Exploring the Molecular Complexity of Protostellar Environments with ASAI.

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

B. Lefloch (IPAG), R. Bachiller (OAN)
and the ASAI team

The IRAM Large Program ASAI

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

PI : B. Lefloch (IPAG) & R. Bachiller (OAN)

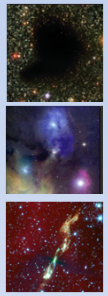
Two Main Goals :

to obtain an evolutive view of chemistry

to constrain the influence of environmental conditions

Unbiased spectral surveys 80-272 GHz of a sample of 10 template sources of the different stages of solar-type star formation

Prestellar cores: young / evolved
Class 0 : Early / Hot Corino / WCCC
Class I
Class II
Shocks



1. Census of the molecular composition:

source intercomparison → time, environmental conditions

2. Derive chemical composition/structure of the sources

comparison with models → quantify chemical differentiation : how and when

3. Characterize the physical and chemical processes at work

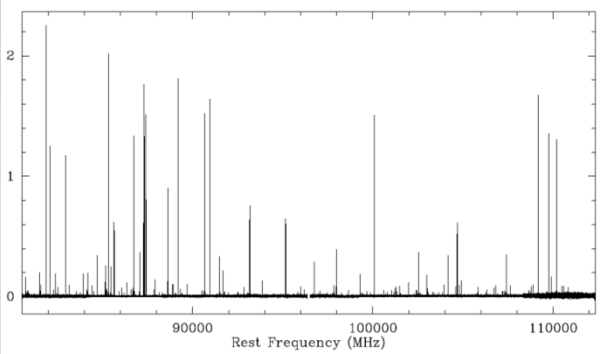
constraints on formation pathways

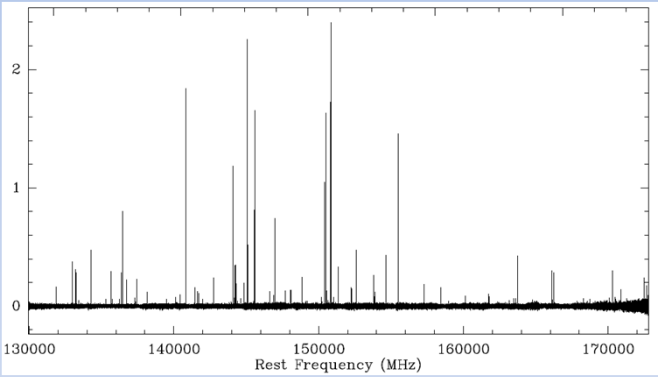
Present status

Data acquisition : completed (10 sources)
Reduction + calibration + line id.: ongoing

Dataset + line catalogues to be released early 2016

Class 0 Protostar L1527 (WCCC)



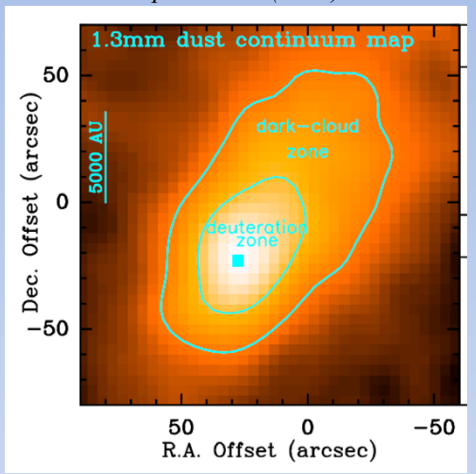


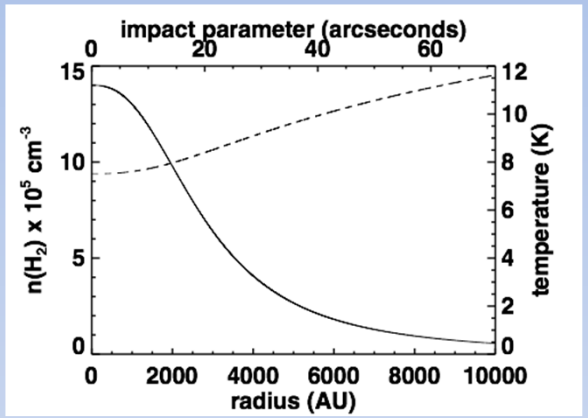
L1527	σ (mK)	Nb Lines (4 σ)	U-Lines	Line density (GHz $^{-1}$)
80-116	3	237	38	7.8
130 - 174	5	153	18	3.7
200-272	5	180	30	2.5
Total		570	86 (15%)	4.0

