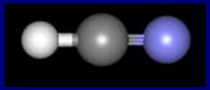
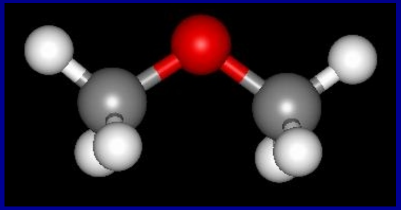
Astrochemistry

and its uses in astronomy



Ewine F. van Dishoeck

Leiden Observatory/
Max-Planck Institüt fur
Extraterrestrische Physik



January 7, 2008   ISSI workshop

Introduction

- Is interstellar chemistry useful? (Dalgarno 1986)
- Purpose of this talk: show that answer to this question is indeed YES!
- Molecular astrophysics forms an integral part in understanding formation of galaxies, stars, planets and perhaps even prebiotic material
- Illustrate here with a few examples

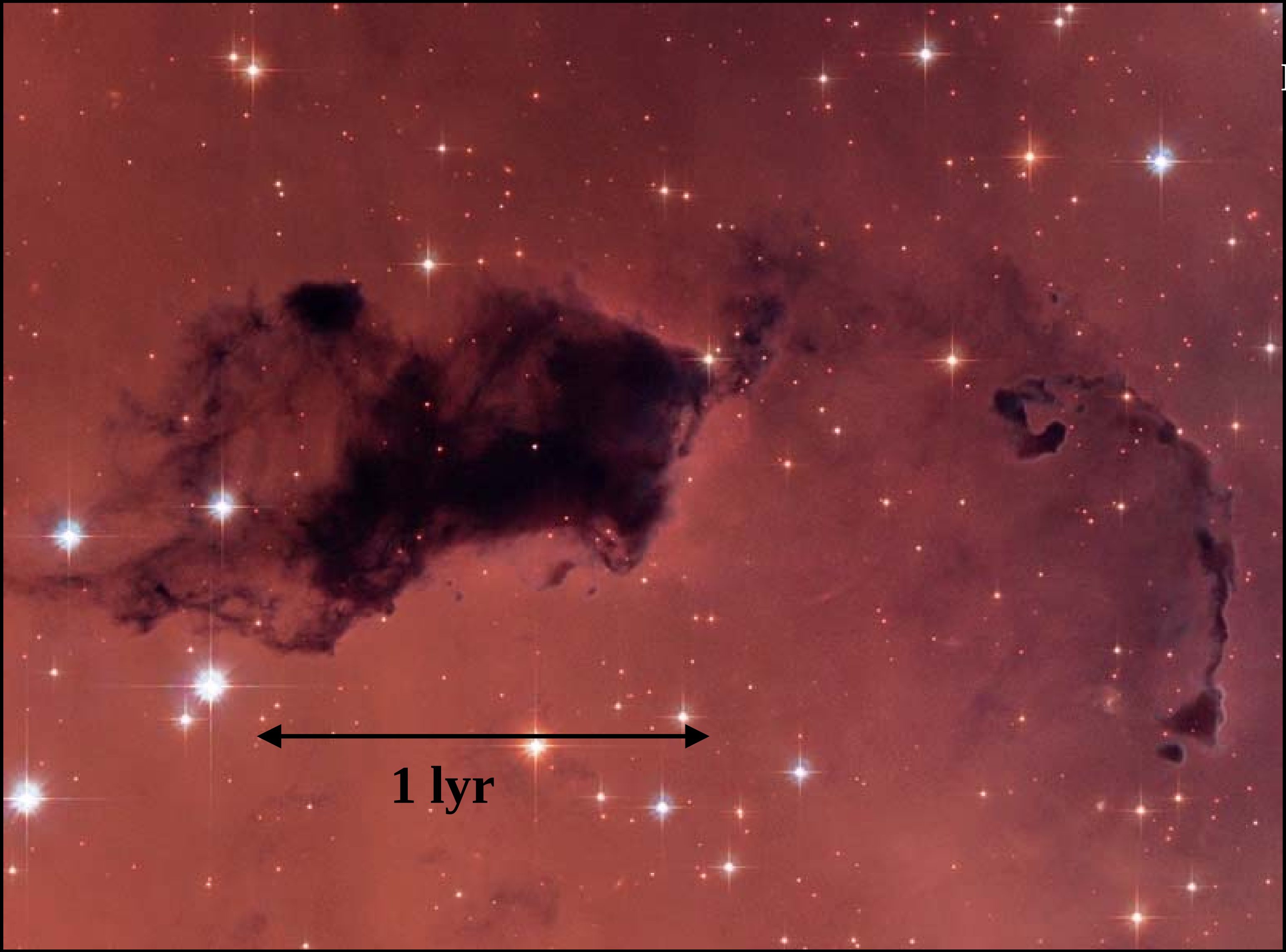
Where do we find molecules?

Orion
HST image

Horsehead nebula

AAT

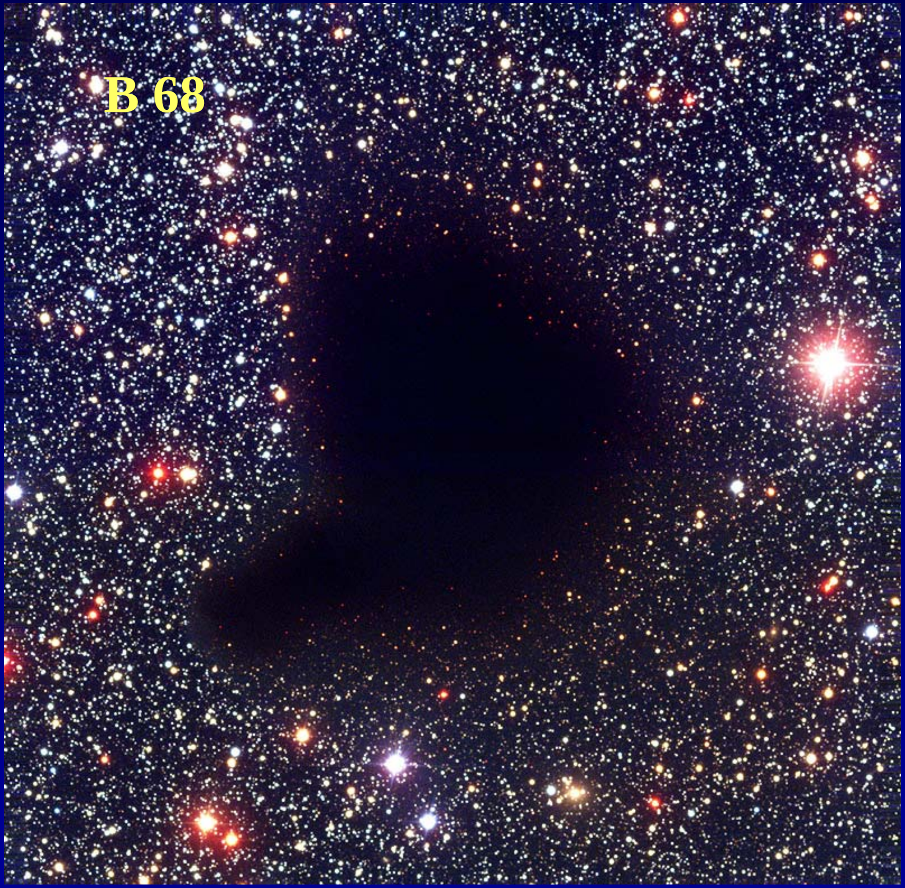
Dark clouds: sites of star formation



NGC 281

Mass of cloud can be as large as $10^4 - 10^6\ M_{Sun}$

Dark clouds: 'coal sacks'

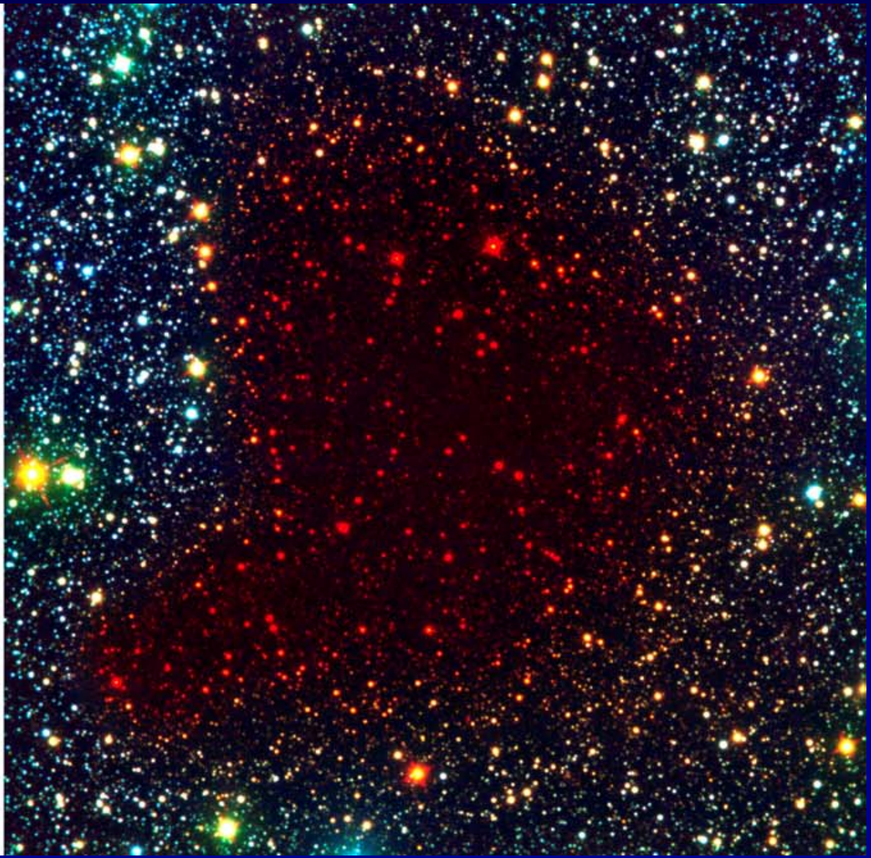


- 99% gas (H_2)
  1% dust (0.1 μm silicates+carbonaceous)
- Temperature: ~10 K
- Density: ~10^4 particles per cubic cm

→ Unique chemical laboratory!

How do we study what is happening inside clouds?

Optical **Infrared**



Long wavelengths!

Alves et al. 2001

From visible to infrared light

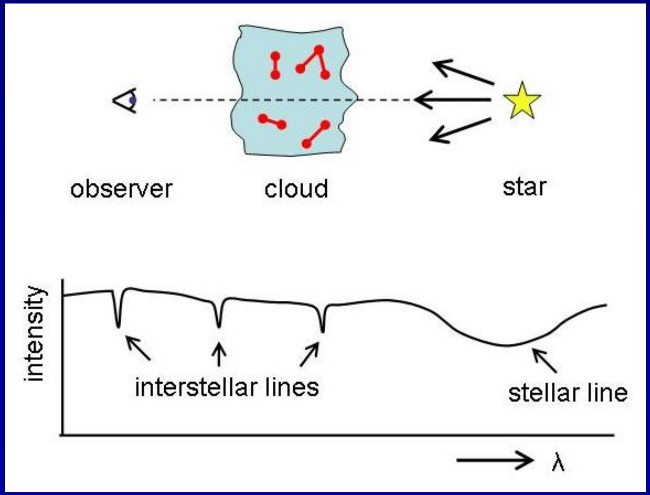
HH 46 star-forming region

Types of clouds

- **Diffuse and translucent clouds**
  - **Observed primarily by absorption lines at visible (since 1900's) and UV wavelengths (since 1970's)**
- **PDRs**
  - **Dense clouds exposed to intense UV radiation, typically at least 100x average interstellar radiation field**
  - **Observed by far-infrared and submm emission lines**
- **Cold dark clouds**
  - **Observed by mm emission lines**
- **Warm star-forming regions/hot cores**
  - **Observed by submm/mm emission lines**
  - **IR absorption for ices**
- **Shocks**
  - **Observed by IR and submm/mm emission**
- **Circumstellar shells evolved stars**
- **Protoplanetary disks**
- **Comets, planetary atmospheres**

T~8-2000 K, $n(H_2)$~10^2-10^{13} cm^{-3}

I_{UV}~0.2-10^7



NGC 1333 outflows

Q: effects of outflows, jets, shocks on chemistry?

Ha, [SII]
Walawender, Bally, Reipurth 2006

Spitzer/IRAC
Jørgensen et al. 2006

Ingredients of clouds

Element	Abundance	Element	Abundance
H	1.00	Mg	4.2×10^{-5}
He	0.075	Al	3.1×10^{-6}
C	2.5×10^{-4}	Si	4.3×10^{-5}
N	6.3×10^{-5}	S	1.7×10^{-5}
O	4.5×10^{-4}	Ca	2.2×10^{-6}
Na	2.1×10^{-6}	Fe	4.3×10^{-5}

Note: abundances of C,N,O recently revised downward by almost factor of 2; other elements TBD

