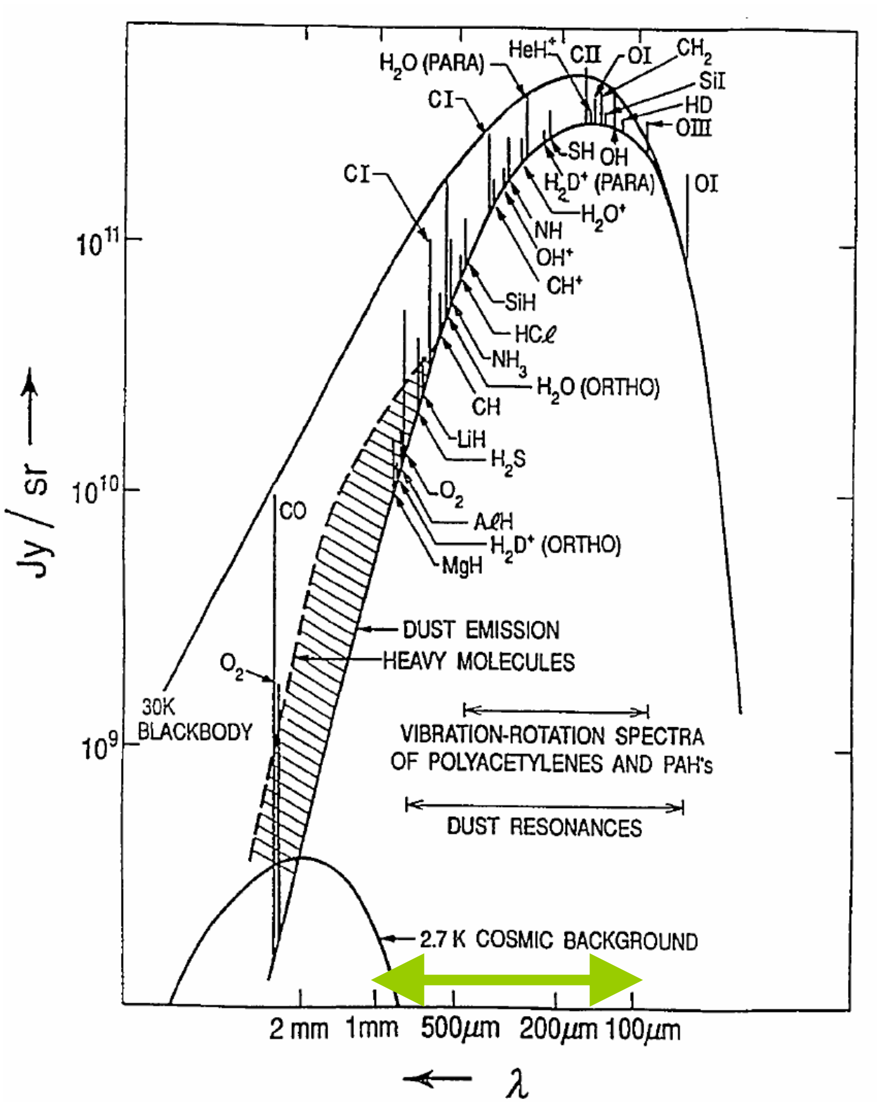
Submillimeter Absorption Spectroscopy

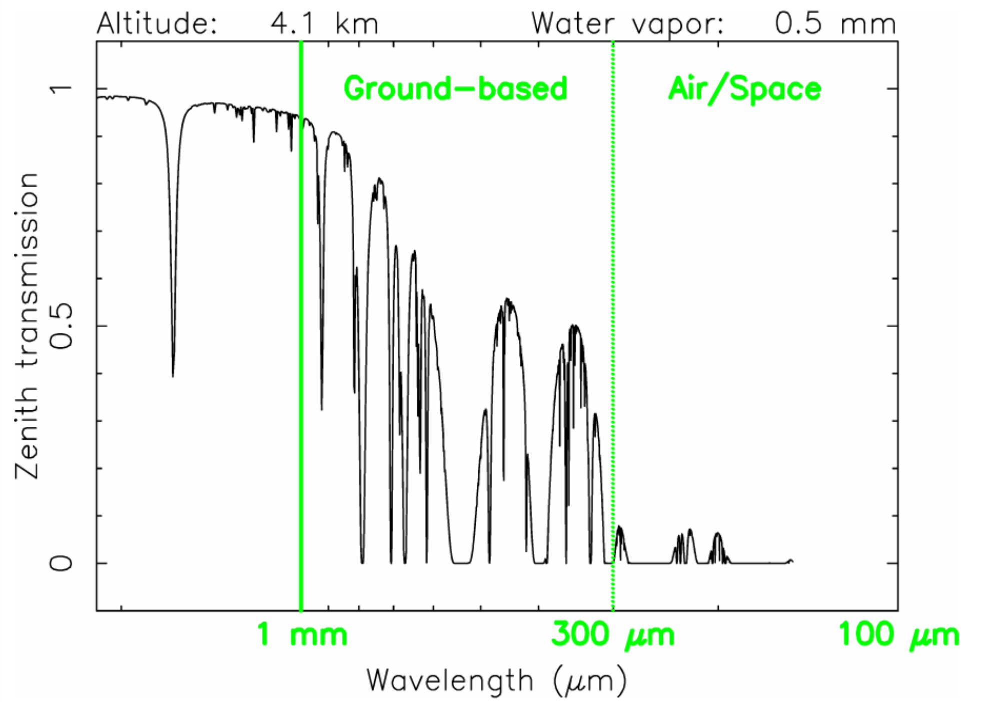
Darek Lis (Caltech)

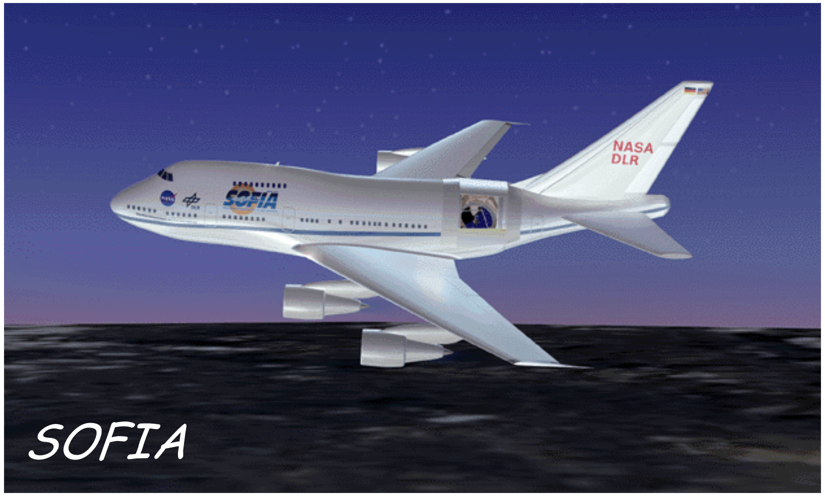
Nizhnij Arkhyz, Russia, August 8, 2008

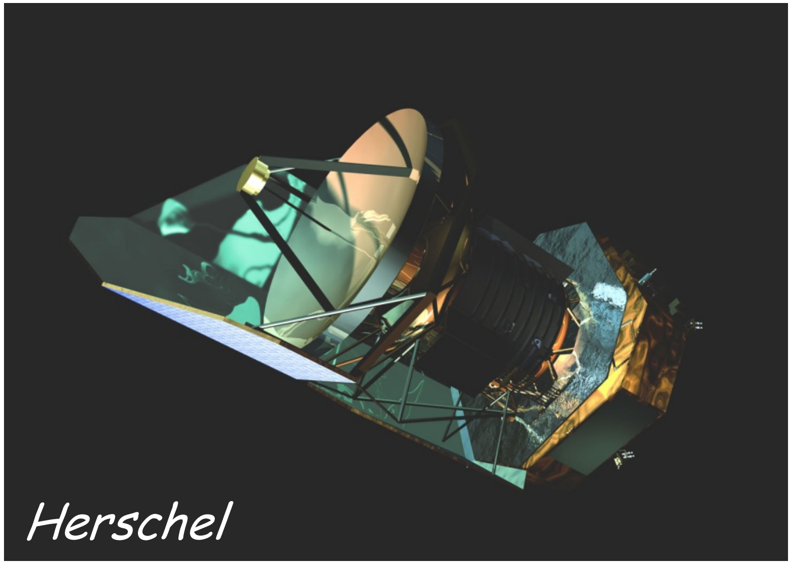
Submillimeter Astrophysics



Phillips & Keene 1992

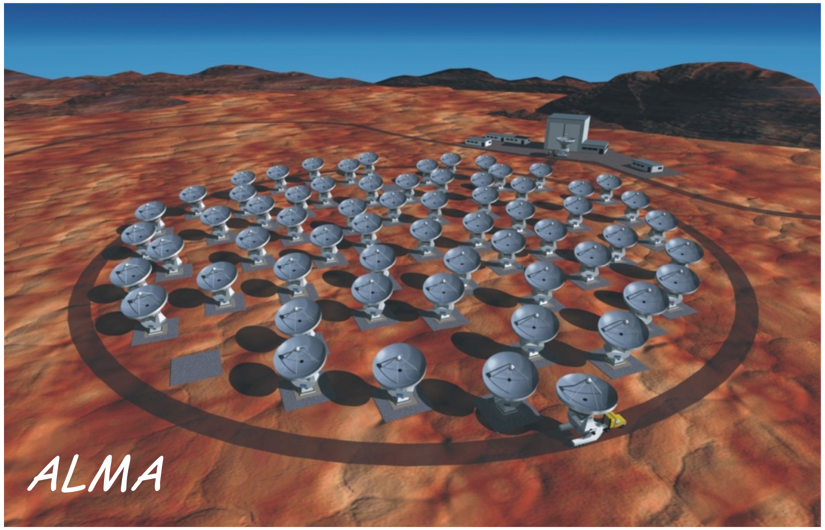


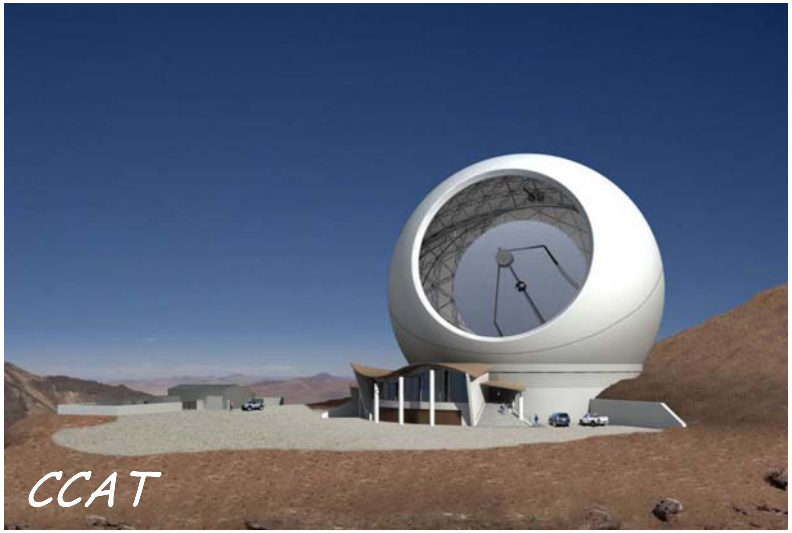




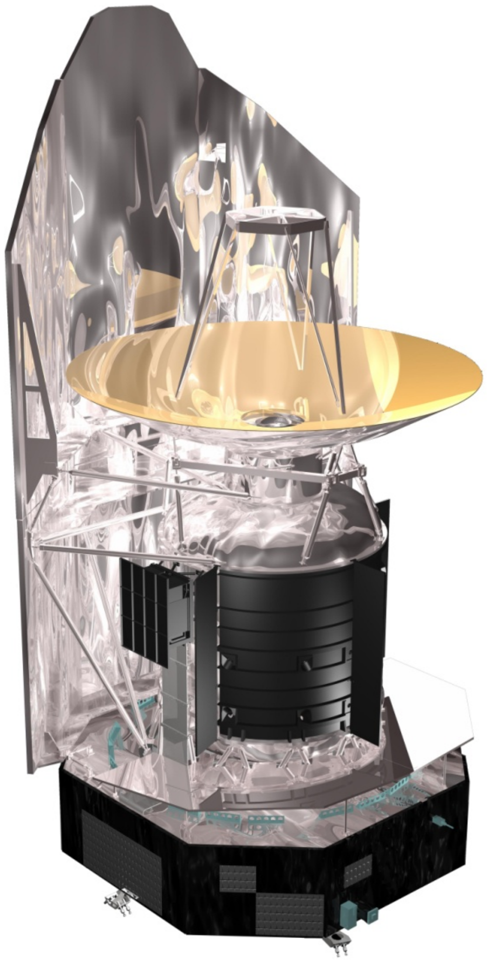
New Submillimeter Facilities

Testimony to the Importance of the Field





Herschel Space Observatory



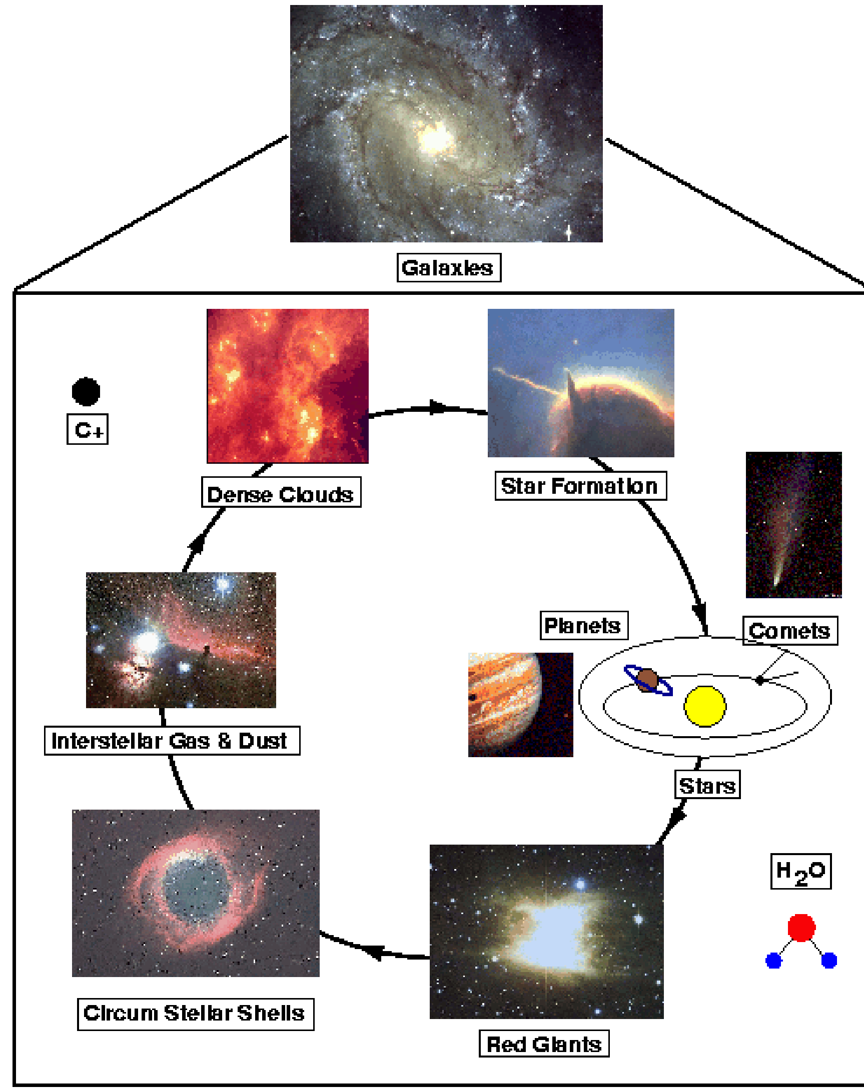
- ESA cornerstone mission; first space facility to completely cover the 60–670 μm spectral range
- Telescope: 3.5 m diameter, passively cooled to ~80 K
- Orbit: Lissajous around L2; very stable and low background
- Larger telescope than other missions (IRAS, ISO, SWAS, Spitzer, Akari,…)
- Colder aperture, better 'site', more observing time than balloon and airborne instruments (~1000 SOFIA flights/year)
- Lifetime: >3 years; Ariane 5; early-2009
- Three cryogenically cooled instruments, PACS, SPIRE (bolometers), and **HIFI** (heterodyne)

