



PCMI 2012  
Session Complexification moléculaire :  
lien vers la chimie prébiotique

# Molecular spectral surveys from millimeter range to far infrared.

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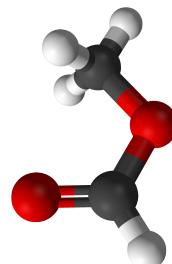
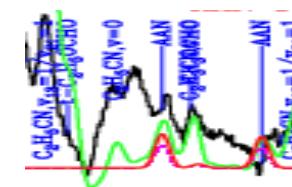
## 1. Telescopes & frequencies



## 2. Main « prototype » surveys

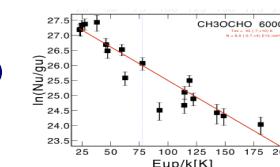
see : <http://www.gb.nrao.edu/~thunter/terahertzLineList.html> (*T. Hunter*)

## 3. Line identification

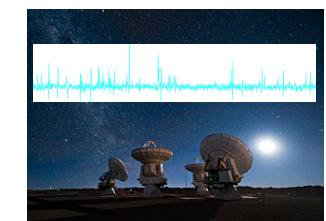


## 4. Molecular content

see : <http://www.astro.uni> (*H.S.P. Müller*)



## 5. What can we learn ?



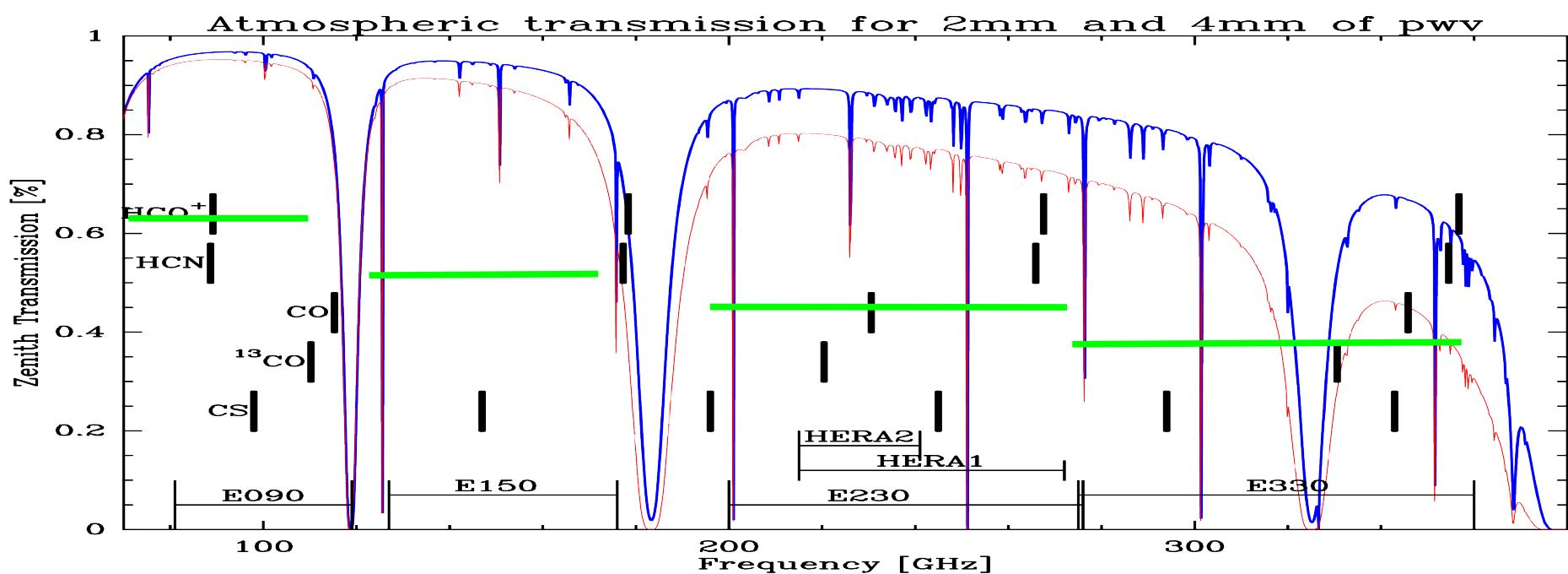
## 6. Perspectives, prospective



# Telescopes and frequencies (1)



receiver	Frequency(GHz)	Width(GHz)	Trec (K)
E0	83 - 117	8 (0.5)	50
E1	129 - 174	4 (0.5)	50
E2	202 - 274	8 (0.5)	80
<b>E3</b>	<b>277 - 358</b>	<b>8 (0.5)</b>	80

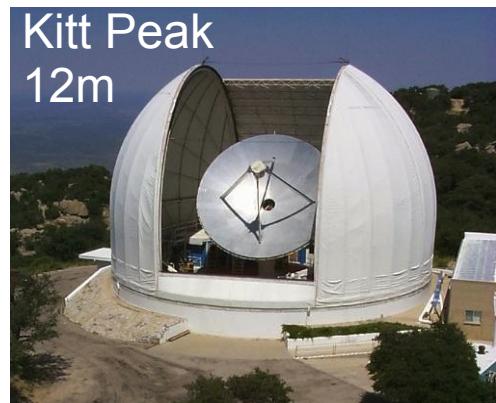




# Telescopes and frequencies (2)



Frequency	Band Width (GHz)
0.3 – 1.2 GHz	0.240
1 – 15 GHz	1 - 3
18 – 50 GHz	4



Frequency (GHz)	Band width (MHz)
83 - 116*	≤ 600
68 - 90	≤ 600
90 - 116	≤ 600
133 - 180	≤ 600

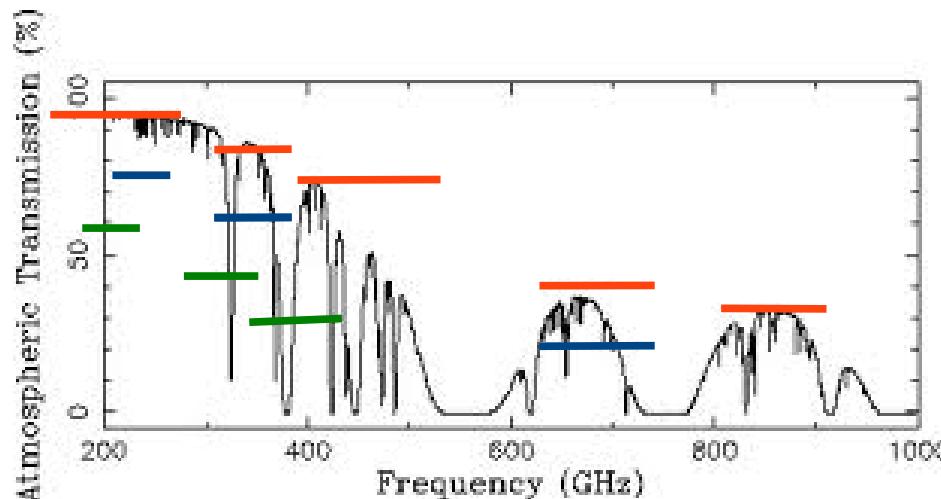
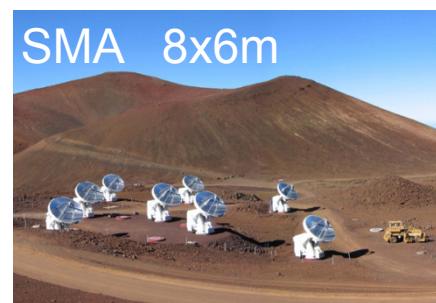
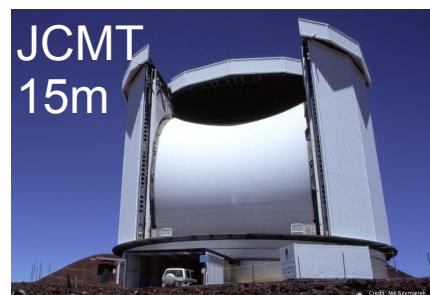
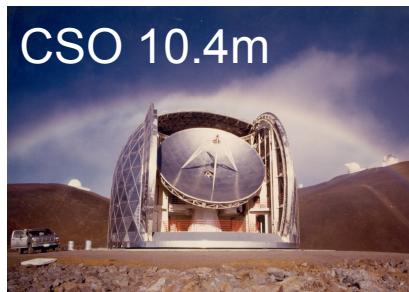
\* type ALMA Band 3



Frequency (GHz)	Band width
20.0 - 25.0	4 MHz to 2 GHz
42 - 44	4 MHz to 2 GHz
35 - 50	4 MHz to 2 GHz
72 - 120	4 MHz to 2 GHz



# Telescopes and frequencies (3)



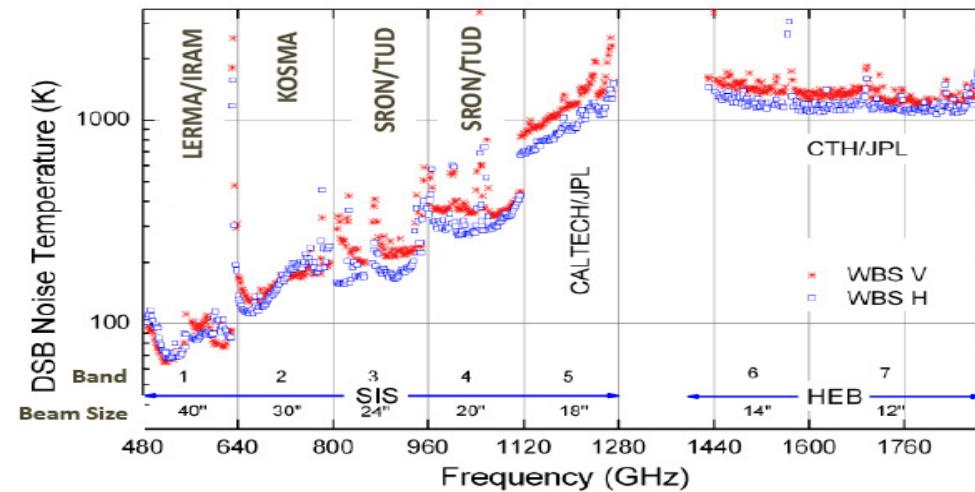
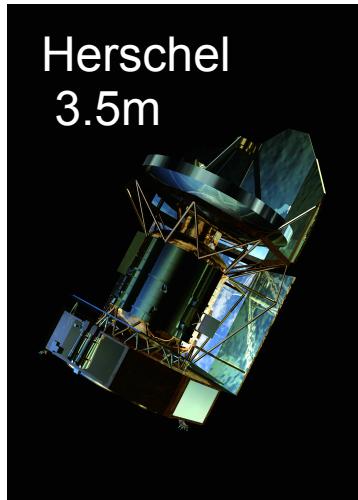
CSO receivers(GHz)
177 - 286
315 - 380
382 - 532
620 - 730
810 - 900

JCMT receivers(GHz)
211 - 272
315 - 375
630 - 710

Receiver	Frequency (GHz)	1984 Noise (K)	1992 Noise (K)	CSO 2012
230	186-242	300	60	40 K
345	272-350	900	150	90 K
400	330-420			
460	425 - 510	2000	200	40 K
650	600 - 720	5000		230 K
850	800 - 900	8000	750	400 K