First publications in 2014:
Complex (n > 6) Organic Molecules

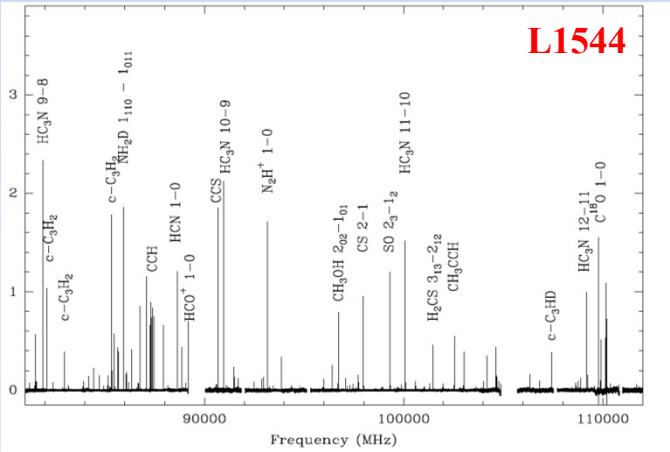
Complex Organic Molecules in L1544

Ward-Thompson et al. (1999)





Crapsi et al. (2007), Caselli et al. (2012)



50 kHz resolution (0.15 km/s) rms : 2-4 mK
$\sigma \simeq 10$ GHz $^{-1}$

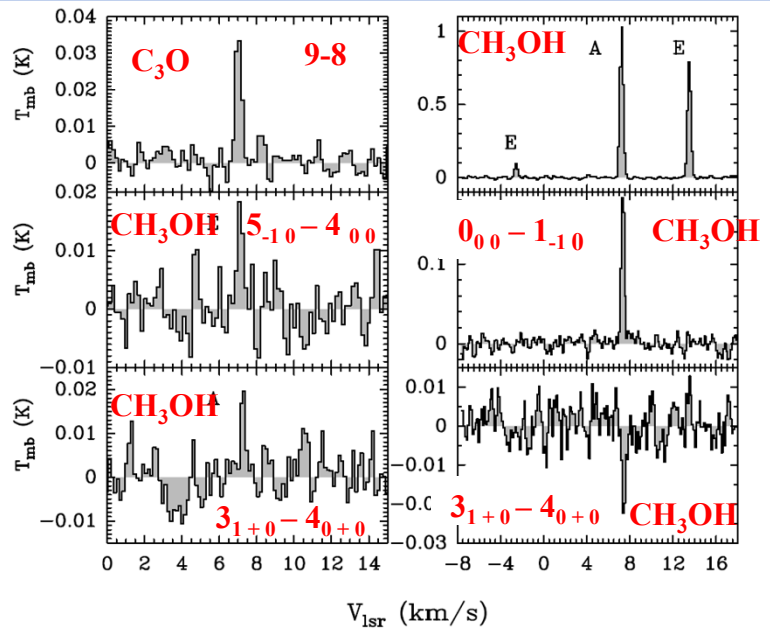
C-chains, Cyanopolyynes, Deuterated species

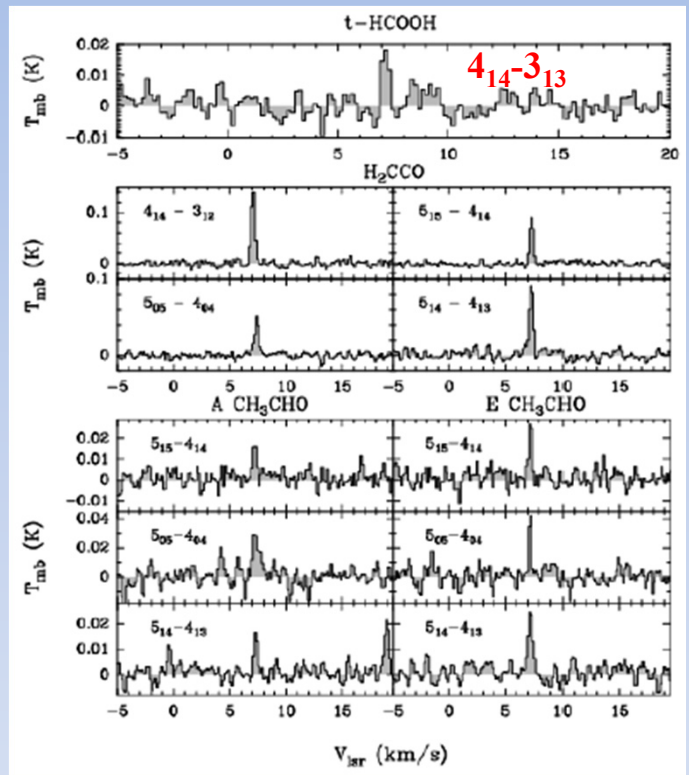
Complex Organic Molecules: N-, C-, O-bearing

