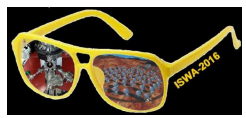
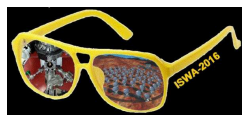
line analysis and chemical modelling the case of NH_2CHO

Edgar Mendoza
IAG/USP, São Paulo

International Symposium and Workshop on Astrochemistry

Campinas
07/07/2016




ISWA 2016

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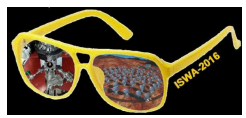
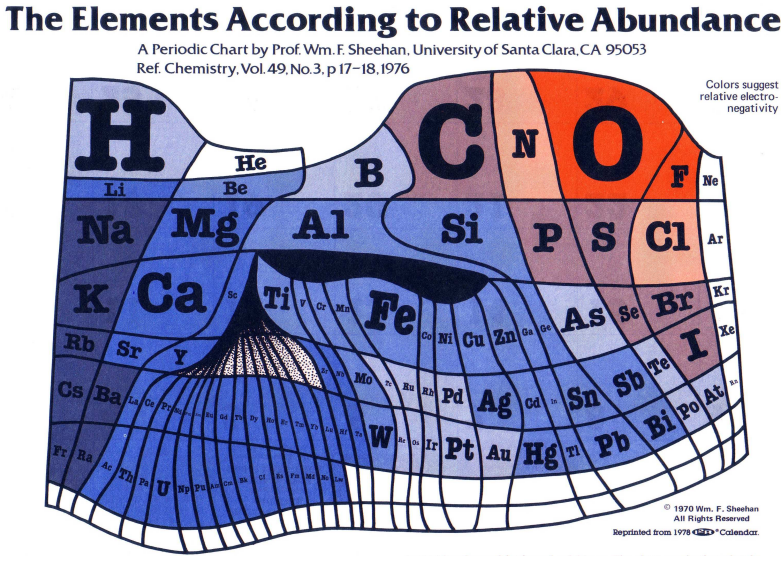
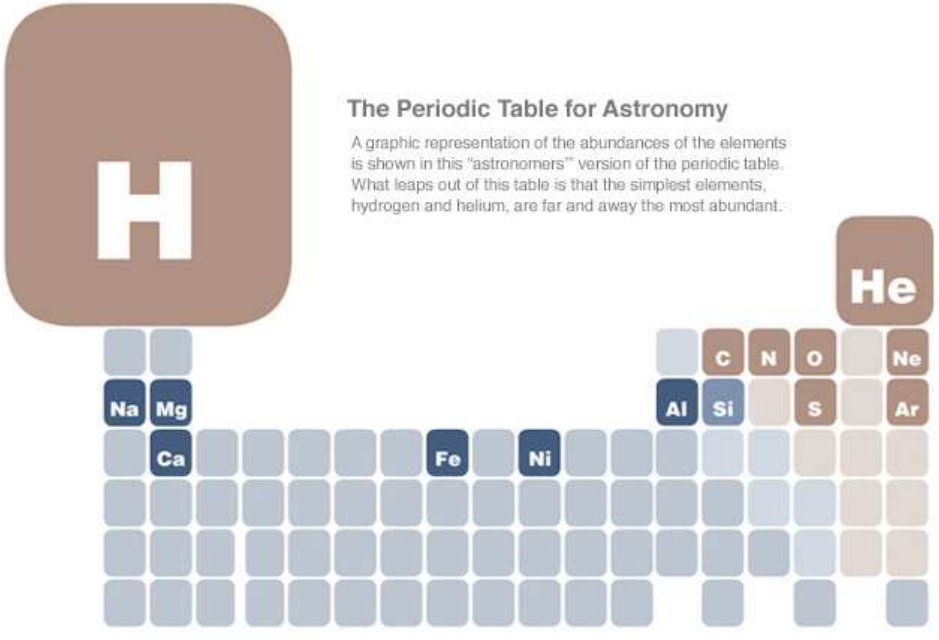
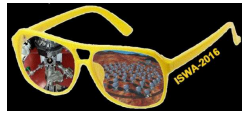


atoms and molecules





Thaddeus et al. 2008 and references therein.

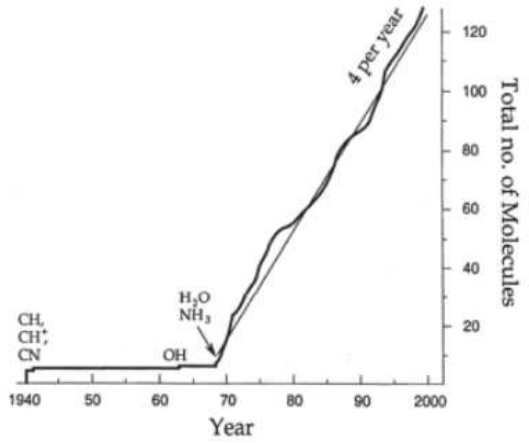


atoms and molecules

Known Interstellar and Circumstellar Molecules (July 2000)

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_2O^+	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≡CCN	CH_3NC	CH_2CHCN	C_7H	$H(C≡C)_3CN$
SiO	HNO	HNCO	CH_2NH	CH_3SH	HC_4CN	H_2C_6	$H(C≡C)_2CH_3$
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^-?		
HCl	NNO	CCCH	c-C_3H_2	H_2CCCC			
NaCl	HCO	c-CCCH	CH_2CN	HC_3NH^+			
KCl	HCO^+	CCCO	C_5	C_5N			
AlCl	OCS	CCCS	SiC_4	C_5S?			
AlF	CCH	HCCH	H_2CCC				
PN	HCS^+	$HCNH^+$	HCCNC				
SiN	c-SiCC	HCCN	HNCCC				
NH	CCO	H_2CN	H_3CO^+				
CH	CCS	c-SiC_3					
CH^+	C_3	CH_3					
CN	MgNC	CH_2D^+?					
CO	NaCN						
CS	CH_2						
C_2	MgCN						
SiC	HOC^+						
CP	HCN						
CO^+	HNC						
HF	SiCN						
	KCN?						

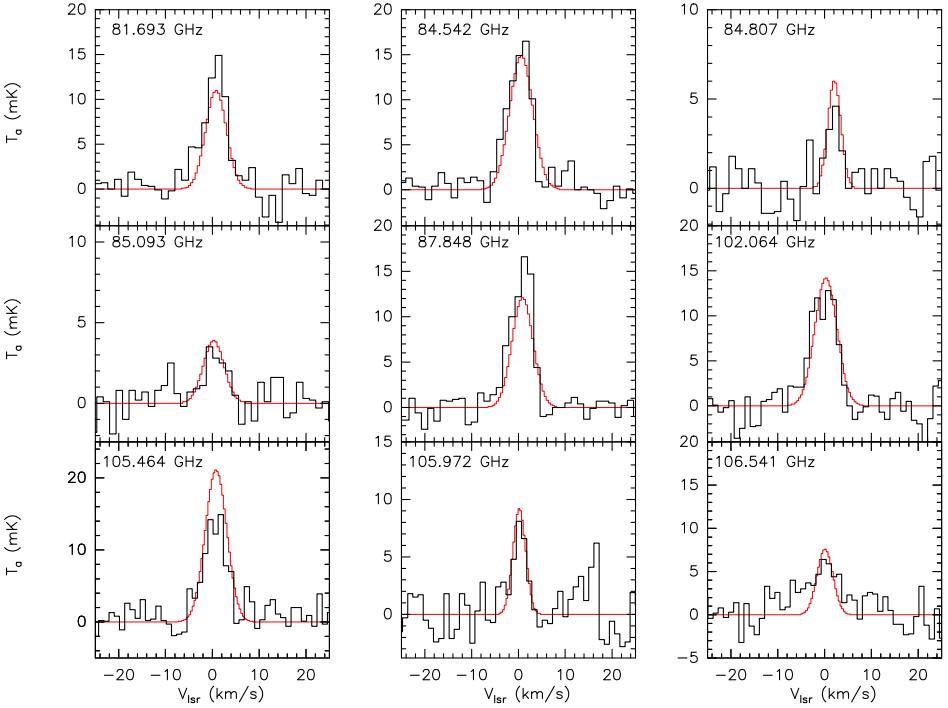
Carbon chains
Complex Organic Molecules
Tracers of shocks and UV-irradiation

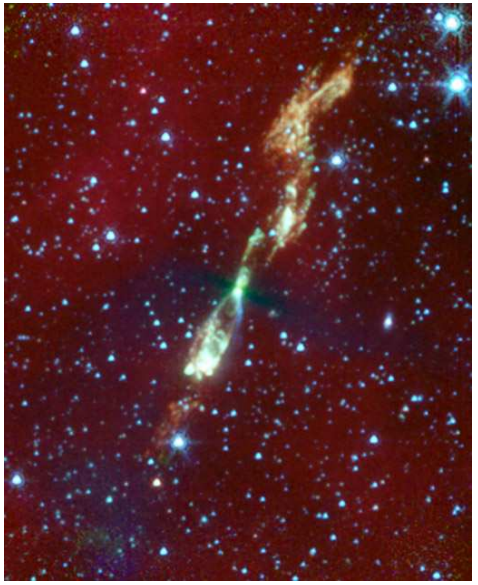


Thaddeus et al. 2008 and references therein.

detection and analysis of NH_2CHO in L1157-B1

- ✓ Identification of lines
- ✓ Analysis: GILDAS + CASSIS
- ✓ Physical conditions: Rotational diagram
- ✓ Chemical modelling: ASTROCHEM

