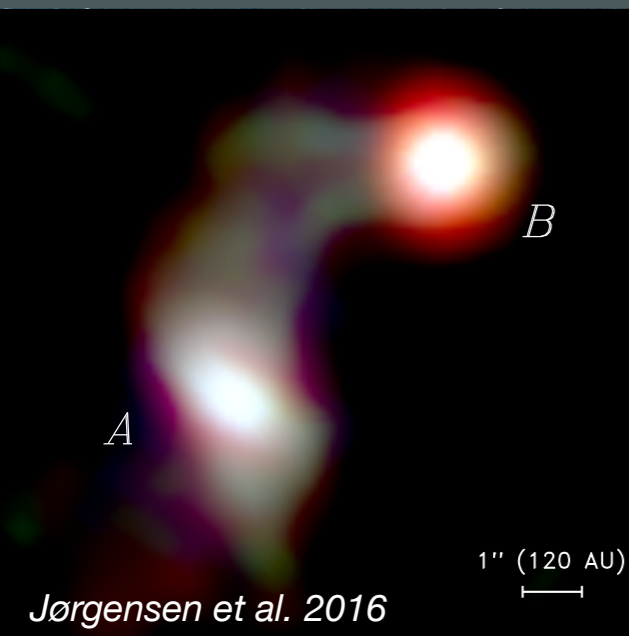


The PILS program: a large spectral survey of the solar-type protostar IRAS 16293-2422 with ALMA

Audrey Coutens (IRAP)

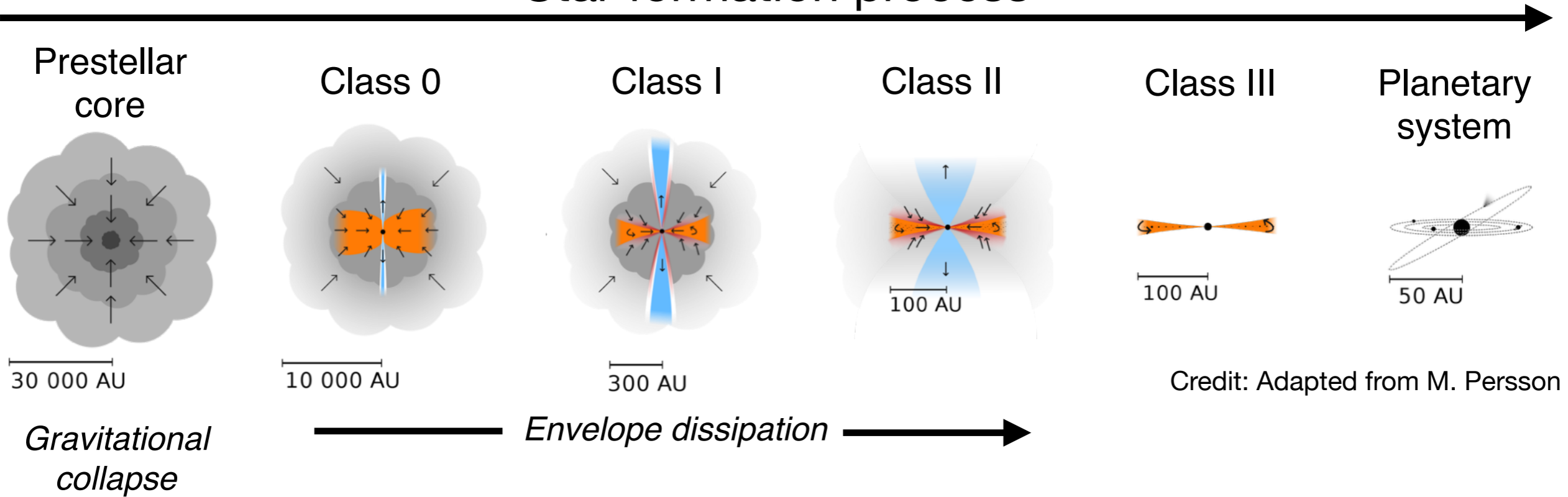
PILS team : J.K. Jørgensen (PI), Per Bjerkeli, Tyler Bourke, Hannah Calcutt, Audrey Coutens, Maria Drozdovskaya, Edith Fayolle, Rob Garrod, Steffen Jacobsen, Niels Ligterink, Julie Lykke, Sebastien Manigand, Holger Müller, Nadia Murillo, Karin Öberg, Magnus Persson, Gwendoline Stephan, Matthijs van der Wiel, Ewine van Dishoeck, Susanne Wampfler & Eric Willis