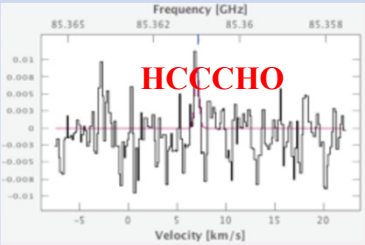
A large degree of molecular complexity degree is already present in the prestellar phase

Complex Organic Molecules in L1544

Census of O-bearing COMs







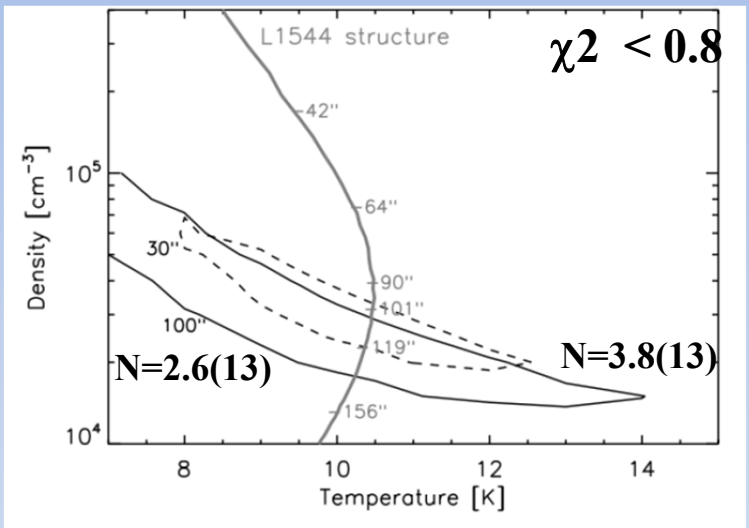
Firm detections	X
CH_3OH (7)	6(-9)
CH_3CHO (8)	1(-10)
t-HCOOH (1)	1(-10)
H_2CCO (4)	1(-9)
HCCCHO (3)	

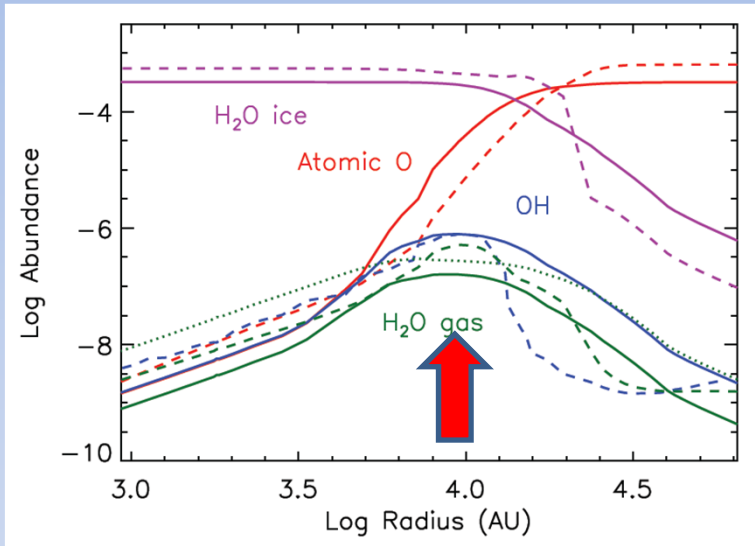
E_{up}= 5 – 30K

Upper Limits	X
CH_3OCH_3	< 2(-10)
$HCOOCH_3$	< 1.5(-9)
CH_3O	< 1.5(-10)

Origin of COM Emission

Comparison with the radial structure of L1544 *(Caselli et al. 2012)*





Best fit solution

Size > 30'' : $n(H_2)$= (1-3)(4) cm^{-3} T= 10-11K N= (2.6-3.8)(13) cm^{-2}

Keto et al. (2014)

CH_3OH (and other COM) arise from the low-density, outer layers at 7000-1000 AU from the core center, where strong UV-photodesorption of water ice is observed.