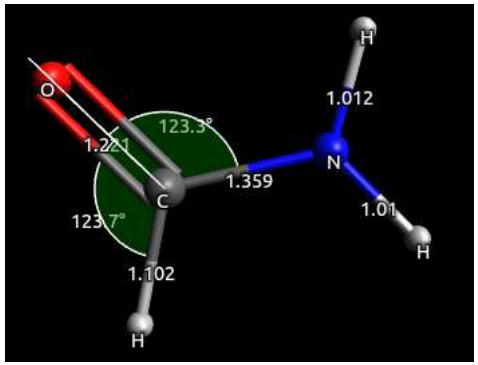


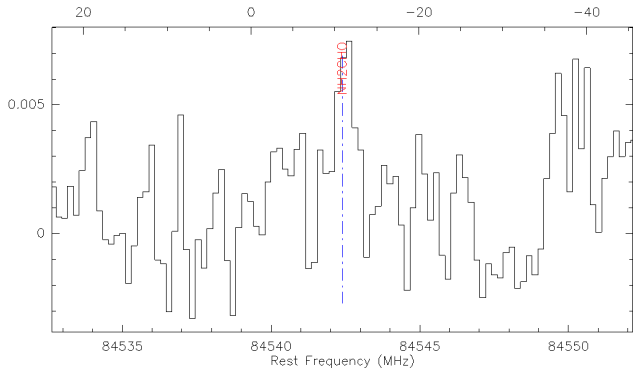


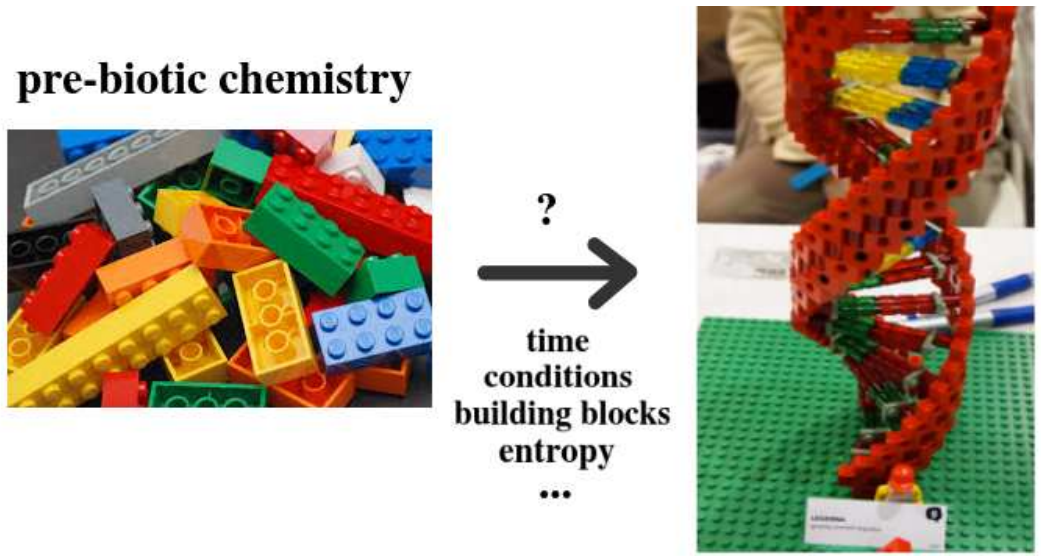
L1157 image (Spitzer Space Telescope IRAC).

Why formamide?

NH_2CHO and HNCO are the simplest molecules with H, C, N and O.







Importance of NH_2CHO as a building block (Saladino et al. 2012).

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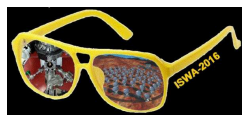


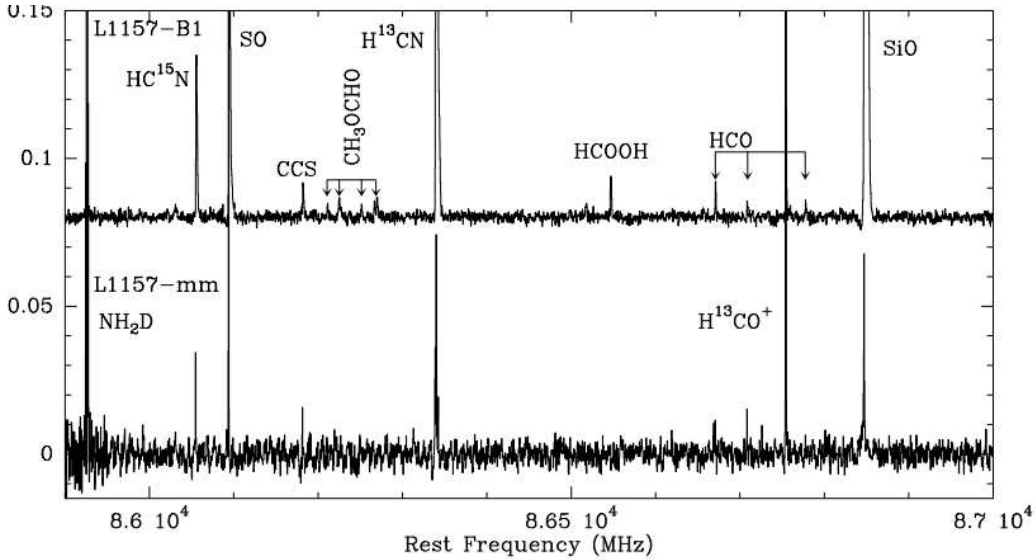
ASAI: Astrochemical Surveys At IRAM

Through ASAI was proposed an unbiased spectral exploration of a carefully selected sample of sources, which cover the full formation processes of solar-type stars.
PIs: Lefloch & Bachiller (350 h with IRAM-30m)

The need for systematic spectral surveys

- Powerful diagnostic to study the chemical evolution of star-forming regions
- It is possible to probe the chemical differentiation along the line of sight of several sources

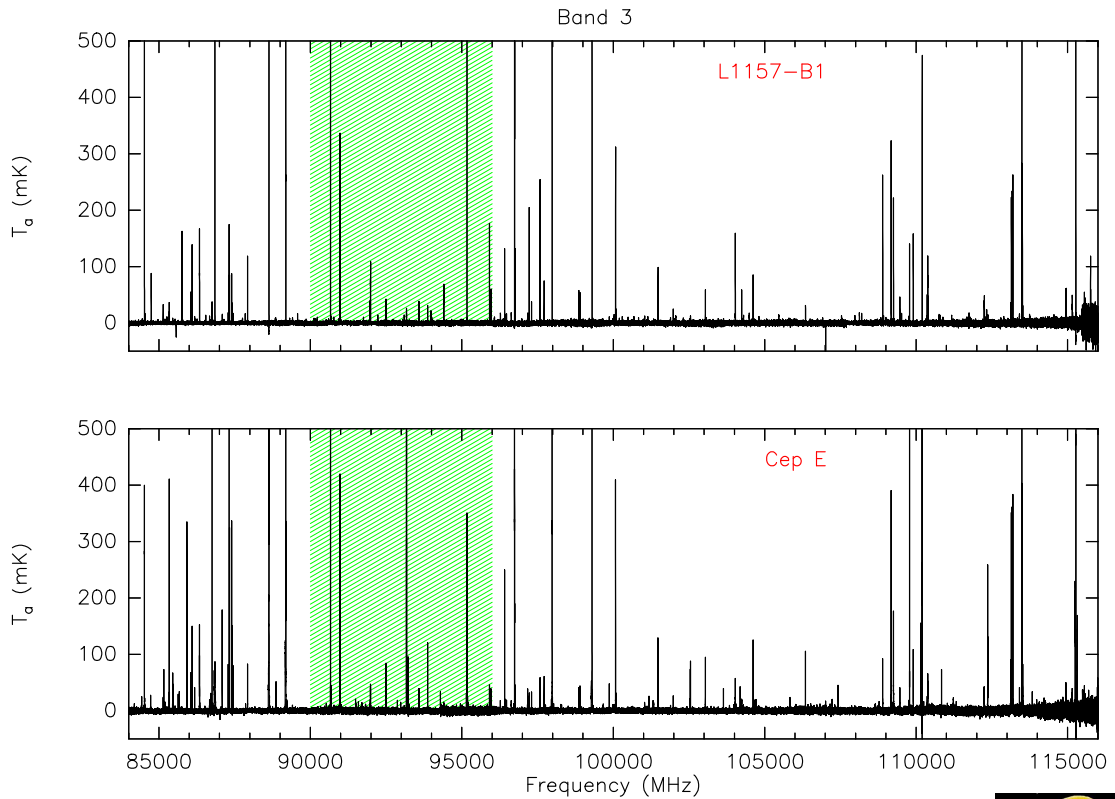
Lefloch (IPAG) & Bachiller (OAN) 2015

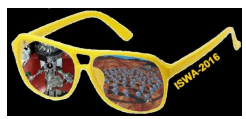


The ASAI large program

Astrochemical Surveys At Iram: 350 hours of observation at IRAM-30m (PIs: Lefloch & Bachiller 2014)
Sources: Samples that cover all the evolutionary phases of solar type protostars

Frequencies observed through ASAI:
3 mm: 80 - 116 GHz
2 mm: 130 - 170 GHz
1.3 mm: 200 - 320 GHz
0.8 mm: 329 - 350 GHz





Data reduction

The data reduction was performed using the GILDAS/CLASS90 package.