http://herschel.esac.esa.int/overview.shtml

HIFI Specifications

- Heterodyne spectrometer
- Wide frequency coverage:
  - Bands 1-5 (SIS) : 480-1250 GHz (625-240 μm)
  - Bands 6-7 (HEB): 1410-1910 GHz (212-157 μm)
- Wide instantaneous IF bandwidth:
  - 4 GHz in 2 polarizations (2.4 GHz for Bands 6-7)
- High frequency resolution:
  - WBS: 1 MHz (0.63 km/s at 480 GHz, 0.16 km/s at 1910 GHz)
  - HRS: 140/280 kHz
- High sensitivity (state of the art mixers)

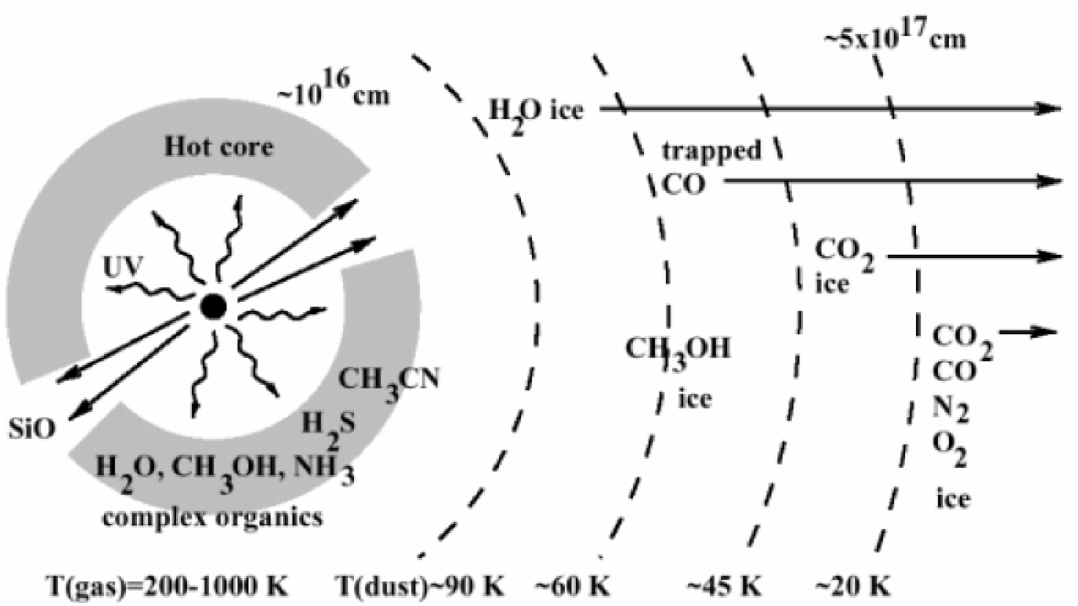
Science: Life Cycle of Gas and Dust



http://herschel.esac.esa.int/science_instruments.shtml

Spectral 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)

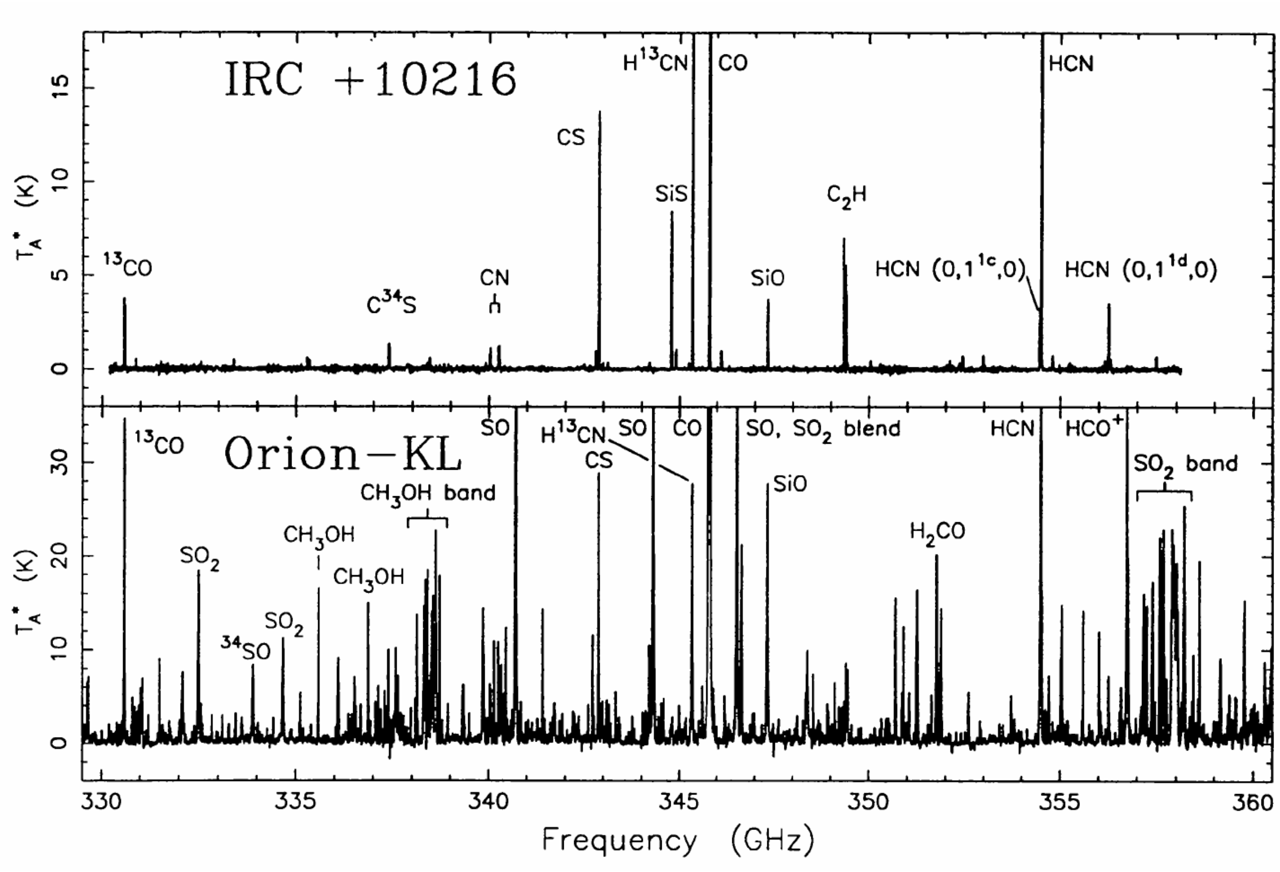


van Dishoeck 1998

Fundamental questions:

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

Molecular Complexity: ISM

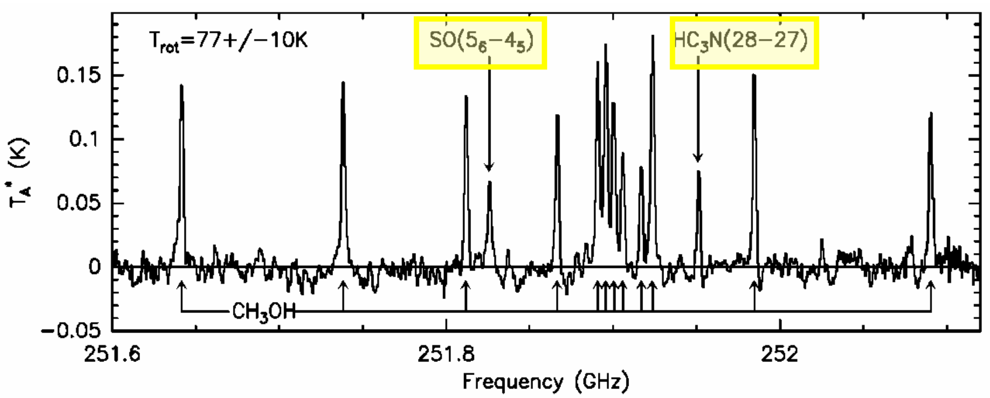


Groesbeck et al. 1994
Schilke et al. 1997

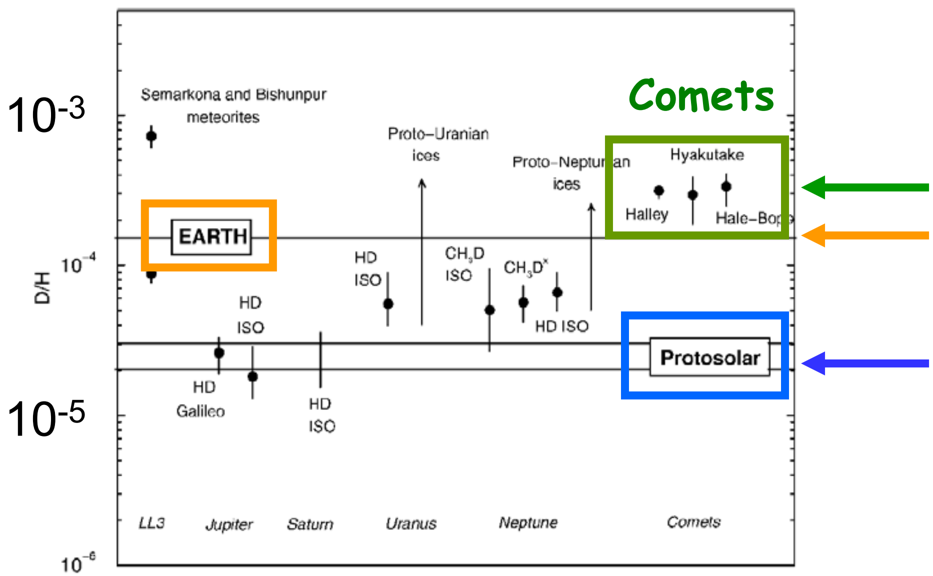
Line Contribution to Broadband Continuum Flux

Source	Line Flux
Orion KL 0.8–1 mm	50%
Orion KL 450 μm	15%
Orion S	8%
IRAS 16293	5%
IRC +10216	65%
VY CMA	27%
OH 231.8	23%

Molecular Complexity: Comets



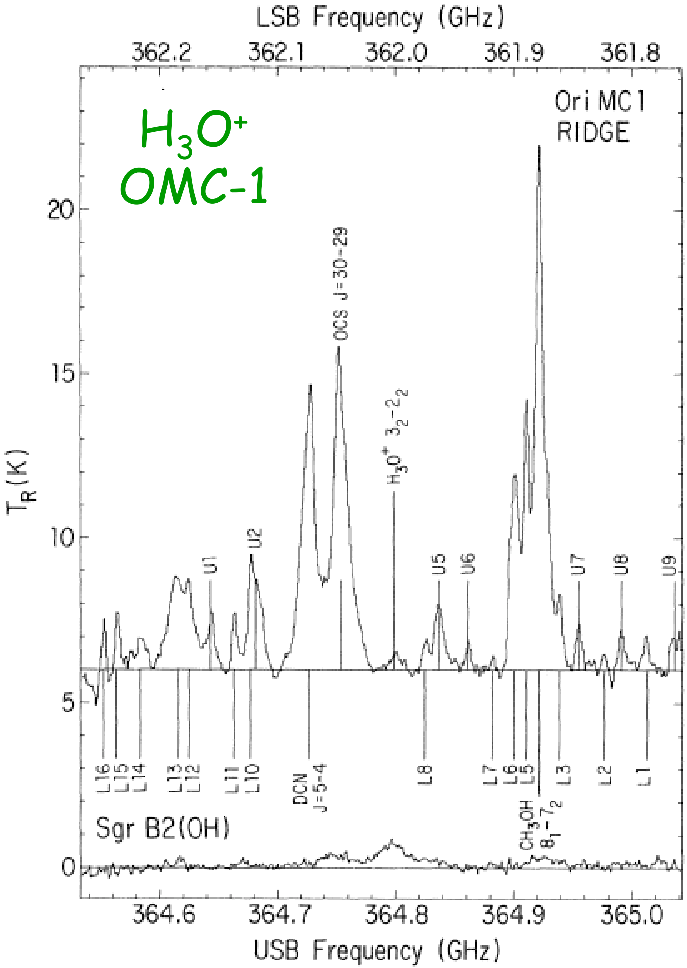
Hale-Bopp: *Lis et al. 1999*



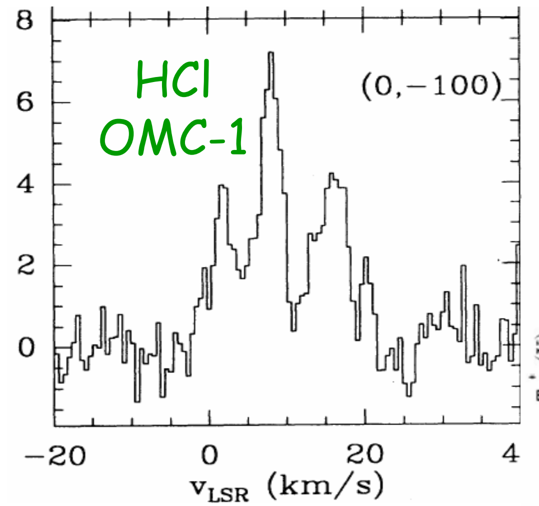
Altwegg & Bockelée-Morvan 2002

- Over two dozen species detected in cometary atmospheres, primarily using radio techniques
- Some complex species, such as methyl formate ($HCOOCH_3$) and ethylene glycol ($HOCH_2CH_2OH$)
- The (sub)millimeter wavelength range is well matched to the cold environments of cometary atmospheres (T~40—100 K)
- Heterodyne techniques allow velocity-resolved kinematic studies
- Measurements of isotopic ratios (e.g., D/H)