Gas Phase Modelling

The detection of COMs at T=10K is a challenge for models : Formation/Desorption

NAHOON : time-dependent gas phase chemistry code ***(Wakelam et al. 2012)***

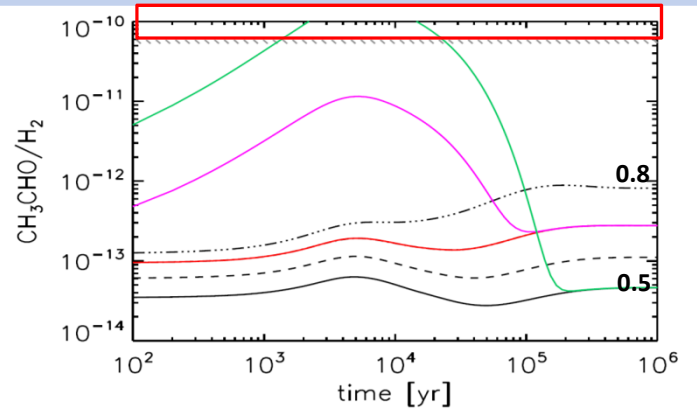
Chemical network : kida.uva.2011: 6680 reactions, 486 species – *Loison et al. (2014)*

Step 1 : Steady-state : C/O= 0.5(0.1)0.8

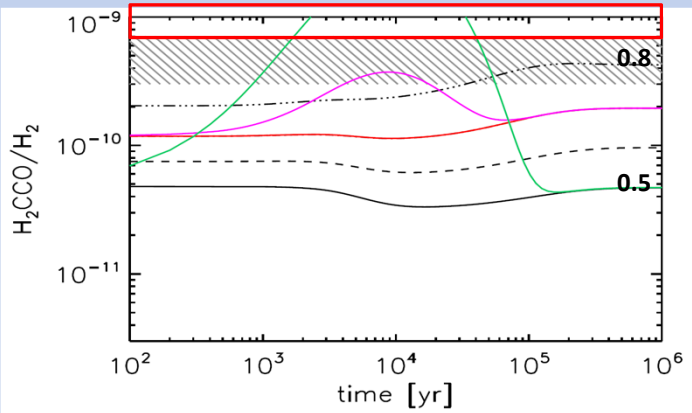
Physical conditions : T=10K, $n(H_2)= 2x10^4$ cm^{-3} $N(H_2)= 10^{22}$ cm^{-2} $\zeta= 3x10^{-17}$ s^{-1}

Step 2 : $[CH_3CHO]$ and $[C_2H_4]$ are increased

CH_3CHO



H_2CCO



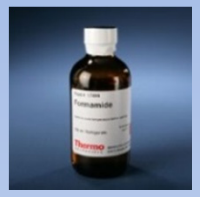
C/O= 0.5
CH_3OH : 1e-8
C_2H_4 : 0, 5e-9, 5e-8

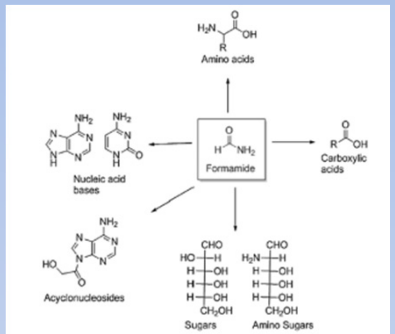
Non-thermal (FUV) desorption of a small amount of CH_3OH and C_2H_4 from grain mantles followed by gas phase reactions could account for the formation of COMs *in the gas phase*

Pre-biotic molecules: Formamide

NH_2CHO: A starting point for prebiotic chemistry ?

