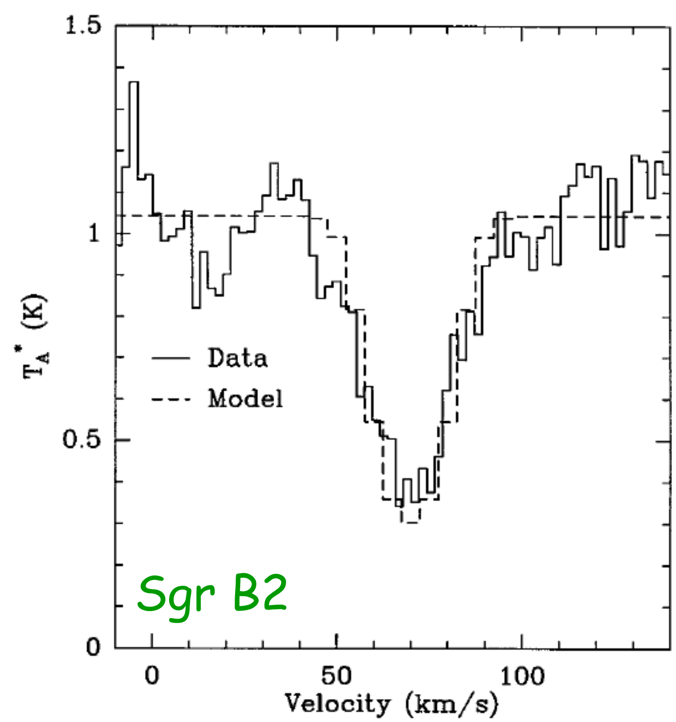
HCl, once formed, is destroyed by

$$\mathrm{HCl + H_3^+ \rightarrow H_2Cl^+ + H_2} \quad (5)$$

Schilke 1995

- Chemistry of Cl is fairly simple in dense interstellar clouds, with Cl and HCl as the only significant species (Blake et al. 1986; Schilke et al. 1995)
- HCl/Cl ratio is determined by the branching ratio of reaction (3) and the relative importance of reactions (3) and (4)
- At high densities (4) dominates and HCl/Cl rises
- In OMC-1, HCl contains about one third of available gas-phase chlorine (Schilke et al. 1995)
- Funded Herschel theory program to reanalyze Cl and F chemistry (Neufeld)



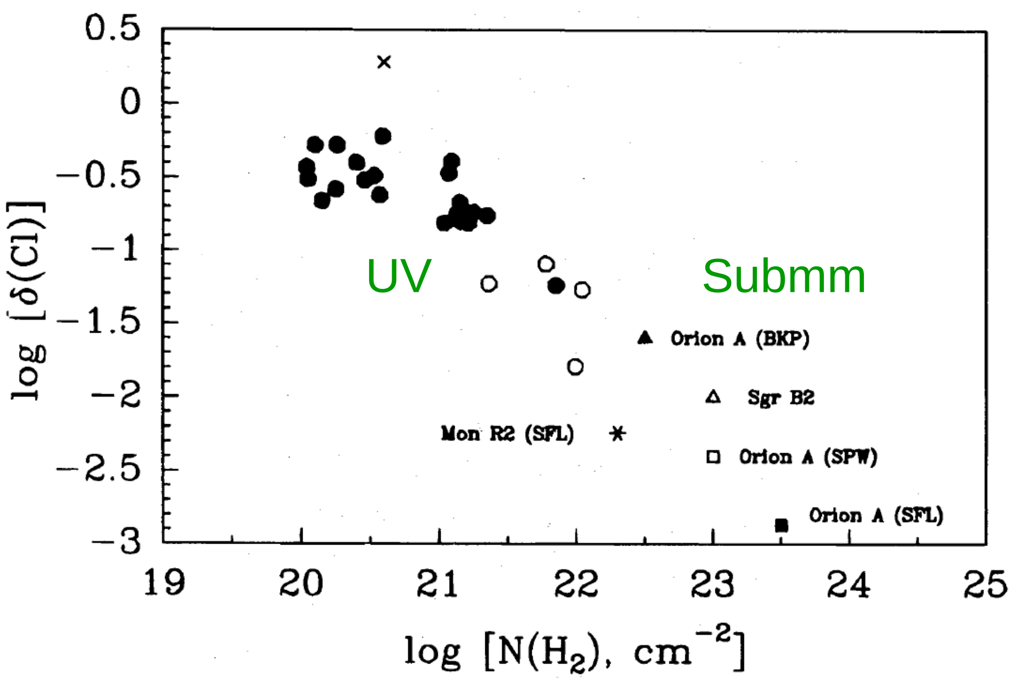


HCl Observations

- HCl 1—0 transition at 625.9 GHz has a very high critical density (4×10^7 cm^{-3}) and is well suited for absorption studies against bright submm sources
- Transition split into three hyperfine components (determination of the optical depth)
- Observations of the corresponding $H^{37}Cl$ transition at 625.0 GHz allow for determination of the $^{35}Cl/^{37}Cl$ isotopic ratio (metallicity gradients)