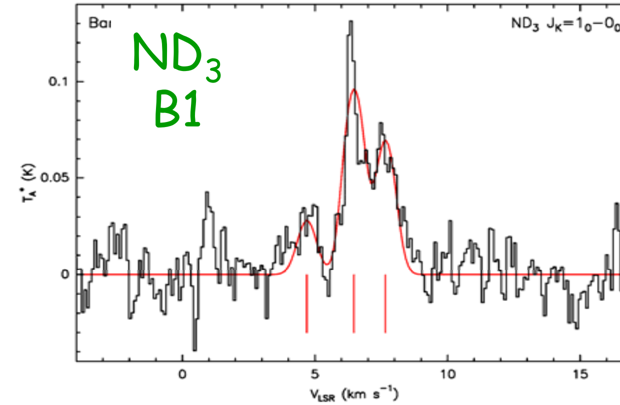
Hydrides and Deuterides



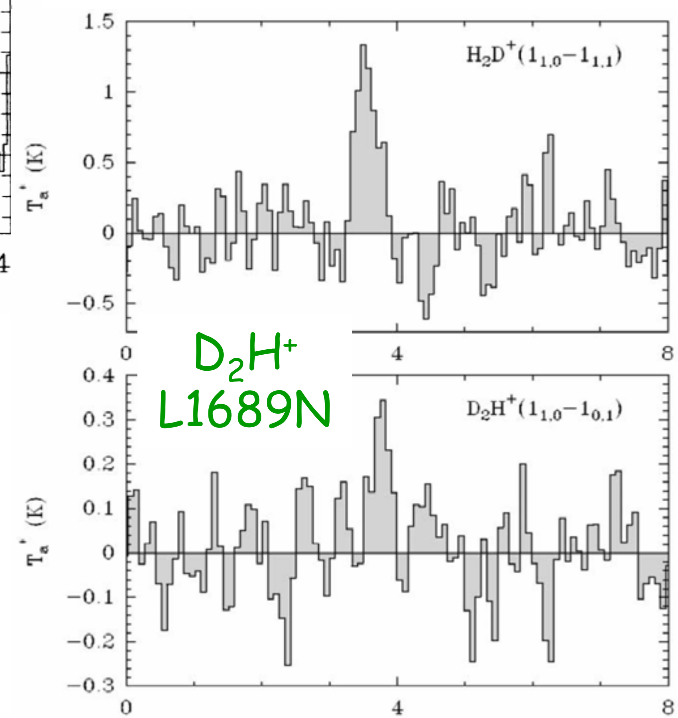
Wootten et al. (1991)



Schilke et al. (1995)



Lis et al. (2002)

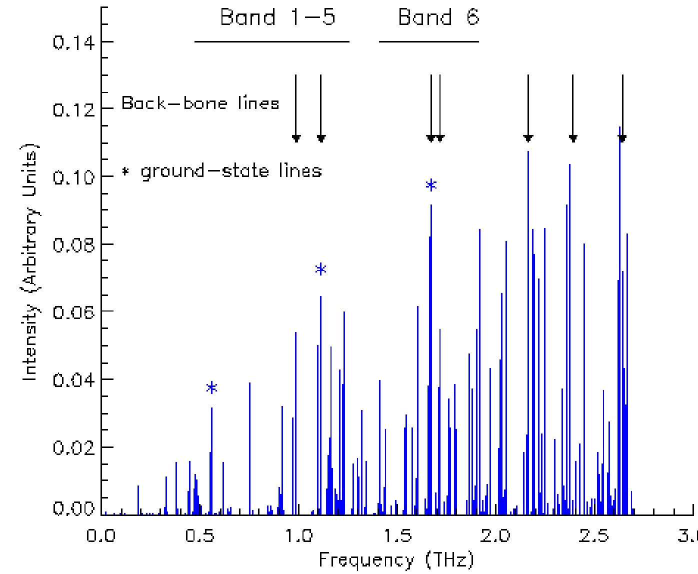


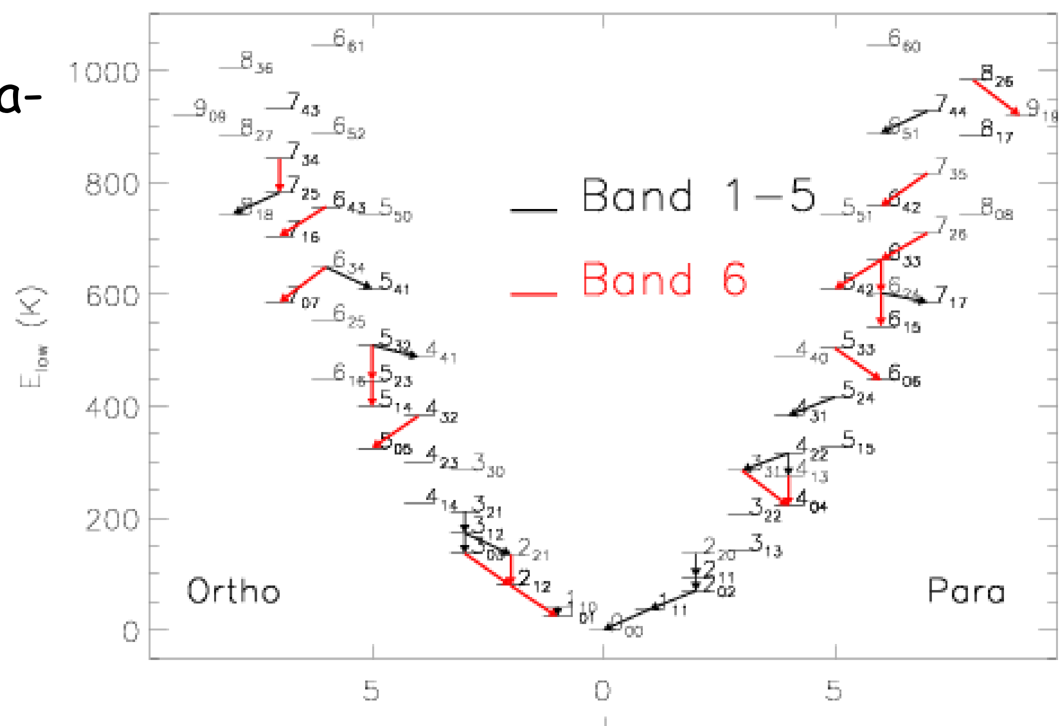
Vastel et al. (2004)

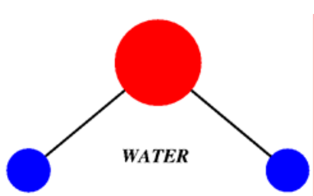
Also submm water masers (Menten et al. 1990), NH_2 (Gerin et al. 2008)…

The Water Universe

- HIFI will provide a comprehensive view of the water Universe, not obscured by Earth's atmosphere
- Multiple lines, including ground-state and back-bone lines of both ortho- and para-water
- Water isotopologues, OH and H_3O^+ for detailed investigation of water chemistry
- Half of HIFI water lines are in Bands 6—7

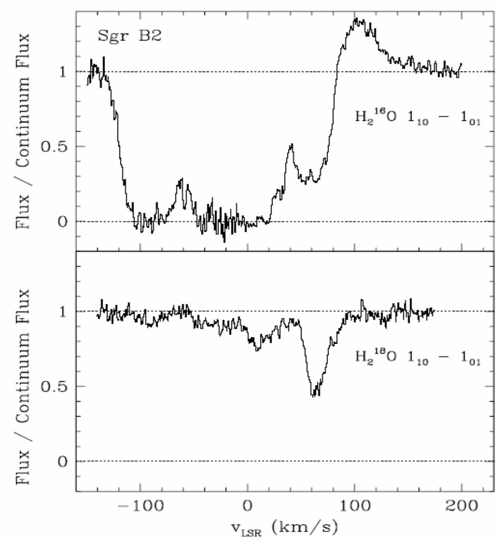




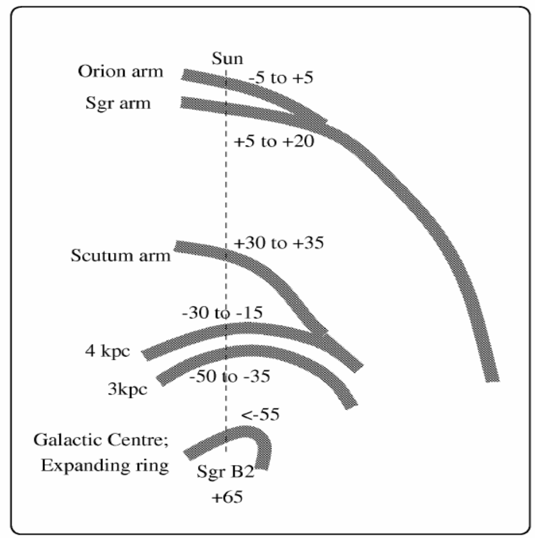


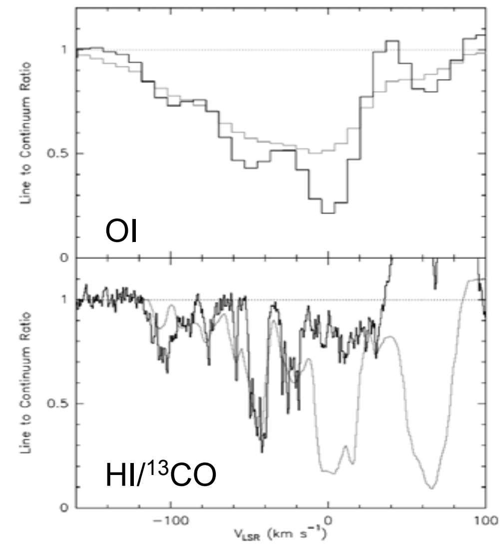
http://www.strw.leidenuniv.nl/WISH/

Absorption Spectroscopy



Neufeld et al. 2000





Lis et al. 2001

- At submm wavelengths, the line forest of heavy molecules gives way to fundamental transitions of light hydrides and deuterides
- Lines can often be seen in absorption toward bright cont sources
- This allows detailed investigations of the physics and chemistry of the l-o-s clouds with a wide range of physical conditions

PRISMAS and HEXOS GT KPs

(PIs Gerin and Bergin)

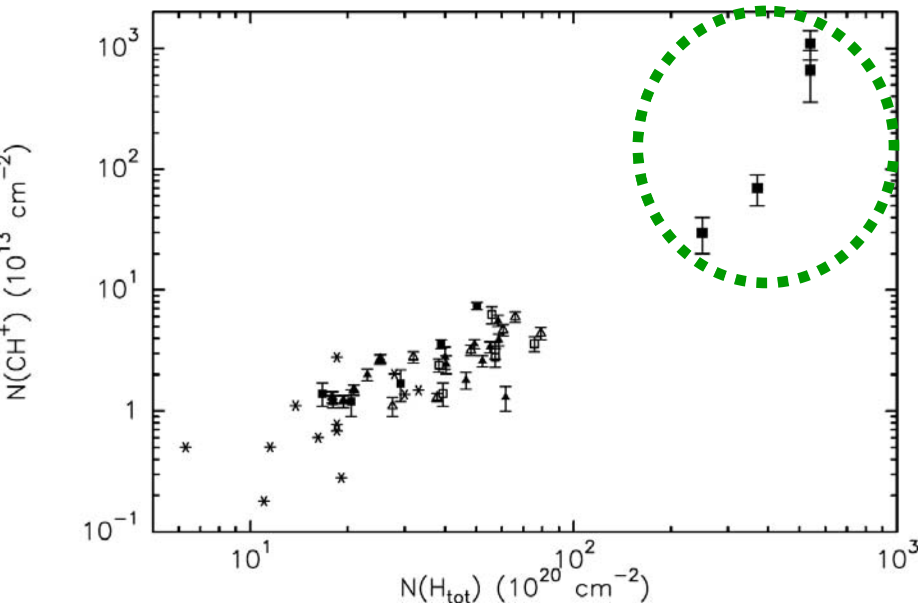
- Carbon chemistry: CI (492 GHz), CH (537 GHz), CH^+ (835 GHz), ^{13}CH, $^{13}CH^+$, CH_2 (1910 GHz)
- Oxygen chemistry: H_2O (o/p 557, 1113 GHz), $H_2{}^{18}O$ (o/p 548, 1101 GHz), HDO (894 GHz), D_2O (607 GHz), OH^+ (972 GHz), H_3O^+ (985, 1656 GHz), H_2O^+
- Nitrogen chemistry: NH (974 GHz), NH^+ (1013 GHz), ND (491 GHz), NH_2 (953 GHz), NH_3 (572 GHz), NH_2D (494 GHz)
- Hydrides: FeH (1411 GHz), HCl (625 GHz), HCl^+ (?), HF (1233 GHz), DF (651 GHz), D_2H^+ (691, 1477 GHz), SD (725 GHz)