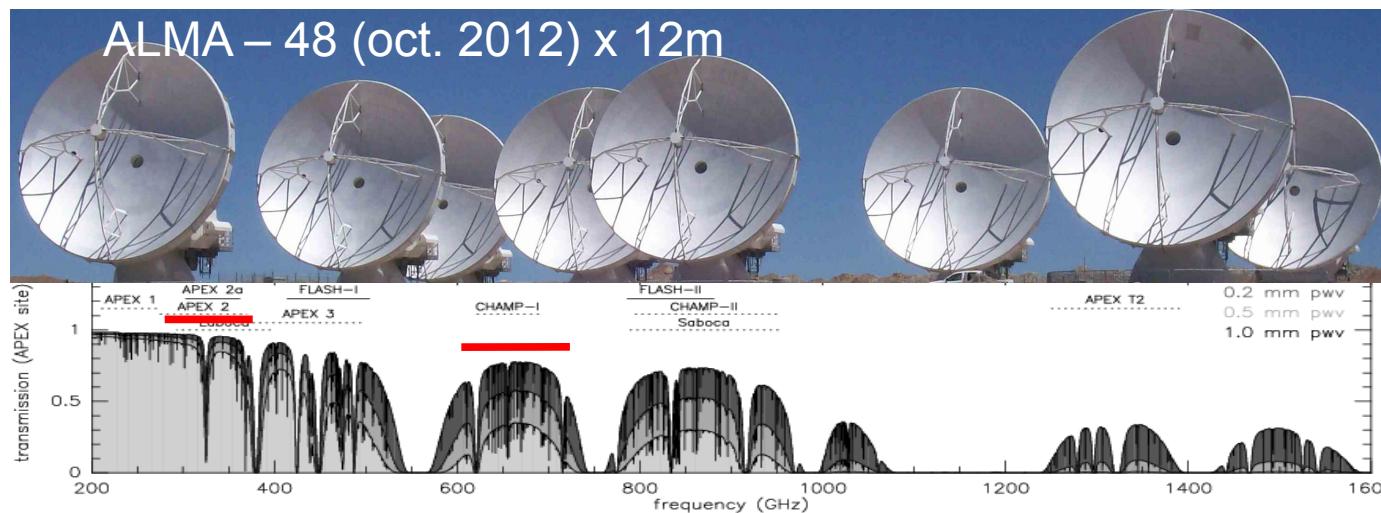


# Telescopes and frequencies (4)



**Herschel HiFi receivers(GHz)**

#1 : 480 – 640
#2 : 640 – 800
#3 : 800 – 960
#4 : 960 – 1120
#5 : 1120 – 1250
#6 : 1410 – 1703
#7 : 1703 – 1910



**ALMA receivers(GHz)**

#3 : 84 - 116
#6 : 211 - 215
#7 : 275 - 373
#9 : 602 - 720

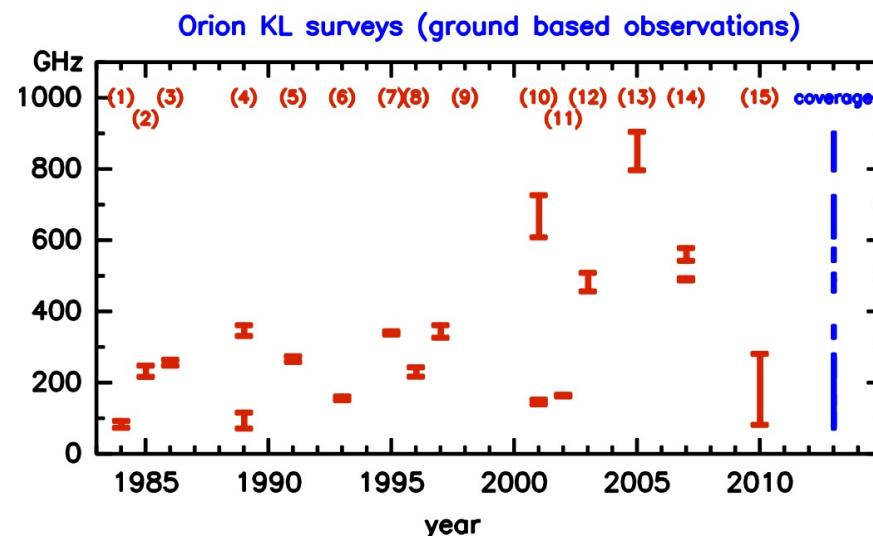


# Prototypical surveys (1)

**Orion K-L: closest massive star forming region, 4 main components**



- > 15 surveys in the mm range published since 1984
- Complete frequency coverage from earth : 72 – 930 GHz
- Herschel survey (HEXOS, ref. 16) : 490-1240, 1430-1900 GHz
- 2D spectral survey IRAM 30m, 200-282 GHz (ref. 17)
- ALMA SV : band #6 (211 – 215 GHz)
- Molecule searches : 29 first identifications

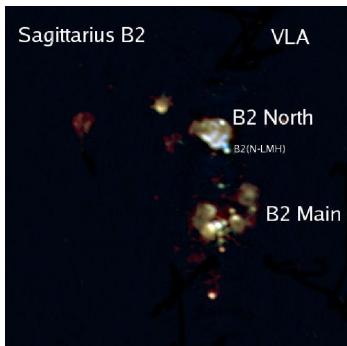


- |                       |                           |
|-----------------------|---------------------------|
| (1) Onsala 20m        | Johansson et al. 1984     |
| (2) OVRO 10.4m        | Sutton et al. 1985        |
| (3) OVRO 10.4m        | Blake et al. 1986         |
| (4) KP 12m            | Turner 1989               |
| (5) JCMT 15m          | Greaves et al. 1991       |
| (6) FCRAO 14m         | Ziurys et al. 1993        |
| (7) JCMT 15m          | Sutton et al. 1995        |
| (8) OVRO Array        | Blake et al. 1996         |
| (9) CSO 10.4m         | Schilke et al. 1997       |
| (10) CSO 10.4m        | Schilke et al. 2001       |
| (11) TRAO 14m         | Lee et al. 2001, 2002     |
| (12) JCMT 15m         | White et al. 2003         |
| (13) CSO 10.4m        | Comito et al. 2005        |
| (14) Odin 1.1m        | Olofsson et al. 2007      |
| (15) IRAM 30m         | Tercero et al. 2010, 2011 |
| (16) Herschel (HEXOS) | Bergin et al 2010         |
| (17) IRAM 30m         | Marcelino et al. 2012     |

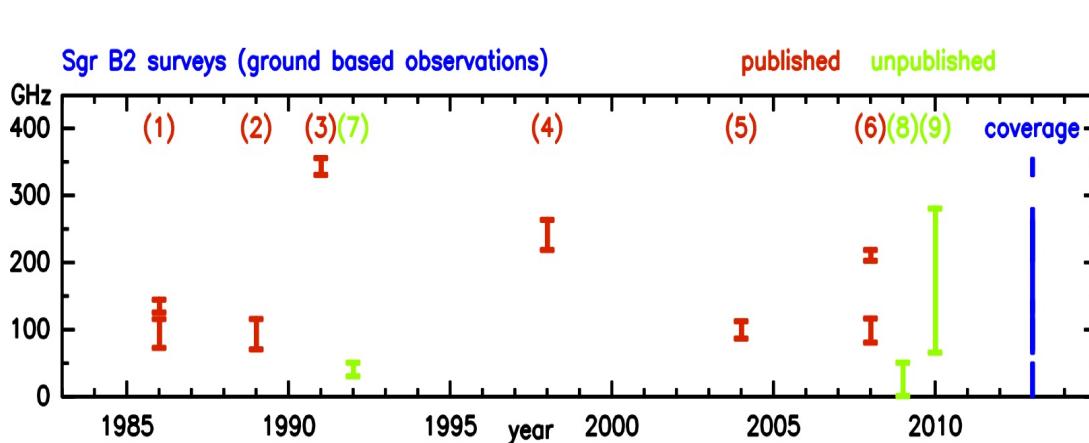


# Prototypical surveys (2)

**SgrB2 : massive star forming region, complex geometry and velocity structures, 2 main cores (M,N), foreground clouds**



- 5 surveys in the mm-range published since 1986
- Almost complete frequency coverage from 72 to 355 GHz
- GBT survey: 0.3-50 GHz (<http://www.cv.nrao.edu/~aremijan/PRIMOS>)
- Herschel survey (HEXOS, ref. 10) : 714 – 801 GHz
- Molecular searches : 66 first identifications



(1) BTL 7m	Cummins et al. 1986
(2) KP 12m	Turner 1989
(3) CSO 10.4m, JCMT 15m	Sutton et al. 1991
(4) SEST 15m	Nummeling et al. 1998
(5) KP 12m	Friedel et al. 2004
(6) IRAM 30m	Belloche et al. 2008
(7) NRO 45m	Ohishi 1992 (unpublished)
(8) GBT 100m	Remijan 2009 (unpublished)
(9) KP 12m	Halfen 2010 (unpublished)
(10) Herschel (HEXOS)	Neill 2012 (unpublished)

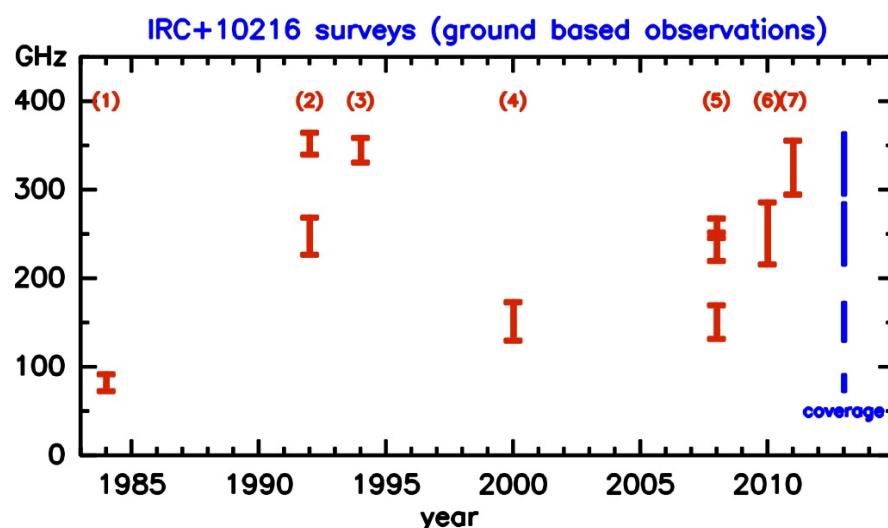


# Prototypical surveys (3)

## IRC+10216 : closest AGB star (C-rich)



- 7 surveys in the mm-range published since 1984
- Frequency coverage from earth : 72 – 364 GHz
- Herschel survey (ref. 8) : 488 to 1901 GHz
- Molecule searches : 42 first identifications



- |                |                        |
|----------------|------------------------|
| (1) Onsala 20m | Johansson et al. 1984  |
| (2) JCMT 15m   | Avery et al. 1992      |
| (3) CSO 10.4m  | Groesbeck et al 1994   |
| (4) IRAM 30m   | Cernicharo et al. 2000 |
| (5) KP 12m     | He et al. 2008         |
| (6) SMT 10m    | Tenenbaum et al. 2010  |
| (7) <b>SMA</b> | Patel et al. 2011      |
| (8) Herschel   | Cernicharo et al. 2010 |