Schilke 1995; Zmuidzinas 1995

Chlorine Depletion



Salez 1996

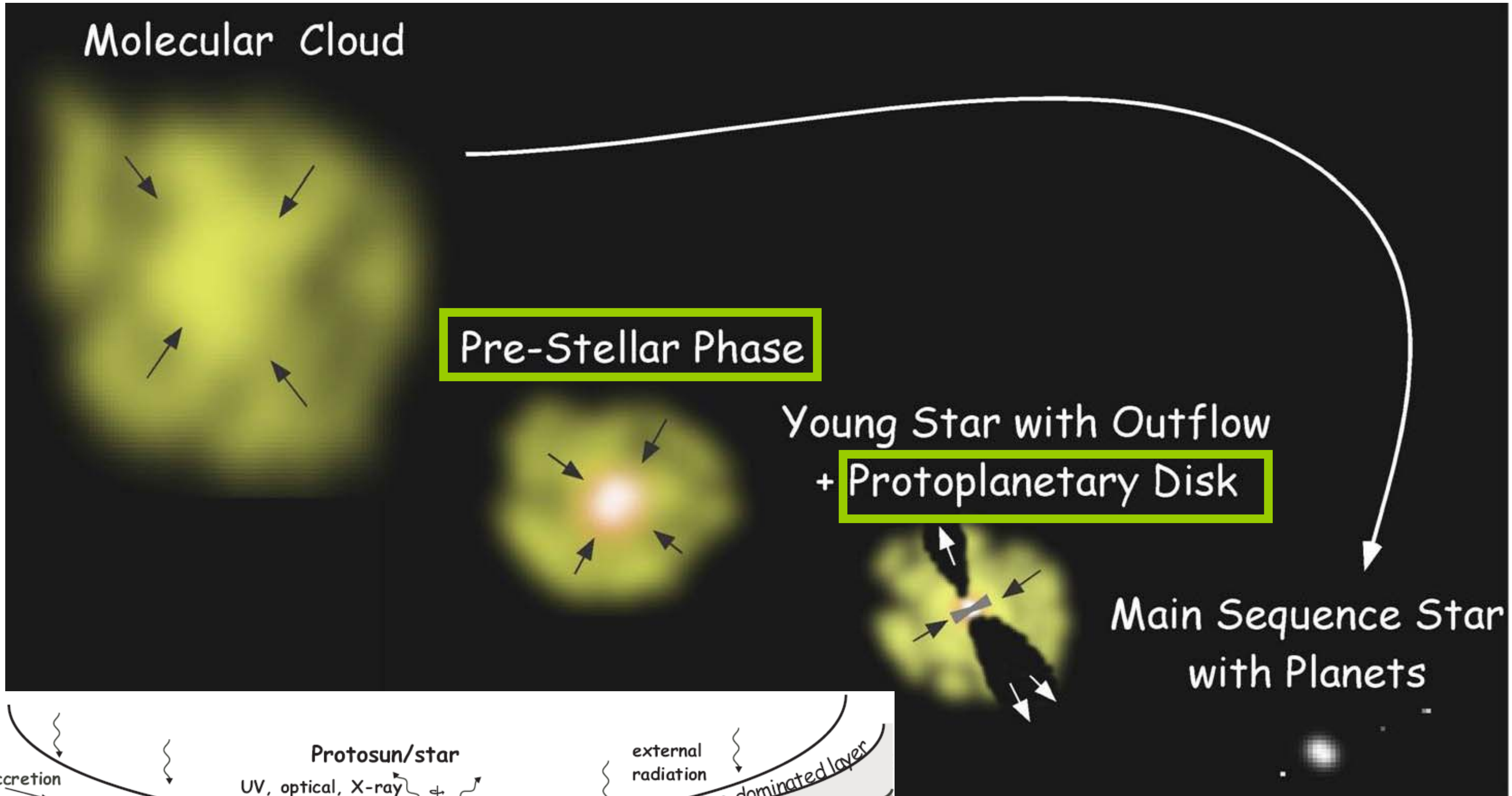
- Measurements of HCl abundance can serve as a valuable probe of depletion (as is the case for HF)
- In diffuse ISM chlorine is depleted by a factor of 2—3
- Depletion increases steeply with density
- In the shielded, high-density regions both chlorine atoms and HCl are depleted
- However, if the dust is moderately warm (15—30 K), only the highly polar HCl can remain on the grains (Bergin et al. 1995)

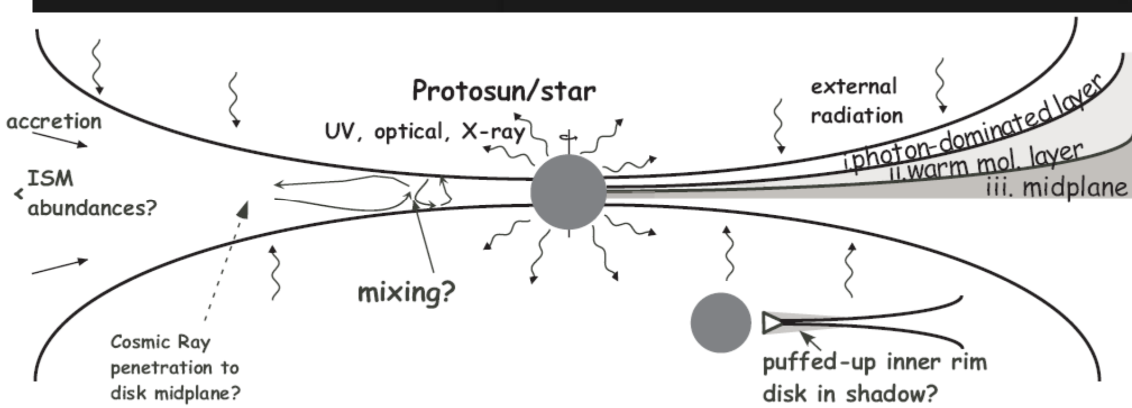
Deuterated Molecules

- Astrochemist's perspective
  - Peculiar, non-LTE low-temperature chemistry (fractionation)
- Astrophysicist's perspective
  - Excellent tracers of early stages of star formation
  - Dust: good mass tracer, but carries no velocity information
  - Molecules: often depleted onto dust grains in cold regions, except some deuterated species

Chemistry imposes a limit where the molecules can probe.