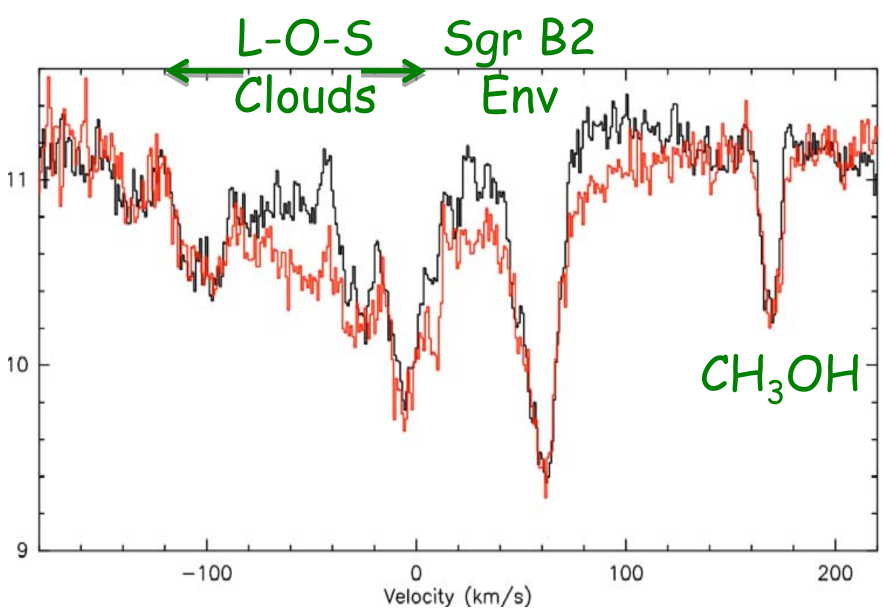
http://astro.ens.fr/index.cgi?cm=34&cv=1350&ua=1

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) and slow at the diffuse cloud temperatures, yet CH^+ is found associated with the CNM (based on velocities and linewidths; absorption spectroscopy in the visible)
- Measured CH^+ column densities are inconsistent with predictions of steady-state low-temperature chemistry (too high)
- 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; Joulain et al. 1998; Falgarone et al. 2005)
- MHD shocks or bursts of turbulent dissipation that locally heat gas to temperatures ~1000 K have been suggested

$^{13}CH^+$





Falgarone et al. 2008

- 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 been detected in absorption toward G10.6 (Falgarone et al. 2005)
- New observations in Sgr B2, W51e, W49N, G34.3… (CSO)
- New avenue for investigations of the high-temperature chemistry in *high-extinction* regions

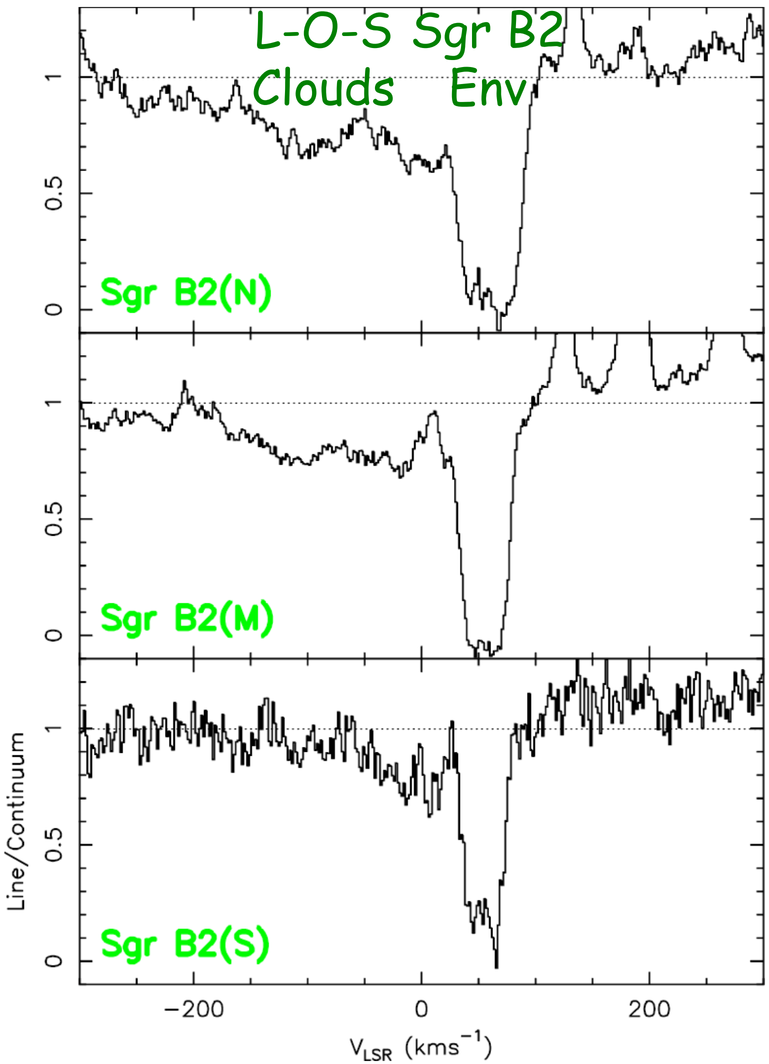
Oxygen Chemistry

- High H_2O abundances in hot cores and outflows (Boonman et al. 2003; Cernicharo et al. 2006) consistent with theoretical models
- Why is H_2O abundance so small in cold, quiescent molecular clouds (e.g., Bergin et al. 2001)—ice mantle formation at A_v of a few?
- Why is O_2 abundance so small? What is the oxygen reservoir?
- Why is OH/H_2O ratio variable in diffuse clouds—both molecules formed by the dissociative recombination of H_3O^+? Why good correlation of H_2O and HCO^+?
- Additional formation mechanisms of OH or H_2O needed
  - Endothermic neutral-neutral chemistry in regions with temperature enhanced by shocks or turbulence?
  - Grain catalysis, O atoms stick to grain surfaces, react with H to form OH, then H_2O, and are photo-desorbed by UV photons?
- HIFI gives access to both ortho- and para-H_2O lines, $H_2{}^{18}O$, as well as molecular ions OH^+, H_2O^+ and H_3O^+, which probe directly the ion-molecule route to OH and H_2O formation
- PACS gives access to OI (63 and 145 μm) and OH lines (both ground state and excited)

Nitrogen Chemistry

- Nitrogen chemistry through ammonia is still somewhat uncertain and data on nitrogen hydrides are scarce, with only a few reported detections (e.g. Goicoechea et al. 2004; ISO)
- Ammonia chemistry is unique, as it is driven by *neutral-neutral* reactions, starting with the synthesis of N_2
- Once sufficient quantity of N_2 builds up, the atomic nitrogen ion N^+ can be formed, in reaction with abundant He^+
- Formation of ammonia starts with the weakly endothermic reaction $N^+ + H_2 \rightarrow NH^+ + H$, which can be powered at low temperatures by the fine structure excitation of N^+, or by the ortho spin modification of H_2
- Subsequent hydrogen atom-transfer reactions with H_2 lead to NH_2^+ and NH_3^+
- The final reaction $NH_3^+ + H_2 \rightarrow NH_4^+ + H$ is slow at room temperature, but the rate increases at T<100 K

NH and NH_2



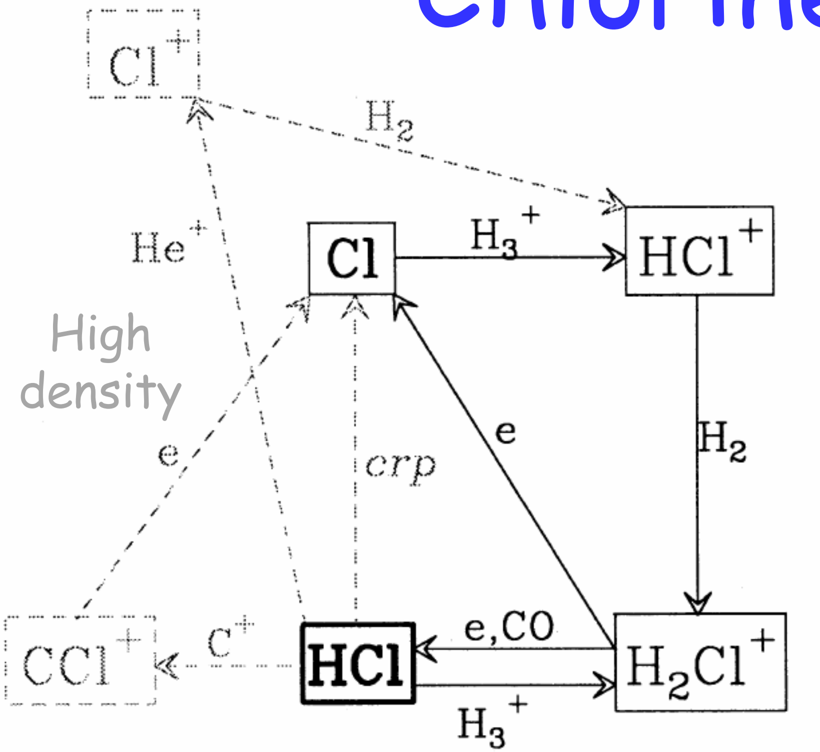
Gerin et al. 2008

- NH in diffuse clouds is often ascribed to a surface formation mechanism, but the assignment is very uncertain
- HIFI observations of NH and NH^+ will help to evaluate the relative importance of gas phase vs. grain surface processes
- NH_2, another building block of ammonia, has a fundamental transition at 462 GHz, recently detected using CSO—provides additional constraints
- NH_2 excitation analysis under way (M. Schmidt, Torun)

Fluorine Chemistry

- Fluorine is expected to be the heavy element, which shows the greatest tendency toward molecule formation (undergoes an exothermic reaction with H_2; HF detected by ISO)
- In diffuse clouds of small extinctions, the predicted HF abundance can exceed that of CO (Neufeld et al. 2005)
- HF should be detectable with HIFI in clouds with a visual extinction of ~0.1 mag—only molecules detected in such clouds to date are H_2 and HD
- Absorption spectroscopy of FIR continuum sources with HIFI may reveal a component of foreground molecular gas that is observable exclusively my means of HF!
- HF abundance can be used as a powerful probe of the freeze-out of atoms and molecules onto dust grains in dense gas ($HF/H_{tot} \sim F/H_{tot}$)
- HF absorption in quasar spectra is a potential probe of molecular gas at high redshifts (ALMA)

Chlorine Chemistry



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

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

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

or

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

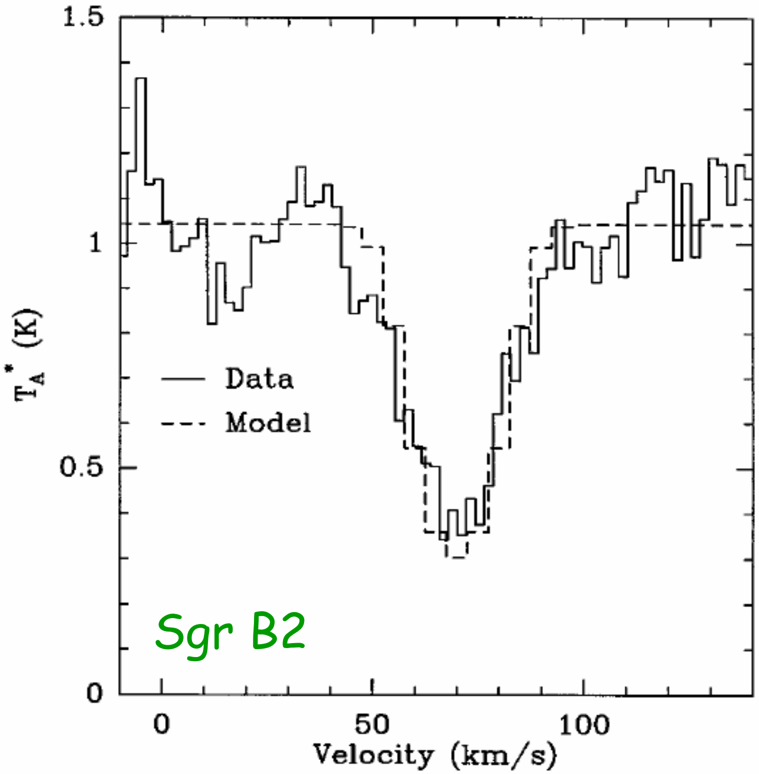
HCl, once formed, is destroyed by

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

Schilke et al. 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)
- New, funded Herschel theory program to reanalyze Cl and F chemistry (NASA; PI Neufeld)
- Strong interest in lab measurements of H_2Cl^+

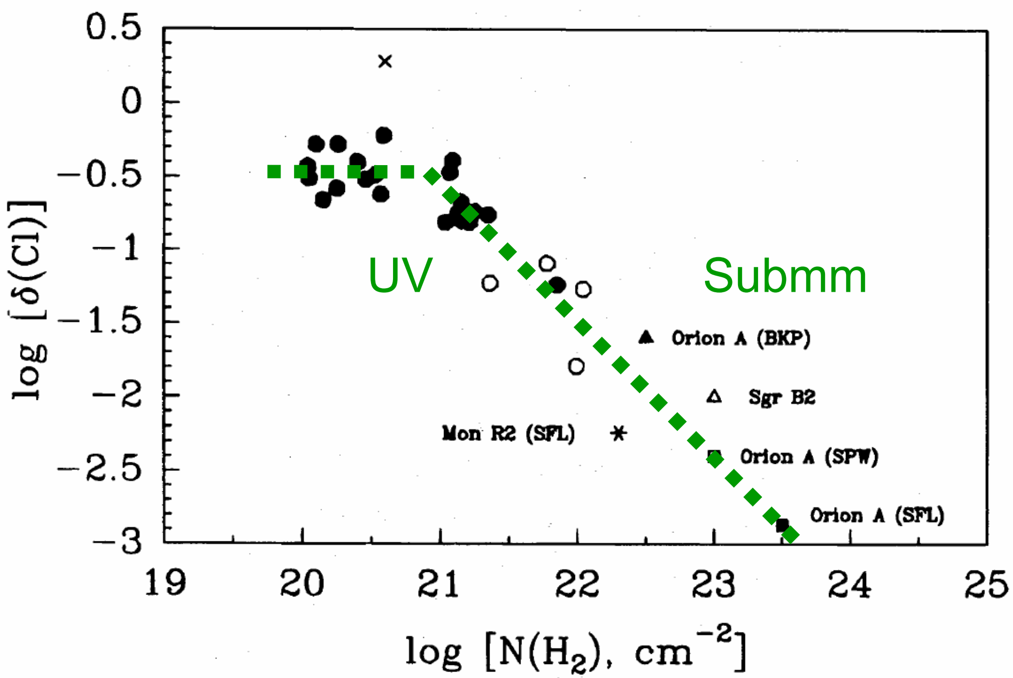
HCl Observations



Zmuidzinas et al. 1995

- 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)