Approach

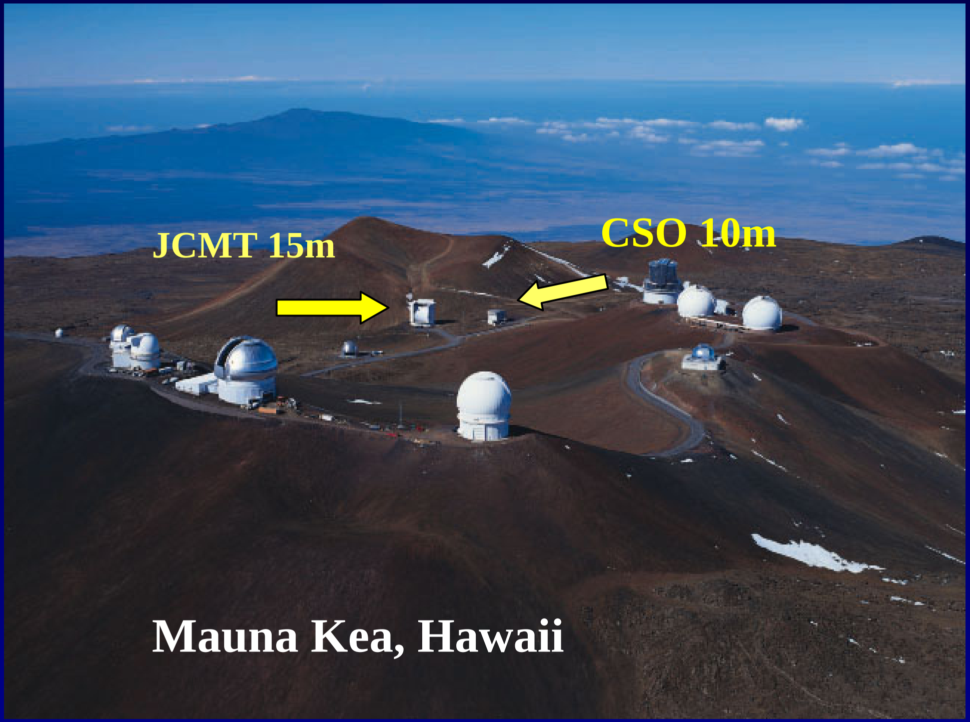
Observations + Instrumentation

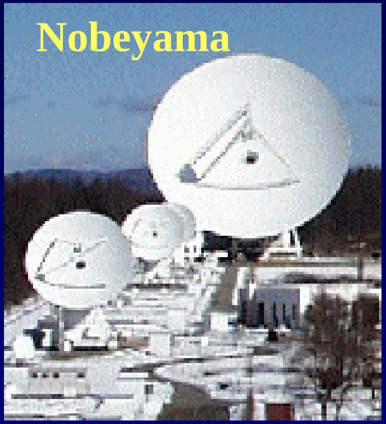
Models

C+ ¬> C ¬> CO

Laboratory

Submillimeter telescopes





Pico Valeta, Spain

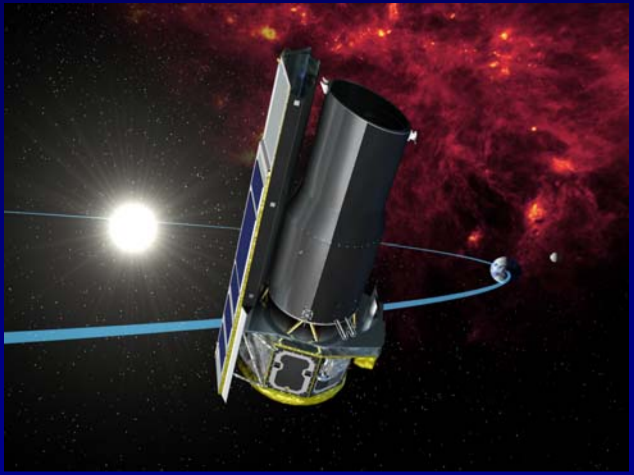
APEX
Chajnantor

Infrared telescopes

Very Large Telescope, ESO, Paranal

Space observatories

ISO

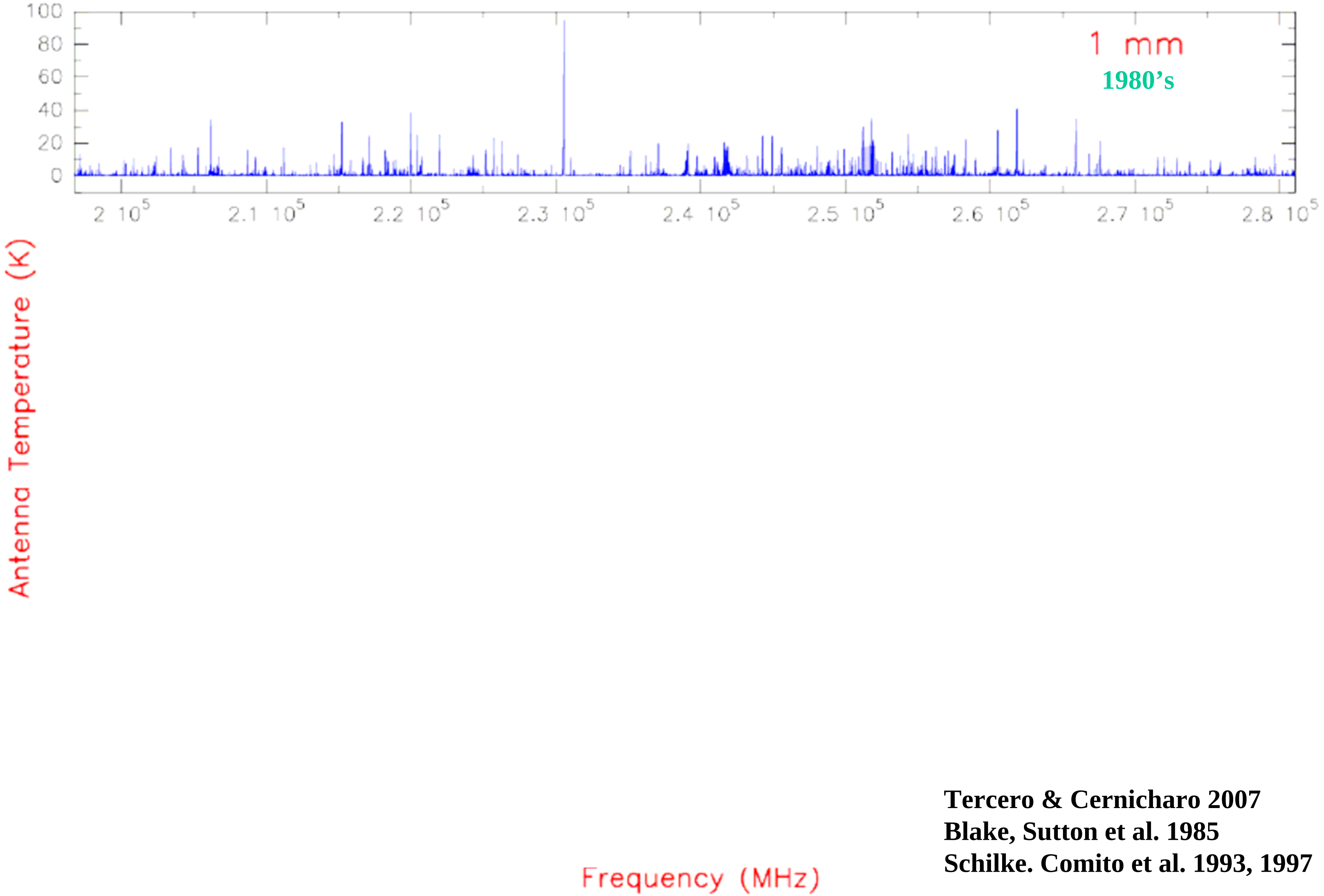


Spitzer

SWAS/ODIN

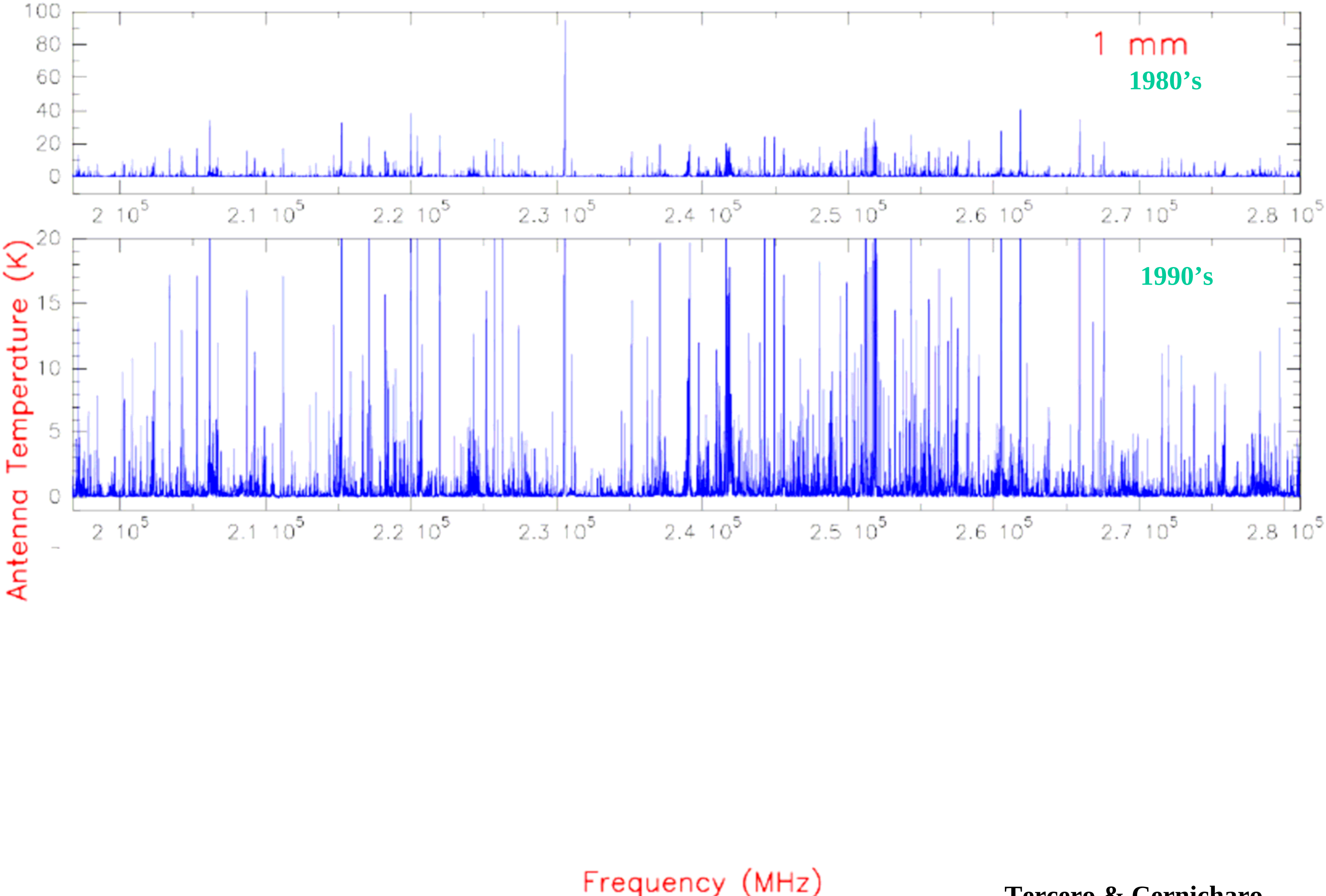
Large part of infrared and submm blocked by atmosphere (i.p. H_2O, O_2 and CO_2)

Orion line surveys



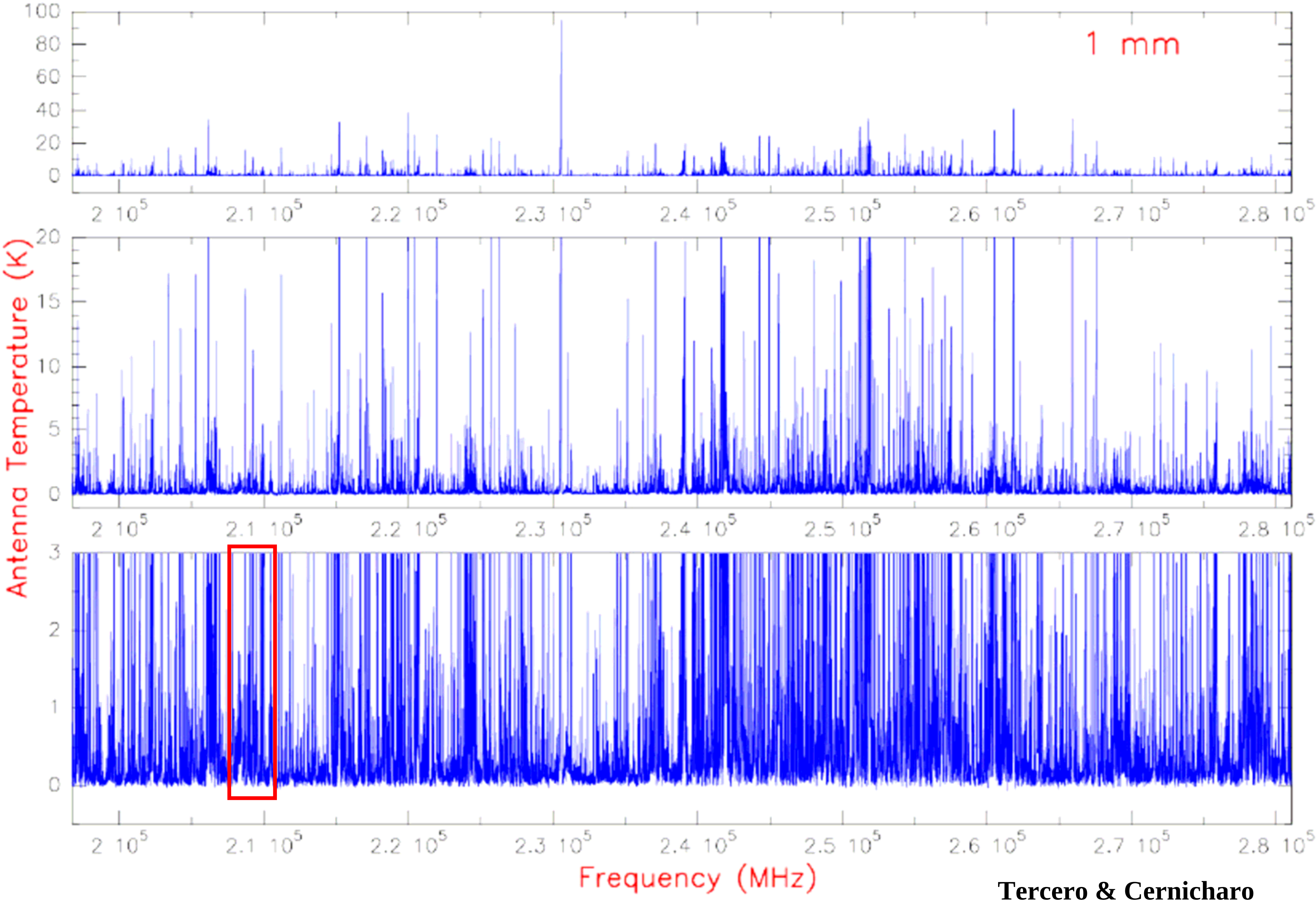
Tercero & Cernicharo 2007
Blake, Sutton et al. 1985
Schilke. Comito et al. 1993, 1997
….

Orion line surveys

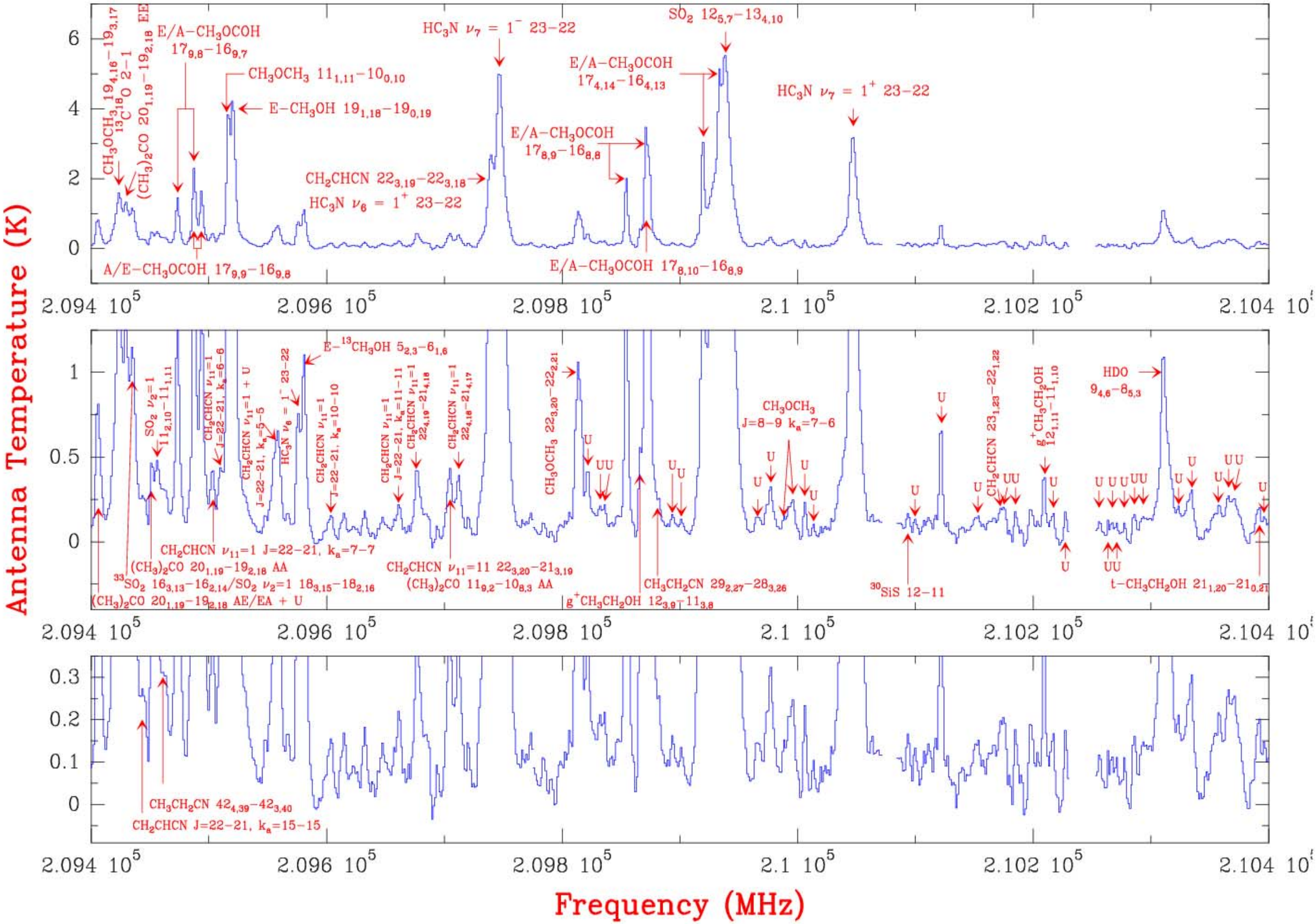


Tercero & Cernicharo

Orion line surveys



Tercero & Cernicharo



Q: how far does chemical complexity go? Prebiotic molecules?