Star Formation



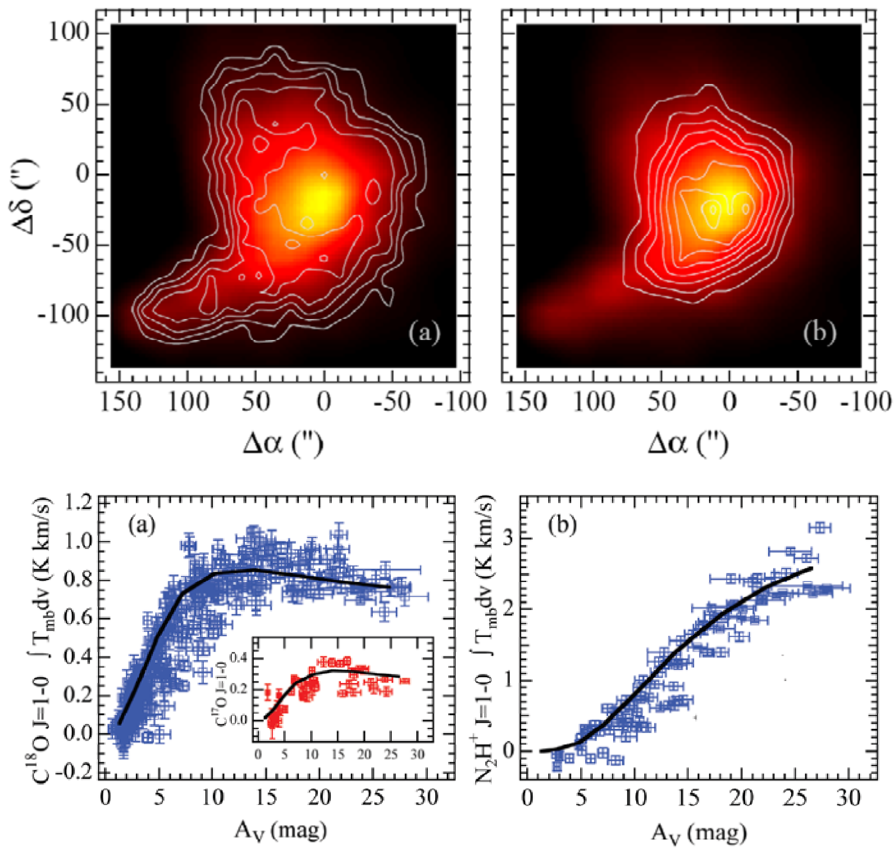


Cold disk midplane

Bergin 2006

Molecular Differentiation in Starless Cores

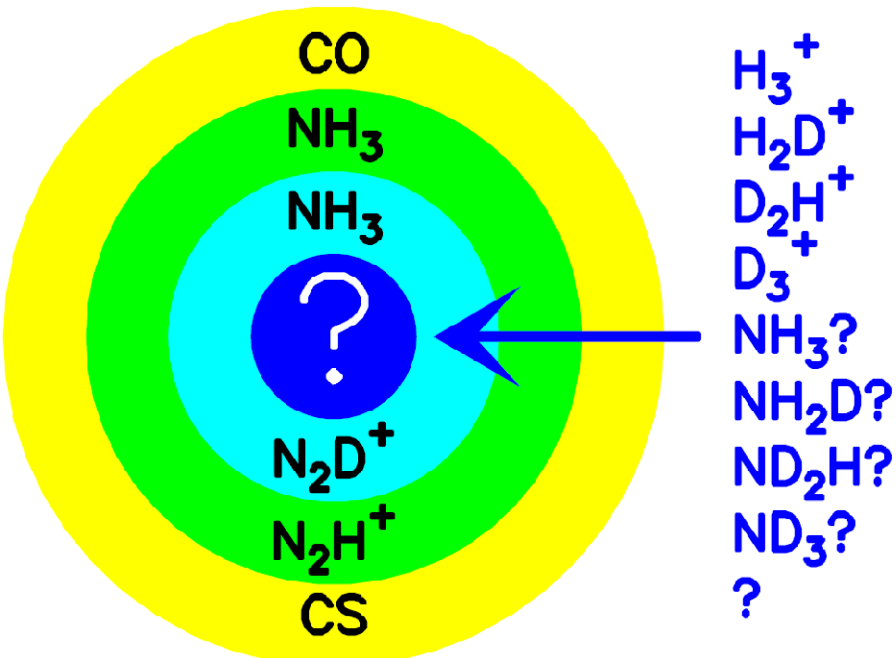
$C^{18}O$ – contours – N_2H^+



B68: *Bergin et al. 2002*

- CO, CS depleted at densities above a few $\times 10^4$ cm^{-3}
- N_2H^+ unaffected up to a few 10^5 – 10^6 cm^{-3} (complicated hyperfine pattern)
- NH_3 abundance may actually be enhanced in the central regions (e.g., Tafalla et al. 2002, 2004)

"Complete Freeze-out" Models



- Recent chemical calculations (e.g. Walmsley et al. 2004) suggest that at densities above ~10^6 cm^{-3} even the N-bearing species should eventually condense onto dust grains
- Under such conditions, H_3^+ and its deuterated isotopologues become the only tracers of H_2
- Density threshold time and model dependent
- Good observational constraints needed

Revised D Chemistry

$$H^+ + D \quad = H + D^+$$

$$D^+ + H_2 \quad = HD + H^+ + \Delta E_1$$

$$D^+ + HD \quad = D_2 + H^+ + \Delta E_2$$

Also

$$H_3^+ + HD \quad = \quad H_2D^+ + H_2 + \Delta E_a$$

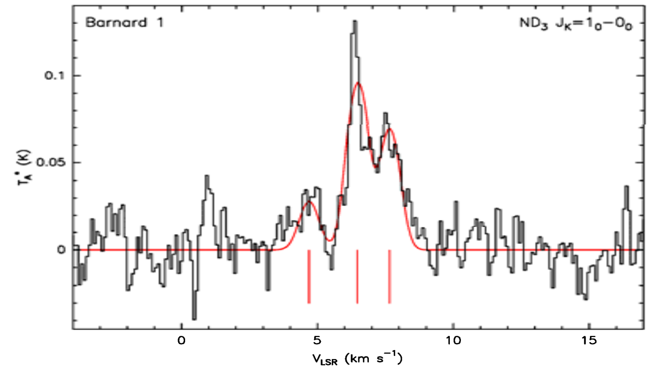
$$\boxed{\begin{array}{l} H_2D^+ + HD \; = \; D_2H^+ + H_2 + \Delta E_b \\ D_2H^+ + HD \; = \; D_3^+ + H_2 + \Delta E_c \end{array}}$$

Presence of D_2 at ~ 10^{-6} $[H_2]$?