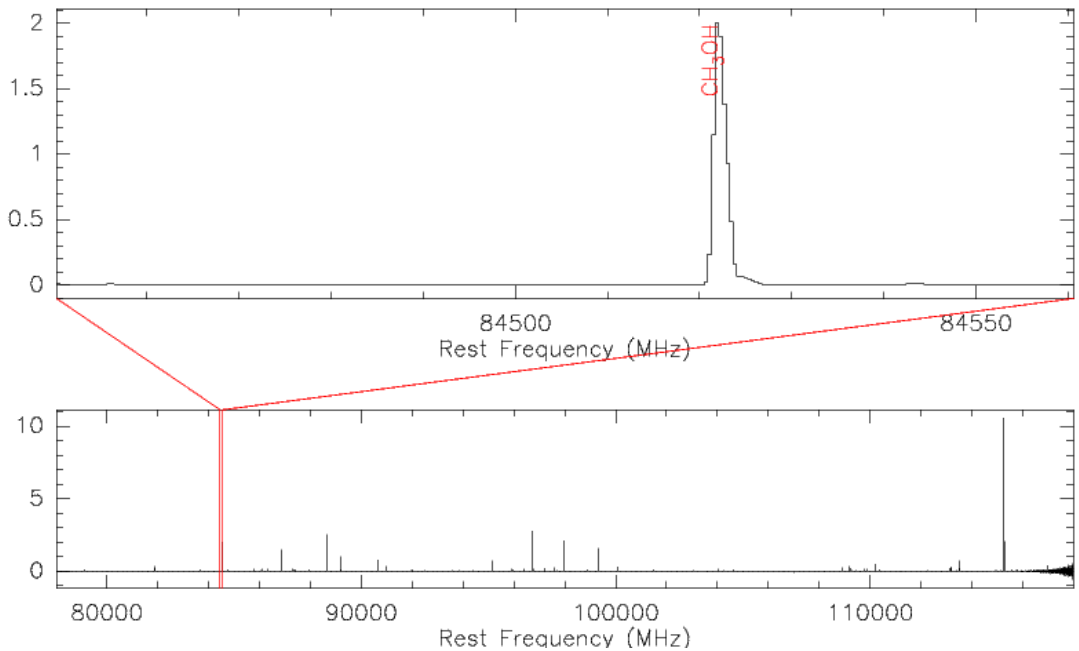
http://www.iram.fr/IRAMFR/GILDAS/

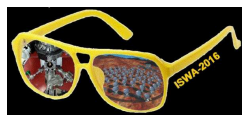
The CDMS and JPL spectroscopy databases were used to identify lines

http://www.astro-uni-koel.de/cgi-bin/cdmssearch
http://spec.jpl.nasa.gov/ftp/pub/catalog/catform.html

The telescope and receiver paramenters:

http://www.iram.es/IRAMES/mainWiki/Iram30mEfficiencies

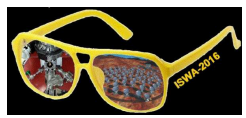




CLASS + Weeds

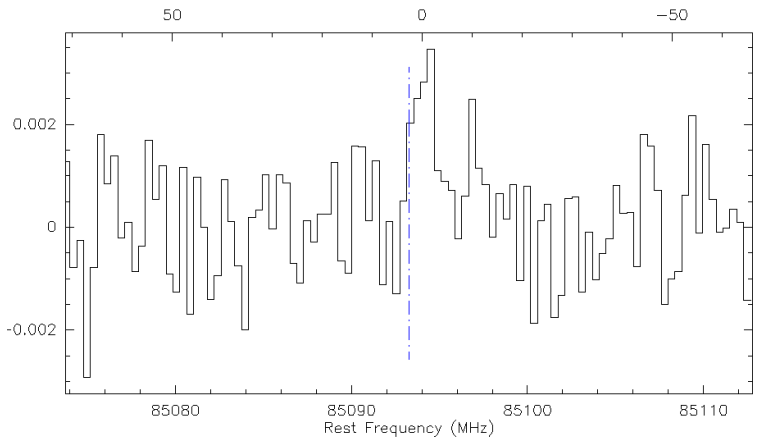
✓Line analysis
✓Modelling considering LTE conditions
✓Databases as CDMS and JPL
https://www.iram.fr/IRAMFR/GILDAS/doc/html/weeds-html/weeds.html
look for weeds.pdf

```
...
* Welcome to CLASS
...
* Loaded extensions
weeds (S.Maret, P.Hily-Blant, J.Pety, S.Bardeau, E.Reynier)
...
Available commands:
LID Identify lines on the current spectra
LFIND Find lines from a species within a frequency range
LLIST List lines from the line index
LGET Get a line from the line index
LPLOT Plot a line from the current line index
MODSOURCE Model the emission of a source at the LTE
MODSHOW Show the results of MODSOURCE
```



Formamide in L1157-B1/ASAI

```
LAS> select /freq 84000 85000
I-SELECT, 3123 lines found in the frequency range 84000.0 to 85000.0 MHz
LAS > select /freq 84541.829 84546.088
I-SELECT, 6 lines found in the frequency range 84541.829 to 84546.088
MHz
LAS> llist
(...)
LAS> lget 2 I-LGET, Found line frequency in the current scan
Species Freq[MHz] Err[MHz] Eup[K] Gup Aij[s-1] Upper level - Lower level
Origin
1 HC(O)NH2, v=0   84542.330   0.000   10.2   9   4.09e-05   4 0 4 - 3 0
3 cdms
```



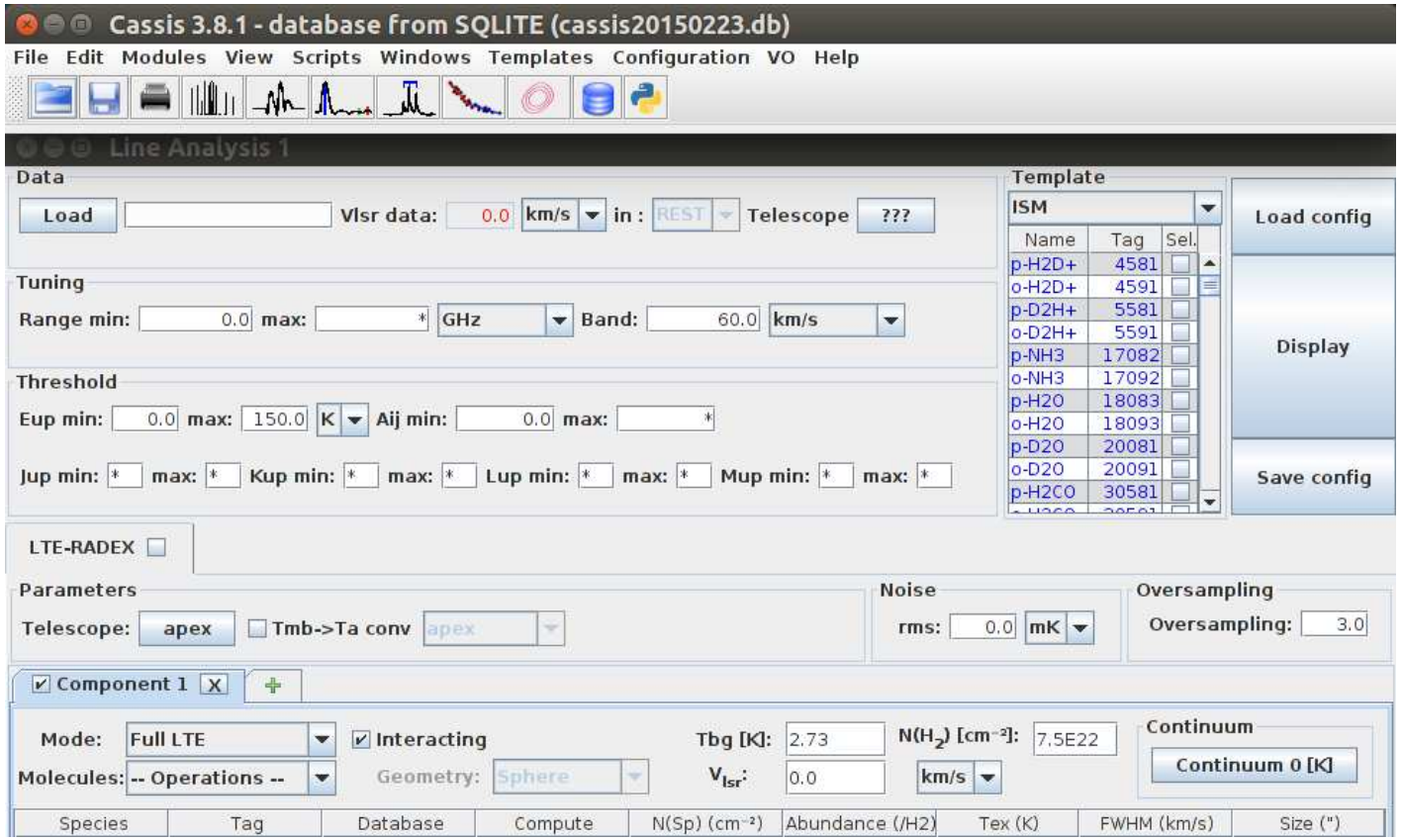

```
LAS> select /freq 85090.609 85097.065
I-SELECT, 32 lines found in the frequency range 85090.609 to 85097.065
MHz
```

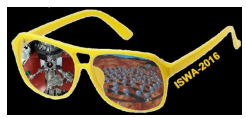
CASSIS

✓ An easy and interactive software to analyse lines

✓ CASSIS is useful to identify and reproduce lines using databases as CDMS, JPL and NIST