Saladino et al. 2012, *Chem. Soc. Rev.* 41, 5526





First detections: SgrB2 (Rubin et al. 1971), Orion KL (Blake 1986), Hot Cores (Bisschop et al. 2007), Hale-Bopp (Bockelee-Morvan 2000), I16293 (Kahane 2013)

Source sample

	Source	d (pc)	M ($M_\odot$)	L_{bol} ($L_\odot$)	Type
pre-stellar	TMC1	140	21	—	PSC - young
	L1544	140	2.7	1.0	PSC - evolved
protostar	B1	200	1.9	1.9	Class 0 - early
	L1527	140	0.9	1.9	Class 0, WCCC
	L1157-mm	325	1.5	4.7	Class 0, WCCC?
	IRAS 4A	235	5.6	9.1	Class 0, HC
	SVS 13A	235	0.34	21	Class 0/1
intermediate mass	OMC-2 FIR 4	420	30	100	IM proto-cluster
	Cep E	730	35	100	IM protostar
outflow shock	L1157-B1	250	—	—	outflow shock

Mendoza et al. 2014, MNRAS 445, 151

López-Sepulcre et al. (*in preparation*)

NH_2CHO detections

	Source	d (pc)	M ($M_\odot$)	L_{bol} ($L_\odot$)	Type
Not detected	TMC1	140	21	—	PSC - young
	L1544	140	2.7	1.0	PSC - evolved
	B1	200	1.9	1.9	Class 0 - early
	L1527	140	0.9	1.9	Class 0, WCCC
	L1157-mm	325	1.5	4.7	Class 0, WCCC?
Detected	IRAS 4A	235	5.6	9.1	Class 0, HC
	SVS 13A	235	0.34	21	Class 0/1
	OMC-2 FIR 4	420	30	100	IM proto-cluster
	Cep E	730	35	100	IM protostar
	L1157-B1	250	—	—	outflow shock

Colder and/or less-evolved regions do not produce enough NH_2CHO to be detectable

First detection of NH_2CHO in shocks : $X \simeq 1(-8)$

NH_2CHO Formation routes

Gas Phase :

Neutral-neutral reactions *(Garrod 2008; Redondo 2014)*

$$NH_2 + H_2CO \rightarrow NH_2CHO + H$$

Radiative association & ion-molecule + e- recombination H_2CO and NH_4^+ (Quan & Herbst; Halfen 2011)

$$H_2CO + NH_4^+ \rightarrow NH_3CHO^+ + H_2$$
$$NH_3CHO^+ + e^- \rightarrow NH_2CHO + H$$

Grain mantles:

Jones (2011) :

$$NH_3 \rightarrow NH_2 + H$$
$$H + CO \rightarrow HCO$$
$$HCO + NH_2 \rightarrow NH_2CHO$$

Raunier (2004), Garrod (2008)

$$HNCO + H \rightarrow H_2NCO$$
$$H_2NCO + H \rightarrow NH_2CHO$$

Link between HNCO and NH_2CHO ?

NH_2CHO Formation routes

Gas Phase :

Neutral-neutral reactions *(Garrod 2008; Redondo 2014)*

$$NH_2 + H_2CO \rightarrow NH_2CHO + H$$

Activation barrier

Radiative association & ion-molecule + e- recombination H_2CO and NH_4^+ *(Quan & Herbst; Halfen 2011)*

$$H_2CO + NH_4^+ \rightarrow NH_3CHO^+ + H_2$$
$$NH_3CHO^+ + e^- \rightarrow NH_2CHO + H$$

Theory/experiments needed

Grain mantles:

Jones (2011) :

$$NH_3 \rightarrow NH_2 + H$$
$$H + CO \rightarrow HCO$$
$$HCO + NH_2 \rightarrow NH_2CHO$$

