line analysis and chemical modelling
the case of NH$_2$CHO

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Introduction

Tools of spectral line analysis

Tools of chemical modelling
atoms and molecules

The Elements According to Relative Abundance
A Periodic Chart by Prof. Wm. F. Sheehan, University of Santa Clara, CA 95053

The Periodic Table for Astronomy
A graphic representation of the abundances of the elements is shown in this “astronomers” version of the periodic table.
What leaps out of this table is that the simplest elements, hydrogen and helium, are far and away the most abundant.

Thaddeus et al. 2008 and references therein.
**Atoms and molecules**

**Known Interstellar and Circumstellar Molecules (July 2000)**

<table>
<thead>
<tr>
<th>Number of Atoms</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
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</thead>
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<tr>
<td>H₂</td>
<td>H₂O</td>
<td>NH₃</td>
<td>SIH₄</td>
<td>CH₃OH</td>
<td>CH₃CHO</td>
<td>CH₃CO₂H</td>
<td>CH₃CH₂OH</td>
<td></td>
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<tr>
<td>OH</td>
<td>H₂S</td>
<td>H₂O⁺</td>
<td>CH₄</td>
<td>NH₂CHO</td>
<td>CH₃NH₂</td>
<td>HCO₂CH₃</td>
<td>(CH₃)₂O</td>
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<tr>
<td>SO</td>
<td>SO₂</td>
<td>H₂CO</td>
<td>CH₂CN</td>
<td>CH₃CN</td>
<td>CH₃CCH</td>
<td>CH₃CN</td>
<td>CH₃CH₂CN</td>
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</tr>
<tr>
<td>SO⁺</td>
<td>HN₂⁺</td>
<td>H₂CS</td>
<td>HC≡CCN</td>
<td>CH₃NC</td>
<td>CH₂CHCN</td>
<td>C₇H</td>
<td>H(C≡C)₂CN</td>
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<tr>
<td>SIO</td>
<td>HNO</td>
<td>HNCO</td>
<td>CH₂NH</td>
<td>CH₂SH</td>
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<td>SiH₂?</td>
<td>HNCS</td>
<td>NH₂CN</td>
<td>C₃H</td>
<td>C₅H</td>
<td>C₆H</td>
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<td>CCCN</td>
<td>H₂CCO</td>
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<td>C-CH₃OCH₂</td>
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<tr>
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<td>H⁺</td>
<td>HCNT⁺</td>
<td>CH₂ = CH₂</td>
<td>C₇?</td>
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<td></td>
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<td>HCO</td>
<td>c-CCCH</td>
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<td>H₂CNH⁺</td>
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<td>HCNH⁺</td>
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<tr>
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<td>MgNC</td>
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<tr>
<td>C₂</td>
<td>MgCN</td>
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</tr>
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<td></td>
</tr>
<tr>
<td>KCN?</td>
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</tr>
</tbody>
</table>

Thaddeus et al. 2008 and references therein.
detection and analysis of NH$_2$CHO in L1157-B1

✓ Identification of lines
✓ Analysis: GILDAS + CASSIS
✓ Physical conditions: Rotational diagram
✓ Chemical modelling: ASTROCHEM
Why formamide?
NH$_2$CHO and HNCO are the simplest molecules with H, C, N and O.

Importance of NH$_2$CHO as a building block (Saladino et al. 2012).
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Introduction

Tools of spectral line analysis

Tools of chemical modelling
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

The telescope and receiver parameters:

http://www.iram.es/IRAMES/mainWiki/Iram30mEfficiencies
CLASS + Weeds
✓ Line analysis
✓ Modelling considering LTE conditions
✓ Databases as CDMS and JPL

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
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

Astrophysical template
(fixed parameters N, T, \( T_\text{ex} \), \( N_\text{H}_2 \), \( \Delta v \), choice of the molecule...)

Observed spectra
(laboratory or telescope)

CASSIS

- LTE model and Radex
- Parameters to vary: N, \( T_k \), \( T_\text{ex} \), \( n_\text{H}_2 \), \( \Delta v \), choice of the molecule and telescope, beam dilution...

Spectroscopic and molecular databases
(JPL, CDMS, HITRAN, Basecol, LAMDA, NIST)

Synthetic spectra, Line identification,
Adjustment of the source parameters

<table>
<thead>
<tr>
<th>Frequência (MHz)</th>
<th>( E_u ) (K)</th>
<th>( \int T_{mb}dv ) (mK km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>81505.17</td>
<td>15.4</td>
<td>201 ± 4</td>
</tr>
<tr>
<td>86181.39</td>
<td>23.3</td>
<td>6629 ± 3</td>
</tr>
<tr>
<td>90686.38</td>
<td>26.1</td>
<td>7489 ± 4</td>
</tr>
<tr>
<td>93870.11</td>
<td>19.9</td>
<td>175 ± 3</td>
</tr>
<tr>
<td>99866.52</td>
<td>28.1</td>
<td>8043 ± 3</td>
</tr>
<tr>
<td>103640.75</td>
<td>31.1</td>
<td>6543 ± 2</td>
</tr>
<tr>
<td>106347.72</td>
<td>24.9</td>
<td>154 ± 4</td>
</tr>
<tr>
<td>113410.19</td>
<td>33.6</td>
<td>6158 ± 5</td>
</tr>
</tbody>
</table>

http://cassis.irap.omp.eu/?page=cassis
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