All the documentation and information at
http://cassis.irap.omp.eu/?page=cassis





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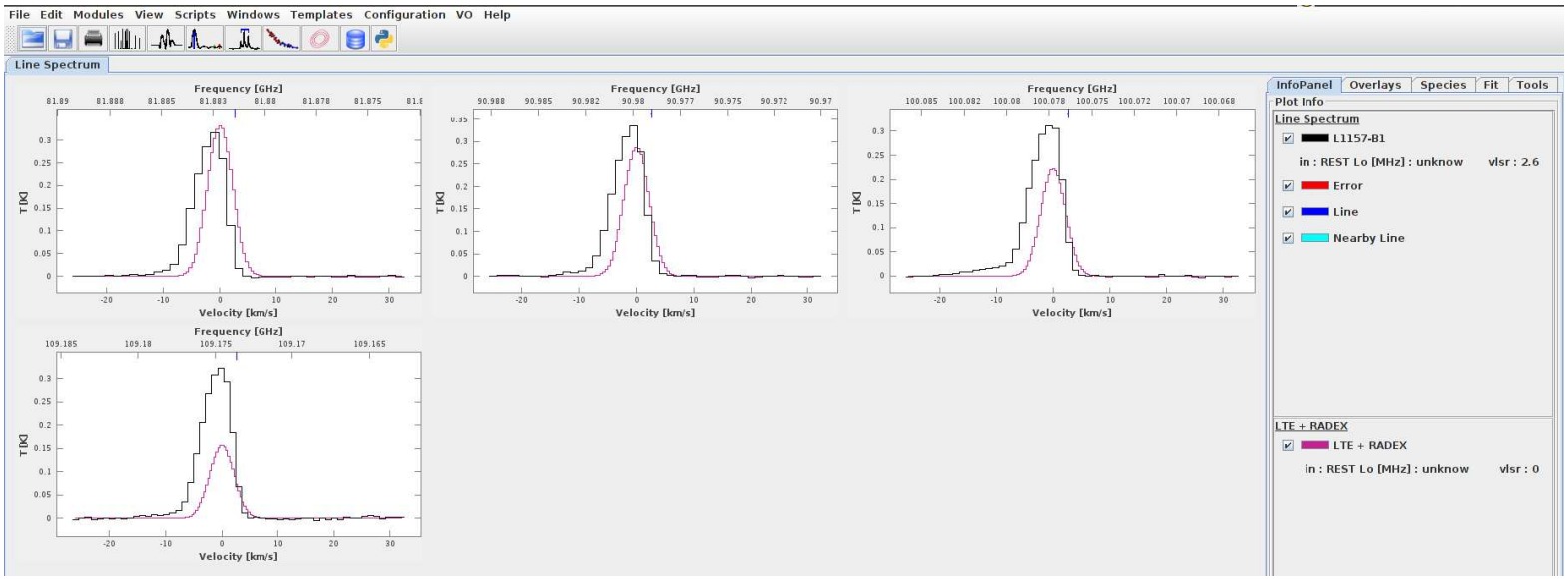
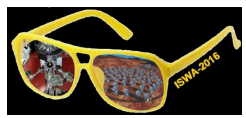
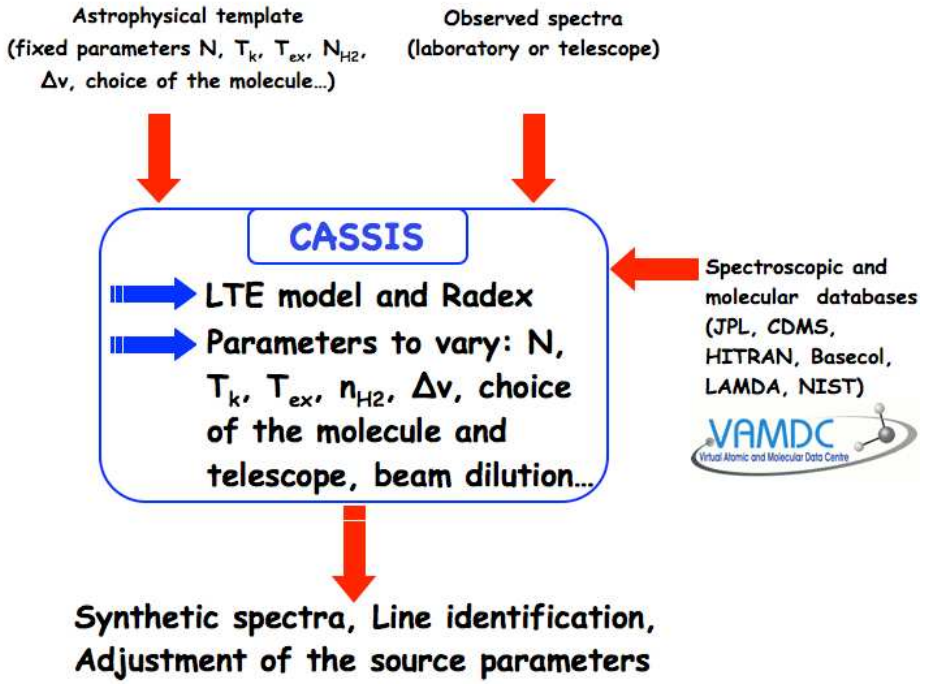
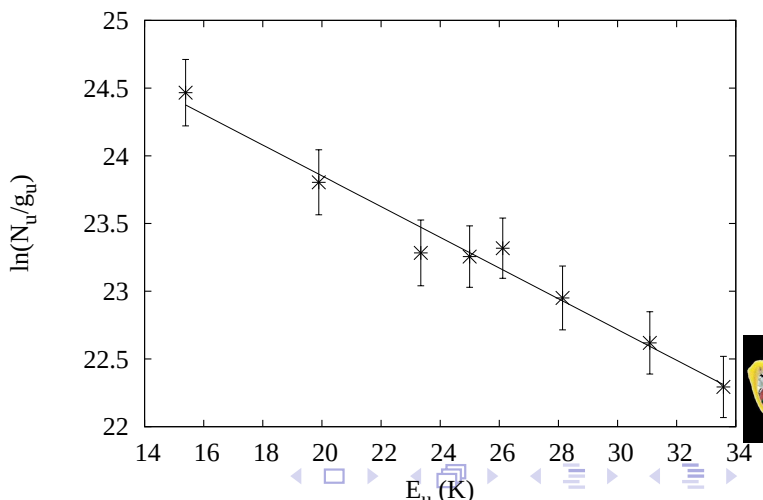


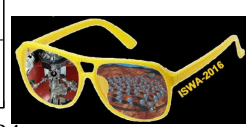


CASSIS functionalities



Frequência MHz	E_u K	$\int T_{mb} dv$ mK km s^{-1}
81505.17	15.4	201 ± 4
86181.39	23.3	6629 ± 3
90686.38	26.1	7489 ± 4
93870.11	19.9	175 ± 3
99866.52	28.1	8043 ± 3
103640.75	31.1	6543 ± 2
106347.72	24.9	154 ± 4
113410.19	33.6	6158 ± 5





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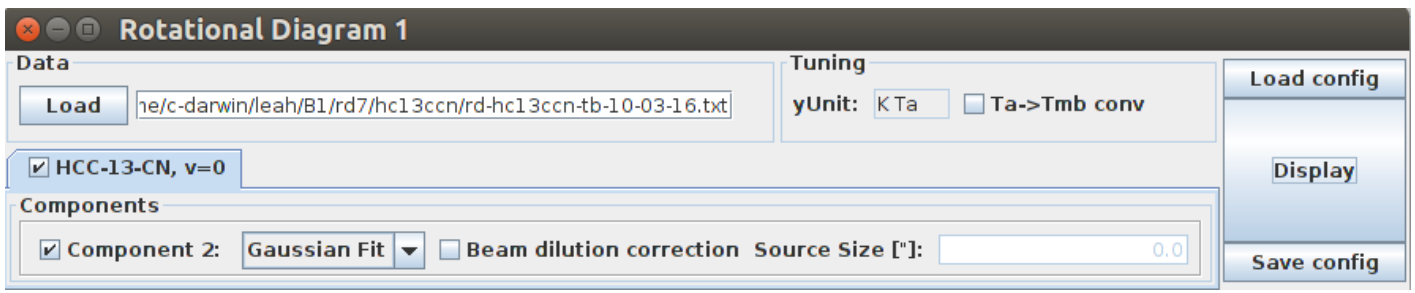
CASSIS Modules: Rotational diagram

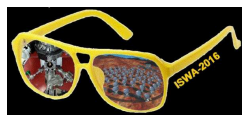
- ✓ Rotational diagram: An important technique to analyse properties from molecular line emission (see Goldsmith et al. 1999).
- ✓ In LTE conditions, the temperature obtained should be expected to be equal to the kinetic temperatures if all the level were thermalized

$$\ln \frac{N_u}{g_u} = -\frac{1}{T_{rot}} \left(\frac{E_u}{k} \right) + [\ln N_T - \ln Q(T_{rot})] \quad \rightarrow \rightarrow \rightarrow N_u = \frac{8\pi h \nu^2 A}{hc^3 A_{ul}}$$

A simple analysis of $HC^{13}CCN$



LTE conditions: 1. Excitation temperatures 2. FWHM 3. Column densities...