Credit: ESO/C. Malin

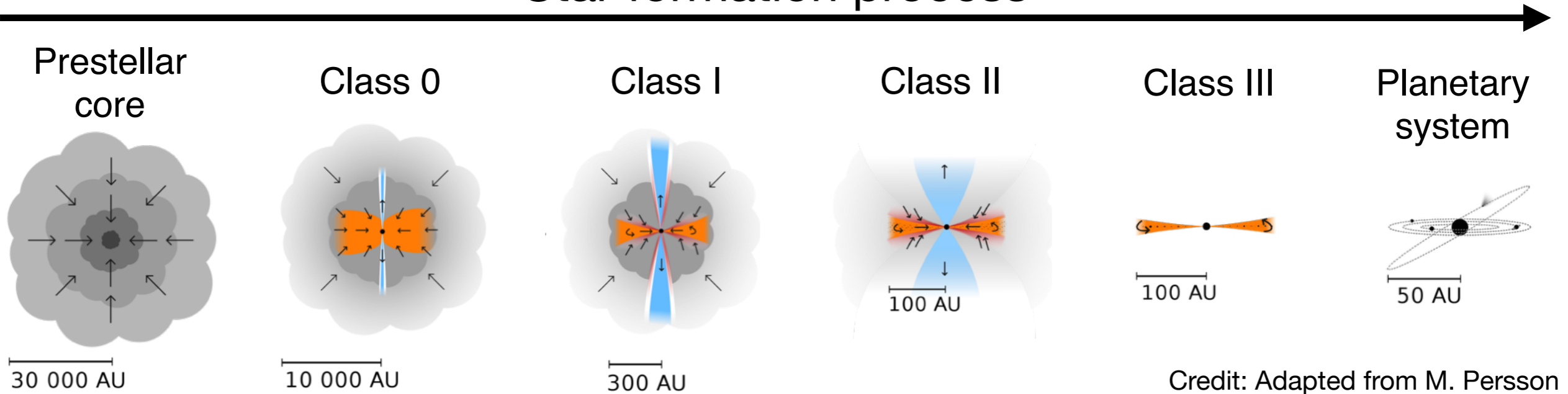
Star and planet formation

Star formation process



Star and planet formation

Star formation process



Gravitational collapse

Envelope dissipation

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

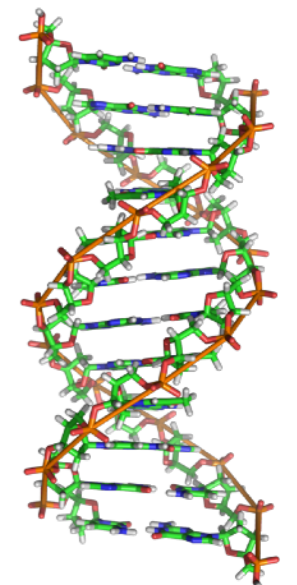
Churyumov-
Gerasimenko



Murchison
Meteorite

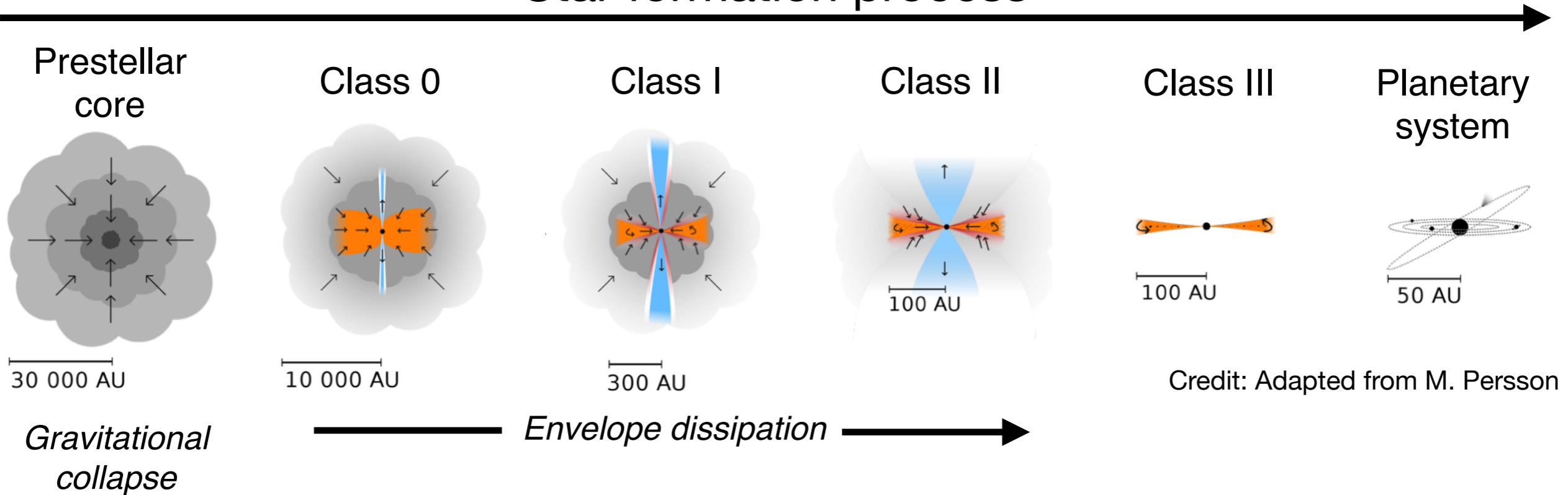


DNA



Star and planet formation

Star formation process



Credit: Adapted from M. Persson

* Origin of the molecular complexity ?

* What is the level of molecular complexity in star-forming regions ?