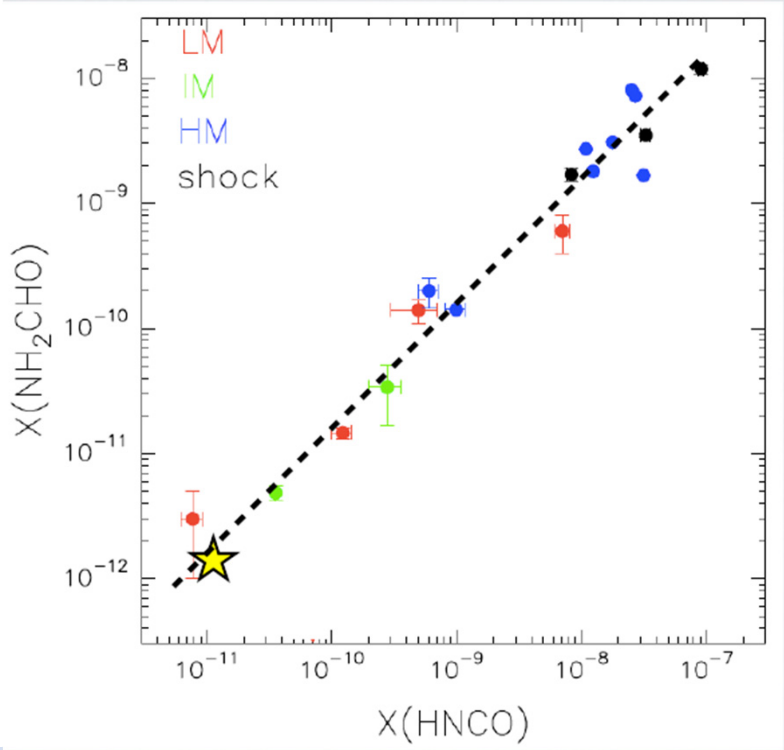
Raunier (2004), Garrod (2008)

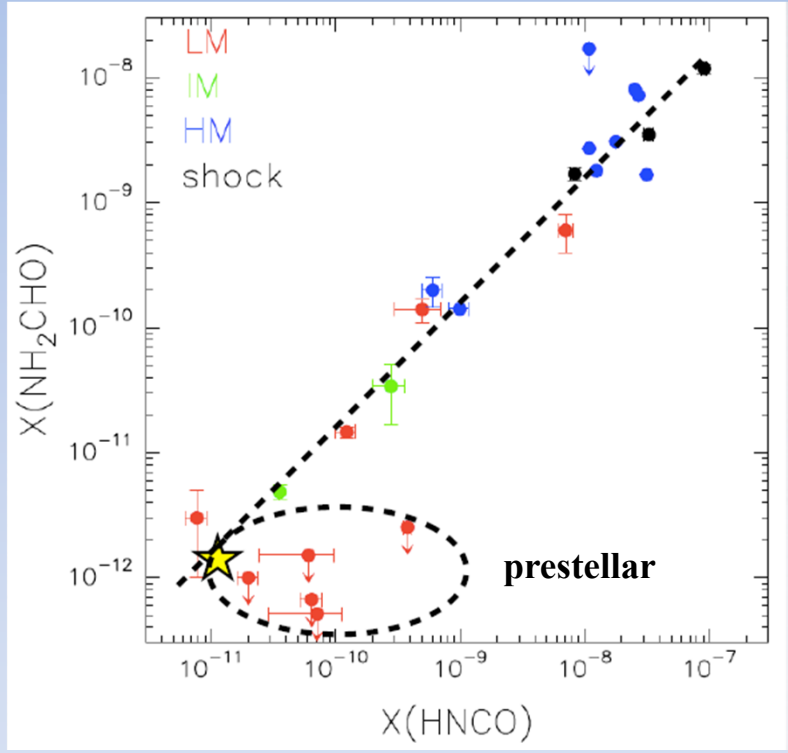
$$HNCO + H \rightarrow H_2NCO$$
$$H_2NCO + H \rightarrow NH_2CHO$$

Link between HNCO and NH_2CHO ?

The link between NH_2CHO and HNCO

Linear relation : Rd ≃ 10





(a) One forms from the other, e.g. hydrogenation of HNCO
(b) Both formed from the same parent molecular species

Excess HNCO: formed in gas phase (Marcelino et al. 2009)
NH_2CHO formation on icy grain mantles, then evaporated

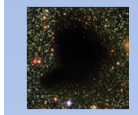
Conclusions and Perspective

Exploitation of ASAI is just starting : about 15% of lines remain to be identified: help from spectroscopists needed !

Comprehensive study of Complex Organic Molecules in prestellar cores:
A puzzle resolved ? Emission from outer layers.
FUV photodesorption + gas phase reactions could account for COM formation. Theoretical work and modelling needed to quantify its efficiency.

First comprehensive study of NH_2CHO in solar-type environments:
Observations suggest NH_2CHO formation on dust grains, possibly from hydrogenation of HNCO and subsequent sublimation/sputtering in the gas phase. Actual formation route remains speculative : more experimental/theoretical studies are needed.