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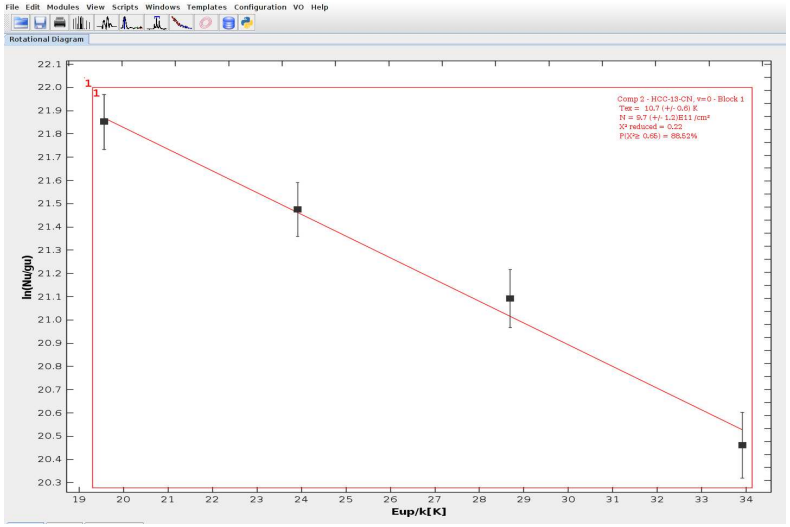

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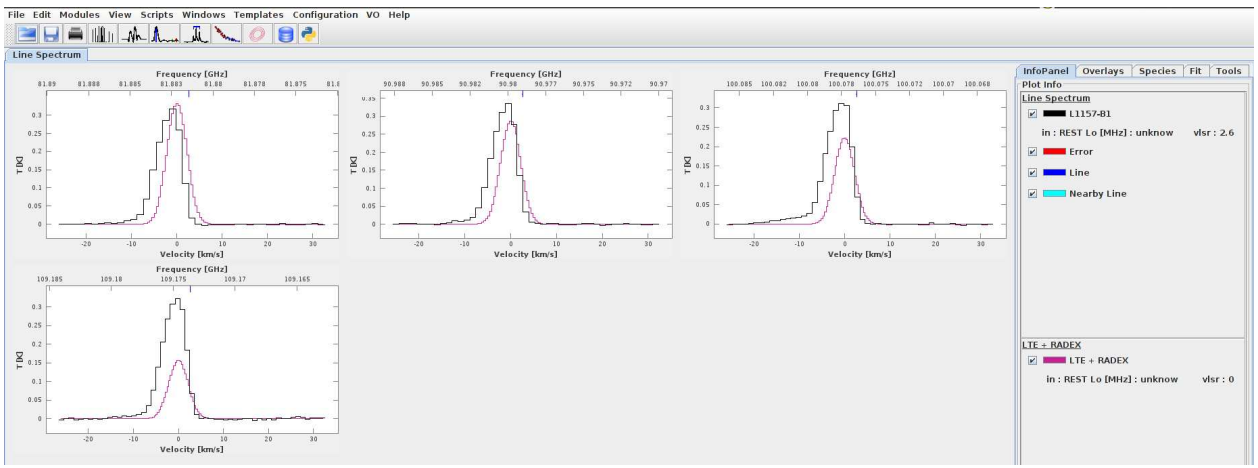

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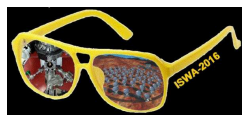

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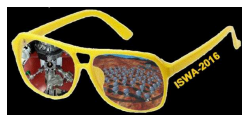
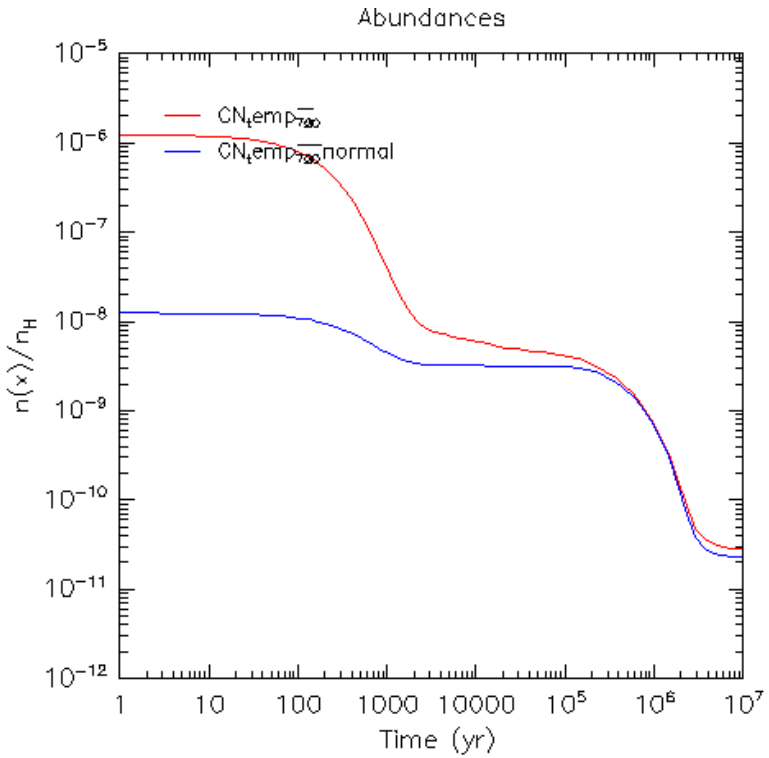


1. Astrochem

http://smaret.github.io/astrochem/

The code compute the abundances of chemical species, as a function of time, in the interstellar medium.



Chemical processes:

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C} + \mathrm{D}$$
$$\mathrm{AB} + h\nu \longrightarrow \mathrm{A} + \mathrm{B}$$
$$\mathrm{A} + h\nu \longrightarrow \mathrm{A}^{+} + e^{-}$$
$$\mathrm{A}^{+} + \mathrm{B} \longrightarrow \mathrm{C}^{+} + \mathrm{D}$$
$$\mathrm{A}^{+} + e^{-} \longrightarrow \mathrm{C} + \mathrm{D}$$

The code reads a network of chemical reactions: OSU database (http://faculty.virginia.edu/ericherb/research.html)

- Molecular abundances as a function of time
- Routes of formation and destruction
- Formulating the problem: Physical condition + chemical abundances

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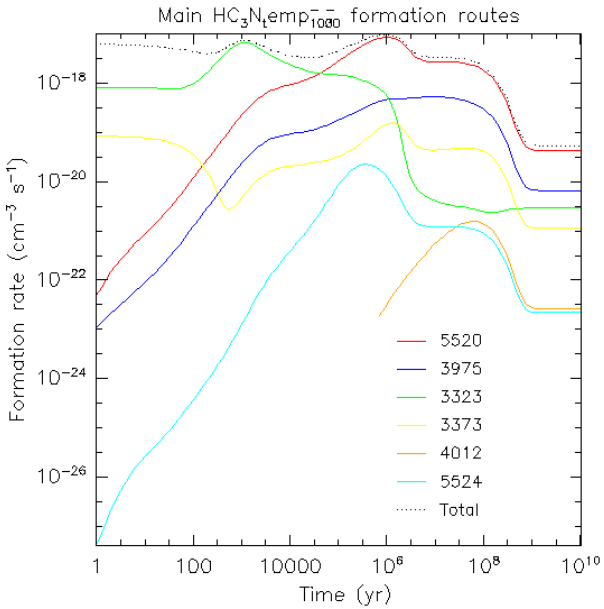

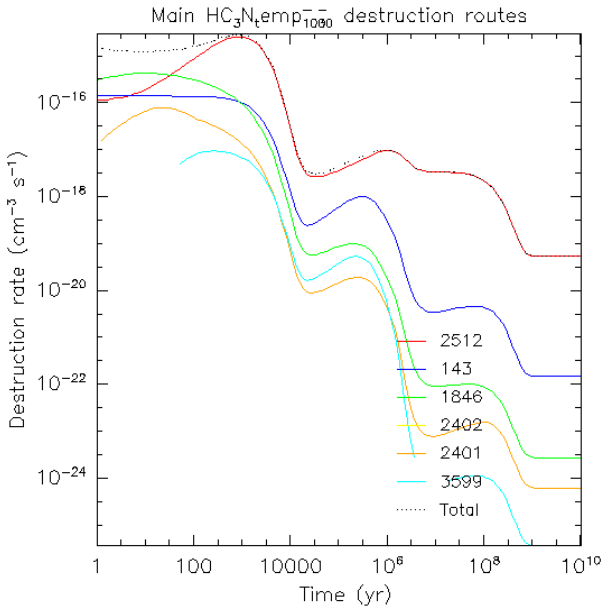

Chemical processes:

$$A + B \longrightarrow C + D$$
$$AB + h\nu \longrightarrow A + B$$
$$A + h\nu \longrightarrow A^+ + e^-$$
$$A^+ + B \longrightarrow C^+ + D$$
$$A^+ + e^- \longrightarrow C + D$$

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- Routes of formation and destruction
- Formulating the problem: Physical condition + chemical abundance

Physical conditions

Properties as temperature, density and visual extinction can be introduced in an input file with extension .mdl

```
# -----------------------------------------------
# Source model file example
# shell number, Av [mag], nH [cm-3], Tgas [K], Tdust [K]
0        0          0.e0          0          0
# -----------------------------------------------
```

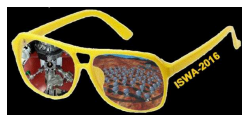
Chemical properties

Chemical abundance with respect to H can be introduced in an input file with extension .ini

```
[files]
source = input-file.mdl
chem = osu2009.chm
# Physical paramaters
[phys]
chi = 0.0
cosmic = 0.0000000e-00
grain-size = 0.0
# Solver parameters
ti = 0e-0
tf = 0e0
```

```
# Initial abundances [abundances]
C(+) = 0.0e+0
H2O = 0.0e+0
NH2CHO = 0.0e+0
# Output
[output]
abundances =
suffix = model-name
time-steps = 0
trace-routes = 0
```

http://smaret.github.io/astrochem/



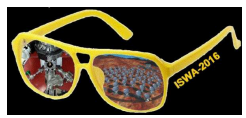
Chemical networks of Astrochem

osu2009.chm: the network contains the reactions and coefficients of the Ohio State University. The network is composed by around 6000 reactions and 460 chemical species