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

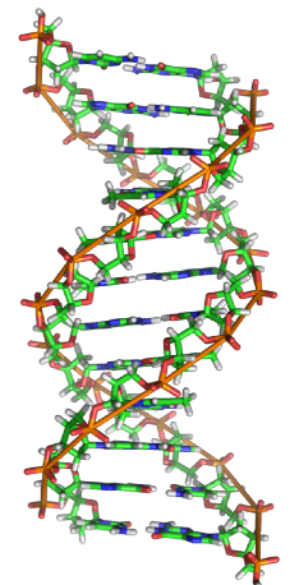
Churyumov-
Gerasimenko



Murchison
Meteorite

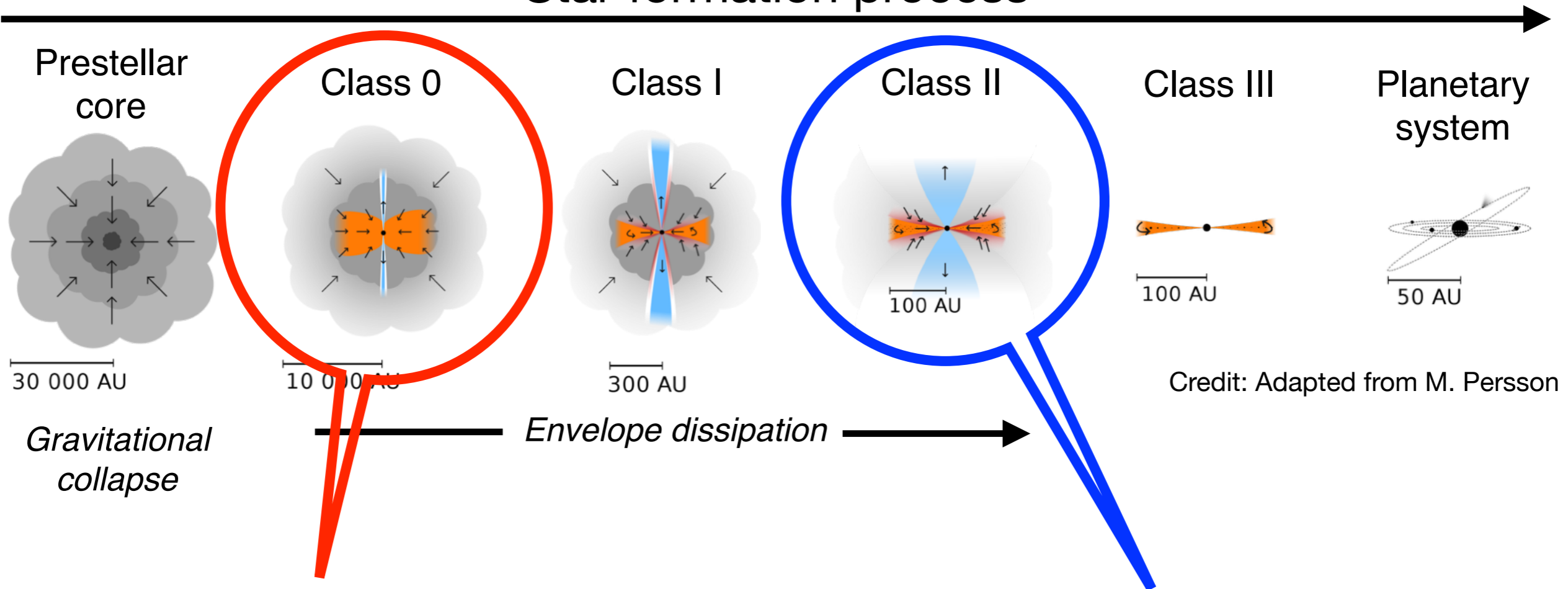


DNA



Star and planet formation

Star formation process



Credit: Adapted from M. Persson

HOT CORINOS

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

COLD DISK

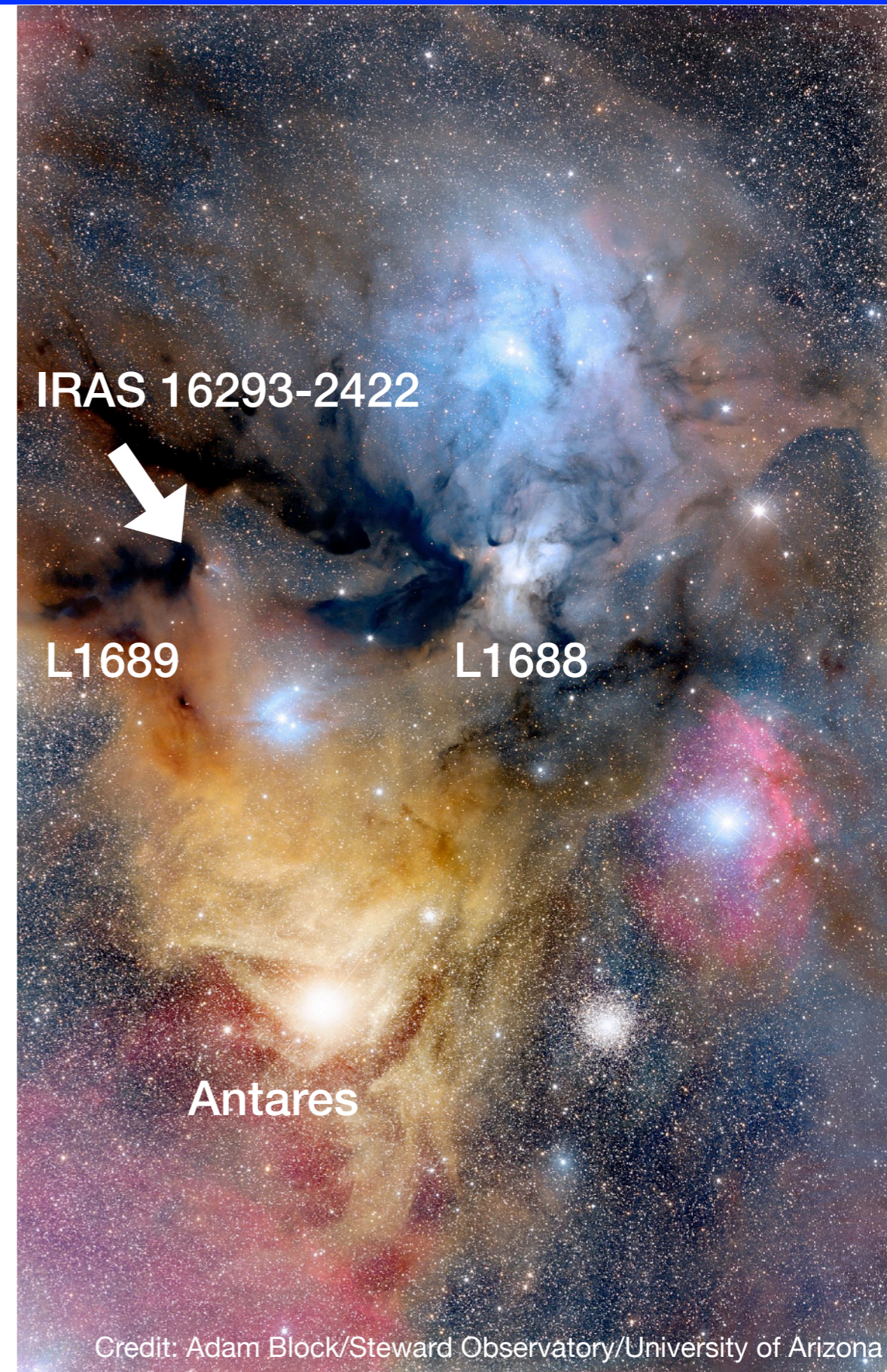
Most molecules in solid phase

The solar-type protostar IRAS 16293-2422

- Class 0 protostellar system
- Ophiuchus molecular cloud, $d \sim 160$ pc
- First solar-type protostar with COMs detection (*Cazaux et al. 2003*)
- High deuteration

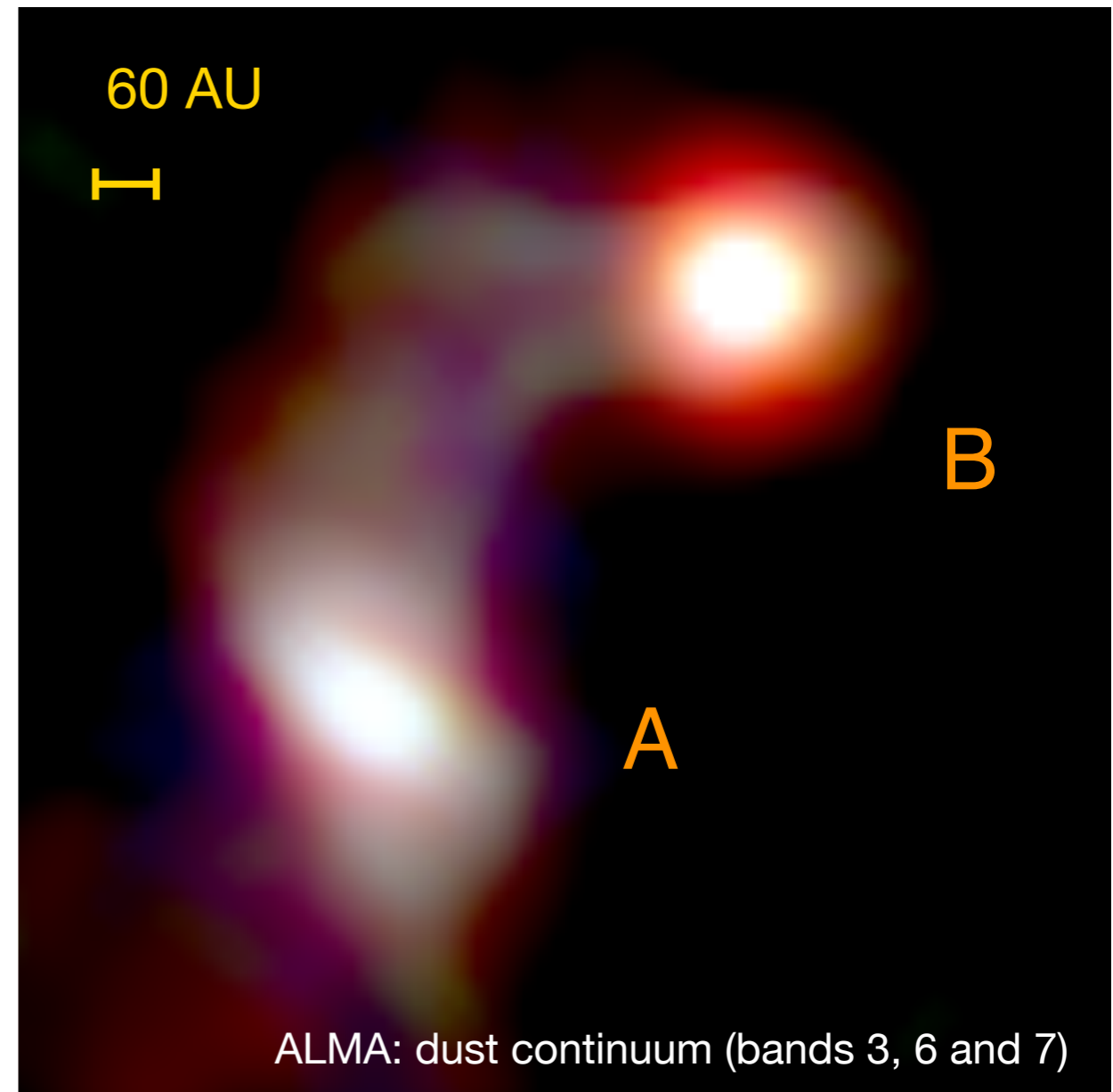
Spectral surveys :