Chlorine Depletion



Salez 1996

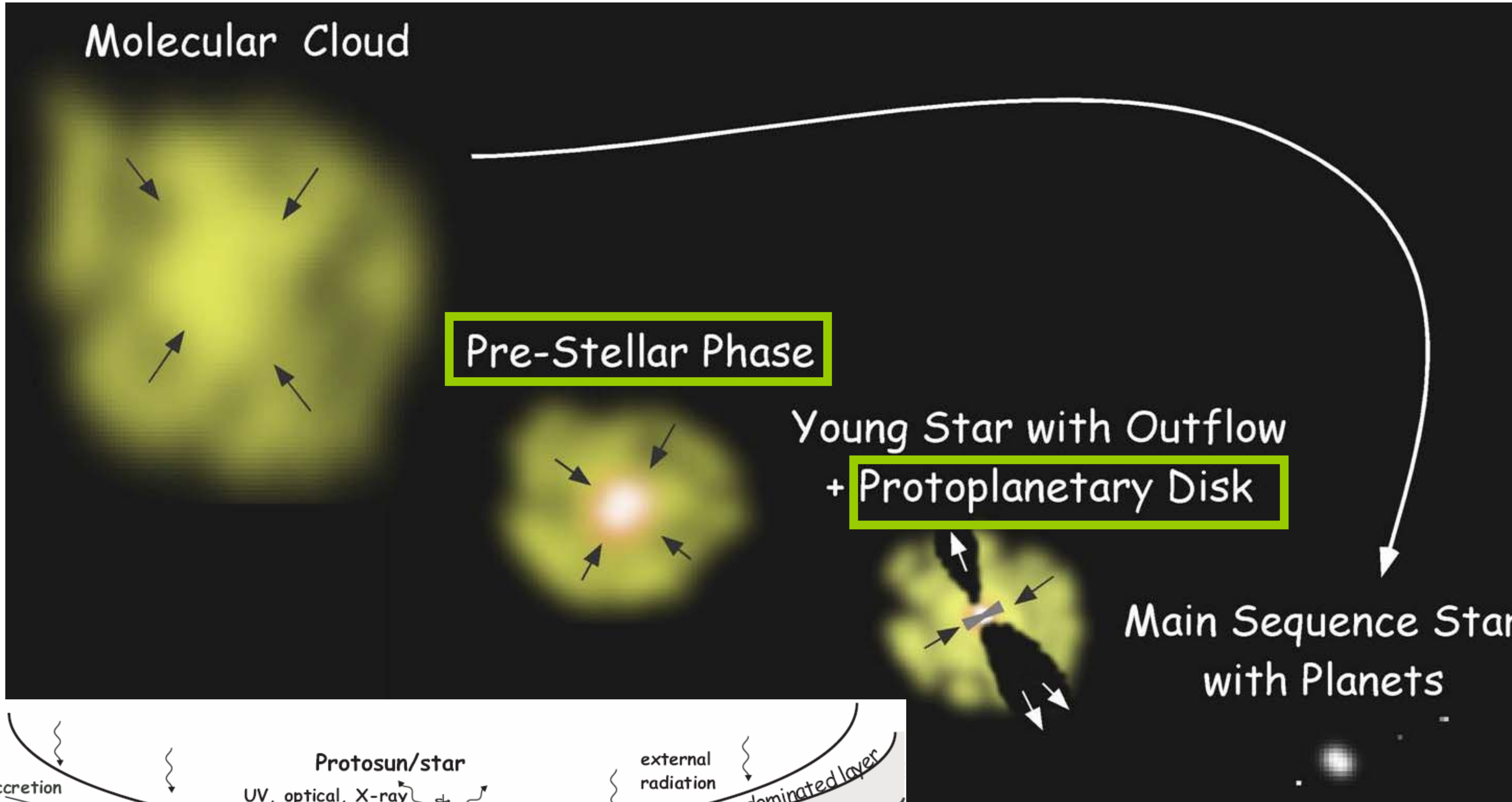
- Measurements of HCl abundance can serve as a valuable probe of depletion (as is the case for HF)
- In diffuse ISM chlorine is depleted by a factor of 2—3
- Depletion increases steeply with density
- In the shielded, high-density regions both chlorine atoms and HCl are depleted
- However, if the dust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

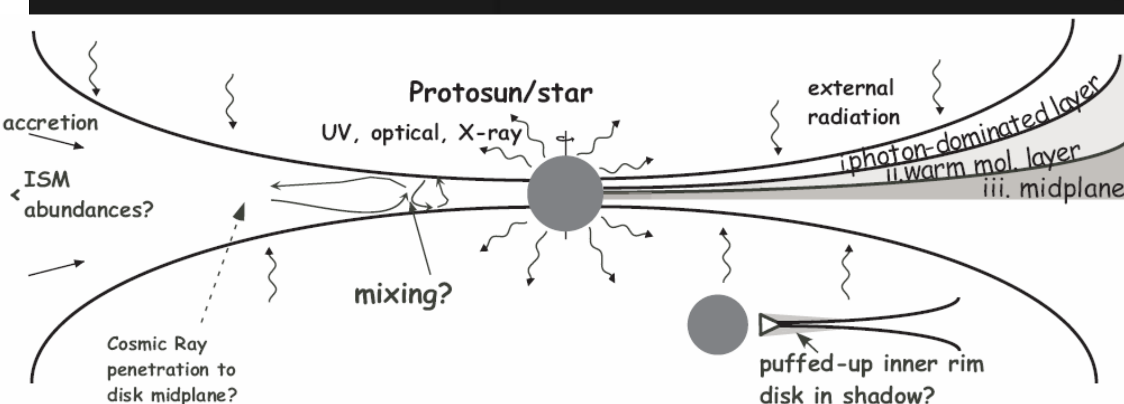
Deuterated Molecules

- 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



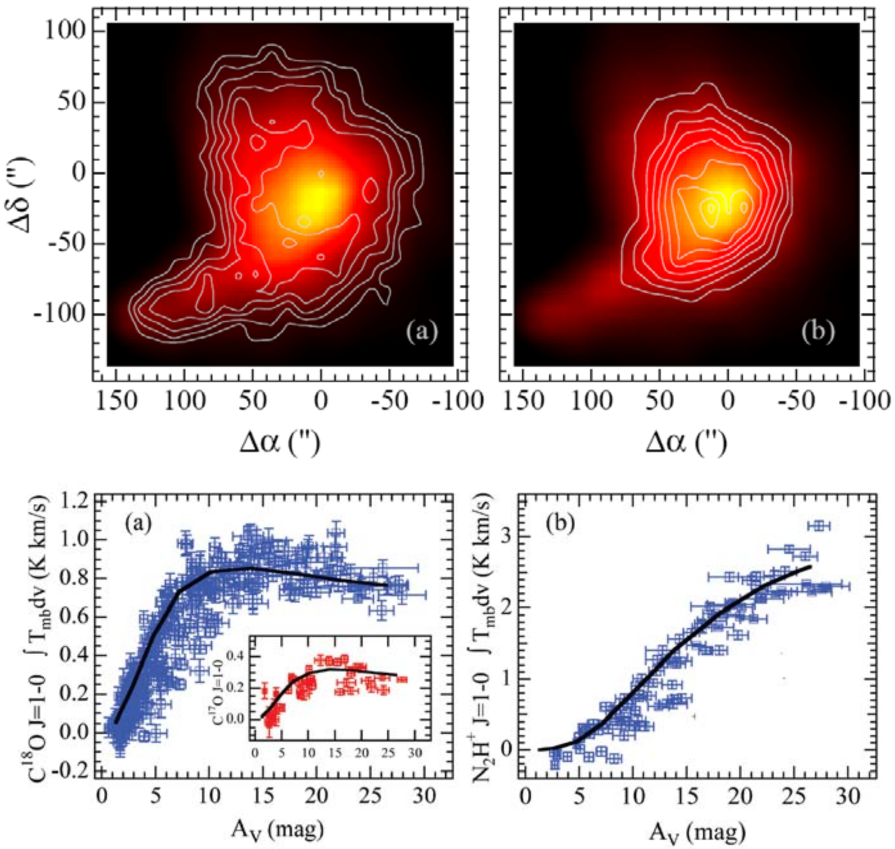


Cold disk midplane

Bergin 2006

Molecular Differentiation in Starless Cores

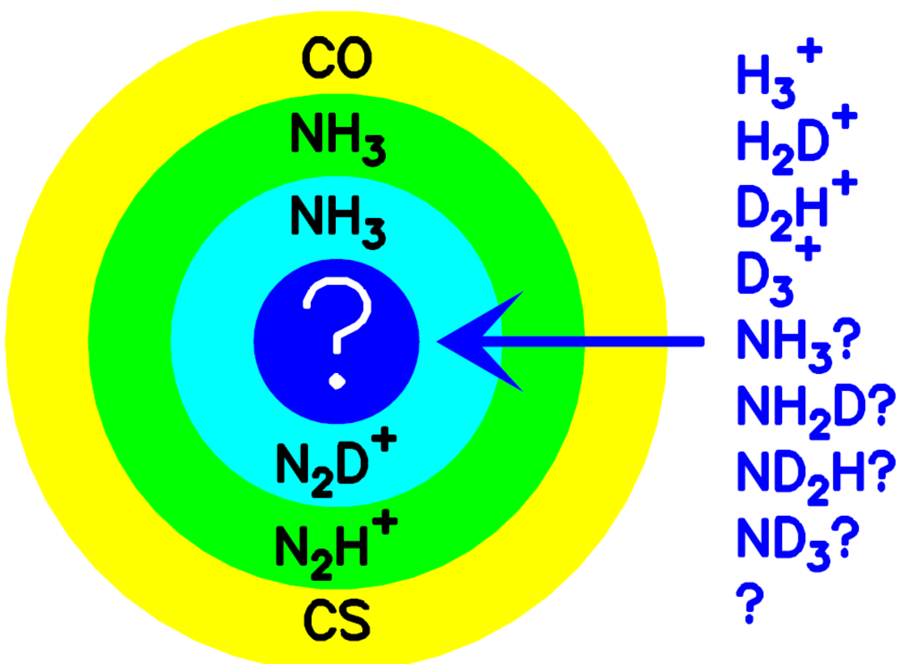
$C^{18}O$ – contours – N_2H^+



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 (H_2D^+ and D_2H^+) become the only tracers of H_2
- Density threshold time and model dependent
- Good observational constraints needed

Revised D Chemistry

$$H^+ + D = H + D^+$$

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

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

Also

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

$$H_2D^+ + HD = D_2H^+ + H_2 + \Delta E_b$$

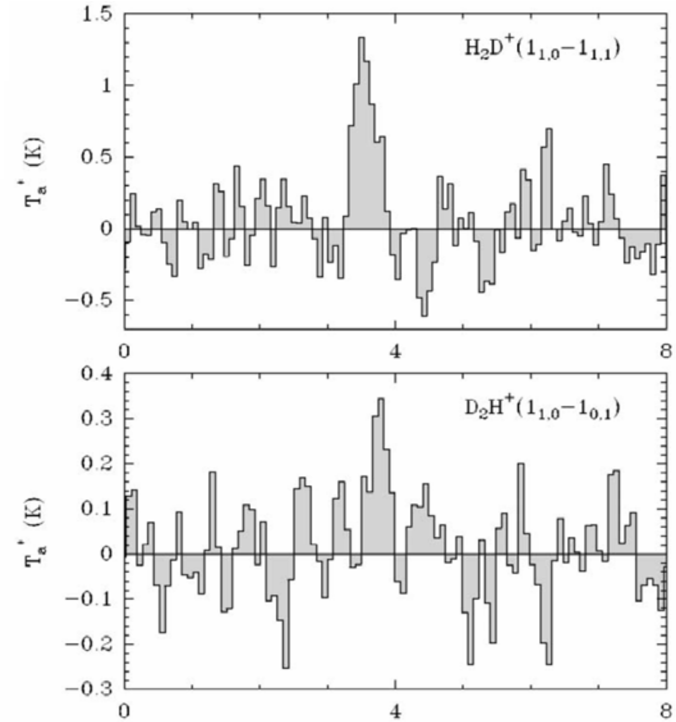
$$D_2H^+ + HD = D_3^+ + H_2 + \Delta E_c$$

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

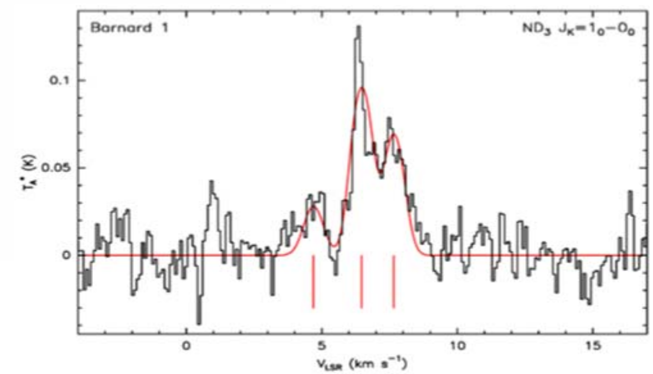
D_2H^+, D_3^+ ?

