The PILS program: a large spectral survey of the solar-type protostar IRAS 16293-2422 with ALMA

Audrey Coutens (IRAP)

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Fig. 1. Methodology for continuum subtraction illustrated with data from two representative pixels toward IRAS 16293A (upper) and IRAS 16293B (lower): shown are the flux distributions for the two pixels (histogram) with the resulting fit overlaid (red line).

4. Results

4.1. Continuum emission

Much can be learned about the structure of the IRAS 16293-2422 system by straightforward inspection of the dust continuum maps. Figure 3 shows a three-color composite of the continuum toward the system in the 3.0 mm, 1.3 mm, and 0.87 mm bands, while Fig. 4 shows the continuum at the three different wavelengths separately at the angular resolution of each individual dataset. The extended emission connecting the two sources, also noted in the science verification data (Pineda et al. 2012), is clearly seen. It shows a characteristic bend toward the north of IRAS 16293A/east of IRAS 16293B. East of IRAS 16293B two separate stream-lines pointing away from the source are seen. Toward IRAS 16293A additional extended continuum emission is observed toward the southwest. This extension coincides with the N$_2$D$^+$ emission picked up in SMA observations (Jørgensen et al. 2011) and likely reflects cold material with a high column density. Another very striking feature of the maps is the clear differences in the morphologies and colors of the emission toward the two protostars. IRAS 16293A appears clearly elongated in the northeast/southwest direction (with an aspect ratio of 1.9). Chandler et al. (2005) used continuum maps at 305 GHz from the SMA to study the system: in super-resolution images (images for which higher weight was given to the longer baselines and subsequently restored with a beam slightly smaller than the usual synthesized beams), they noted a similar extension, but also found that the source broke up into two separate components named "Aa" and "Ab". These separate components are not seen in our images even though the beam in the ALMA observations (with regular weighting) is comparable to those super-resolution images. Our images are therefore more in...
Star and planet formation

Star formation process

Prestellar core → Class 0 → Class I → Class II → Class III → Planetary system

Gravitational collapse → Envelope dissipation

Credit: Adapted from M. Persson
Star and planet formation

Star formation process

- Prestellar core
- Class 0
- Class I
- Class II
- Class III
- Planetary system

Gravitational collapse → Envelope dissipation

Comets & asteroids (meteorites) rich in amino acids and sugars

DNA

Credit: Adapted from M. Persson
Origin of the molecular complexity?

What is the level of molecular complexity in star-forming regions?
Star and planet formation

Star formation process

- Prestellar core
- Class 0
- Class I
- Class II
- Class III
- Planetary system

Gravitational collapse → Envelope dissipation

HOT CORINOS
Warm inner regions of protostellar envelopes
(T > 100 K, ~ 100 au)
in which COMs are detected

COLD DISK
Most molecules in solid phase

Credit: Adapted from M. Persson
• Class 0 protostellar system

• Ophiuchus molecular cloud, d ~ 160 pc

• First solar-type protostar with COMs detection (Cazaux et al. 2003)

• High deuteration

Spectral surveys:

• CSO + JCMT (239-250 GHz and 338-347 GHz) van Dishoeck et al. 1995

• TIMASSS : IRAM-30m + JCMT (0.9-3 mm) Caux et al. 2011

• SMA (~0.9 and ~1 mm) Jørgensen et al. 2011

Credit: Adam Block/Steward Observatory/University of Arizona
The ALMA-PILS survey

- PILS = *Protostellar Interferometric Line Survey*

- ALMA band 7 (329-363 GHz)

- Complementary observations in bands 3 and 6

- ALMA 12m array (13 h) + ACA (53 h)

- Spectral resolution ~ 0.2 km/s

- Angular resolution ~ 0.5” (60 AU)

- rms ~ 5 mJy (1 km/s)

*Jørgensen et al. 2016*
10,000 lines: 1 per 3 km/s
Characterizing the molecular content in protostars

- Spectroscopy (CDMS, JPL, …)
  - Frequencies
  - Relative intensities

- Radiative transfer modeling
  - Line identification
  - Abundance, temperature, …
  - Kinematics (infall, rotation, …)
• The bridge arc could be a remnant of filamentary substructure in the protostellar envelope material from which protostellar sources A and B have formed