First Results of the ASAI Team



Prestellar Phase

Tentative detection of the nitrosylium ion NO^+ in Barnard 1, J. Cernicharo, S. Bailleux, E. Alekseev, A. Fuente, E. Roueff, M. Gerin, B. Tercero, S.P. Trevino-Morales, N. Marcelino, R. Bachiller, B. Lefloch, 2014, ApJL, 794

The origin of complex organic molecules in prestellar cores , C. Vastel, C. Ceccarelli, B. Lefloch, R. Bachiller, 2014, ApJL,

The ionic content of Barnard 1 , J. Cernicharo, A.Fuente et al, in prep

Protostellar Phase

First results from the IRAM Large Programme ASAI: Formamide (NH_2CHO) in star-forming regions, A.Lopez-Sepulcre, E. Mendoza, A. A. Jaber, B. Lefloch, C. Ceccarelli, E. Caux, C. Codella, M. Tafalla, C. Vastel, R. Bachiller, submitted

Jets and Shocks

Molecular ions in the protostellar shock L1157-B1, Podio L., Lefloch B., Ceccarelli C., Codella C., and Bachiller R., 2014, A&A, 565, 64

The density structure of the L1157 protostellar outflow Gomez-Ruiz, A., Codella, C., Lefloch, B., Benedettini, M., Busquet, G., Ceccarelli, C., Nisini, B., Podio, L., Viti, S., 2014, MNRAS, in press

Molecules with a peptide link in protostellar shocks: a comprehensive study of L1157-B1 E. Mendoza, A. Lopez-Sepulcre, C. Ceccarelli, C. Codella, H. M. Boechat-Roberty, R. Bachiller, 2014, MNRAS, 445, 151

A fast molecular jet from L1157-mm, *M. Tafalla , R. Bachiller, B. Lefloch, N.Rodriguez-Fernandez, C. Codella, A. Lopez-Sepulcre, L. Podio, 2014, in prep*

Protoplanetary disk

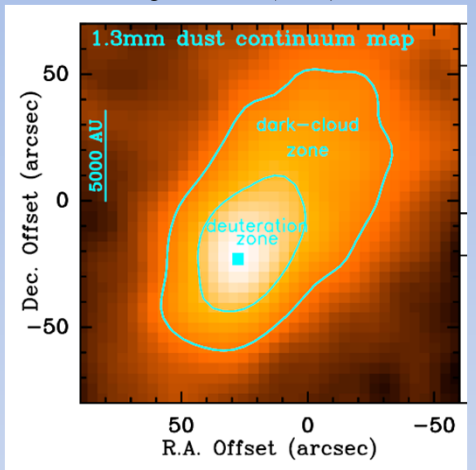
ASAI first results of the chemical composition of the circumstellar disk around AB Aurigae, S. Pacheco-Vázquez, A. Fuente, M. Agúndez, C. Pinte, T. Alonso-Albi, R. Neri, J. Cernicharo, J. Goicoechea, O.Berné, L.Wiesenfeld, R.Bachiller, and B.Lefloch, 2014, in prep

More to come soon !

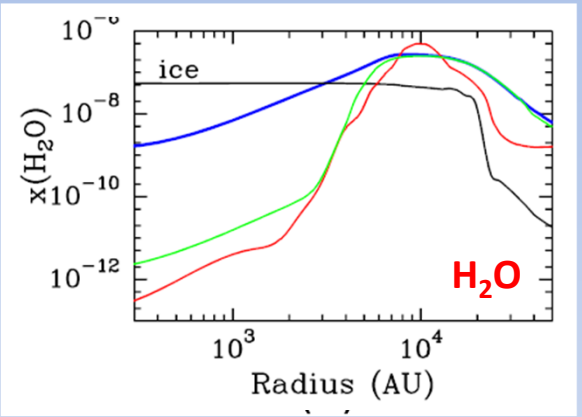
Complex Organic Molecules in L1544

Vastel et al. (2014)