Inventory of gas-phase molecules

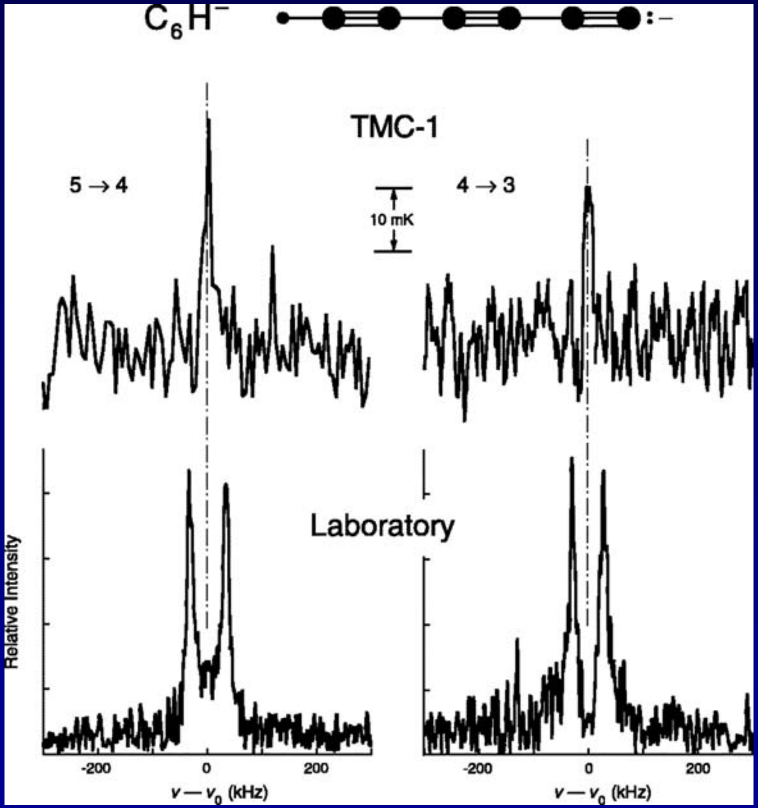
Number of Atoms										
2	3	4	5	6	7	8	9	10	11	13
H_2	C_3	c-C_3H	C_5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N?	HC_9N	$HC_{11}N$
AlF	C_2H	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$		
AlCl	C_2O	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH?	$(CH_3)_2O$	NH_2CH_2COOH?		
C_2	C_2S	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH			
CH	CH_2	C_3S	c-C_3H_2	CH_3NC	$HCOCH_3$	H_2C_6	HC_7N			
CH^+	HCN	C_2H_2	CH_2CN	CH_3OH	NH_2CH_3		C_8H			
CN	HCO	CH_2D^+?	CH_4	CH_3SH	c-C_2H_4O					
CO	HCO^+	HCCN	HC_3N	HC_3NH^+						
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO						
CP	HOC^+	HNCO	HCOOH	NH_2CHO						
CSi	H_2O	HNCS	H_2CHN	C_5N						
HCl	H_2S	$HOCO^+$	H_2C_2O							
KCl	HNC	H_2CO	H_2NCN							
NH	HNO	H_2CN	HNC_3							
NO	MgCN	H_2CS	SiH_4							
NS	MgNC	H_3O^+	H_2COH^+							
NaCl	N_2H^+	NH_3								
OH	N_2O	SiC_3								
PN	NaCN									
SO	OCS									
SO^+	SO_2									
SiN	c-SiC_2									
SiO	CO_2									
SiS	NH_2									
CS	H_3^+									
HF										

-Abundances vary from 10^{-4} to 10^{-11} w.r.t. H_2

-Abundances vary from region to region

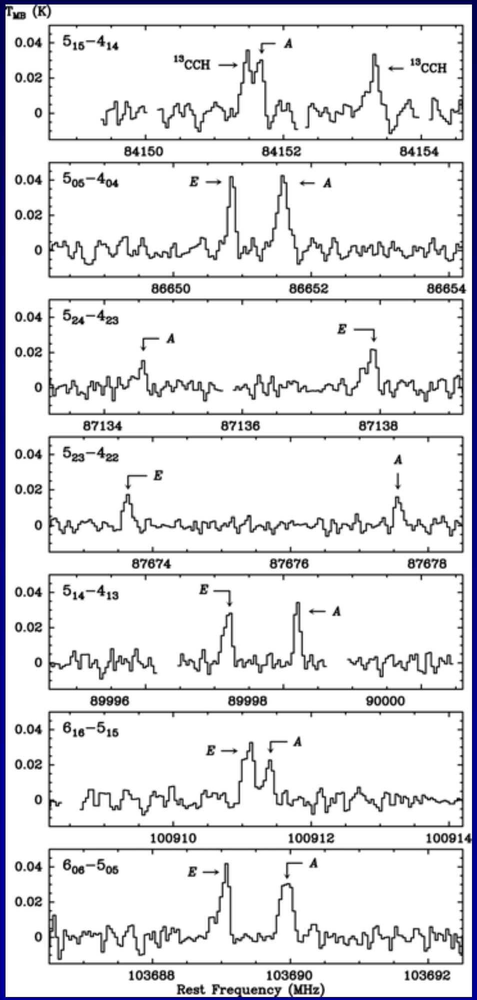
Some recent detections

Negative ions

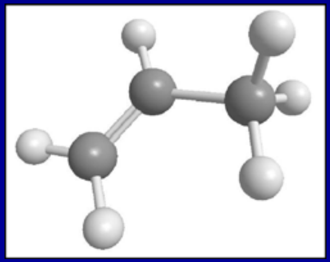


McCarthy et al. 2006

Propene in TMC-1



Marcelino et al. 2007

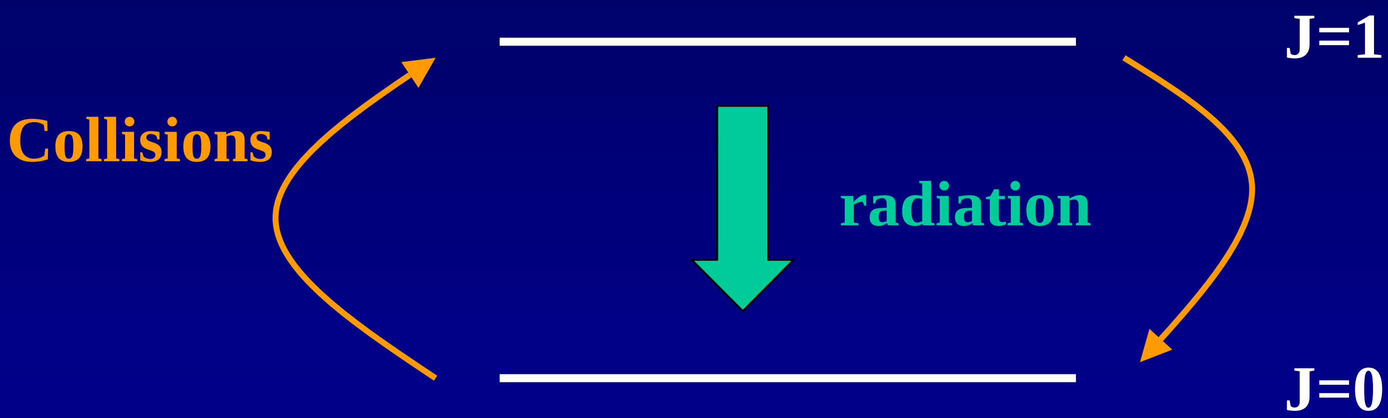


Importance of molecules

- **Molecules as *physical* diagnostics of temperature, density, mass, velocity, redshift, star-formation activity,…**
- **Molecules as *chemical* diagnostics of ionization rate, temperature (history), evolutionary state protostars, …**
- **Astrochemical evolution clouds => planets**
- **Molecules as coolants**
- **Basic chemistry under exotic conditions**

$$\mathrm{CO\ (J=0)} \xrightarrow{\text{Collisions}} \mathrm{CO(J=1)} \xrightarrow{\text{Radiation}} \mathrm{CO(J=0)}$$

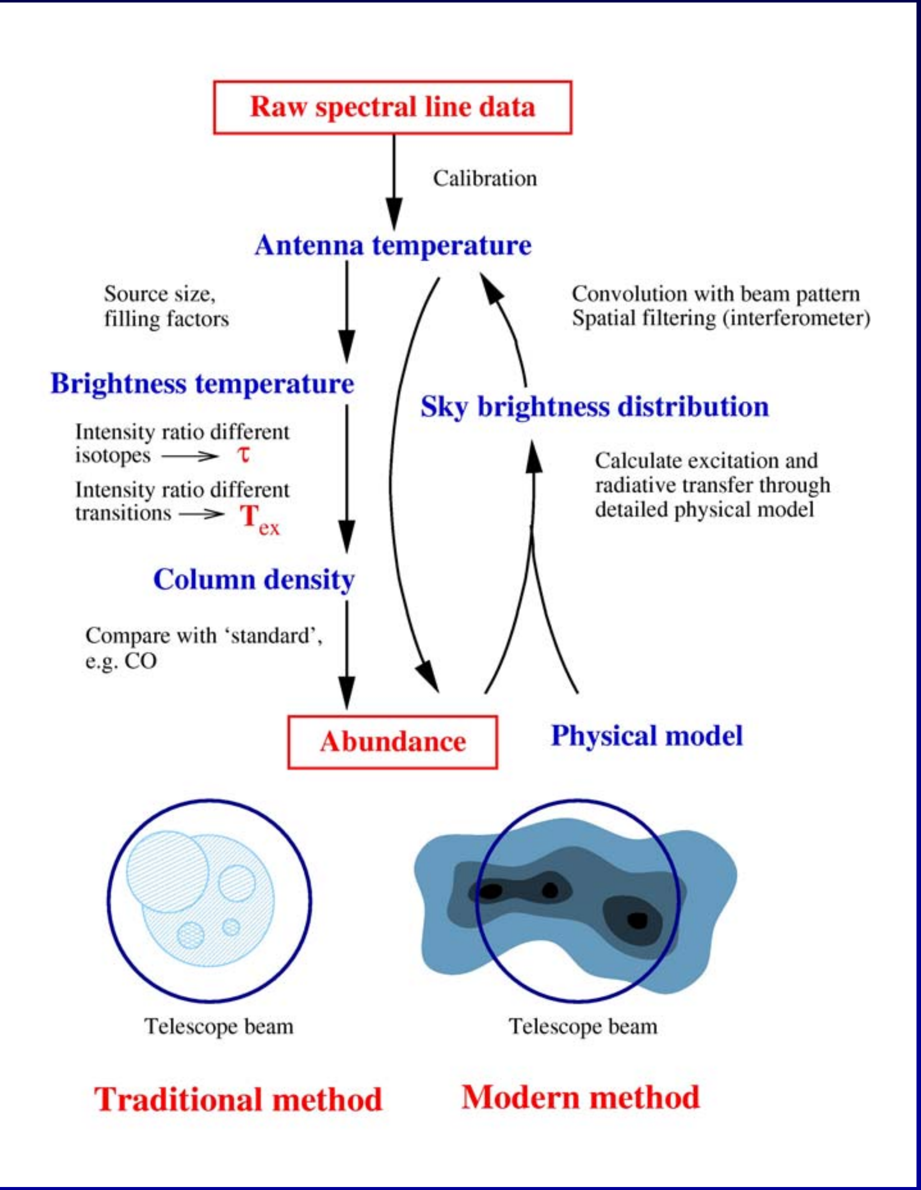
Molecules as physical diagnostics



Pure rotational transitions

Higher transitions probe higher temperatures and densities

Derivation of abundances

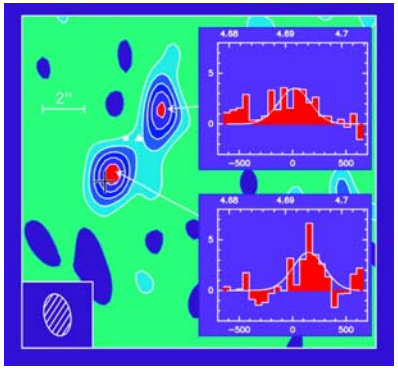


Abundance can vary with position in cloud

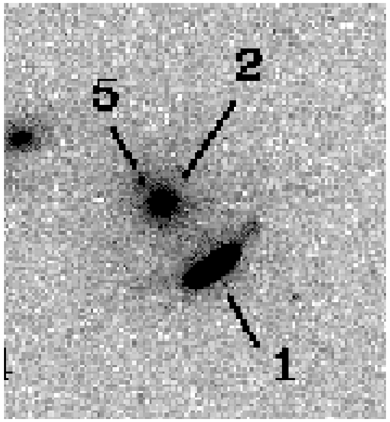
Molecules as probe of star- and galaxy formation at high redshifts

From z ~ 0 to z ~ 5

in just 5 years

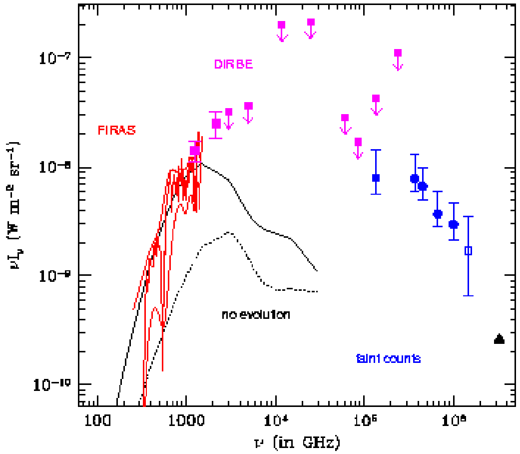


CO at *z* = 2



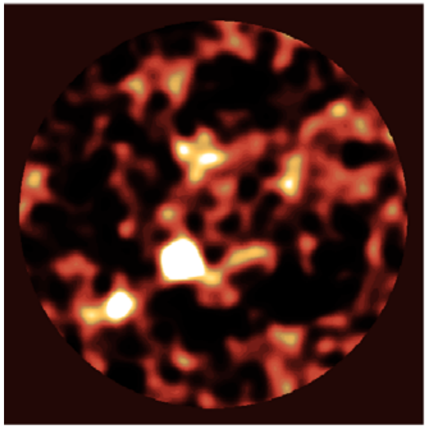
(Eisenhardt et al. 1996)

FIR background



(Guiderdoni et al. 1999)

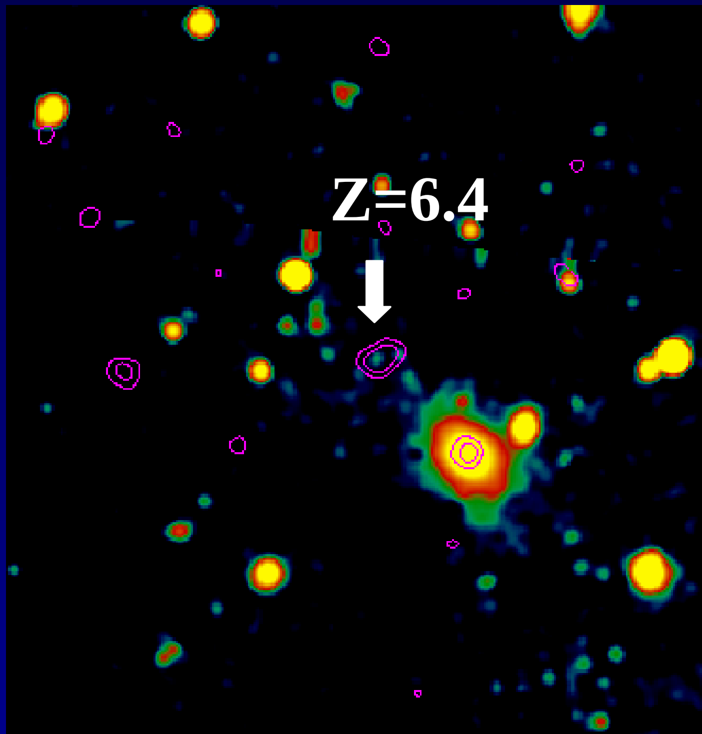
SCUBA sources

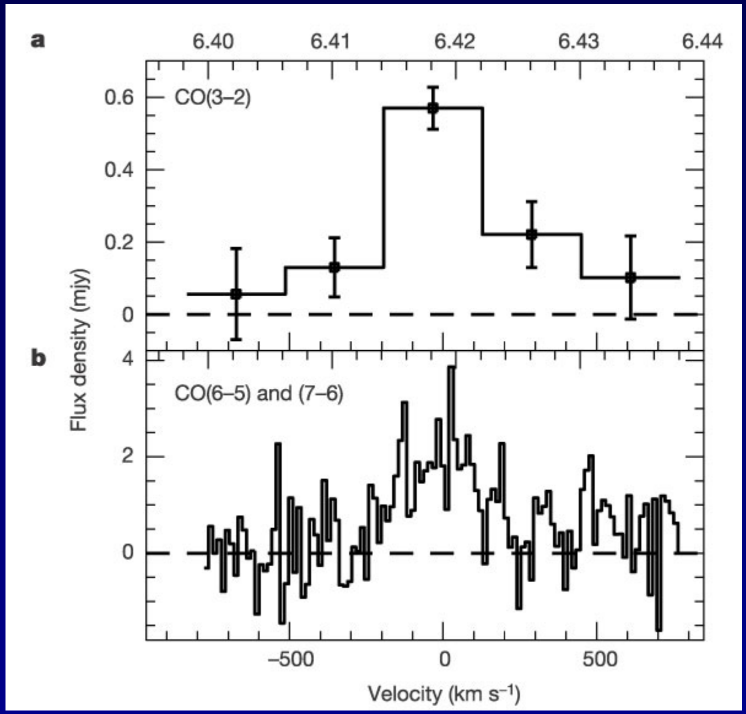


(Hughes et al. 1998)

P. Shaver

Dust, CO and [C II] at z=6.4!





