OAA

Astrochemistry with ALMA: Hot cores and hot corinos

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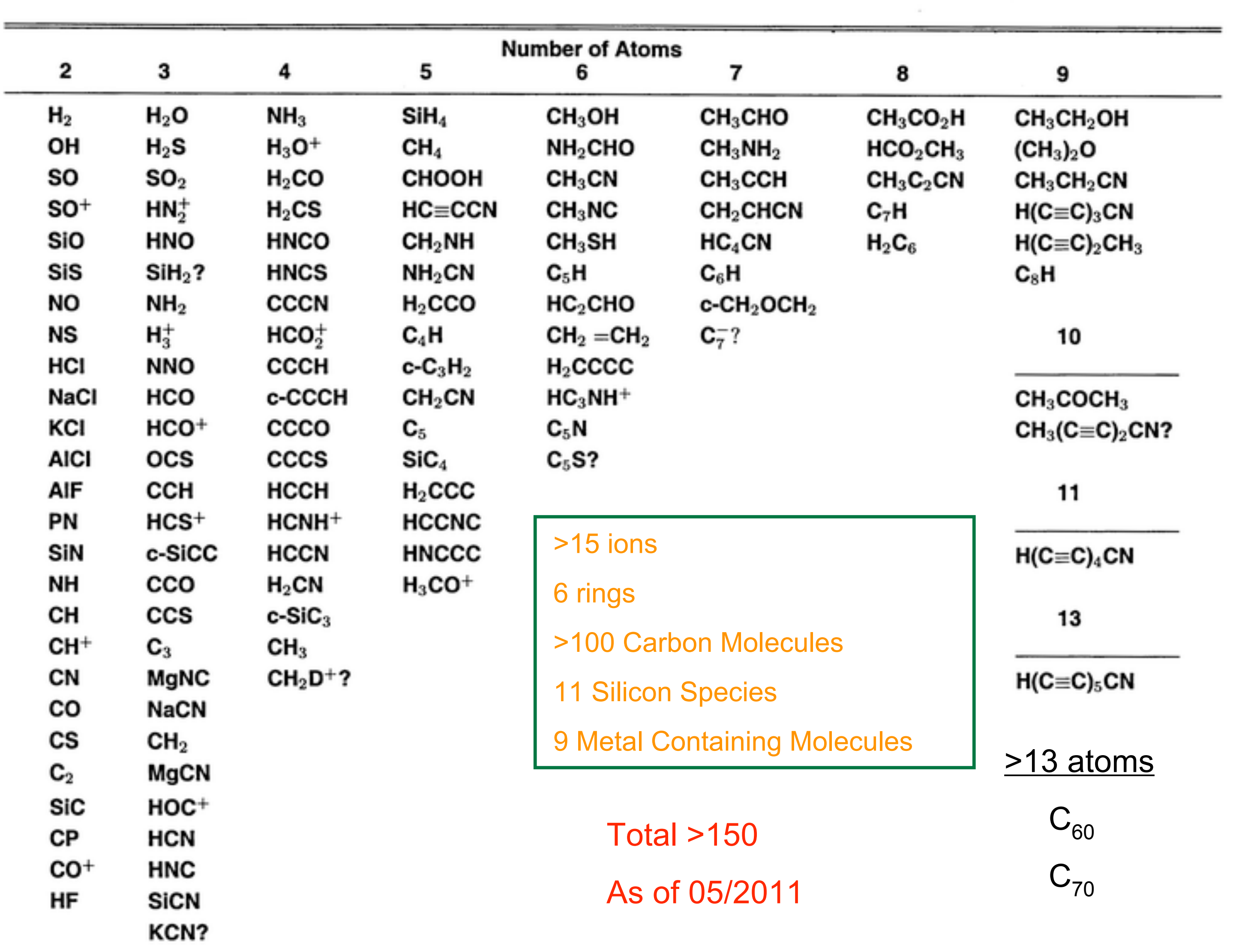
NGC 3603

Interstellar molecules



				Number of Atoms			
2	3	4	5	6	7	8	9
H_2	H_2O	NH_3	SiH_4	CH_3OH	CH_3CHO	CH_3CO_2H	CH_3CH_2OH
OH	H_2S	H_3O^+	CH_4	NH_2CHO	CH_3NH_2	HCO_2CH_3	$(CH_3)_2O$
SO	SO_2	H_2CO	CHOOH	CH_3CN	CH_3CCH	CH_3C_2CN	CH_3CH_2CN
SO^+	HN_2^+	H_2CS	$HC{\equiv}CCN$	CH_3NC	CH_2CHCN	C_7H	$H(C{\equiv}C)_3CN$
SiO	HNO	HNCO	CH_2NH	CH_3SH	HC_4CN	H_2C_6	$H(C{\equiv}C)_2CH_3$
SiS	SiH_2?	HNCS	NH_2CN	C_5H	C_6H		C_8H
NO	NH_2	CCCN	H_2CCO	HC_2CHO	c-CH_2OCH_2		
NS	H_3^+	HCO_2^+	C_4H	$CH_2{=}CH_2$	C_7^-?		**10**
HCl	NNO	CCCH	c-C_3H_2	H_2CCCC			
NaCl	HCO	c-CCCH	CH_2CN	HC_3NH^+			CH_3COCH_3
KCl	HCO^+	CCCO	C_5	C_5N			$CH_3(C{\equiv}C)_2CN$?
AlCl	OCS	CCCS	SiC_4	C_5S?			
AlF	CCH	HCCH	H_2CCC				**11**
PN	HCS^+	$HCNH^+$	HCCNC				
SiN	c-SiCC	HCCN	HNCCC				$H(C{\equiv}C)_4CN$
NH	CCO	H_2CN	H_3CO^+				
CH	CCS	c-SiC_3					**13**
CH^+	C_3	CH_3					
CN	MgNC	CH_2D^+?					$H(C{\equiv}C)_5CN$
CO	NaCN						
CS	CH_2						
C_2	MgCN						
SiC	HOC^+						
CP	HCN						
CO^+	HNC						
HF	SiCN						
	KCN?						

>15 ions

6 rings

>100 Carbon Molecules

11 Silicon Species

9 Metal Containing Molecules

>13 atoms

C_{60}

C_{70}

Total >150

As of 05/2011

http://www.astro.uni-koeln.de/cdms/molecules

Complex organic molecules

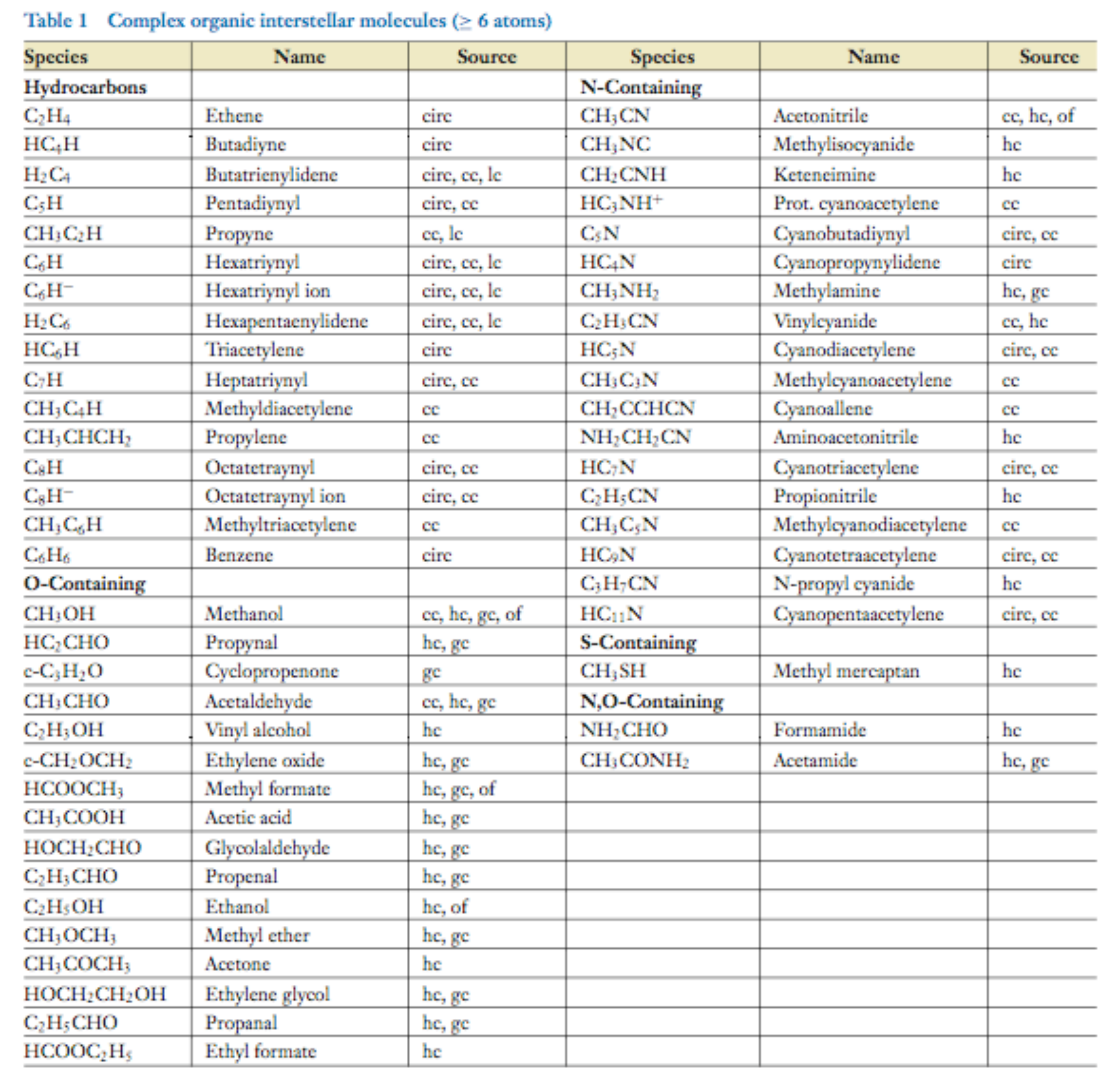
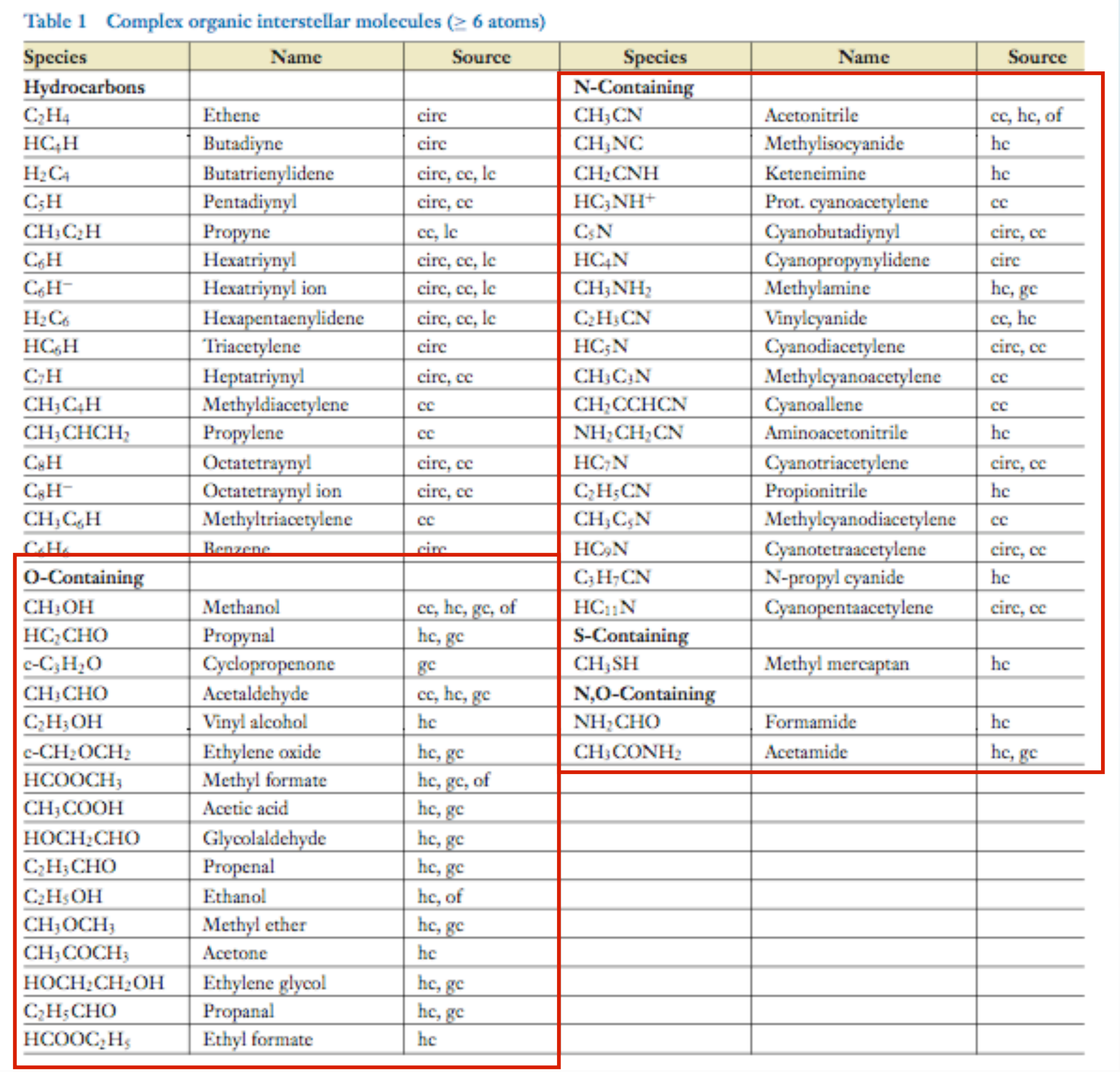


Table 1 Complex organic interstellar molecules (≥ 6 atoms)