Roberts et al. (2003) Phillips & Vastel (2003)

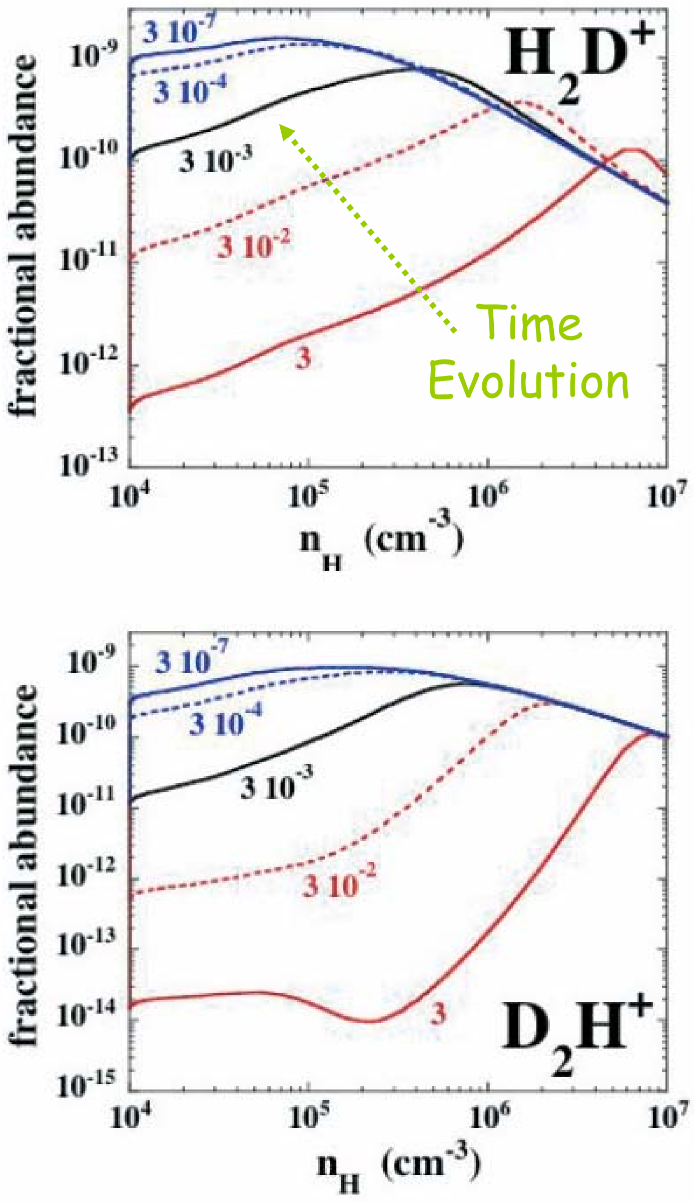
Submm: emission; FIR: absorption
(Goicoechea et al. 2007; ISO LWS)



D_2H^+: *Vastel 2004*



ND_3: *Lis 2002*

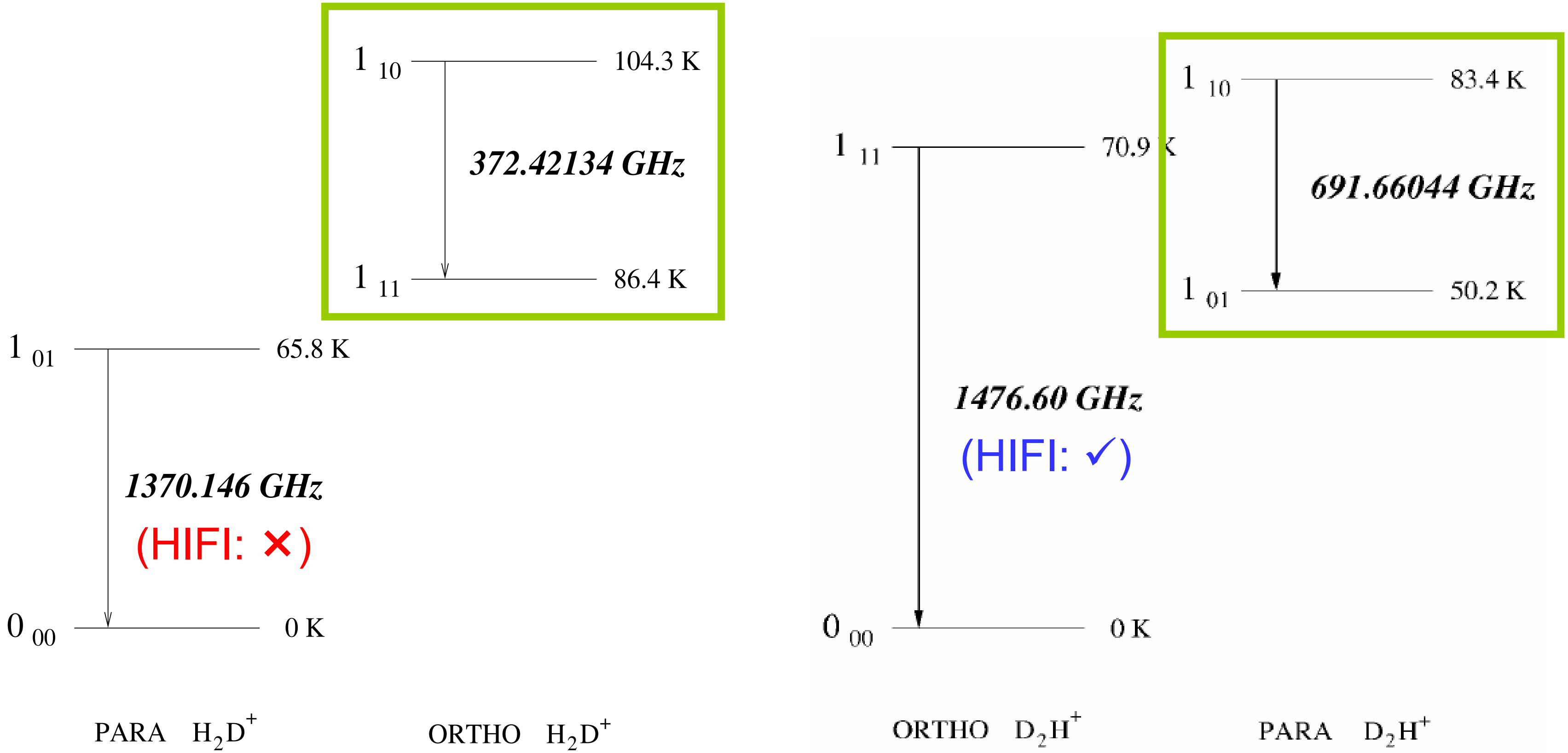


Importance of the o/p H_2 Ratio

- 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

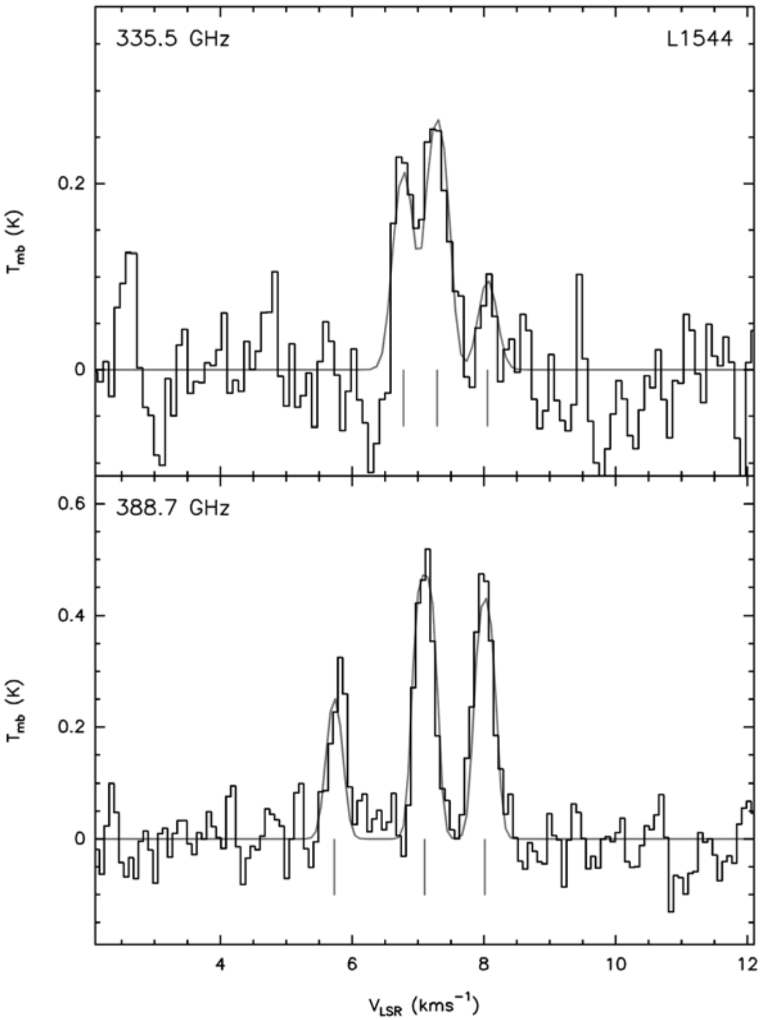
Flower et al. 2006; also Roueff, Pagani 2008, Arcachon meeting

Nuclear Spin Statistics



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

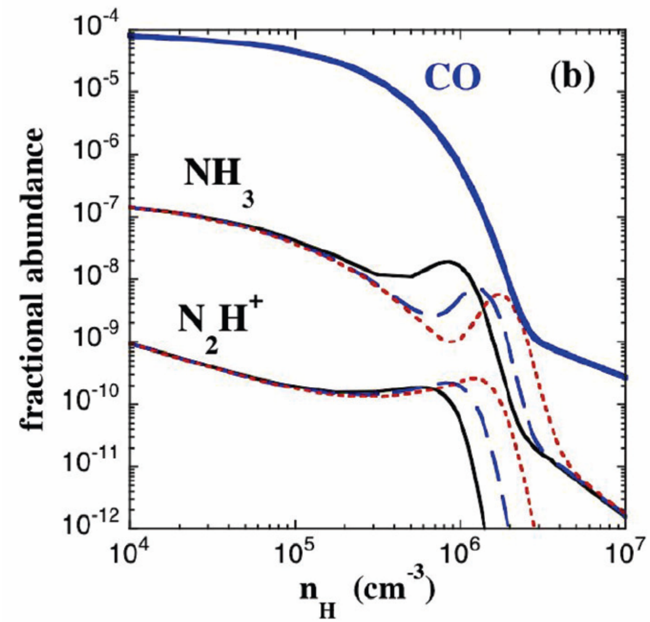
Deuterated Ammonia



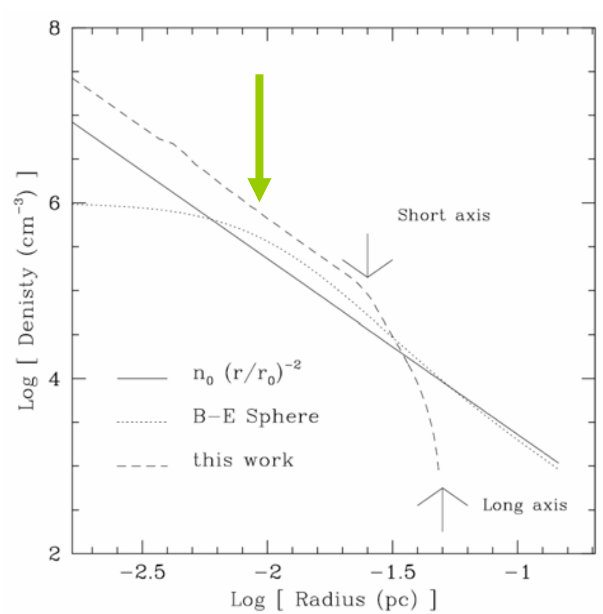
ND_2H: Lis et al. 2006

- H_2D^+ and D_2H^+ not affected by depletion, but difficult to observe from the ground (atmosphere)
- 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 excellent for absorption studies (e.g. ND^2H 336/389 GHz)
- NH_2D abundant, fundamental transitions at 470/494 GHz—completely unexplored

Onset of Ammonia Depletion



Flower et al. 2006

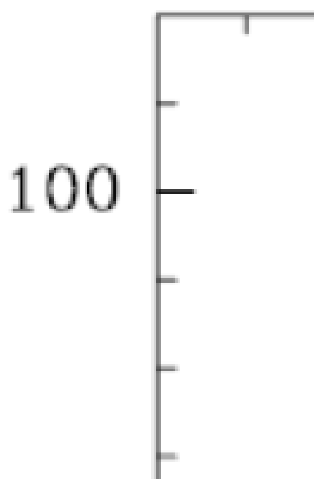


Doty et al. 2005

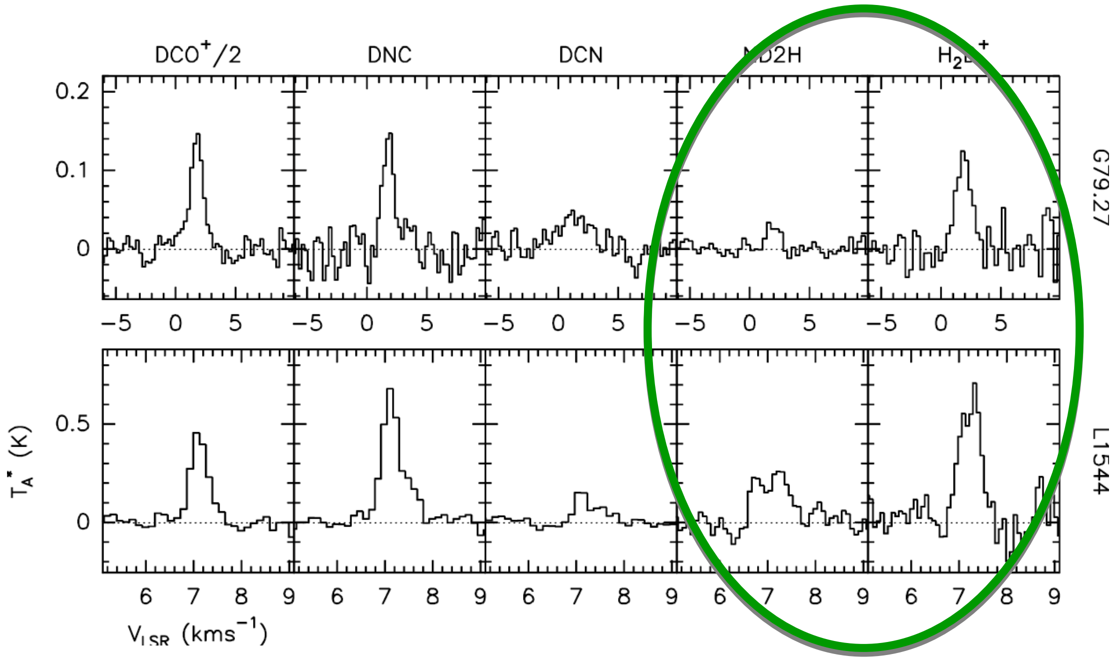
- Ammonia starts depleting at densities just above 10^6 cm^{-3} (e.g., Flower et al. 2006)
- This corresponds to ~0.01 pc or 15" in the dense, centrally peaked pre-stellar core L1544 (Doty et al. 2005)
- Recent PdB observations (Crapsi et al. 2007): no NH_2D hole in L1544, but N_2H^+ hole in class 0 source IRAM04191 (Belloche et al. 2004)
- Depletion is not a factor in more diffuse clouds

H_2D^+ and Ammonia in IRDCs

- IRDCs denser but more turbulent than low-mass cores
- How does this affect deuteration and depletion?
- G79.27—very similar to L1544 in terms of H_2D+ emission and DNC/DCN ratio, *but* weak ND_2H emission
- Do we finally see ammonia depletion?