osu2009.chm ×

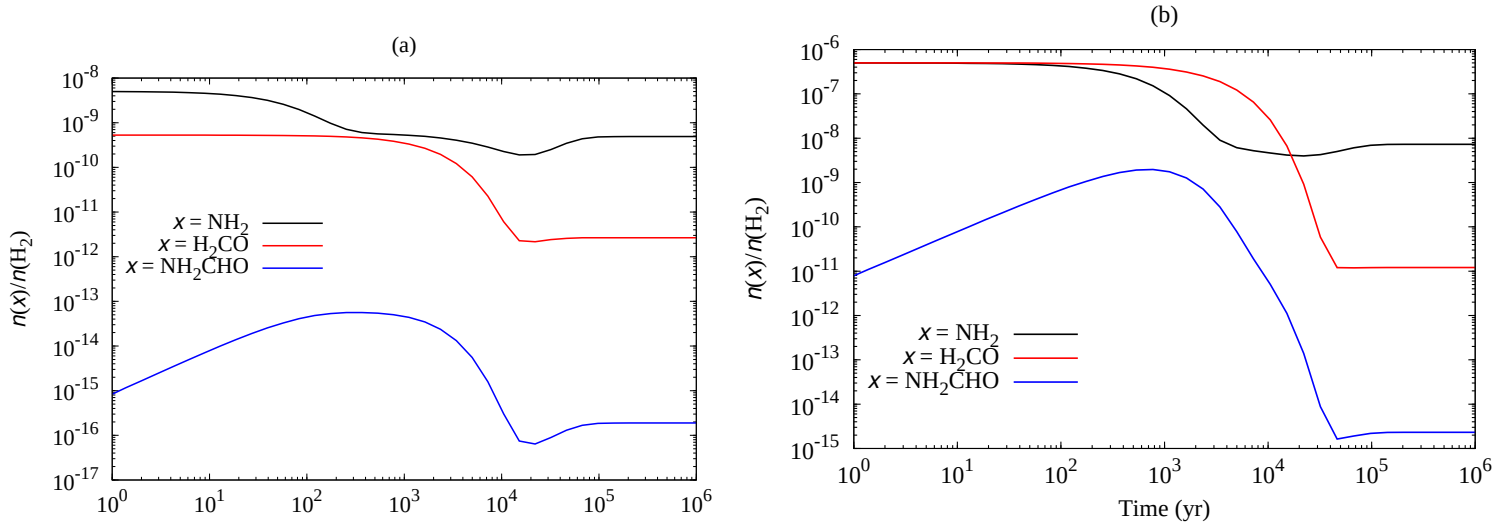
```
H          + H                -> H2                                    4.95e-17  5.00e-01  0.00e
+00  0    1
e(-)       + grain            -> grain(-)                              6.90e-15  5.00e-01  0.00e
+00 -1    2
C(+)       + grain(-)         -> C          + grain                    4.90e-17  5.00e-01  0.00e
+00 -1    3
Fe(+)      + grain(-)         -> Fe         + grain                    2.30e-17  5.00e-01  0.00e
+00 -1    4
H(+)       + grain(-)         -> H          + grain                    1.70e-16  5.00e-01  0.00e
+00 -1    5
He(+)      + grain(-)         -> He         + grain                    8.50e-17  5.00e-01  0.00e
+00 -1    6
Mg(+)      + grain(-)         -> Mg         + grain                    3.70e-17  5.00e-01  0.00e
+00 -1    7
N(+)       + grain(-)         -> N          + grain                    4.70e-17  5.00e-01  0.00e
+00 -1    8
Na(+)      + grain(-)         -> Na         + grain                    3.60e-17  5.00e-01  0.00e
+00 -1    9
O(+)       + grain(-)         -> O          + grain                    4.40e-17  5.00e-01  0.00e
+00 -1   10
S(+)       + grain(-)         -> S          + grain                    3.00e-17  5.00e-01  0.00e
+00 -1   11
Si(+)      + grain(-)         -> Si         + grain                    3.30e-17  5.00e-01  0.00e
+00 -1   12
H3(+)      + grain(-)         -> H2         + H          + grain       1.00e-16  5.00e-01  0.00e
+00 -1   13
HCO(+)     + grain(-)         -> H          + CO         + grain       3.10e-17  5.00e-01  0.00e
+00 -1   14
C          + cosmic-ray       -> C(+)       + e(-)                     1.02e+03  0.00e+00  0.00e
+00  1   15
Cl         + cosmic-ray       -> Cl(+)      + e(-)                     3.00e+03  0.00e+00  0.00e
+00  1   16
Fe         + cosmic-ray       -> Fe(+)      + e(-)                     1.50e+03  0.00e+00  0.00e
+00  1   17
H          + cosmic-ray       -> H(+)       + e(-)                     4.60e-01  0.00e+00  0.00e
```

Hasegawa, Herbst & Leung (1992)



The case of NH_2CHO

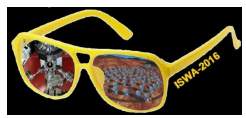
Chemical equations	k(80 K) (cm^3 s^{-1})
Formation processes	
(a) $NH_2 + H_2CO \rightarrow NH_2CHO + H$	1×10^{-10}
(b) $NH_2CH_2O^+ + e^- \rightarrow NH_2CHO + H$	2.9×10^{-7}
Destruction processes	
(c) $H_3^+ + NH_2CHO \rightarrow NH_2CH_2O^+ + H_2$	3.9×10^{-8}
(d) $CH_3^+ + NH_2CHO \rightarrow CH_5N^+ + HCO$	1.9×10^{-8}
(e) $H_3O^+ + NH_2CHO \rightarrow NH_2CH_2O^+ + H_2O$	1.8×10^{-8}
(f) $H^+ + NH_2CHO \rightarrow NH_4^+ + CO$	1.7×10^{-8}



Two cases:

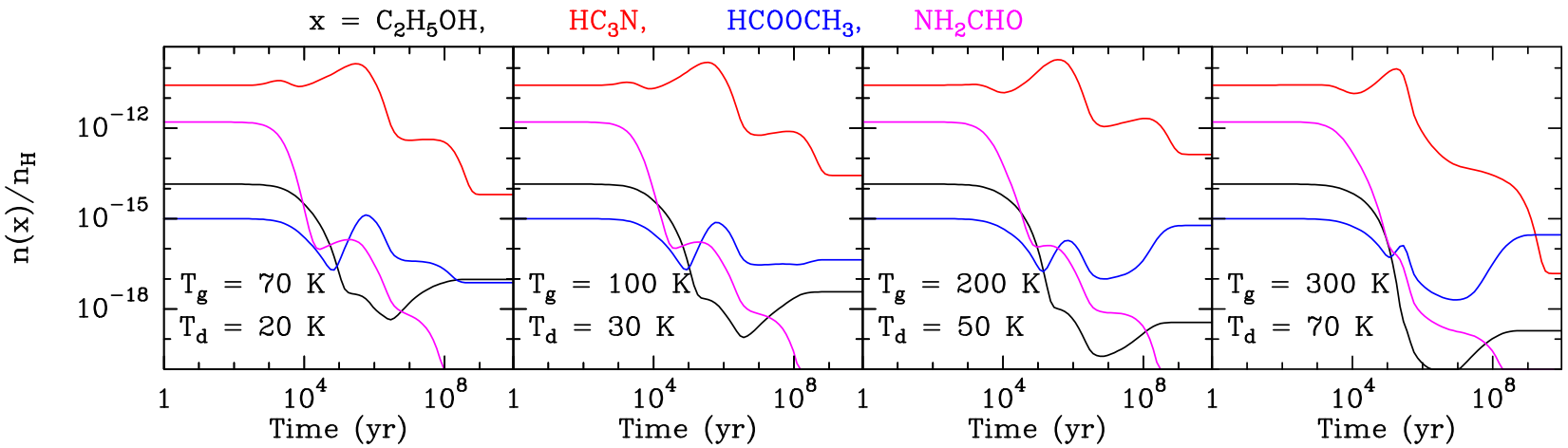
a. Typical abundances of NH_2 and H_2CO in interstellar conditions

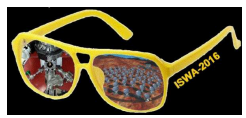
b. Considering abundances of NH_2 and H_2CO higher by a factor 1000



Chemical behaviour of COMs: Several possibilities

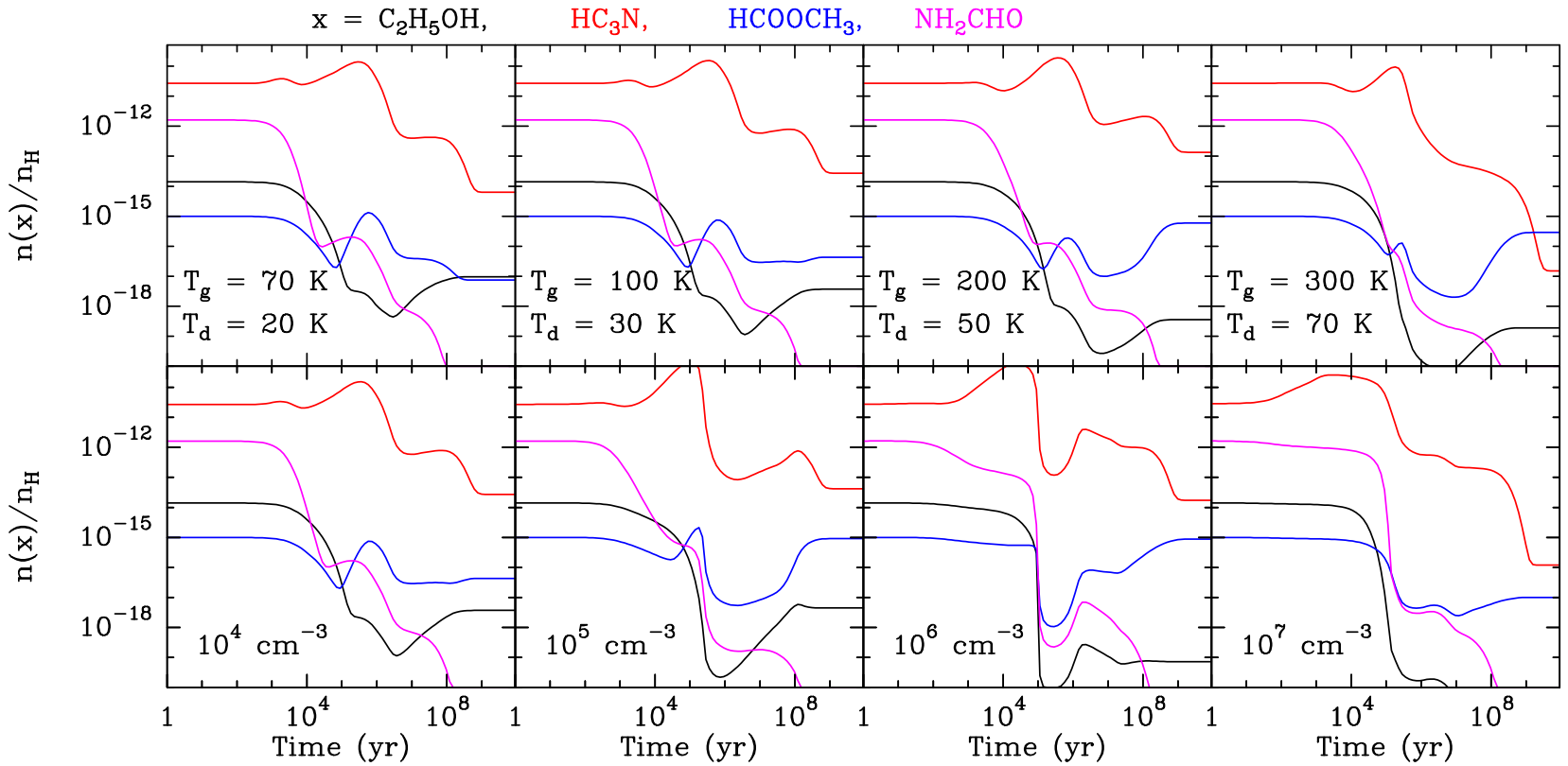
Chemical networks can be explored changing easily physical properties