Species	Name	Source	Species	Name	Source
Hydrocarbons			**N-Containing**		
C_2H_4	Ethene	circ	CH_3CN	Acetonitrile	cc, hc, of
HC_4H	Butadiyne	circ	CH_3NC	Methylisocyanide	hc
H_2C_4	Butatrienylidene	circ, cc, lc	CH_2CNH	Keteneimine	hc
C_5H	Pentadiynyl	circ, cc	HC_3NH^+	Prot. cyanoacetylene	cc
CH_3C_2H	Propyne	cc, lc	C_5N	Cyanobutadiynyl	circ, cc
C_6H	Hexatriynyl	circ, cc, lc	HC_4N	Cyanopropynylidene	circ
C_6H^-	Hexatriynyl ion	circ, cc, lc	CH_3NH_2	Methylamine	hc, gc
H_2C_6	Hexapentaenylidene	circ, cc, lc	C_2H_3CN	Vinylcyanide	cc, hc
HC_6H	Triacetylene	circ	HC_5N	Cyanodiacetylene	circ, cc
C_7H	Heptatriynyl	circ, cc	CH_3C_3N	Methylcyanoacetylene	cc
CH_3C_4H	Methyldiacetylene	cc	CH_2CCHCN	Cyanoallene	cc
CH_3CHCH_2	Propylene	cc	NH_2CH_2CN	Aminoacetonitrile	hc
C_8H	Octatetraynyl	circ, cc	HC_7N	Cyanotriacetylene	circ, cc
C_8H^-	Octatetraynyl ion	circ, cc	C_2H_5CN	Propionitrile	hc
CH_3C_6H	Methyltriacetylene	cc	CH_3C_5N	Methylcyanodiacetylene	cc
C_6H_6	Benzene	circ	HC_9N	Cyanotetraacetylene	circ, cc
O-Containing			C_3H_7CN	N-propyl cyanide	hc
CH_3OH	Methanol	cc, hc, gc, of	$HC_{11}N$	Cyanopentaacetylene	circ, cc
HC_2CHO	Propynal	hc, gc	**S-Containing**		
$c\text{-}C_3H_2O$	Cyclopropenone	gc	CH_3SH	Methyl mercaptan	hc
CH_3CHO	Acetaldehyde	cc, hc, gc	**N,O-Containing**		
C_2H_3OH	Vinyl alcohol	hc	NH_2CHO	Formamide	hc
$c\text{-}CH_2OCH_2$	Ethylene oxide	hc, gc	CH_3CONH_2	Acetamide	hc, gc
$HCOOCH_3$	Methyl formate	hc, gc, of			
CH_3COOH	Acetic acid	hc, gc			
$HOCH_2CHO$	Glycolaldehyde	hc, gc			
C_2H_3CHO	Propenal	hc, gc			
C_2H_5OH	Ethanol	hc, of			
CH_3OCH_3	Methyl ether	hc, gc			
CH_3COCH_3	Acetone	hc			
$HOCH_2CH_2OH$	Ethylene glycol	hc, gc			
C_2H_5CHO	Propanal	hc, gc			
$HCOOC_2H_5$	Ethyl formate	hc			

Herbst & van Dishoeck 2009

Complex organic molecules



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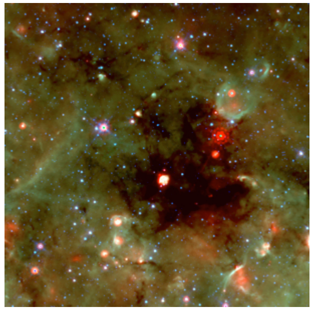
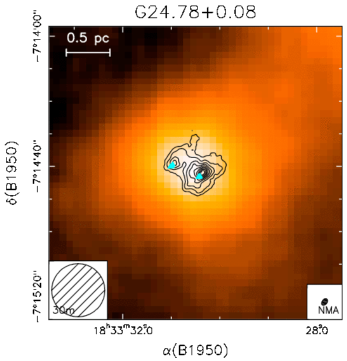
$HCOOC_2H_5$	Ethyl formate	hc			

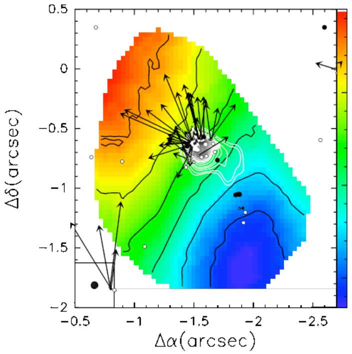
Herbst & van Dishoeck 2009

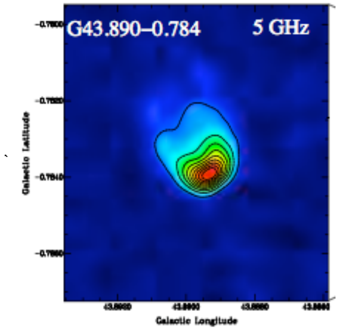
Evolutionary sequence for high-mass stars

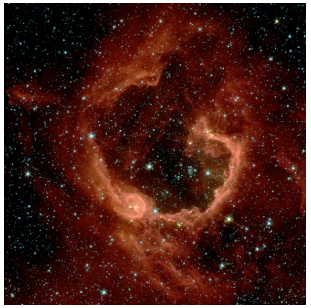
IR-dark cloud **Hot Molecular Core** **HC HII** **UC HII** **Extended HII**











fragmentation *Infall+rotation +outflow* *accretion* *expansion*

Hot Molecular Cores

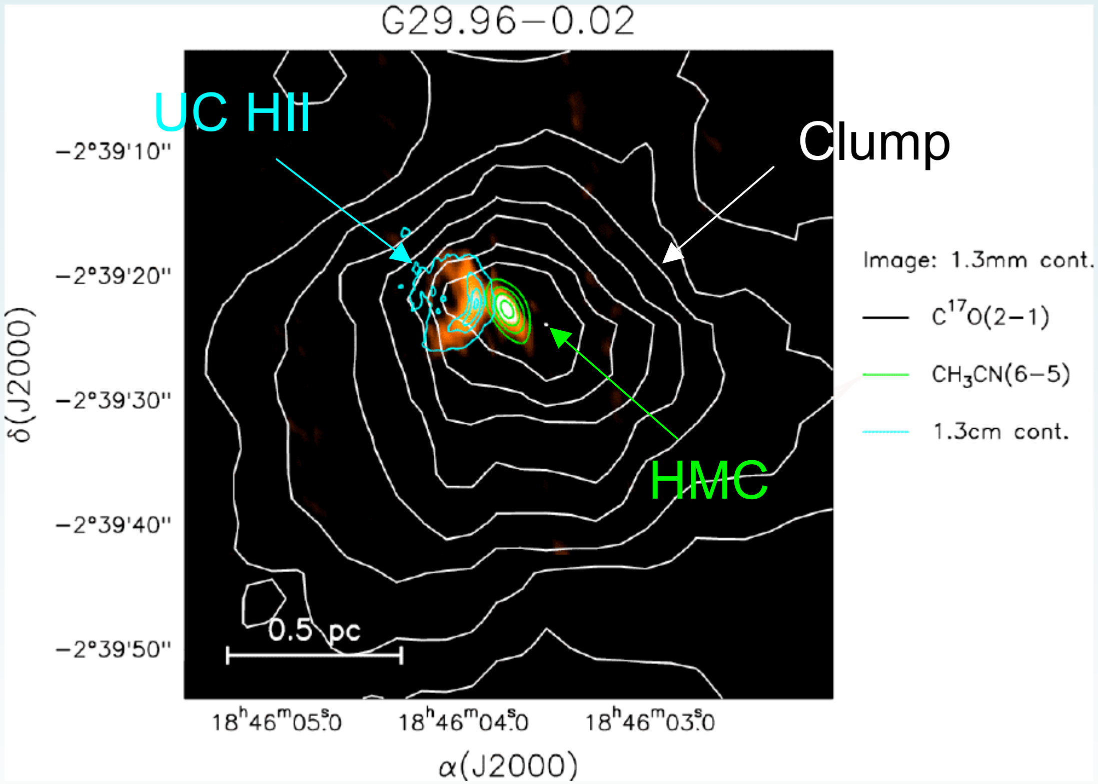
- ❑ Hot molecular cores, the cradles of OB stars, have sizes <0.1 pc

  T >100 K

  n~10^7 cm^{-3}

  L >10^4 $L_\odot$

- ❑ Sometimes associated with embedded HC / UC HII regions



Hot Molecular Cores

- Hot molecular cores, the cradles of OB stars, have sizes <0.1 pc

  T >100 K

  $n \sim 10^7$ cm^{-3}

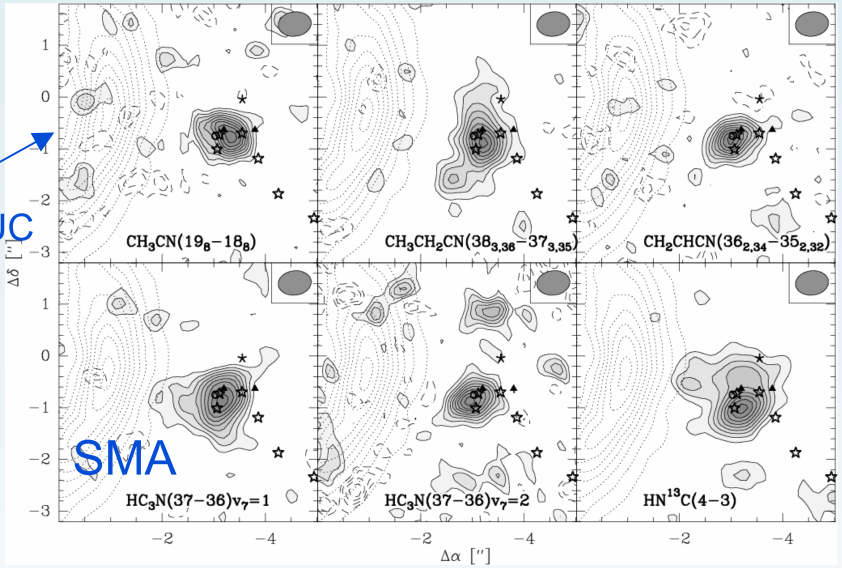
  $L > 10^4 L_\odot$

- Sometimes associated with embedded HC / UC HII regions

- Rich chemistry : evaporation of dust grain mantles

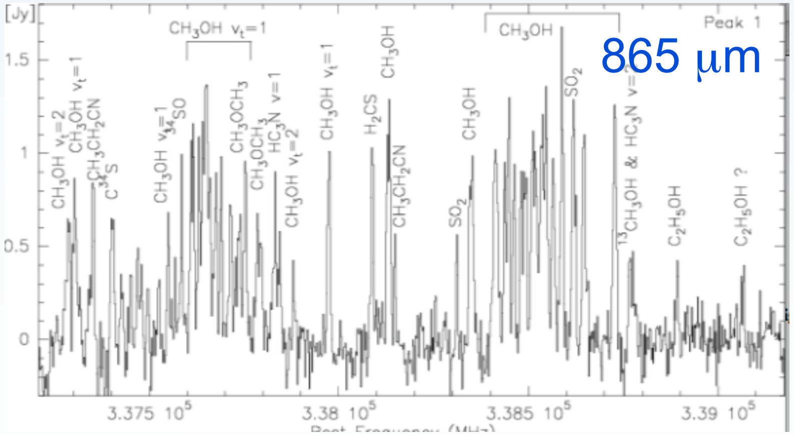
- Associated with outflow, infall, and rotation