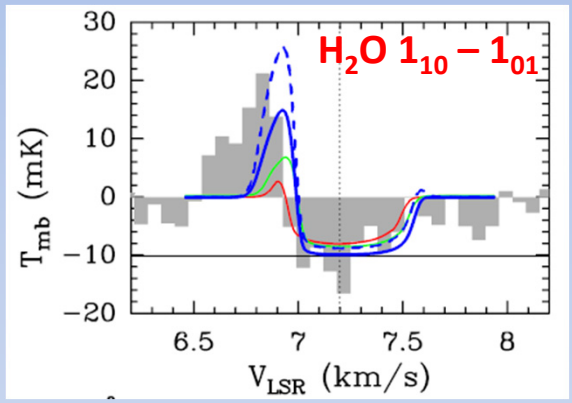
Ward-Thompson et al. (1999)



Crapsi et al. (2007), Caselli et al. (2012)



Caselli et al. (2012) Keto et al. (2014)



Gravitational contraction of the envelope

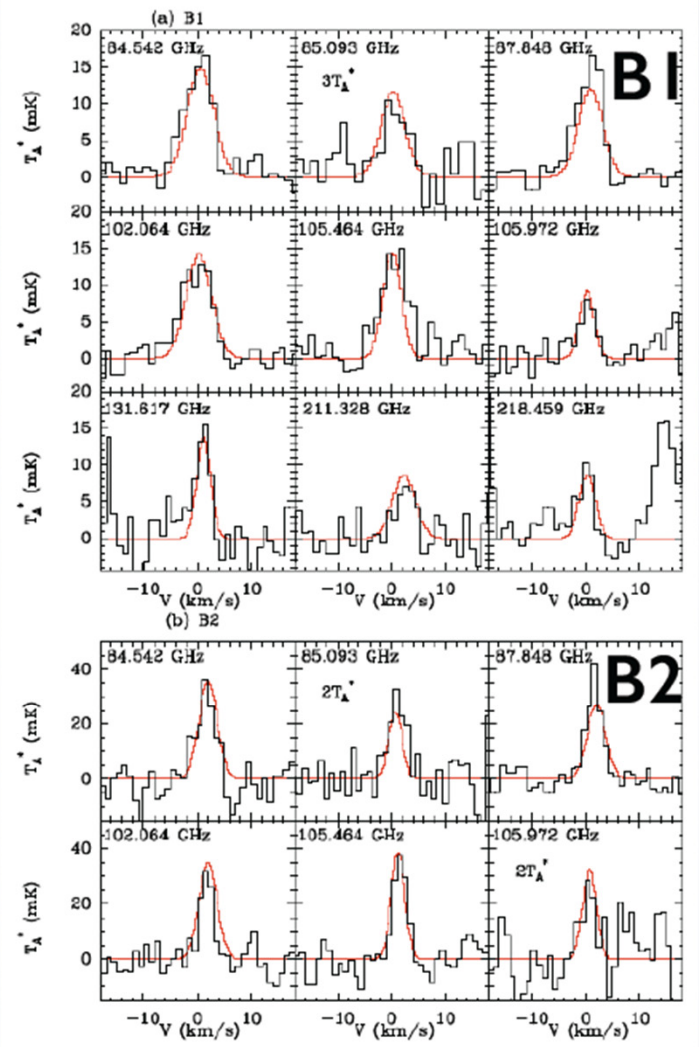
H_2O : Abundances Xi ≈ 10^{-9} Xe ≈ 10^{-7}

Photodesorption of H_2O ices due to :

FUV photons in the external envelope (r > 5000 AU)

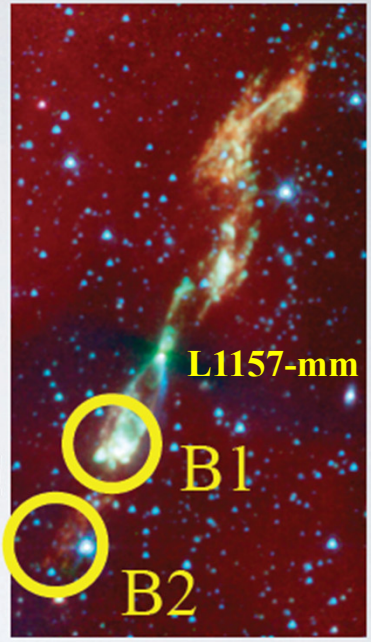
CR-H_2 interaction → dim FUV field ≈ 10^{-3} G_0

Formamide in protostellar shocks



Detections:
B1: 23 lines
B2: 6 lines

$X \sim 10^{-9} - 10^{-8}$
similar to high-mass!



First discovery of NH_2CHO in protostellar shocks

Mendoza et al. (2014)