- 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*



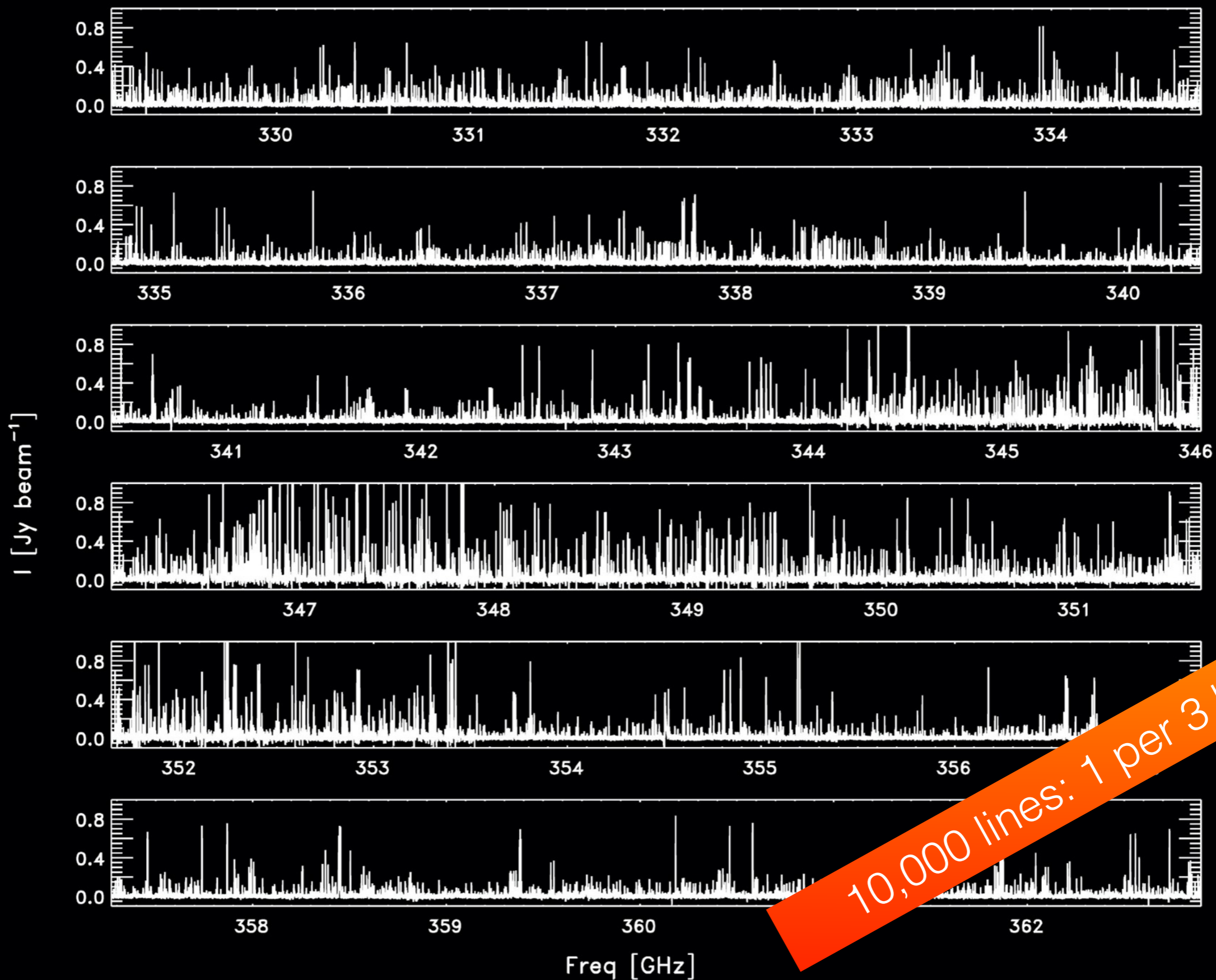
The ALMA-PILS survey

- 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 $\sim 0.5''$ (60 AU)
- rms ~ 5 mJy (1 km/s)



Jørgensen et al. 2016

The ALMA-PILS survey



10,000 lines: 1 per 3 km/s

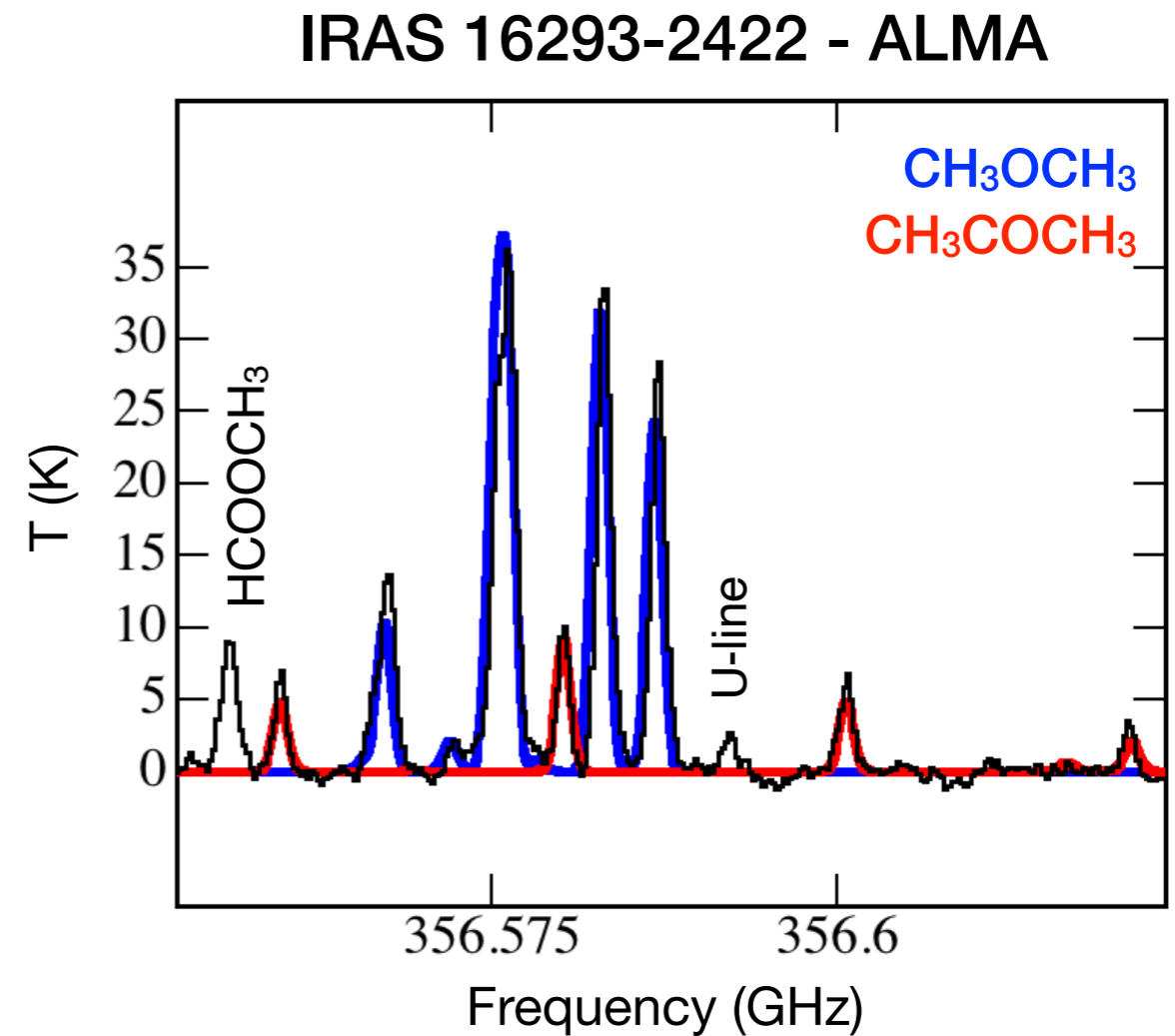
Characterizing the molecular content in protostars

❖ Spectroscopy (CDMS, JPL, ...)