G29.96-0.02



cometary UC HII region

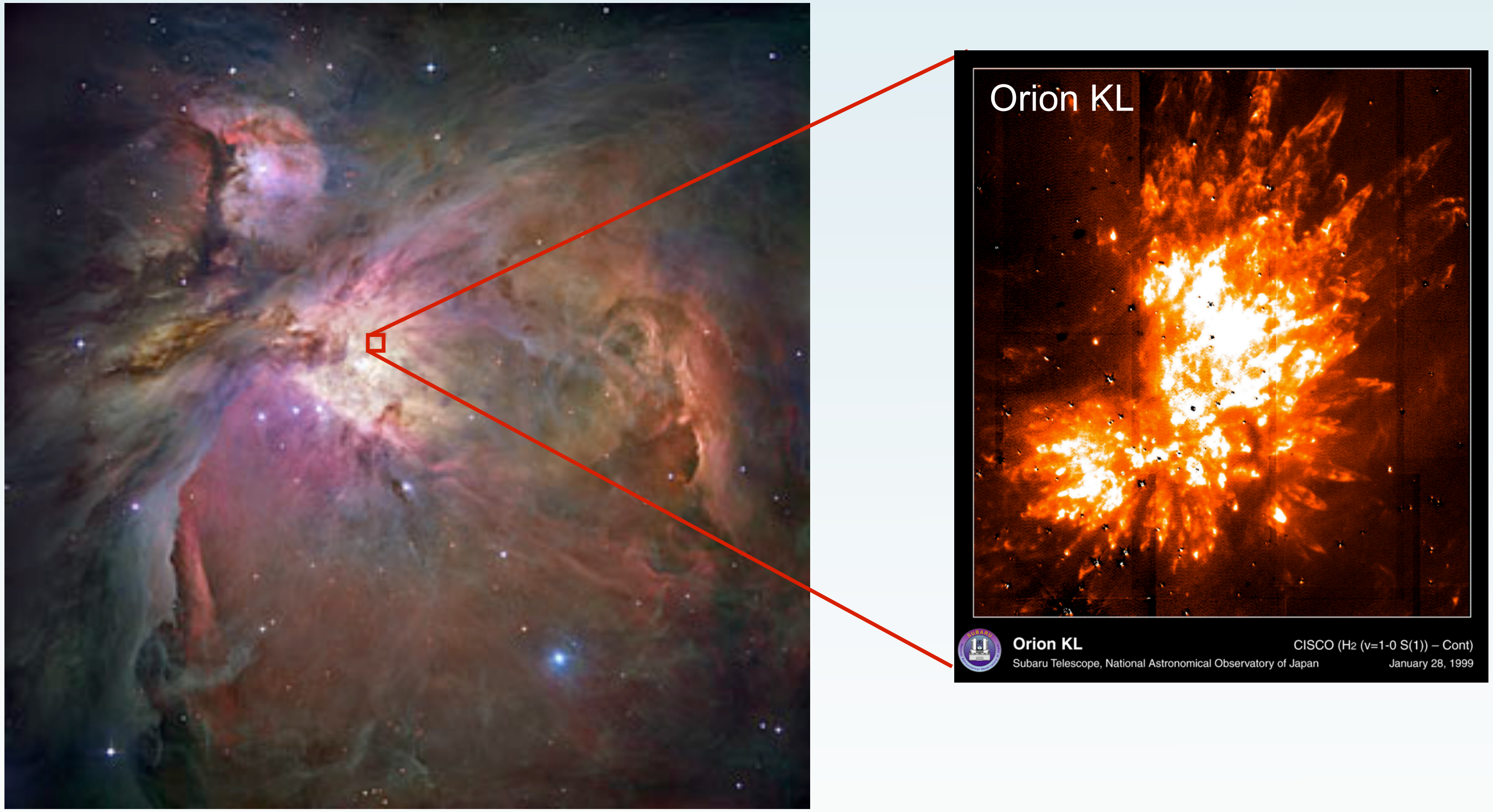
SMA



865 μm

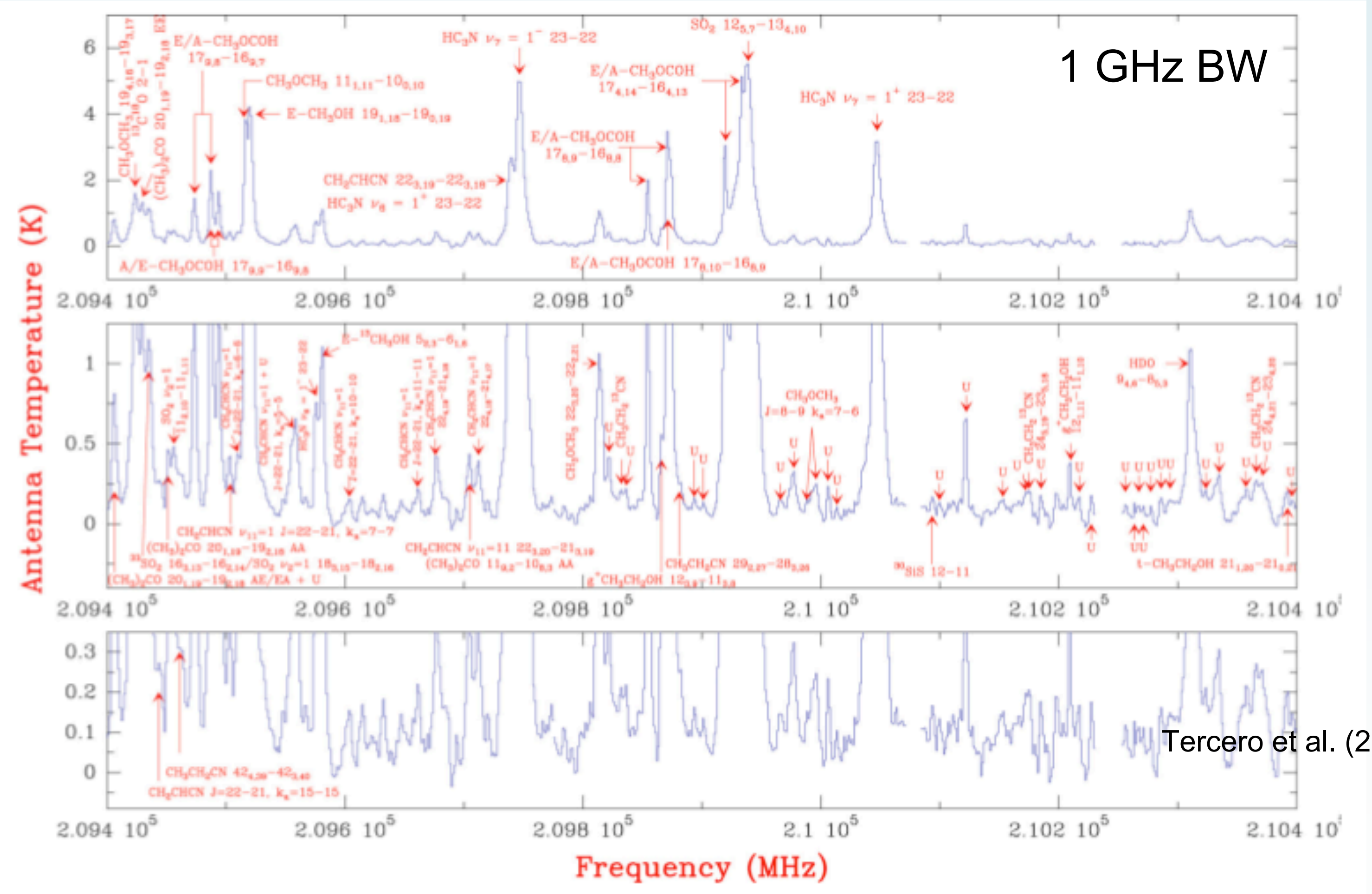
Beuther et al. (2007)

Hot Molecular Cores



Hot Molecular Cores

Orion KL



Tercero et al. (2010)

- Many lines (almost all peaks are real lines)
- Many unidentified

Hot Molecular Cores

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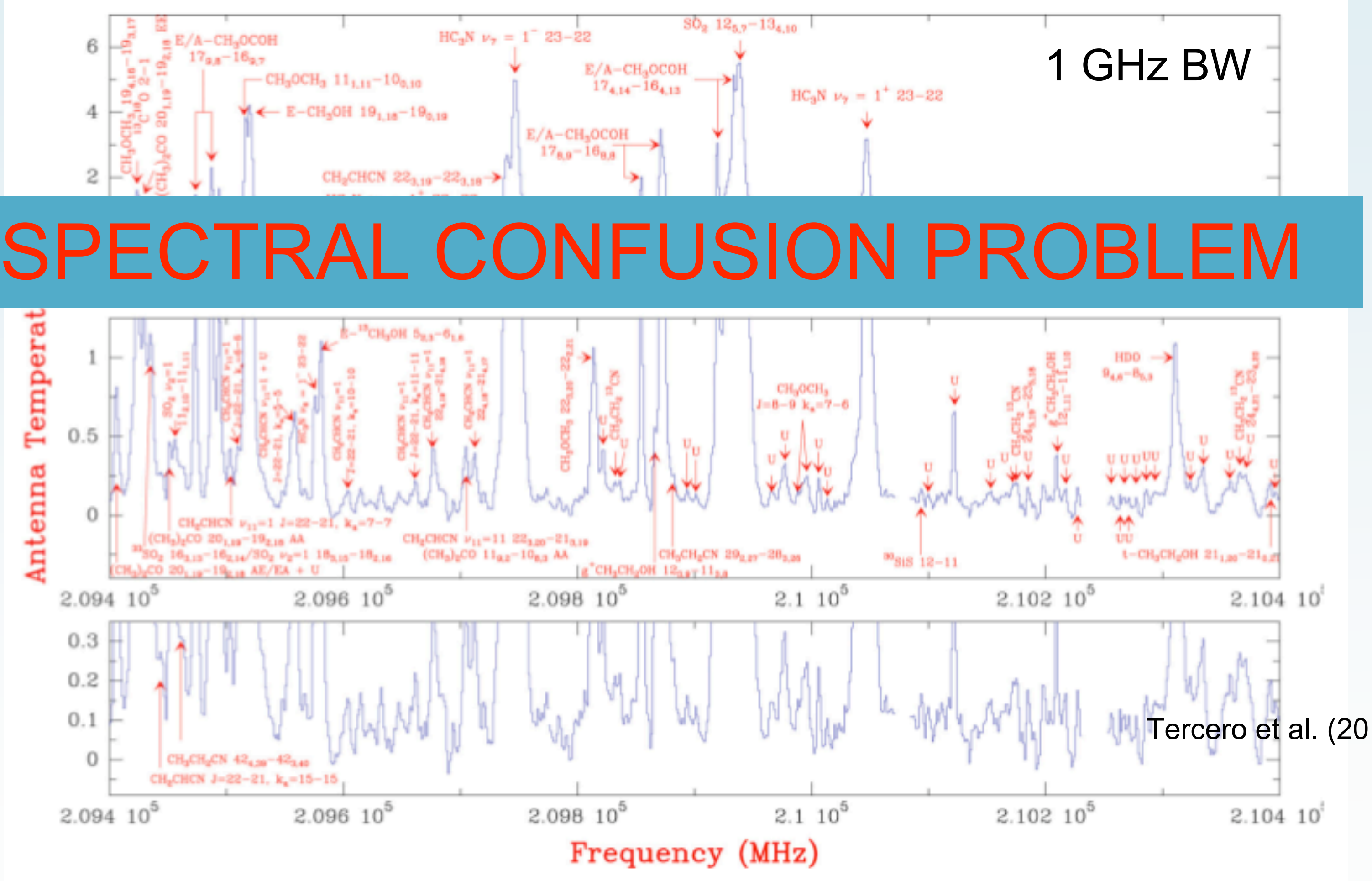


SPECTRAL CONFUSION PROBLEM

1 GHz BW

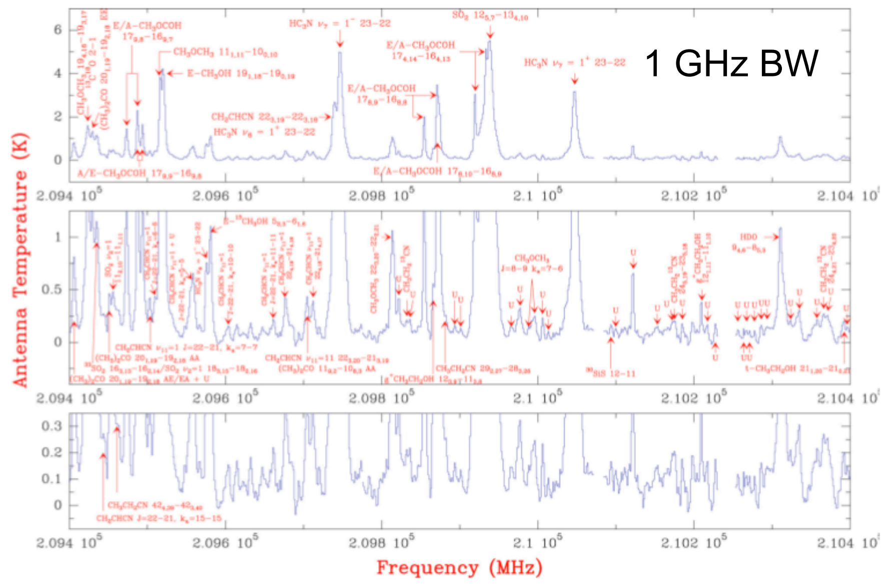
Tercero et al. (2010)

- Many lines (almost all peaks are real lines)
- Many unidentified

Hot Molecular Cores

- ALMA will see hundreds of Orion-like sources.
- ALMA, with its gain in sensitivity and angular resolution with respect to any available facility, will unveil a real forest of lines in all spectral observations.
- Is ALMA useless for chemistry studies?

Orion KL



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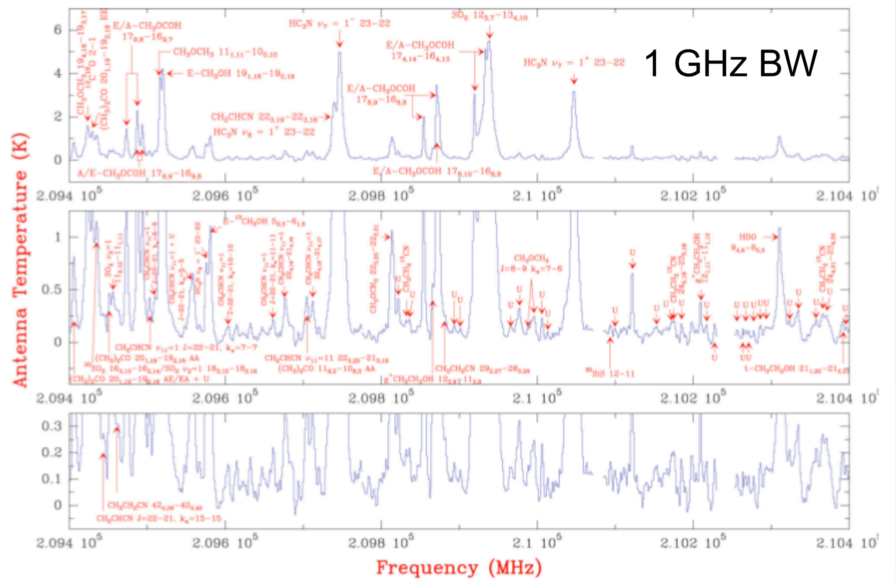
ALMA may reduce (in part) the confusion problem

Orion KL



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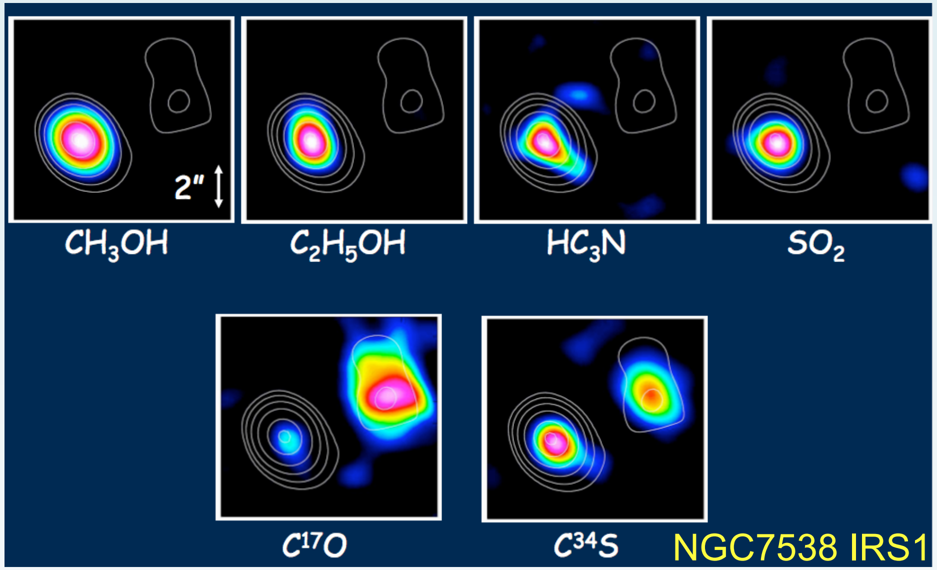
SPATIAL RESOLUTION



Courtesy of C. Brogan

- Interferometers additionally filter out spectral line originated from extended structures which may otherwise blank or confuse weak target lines in single-dish telescope surveys.

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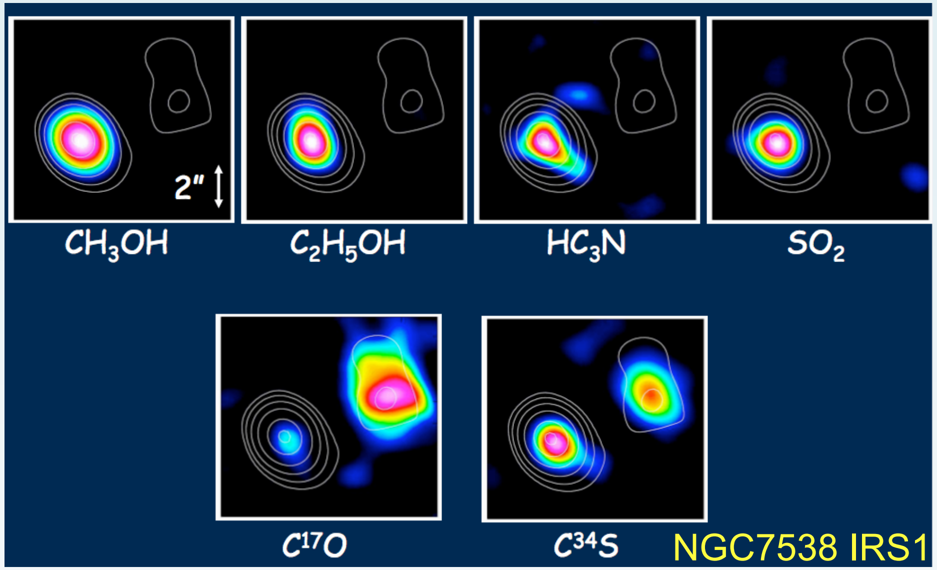

Courtesy of C. Brogan

➔ ALMA will have 10-100 times better angular resolution compared to current millimeter interferometers