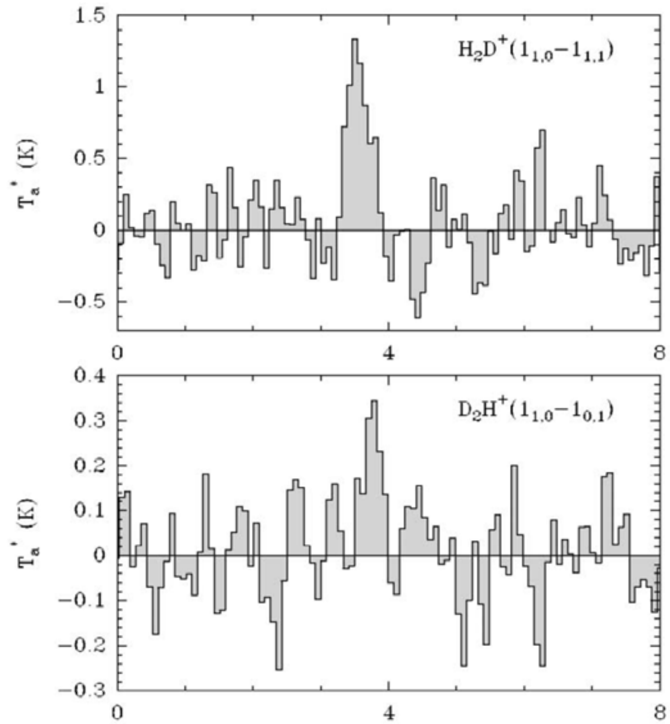
D_2H^+, D_3^+ ?

Roberts et al. (2003)

Phillips & Vastel (2003)