• Infalling rotating collapse or protoplanetary disk

• Source A at least 3 times (18 \( L_{\text{sol}} \)) more luminous than B (3 \( L_{\text{sol}} \))
• Müller, H. S. P. et al. "Rotational spectroscopy of mono-deuterated oxirane (c-C\textsubscript{2}H\textsubscript{2}DO) and its detection towards IRAS 16293-2422 B", 2022 A&A in press
• Coutens, A., et al., "The ALMA-PILS survey: First tentative detection of 3-hydroxypropenal (HOCH\textsubscript{2}CHO) in the interstellar medium and chemical modeling of the \textsubscript{3}C\textsubscript{2}H\textsubscript{4}O\textsubscript{2} isomers", 2022, A&A 660, L6
• Richard, C., et al. "Torsional-rotational spectrum of doubly-deuterated dimethyl ether (CH\textsubscript{3}OCHD\textsubscript{2}): first ALMA detection in the interstellar medium", 2021, A&A
• Manigand, S., et al. "The ALMA-PILS survey: First detection of the unsaturated 3-carbon molecules Propenal (C\textsubscript{2}H\textsubscript{5}CHO) and Propylene (C\textsubscript{3}H\textsubscript{6}) towards IRAS 16293-2422 B", 2021, A&A 645, A53
• Müller, H. S. P. et al. "Rotational spectroscopy of mono-deuterated oxirane (c-C₃H₆DO) and its detection towards IRAS 16293-2422 B", 2022 A&A in press
• Ligterink, N. F. W., et al. "The ALMA-PILS survey: Detection of CH₃NCO toward the low-mass protostar IRAS 16293-2422 and laboratory constraints on its formation", 2017, MNRA, 469, 2219
Why do all these detections matter?

- Knowledge of the chemistry at an early stage of the star formation process
- Comparison with comets (e.g., 67P - Rosetta)
- Tests of chemical networks through the comparison between the observed and predicted abundances
- Updates of chemical networks for the species which were not previously included
- Comparisons between star forming regions: chemical differentiation? Evolution or environment?
First detections in solar-type protostars

- Ethylene oxide (c-C$_2$H$_4$O)
- Acetone (CH$_3$COCH$_3$)
- Propanal (CH$_3$CH$_2$CHO)
- Propylene (C$_3$H$_6$)
- Propanal (CH$_2$CHCHO)
- Propenal (CH$_2$CHCHCHO)
- Propylene (C$_3$H$_6$)
- Acetone (CH$_3$COCH$_3$)
- Ethylene oxide (c-C$_2$H$_4$O)
- Methyl isocyanate (CH$_3$NCO)
- Methoxymethanol (CH$_3$OCH$_2$OH)
- Trans-ethyl methyl ether (t-C$_2$H$_5$OCH$_3$)
- Vinyl cyanide (CH$_2$CHCN)
- Methyl isocyanide (CH$_3$NC)
- Methanimine (CH$_2$NH)
- Cyanamide (NH$_2$CN)
- Nitrous oxide (N$_2$O)

References:
- Ligterink et al. 2017
- Martin-Domenech et al. 2017
- Ligterink et al. 2018
- Coutens et al. 2018
- Manigand et al. 2020
- Lykke et al. (2017)
- Manigand et al. 2021
- Calcutt et al. 2018
First detections in solar-type protostars

- Acetone (CH₃COCH₃)
- Ethylene oxide (c-C₂H₄O)
- Methyl isocyanate (CH₃NCO)
- Methoxymethanol (CH₃OCH₂OH)
- Propylene (C₃H₆)
- Propenal (CH₂CHCHO)
- Trans-ethyl methyl ether (t-C₂H₅OCH₃)
- Propanal (CH₃CH₂CHO)
- Methanimine (CH₂NH)
- Nitrous oxide (N₂O)
- Cyanamide (NH₂CN)
- Methyl isocyanide (CH₃NC)
- Vinyl cyanide (CH₂CHCN)

First detections in solar-type protostars:

- Lykke et al. (2017)
- Manigand et al. 2020
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First detections in solar-type protostars

Ethylene oxide (c-C\textsubscript{2}H\textsubscript{4}O)

Acetone (CH\textsubscript{3}COCH\textsubscript{3})

Propanal (CH\textsubscript{3}CH\textsubscript{2}CHO)  
*Lykke et al. (2017)*

**Notes.**

Table 2. Relative abundances in different sources.