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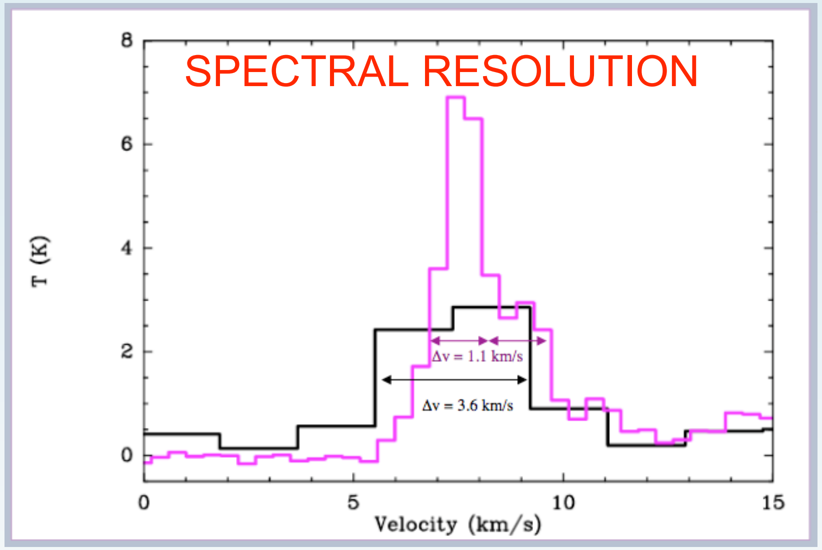
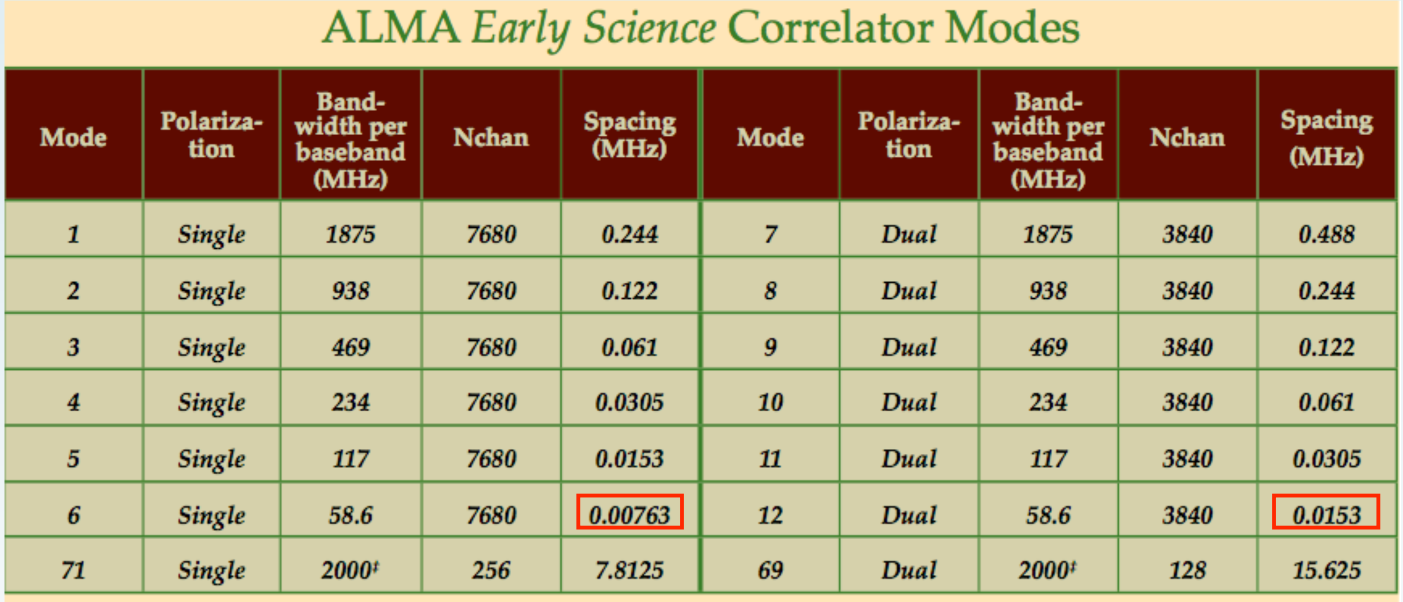


Hot Molecular Cores



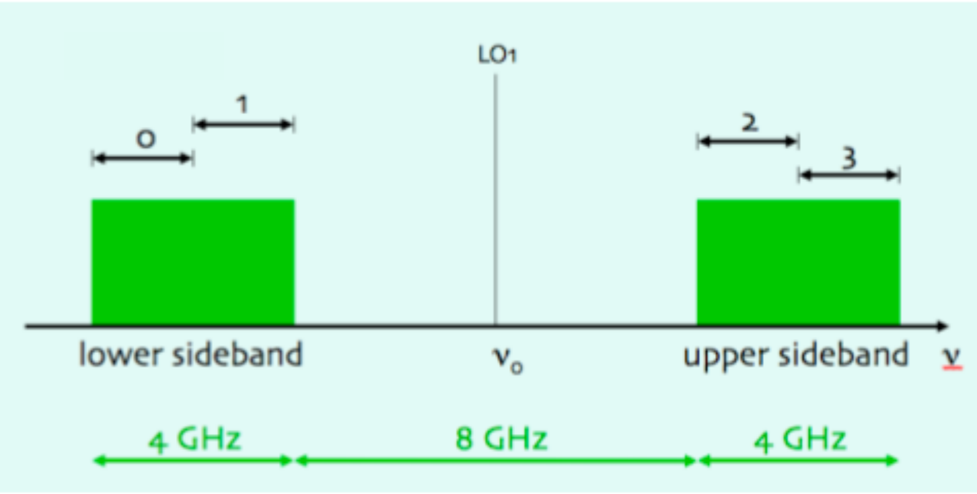
ALMA *Early Science* Correlator Modes

Mode	Polarization	Bandwidth per baseband (MHz)	Nchan	Spacing (MHz)	Mode	Polarization	Bandwidth per baseband (MHz)	Nchan	Spacing (MHz)
1	*Single*	*1875*	*7680*	*0.244*	*7*	*Dual*	*1875*	*3840*	*0.488*
2	*Single*	*938*	*7680*	*0.122*	*8*	*Dual*	*938*	*3840*	*0.244*
3	*Single*	*469*	*7680*	*0.061*	*9*	*Dual*	*469*	*3840*	*0.122*
4	*Single*	*234*	*7680*	*0.0305*	*10*	*Dual*	*234*	*3840*	*0.061*
5	*Single*	*117*	*7680*	*0.0153*	*11*	*Dual*	*117*	*3840*	*0.0305*
6	*Single*	*58.6*	*7680*	*0.00763*	*12*	*Dual*	*58.6*	*3840*	*0.0153*
71	*Single*	*2000‡*	*256*	*7.8125*	*69*	*Dual*	*2000‡*	*128*	*15.625*

Spectral Resolution (km/s)			
Frequency (GHz)	Dual Polarization	Single Polarization	Band
100	0.046	0.023	3
250	0.018	0.009	6
350	0.012	0.006	7
700	0.006	0.003	9

Hot Molecular Cores

- ❑ ALMA will see hundreds of Orion-like sources.
- ❑ ALMA, with its gain in sensitivity and angular resolution with respect to any available facility, will unveil a real forest of lines in all spectral observations.
- ❑ ALMA wide bandwidth will allow to simultaneously observe several transitions of a same species
- ❑ Spanning the survey over the whole frequency range of ALMA will cover a large range of excitation conditions.
- ❑ Most of the emission will arise from isotopic species and vibrationally excited states of already known molecules.



- ❑ Up to 4x1.875 GHz bandwidth simultaneously with 0.244 MHz spectral resolution (single polarization)

Hot Molecular Cores

➔ a complete and accurate molecular line database will be required

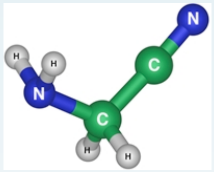
➔ The interpretation of molecular ALMA data will also need additional molecular physics information, like collisional rates, quantum chemistry calculations, etc.

➔ Laboratory investigation to produce synthetic spectra of selected species

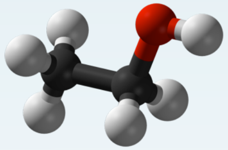
Complex molecules in HMCs

- First discoveries of “large organic” (and prebiotic) molecules in space: formaldehyde (H_2CO) in 1969 and methanol (CH_3OH) in 1970
- Some “exotic” molecules in interstellar clouds (most towards the Galactic Center):

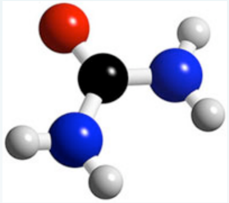
  - formic acid ($HCOOH$)



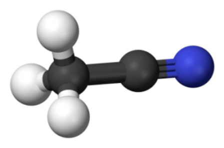
  - ethanol (CH_3CH_2OH)



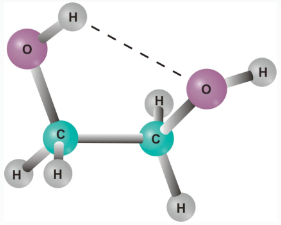
  - urea (H_2NCONH_2)



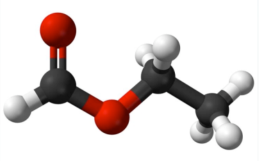
  - methyl cyanide (CH_3CN)



  - acetone (CH_3COOCH_3)
  - ethylene glycol (a.k.a interstellar antifreeze) ($HOCH_2CH_2OH$)



  - ethyl formate (C_2H_5OCHO) (flavour of berries)



Formation mechanism in HMCs

❑ Cold gas in the interstellar medium ‘made up’ of simple molecules (e.g. CO, HCN, N_2, O_2 etc) frozen onto dust grains

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❑ Accretion of atoms and molecules on dust + surface reactions form more complex molecules: CO_2, CH_3OH, H_2O etc (ices)

REACTANTS: ATOMS AND RADICALS

A + B → AB association

$$H + H \rightarrow H_2$$

$$H + X \rightarrow XH \quad (X = O, C, N, CO, \text{etc.})$$

Conversion

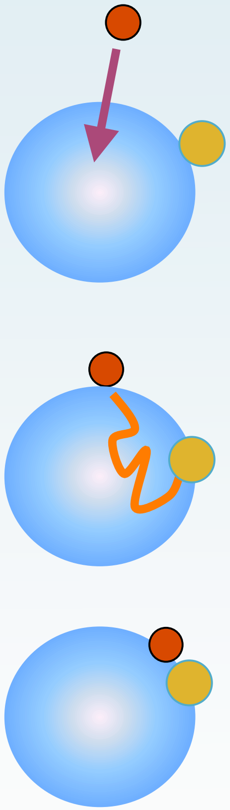
$$O \rightarrow OH \rightarrow H_2O$$

$$C \rightarrow CH \rightarrow CH_2 \rightarrow CH_3 \rightarrow CH_4$$

$$N \rightarrow NH \rightarrow NH_2 \rightarrow NH_3$$

$$CO \rightarrow HCO \rightarrow H_2CO \rightarrow H_3CO \rightarrow CH_3OH$$

Surface reactions: hydrogenation



Courtesy of S.Viti

Formation mechanism in HMCs

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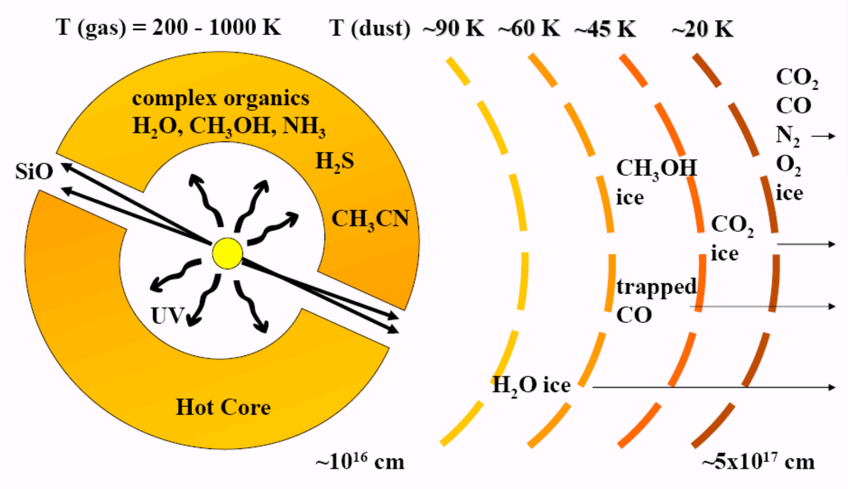
- Accretion of atoms and molecules on dust + surface reactions form more complex molecules: CO_2, CH_3OH, H_2O etc (ices)
- Back into the gas phase when dust heats up (e.g. by a star) → Evaporated ices: precursors of larger organic molecules
- Production of organic molecules can be enriched by thermal and energetic processing (UV and cosmic rays) in the gas phase (and possibly in the solid phase)

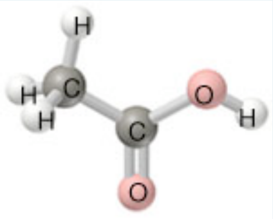
SCHEMATIC OF A HOT CORE



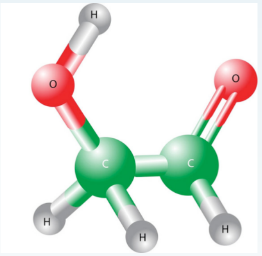
Pre-biotic molecules in HMCs

❑ Biologically important: pre-biotic molecules or building blocks of life

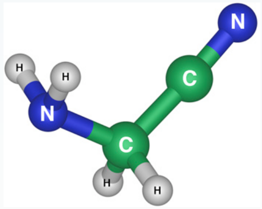
- ❑ acetic acid (vinegar) (CH_3COOH)



- ❑ glycolaldehyde (CH_2OHCHO)



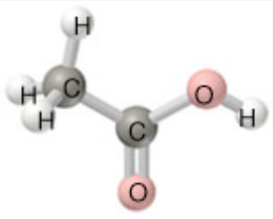
- ❑ amino acetonitrile (NH_2CH_2CN) (direct precursor of glycine??)



Pre-biotic molecules in HMCs

- Biologically important:

  - acetic acid (vinegar) (CH_3COOH)



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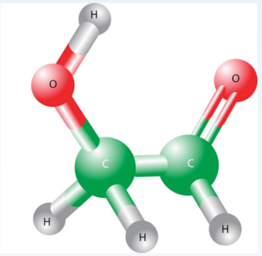
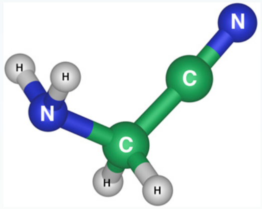
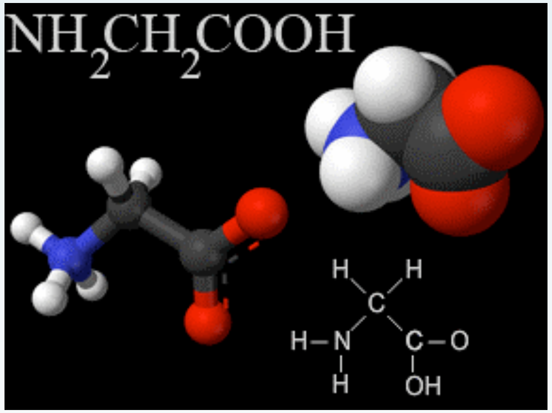


  - amino acetonitrile (NH_2CH_2CN) (direct precursor of glycine??)