# Prototypical surveys (4)

## IRAS16293-2422 : close low mass binary protostar, prototype of super-deuteration & « hot corino »



- 3 surveys in the mm-range since 1994
- Frequency coverage from earth : 72 – 364 GHz
- Herschel CHESS survey (ref. 4) : 488 to 1901 Ghz
- ALMA SV : band #6 (211 – 215) & band #9 (602 - 720)
- Molecule searches : no first identifications (except D-isotopes)

(1) JCMT 15m, CSO 10.4m Blake et al. 1994  
(3) SMA 8x6m Jorgensen et al. 2011

(2) IRAM 30m, JCMT 15m Caux et al. 2011  
(4) Herschel (CHESS) Ceccarelli et al. 2010

## TMC1 : cold dark cloud, low mass star forming region



- 1 survey in the mm-range published to date (Kaifu et al. 2004)
- Frequency coverage : 8.8 - 50 GHz with NRO 45m
- Molecule searches : 29 first identifications



# Other recent & on going surveys (1)



Herschel HiFi KP

L1544	« Cold » pre-stellar core	→ See also A. Bacmann (poster n°1)
I16293E	« Warm » pre-stellar core	
L1157-B1	outflow shock spot	→ See B. Le Floch 's talk
IRAS 16293	Class 0 low mass protostar	
OMC2-FIR4	Intermediate mass protostar	→ See A. Sepulcre 's poster n°41
AFGL 2591	High mass protostar	
NGC 6334I	High mass protostar	
W51e	High mass protostar	

*The global nightmare !*



**HEXOS** : Herschel HiFi KP : survey of Ori-KL and SgrB2

See also D. Despois (poster n°18)

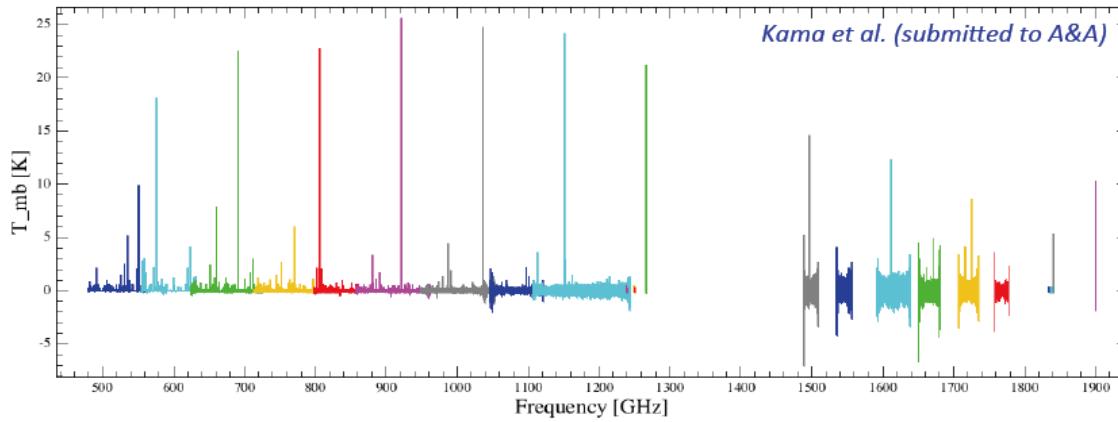
**JCMT Spectral Legacy Survey:** 330-360 GHz 2D + complementary maps 360-373 GHz  
4 targets : Orion Bar, NGC1333-IRAS4A, W49, AFGL2591

**ASAI** : IRAM 30m Large Program (survey on 10 sources) → See this talk

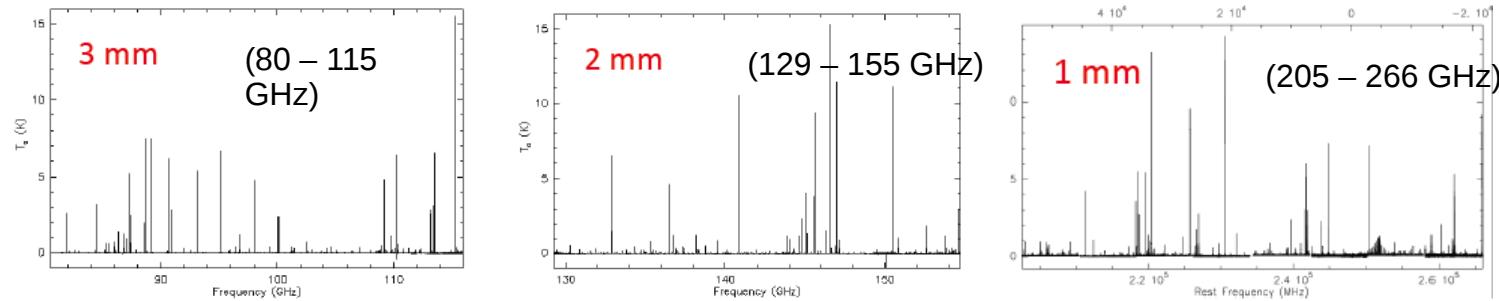


# OMC2 – FIR4 surveys

## CHESS HiFi survey



718 lines identified :  
 58% from CH<sub>3</sub>OH ! 10%  
 from H<sub>2</sub>CO !  
 26 species (+ 14 isotopes)  
 Eup = 24 – 752 K  
 Several kinematical  
 components

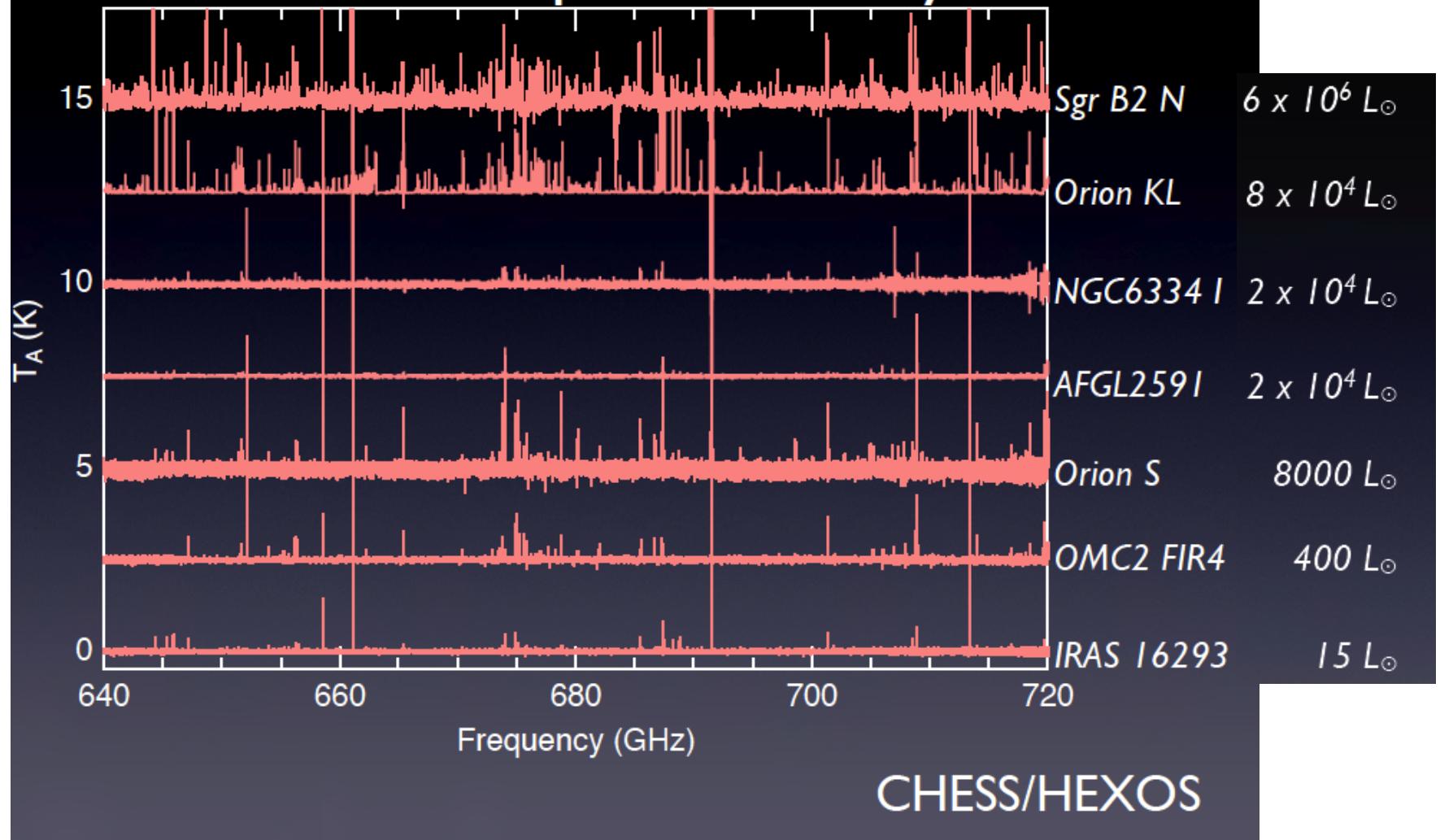


## IRAM 30-m spectral survey

(A. López-Sepulcre et al., in preparation)



## Herschel Spectral Surveys





# Other recent & going on surveys (2)

## Galactic surveys

- The Horsehead WHISPER line survey
- Ultra compact HII region (MonR2) : IRAM 30m, 1mm & 2mm survey  
(Ginard et al. 2012)
- NRO 45m line surveys in the 3mm range : low mass protostars  
(L1157B1, L1527), IR dark cloud (G28.34+0.06)

See Gratier's talk and  
→ V. Guzman's poster n°30

## Extra Galactic surveys

- Starburst galaxy (NGC 253) : IRAM 30m, 2mm survey (Martin et al. 2006)
- ULIR galaxy (Arp 220) : SMA, 1mm survey (Martin et al. 2011)
- Starburst galaxy (M82) : IRAM 30m, 1mm & 2mm survey (Aladro et al. 2011)
- NRO 45m line survey in the 3mm range : NGC 1068, NGC 253.