- Frequencies
- Relative intensities

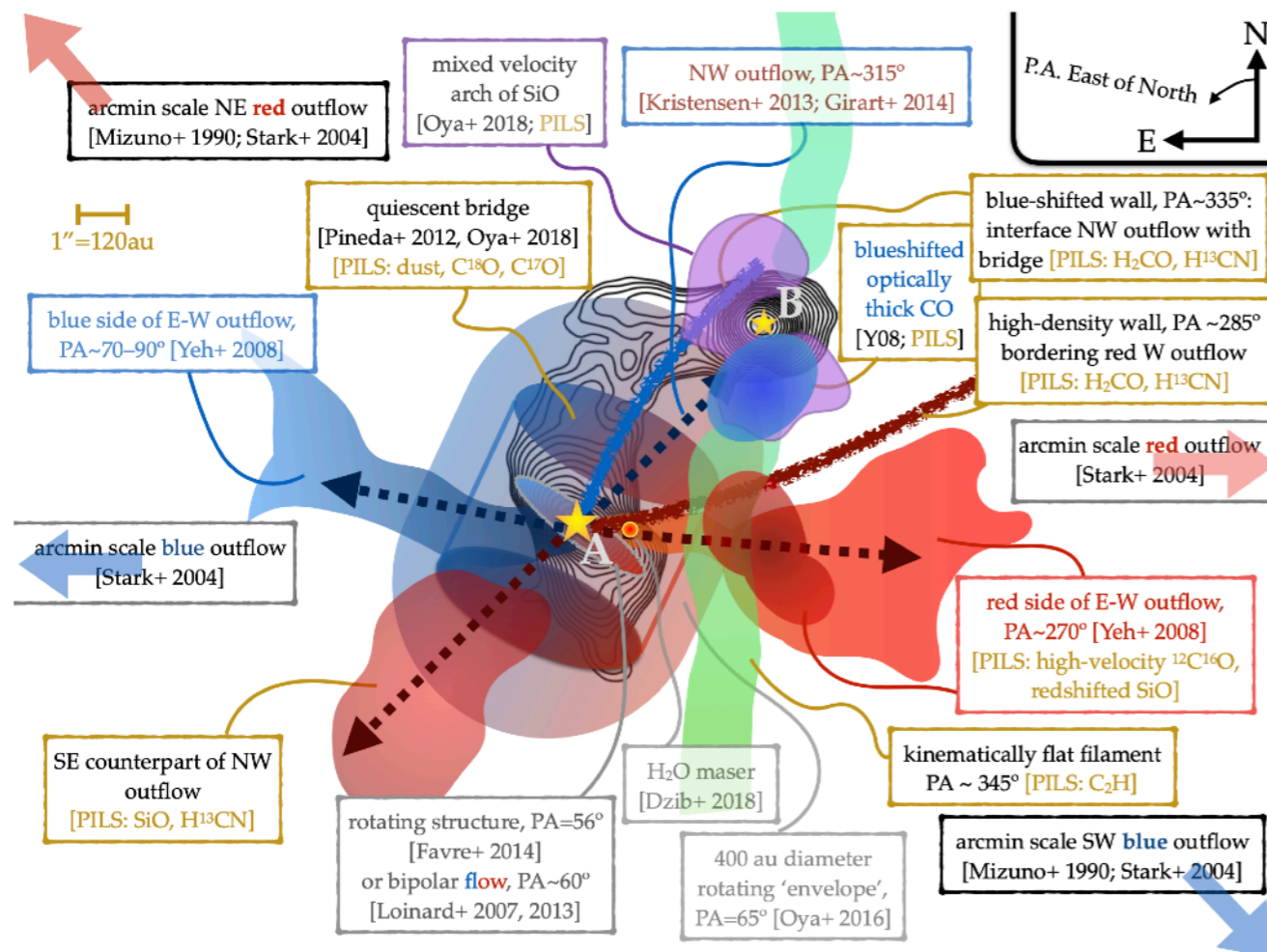
❖ Radiative transfer modeling

- Line identification
- Abundance, temperature, ...
- Kinematics (infall, rotation, ...)

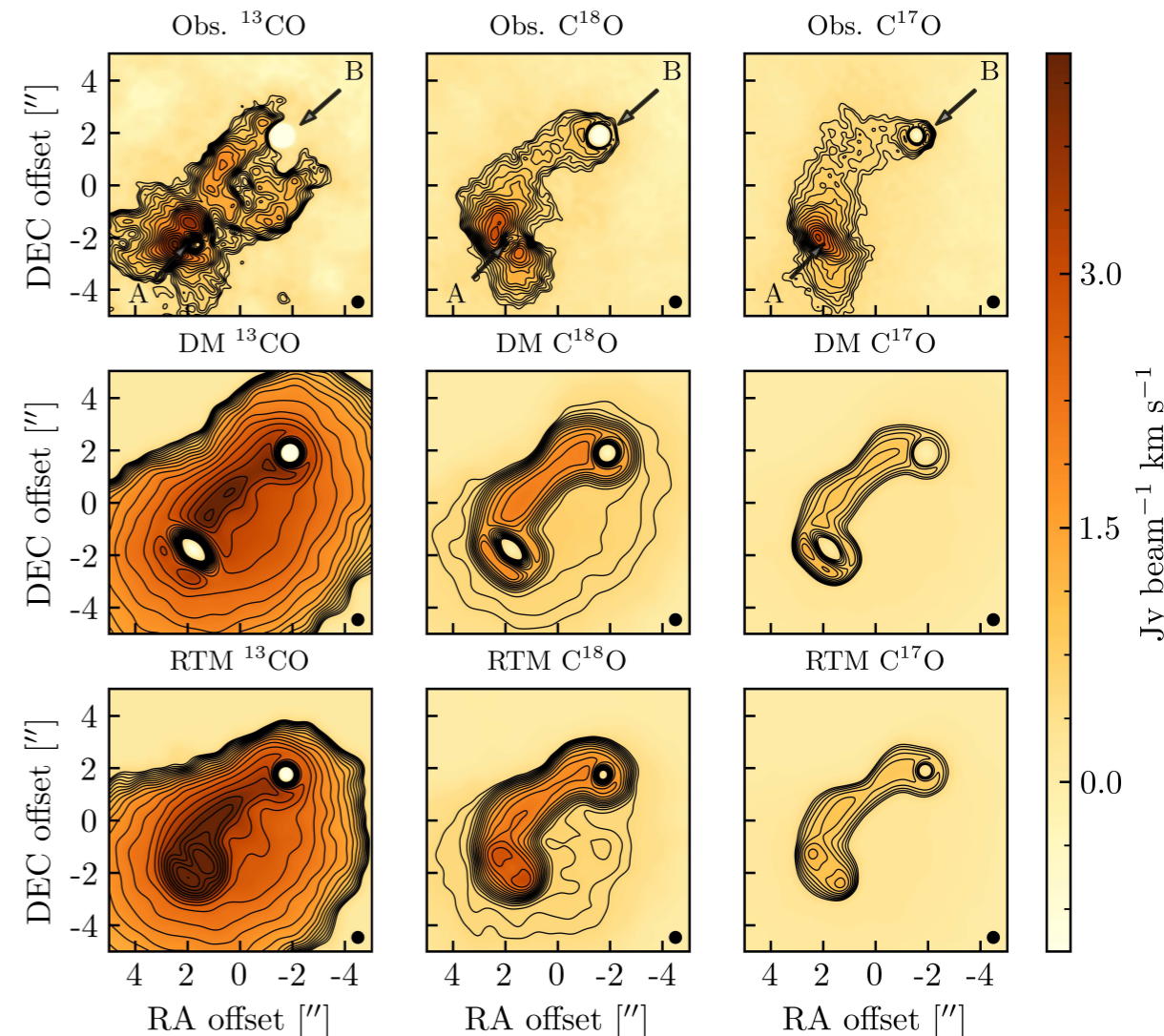


Kinematic and modeling study of IRAS 16293-2422

- 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 ($3 L_{\text{sol}}$)