**Fig. 3.** Chemical model of hot cores – 1

Chemical model: peak grain-surface 0.37: 2.3: 0.39
Chemical model: peak gas-phase 0.22: 0.83: 0.07

Survey of massive SF regions – 1

Sgr B2(N)

Source CH\textsubscript{3}COCH\textsubscript{3} (Hollis et al. 2001) is indicated by the hatched area. For the CH\textsubscript{3}CHO (Garrod et al. 2013) peak grain-surface 0.37: 2.3: 0.39, 2.3: 0.37: 2.3, and 2.3: 0.37: 2.3 for rotational, first torsionally (Lykke et al. 2017), and fast model, respectively.

*Lykke et al. (2017)*
First detections in solar-type protostars

- Ethylene oxide (c-C\textsubscript{2}H\textsubscript{4}O)
- Acetone (CH\textsubscript{3}COCH\textsubscript{3})
- Propylene (C\textsubscript{3}H\textsubscript{6})
- Propanal (CH\textsubscript{3}CH\textsubscript{2}CHO)
- Propenal (CH\textsubscript{2}CHCHO)
- Nitrous oxide (N\textsubscript{2}O)
- Methanimine (CH\textsubscript{2}NH)
- Cyanamide (NH\textsubscript{2}CN)
- Methyl isocyanide (CH\textsubscript{3}NC)
- Meoxymethanol (CH\textsubscript{3}OCH\textsubscript{2}OH)
- Trans-ethyl methyl ether (t-C\textsubscript{2}H\textsubscript{5}OCH\textsubscript{3})
- Vinyl cyanide (CH\textsubscript{2}CHC\textsubscript{2}N)

Source:
- Lykke et al. (2017)
- Martin-Domenech et al. 2017
- Ligterink et al. 2018
- Ligterink et al. 2017
- Coutens et al. 2018
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- Martin-Domenech et al. 2017
- Coutens et al. 2018
- Lykke et al. (2017)
- Manigand et al. 2021
First detections in solar-type protostars

- Gas-grain chemistry model
- Possible formation of NH$_2$CN through the NH$_2$ + CN reaction on grains

Coutens et al. 2018
First detections in solar-type protostars

Ethylene oxide (c-C\textsubscript{2}H\textsubscript{4}O)

Acetone (CH\textsubscript{3}COCH\textsubscript{3})

Propenal (CH\textsubscript{2}CHCHO)

Propylene (C\textsubscript{3}H\textsubscript{6})

Methyl isocyanate (CH\textsubscript{3}NCO)

Methoxymethanol (CH\textsubscript{3}OCH\textsubscript{2}OH)

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Methyl isocyanide (CH\textsubscript{3}NC)

Coutens et al. 2018

Lykke et al. (2017)

Manigand et al. 2020

Vinyl cyanide (CH\textsubscript{2}CHCN)

Calcutt et al. 2018
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- Propylene (C\textsubscript{3}H\textsubscript{6})
- Propenal (CH\textsubscript{2}CHCHO)
- Propanal (CH\textsubscript{3}CH\textsubscript{2}CHO)
- Trans-ethyl methyl ether (t-C\textsubscript{2}H\textsubscript{5}OCH\textsubscript{3})
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- Propenal (CH\textsubscript{2}CHCHO)
- Vinyl cyanide (CH\textsubscript{2}CHCN)

Sources:
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- Coutens et al. 2018
- Manigand et al. 2020
- Lykke et al. (2017)
- Manigand et al. 2021
- Calcutt et al. 2018
First detections in solar-type protostars

- Laboratory experiments
- VUV irradiation of CH₄:HNCO mixtures at 20 K
- Formation on grains through CH₃ and (H)NCO recombinations

Ligterink et al. 2017

Methyl isocyanate (CH₃NCO)
First detections in the ISM

Methyl chloride (CH₃Cl)  
*Fayolle et al. 2017*

Nitrous acid (HONO)  
*Coutens et al. 2019*

3-hydroxypropanal (HOCHCHCHO)  
*Coutens et al. 2022*

+ a lot of isotopologues!
First detections in the ISM

Methyl chloride (CH$_3$Cl)  
*Fayolle et al. 2017*

Nitrous acid (HONO)  
*Coutens et al. 2019*

3-hydroxypropenal (HOCHCHCHO)  
*Coutens et al. 2022*

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**Fig. 1.** Chemical representation of the tautomers of malonaldehyde. The CHO group, thus exchanging the positions of the two groups. We conclude in Section 5.