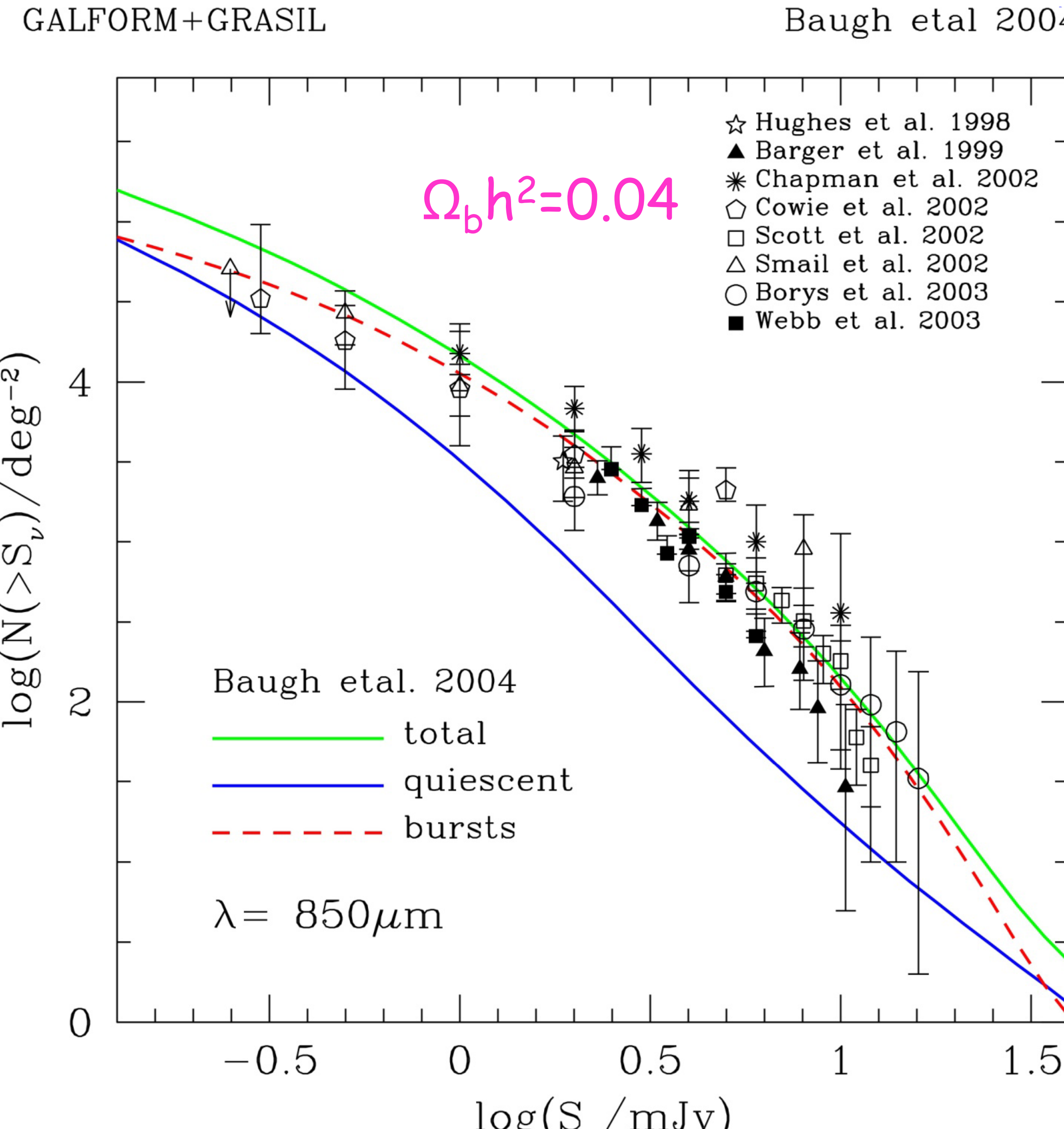


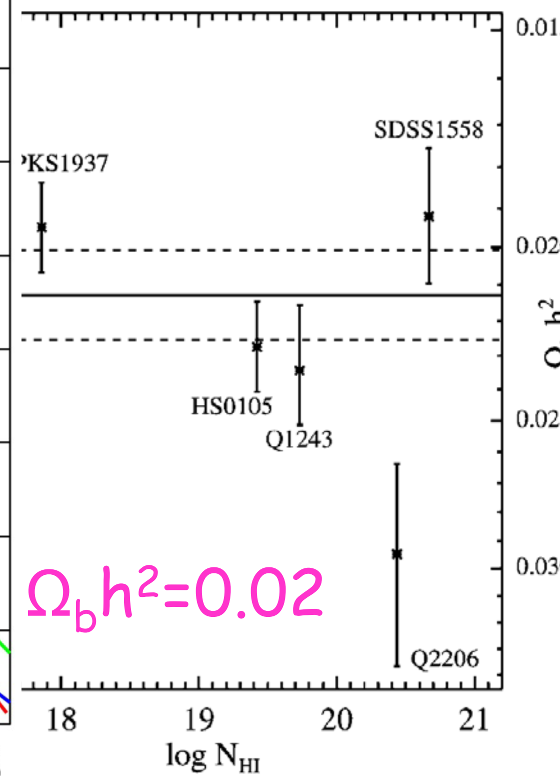
Vastel et al. 2006



Lis et al. 2008

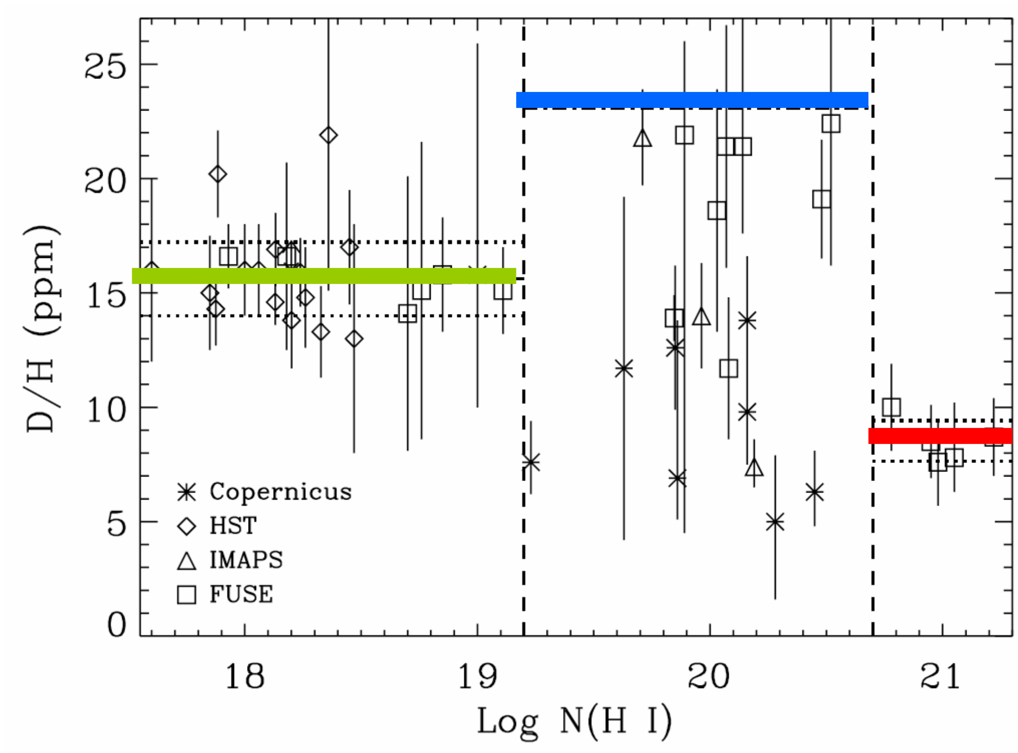
H and the smological yon Density





’Meara et al. 2006

D/H Variations in Diffuse ISM

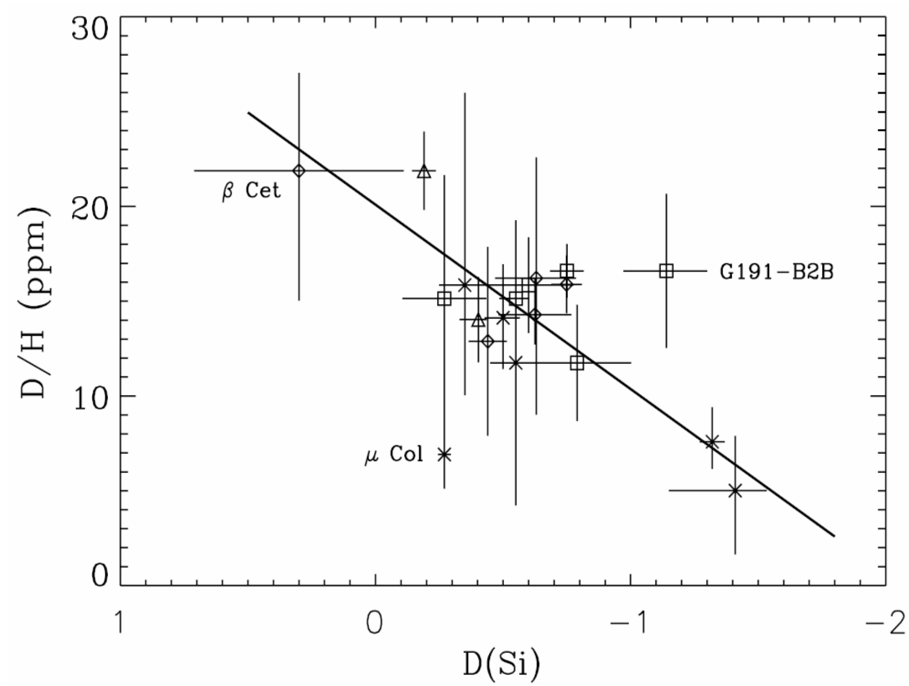


Linsky et al. 2006

- Within the Local Bubble: D/H=15.6±0.4 ppm
- Outside the Local Bubble, a factor of 4-5 variations
- Large scatter explained by spatial variations in the depletion of deuterium onto dust grains
- The highest points give the correct D/H ratio in the local Galactic disk: D/H=23.1±2.4 ppm

Variable D Depletion Model

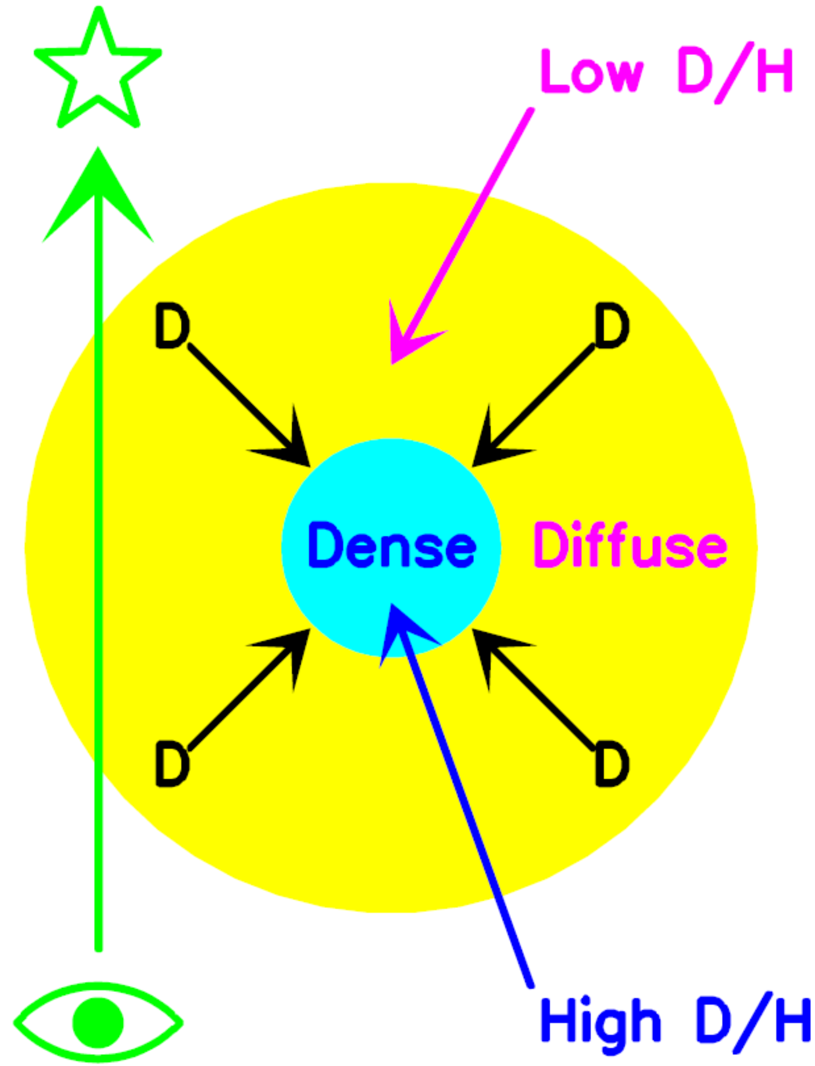
- Local Bubble: last reheated or shocked 1—2 Myr ago; D-bearing grains only partially evaporated
- Intermediate regime: a mixture of recently shocked and quiescent gas
- Distant regime: mostly cool HI gas
- Correlation with depletion of refractory metals (Si, Fe) and H2 rotational temperature