# Species identification (1)

**From a small number of lines** ... can still be efficient when

- Lines are strong ... or S/N large
- Lines are isolated ... or good spectral resolution available
- Molecular spectrum is simple ... or spectroscopy well known

- **Exemple of C<sub>5</sub>H** (IRC+10216, Cernicharo et al. 1986)

Telescope

- Prediction
- Observations
- Confirmation

Chemistry

C<sub>5</sub>H is likely to be **abundant** enough  
**accurate spectrum** can be predicted

6 doublets (2 partially blended) : « **tentative** » detection

Spectroscopy

**Laboratory** observation of C<sub>5</sub>H spectrum

**Additional** space observations (more lines, different source)

- Recent exemples : anions identification

C<sub>6</sub>H<sup>-</sup> : identification in 2006, but 1st observation in 1995 (« B1335 ») ; C<sub>4</sub>H<sup>-</sup> (2007),  
C<sub>8</sub>H<sup>-</sup> (2007), C<sub>3</sub>N<sup>-</sup> (2008), C<sub>5</sub>N<sup>-</sup> (2008). cf. posters : K. Béroff (n°2), L. Biennier (n°5)  
F. Lique (n°41)



# Species identification (2)

**From a large number of lines** ... is more and more often mandatory because, for not yet identified species,

- Lines are weak ... or S/N low
  - Lines are blended ... or spectral resolution limited
  - Molecular spectrum is complex ... and spectroscopy tricky

## Exemple of acetone ( $\text{CH}_3)_2\text{CO}$

**15 yrs !**

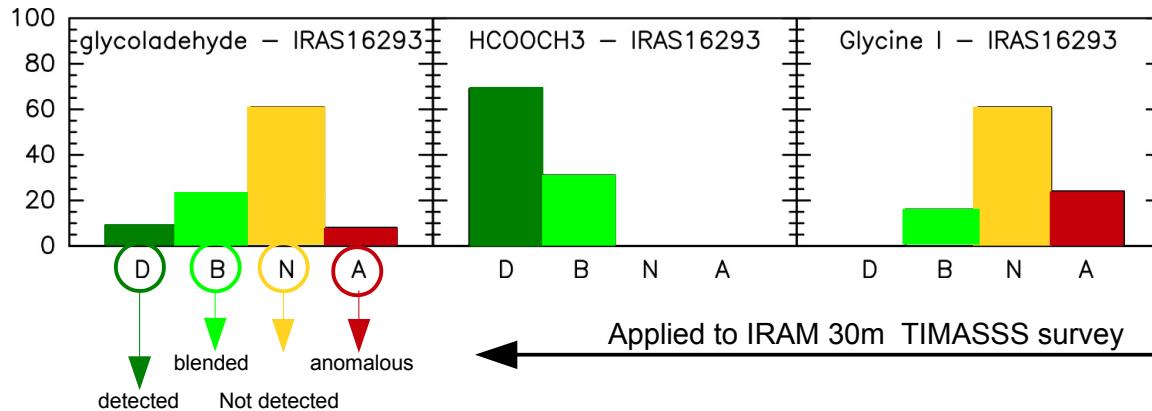
- 1987 (Combes et al.) lab. frequencies ; 4 lines (IRAM30m, KP12m) : **detection**  
LTE model : abundance  $5 \cdot 10^{-11}$  ; formation :  $\text{CH}_3^+ + \text{CH}_3\text{CHO}$
  - 1990 (Herbst et al.) : new calculations + measurements of the rate  
reaction too slow / observed abundance ; role of **grain chemistry** ?
  - 2002 (Snyder et al.) : new measured + calculated frequencies  
32 new lines (KP12 m + BIMA) : **confirmation** of identification
  - 2008 ... Torsional states, **spectro**, **telescope** formation in plasma decharge ...



# Species identification (3)

- LTE modelisation of molecular emission : which detection criterion ?

ex : glycolaldehyde ((HCOCH<sub>2</sub>OH) in IRAS 16293-2422

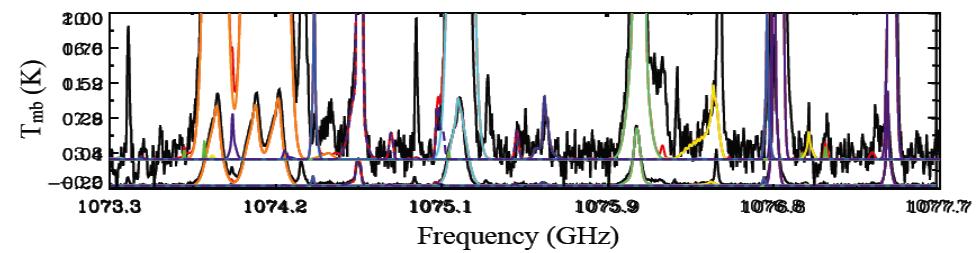
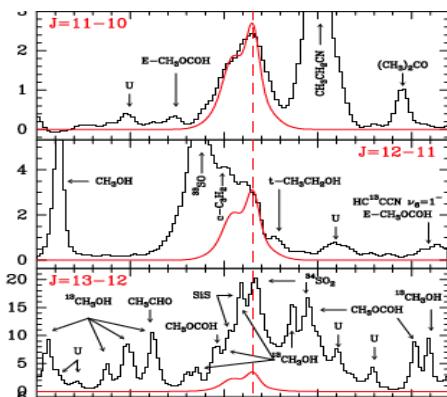


glycolaldehyde detection ?

- 2000 SgrB2 : 6 +/- blended lines (KP12m)
- 2001 SgrB2 : Extended emission of 1 line (BIMA)
- 2003 SgrB2 : predicted lines are missing (KP12m)  
Ori : 8 lines but doubtful extrapolated freq.
- 2004 SgrB2 : 40 lines observed (KP12m) :  
8 lines D (20%) ; 32 lines B + N (80%).
- 2008 GC MC : detection of 3 lines / 4 observed freq.
- 2009 Hot core : 2 or 3 detections / 3 observed freq.
- 2012 IRAS16293 : detection of 13 transitions (ALMA)  
LTE modelling

- Global modelisation : multiple components / species (cf. J. Cernicharo's talk)

SiS in Orion-KL  
(IRAM 30m survey)  
Modeling :  
Hot core (LTE) +  
plateau (LVG) +  
narrow feature (LVG)  
from Tercero et al. 2011

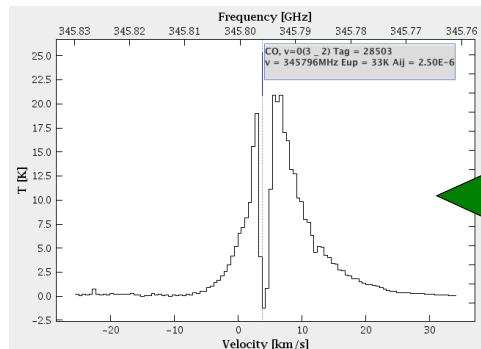


HEXOS survey in Orion-KL : detail of Band 4b  
Simultaneous modeling of 64 species (isotopes included)  
Here : CH<sub>3</sub>OH, SO<sub>2</sub>, <sup>33</sup>SO<sub>2</sub>, SO, C<sub>2</sub>H<sub>5</sub>OH, CH<sub>3</sub>OCH<sub>3</sub>, CS, H<sub>2</sub>CS, HNCO  
from Crockett 2012 (Herschel meeting in Grenoble)



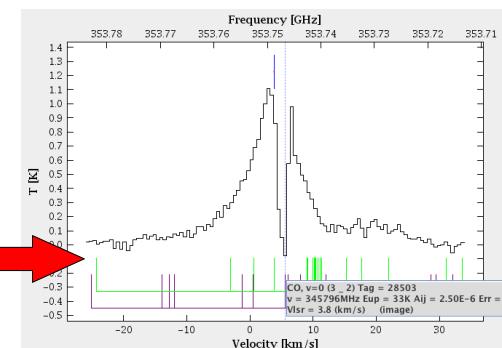
# Species identification (4)

## Some frequent tricks



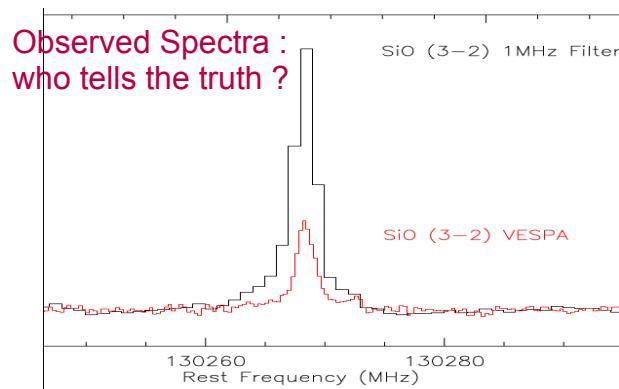
### Lines from the image band

With a rejection of 13dB ...  
a line of 20 K in the signal band  
is a line of 1 K in the image band !  
*Shifted spectra are useful !*

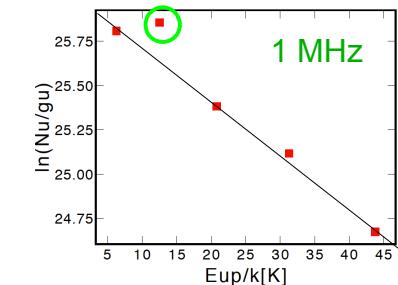
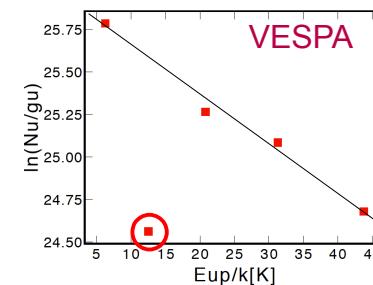


### Calibration problems

not always easy to detect and solve !  
*Calibrators are useful !*



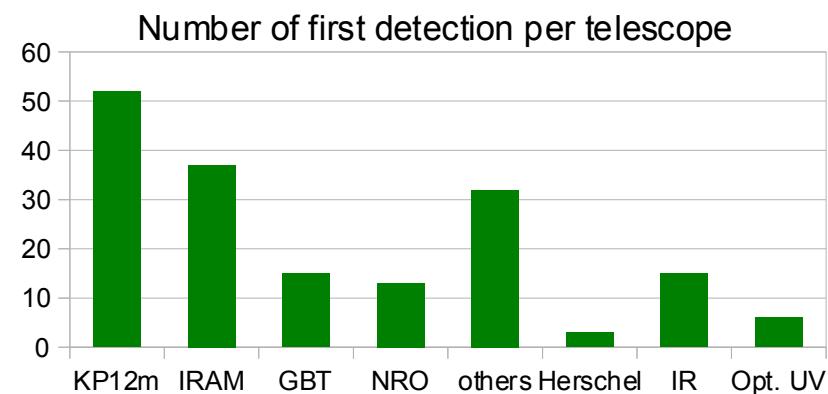
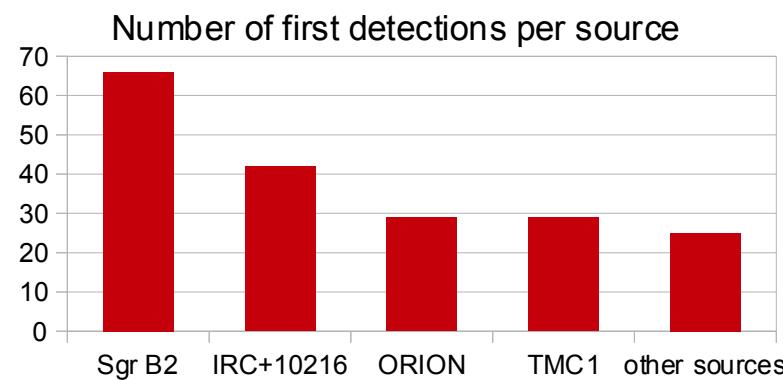
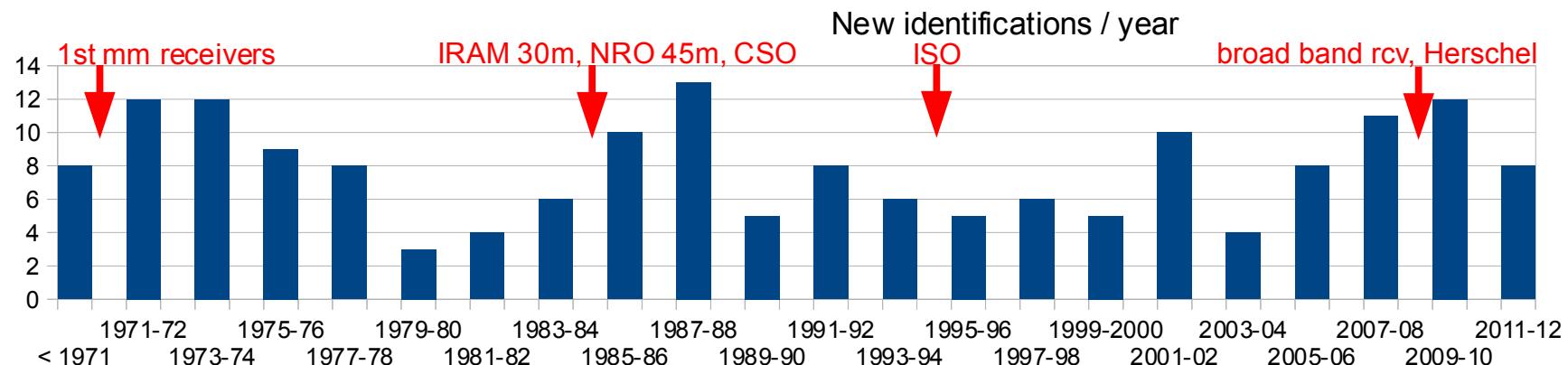
LTE modeling  
(Rotational diagrams)  
helps to know  
(not always so simple!)