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**Table 1.** The abundances of HOCHCHCHO and its isomers in Section 4.
First detections in the ISM

Methyl chloride (CH₃Cl)  
**Fayolle et al. 2017**

Nitrous acid (HONO)  
**Coutens et al. 2019**

3-hydroxypropanenal (HOCHCHCHO)  
**Coutens et al. 2022**

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Formula</th>
<th>Nₜot (cm⁻²)</th>
<th>Tₑₓ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrous acid</td>
<td>HONO</td>
<td>(9 ± 5) × 10¹⁴</td>
<td>100</td>
</tr>
<tr>
<td>Nitric oxide†</td>
<td>NO</td>
<td>(2.0 ± 0.5) × 10¹⁶</td>
<td>40–150</td>
</tr>
<tr>
<td>Nitrous oxide‡</td>
<td>N₂O</td>
<td>≥4.0 × 10¹⁶</td>
<td>25–350</td>
</tr>
<tr>
<td>Hydroxylamine‡</td>
<td>NH₂OH</td>
<td>≤4 × 10¹⁴</td>
<td>[100]</td>
</tr>
<tr>
<td>Nitrosyl hydride</td>
<td>HNO</td>
<td>≤3 × 10¹⁴</td>
<td>[100]</td>
</tr>
<tr>
<td>Nitrogen dioxide</td>
<td>NO₂</td>
<td>≤2 × 10¹⁶</td>
<td>[100]</td>
</tr>
<tr>
<td>Nitrosyl cation</td>
<td>NO⁺</td>
<td>≤2 × 10¹⁴</td>
<td>[100]</td>
</tr>
<tr>
<td>Nitric acid</td>
<td>HNO₃</td>
<td>≤5 × 10¹⁴</td>
<td>[100]</td>
</tr>
</tbody>
</table>

- Production on grains through s-O + s-HNO, s-H + s-NO₂, and s-OH + s-NO surface reactions

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(For references and further details, see the cited sources.)

**Notes:**
- †: Tentative identification
- ‡: Tentative identification
- §: Tentative identification

**Abbreviations:**
- PILS: Plateau de l′Observatoire de la SAG-basse
- ALMA: Atacama Large Millimeter/Sub millimeter Array
- CDMS: Cologne Database for Molecular Spectroscopy
- LTE: Local Thermodynamic Equilibrium
First detections in the ISM

Methyl chloride (CH$_3$Cl)
*Fayolle et al. 2017*

Nitrous acid (HONO)
*Coutens et al. 2019*

3-hydroxypropenal (HOCHCHCHO)
*Coutens et al. 2022*
The chemistry of 3-carbon species

Major update of the chemical network to include 3-carbon species (J.-C. Loison, ISM)