van der Wiel et al. 2019



Jacobsen et al. 2018

Publications

- Müller, H. S. P. et al. "Rotational spectroscopy of mono-deuterated oxirane ($c\text{-C}_2\text{H}_3\text{DO}$) and its detection towards IRAS 16293-2422 B", 2022 A&A in press
- Koucky, J, et al., "Millimetre-wave spectroscopy of 2-hydroxyprop-2-enal and an astronomical search with ALMA", 2022, A&A in press
- Coutens, A, et al., "The ALMA-PILS survey: First tentative detection of 3-hydroxypropenal (HOCHCHCHO) in the interstellar medium and chemical modeling of the $\text{C}_3\text{H}_4\text{O}_2$ isomers", 2022, A&A 660, L6
- Richard, C., et al. "Torsional-rotational spectrum of doubly-deuterated dimethyl ether (CH_3OCHD_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 ($\text{C}_2\text{H}_3\text{CHO}$) and Propylene (C_3H_6) towards IRAS 16293-2422 B", 2021, A&A 645, A53
- Jørgensen, J. K, Belloche, A., & Garrod, R., "Astrochemistry During the Formation of Stars", 2020, ARA&A, 58,727
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- Coutens, A., et al. "The ALMA-PILS survey: First detection of nitrous acid (HONO) in the interstellar medium", 2019, A&A, 623, A93
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- Manigand, S., et al. "The ALMA-PILS survey: The first detection of doubly-deuterated methyl formate (CHD_2OCHO) in the ISM", 2019, A&A, 623, A69
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- Ligterink, N. F. W., et al. "The formation of peptide-like molecules on interstellar dust grains", 2018, MNRAS, 480, 3628
- Ligterink, N. F. W., et al. "The ALMA-PILS survey: Stringent limits on small amines and nitrogen-oxides towards IRAS 16293-2422B", 2018, A&A, 619, A28
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- Coutens, A., et al. "First detection of cyanamide (NH_2CN) towards solar-type protostars", 2018, A&A, 612, 107
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- Persson, M. V., et al. "The ALMA-PILS survey: Formaldehyde deuteration in warm gas on small scales toward IRAS 16293-2422B", 2018, A&A, 610, A45
- Fayolle, E. C., et al. "Protostellar and Cometary Detections of Organohalogens", 2017, Nature Astronomy, 1, 703
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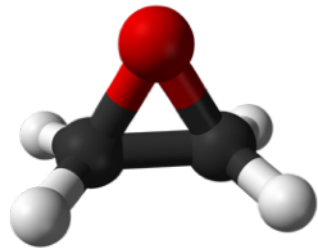
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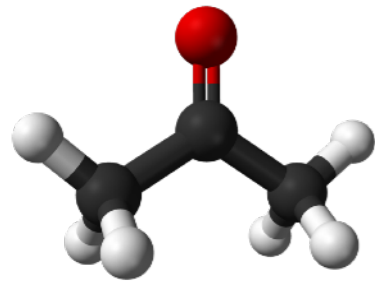
Why do all these detections matter ?

- 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?

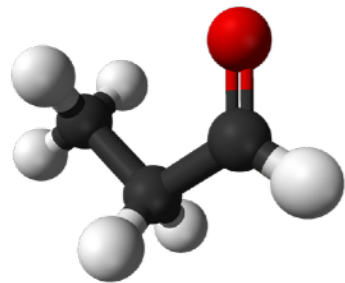
First detections in solar-type protostars



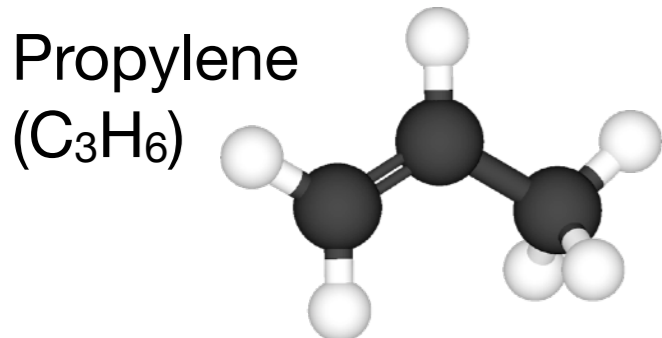
Ethylene oxide (c-C₂H₄O)



Acetone (CH₃COCH₃)



Propanal (CH₃CH₂CHO)
Lykke et al. (2017)

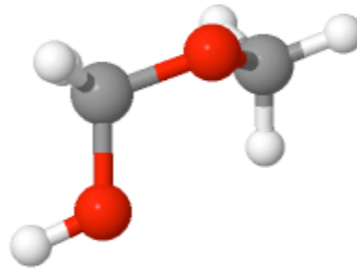


Propylene
(C₃H₆)

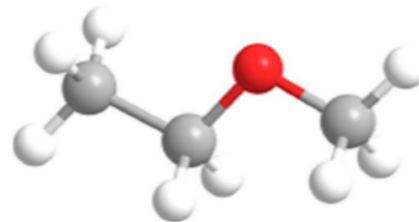


Ligterink et al. 2017
Martin-Domenech et al. 2017

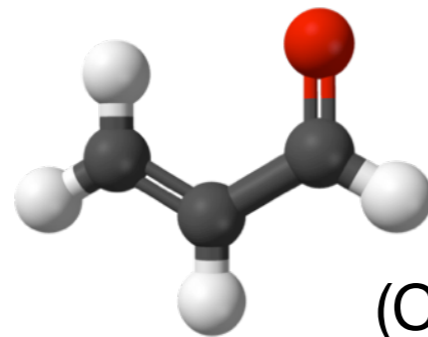
Methyl isocyanate (CH₃NCO)



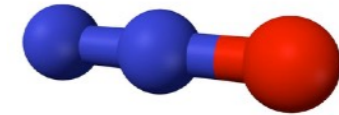
Methoxymethanol (CH₃OCH₂OH)



Trans-ethyl methyl ether (t-C₂H₅OCH₃)
Manigand et al. 2020

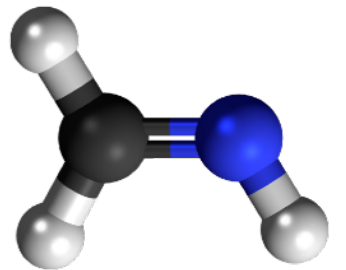


Propenal (CH₂CHCHO)
Manigand et al. 2021

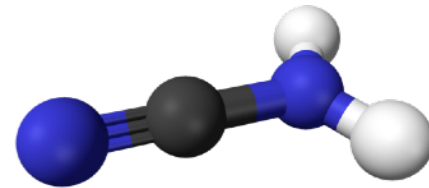


Nitrous oxide (N₂O)

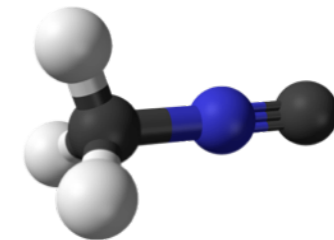
Methanimine
(CH₂NH)



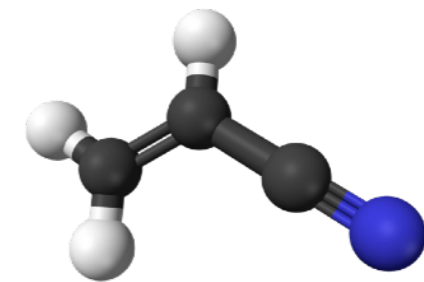
Ligterink et al. 2018



Cyanamide (NH₂CN)
Coutens et al. 2018



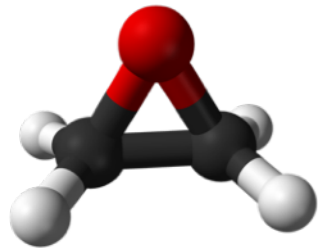
Methyl
isocyanide
(CH₃NC)



Vinyl
cyanide
(CH₂CHCN)

Calcutt et al. 2018

First detections in solar-type protostars

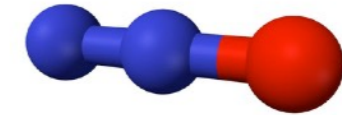


Ethylene oxide (c-C₂H₄O)

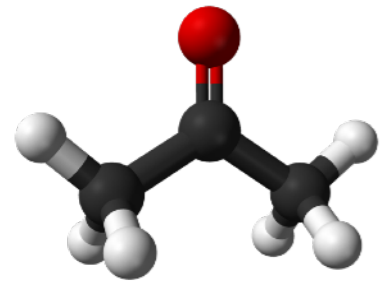


Ligterink et al. 2017
Martin-Domenech et al. 2017

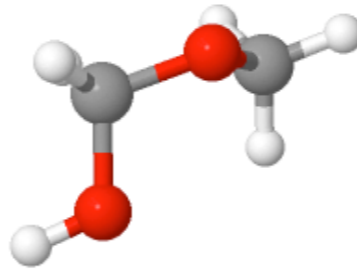
Methyl isocyanate (CH₃NCO)



Nitrous oxide (N₂O)