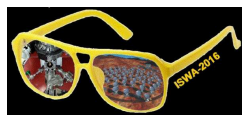




Chemical behaviour of COMs: Several possibilities

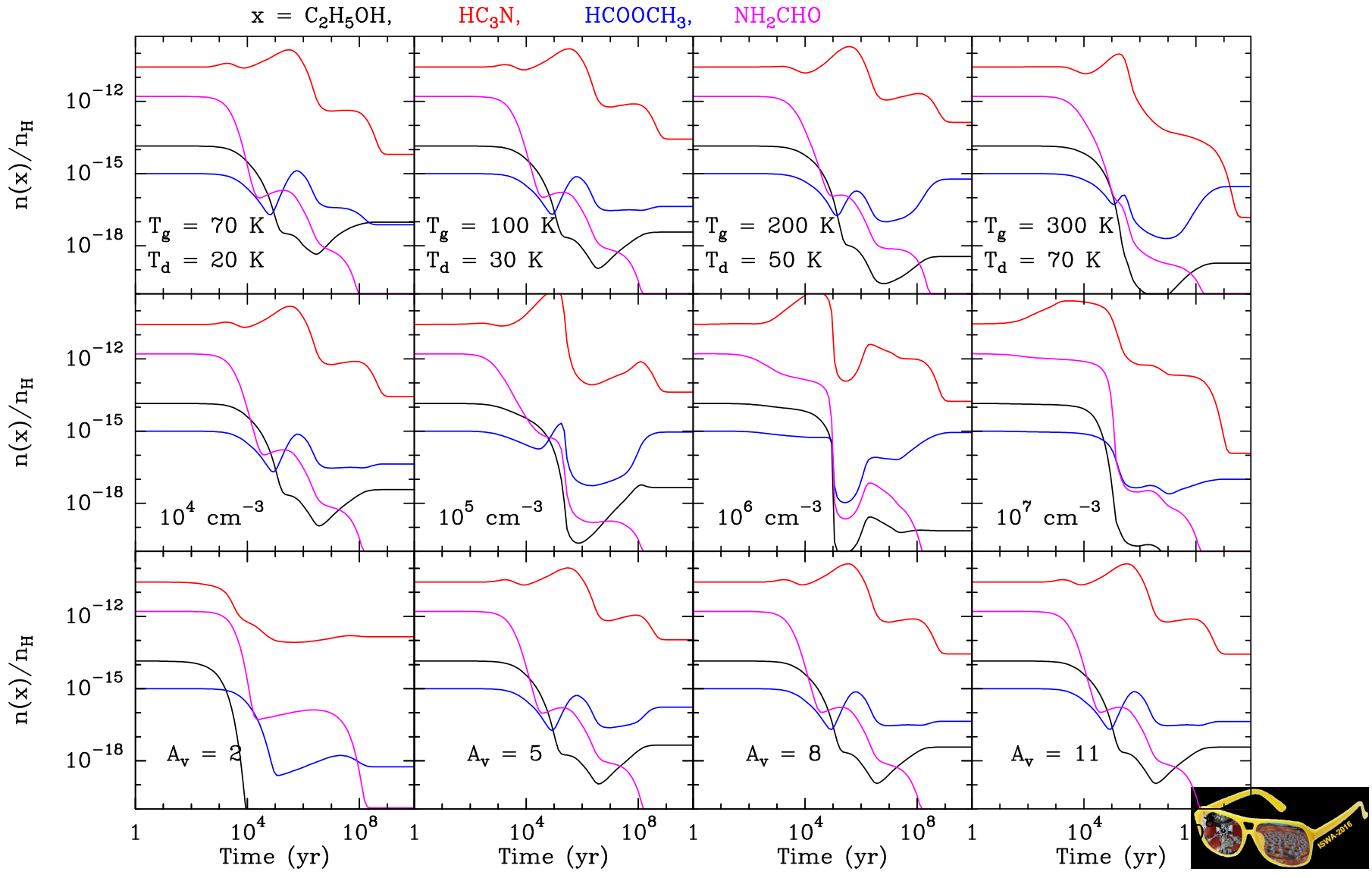
Chemical networks can be explored changing easily physical properties





Chemical behaviour of COMs: Several possibilities

Chemical networks can be explored changing easily physical properties



Tools of chemical modelling: Nahoon

✓ Nahoon computes the chemical abundances as a function of time considering a gas-phase chemical model (Wakelam et al. 2012)

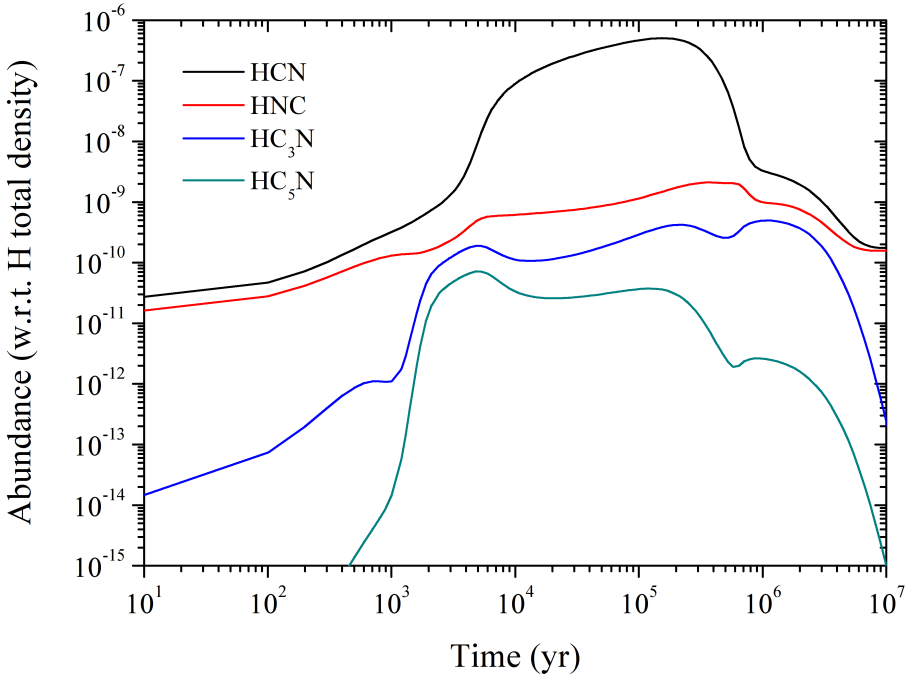
✓ The code is written in Fortran 90 and is available on KIDA to compute gas-phase chemistry

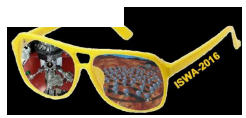
More info: Wakelam et al. 2012 and references therein

http://kida.obs.u-bordeaux1.fr/models/

Chemical reactions

- ✓ Bimolecular reactions
- ✓ Electronic recombinations
- ✓ Direct cosmic-ray processes
- ✓ Photo-processes
- ✓ ...