# Galactic molecular census (1) (oct 2012)

## Methods : survey or / and dedicated observations





# Galactic Molecular Census (2)

(173 detections, oct. 2012)

Molecules in the Interstellar Medium or Circumstellar Shells (as of 10/2012)												
2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	13 atoms	
38	36	24	20	16	9	10	9	4	3	3	1	
CH	H <sub>2</sub> O	NH <sub>3</sub>	HC <sub>3</sub> N	CH <sub>3</sub> CN	CH <sub>3</sub> CHO	HC(O)OCH <sub>3</sub>	(CH <sub>3</sub> ) <sub>2</sub> O	CH <sub>3</sub> C <sub>5</sub> N	HCSN	c-C <sub>8</sub> H <sub>6</sub> *	HC <sub>11</sub> N	
CH+	HCN	H <sub>2</sub> CO	HCOOH	CH <sub>3</sub> OH	CH <sub>3</sub> NH <sub>2</sub>	CH <sub>3</sub> C <sub>3</sub> N	CH <sub>3</sub> CH <sub>2</sub> OH	(CH <sub>3</sub> ) <sub>2</sub> CO	CH <sub>3</sub> C <sub>6</sub> H	C <sub>2</sub> H <sub>5</sub> OCH <sub>3</sub> ?		
CN	OCS	HNCO	H <sub>2</sub> CNH	NH <sub>2</sub> CHO	CH <sub>2</sub> CHCN	CH <sub>3</sub> COOH	CH <sub>3</sub> CH <sub>2</sub> CN	(CH <sub>2</sub> OH) <sub>2</sub>	C <sub>2</sub> H <sub>5</sub> OCHO	n-C <sub>3</sub> H <sub>7</sub> CN		
OH	H <sub>2</sub> S	H <sub>2</sub> CS	H <sub>3</sub> NCN	CH <sub>3</sub> SH	HC <sub>5</sub> N	C <sub>7</sub> H	HC <sub>7</sub> N	CH <sub>3</sub> CH <sub>2</sub> CHO				
CO	HNC	C <sub>2</sub> H <sub>2</sub> *	H <sub>2</sub> C <sub>2</sub> S	C <sub>2</sub> H <sub>4</sub>	CH <sub>3</sub> C <sub>2</sub> H	C <sub>6</sub> H <sub>2</sub>	CH <sub>3</sub> C <sub>4</sub> H					
SiO	HNO	HNC <sub>5</sub>	C <sub>4</sub> H	C <sub>5</sub> H	C <sub>8</sub> H	-HC <sub>8</sub> H *	C <sub>8</sub> H					
CS	C <sub>2</sub> H	C <sub>3</sub> N	CH <sub>4</sub> *	CN <sub>3</sub> NC	c- <sub>2</sub> H <sub>4</sub> O	CH <sub>2</sub> CHCHO (?)	CH <sub>3</sub> C(O)NH <sub>2</sub>					
H <sub>2</sub>	HCO+	HOCO+	SiH <sub>4</sub> *	HC <sub>2</sub> CHO	H <sub>2</sub> CCOH	CH <sub>2</sub> CCHCN	C <sub>8</sub> H-					
SO	N <sub>2</sub> H <sub>2</sub>	C <sub>3</sub> O	c-C <sub>3</sub> H <sub>2</sub>	L-H <sub>2</sub> O <sub>4</sub>	C <sub>8</sub> H-	H <sub>2</sub> NCH <sub>2</sub> CN	P <sub>3</sub> H <sub>6</sub>					
HD	SO <sub>2</sub>	I-C <sub>3</sub> H	H <sub>2</sub> CCN	HC <sub>3</sub> NH <sub>2</sub>			CH <sub>2</sub> ORCHO					
NS	HCS	HCN <sub>2</sub>	HCN <sub>2</sub> +	C <sub>5</sub> *	C <sub>5</sub> N							
SiS	c-SiC <sub>2</sub>	H <sub>3</sub> O+	C <sub>4</sub> Si	I-HC <sub>4</sub> H	*							
C <sub>2</sub> **	C <sub>2</sub> O	c-C <sub>3</sub> H	I-C <sub>3</sub> H <sub>2</sub>	I-HC <sub>4</sub> N								
NO	HCO	C <sub>3</sub> S	HC <sub>2</sub> NC	c-H <sub>2</sub> C <sub>3</sub> O								
HC	Mg <sub>2</sub> N	HCCN	HNC <sub>3</sub>	H <sub>2</sub> CC <sub>2</sub> NH (?)								
Al	C <sub>2</sub> S	H <sub>2</sub> CN	H <sub>2</sub> COH <sub>2</sub>	C <sub>5</sub> N-								
HCl	C <sub>3</sub> *	c-SiC <sub>3</sub>	C <sub>4</sub> H-									
CI	CO <sub>2</sub> *	CH <sub>3</sub> *	HC(O)CN									
NaCl	NH <sub>2</sub>	C <sub>3</sub> N-	HNCNH									
PN	N <sub>2</sub> O	PH <sub>3</sub> ?	CH <sub>3</sub> O									
SiC	NaCN	HCNO										
CP	CH <sub>2</sub>	HOCH										
NH	HOC+	HSCN										
SO+	MgCN	H <sub>2</sub> O <sub>2</sub>										
SIN	H <sub>2</sub> D+											
CO+	SiCN											
HF	AlNC											
SiH ?	SiNC											
FeO ?	HCP											
D <sub>2</sub>	CCP											
CF+	AlOH											
PO	H <sub>2</sub> O <sub>2</sub>											
AlO	H <sub>2</sub> C <sub>2</sub> +											
OH+	KCN											
CN-	eCN											
SH+	HO <sub>2</sub>											
SH												
HCl+												

Complex Organic Molecules « COMs »

metal-bearing

Carbon chains

anions

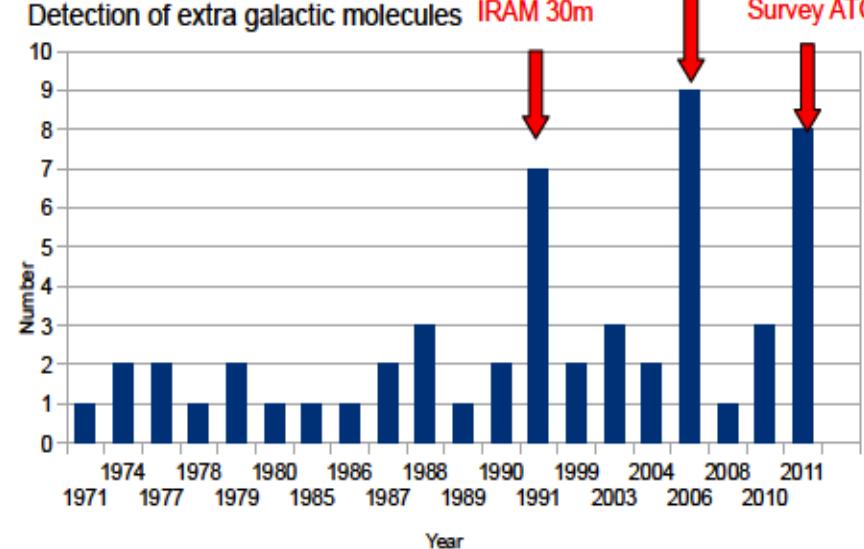
Orion      IRC+10216  
 SgrB2      TMC1  
 Orion + SgrB2      IRC + TMC1



# Extra galactic molecular census

(54 at the end of 2011)

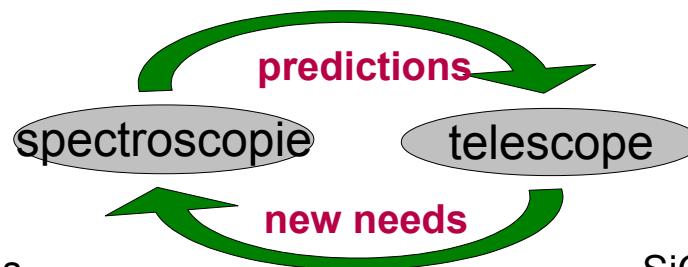
<b>2 atoms</b>	date	<b>3 atoms</b>	date	<b>4 atoms</b>	date	<b>5 atoms</b>	date	<b>6 atoms</b>	date	<b>7 atoms</b>	date	<b>8 atoms</b>	date	<b>&gt;8 atoms</b>	date
16		13		9		8		3		3		1		1	
OH	1971	H2O	1977	H2CO	1974	c-C3H2	1986	CH3OH	1987	CH3CCH	1991	HC6H	2006	c-C6H6 *	2006
CO	1974	HCN	1977	NH3	1979	HC3N	1990	CH3CN	1991	CH3NH2	2011				
H2 *	1978	HCO+	1979	HNCO	1990	CH2NH	2006	HC4H *	2006	CH3CHO	2011				Survey NGC253 IRAM 30m
CH	1980	C2H	1988	C2H2 *	1999	NH2CN	2006								
CS	1985	HNC	1988	H2CS ?	1999	I-C3H2	2011								Detection of extra galactic molecules IRAM 30m
CH+ **	1987	H2S	1989	HOCO+	2006	H2CCN	2011								
CN	1988	N2H+	1991	c-C3H	2006	H2CCO	2011								
SO	1991	OCS	1991	H3O+	2008	C4H	2011								
SiO	1991	HCO	1991	I-C3H	2011										
NO	2003	SO2	2003												
NS	2003	HOC+	2004												
NH	2004	C2S	2006												
CO+	2006	H2O+	2010												
OH+	2010														
HF	2010														
SO+	2011														