Sloan survey optical image
Contours: dust

IRAM 30m MAMBO

Bertoldi et al. 2003

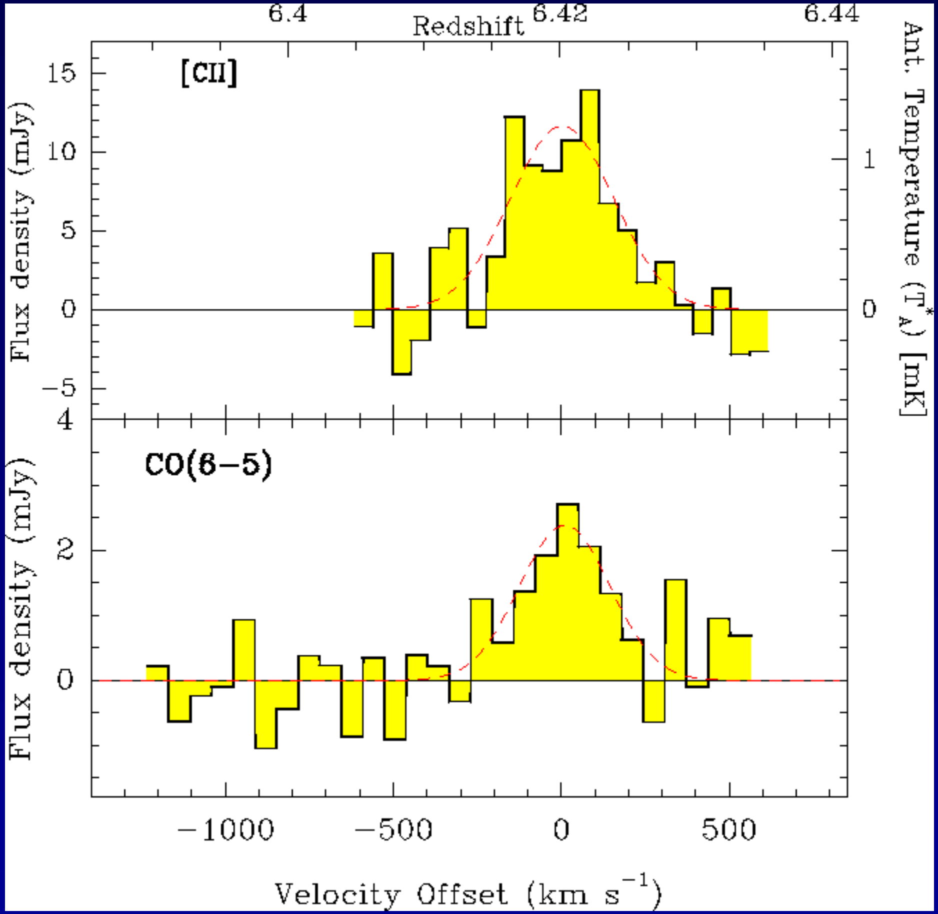
VLA and IRAM PdB

Walter et al. 2003

=> *- Molecular astrophysics started shortly after Big Bang*

- Dust and molecules are tracers of mass, dynamics, T, star formation activity of earliest galaxies

[C II] detection at z=6.4!

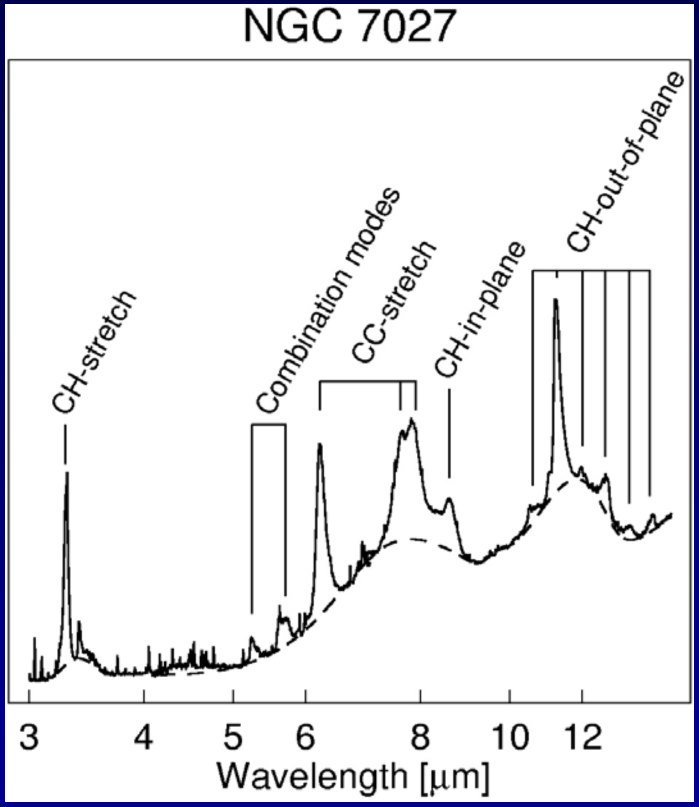


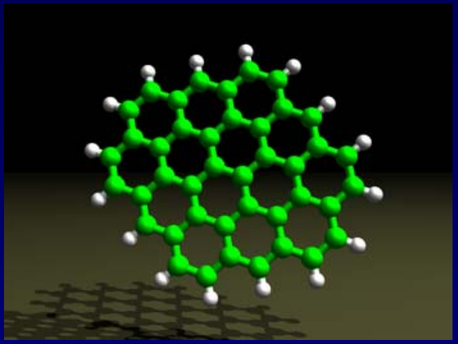
Rest wavelength 157 μm

- [C II] will be primary probe of z>7 galaxies, when bright CO lines have shifted out of ALMA frequency range
- Luminosity 0.1-1% of L_{FIR}

Maiolino et al. 2005

Ubiquitous PAH emission



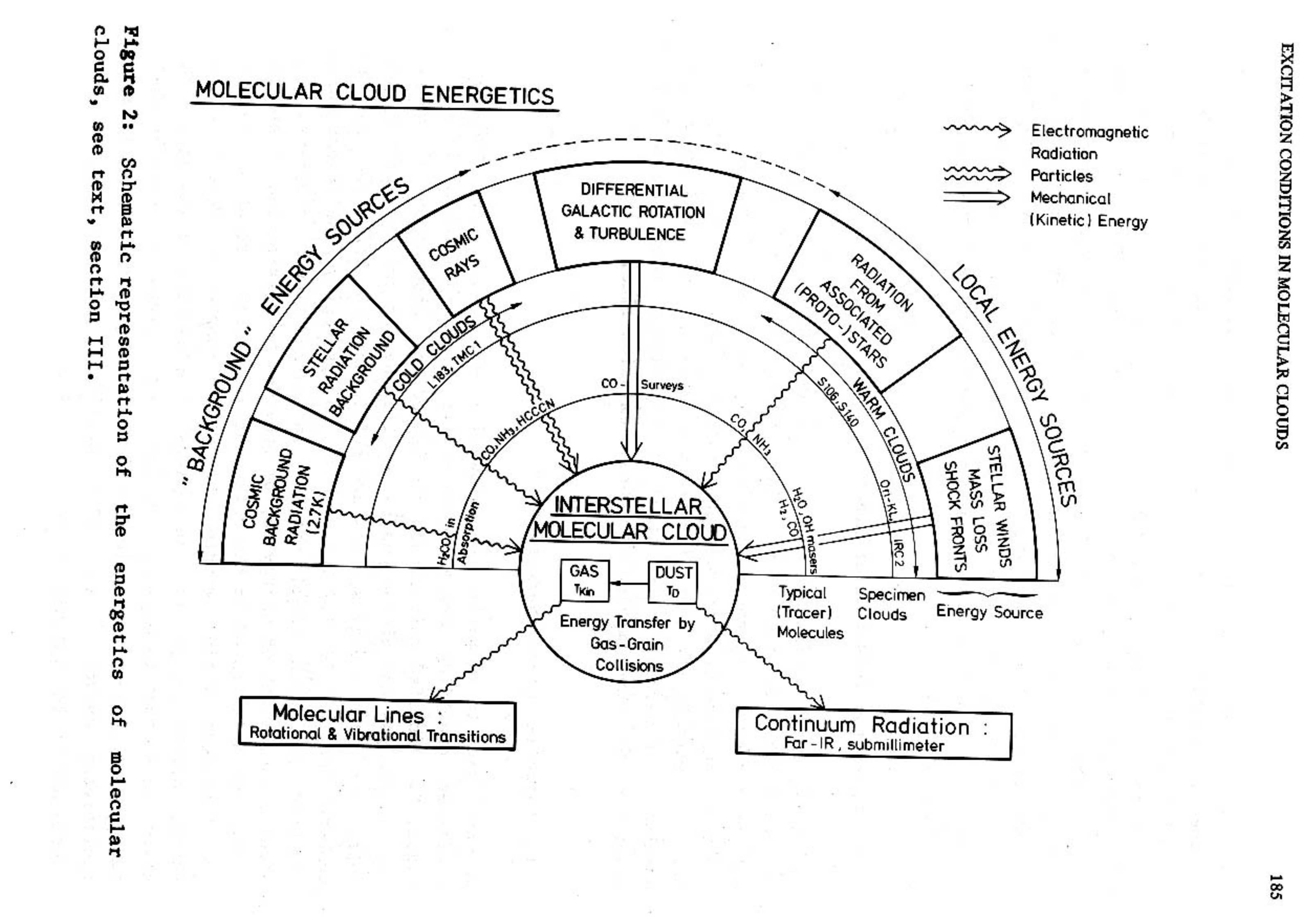


ISO-SWS

- PAH's dominate mid-IR spectra => redshift indicators
- PAH emission requires UV for excitation => diagnostic starburst vs. AGN

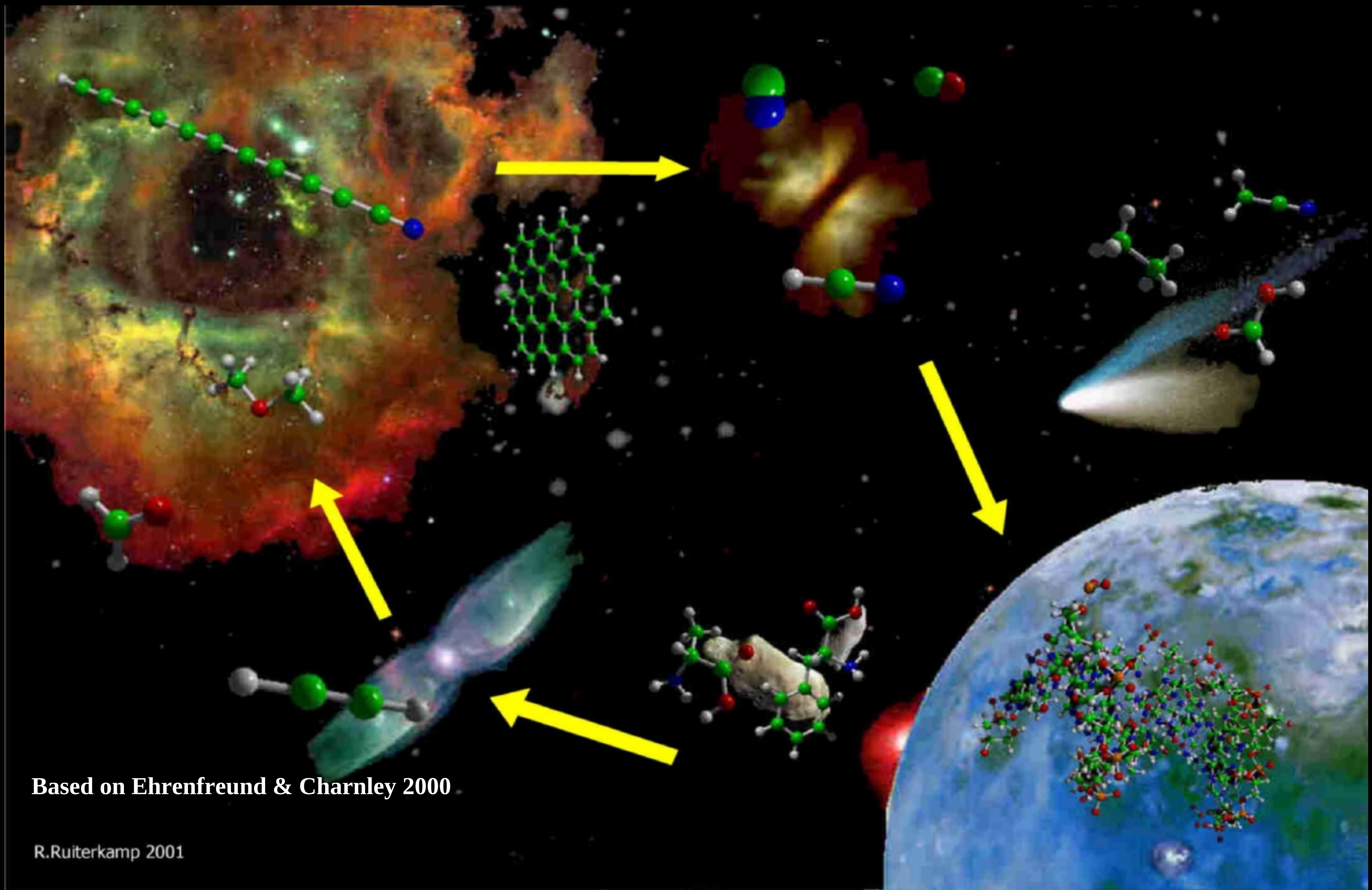
Allamandola , Tielens et al.
Léger, Puget

Role of molecular clouds in galaxy



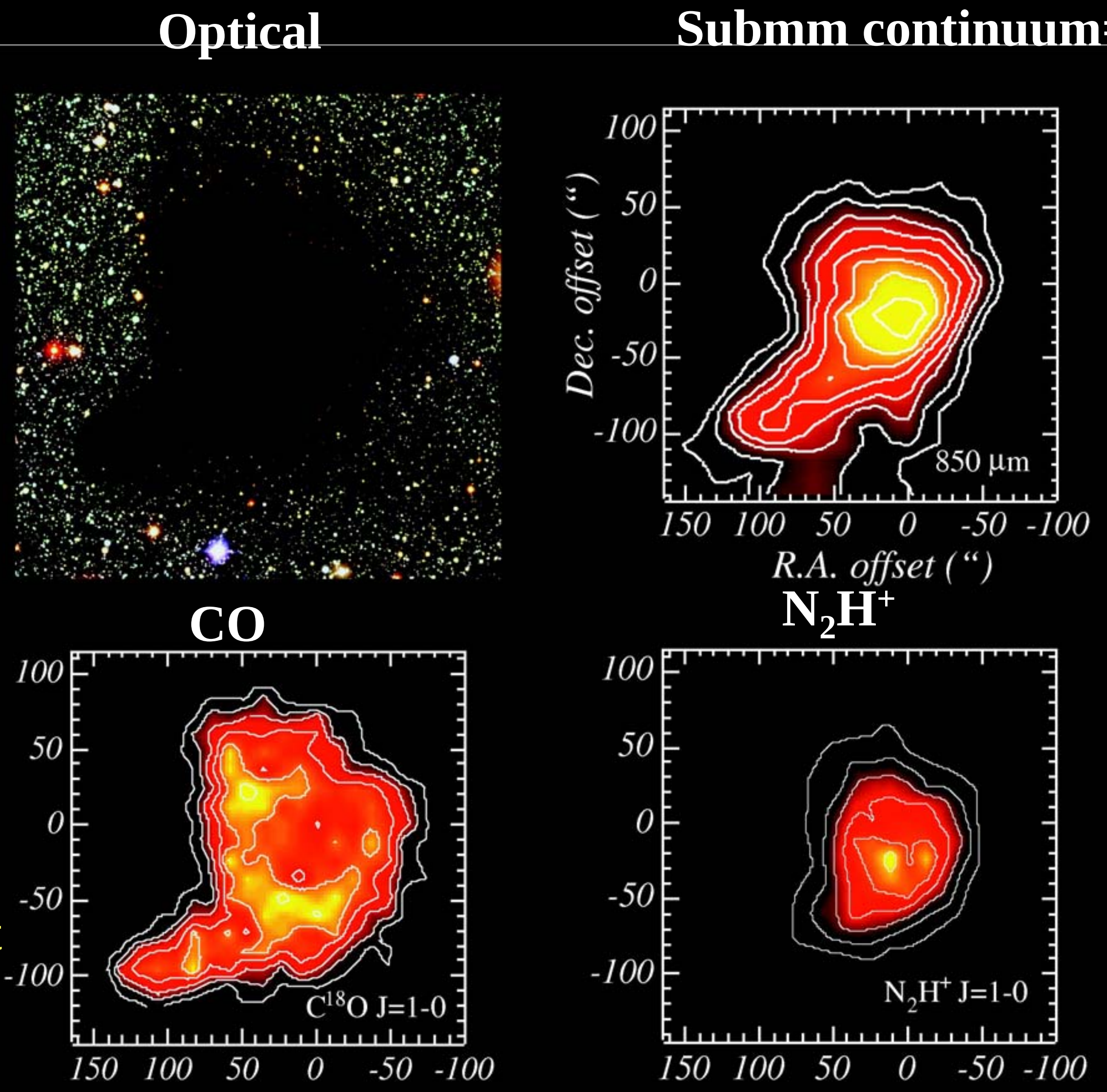
Winnewisser et al. 1984

Detection of exoplanets: renewed interest in lifecycle of gas and dust



Based on Ehrenfreund & Charnley 2000

Cold cores: heavy freeze-out



More than 90% of all molecules except most volatile species frozen out on T~10 K grains

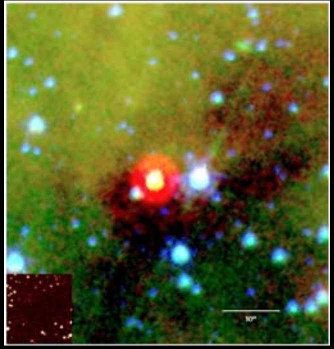
CO avoids densest, coldest part of core

Bergin et al. 2002
Caselli et al. 2002

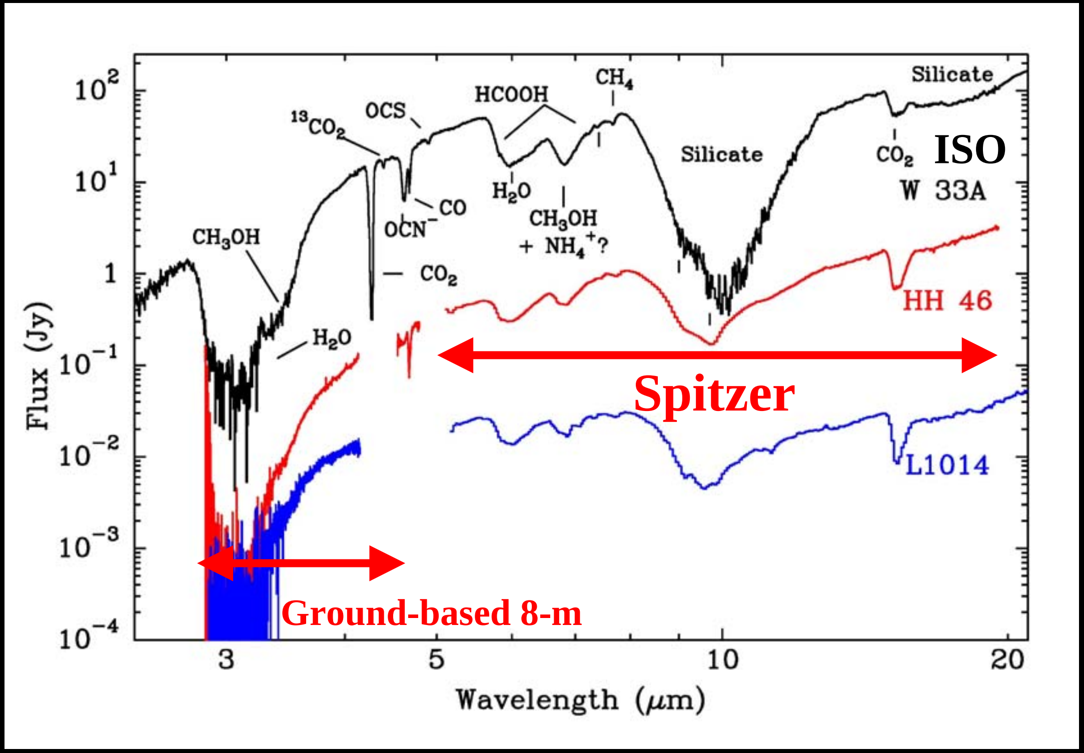
Direct detection ices at infrared

HH 46: solar-mass YSO

L1014: substellar YSO



From 10^5 to $<0.1\ L_{sun}$ objects!