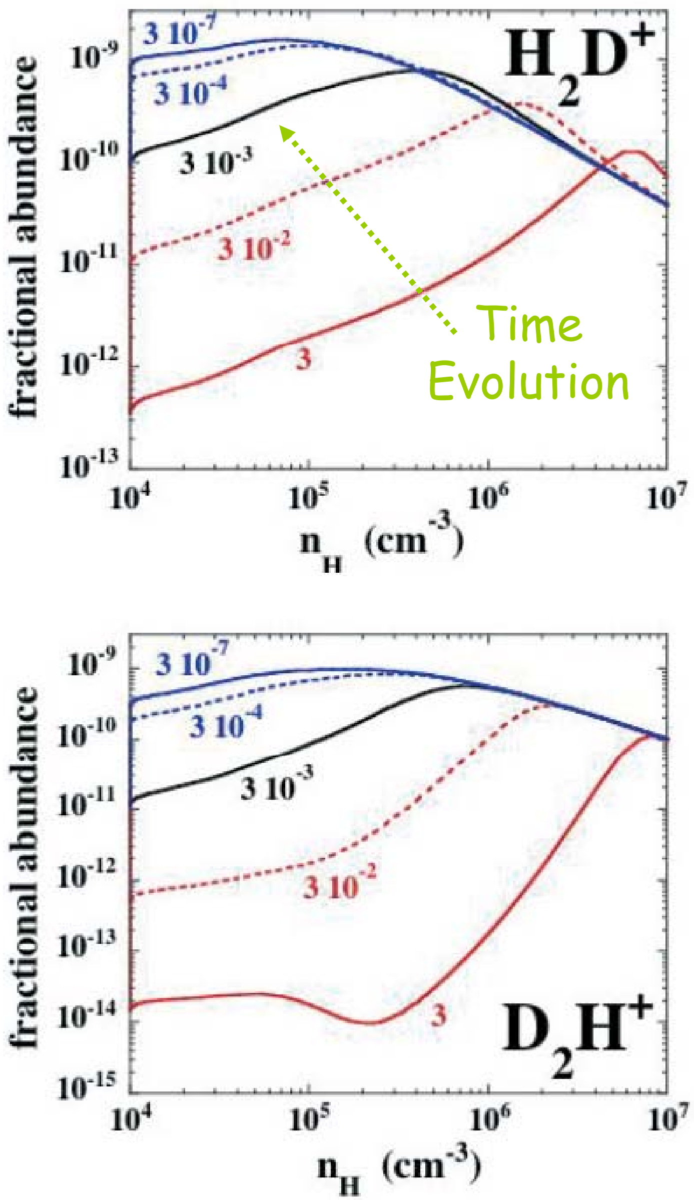


ND_3: *Lis 2002*



D_2H^+: *Vastel 2004*

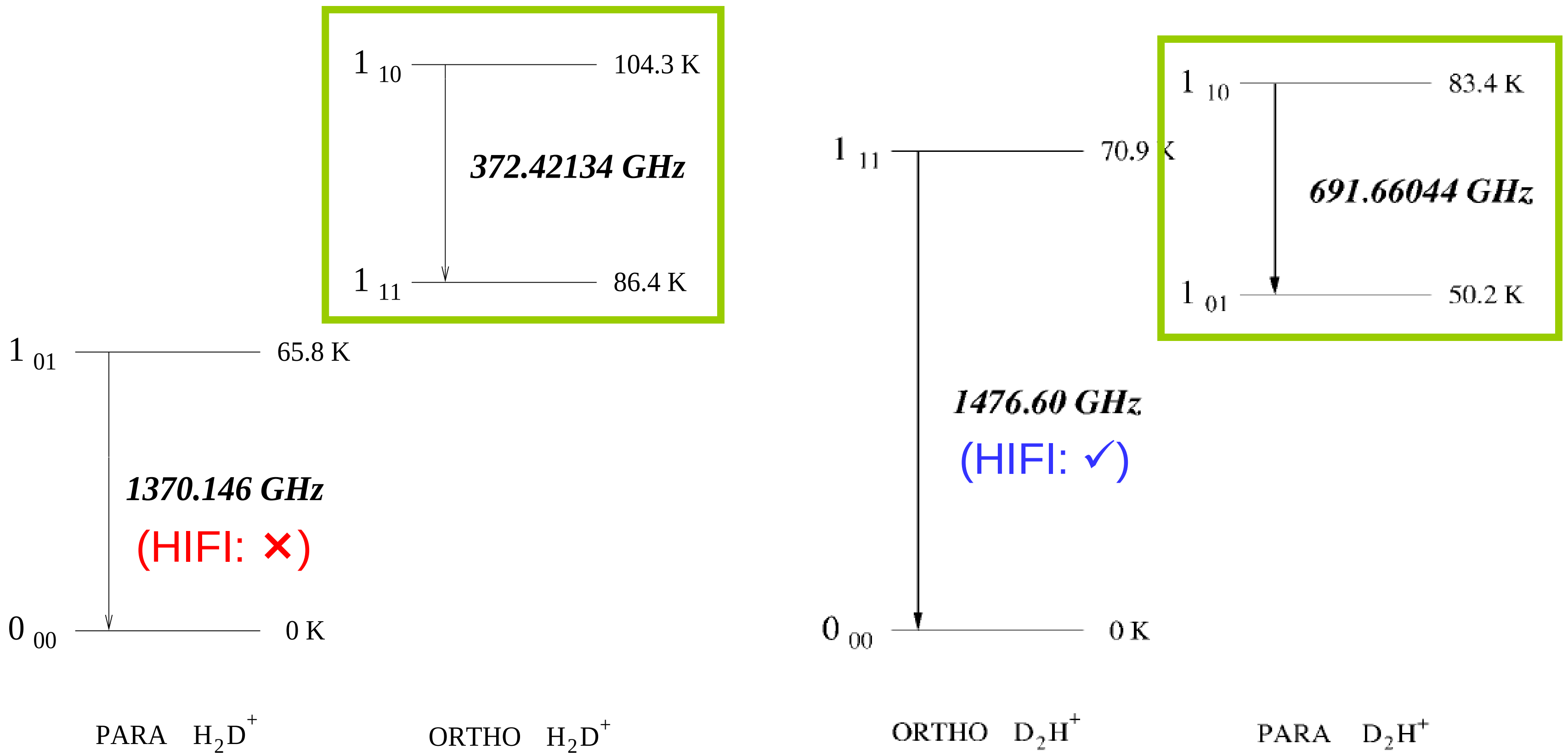
Importance of the o/p H_2 Ratio



Flower 2006

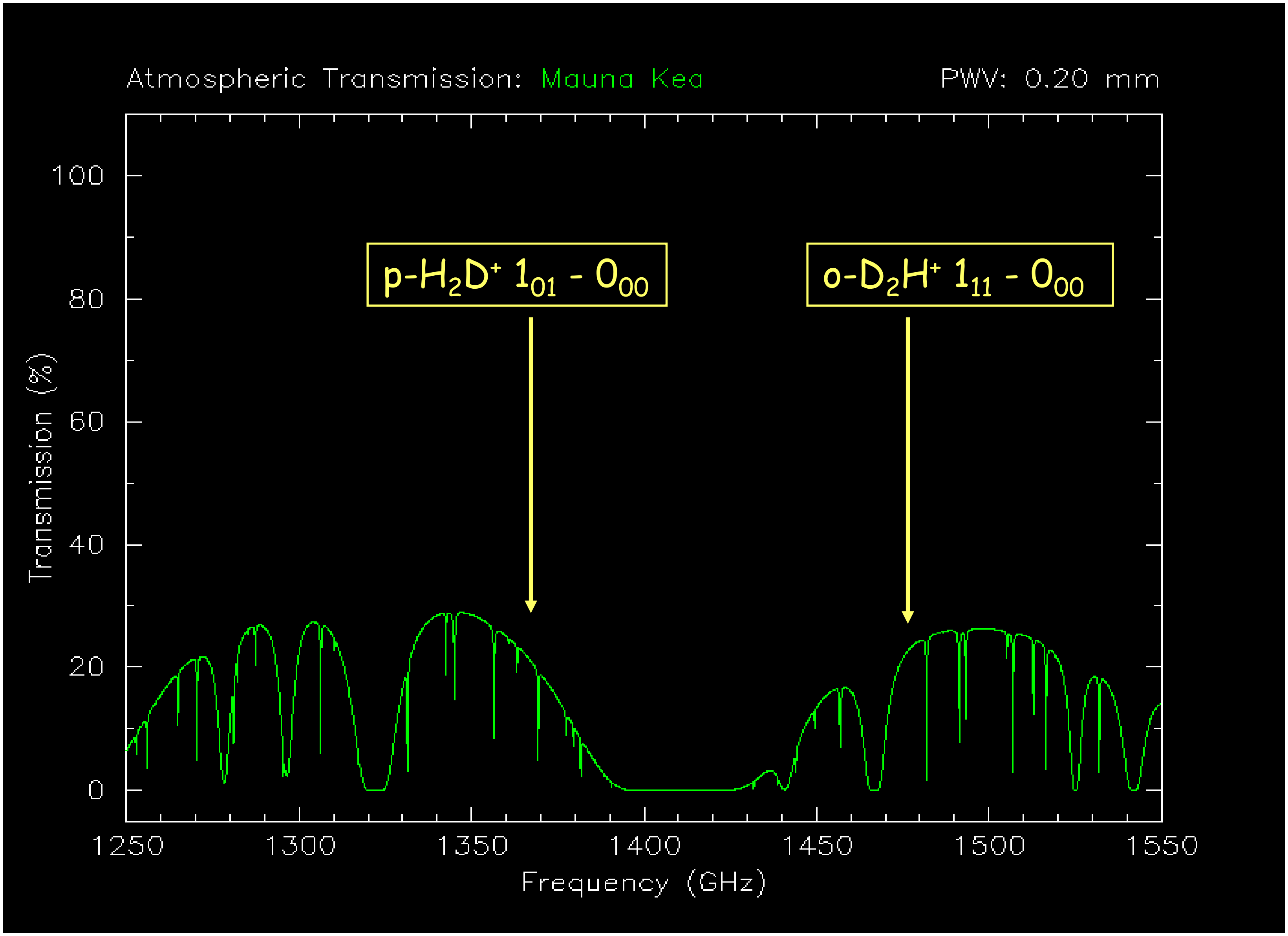
- Degree of deuteration of molecular ions and neutrals is sensitive to the o/p ratio in H_2 and hence the chemical and thermal history of the gas
- Protostars forming in young (<10^6 yr) clouds *should not* display high levels of deuteration (high o/p H_2 ratio)
- Important to observe both ortho and para transitions to derive *total* column densities