<table>
<thead>
<tr>
<th>Species</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ (cm$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C$_2$H$_3$CHO</td>
<td>125 ± 25</td>
<td>$3.4 \pm 0.7 \times 10^{14}$</td>
</tr>
<tr>
<td>C$_3$H$_6$</td>
<td>75 ± 15</td>
<td>$4.2 \pm 0.8 \times 10^{16}$</td>
</tr>
<tr>
<td>HCCCHO</td>
<td>100$^{(a)}$</td>
<td>&lt;$5.0 \times 10^{14}$</td>
</tr>
<tr>
<td>$n$-C$_3$H$_7$OH</td>
<td>100$^{(a)}$</td>
<td>&lt;$3.0 \times 10^{15}$</td>
</tr>
<tr>
<td>$i$-C$_3$H$_7$OH</td>
<td>100$^{(a)}$</td>
<td>&lt;$3.0 \times 10^{15}$</td>
</tr>
<tr>
<td>C$_3$O</td>
<td>100$^{(a)}$</td>
<td>&lt;$2.0 \times 10^{13}$</td>
</tr>
<tr>
<td>cis-HC(O)CHO</td>
<td>100$^{(a)}$</td>
<td>&lt;$5.0 \times 10^{13}$</td>
</tr>
<tr>
<td>C$_3$H$_8$</td>
<td>100$^{(a)}$</td>
<td>&lt;$8.0 \times 10^{16}$</td>
</tr>
<tr>
<td>CH$_3$CCH</td>
<td>100 ± 20</td>
<td>$1.1 \pm 0.2 \times 10^{16}$</td>
</tr>
<tr>
<td>C$_2$H$_5$CHO</td>
<td>125 ± 25</td>
<td>$2.2 \pm 1.1 \times 10^{15}$  $^{(\dagger)}$</td>
</tr>
<tr>
<td>CH$_3$CHO</td>
<td>125 ± 25</td>
<td>$7.0 \pm 3.5 \times 10^{16}$  $^{(\dagger)}$</td>
</tr>
<tr>
<td>CH$_3$COCH$_3$</td>
<td>125 ± 25</td>
<td>$1.7 \pm 0.8 \times 10^{16}$  $^{(\dagger)}$</td>
</tr>
<tr>
<td>C$_2$H$_5$OCH$_3$</td>
<td>100 ± 20</td>
<td>$1.8 \pm 0.2 \times 10^{16}$  $^{(\dagger)}$</td>
</tr>
</tbody>
</table>

Unsaturated 3-carbon molecules

Propylene (C$_3$H$_6$)  Propenal = Acrolein (CH$_2$CHCHO)

Detection towards IRAS 16293 B

Manigand et al. 2021, Lykke et al. 2017
The chemistry of 3-carbon species

- Three-phase chemistry code Nautilus (PI: V. Wakelam)

- Prestellar phase followed by a 1D hydrodynamical collapse (Masunaga & Inutsuka 2000)

- Tests of different formation pathways (successive hydrogenation of C\(_3\) and C\(_3\)O and radical-radical additions on grain surfaces) to assess which are the dominant formation mechanisms

Ruaud et al. 2016
The chemistry of 3-carbon species

S. Manigand et al.: First detection of $\text{C}_2\text{H}_3\text{CHO}$ and $\text{C}_3\text{H}_6$ towards IRAS 16293–2422 B

Fig. 6. Final abundances reached at the end of each simulation run for the targeted species. The dashed blue line shows the observed abundance of the species towards IRAS 16293B. The error bars and the blue area correspond to one half order of magnitude confidence limit, thus a $1\times$-difference between observations and simulations corresponds to one order of magnitude. The dashed blue region represents the abundance values that are consistent with the corresponding upper limit. The abundance scale of $\text{C}_3\text{O}$ is lower than the other plots. The abundance upper limit of $\text{HC(O)}\text{CHO}$ is $< 2.6 \times 10^4$ relative to $\text{CH}_3\text{OH}$, therefore, there is no observational constraint on the abundance of $\text{HC(O)}\text{CHO}$. The abundance upper limit of $\text{C}_3\text{H}_7\text{OH}$ is the sum of n-$\text{C}_3\text{H}_7\text{OH}$ and i-$\text{C}_3\text{H}_7\text{OH}$ abundance upper limits. Production of saturated ones. The agreement of this run with observations is better than for the fiducial chemical network in terms of abundances of $\text{CH}_2\text{(OH)}\text{CHO}$, $\text{(CH}_2\text{OH)}^2$, $\text{C}_3\text{H}_6\text{OCHO}$, and $\text{CH}_3\text{OCH}_2\text{OH}$, suggesting that hydrogenation reactions play an important role in formation of such COMs in hot corino regions. The hydrogenation of $\text{CH}_3\text{OCHO}$ has been recently studied in laboratory by Krim et al. (2018). They reported a calculated energy barrier of 32.7 kJ mol$^{-1}$ for the ice-surface reaction s-H + s-$\text{CH}_3\text{OCHO}$ and concluded that this pathway did not seem to contribute to the formation of $\text{CH}_3\text{OCH}_2\text{OH}$. The experimental result of Krim et al. mainly shows that this reaction is slower than the s-H + s-H$_2$CO $\rightarrow$ s-$\text{CH}_3\text{O}$ reaction.
The chemistry of 3-carbon species