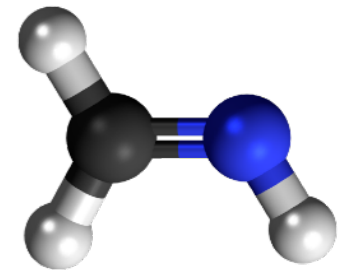


Acetone (CH₃COCH₃)

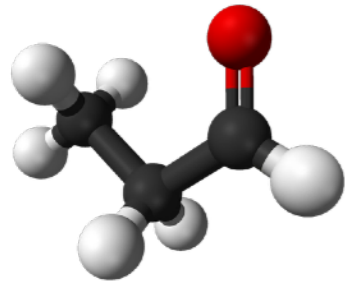


Methoxymethanol (CH₃OCH₂OH)

Methanimine (CH₂NH)

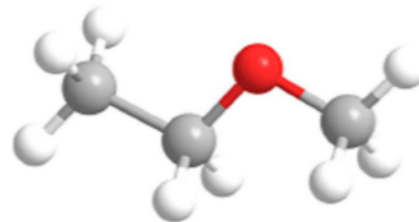


Ligterink et al. 2018



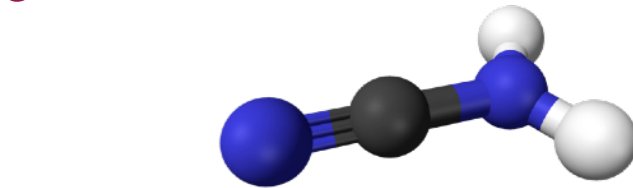
Propanal (CH₃CH₂CHO)

Lykke et al. (2017)



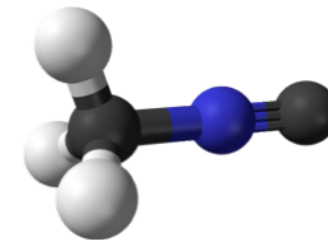
Trans-ethyl methyl ether (t-C₂H₅OCH₃)

Manigand et al. 2020



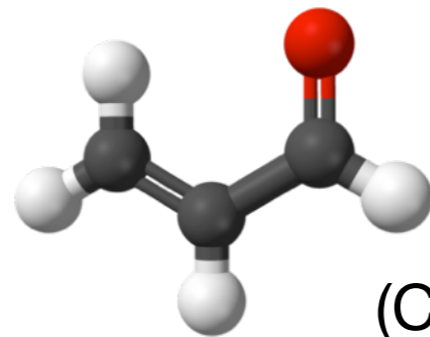
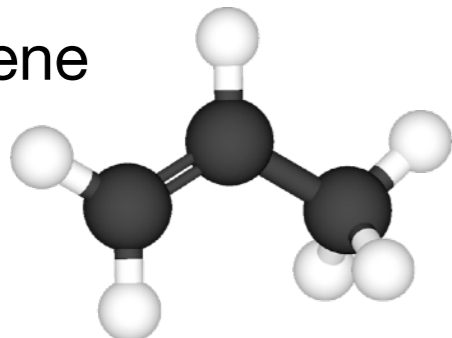
Cyanamide (NH₂CN)

Coutens et al. 2018



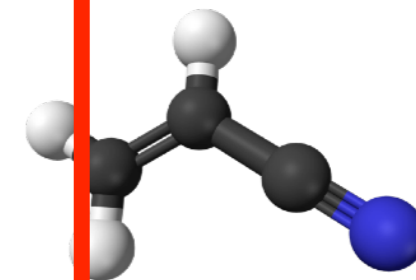
Methyl isocyanide (CH₃NC)

Propylene (C₃H₆)



Propenal (CH₂CHCHO)

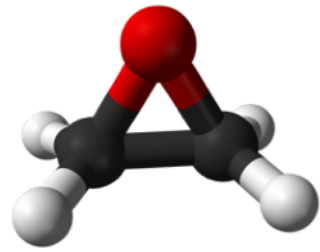
Manigand et al. 2021



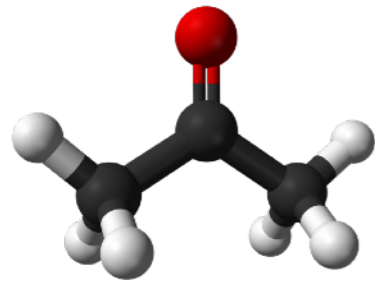
Vinyl cyanide (CH₂CHCN)

Calcutt et al. 2018

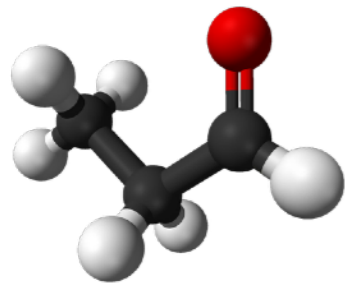
First detections in solar-type protostars



Ethylene oxide (c-C₂H₄O)



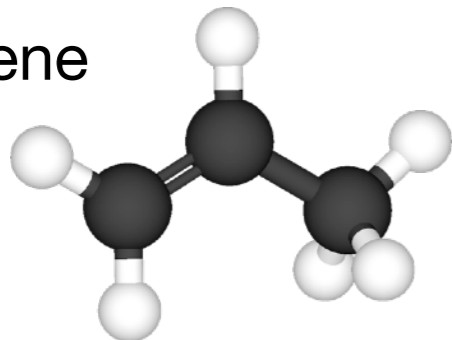
Acetone (CH₃COCH₃)



Propanal (CH₃CH₂CHO)

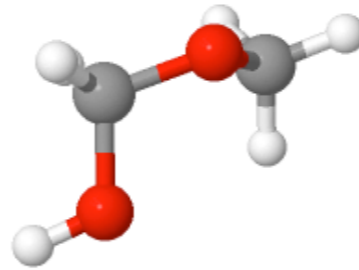
Lykke et al. (2017)

Propylene
(C₃H₆)

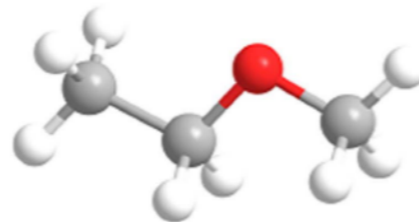


Methyl isocyanate (CH₃NCO)

Ligterink et al. 2017
Martin-Domenech et al. 2017

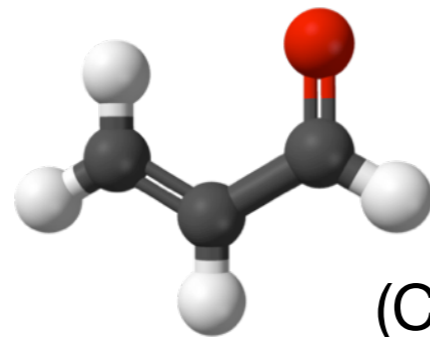


Methoxymethanol (CH₃OCH₂OH)



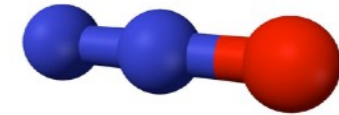
Trans-ethyl methyl ether (t-C₂H₅OCH₃)

Manigand et al. 2020



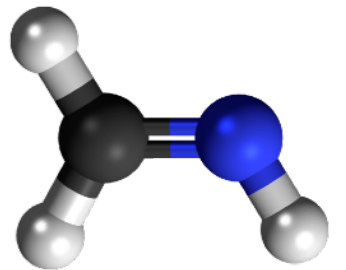
Propenal (CH₂CHCHO)

Manigand et al. 2021

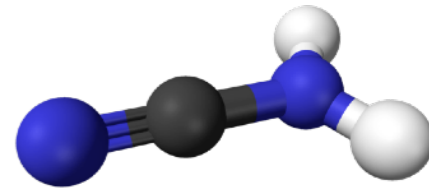


Nitrous oxide (N₂O)