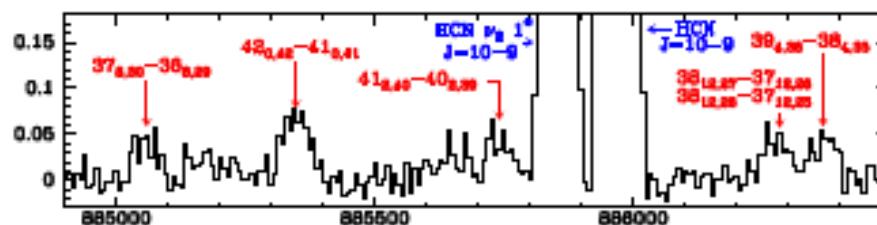


# What can we learn from surveys ? (1)

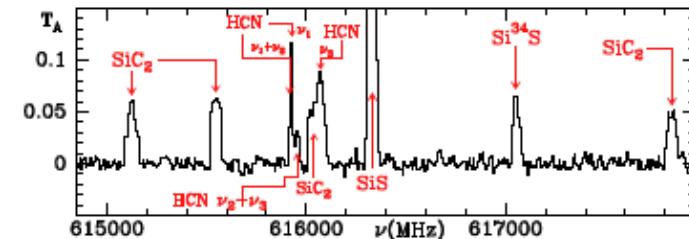
- **Line frequencies** (see also J. Cernicharo's talk)



$\text{CH}_3\text{CH}_2\text{CN}$  excited lines  
in Orion (HEXOS) *Muller et al. 2012*



$\text{SiC}_2$  lines in IRC+10216  
(Herschel-HiFi) *Cernicharo et al. 2010*



<b>Need for</b>	- New species frequencies (including isotopes) - High excitation frequencies (torsion, vibration)	poster n°7 A. Bouchez-Giret
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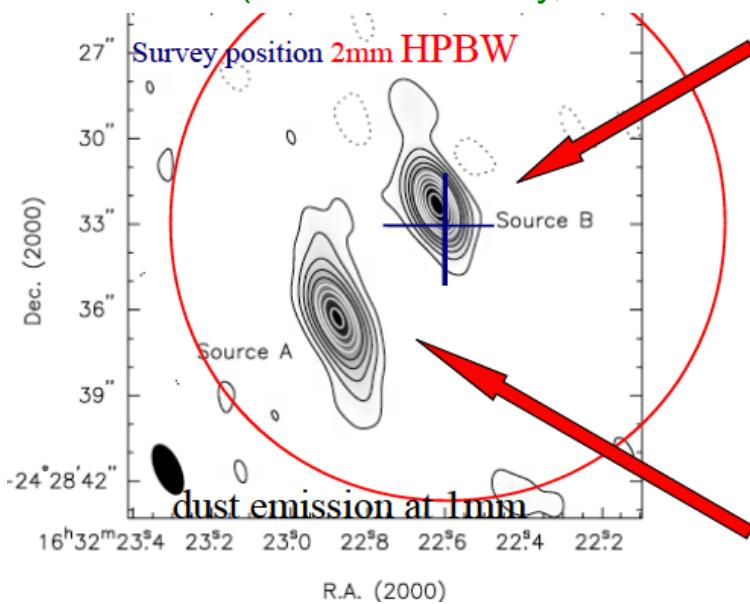


# What can we learn from surveys ? (2)

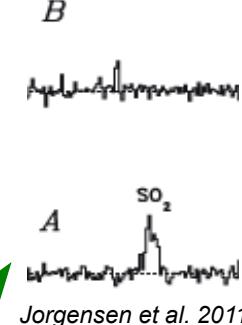
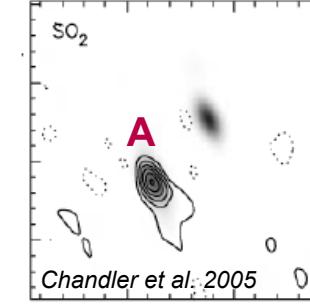
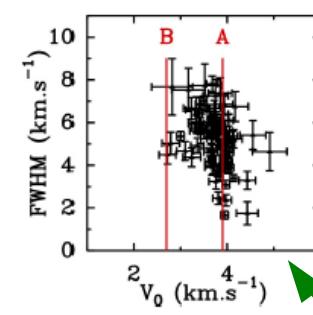
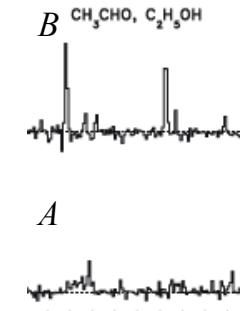
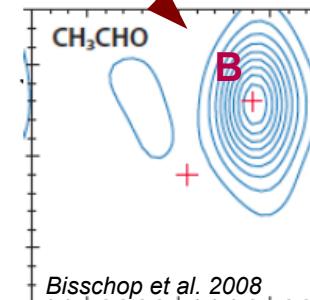
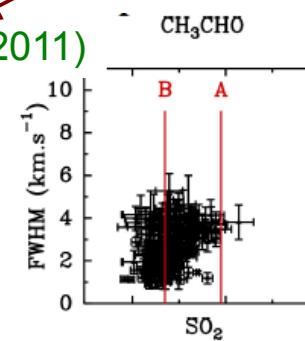
- **Gas kinematics** (see also B. Lefloch's talk)

*Super spectral and spatial resolutions !*

IRAS16293 (TIMASSS survey, Caux et al. 2011)



Origin of dominant emission



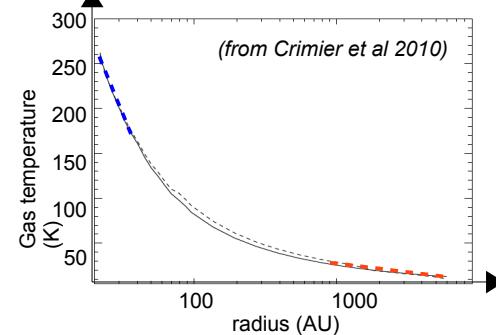
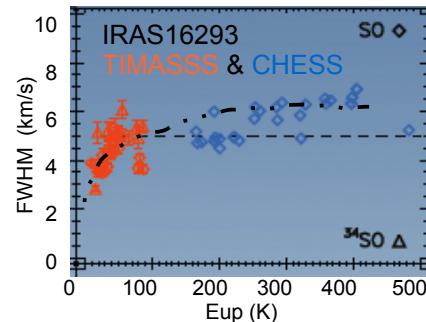
Line kinematical signature



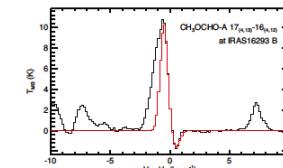
# What can we learn from surveys ? (3)

- **Gas excitation and dynamics** (see also B. Lefloch's talk)

**IRAS16293 : free fall hot corino ? Rotating disk ?**



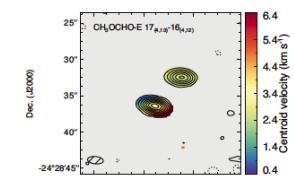
**ALMA SV (band 6)**



Core B : inverse  
P Cygni = free fall

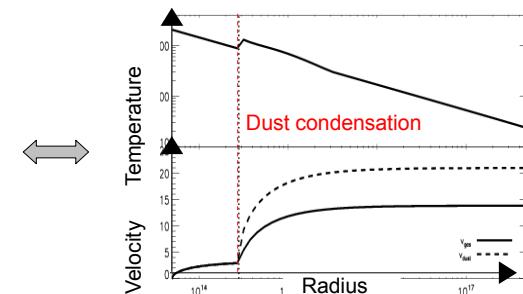
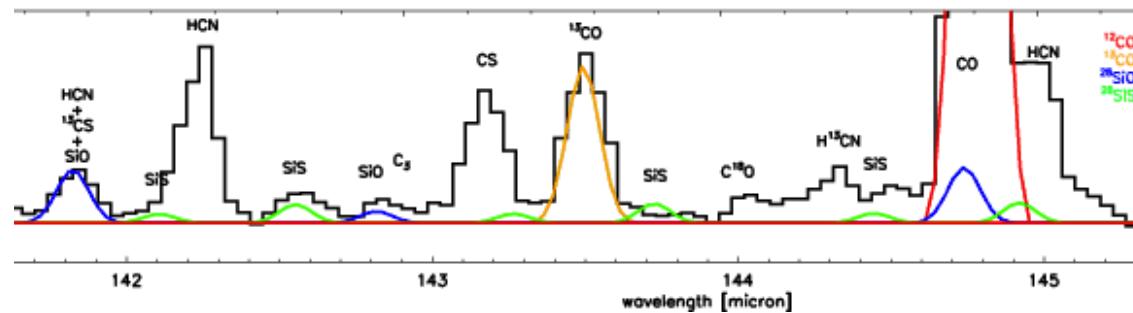
Core A : velocity gradient  
rotating disk ?

(Pineda et al 2010)



**Multi line modeling may help to estimate the source size**

**Gas acceleration in the inner envelope of IRC+10216**



from Decin et al 2010, Herschel « MESS » KP



# What can we learn from surveys ? (4)

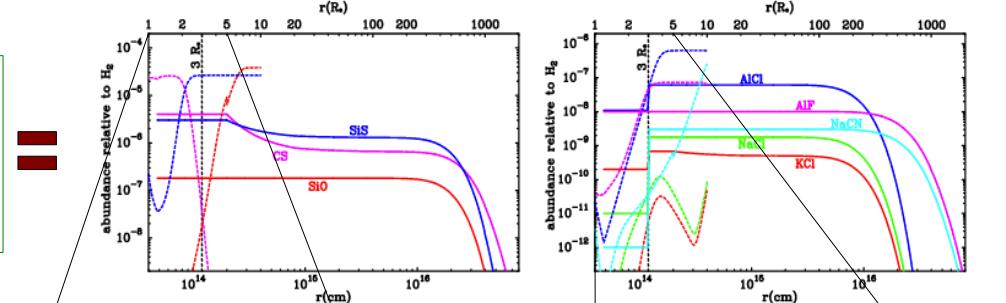
- Molecular abundances & chemistry**

## IRC+10216 – IRAM 30m survey (80 – 357.5 GHz)

(Agundez et al. 2012)

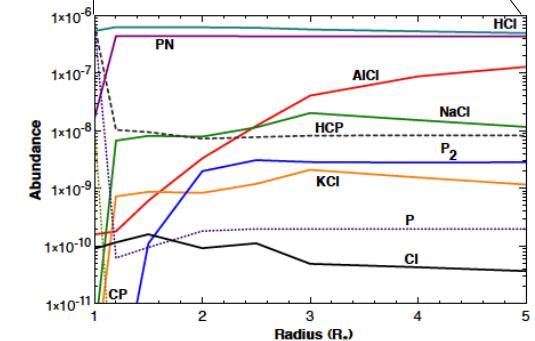
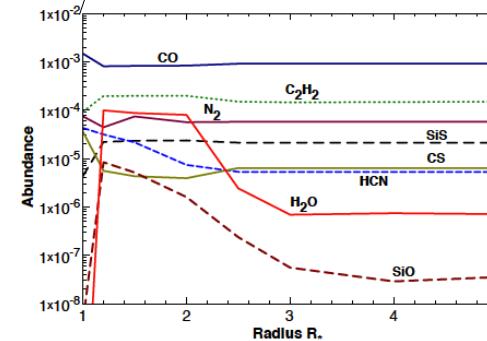
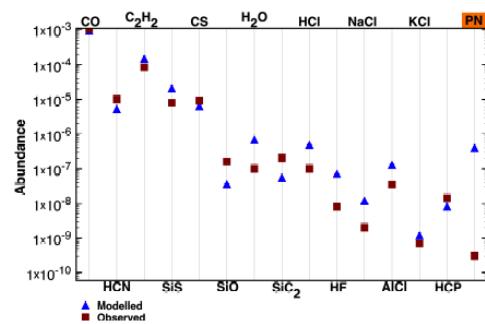
CS, SiO, SiS, NaCl, KCl, AlCl, AlF, NaCN observations of rotational lines  $v=0, v=1, v=2, v=3$