+ comparison with 2C-species

Manigand et al. 2021
Main conclusions of Manigand et al. 2021

• Impact of the duration of the prestellar phase on the abundances of the saturated vs unsaturated COMs

• Formation of C$_2$H$_3$CHO and C$_2$H$_5$CHO through both:
  ‣ successive hydrogenation reactions on ice surfaces of C$_3$O, with a formation of C$_3$O in the gas phase (C$_3$ + OH $\rightarrow$ C$_3$O + H)
  ‣ radical-radical additions of HCO and C$_2$H$_3$ or C$_2$H$_5$ on ice surfaces

• Rate of 10$^{-12}$ cm$^3$ s$^{-1}$ for the gas phase reaction C$_3$ + O $\rightarrow$ C$_2$ + CO necessary to fit the observed abundances

• Other missing consumption pathways of C$_3$ (PAHs) ?
Tentative detection of 3-hydroxypropenal

3-hydroxypropenal: biomarker to measure the level of oxidative stress in living organisms

Antoine Boulanger’s internship
Predicted towards source B with a Convolutional Neural Network on a large set of multi-species synthetic spectra assuming LTE (Boulanger et al. 2022)

Confirmation with the classical method

Coutens et al. 2022
3-hydroxypropenal and isomers

**Tautomers**

- 3-hydroxypropenal (enol)
- Propanedial (dialdehyde)

**Tautomeration**

**Isomers**

- 2-propenoic acid ($\text{C}_2\text{H}_3\text{COOH}$)
- Methyl glyoxal ($\text{CH}_3\text{COCHO}$)
- 2-hydroxypropenal ($\text{CH}_2\text{COHCHO}$)
- Vinyl formate ($\text{C}_2\text{H}_3\text{OCHO}$)
Chemical modeling of the $C_3H_4O_2$ isomers

- Same physical model as in Manigand et al. 2021
- Update of the chemical network by including the reactions producing and consuming the $C_3H_4O_2$ isomers and some radical species linked to $C_3H_4O_2$
- Our model reproduces the abundance of HOCHCHCHO with respect to CH$_3$OH within the uncertainties (~10)
- $CH_2CHO + HCO \rightarrow HCOCH_2CHO$
- $HCOCH_2CHO \rightarrow HOCHCHCHO$

$Coutens$ et al. 2022
Importance of spectroscopic studies

<table>
<thead>
<tr>
<th>Isomer</th>
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- Upper limits in agreement for vinyl formate and 2-propenoic acid
## Importance of spectroscopic studies

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Spectroscopic studies are needed:

- to search for propanedial, methyl glyoxal and 2-hydroxyprop-2-enal in IRAS16293 and other sources

- to test the chemical network
2-hydroxyprop-2-enal

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First detections of isotopologues in the ISM

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<th>Compound</th>
<th>Isotopologues</th>
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<tbody>
<tr>
<td>Formamide</td>
<td>NH$_2$CDO</td>
</tr>
<tr>
<td></td>
<td>cis-NHDCHO</td>
</tr>
<tr>
<td></td>
<td>trans-NHDCHO</td>
</tr>
<tr>
<td>Glycolaldehyde</td>
<td>CHDOHCHO</td>
</tr>
<tr>
<td></td>
<td>CH$_2$ODCHO</td>
</tr>
<tr>
<td></td>
<td>CH$_2$OHCDNO</td>
</tr>
<tr>
<td></td>
<td>$^{13}$CH$_2$OHOCHO</td>
</tr>
<tr>
<td></td>
<td>CH$_2$OH$^{13}$CHO</td>
</tr>
<tr>
<td>Acetaldehyde</td>
<td>CH$_3$CDO</td>
</tr>
<tr>
<td></td>
<td>$^{13}$CH$_3$CHO</td>
</tr>
<tr>
<td>Formic acid</td>
<td>H$^{13}$COOH</td>
</tr>
<tr>
<td></td>
<td>t-DCOOH</td>
</tr>
<tr>
<td></td>
<td>t-HCOOD</td>
</tr>
<tr>
<td>Formaldehyde</td>
<td>H$_2$C$^{17}$O</td>
</tr>
<tr>
<td></td>
<td>D$_2$$^{13}$CO</td>
</tr>
<tr>
<td>Isocyanic acid</td>
<td>DNCO</td>
</tr>
<tr>
<td>Cyanamide</td>
<td>NHDCN</td>
</tr>
<tr>
<td></td>
<td>NH$_2^{13}$CN</td>
</tr>
<tr>
<td>Ethanol</td>
<td>a-a-CH$_2$DCH$_2$OH</td>
</tr>
<tr>
<td></td>
<td>a-s-CH$_2$DCH$_2$OH</td>
</tr>
<tr>
<td></td>
<td>CH$_3$CHDOH</td>
</tr>
<tr>
<td>Oxyrane</td>
<td>c-C$_2$H$_3$DO</td>
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<td>Ketene</td>
<td>$^{13}$CH$_2$CO</td>
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<td>CH$_2^{13}$CO</td>
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<tr>
<td></td>
<td>CHDCO</td>
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<tr>
<td>Methyl cyanide</td>
<td>CHD$_2$CN</td>
</tr>
<tr>
<td>Methyl formate</td>
<td>HCOOCHD$_2$</td>
</tr>
<tr>
<td>Dimethyl ether</td>
<td>CH$_3$OCHD$_2$</td>
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Deuteration of molecules