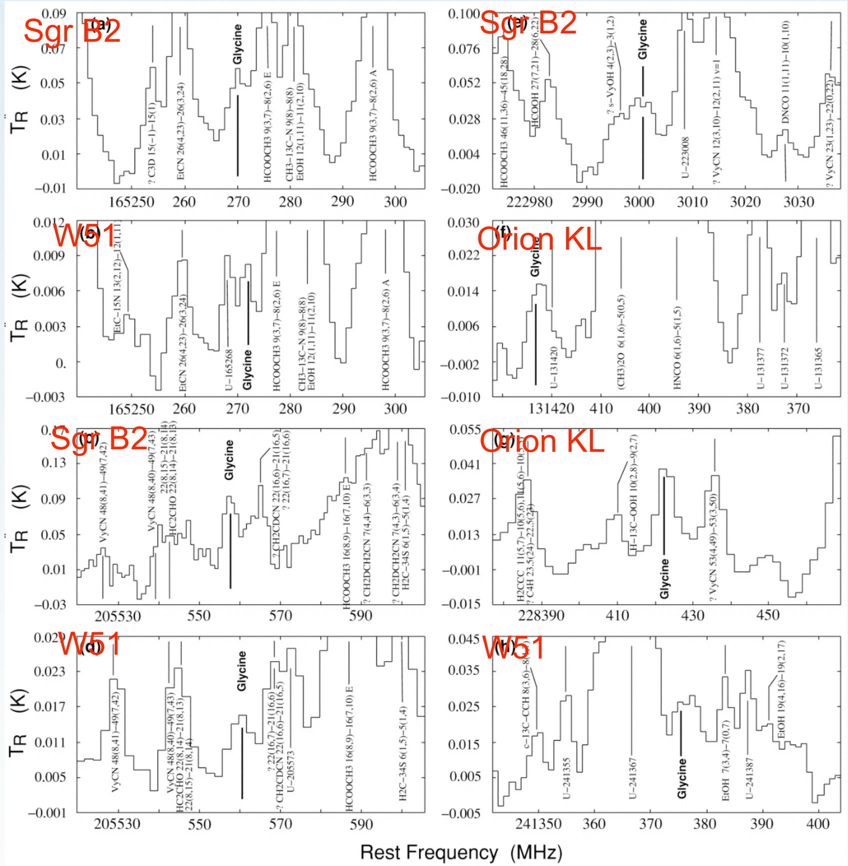
Not YET detected

- glycine (NH_2CH_2COOH), the simplest amino acid



Glycine

- Glycine is the simplest of the 20 amino acids commonly found in proteins
- Kuan et at. (2003) claimed to have detected 27 spectral lines of glycine in the hot cores Sgr B2(N), Orion KL, and W51 e1/e2.
- Snyder et al. (2005) disputed the claim and concluded that the identified lines are more likely due to weeds such as C_2H_5CN, C_2H_3CN, and *gauche*-ethanol. The analysis of these researchers was based partially on the fact that the observation of some lines of a candidate species implies the existence of other lines, and that some intense lines of glycine were missing.



Kuan et al. (2003)

What constitutes a firm detection

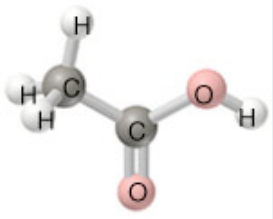
❑ The currently accepted procedure for unequivocally identifying new molecules requires that at least the following criteria are met (Belloche et al. 2008; Snyder et al. 2005; Ziurys & Apponi 2005):

1) Rest frequencies are accurately known to 1:10^7, either from direct laboratory measurements or from a high-precision Hamiltonian model
2) Observed frequencies of clean, non-blended lines agree with rest frequencies for a single well-determined velocity of the source
3) All predicted lines of a molecule based on an LTE spectrum at a well-defined rotational temperature and appropriately corrected for beam dilution are present in the observed spectrum at roughly their predicted relative intensities. A single anti-coincidence (that is, a predicted line missing in the observational data) is a much stronger criterion for rejection than hundreds of coincidences are for identification.
4) Other criteria: to obtain interferometric images of the source and show that all lines of the new molecule originate from the same location.

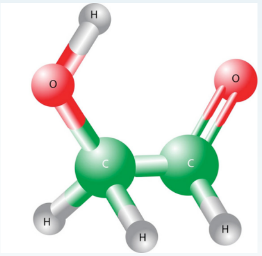
Pre-biotic molecules in HMCs

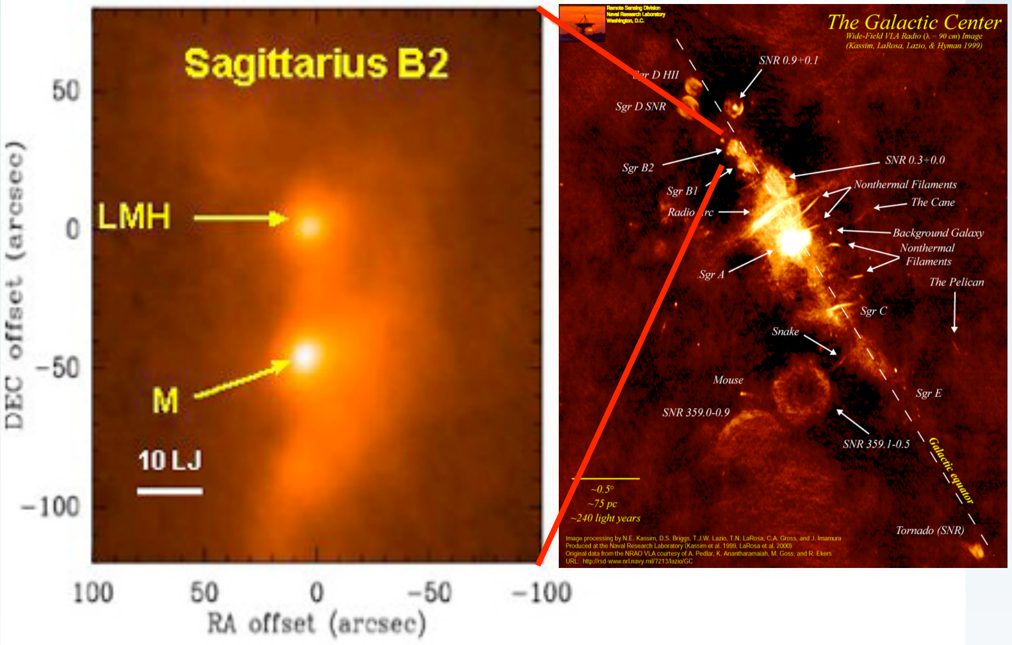
- ❑ Biologically important:

  - ❑ acetic acid (vinegar) (CH_3COOH)

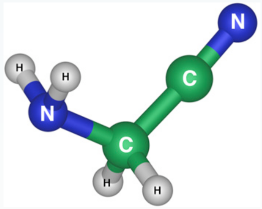


  - ❑ glycolaldehyde (CH_2OHCHO)





  - ❑ amino acetonitrile (NH_2CH_2CN) (direct precursor of glycine??)



Glycolaldehyde

❑ Glycolaldehyde is the simplest of the monosaccharide sugars

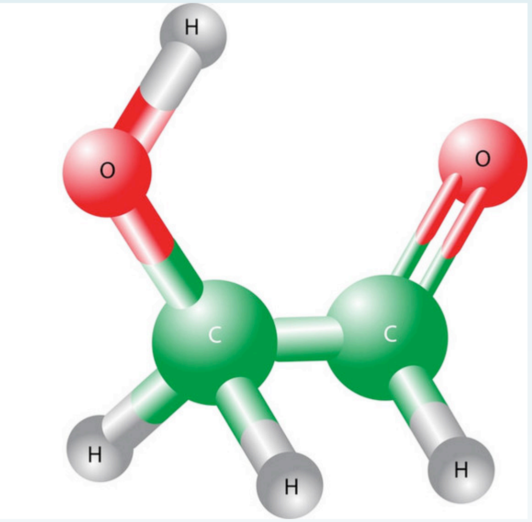
❑ Monosaccharide sugars are carbohydrates with the following empirical chemical expression:

$$C_nH_{2n}O_n$$

where $n \geq 2$, is the number of carbon or oxygen atoms present.

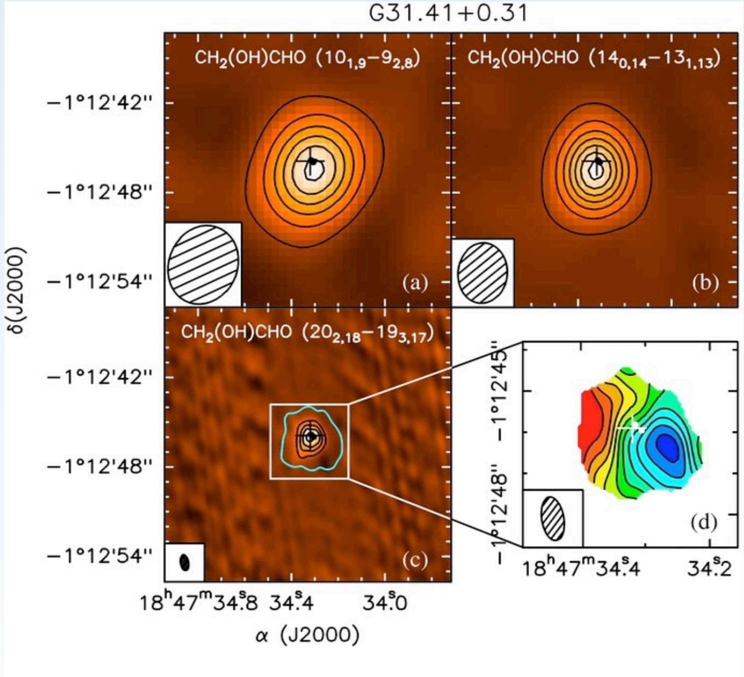
❑ Glycolaldehyde with n=2 is composed of 2 oxygen atoms, 2 carbon atoms and 4 hydrogen atoms

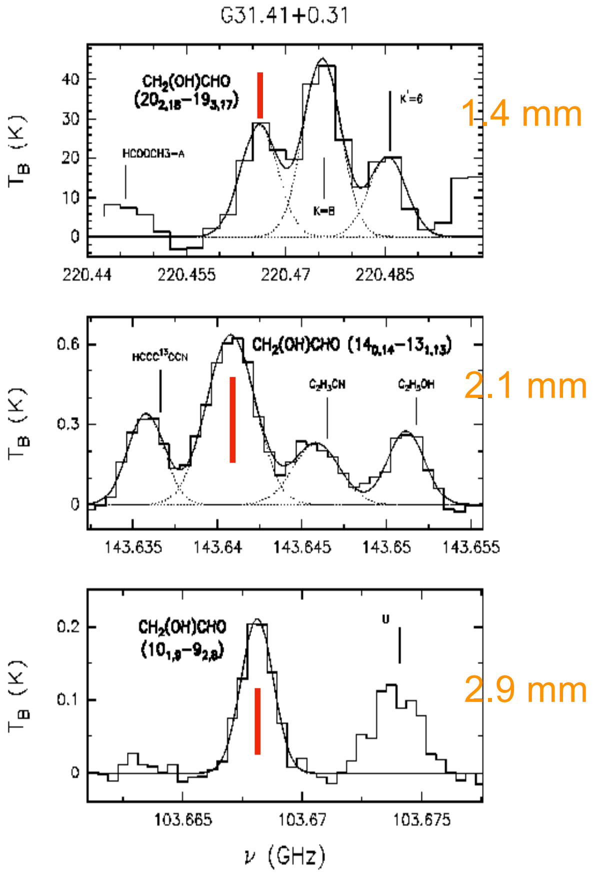
❑ Glycolaldehyde can be incorporated into larger sugar molecules. It can react with a 3-carbon sugar to produce a 5-carbon sugar called ribose ($C_5H_{10}O_5$), the central constituent of RNA



Glycolaldehyde in G31.41+0.31

☐ Glycolaldehyde has been detected for the first time towards a hot molecular core OUTSIDE the Galactic Center: G31.41+0.31 (Beltrán et al. 2009).





Beltrán et al. (2009)

☐ Very compact emission (~1.3", ~10,000 AU) unlike in Sgr B2, arising from the hottest and densest gas in the surroundings of the newly formed star(s).

☐ No direct determination of its temperature and abundance (rotational diagram flat ➔ optically thick emission): $N_{glycol} > 1 \times 10^{17}$ cm^{-2}

Origin of glycolaldehyde

- Following the Viti's HMC model (Viti et al. 2004), Beltrán et al. (2009) adopted a formation route based on the formation of glycolaldehyde on ices via surface reactions of HCO with CH_3OH and H_2CO. The model already included hydrogenation on grains.

- The best -fit model implies an age of the HMC of a few 10^5 yr and low CO conversion efficiencies and probabilities: only 10-15% of CO needs to be processed on grains

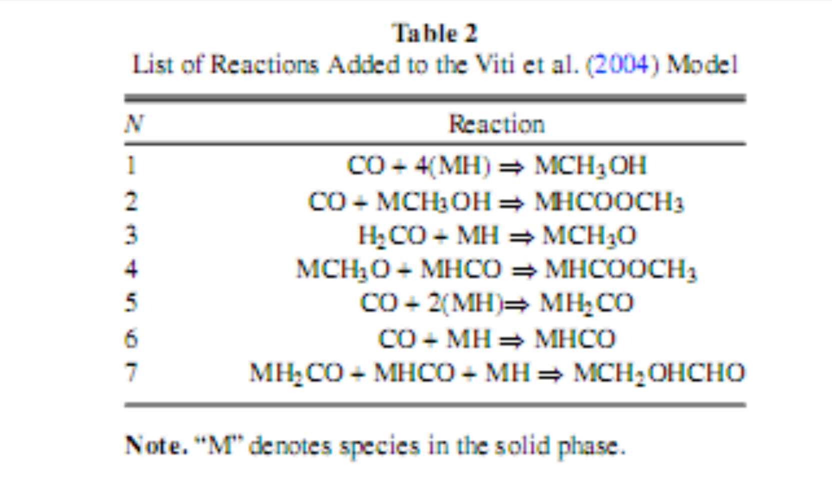


Table 2

List of Reactions Added to the Viti et al. (2004) Model

N	Reaction
1	$CO + 4(MH) \Rightarrow MCH_3OH$
2	$CO + MCH_3OH \Rightarrow MHCOOCH_3$
3	$H_2CO + MH \Rightarrow MCH_3O$
4	$MCH_3O + MHCO \Rightarrow MHCOOCH_3$
5	$CO + 2(MH) \Rightarrow MH_2CO$
6	$CO + MH \Rightarrow MHCO$
7	$MH_2CO + MHCO + MH \Rightarrow MCH_2OHCHO$

Note. "M" denotes species in the solid phase.