+ LVG modeling including  
Inelastic collision rates  
Infra red pumping  
Rotational transitions & ro-vibration transitions



## Inner wind chemistry (Cherchneff 2012)

- Model : shock induced non equilibrium chemistry ( $1R_*$  to  $5R_*$ )
- Results : very good agreement with abundances derived from surveys

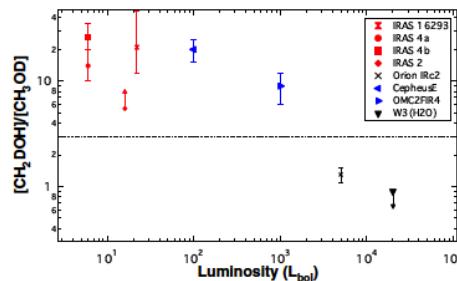




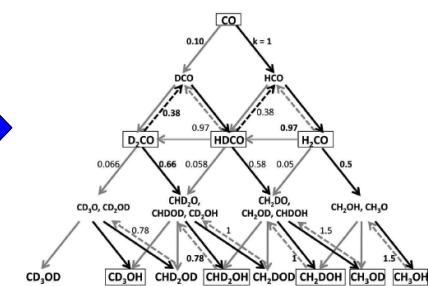
# What can we learn from surveys ? (5)

- ## • Isotopic ratios & chemistry (see also V. Taquet's talk)

## Methanol D/H ratio

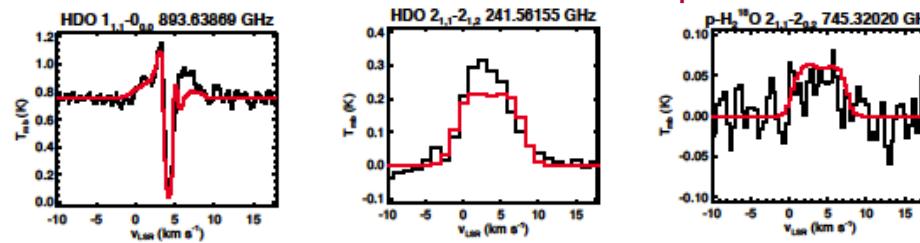


## Laboratory experiments on gas-surface exchanges



#### Observations (*from Ratajczak et al. 2011*)

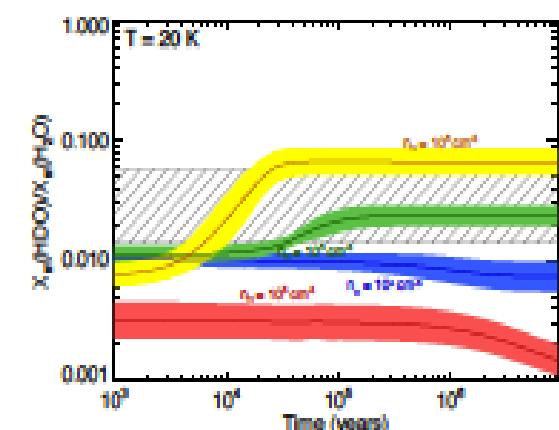
**Water D/H ratio in IRAS16293** Cf. aussi poster A. Coutens (n°14)



## Collision rates

	Hot corino		Outer envelope		Photodesorption layer
	Best fit	$3\sigma$	Best fit	$3\sigma$	$A_V \sim 1 - 4 \text{ mag}$
HDO	$1.7 \times 10^{-7}$	$1.5 - 2.2 \times 10^{-7}$	$8 \times 10^{-11}$	$4.6 - 10.0 \times 10^{-11}$	$\sim 0.6 - 2.4 \times 10^{-8}$
H <sub>2</sub> O	$5 \times 10^{-6}$	$3.8 - 10.5 \times 10^{-6}$	$1.5 \times 10^{-8}$	$4.5 - 24.5 \times 10^{-9}$	$\sim 1.3 - 5.3 \times 10^{-7}$
HDO/H <sub>2</sub> O	3.4%	1.4% - 5.8%	0.5%	0.2% - 2.2%	$\sim 4.8\%^a$

CHESS and TIMASSS observations (*from Coutens et al. 2012*)



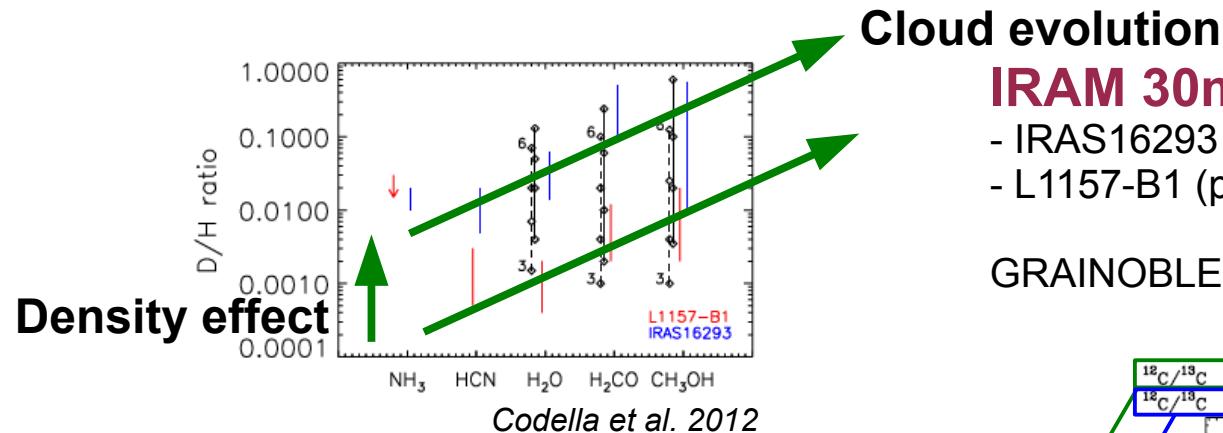
Gas-Grain chemistry (from Taquet et al. 2012c)



# What can we learn from surveys ? (6)

- Abundances & source history**

## D/H ratios as star formation fossils



## IRAM 30m + CHESS surveys

- IRAS16293 (hot corino)
- L1157-B1 (pre shock gas)

+

GRAINOBLE chemical model

## 12C/13C ratios as AGB evolution tracers

### IRAM 30m survey of CRL 618

80-116 GHz, 131-179 GHz, 204-275 GHz.

AGB star

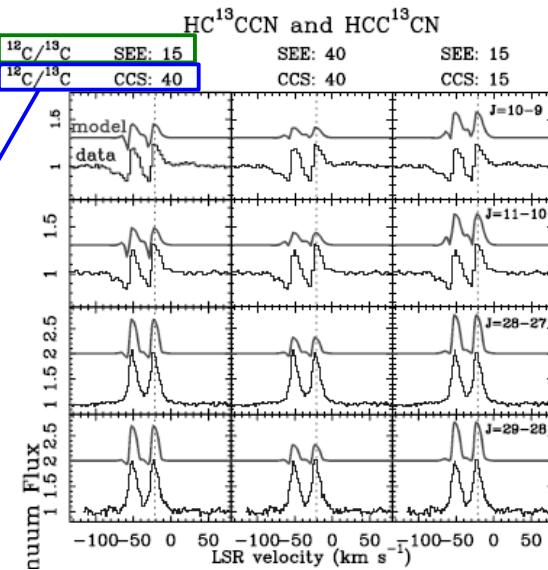
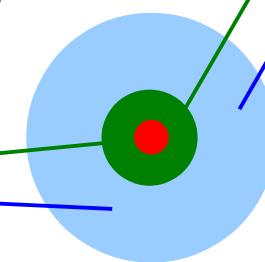
LTE modeling with 2 components

13C enrichment  
By AGB pulse ?

SEE : slowly expanding envelope

CCS : cold circumstellar shell

(Pardo et al. 2004, 2005, 2007)

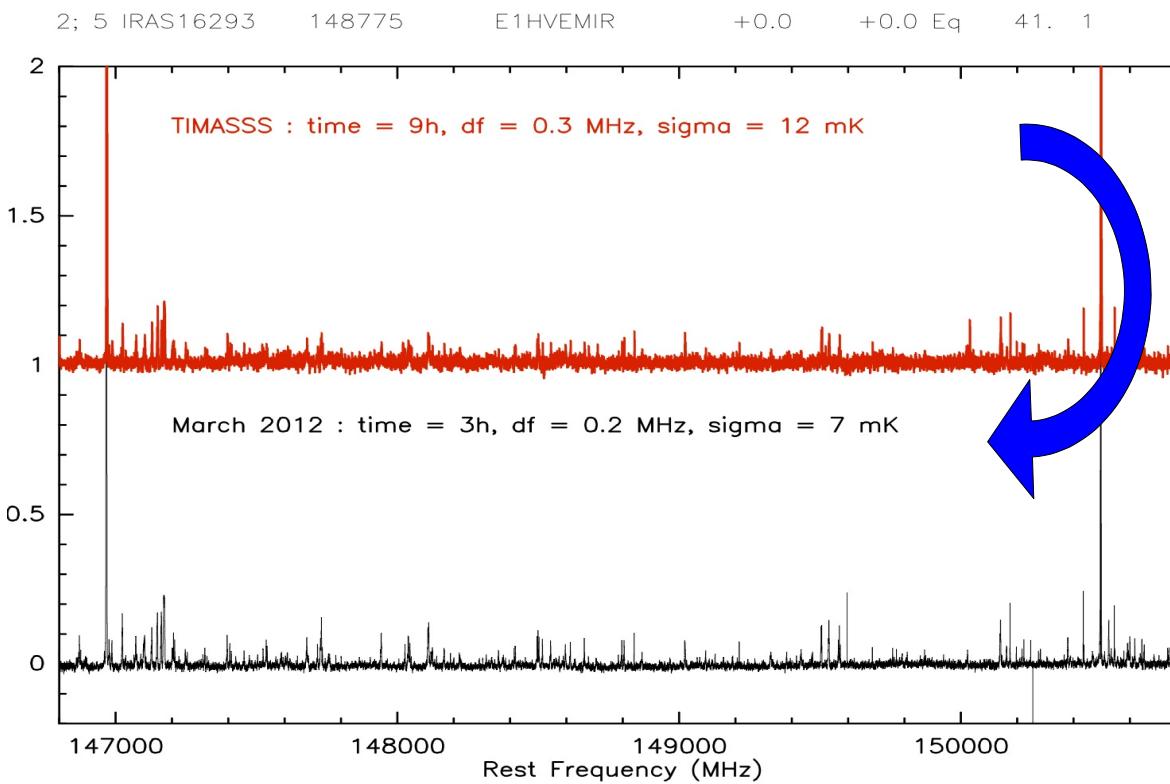




# Perspectives and Prospective (1)

- **Spectral surveys on many more objects**

Huge gains in receivers sensitivity and band widths



IRAM 30m telescope  
from 2005 to 2012,

gain of a factor 12 !