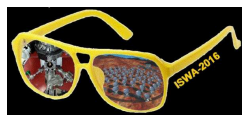
Nahoon: input files

* Chemical network: KIDA (http://kida.obs.u-bordeaux1.fr)

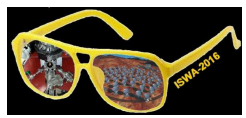
```
...
CN C2H2 H HC3N 2.720e-10 -5.200e-01 1.900e+01 1.25e+00 0.00e+00 logn 4
10 300 3 904 1 1
...
```

kida.uva.2014 ×

```
0.00e+00 logn  2  -9999   9999  1   129 1  1
l-C3H2     CRP                    H          l-C3H                    5.000e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   130 1  1
C4H        CRP                    H          C4                       5.000e+03  0.000e+00  0.000e+00 1.25e+00
0.00e+00 logn  2  -9999   9999  1   131 1  1
C4N        CRP                    CN         C3                       1.000e+03  0.000e+00  0.000e+00 1.50e+00
0.00e+00 logn  2  -9999   9999  1   132 1  1
C4P        CRP                    C          C3P                      1.500e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   133 1  1
C4S        CRP                    CS         C3                       1.500e+03  0.000e+00  0.000e+00 1.50e+00
0.00e+00 logn  2  -9999   9999  1   134 1  1
C5         CRP                    C2         C3                       8.500e+02  0.000e+00  0.000e+00 1.25e+00
0.00e+00 logn  2  -9999   9999  1   135 1  3
C5         CRP                    C          C4                       1.500e+02  0.000e+00  0.000e+00 1.25e+00
0.00e+00 logn  2  -9999   9999  1   136 1  3
HCOOH      CRP                    HCOOH+     e-                       6.500e+02  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   137 1  1
HCOOH      CRP                    OH         HCO                      2.490e+02  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   138 1  1
CH2PH      CRP                    H2         HCP                      1.500e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   139 1  1
CH2NH      CRP                    H2         HCN                      4.980e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   140 1  1
CH4        CRP                    H2         CH2                      2.340e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   141 1  1
HC3N       CRP                    CN         CCH                      1.720e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   142 1  1
c-HCCHSi   CRP                    H2         c-SiC2                   1.500e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   143 1  1
SiC3H      CRP                    H          l-SiC3                   1.500e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   144 1  1
SiC4       CRP                    C2         c-SiC2                   1.500e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   145 1  1
SiCH3      CRP                    H          SiCH2                    1.500e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   146 1  1
SiH4       CRP                    H2         SiH2                     1.500e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   147 1  1
HC4N       CRP                    C2         CH         CN            2.000e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   148 1  1
CH3CN      CRP                    CN         CH3                      4.760e+03  0.000e+00  0.000e+00 2.00e+00
0.00e+00 logn  2  -9999   9999  1   149 1  1
CH3CN      CRP                    CH3CN+     e-                       2.240e+03  0.000e+00  0.000e+00 2.00e+00
```

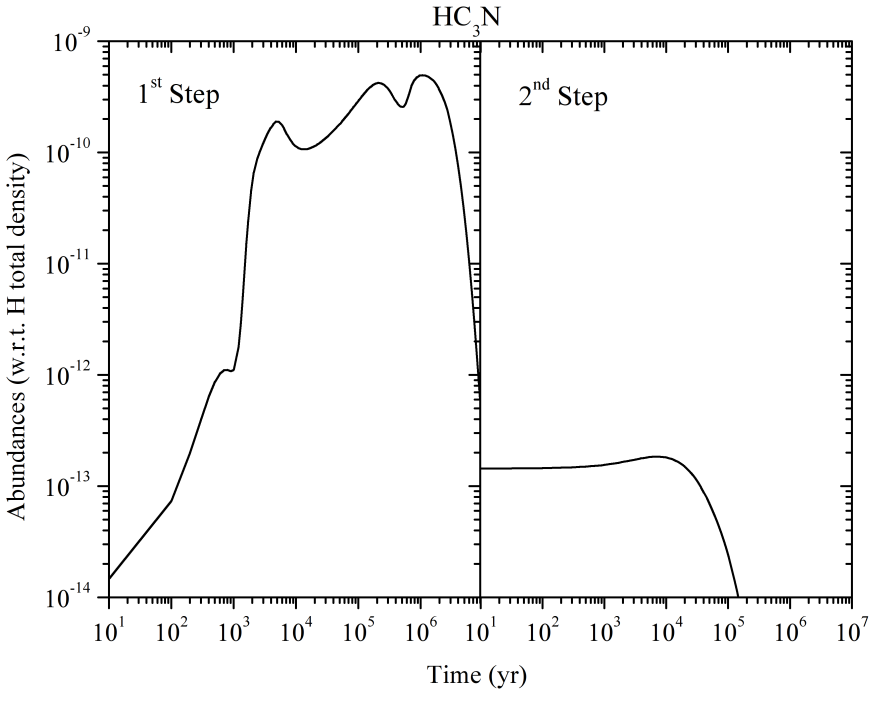


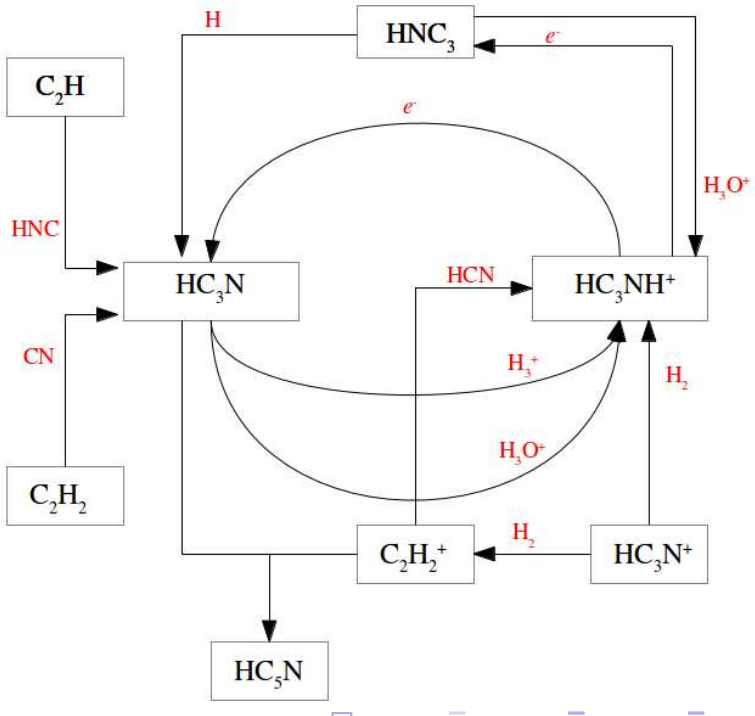
```
* Physical conditions
...
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
N / Do you want to run in the uncertainty mode ? Y or N
0.000D+00 / H tot Density (cm-3) = n(H)+2*n(H2)
0.000D+00 / Temperature (K)
0.000D+00 / Visual extinction
0.063D+00 / Time (in timeres.dat) when you want the output.dat to be
written
0.000D-00 / Cosmic-ray ionization rate (s-1)
0.000D-00 / Dust to gas mass ratio (usually 0.01)
0.000D-00 / Dust grain radius (in cm)
0.000D+00 / grain density (in g cm-3)
...
* Chemistry
JSPACE = 0
1 H 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0.00000000D-00
99 c-C3H2 0 2 0 3 0 0 0 0 0 0 0 0 0 0 0 0.00000000D-00
...
```



testing the chemistry of HC_3N in L1157-B1

1^{st} Step	2^{nd} Step
Chemistry	
Elemental abundances	Abundanes in steady-state
e.g. Wakelam & Herbst 2008	($t = 1 \times 10^6$ yr)
Physics	
n(H) = 2×10^4 cm^{-3}	n(H) = 1×10^5 cm^{-3}
T = 10 K	T = 70 K
A_v = 10 mag	A_v = 10 mag
ξ = 1×10^{-17} s^{-1}	ξ = 1-3 $\times 10^{-16}$ s^{-1}
...	...





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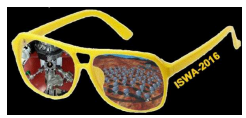
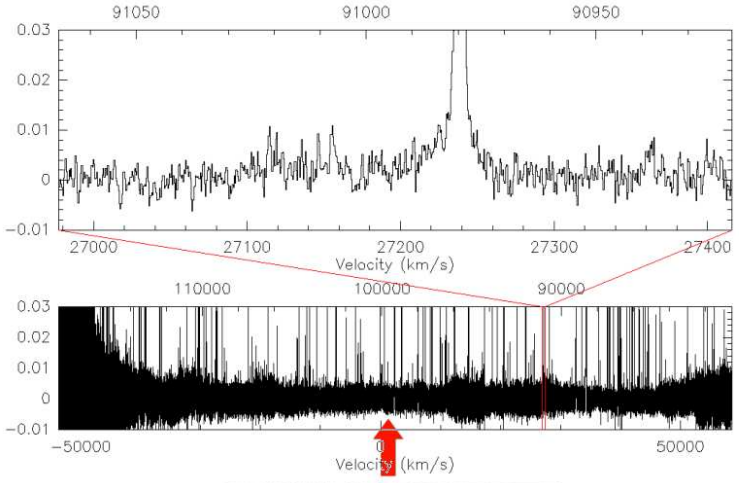


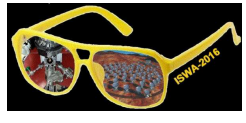
Summarizing

Observations



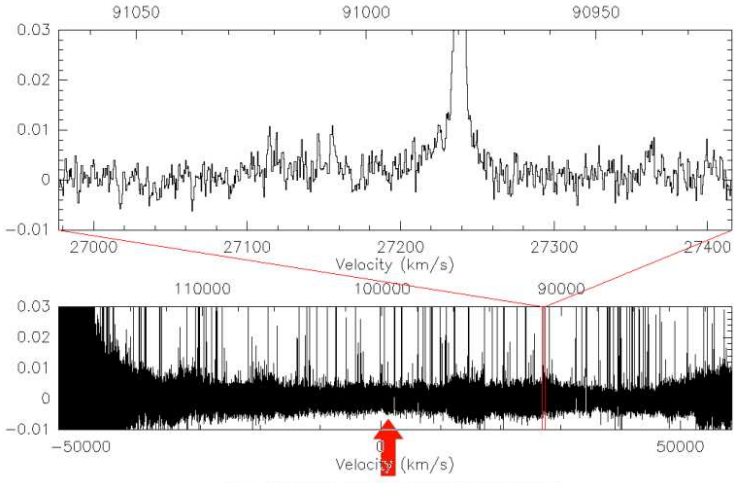
Software
GILDAS
Class
...
CASSIS

Databases: CDMS+JPL+NIST+...



Summarizing

Observations



Software
GILDAS
Class
...
CASSIS

Databases: CDMS+JPL+NIST+...

THANKS!

FAPESP

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