ALMA and glycolaldehyde

Wavelen(mm)	Freq in GHz (Err)	Resolved QNs	Smu2 (D2)	EU (K)
1.42076	211.15530 (0.00013)	21(9,12)-21(8,13)	77.63963	177.72056
1.42038	211.21067 (0.00013)	21(9,13)-21(8,14)	77.63427	177.72034
1.41544	211.94865 (0.00013)	20(9,11)-20(8,12)	72.07920	165.98534
1.41526	211.97444 (0.00013)	20(9,12)-20(8,13)	72.07809	165.98528
1.4124	212.40476 (0.00013)	20(1,19)-19(2,18)	114.70577	112.69783
1.41138	212.55830 (0.00013)	20(2,19)-19(1,18)	114.72447	112.70045
1.41098	212.61805 (0.00013)	19(9,10)-19(8,11)	66.55555	154.82010
1.41091	212.62930 (0.00013)	19(9,11)-19(8,12)	66.54844	154.82007
1.40725	213.18178 (0.00013)	18(9, 9)-18(8,10)	61.05539	144.22315
1.40722	213.18636 (0.00013)	18(9,10)-18(8,11)	61.05273	144.22308
1.40718	213.19187 (0.00013)	21(0,21)-20(1,20)	145.12154	114.69204
1.40717	213.19359 (0.00013)	21(1,21)-20(0,20)	145.11922	114.69212
1.40414	213.65398 (0.00013)	17(9, 8)-17(8, 9)	55.54761	134.19284
1.40413	213.65591 (0.00013)	17(9, 9)-17(8,10)	55.54659	134.19279
1.4039	213.68991 (0.00013)	12(4, 9)-11(3, 8)	28.90103	53.23074
1.40156	214.04719 (0.00013)	16(9, 7)-16(8, 8)	50.03251	124.72764
1.39944	214.37163 (0.00013)	15(9, 6)-15(8, 7)	44.46713	115.82615
1.39873	214.48095 (0.00013)	19(3,17)-18(2,16)	82.01513	109.47204
1.39771	214.63629 (0.00013)	14(9, 5)-14(8, 6)	38.81382	107.48724
1.39633	214.84957 (6.9E-6)	13(9, 4)-13(8, 5)	33.05650	99.70956
1.39633	214.84959 (6.9E-6)	13(9, 5)-13(8, 6)	33.05650	99.70956
1.39523	215.01868 (7.1E-6)	12(9, 3)-12(8, 4)	27.12809	92.49204
1.37865	217.60364 (0.00013)	24(5,19)-23(6,18)	32.75510	187.07989
1.3745	218.26054 (6.8E-6)	20(3,17)-19(4,16)	59.45980	126.14359
1.36842	219.23025 (9.3E-6)	13(4,10)-12(3, 9)	29.94565	60.51624
1.36077	220.46388 (6.8E-6)	20(2,18)-19(3,17)	89.74378	120.05256
1.34921	222.35235 (0.00013)	21(1,20)-20(2,19)	122.27416	123.37164
1.34868	222.43974 (0.00013)	21(2,20)-20(1,19)	122.26227	123.37310

Band 6

50 K < E_u < 200 K

ALMA and glycolaldehyde

Wavelen(mm)	Freq in GHz (Err)	Resolved QNs	Smu2 (D2)	EU (K)
1.34459	223.11622 (7.2E-6)	22(1,22)-21(0,21)	152.60377	125.39985
1.34262	223.44403 (0.00013)	20(3,18)-19(2,17)	89.93252	120.10724
1.34085	223.73863 (0.00013)	14(4,11)-13(3,10)	31.63361	68.35895
1.33178	225.26257 (0.00013)	22(4,18)-21(5,17)	44.11126	155.43126
1.31889	227.46364 (0.00013)	15(4,12)-14(3,11)	34.13716	76.75251
1.30037	230.70369 (0.00013)	16(4,13)-15(3,12)	37.59810	85.68896
1.29927	230.89847 (0.00013)	21(2,19)-20(3,18)	97.67727	131.18857
1.29165	232.26173 (0.00013)	21(3,18)-20(4,17)	68.44724	137.83608
1.29151	232.28603 (0.00013)	22(1,21)-21(2,20)	129.79715	134.52103
1.29124	232.33545 (0.00013)	22(2,21)-21(1,20)	129.80159	134.52196
1.28902	232.73499 (0.00013)	21(3,19)-20(2,18)	97.76795	131.22204
1.28735	233.03736 (0.00013)	23(0,23)-22(1,22)	160.07380	136.58388
1.28735	233.03773 (0.00013)	23(1,23)-22(0,22)	160.07330	136.58389
1.28316	233.79725 (0.00013)	17(4,14)-16(3,13)	42.13068	95.15978
1.26525	237.10813 (0.00013)	18(4,15)-17(3,14)	47.79031	105.15611
1.26135	237.84083 (0.00013)	21(10,11)-21(9,12)	72.74549	189.13494
1.26133	237.84363 (0.00013)	21(10,12)-21(9,13)	72.76055	189.13507
1.25853	238.37354 (0.00013)	20(10,10)-20(9,11)	67.25008	177.42533
1.25852	238.37474 (0.00013)	20(10,11)-20(9,12)	67.24941	177.42539
1.25613	238.82855 (0.00013)	19(10, 9)-19(9,10)	61.75739	166.28204
1.2541	239.21475 (0.00013)	18(10, 8)-18(9, 9)	56.22871	155.70361
1.2524	239.54020 (0.00013)	17(10, 7)-17(9, 8)	50.67200	145.68885
1.2517	239.67413 (0.00013)	11(5, 7)-10(4, 6)	35.29473	51.90368
1.25098	239.81187 (0.00013)	16(10, 6)-16(9, 7)	45.03919	136.23666
1.24981	240.03629 (0.00013)	15(10, 5)-15(9, 6)	39.31876	127.34606
1.24886	240.21917 (0.00013)	14(10, 4)-14(9, 5)	33.47131	119.01588
1.24809	240.36651 (0.00013)	13(10, 3)-13(9, 4)	27.44643	111.24525
1.24538	240.89063 (0.00013)	11(5, 6)-10(4, 7)	35.17052	51.90983
1.24488	240.98694 (0.00013)	19(4,16)-18(3,15)	54.47894	115.66874

Band 6

50 K < E_u < 200 K

ALMA and glycolaldehyde

Wavelen(mm)	Freq in GHz (Err)	Resolved QNs	Smu2 (D2)	EU (K)
1.24413	241.13185 (6.9E-6)	22(2,20)-21(3,19)	105.50426	142.79447
1.23859	242.21148 (7.0E-6)	23(1,22)-22(2,21)	137.31063	146.14624
1.23845	242.23912 (7.0E-6)	23(2,22)-22(1,21)	137.34244	146.14671
1.2384	242.24744 (7.0E-6)	22(3,20)-21(2,19)	105.54823	142.81463
1.23478	242.95779 (7.4E-6)	24(0,24)-23(1,23)	167.54930	148.24396
1.23478	242.95804 (7.4E-6)	24(1,24)-23(0,23)	167.54895	148.24397
1.23003	243.89650 (8.0E-6)	23(4,19)-22(5,18)	52.49221	168.64572
1.22379	245.13994 (0.00013)	22(3,19)-21(4,18)	77.32242	149.97478
1.22095	245.71116 (0.00013)	20(4,17)-19(3,16)	61.98046	126.68940
1.19969	250.06397 (0.00013)	12(5, 8)-11(4, 7)	35.49798	58.61592
1.1941	251.23561 (6.9E-6)	23(2,21)-22(3,20)	113.25240	154.87196
1.19319	251.42632 (8.6E-6)	21(4,18)-20(3,17)	69.99406	138.21010
1.19092	251.90510 (7.0E-6)	23(3,21)-22(2,20)	113.27390	154.88395
1.18985	252.13159 (7.1E-6)	24(1,23)-23(2,22)	144.84711	158.24701
1.18978	252.14700 (7.1E-6)	24(2,23)-23(1,22)	144.82938	158.24731
1.18759	252.61206 (8.8E-6)	12(5, 7)-11(4, 8)	35.21518	58.63059
1.18635	252.87679 (7.5E-6)	25(0,25)-24(1,24)	174.98801	160.38006
1.18635	252.87692 (7.5E-6)	25(1,25)-24(0,24)	174.98782	160.38007
1.17789	254.69353 (9.0E-6)	10(6, 5)- 9(5, 4)	41.84319	52.41040
1.1778	254.71130 (9.0E-6)	10(6, 4)- 9(5, 5)	41.83731	52.41054
1.16678	257.11701 (6.6E-6)	23(3,20)-22(4,19)	85.95630	162.56388
1.16221	258.12876 (8.0E-6)	22(4,19)-21(3,18)	78.22897	150.22421
1.15504	259.73038 (9.1E-6)	13(5, 9)-12(4, 8)	35.57681	65.89988
1.14924	261.04214 (0.00013)	24(4,20)-23(5,19)	61.54166	182.31203
1.14829	261.25807 (0.00013)	24(2,22)-23(3,21)	120.94508	167.42222
1.14654	261.65571 (0.00013)	24(3,22)-23(2,21)	120.96609	167.42936
1.14483	262.04830 (0.00013)	25(1,24)-24(2,23)	152.35659	170.82355
1.14479	262.05684 (0.00013)	25(2,24)-24(1,23)	152.34661	170.82367
1.14158	262.79446 (0.00013)	26(0,26)-25(1,25)	182.47553	172.99205

Band 6

$50\ K < E_u < 200\ K$

ALMA and glycolaldehyde

Wavelen(mm)	Freq in GHz (Err)	Resolved QNs	Smu2 (D2)	EU (K)
1.13473	264.37944 (0.00013)	20(11, 9)-20(10,10)	62.43269	190.11349
1.13356	264.65391 (0.00013)	13(5, 8)-12(4, 9)	34.96472	65.93201
1.13334	264.70481 (0.00013)	19(11, 8)-19(10, 9)	56.87524	178.98570
1.13216	264.98138 (0.00013)	18(11, 7)-18(10, 8)	51.26394	168.42057
1.13116	265.21464 (0.00013)	17(11, 6)-17(10, 7)	45.57828	158.41707
1.13033	265.40880 (0.00013)	16(11, 5)-16(10, 6)	39.77825	148.97426
1.12965	265.56912 (0.00013)	15(11, 4)-15(10, 5)	33.84200	140.09122
1.1291	265.69943 (0.00013)	14(11, 3)-14(10, 4)	27.72524	131.76730
1.12909	265.70082 (0.00013)	23(4,20)-22(3,19)	86.49450	162.72635
1.12739	266.10103 (0.00013)	11(6, 6)-10(5, 5)	42.29937	58.53440
1.12717	266.15416 (0.00013)	11(6, 5)-10(5, 6)	42.29205	58.53450
1.11774	268.39866 (0.00013)	14(5,10)-13(4, 9)	35.54860	73.75677
1.11767	268.41634 (0.00013)	24(3,21)-23(4,20)	94.36479	175.60834
1.11686	268.60998 (0.00013)	9(7, 3)- 8(6, 2)	48.32868	54.74207
1.10607	271.23014 (0.00013)	25(2,23)-24(3,22)	128.60479	180.44628
1.10512	271.46384 (0.00013)	25(3,23)-24(2,22)	128.61947	180.45031
1.10309	271.96232 (0.00013)	26(1,25)-25(2,24)	159.86545	183.87577
1.10308	271.96700 (0.00013)	26(2,25)-25(1,24)	159.85993	183.87585
1.10007	272.71011 (0.00013)	27(0,27)-26(1,26)	189.94789	186.08002
1.09501	273.97028 (7.4E-6)	24(4,21)-23(3,20)	94.68412	175.71231

Band 6

50 K < E_u < 200 K

With BW of ~ 8 GHz, possibility to simultaneously observe several transitions of glycolaldehyde ➔ determine temperature and density (abundance)

Hot Corinos

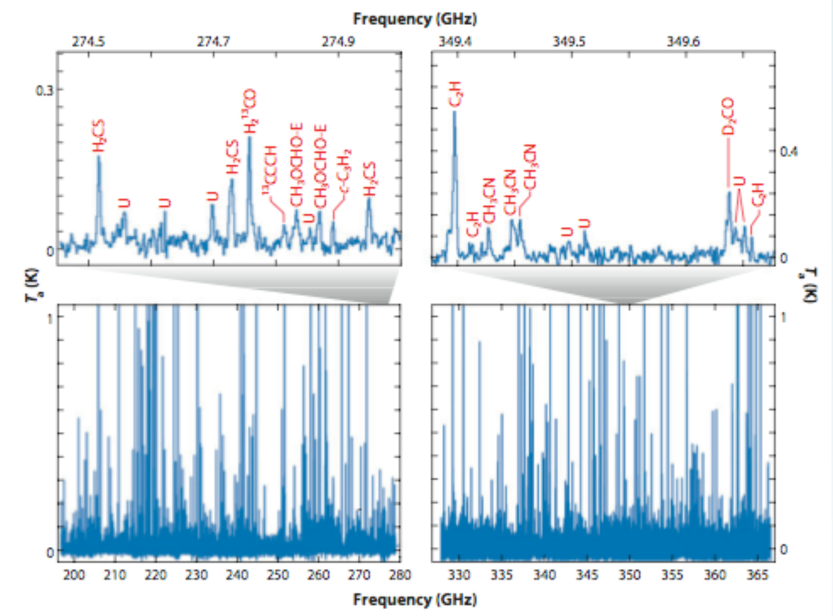
- Organic molecules including CH_3OH, CH_3CN and CH_3C_2H have also been detected in the inner envelopes (≲150 AU) of low-mass deeply embedded Class 0 protostars called hot corinos
- sizes < 150 AU

  $n > 10^8$ cm^{-3}

  T > 100 K

  [H_2CO] and [CH_3OH] has a jump from ~10^{-9} in the outer region to at least 10^{-7} in the inner part where the temperature is above ~90 K (150 AU radius) ➔ supporting the theory that grain mantles sublime in these regions.

IRAS 16293-2422

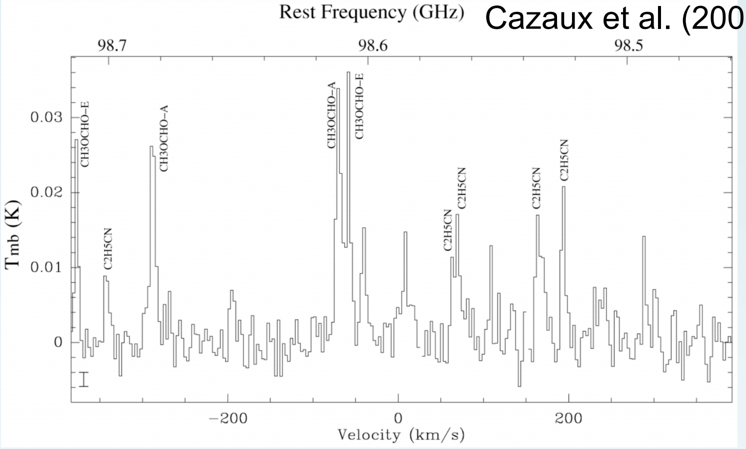


Caux et al. (2005)

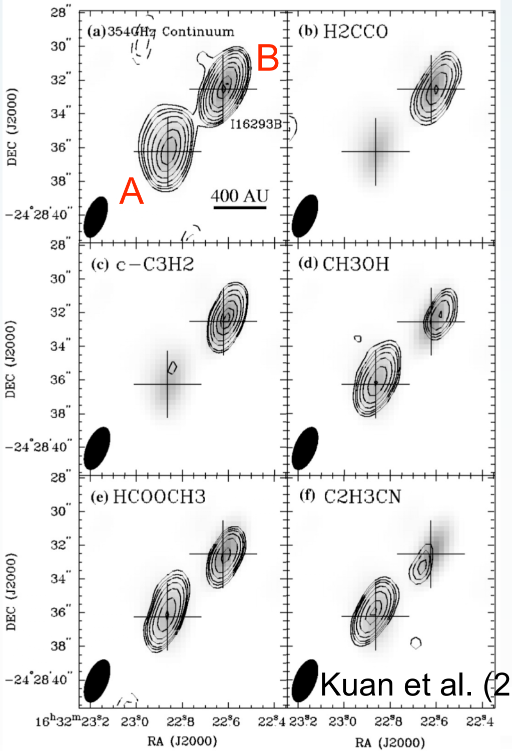
- The gravitational energy from the infalling material is released into radiation, and the matter at the center of the infalling envelope warms up (Ceccarelli et al. 1996). As with the hot cores, where the dust temperature is larger than about 100 K, the grain mantles are sublimated and all their components are injected into the gas phase.
- Alternatively, jets and shocks could responsible for enhancing temperature and abundances (Chandler 2005)