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

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

LTE conditions: 1. Excitation temperatures 2. FWHM 3. Column densities...
CASSIS Modules: Rotational diagram

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\]

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

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

Tools of spectral line analysis

Tools of chemical modelling
1. Astrochem
http://smaret.github.io/astrochem/

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

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

Chemical processes:

A + B → C + D
AB + hν → A + B
A + hν → A⁺ + e⁻
A⁺ + B → C⁺ + D
A⁺ + e⁻ → C + D

![Graph showing abundances over time]
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:

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

[source]
source = input-file.mdl
chem = osu2009.chm

[phys]
chi = 0.0
cosmic = 0.0000000e-00
grain-size = 0.0

[output]
abundances =
suffix = model-name
abundances =
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

Hasegawa, Herbst & Leung (1992)
The case of NH$_2$CHO

| Chemical equations | $k$ (80 K) 
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(cm$^3$ s$^{-1}$)</td>
</tr>
<tr>
<td><strong>Formation processes</strong></td>
<td></td>
</tr>
<tr>
<td>(a) NH$_2$ + H$_2$CO $\rightarrow$ NH$_2$CHO + H</td>
<td>$1 \times 10^{-10}$</td>
</tr>
<tr>
<td>(b) NH$_2$CH$_2$O$^+$ + e$^-$ $\rightarrow$ NH$_2$CHO + H</td>
<td>$2.9 \times 10^{-7}$</td>
</tr>
<tr>
<td><strong>Destruction processes</strong></td>
<td></td>
</tr>
<tr>
<td>(c) H$_3^+$ + NH$_2$CHO $\rightarrow$ NH$_2$CH$_2$O$^+$ + H$_2$</td>
<td>$3.9 \times 10^{-8}$</td>
</tr>
<tr>
<td>(d) CH$_3^+$ + NH$_2$CHO $\rightarrow$ CH$_5$N$^+$ + HCO</td>
<td>$1.9 \times 10^{-8}$</td>
</tr>
<tr>
<td>(e) H$_3$O$^+$ + NH$_2$CHO $\rightarrow$ NH$_2$CH$_2$O$^+$ + H$_2$O</td>
<td>$1.8 \times 10^{-8}$</td>
</tr>
<tr>
<td>(f) H$^+$ + NH$_2$CHO $\rightarrow$ NH$_4^+$ + CO</td>
<td>$1.7 \times 10^{-8}$</td>
</tr>
</tbody>
</table>

Two cases:

a. Typical abundances of NH$_2$ and H$_2$CO in interstellar conditions
b. Considering abundances of NH$_2$ and H$_2$CO higher by a factor 1000
Chemical behaviour of COMs: Several possibilities

Chemical networks can be explored changing easily physical properties

\[ x = \text{C}_2\text{H}_5\text{OH}, \quad \text{HC}_3\text{N}, \quad \text{HCOOCH}_3, \quad \text{NH}_2\text{CHO} \]
Chemical behaviour of COMs: Several possibilities

Chemical networks can be explored changing easily physical properties

\[ x = C_2H_5OH, \quad HC_3N, \quad HCOOCH_3, \quad NH_2CHO \]
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
✓ ...
INTRO

LINE ANALYSIS

MODELLING

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
* Physical conditions
...

Physical conditions...

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 0.00000000D-00
99 c-C3H2 0 2 0 3 0 0 0 0 0 0 0 0 0 0 0.00000000D-00
...
testing the chemistry of HC$_3$N in L1157-B1

<table>
<thead>
<tr>
<th>1$^{st}$ Step</th>
<th>2$^{nd}$ Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td>Abundances in steady-state</td>
</tr>
<tr>
<td>Elemental abundances</td>
<td>(t = 1 $\times$ 10$^6$ yr)</td>
</tr>
<tr>
<td>e.g. Wakelam &amp; Herbst 2008</td>
<td></td>
</tr>
<tr>
<td>Physics</td>
<td></td>
</tr>
<tr>
<td>$n$(H) = 2 $\times$ 10$^4$ cm$^{-3}$</td>
<td>$n$(H) = 1 $\times$ 10$^5$ cm$^{-3}$</td>
</tr>
<tr>
<td>$T$ = 10 K</td>
<td>$T$ = 70 K</td>
</tr>
<tr>
<td>$A_\nu$ = 10 mag</td>
<td>$A_\nu$ = 10 mag</td>
</tr>
<tr>
<td>$\xi$ = 1 $\times$ 10$^{-17}$ s$^{-1}$</td>
<td>$\xi$ = 1-3 $\times$ 10$^{-16}$ s$^{-1}$</td>
</tr>
</tbody>
</table>

...
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Introduction

Tools of spectral line analysis

Tools of chemical modelling
Summarizing

Observations

Databases: CDMS+JPL+NIST+...
Summarizing

Observations

Software
GILDAS
Class
...CASSIS

Databases: CDMS+JPL+NIST+...

THANKS!