Jura 1982
Draine 2004, 2006
Linsky et al. 2006

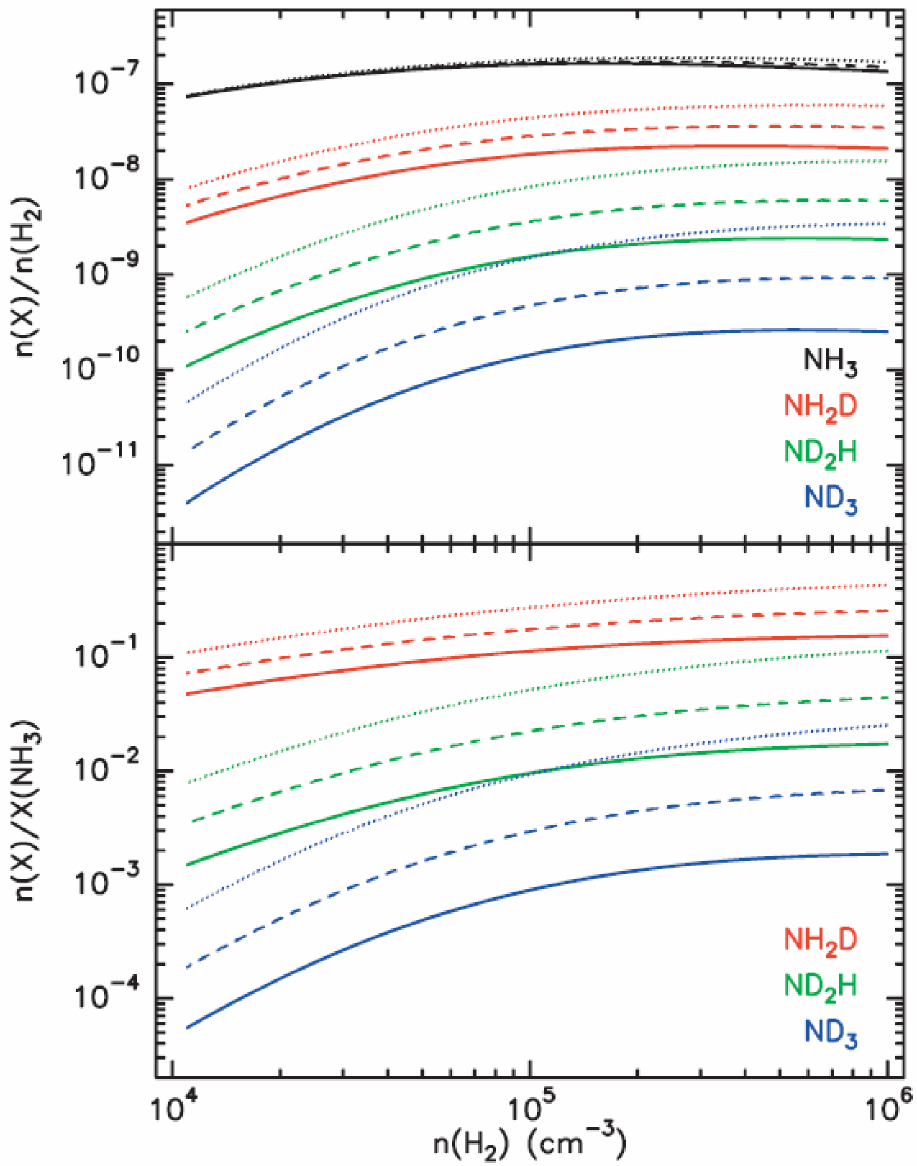
Gas-Phase D/H Variations

- Local variations could be due to proximity to cold, dense regions (Phillips & Vastel 2003)
- Elemental D/H ratio of ~15 ppm typically assumed in the published chemical networks
- If the true D/H ratio in the local disk is ~23 ppm, how is the dense gas chemistry and deuteration affected?



Effects of Enhanced D/H Ratio

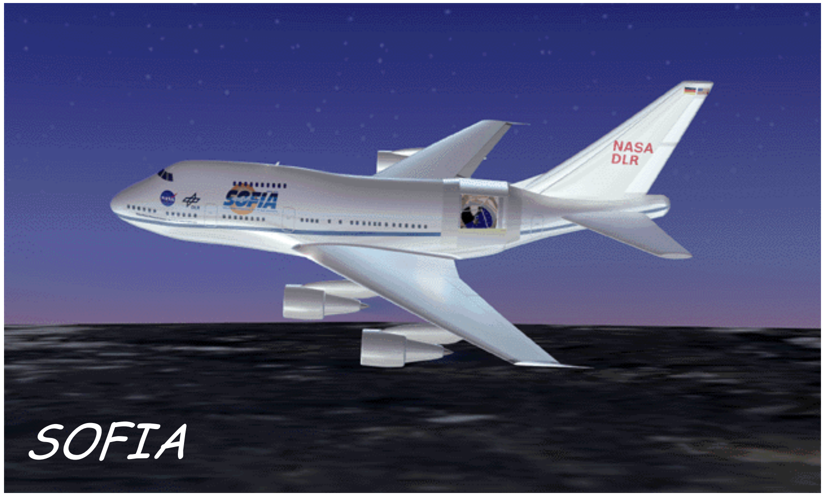
- Increase in fractionation ratio depends on increase in elemental D abundance raised to a power equal to the number of atoms
- For ND_3, $1.5^3=3.4$
- Multiply deuterated isotopologues are a particularly sensitive indicator of changes in the elemental D abundance

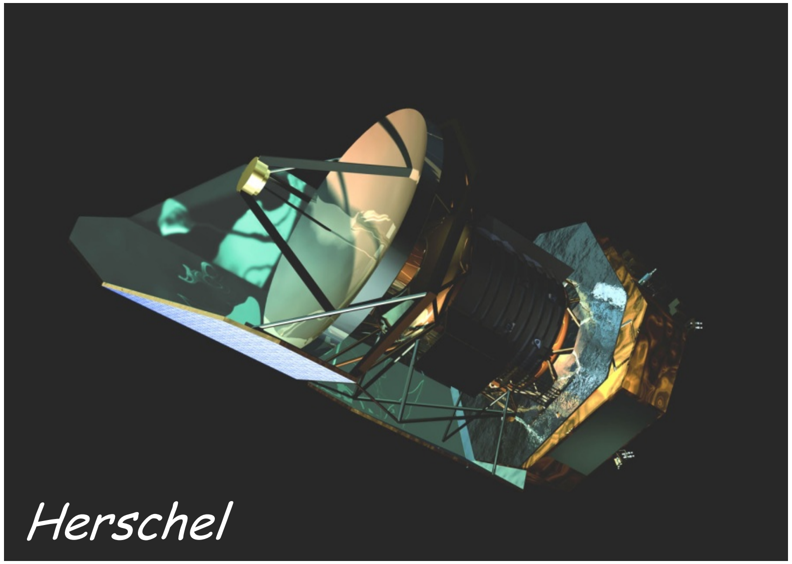


Roueff et al. 2007

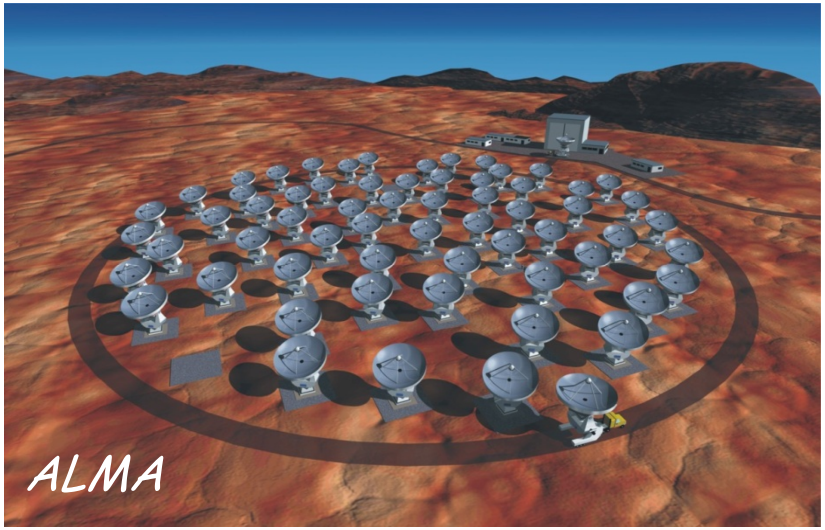
Summary

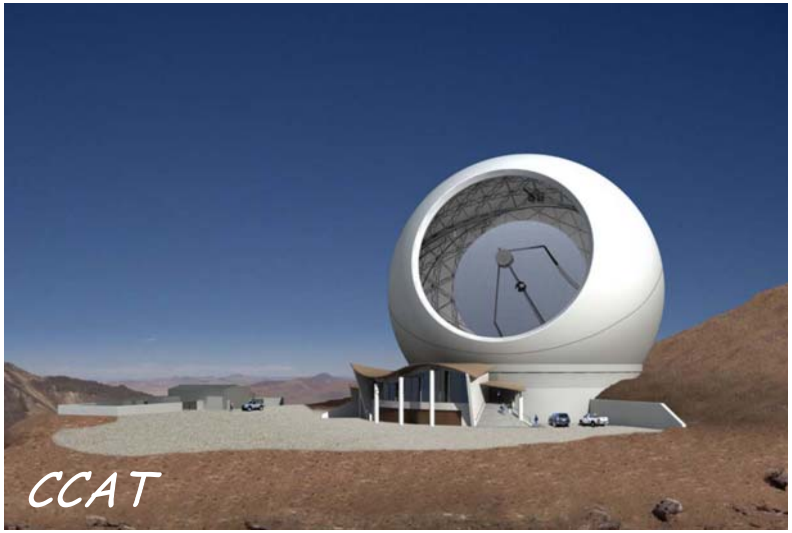
- Submillimeter region is the key for investigations of the chemical composition of cold neutral medium
- Absorption spectroscopy toward bright dust continuum sources allows for measurements of abundances of light hydrides and deuterides sometimes in clouds under 1 mag of visual extinction
- With all the new instruments coming on-line within the next few years, the field is progressing rapidly
- A lot of interesting science to come…



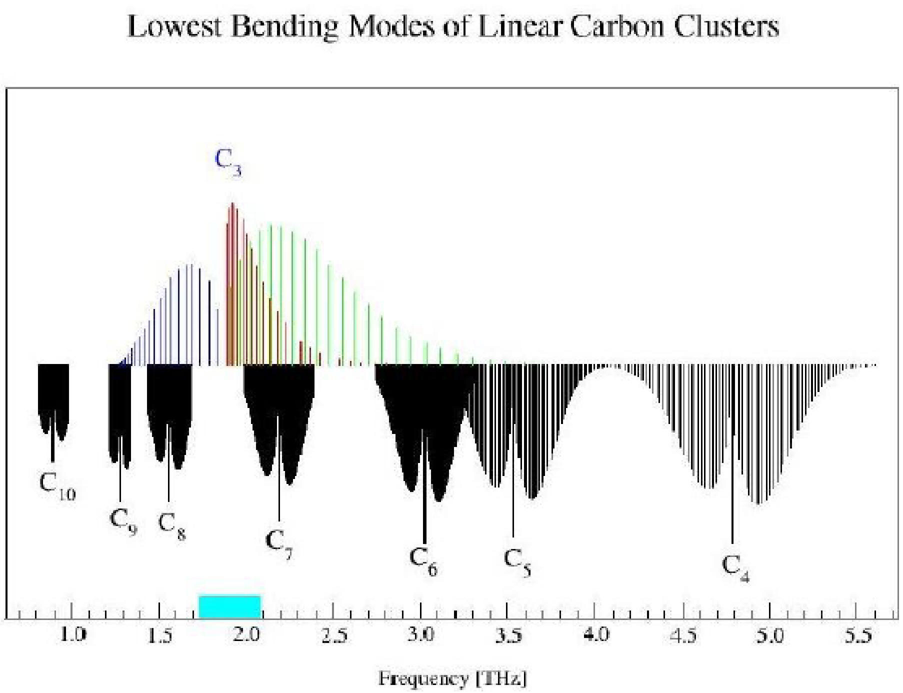


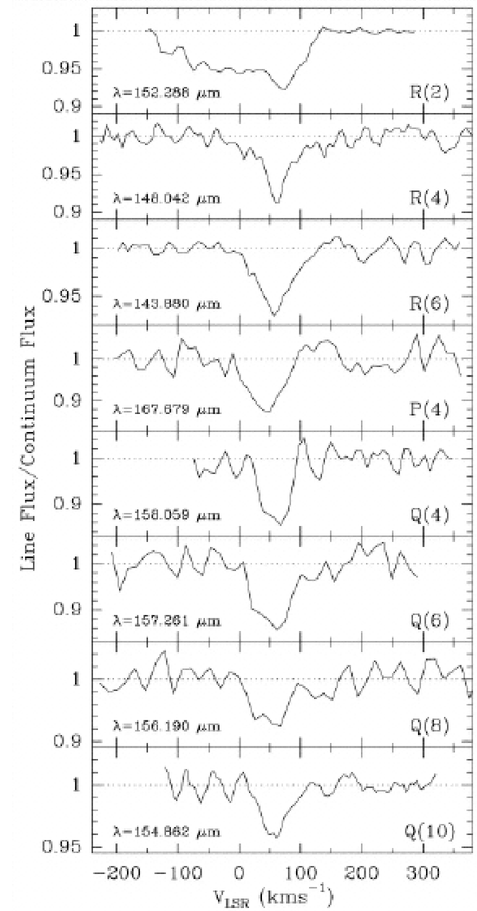
Herschel launch 2009, SOFIA demonstration science 2009, ALMA 2011, CCAT 2012...





PRISMAS—Carbon Clusters





T. Giesen (Priv. comm); Cernicharo et al., 2000, ISO-LWS

PRISMAS—Line List

Name	ν(GHz)	Name	ν(GHz)	Name	ν(GHz)	Name	ν(GHz)
NH_2D	494.454	DF	651.099	OH^+	971.804	FeH	1411.2
	494.455	D_2H^+	691.660	NH	974.462	D_2H^+	1476.606
	494.457	H_2O-para	752.033		974.470	H_3O^+	1655.814
ND	491.934				974.479		
	522.077				999.473		
	546.128	$^{13}CH^+$	830.131				
CH (^{13}CH)	532.724	CH^+	835.079			$H_2{}^{18}O$-ortho	1655.868
	532.793	$HD^{18}O$	883.189			CH	1656.961
	536.761	HDO	893.639	H_3O^+	984.697		
	536.796	D_2O	897.947	H_2O-para	987.927		
$H_2{}^{18}O$-ortho	547.676	NH_2	952.542	NH^+	1012.524	CH^+	1670.16
$H_2{}^{17}O$-ortho	552.021		952.550			H_2O-ortho	1669.905
H_2O-ortho	556.936		952.562	H_2O-ortho	1097.364	CH_2	1907.987
$^{15}NH_3$	572.113		952.572				1912.329
NH_3	572.498		952.573	$H_2{}^{18}O$-para	1101.698		1917.661
D_2O	607.349		952.577	H_2O-para	1113.343		
$H^{37}Cl$	624.964		952.578				
	624.978		952.628			C_3	1914.274
	624.988		959.426	NH_3	1214.859		1890.558
$H^{35}Cl$	625.901		959.512		1215.245		1896.706
	625.919		959.526				1906.337
	625.932		959.562	HF	1232.476		

Sources :

Bright submm/FIR continuum sources, mostly massive star forming regions

W49N	W51	W31C	G34.3
SgrA	NGC6334I	W33A	W28A
W3	DR21	NGC7538	W43S
AFGL7009S	IRAS 15502–5302	IRAS 17455–2800	G008.67–0.36
G10.47+0.03			