Hot Corinos: IRAS 16293-2422

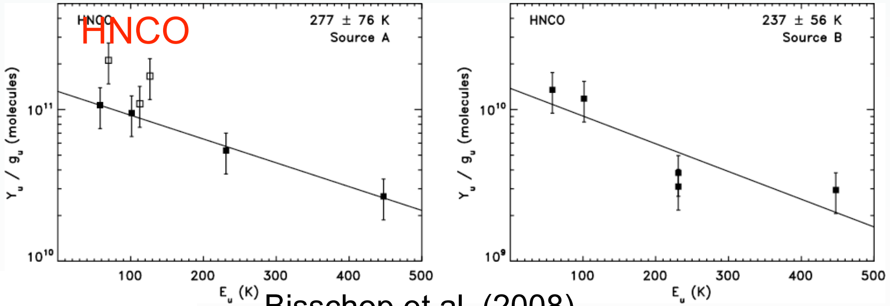
- The first hot corino to be discovered was the protostar IRAS 16293-2422 in Ophiucus ($L = 27\ L_{\odot}$, $M_{\mathrm{env}\ >10\ \mathrm{K}} = 5\ M_{\odot}$, d = 125 pc).
- Single-dish observations by Cazaux et al. (2003) proved that this source is exceptionally rich in organic complex O- and N-bearing molecules such as formic acid, acetaldehyde, methyl formate, dimethyl ether, acetic acid, methyl cyanide, ethyl cyanide, and propyne.
- Interferometric observations show that IRAS 16293-2422 is a proto-binary, with the two YSOs separated by about 800 AU (5”), where each binary component has its own circumstellar disk of radius ~50 AU.
- The temperatures are high enough to evaporate the icy mantles and release organic molecules



Cazaux et al. (2003)

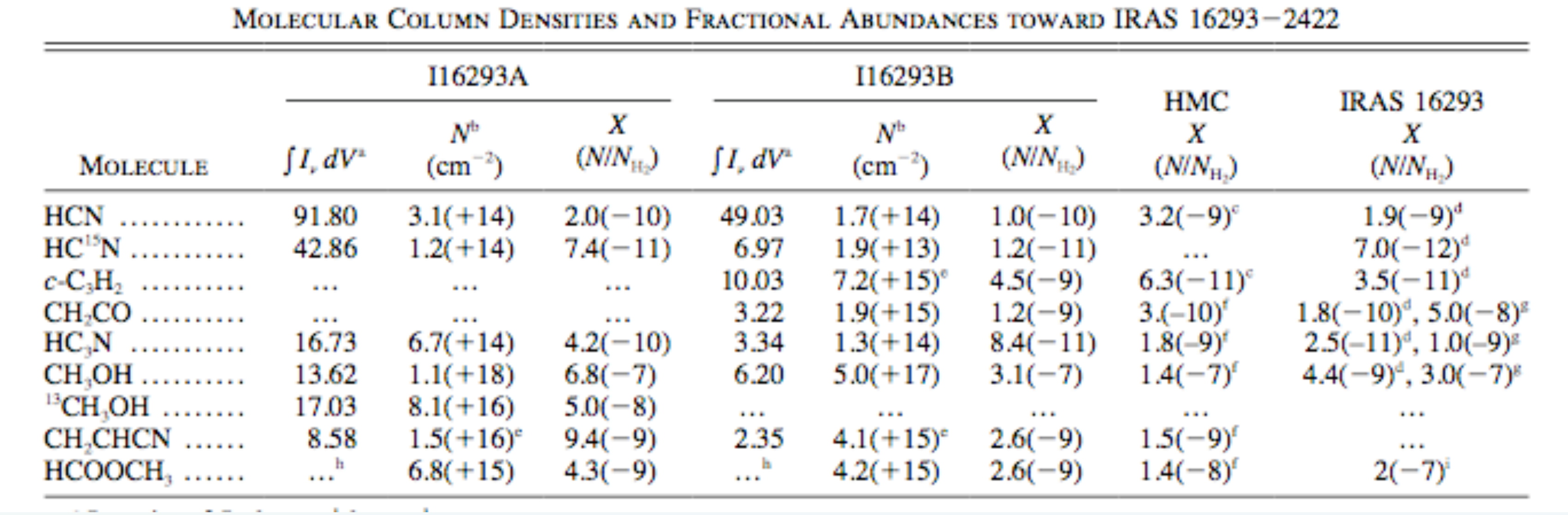


Kuan et al. (2004)



Bisschop et al. (2008)

Hot Corinos: IRAS 16293-2422



MOLECULAR COLUMN DENSITIES AND FRACTIONAL ABUNDANCES TOWARD IRAS 16293−2422

	I16293A			I16293B			HMC	IRAS 16293
MOLECULE	$\int I_\nu\, dV$[a]	N[b] (cm^{-2})	X (N/N_{H_2})	$\int I_\nu\, dV$[a]	N[b] (cm^{-2})	X (N/N_{H_2})	X (N/N_{H_2})	X (N/N_{H_2})
HCN …………	91.80	3.1(+14)	2.0(−10)	49.03	1.7(+14)	1.0(−10)	3.2(−9)[c]	1.9(−9)[d]
$HC^{15}N$ …………	42.86	1.2(+14)	7.4(−11)	6.97	1.9(+13)	1.2(−11)	…	7.0(−12)[d]
c-C_3H_2 …………	…	…	…	10.03	7.2(+15)[e]	4.5(−9)	6.3(−11)[c]	3.5(−11)[d]
CH_2CO …………	…	…	…	3.22	1.9(+15)	1.2(−9)	3.(−10)[f]	1.8(−10)[d], 5.0(−8)[g]
HC_3N …………	16.73	6.7(+14)	4.2(−10)	3.34	1.3(+14)	8.4(−11)	1.8(−9)[f]	2.5(−11)[d], 1.0(−9)[g]
CH_3OH …………	13.62	1.1(+18)	6.8(−7)	6.20	5.0(+17)	3.1(−7)	1.4(−7)[f]	4.4(−9)[d], 3.0(−7)[g]
$^{13}CH_3OH$ ………	17.03	8.1(+16)	5.0(−8)	…	…	…	…	…
CH_2CHCN ……	8.58	1.5(+16)[e]	9.4(−9)	2.35	4.1(+15)[e]	2.6(−9)	1.5(−9)[f]	…
$HCOOCH_3$ ……	…[h]	6.8(+15)	4.3(−9)	…[h]	4.2(+15)	2.6(−9)	1.4(−8)[f]	2(−7)[i]

Kuan et al. (2004)

- ❑ The abundances of the complex molecules change significantly between the two binary components, with the southern component richer in nitrogen-bearing species.
- ❑ The apparent absence of c-C_3H_2 and CH_2CO in I16293A suggests pronounced chemical differentiation between the two cores.
- ❑ The derived fractional abundances and relative column densities are in good agreement with those derived for Orion KL and Sgr B2 massive HMCs

How unique is IRAS 16293-2422?

- ❑ Hot corinos are smaller (≲ 150 AU) than hot cores (≲ 10,000 AU) and harder to detect ➔ only found in a handful of sources
- ❑ CH_3OH is normally detected in low-mass cores, but convincing abundance jumps providing evidence for a hot core not
- ❑ NGC 1333 at 220 pc

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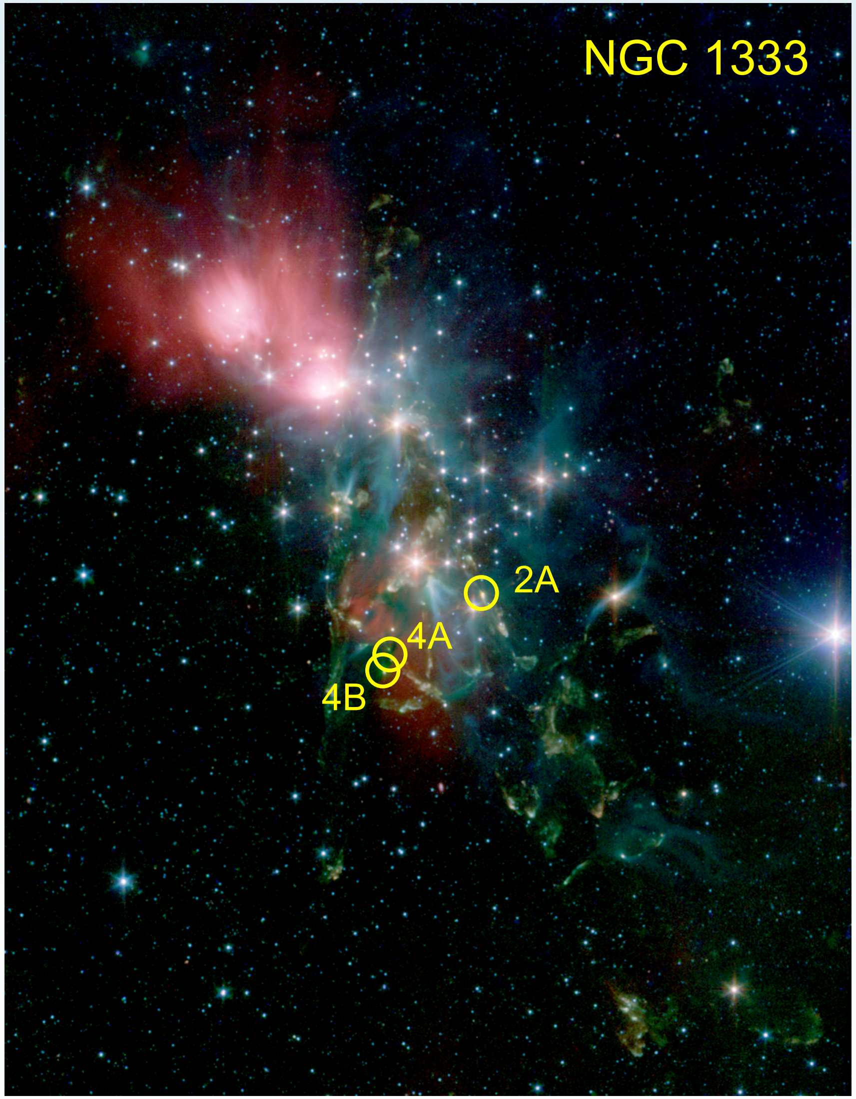
❑ IRAS 2A: $L = 20\ L_\odot$

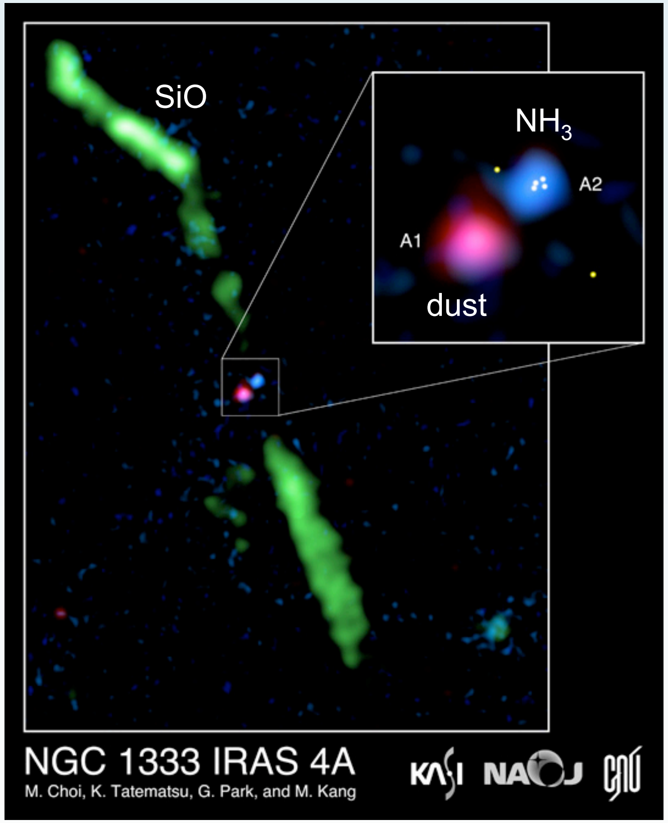
IRAS 4A: $L = 5.8\ L_\odot$

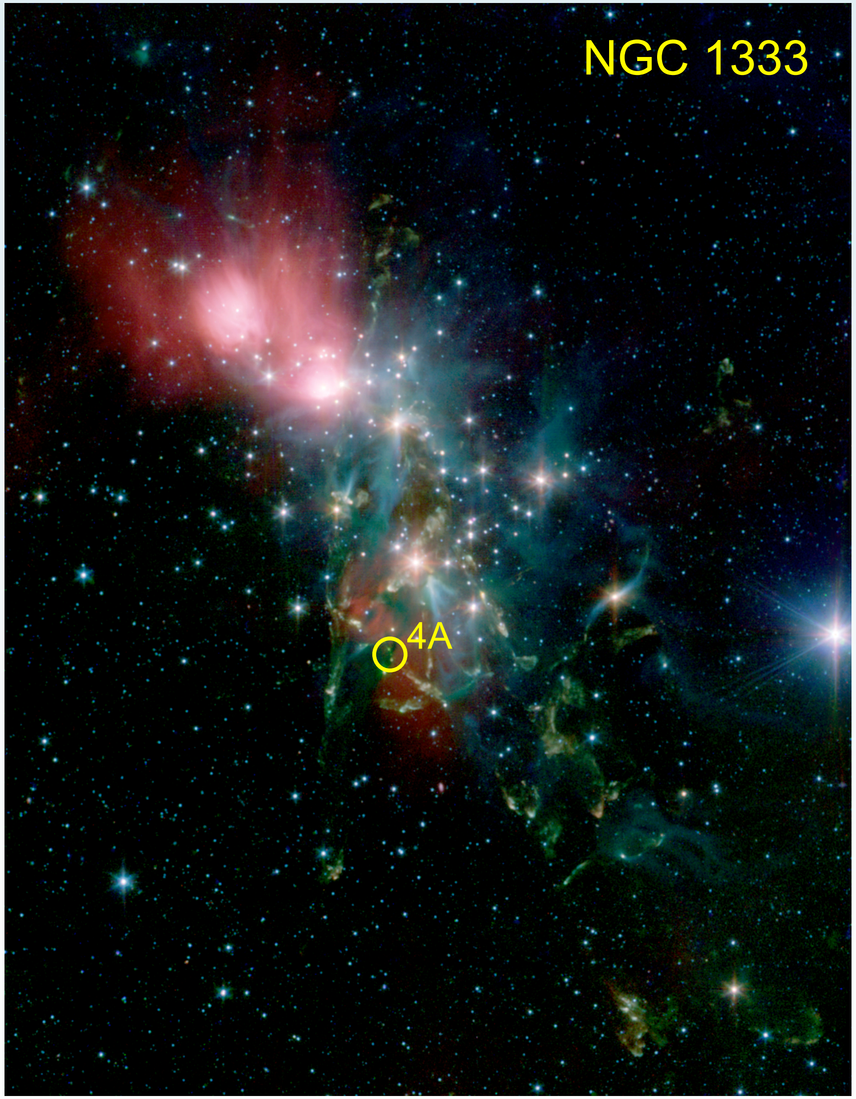
IRAS 4B: $L = 3.8\ L_\odot$



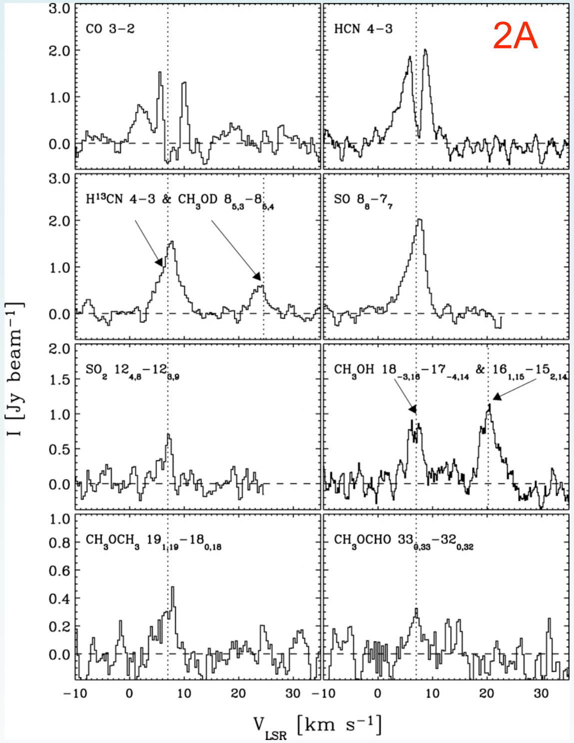
How unique is IRAS 16293-2422?