-Overall ice composition remarkably similar toward high- and low-mass YSOs

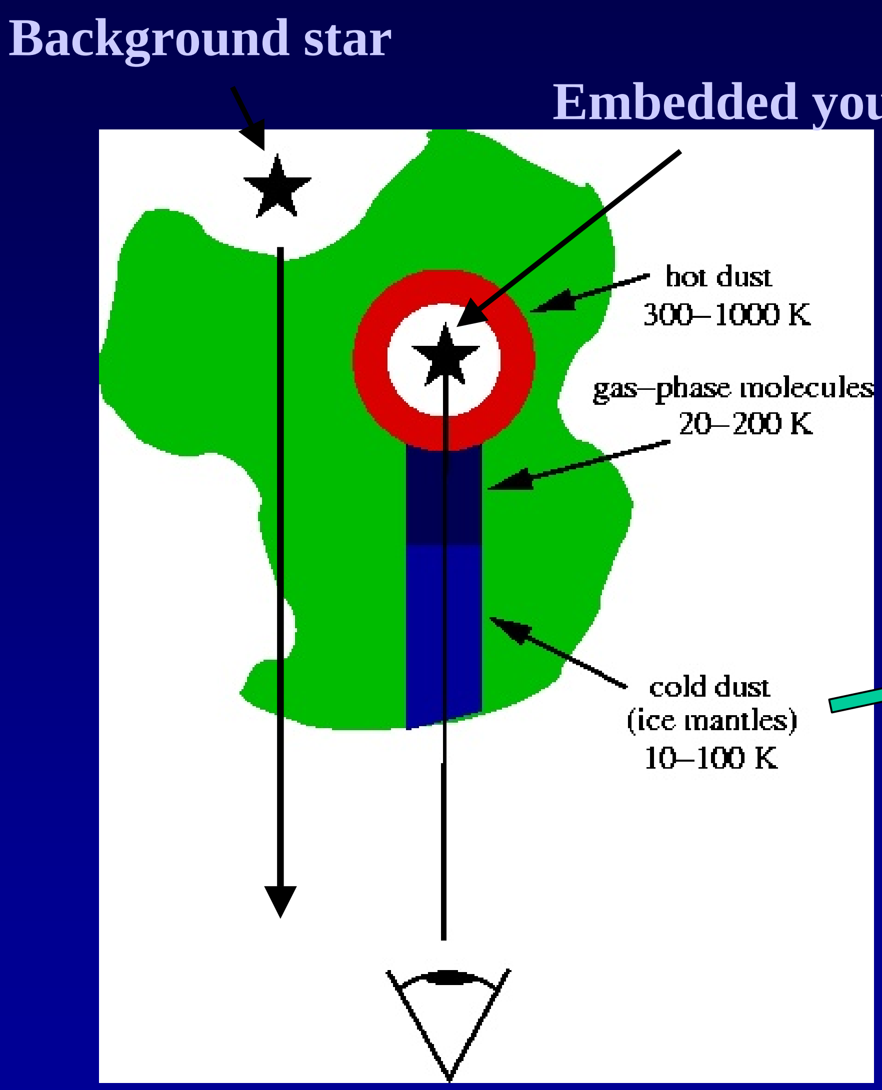
-Large abundance variations in minor species NH_3, OCN^-, CH_3OH on 1000 AU scales

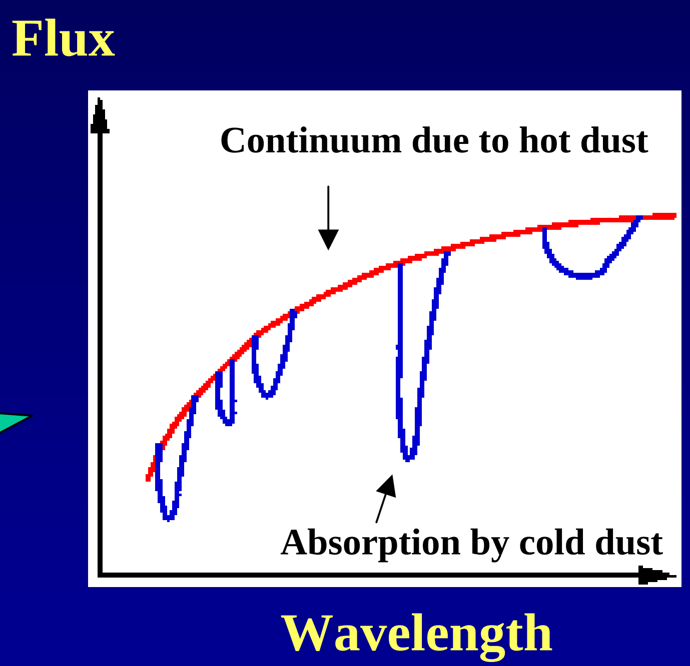
Q: Origin large abundance variations?

Formation complex organics on grains? Is UV needed?

Gibb et al. 2000
Boogert et al. 2004, 2007
Young et al. 2004

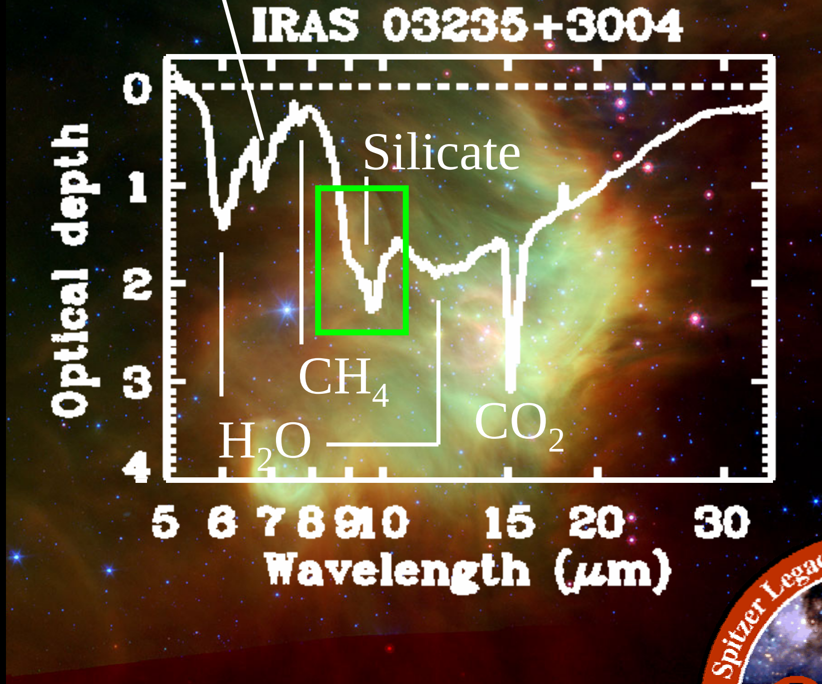
Infrared absorption

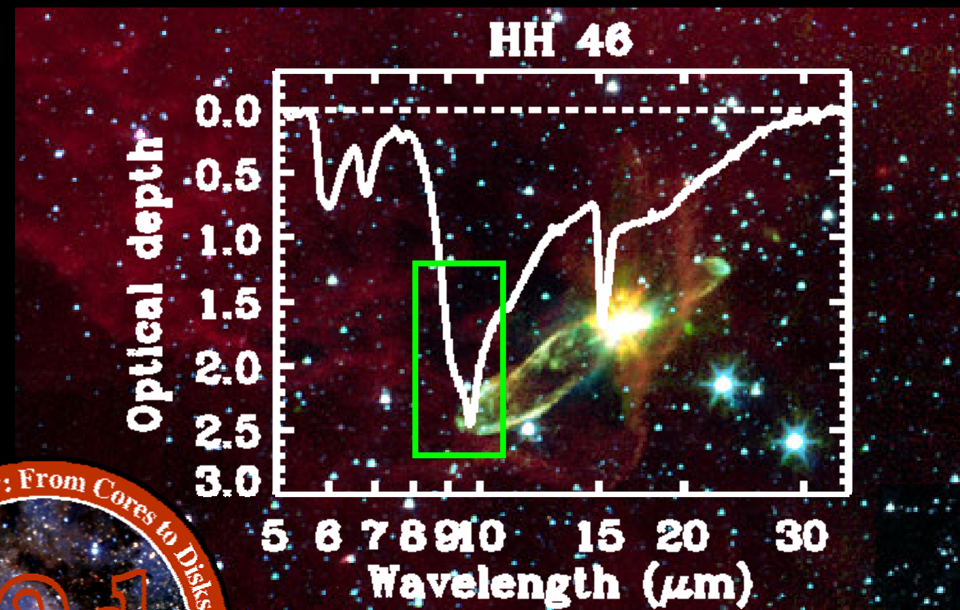


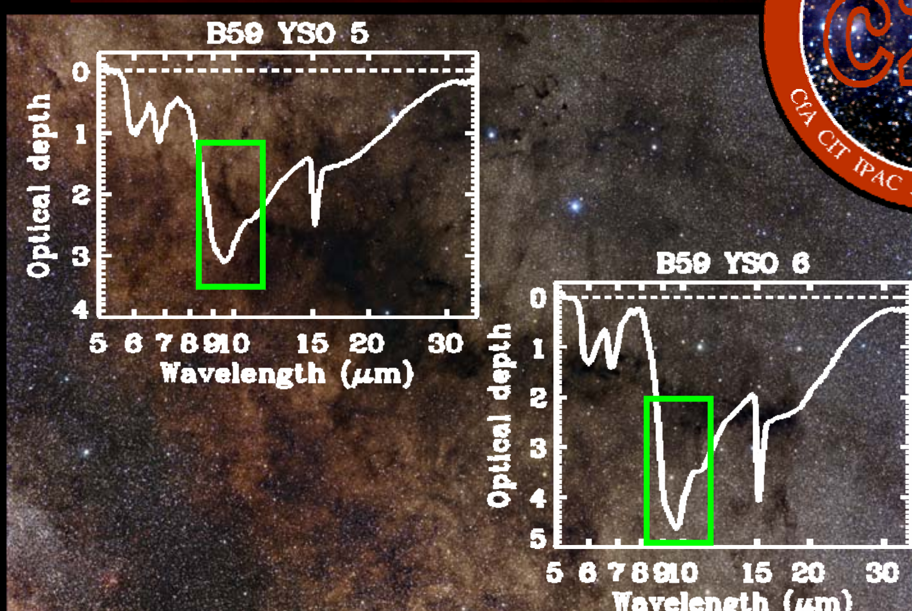


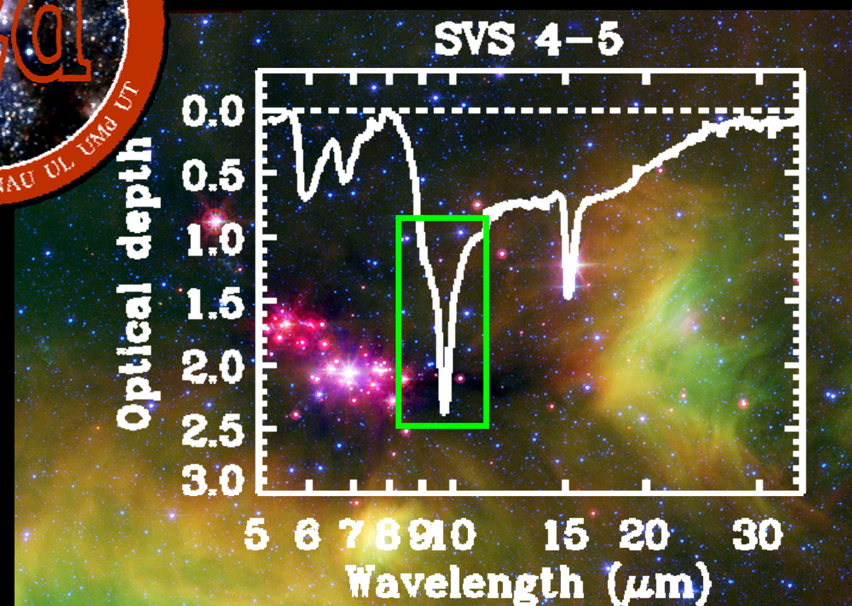
Infrared: vibrational transition of gases and solids