in integration time for  
the same resolution,  
the same bandwidth  
the same sensitivity



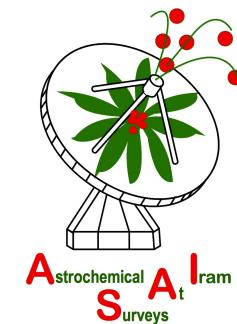
# Perspectives and Prospective (2)

## Astrochemical Surveys At IRAM 30m (ASAI)

*A Legacy Chemical Survey of Star-Forming Regions to study the evolution  
of molecular complexity in protostellar environments*

Large Program (338h, 4 semesters) ; French (Lefloch) & Spanish (Bachiller) PI-ship  
36 participants from 11 institutes : France (20), Spain (9), others (7)

Goal : unbiased surveys (80-280 Ghz), rms=6mK for dV=1km/s (0.25km/s for PSC)  
10 targets sampling different stages of solar-type star formation



Type	Source	Ref.	d (pc)	L ( $L_{\odot}$ )	3mm	2mm	1.3mm	Herschel	Comment
Class 0	L1544	1	140	-	X	-	-	C, W	Evolved: high deuterium
	TMC1	2	140	-	done	X	-	OT1	Young: hydrocarbon rich
	B1	3	200	-	X	X	X	-	Early: no outflow, high deuterium
	IRAS4A	4	250	7.7	X	X	X	C,OT1	Hot Corino
	L1527	5	140	2	done	X	X	W	WCCC
Class I	L1157mm	6	250	4	done	done	X	W	WCCC ? comparison with B1
	SVS13A	7	250	43	X	X	X	W	Evolved
Class I-II	AB Aur	8	145	-	X	X	X	OT1	residual envelope, warm disk
Jet	L1448	9	250	(11.6)	X	X	X	W,OT1	EHV bullets
Bowshock	L1157-B1	10	220	(4)	done	X	done	C,W	MHD shock prototype

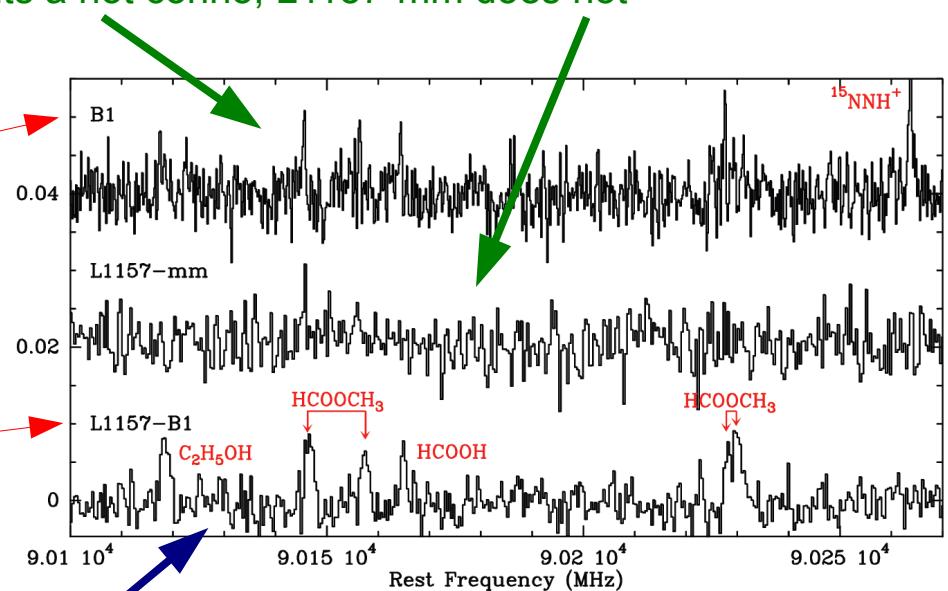
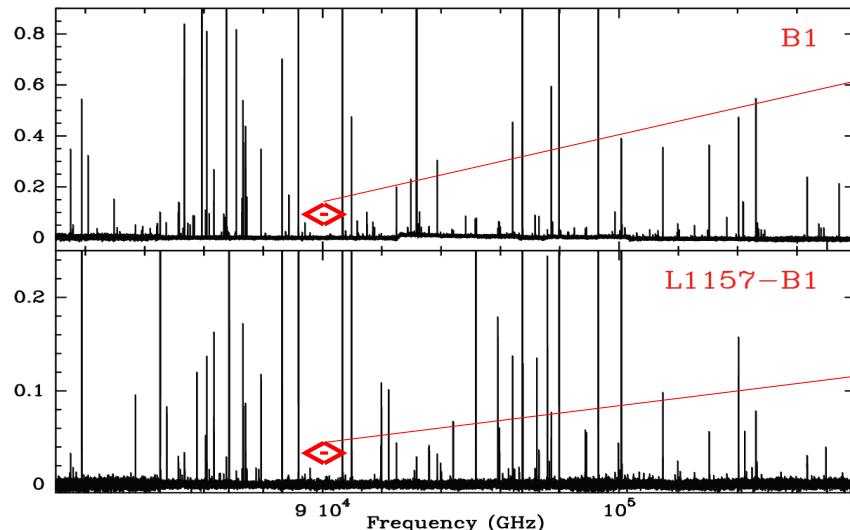


# Perspectives and Prospective (3)

## ASAI first promising results

Aug -Sep 2012 : B1, IRAS4A, L1157mm, L1157-B1, L1527 at 3mm and 2mm

Chemical differentiation between young protostars :  
B1 exhibits a hot corino; L1157-mm does not



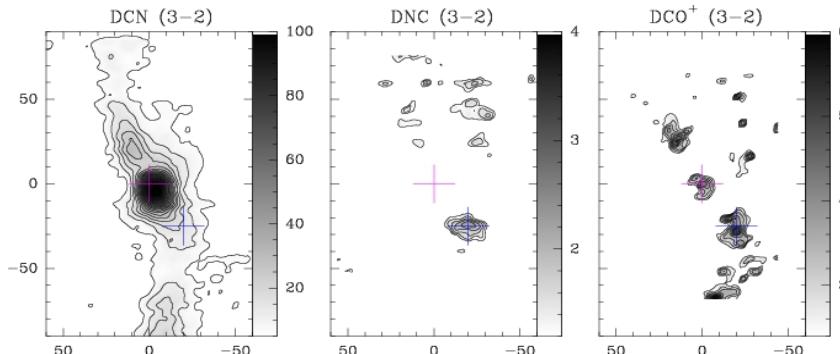
Production of COMs in the protostellar shock L1157-B1



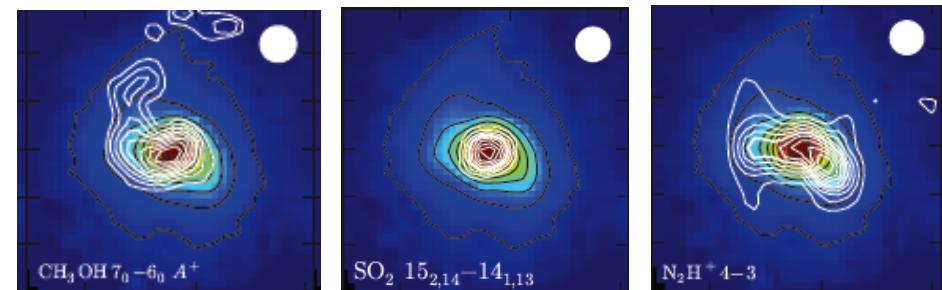
# Perspectives and Prospective (4)

- **Many 2D Spectral surveys become possible**

**Single dish surveys (selected lines mapping) : for extended sources**



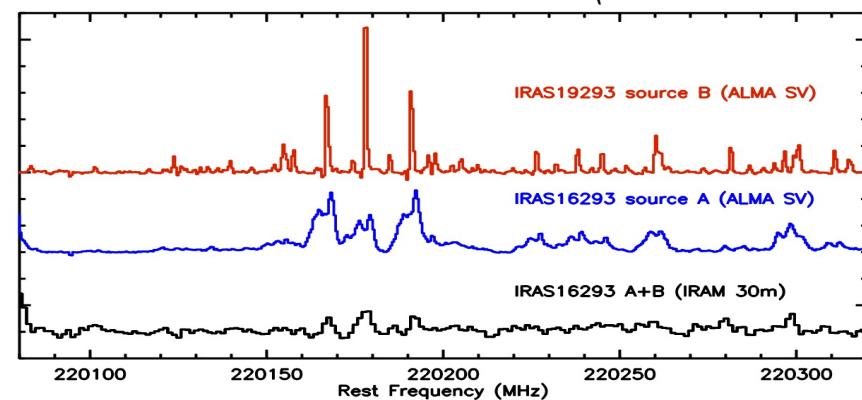
Orion : 2'x2' IRAM 30m survey at 1mm  
(Marcelino et al. 2012)



AFGL2591 : JCMT SLS 2'x2' maps at 330-380 GHz  
(van der Wiel et al. 2011)

**Interferometer surveys :**  
**mandatory for small sources**

→ A lot of projects to come for  
NOEMA, ALMA... !





# Perspectives and Prospective (5)

## Which strategy, why tools to share spectra ?

- Private collaborations : which frame ? financial supports ?
- Public archives : which delay ? (what about IRAM data ?)



**Many Posters to visit !**

### Databases

ML Dubernet n°20, 21

### Collision, reaction rates

Chabot n°11, Capron n°9,  
Denis-Alpizard n°17,  
Dumouchel n°22, Faure n°24  
Hochlaf n°31, Kalugina n°33  
Lanza n°36, Lattelais n°37  
Minisalle n°46, Rist n°55,  
Schneider n°59, Kalugina n°66

### Grain chemistry

Bertin n°4, Bron n°8  
Chaabouni n°10, Congiu n°13,  
Danger n°15, Gavilan n°25, 26  
Noble n°50, Pernet n°51,  
Pilmé n°52, Vinogradoff n°63,  
Teillet-Billy n°61

### Gas chemistry

Ghesquière n°27, Krim n°35,  
LeGal n°39, Mokrane n°47  
Romanzin n°56, Sims n°60  
Thi n°62

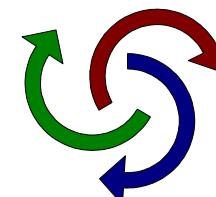
## Which data, which tools to analyze the spectra ?

- Frequency databases (CDMS, JPL, Spatalog, private)
- Spectra analysis tools (CASSIS, CLASS,...)
- Needs for more spectral data



## Which data, which tools to model the lines ?

- Radiative transfer : LTE, LVG codes, 1D to 3D
- Needs for more collision rates



## Which data, which tools to model the chemistry ?

- Chemistry codes : steady-state / time dependant, gas, gas-grain, PDR, shocks...
- Need for reaction rates, radiation / gas / surface interactions