❑ IRAS 4A is a binary with a separation of 1.8” or of 580 AU

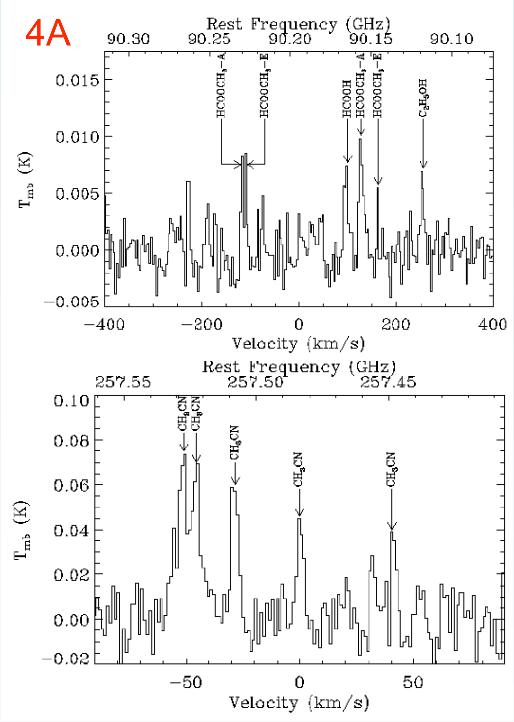




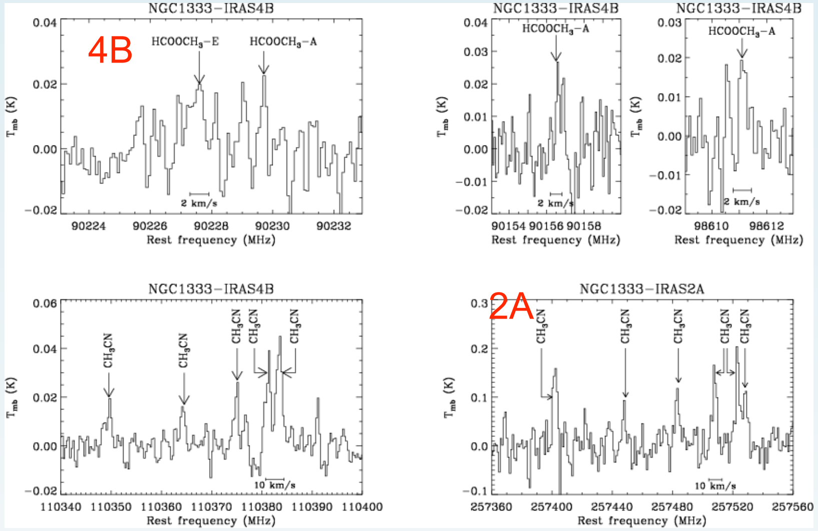
NGC 1333



Jorgensen et al. (2005)

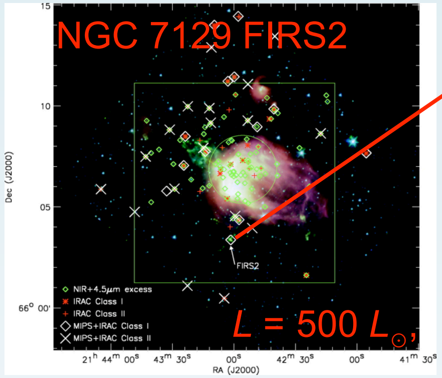


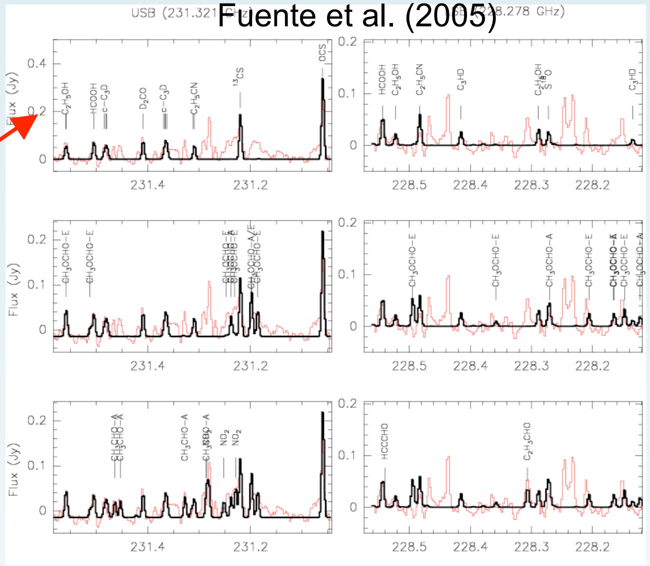
Bottinelli et al. (2004)



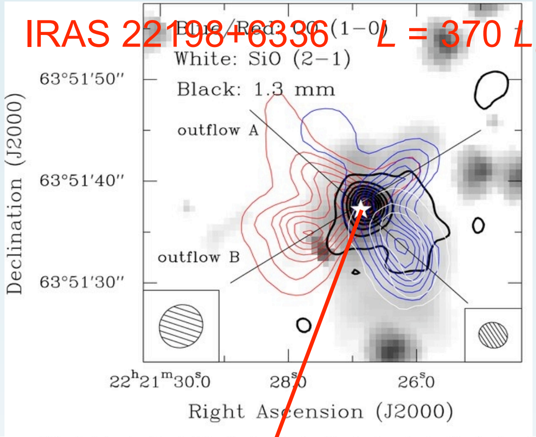
Bottinelli et al. (2007)

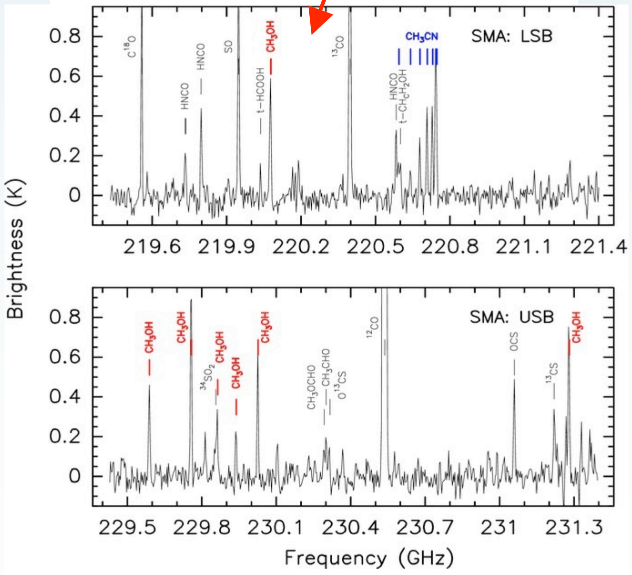
Hot Cores/Corinos in IM protostars



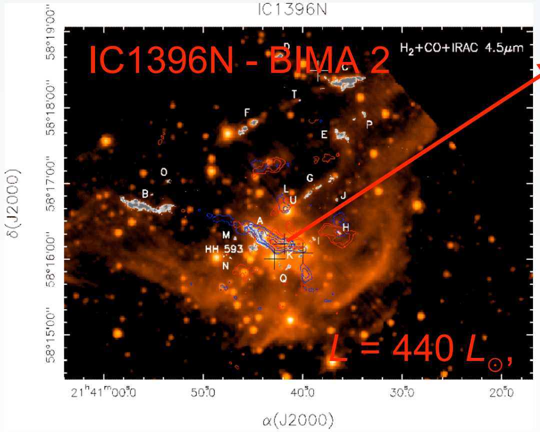


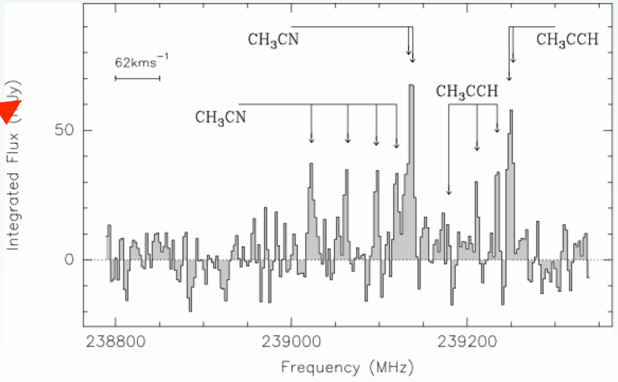
Fuente et al. (2005)





Sánchez-Monge et al. (2010)





Neri et al. (2007)

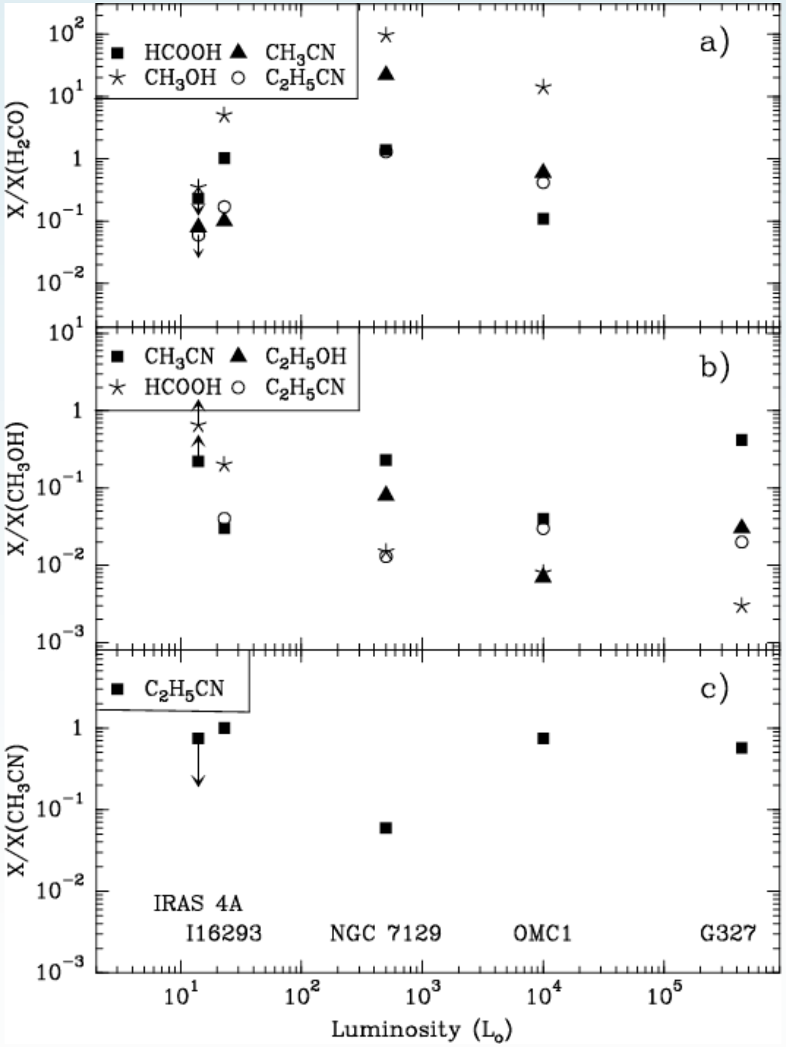
Relative abundances as function of *L*

❑ H_2CO and HCOOH are more abundant in low luminosity sources, while CH_3OH seems to be more abundant in massive objects:

- ➢ $[CH_3OH]/[H_2CO]$, $[CH_3CN]/[H_2CO]$, $[C_2H_5CN]/[H_2CO]$ increases by a factor of ~10 from NGC 1333 IRAS 4A to OMC1. This trend does not present significant differences between O- and N-bearing molecules
- ➢ $[HCOOH]/[CH_3OH]$ decreases by 2 orders of magnitude from NGC 1333 IRAS4 A to G327.3 ➔ the relative abundance of HCOOH seems to decrease with protostellar luminosity
- ➢ $[C_2H_5CN]/[CH_3CN]$ remains quite constant with a dispersion of about a factor <10 between all the sources ➔ the chemistry of both compounds is linked

❑ Possible differences in the grain mantle composition between low and massive SFRs caused by different physical conditions (gas density and dust temperature) during the pre-stellar and accretion phase.

❑ CAVEAT: different spatial scale of observations (0.002 pc NGC 1333 and 0.32 pc OMC1)



Fuente et al. (2005)

Open questions

❑ <u>HOT CORES</u>:

- ➢ which are the abundances and temperatures of complex organic molecules?
- ➢ are the complex organic molecules associated with the inner region of the hot core or with the more external envelope?
- ➢ are glycine and other biologically important molecules present in HMCs?
- ➢ which is formation route for complex molecules? Gas-phase reactions of HCO with methanol and/or formaldehyde? Surface-reactions?

❑ <u>HOT CORINOS</u>:

- ➢ how common are hot corinos?
- ➢ which are the formation mechanisms of complex molecules? Are they released by the sublimation (heating) of icy mantles or by shocks produced by jets and outflows?
- ➢ how do the abundances vary with stellar luminosity?

Open questions

❑ ALMA will resolve hot core/corino regions and map the distribution of molecules on scales smaller than 100 AU

❑ ALMA will allow simultaneous observations of several transitions for the same species and derive temperature and densities

❑ The data will be used to study the physical structure and dynamics of hot cores/corinos necessary to understand their chemistry and the formation of complex organic molecules (thermal evaporation vs. liberation of icy mantles in shocks)

❑ ALMA will allow searches of complex molecules two orders of magnitude deeper (to abundances of $< 10^{-13}$ with respect to H_2) thanks to its much higher sensitivity to compact emission.

❑ ALMA will allow the observation of new complex molecules: in particular, pre-biotic molecules. Systematic search of pre-biotic molecules (glycine, adenine, and other DNA bases) will constrain astro-biological theories: could comets have 'seeded' the primordial Earth with water and other chemical ingredients required to kick start life?