Nuclear Spin Statistics



- Current observations of H_2D^+ and D_2H^+ limited to specific nuclear spin states!

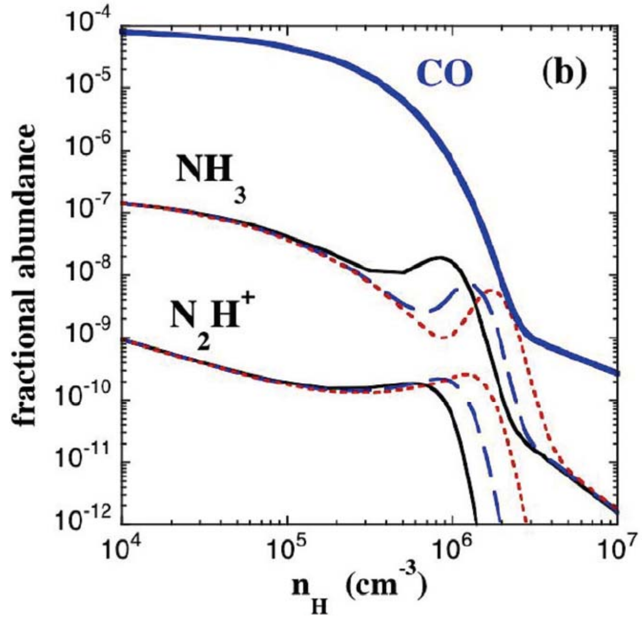
THz Transitions



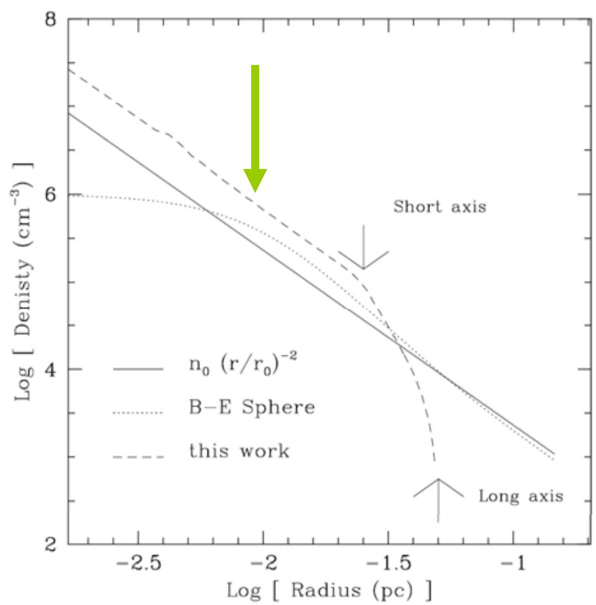
Interstellar Ammonia

- H_2D^+ and D_2H^+ not affected by depletion, but difficult to observe from the ground (atmosphere)
- Are the N-bearing species, in particular NH_3, completely frozen out, if so at what densities?
- Ammonia lines have simple hyperfine patterns and can be used as a tracer of the velocity field
- Submm ground state rotational lines have very high critical densities (>10^7 cm^{-3}) and are only excited in the densest central regions
- Lines of ND_3 and ND_2H (350 GHz window) detected in a number of sources, mapping observations in progress, but lines weak
- NH_2D more abundant, fundamental transitions at 470/494 GHz—completely unexplored