Ices toward low-mass protostars



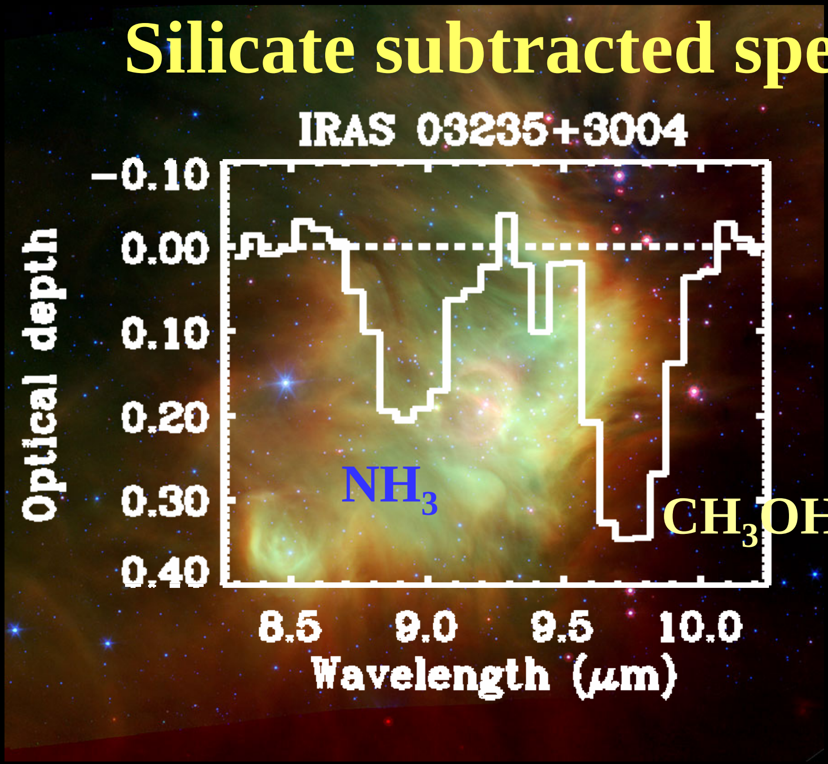


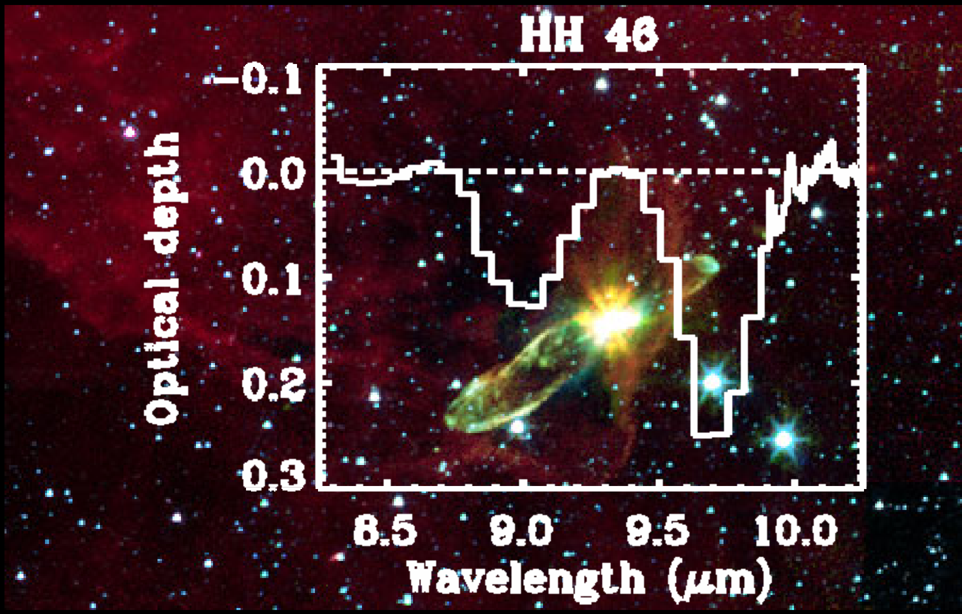


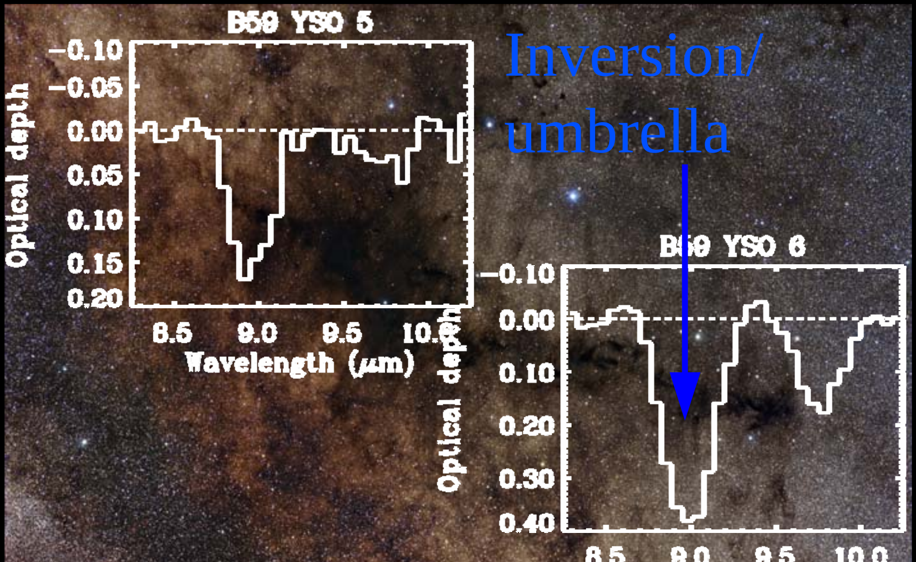


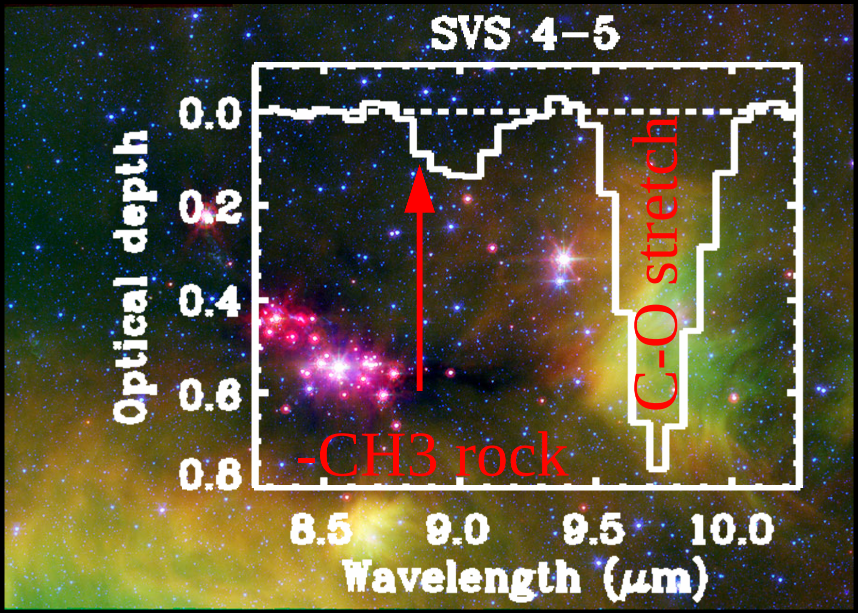
Boogert, Pontoppidan, Oberg, Bottinelli et al. 2007

Silicate subtracted spectra: NH_3 and CH_3OH!









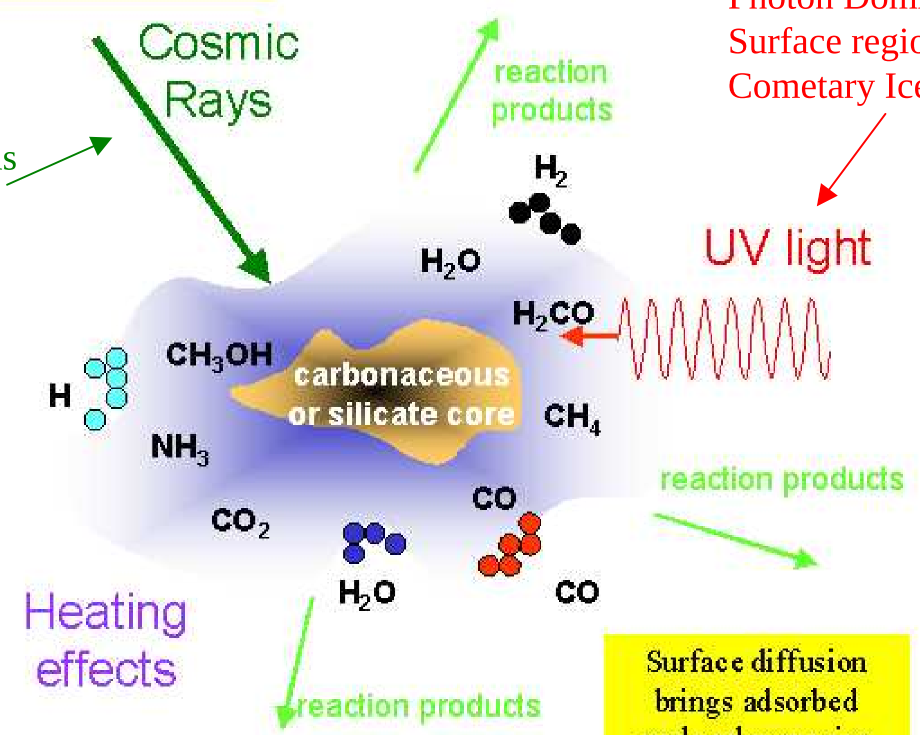
Ingredients for complex organics!

Processing of ices produces complex molecules?

Grain provides a 'catalytic' surface with a weak H-bonded network

Everywhere!
Dense Clouds
Disk Plane

Photon Dominated Regions
Surface regions of dusty disks
Cometary Ices



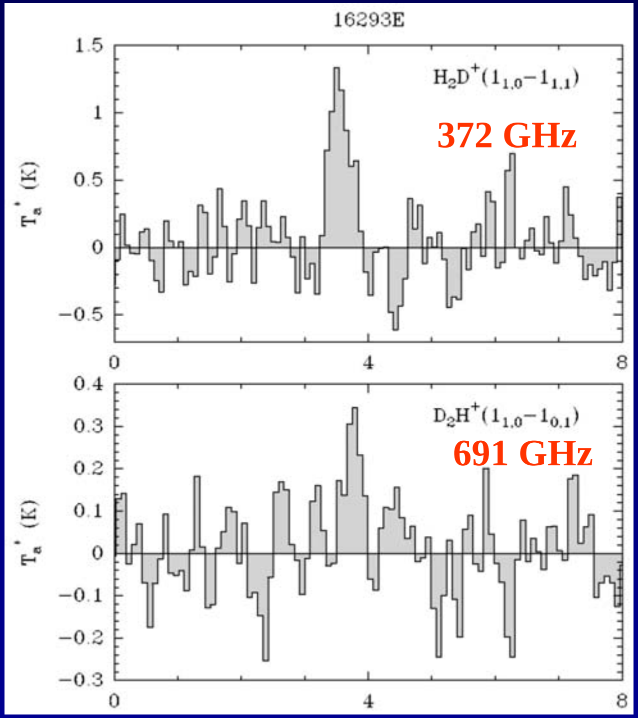
Surface diffusion brings adsorbed molecular species into close contact

Shocked regions (HH objects)
Collapsing Dense Clouds
Turbulent disks

Fraser, Collings & McCoustra
Rev. Sci. Inst. 73, no.5, 2161 (2002)

Cold cores: extreme deuteration: tracer of temperature and freeze-out

Strong H_2D^+ and D_2H^+ in cores

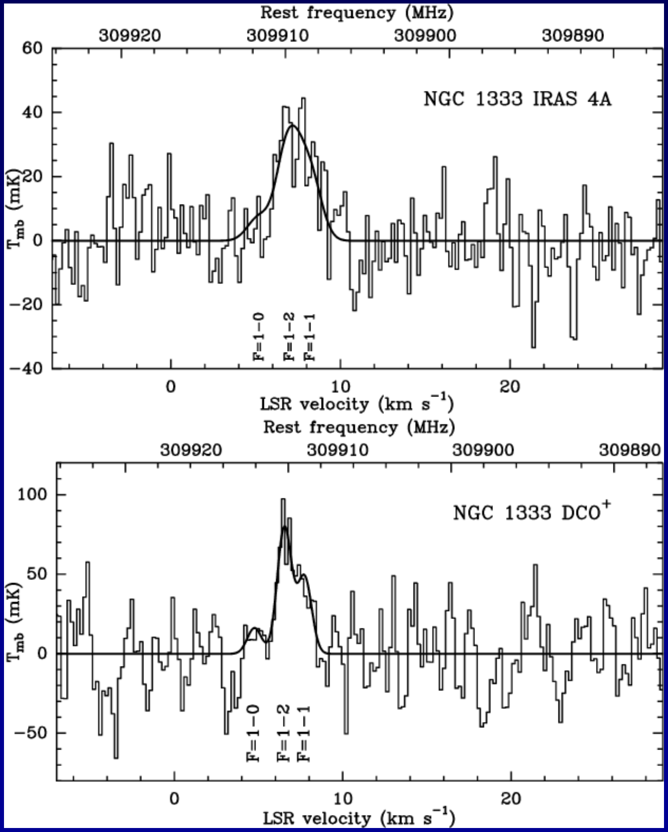


CSO submm

Caselli et al. 2003
Vastel et al. 2006
Stark et al. 1999

H_3^+, D_3^+: IR

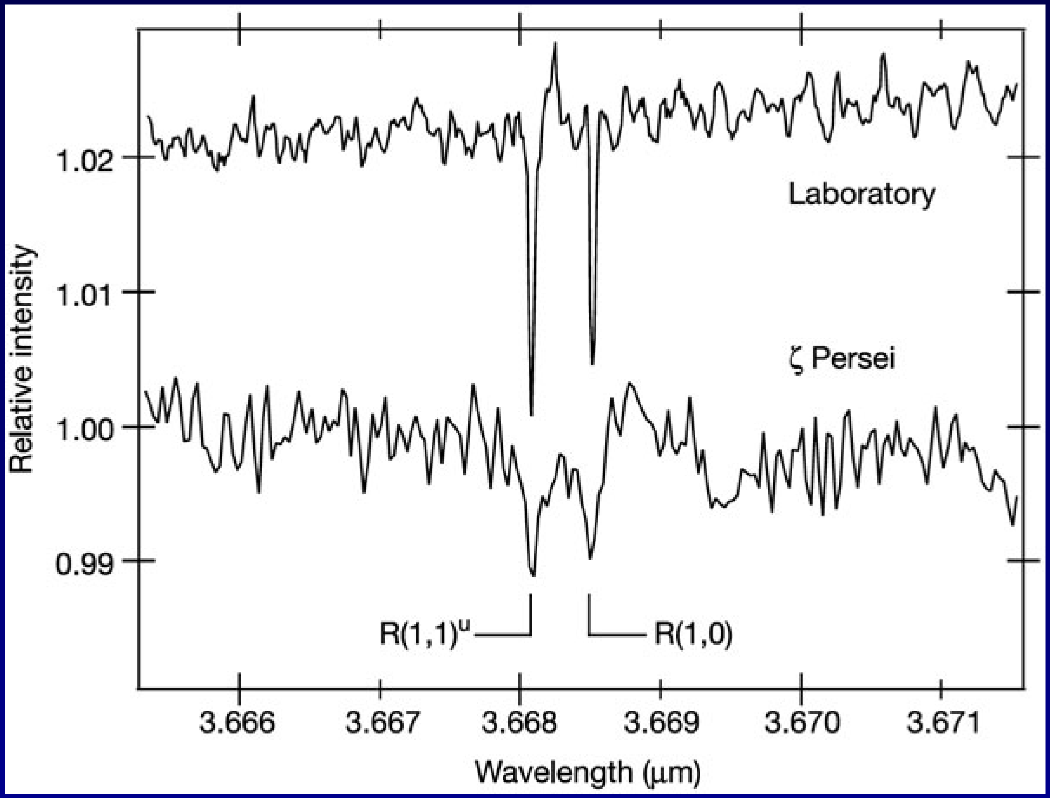
Triply deuterated ammonia: ND_3



CSO submm

Lis et al. 2002
van der Tak et al. 2002

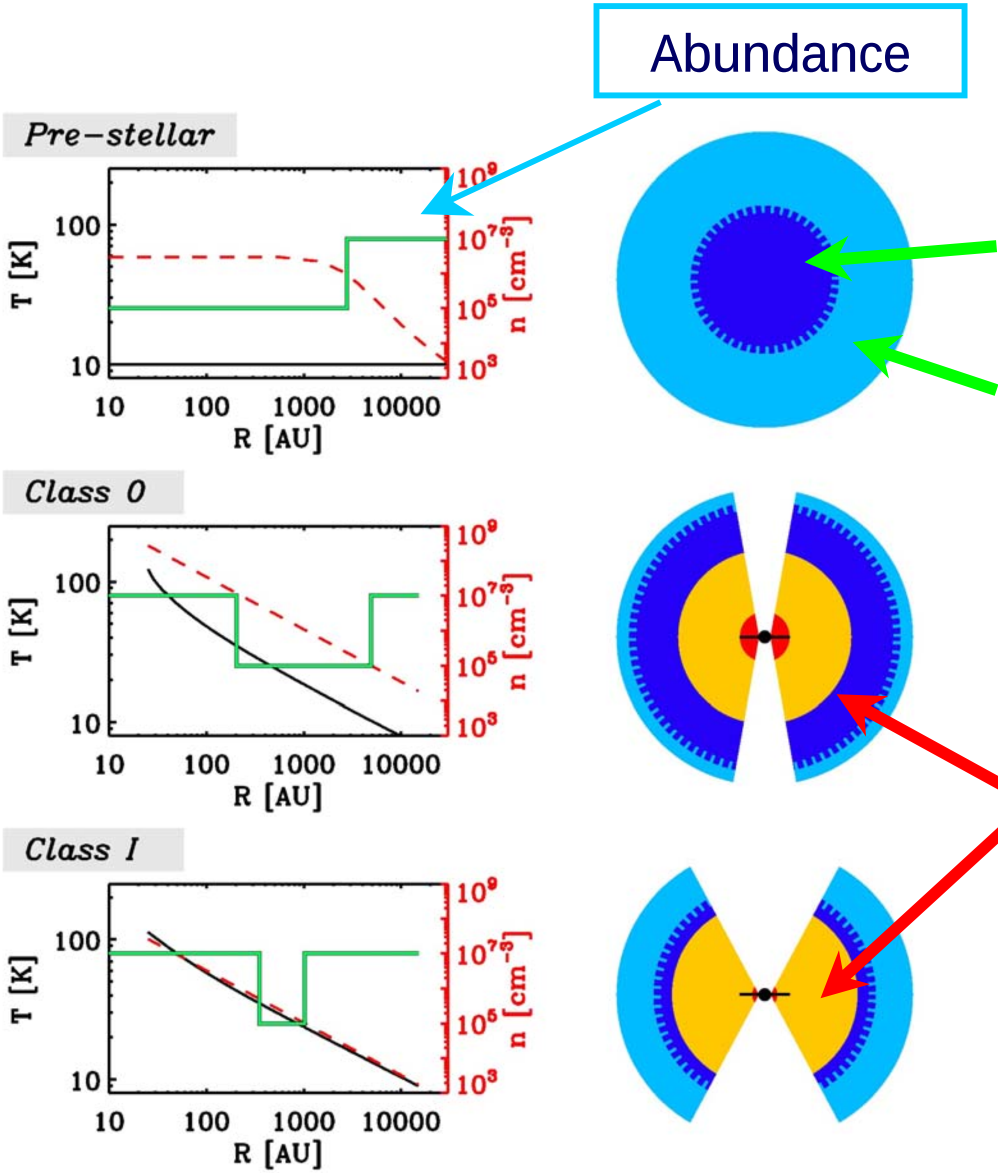
Interstellar H_3^+ as tracer of ionization



Geballe & Oka 1996
McCall et al. 2003
vdTak & vD 2000
Pety et al. 2004

- Cosmic ray ionization rate varies from cloud to cloud?