Formation time?

Jørgensen et al. 2018

$T_{ex}$

300 K

125 K

$D/H$

early

late

300 K

125 K

HNCO
NH$_2$CHO
HCOOH
CH$_3$OH

CH$_2$CO
H$_2$CO

2–3%

4–8%

CH$_3$OCHO
CH$_2$(OH)CHO
CH$_3$CH$_2$OH

CH$_3$CHO
CH$_3$OCH$_3$

Binding energy?
Deuteriation of molecules

Comparison with 3D chemical modeling (*Coutens et al. 2020*)

Formation time?

- Early
- Late

Same initial and final abundances

Cloud B only

$T_{\text{ex}}$

300 K

125 K

Increase of abundances during the collapse

Binding energy?

D/H

2–3%

4–8%

Jørgensen et al. 2018
Analysis of a single position (0.6" north-east of IRAS 16293 A, narrow lines)
Different spatial distribution of the molecules towards A would explain the differences
The less abundant species towards A appear to be more compact
Comparison with other protostars: COMPASS

- ALMA large program (125 h)
- Unbiased line surveys of 11 low-mass protostars (diverse evolutionary stages and different environments)

What are the physical, environmental, and evolutionary regulators of the formation of complex organics?

Is there a universal outcome of interstellar chemistry (COMs)?

How much diversity in organic inventories do we expect for planetary systems?

**PI/co-PIs:**
- Jes Jørgensen
- Audrey Coutens
- Maria Drozdovskaya
- Jeong-Eun Lee
- Adele Plunkett

**co-Is:**
- Arnaud Belloche
- Jenny Bergner
- Daniel Harsono
- Ágnes Kóspál
- Niels Ligterink
- Sheng-Yuan Liu
- Sébastien Maret
- Brett McGuire
- Silvia Spezzano
- Merel van’t Hoff
- Yao-Lun Yang
Comparison with comets

Drozdovskaya et al. 2019
Tools for astrochemical observations

• Characterizing the chemistry of more protostars with ALMA and NOEMA
  ➞ Chemical differentiation
  ➞ Chemical evolution

• Development of tools for an efficient analysis of a large amount of interferometric data

♦ Interface between the CASSIS software (IRAP) and the Aladin software (CDS)

♦ ATOMIS: web interface to search for specific species in the ALMA archive (S. Ben Hmida, J.-M. Glorian)

See poster ATOMIS!

https://aladin.u-strasbg.fr/
• Very rich chemistry in solar-type protostars

• PILS: Large and unbiased spectral survey of IRAS 16293-2422 with ALMA

• A lot of first detections both in solar-type protostars and in the ISM

• Spectroscopic studies are necessary to identify all the lines in the survey

• Chemical models can be improved and tested thanks to the high number of detected species

• Chemical network with molecules with up to 3C atoms (J.-C. Loison)

• Chemical models can also help us determine the most promising species to search for

• More ALMA data coming soon (COMPASS) to investigate the chemical differentiation
Thanks for your attention!