Onset of Ammonia Depletion



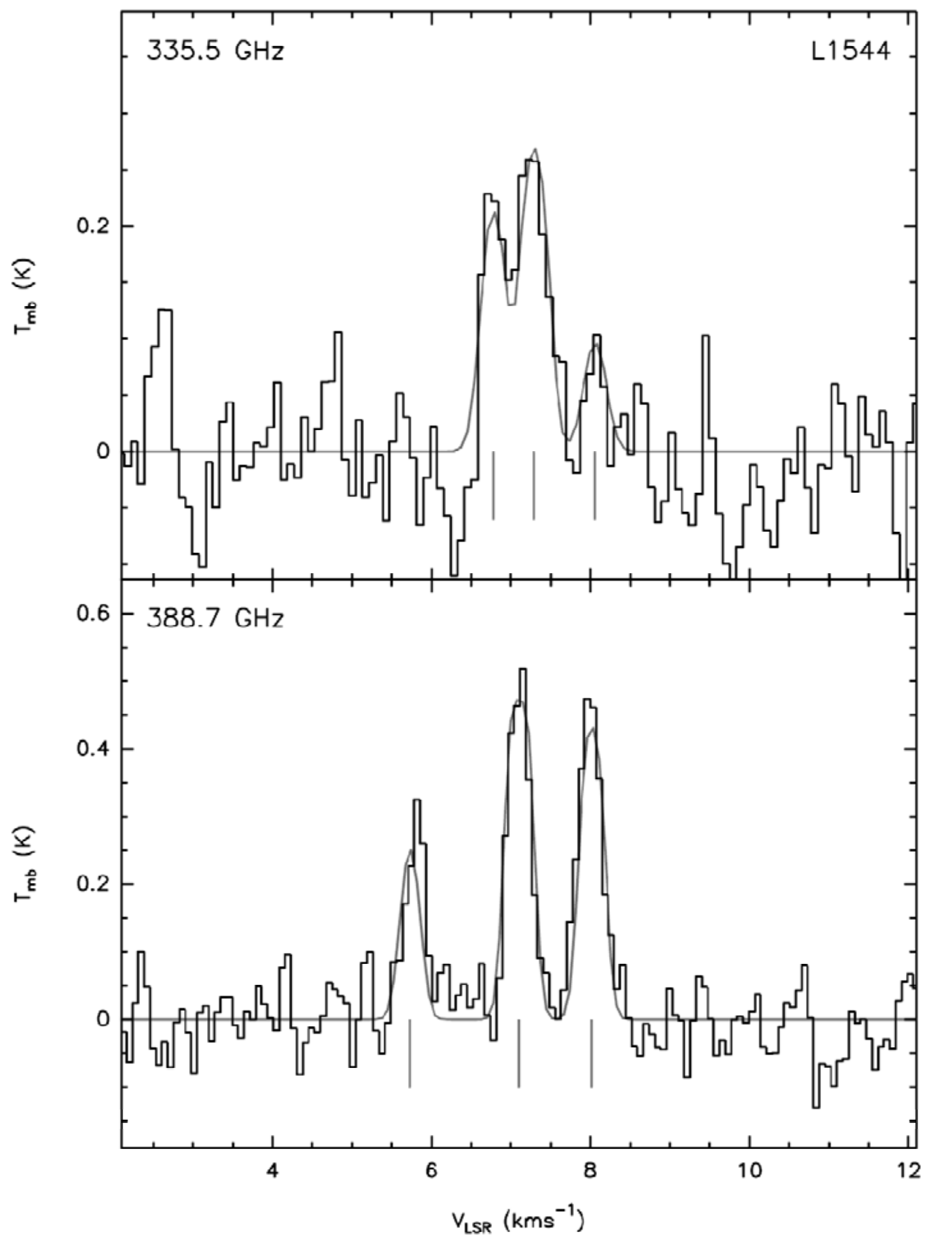
Flower 2006



Doty 2005

- Ammonia starts depleting at densities just above 10^6 cm^{-3} (e.g., Flower et al. 2006)
- In L1544, n=10^6 cm^{-3} corresponds to a radius of ~0.01 pc or 15" (Doty et al. 2005)
- The central depleted region, if present, should be observable with CCAT
- Mapping observations needed

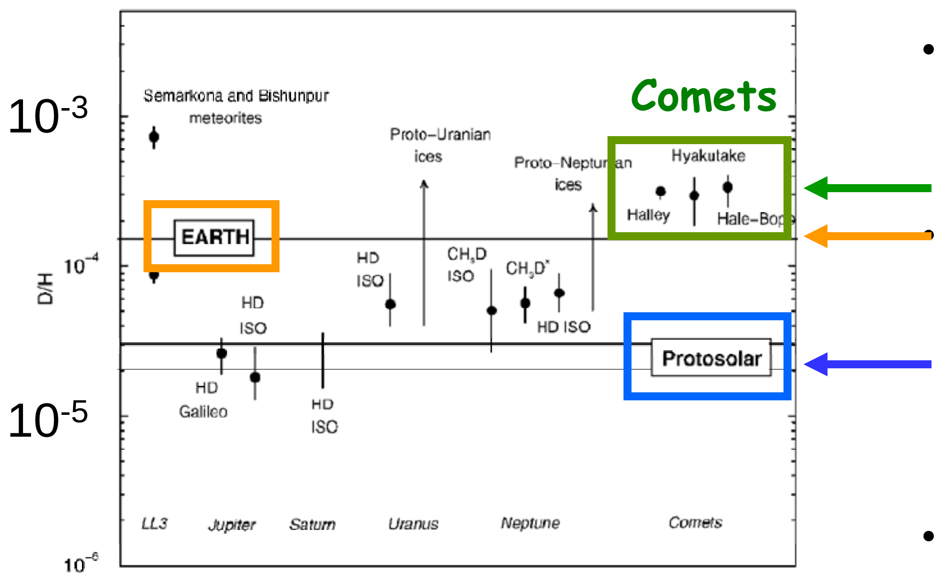
ND_2H in L1544



Lis 2006

- Strong ND_2H emission detected
- Linewidths 0.32/0.26 kms^{-1}
- For T_k=10K, the turbulent linewidth of the 389 GHz ND_2H line is only 0.20 kms^{-1}, compared to 0.5 kms^{-1} for H_2D^+
- ND_2H emission tracing the highest density region, not the low-density envelope
- No mapping observations yet available

D/H Ratio in Comets



Altwegg & Bockelée-Morvan 2002

- Isotopic ratios, in particular D/H ratio, provide important constraints on the origin and thermal history of the gas
- D in cometary water enriched by a factor of 10 compared to the protosolar value
- Cometary water largely preserved the high D/H ratio acquired in the protosolar cloud; only partial mixing occurred in the Solar Nebula
- High cometary D/H values (twice terrestrial) make it difficult to defend a major cometary origin of terrestrial water
- The 894 GHz HDO line *best suited* for cometary studies

Technical Requirements

- For absorption studies need an accurate measurement of the continuum level—chopping or fast switching, several arcmin, ~1 Hz
- Switching between two pixels of the array?
- Submm continuum sources spatially extended: with mapping observations can study *spatial variations* of molecular abundances in the foreground clouds—closely packed array
- The interesting lines spread over *all* submm atmospheric windows—multiple receivers; priorities?
  - 460 GHz: HDO, NH_2D
  - 650 GHz: HCl, p-D_2H^+
  - 850 GHz: HDO, $^{13}CH^+$
  - 1.3/1.5 THz: p-H_2D^+, o-D_2H^+

Can This be Done with ALMA?