- Strong H_3^+ absorption in diffuse clouds implies high cosmic ray ionization rate ~few x 10^{-16} s^{-1}



Pre-stellar core:

- Low temperature
- Depletion toward center
- …but not edge

Protostellar core:

- Central heating ~ temperature gradient
- Thermal desorption toward center
- …outside (low T): depletion/no depletion regions as in pre-stellar stages

Jørgensen et al. 2005

Q: Is this an evolutionary sequence?

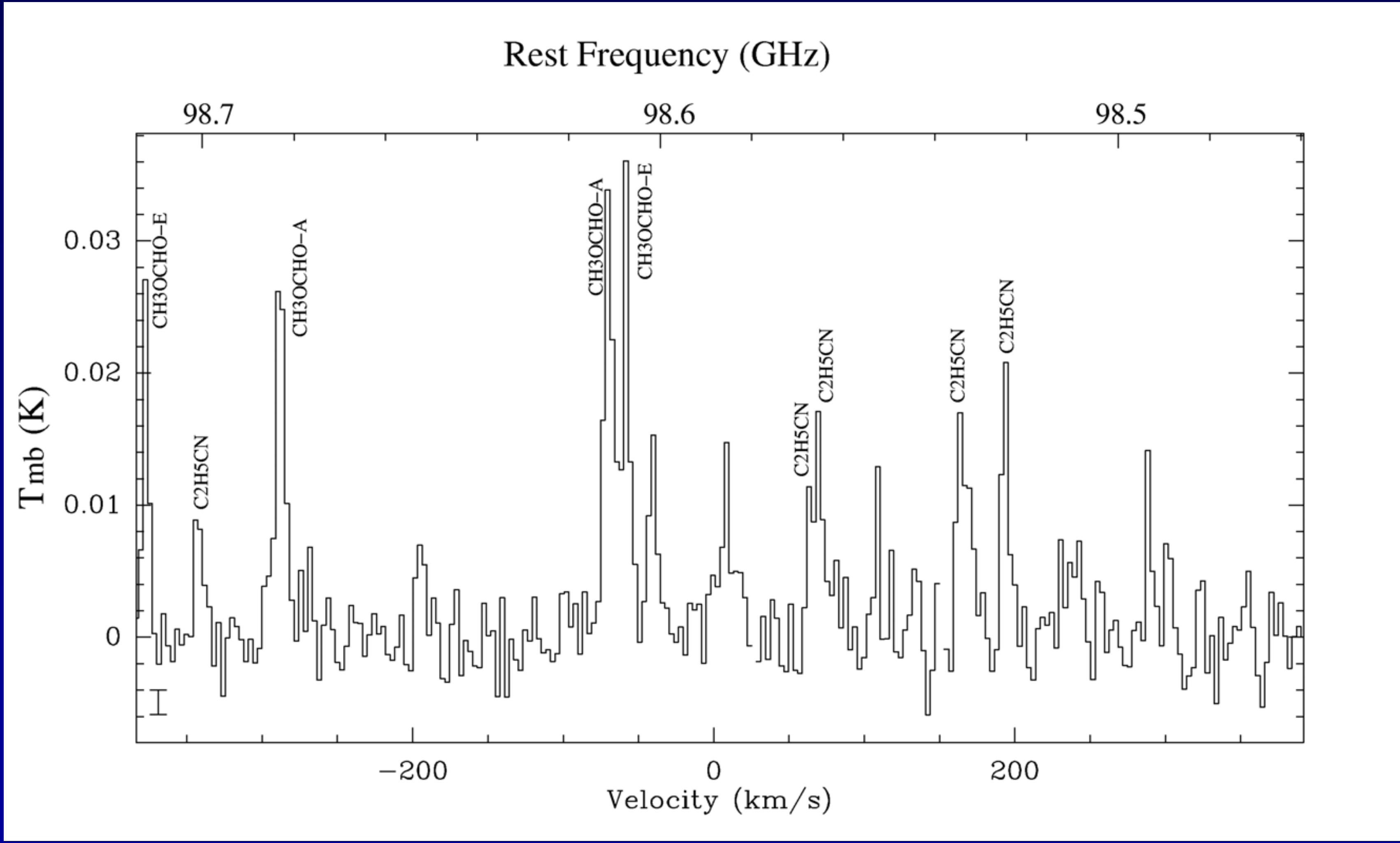
Can chemistry constrain timescales?

Current data suggest phase of heavy depletions (pre-+protostellar) lasts only ~10^5 yr

Hot cores/corinos: Inner envelope chemistry

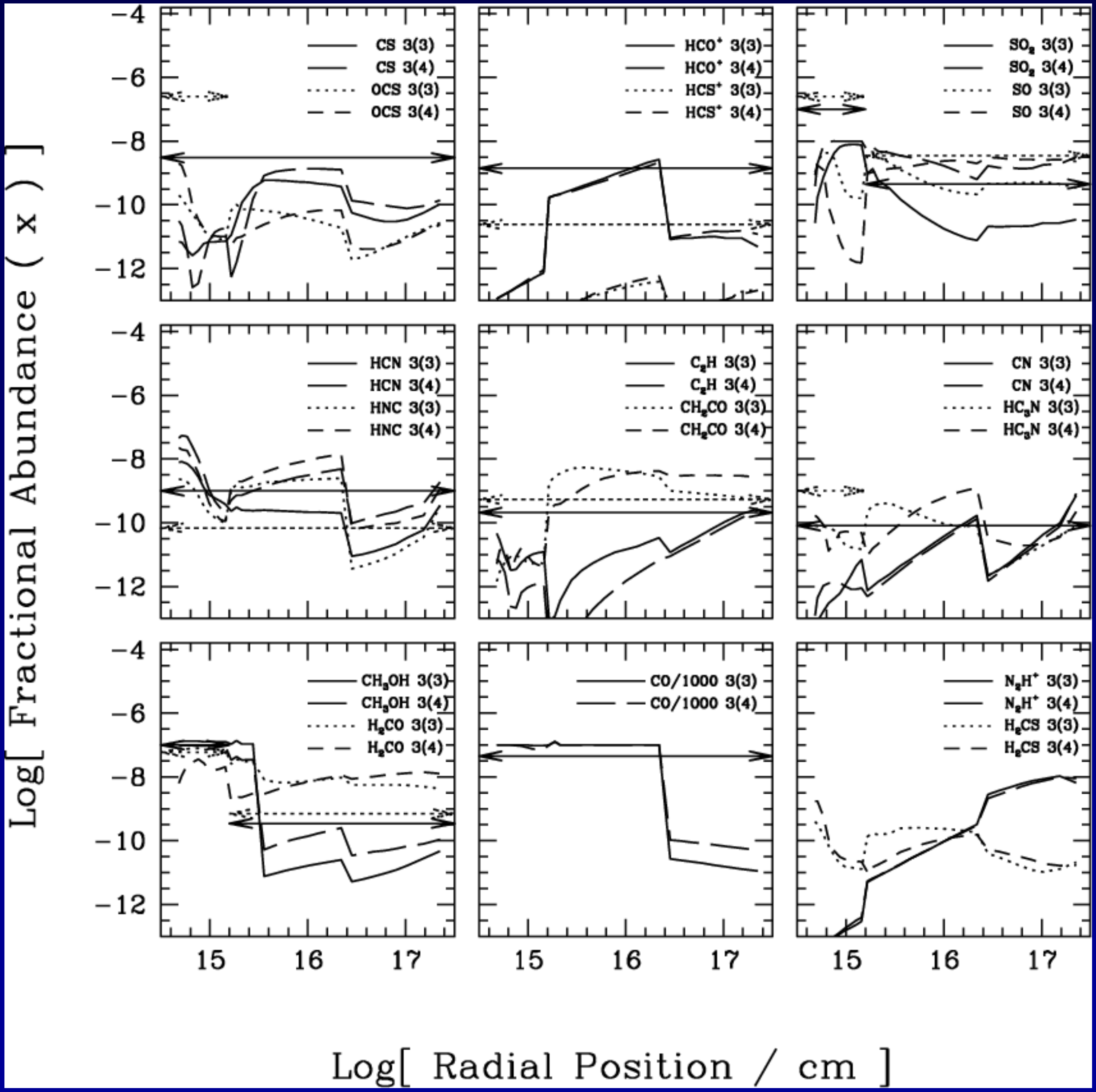
Evaporated ices and complex organics around solar-mass star

IRAS 16293-2422



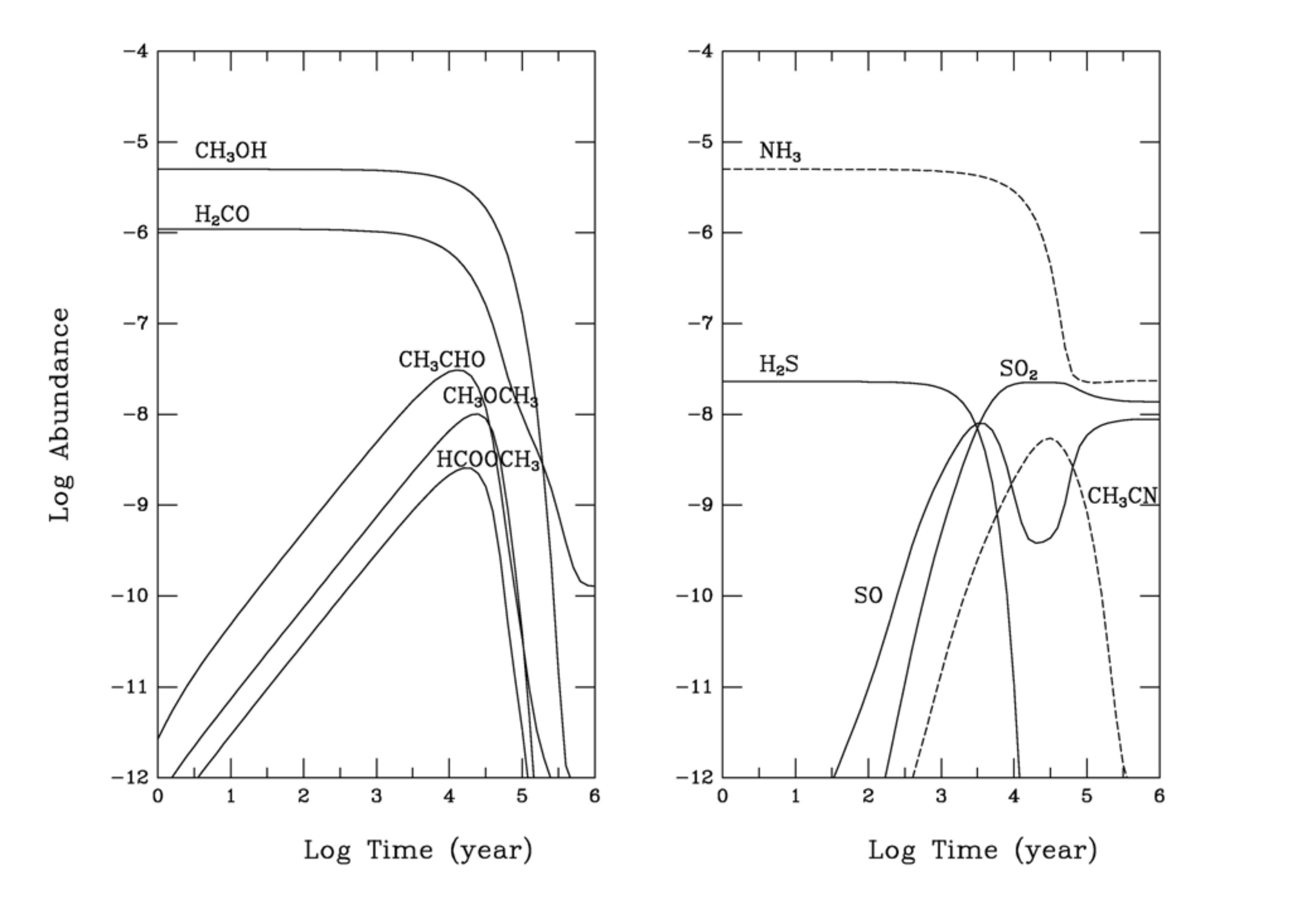
vD et al. 1995, Ceccarelli et al. 2000 **IRAM 30m** **Cazaux et al. 2003**

Abundance profiles



Doty et al. 2004

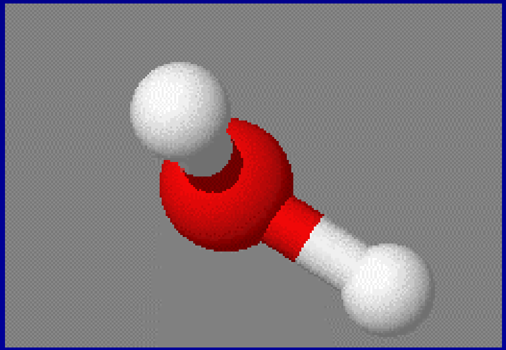
Molecules as chemical clocks



Charnley et al. 1992, 1997
Wakelam et al. 2004, 2006

Importance of water

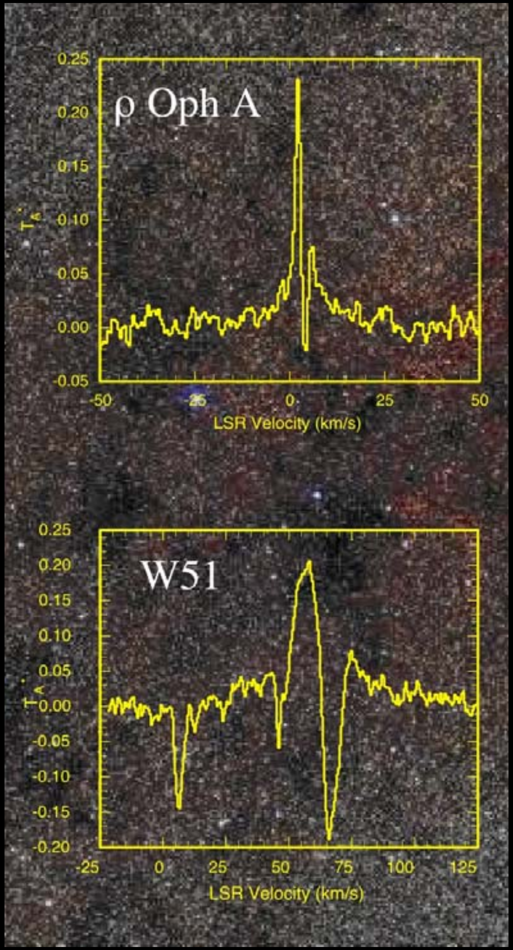
- Dominant form of oxygen => affects all species
- Important role in energy balance as coolant
- Diagnostic for ‘hot spots’
- Origin of water on Earth (through HDO/H_2O)
  - Chemistry of life occurs in water



Gas phase water

o-H_2O 557 GHz
1_{10}-1_{01}

Melnick et al. 2000

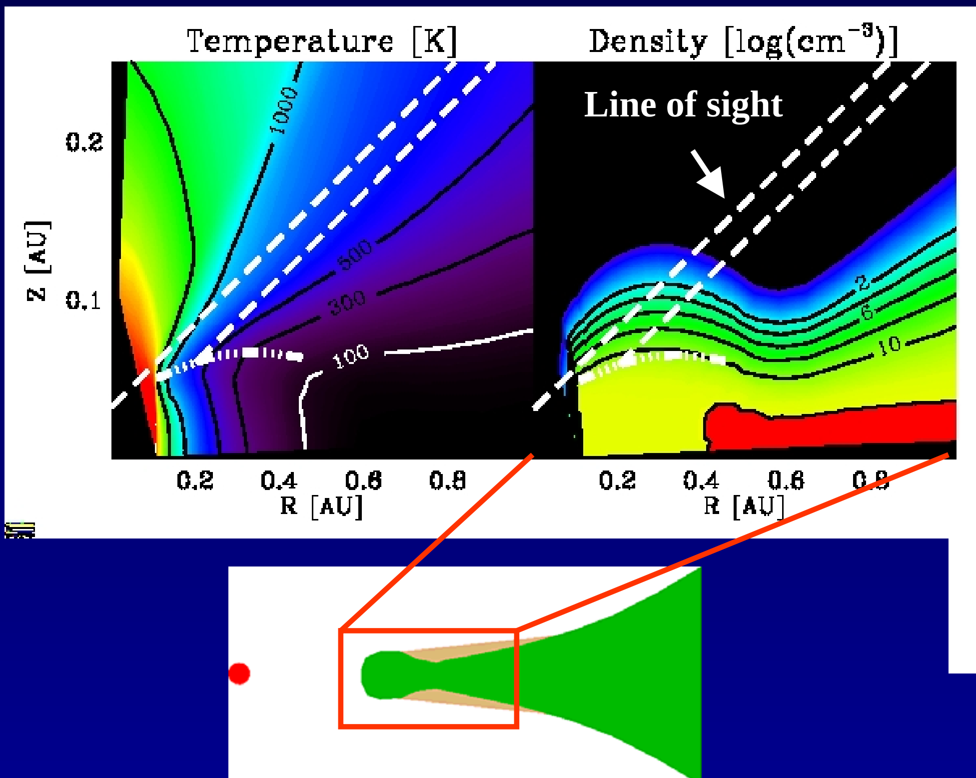


- SWAS and ODIN (~3'):
Water emission is weak =>
most water frozen out on
grains in cold clouds

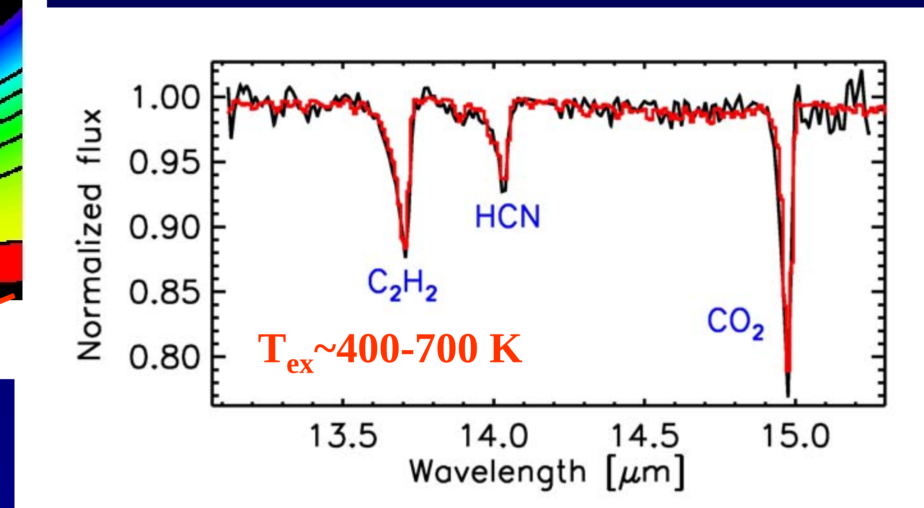
Herschel (10-40'') =>
- zoom in on protostars
- many more lines
- isotopes $H_2{}^{18}O$, $H_2{}^{17}O$, HDO!