- Interferometers generally very good for absorption studies toward point sources (self-cal)
- Filtering of the extended emission (spatial variations in foreground clouds; NH_2D extended; line confusion)
- Interferometry in the high-frequency bands will be challenging
- Band 10 not available at first light (HDO, $^{13}CH^+$, CI…)

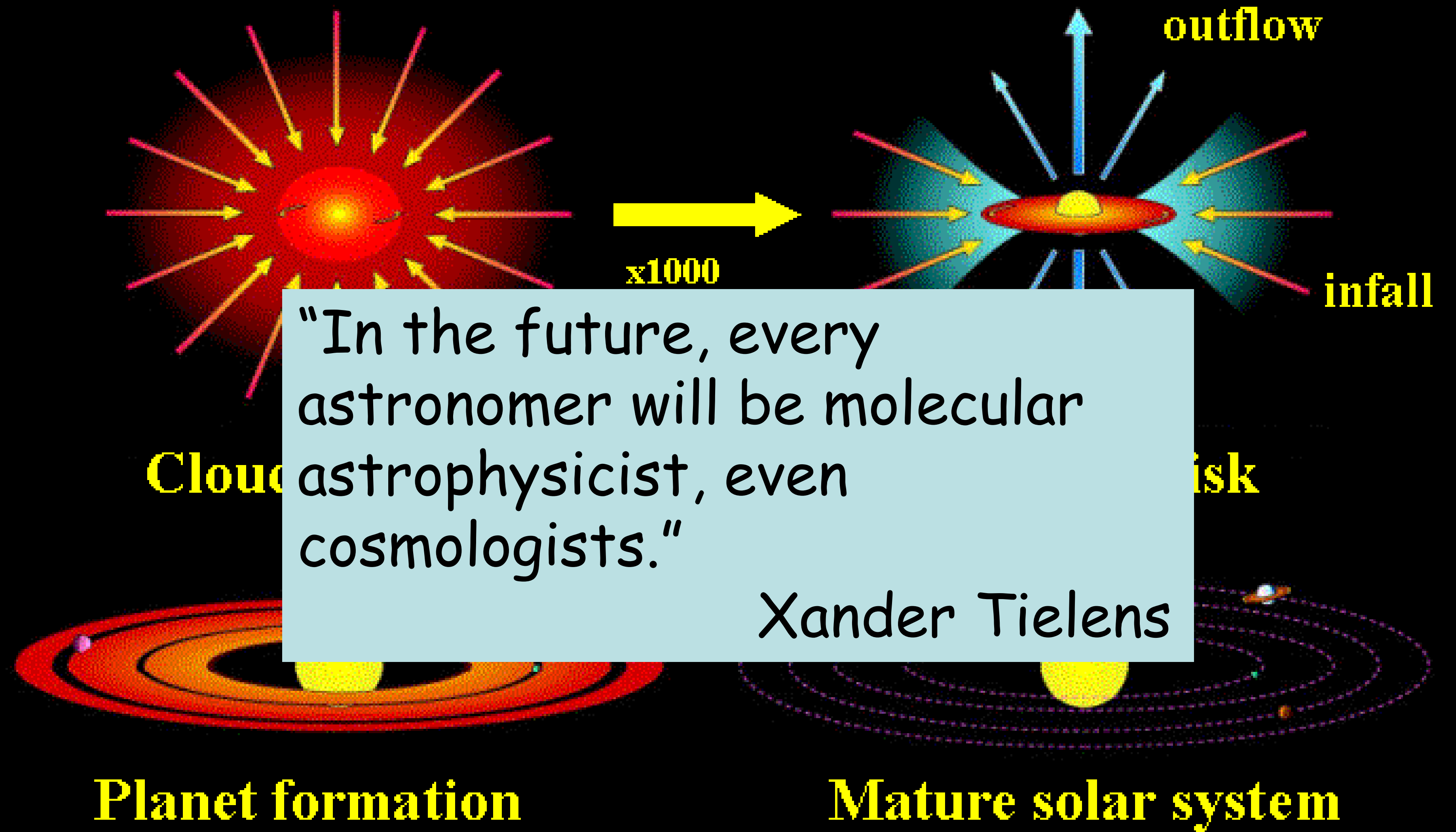
Table 2 Summary of ALMA receivers

Band no.	Frequency range (GHz)	Receiver noise temperature[a] (K)	Mixing scheme	IF Bandwidth
3	84–116	37	2SB	4 GHz
4	125–169	51	2SB	4 GHz
5[b]	163–211	65	2SB	4 GHz
6	211–275	83	2SB	8 GHz
7	275–373	147	2SB	4 GHz
8	385–500	98	2SB	4 GHz
9	602–720	175	DSB	8 GHz
10[b]	787–950	230	DSB	8 GHz

[a]Over 80% of the band, specification. Preproduction units tested to date have been outperforming their specifications

[b]At first light, these bands will be available on fewer than all of the antennas in the array

Molecules are Everywhere



"In the future, every astronomer will be molecular astrophysicist, even cosmologists."

Xander Tielens

Scenario largely from indirect tracers.

Fig. by McCaughrean