Q: what is water cycle from clouds => cores => protostars => disks?

Water and organics in planet-forming zones of disks



Edge-on disk: Oph IRS 46



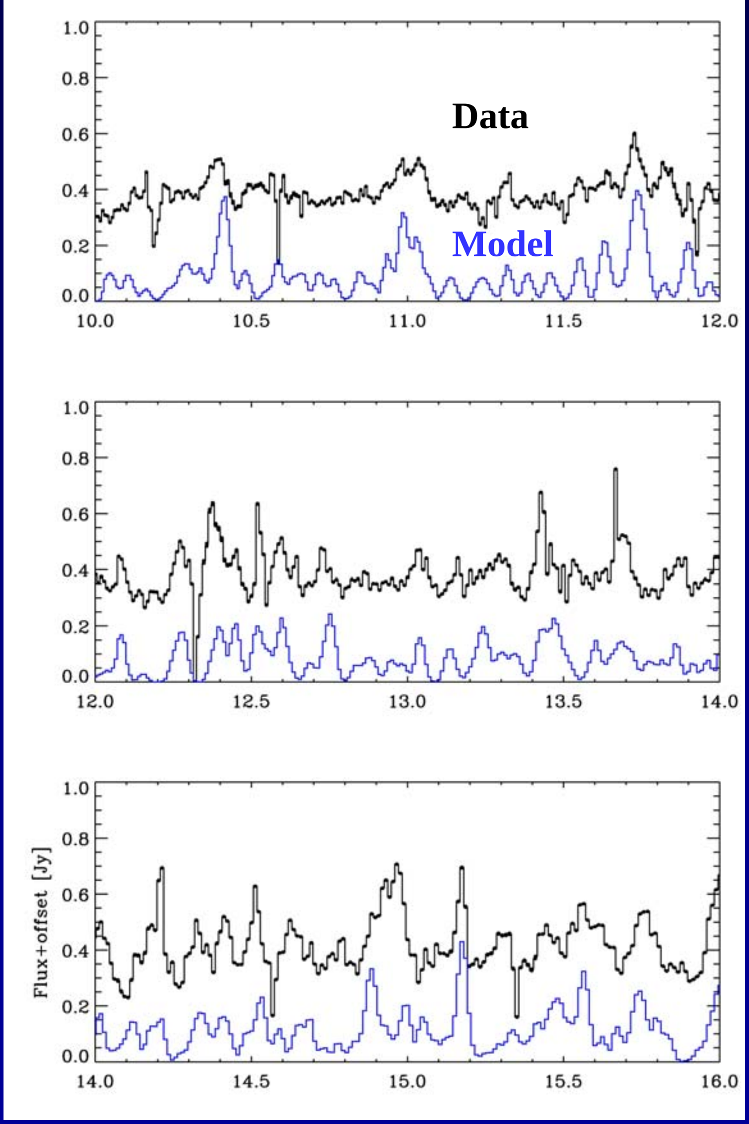
Lahuis et al. 2006

- Probe chemistry in inner 10 AU => planet-forming zones
- Gas is hot: 400-700 K
- Abundances factor 1000 larger than in cold clouds

Hot water emission in disk atmospheres!

T~1000 K
=> 0.1-1 AU

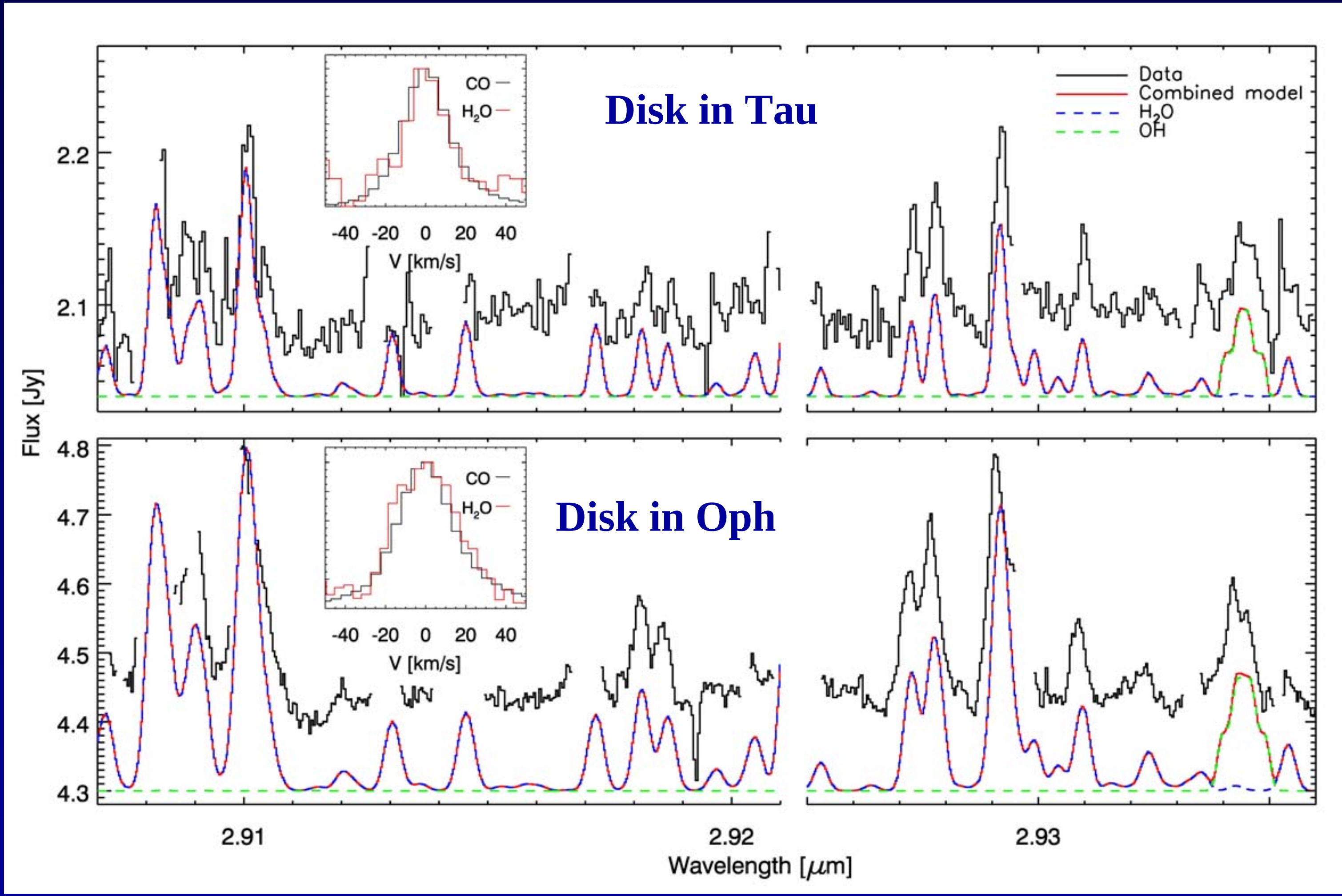
Also hot HCN, C_2H_2
seen in emission



AS 205 disk in Oph
Spitzer observations

Carr & Najita 2008
Salyk, Pontoppidan et al. 2008

Near-IR OH/H_2O from ground



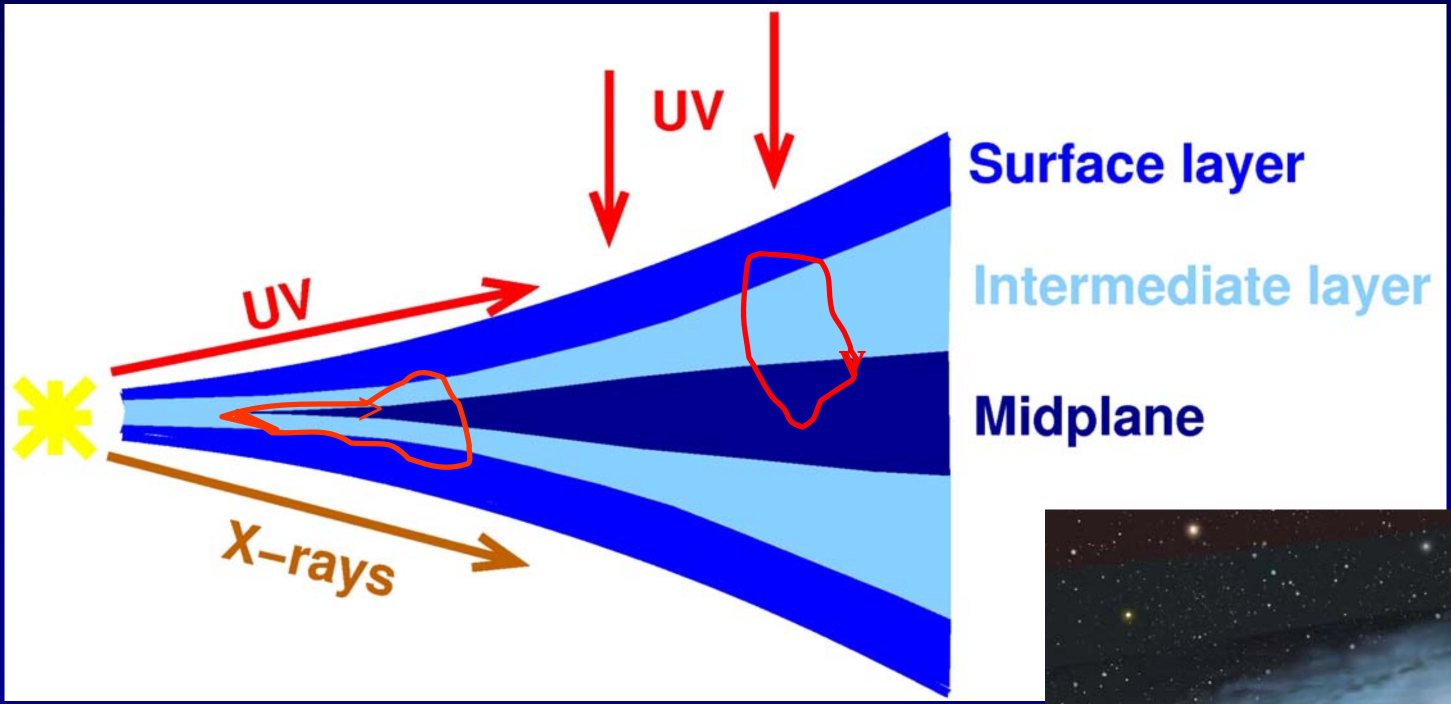
Keck
R=25000

Fully resolved with CRIRES

Note similarity in CO and H_2O line widths!

Salyk et al. 2008

Where is water in protoplanetary disks?

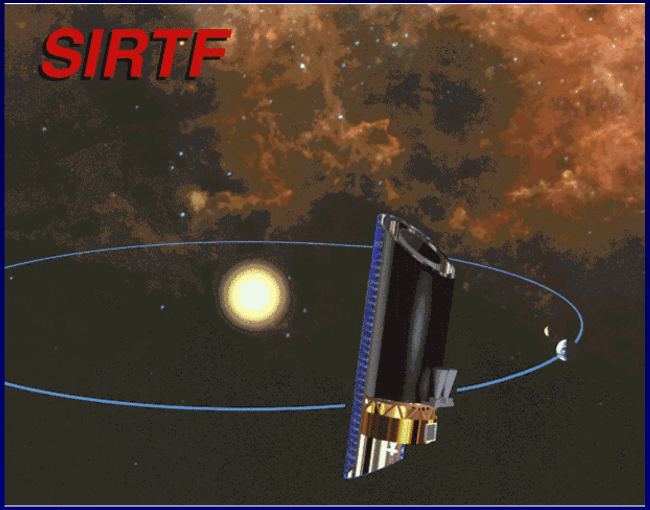


Q: use water as tracer of radial and vertical mixing; 'snow' line?

Future facilities: the best is still to come

Infrared

Far-infrared/THz



SOFIA 2011

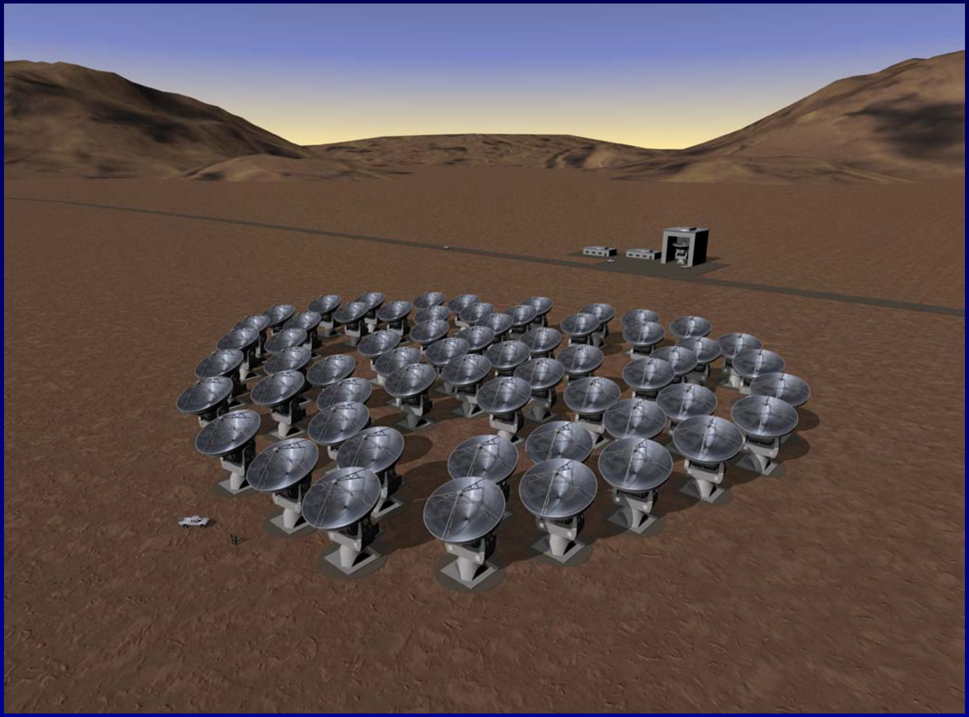
SIRTF 2003

ASTRO-F 2005

Herschel 2008

JWST 2013

ALMA



64 x 12m antenna's; construction started 2003
Early observing 2010; completion 2012

Issues for this workshop

- **Identify most important rates needed to address astrophysical and astrochemical questions**
  - **No use spending a lot of time and money on unimportant rates**
  - **No use spending a lot of time and money on unimportant molecules**
- **Quantify uncertainties as functions of parameters**
  - **Some easy, some difficult**
  - **May vary with temperature, wavelength, ….**
  - ***Critical* evaluation of existing data (latest number is not always the best….)**
- **Educate astrochemists in underlying chemical physics**
  - **Manage their expectations of what can/cannot be achieved**
- **Educate (astro)chemists about proper comparison with observations**
  - **Make sure all relevant processes are included**
  - **Awareness that abundances are not constant with position**
  - **Sometimes physics poorly understood, not chemistry (CH^+)**