Methanimine
(CH₂NH)

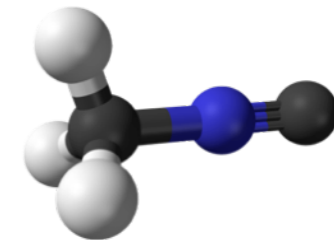


Ligterink et al. 2018

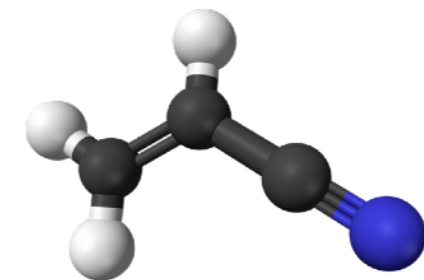


Cyanamide (NH₂CN)

Coutens et al. 2018



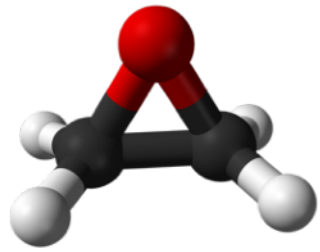
Methyl
isocyanide
(CH₃NC)



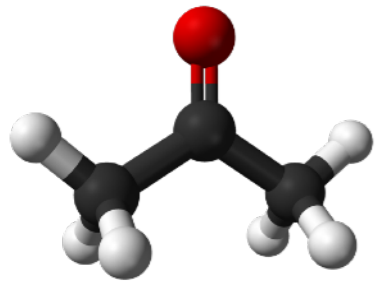
Vinyl
cyanide
(CH₂CHCN)

Calcutt et al. 2018

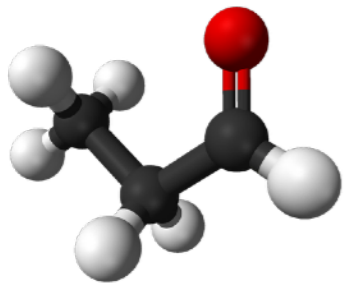
First detections in solar-type protostars



Ethylene oxide (c-C₂H₄O)

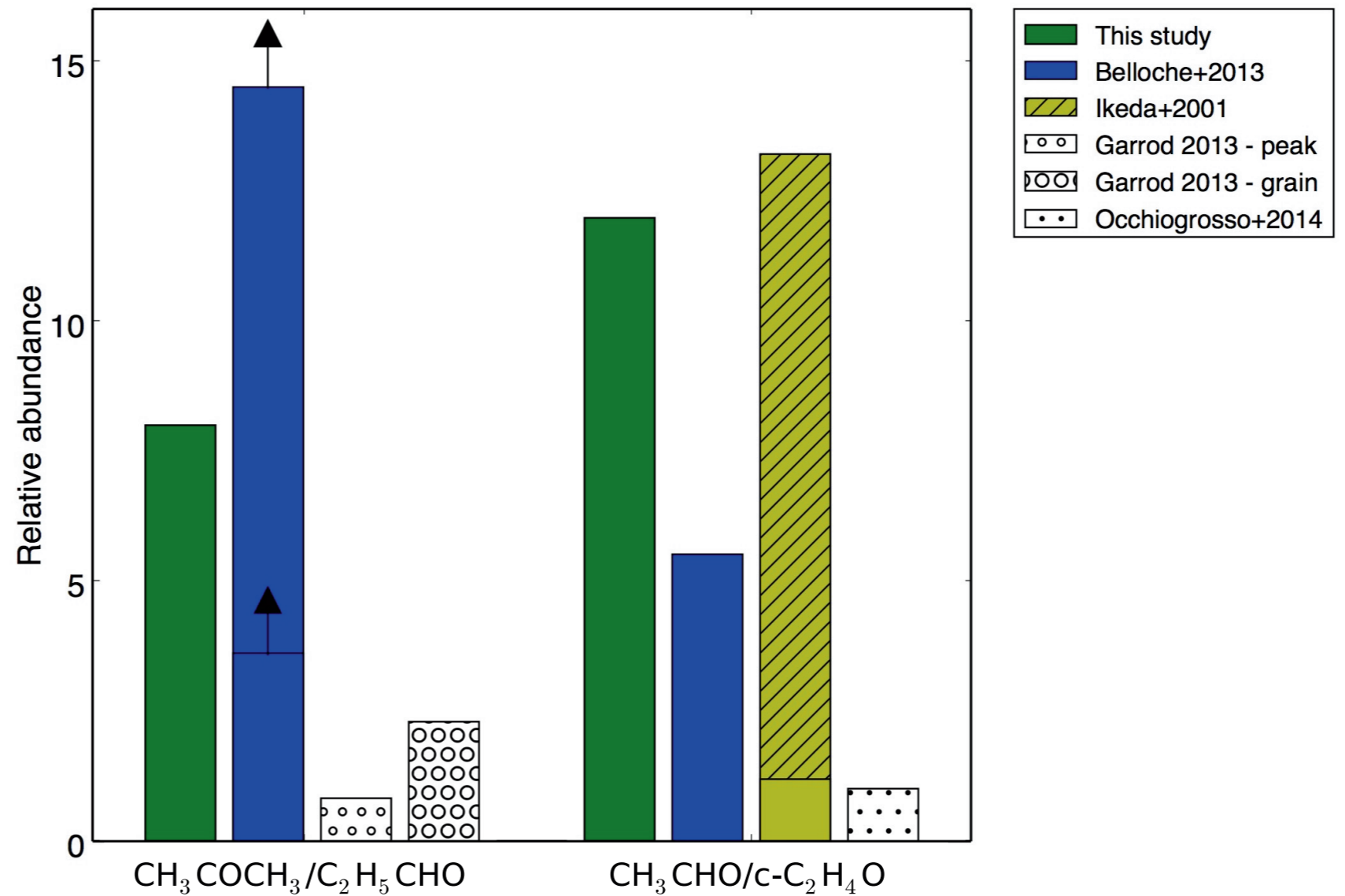


Acetone (CH₃COCH₃)



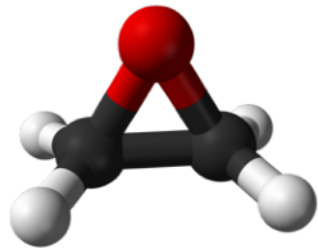
Propanal (CH₃CH₂CHO)

Lykke et al. (2017)

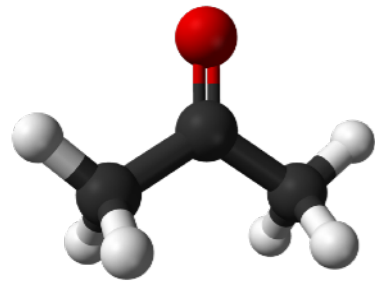


Lykke et al. (2017)

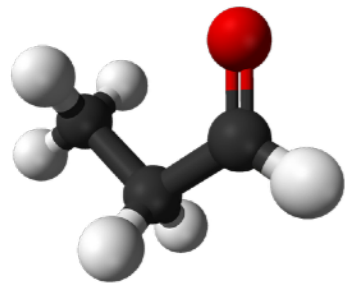
First detections in solar-type protostars



Ethylene oxide (c-C₂H₄O)



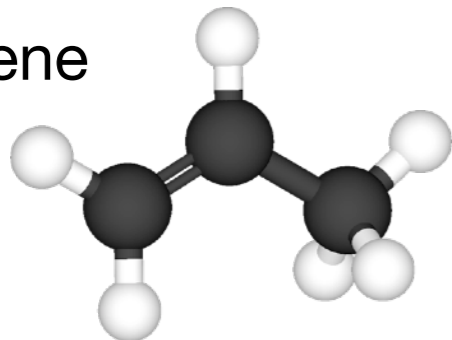
Acetone (CH₃COCH₃)



Propanal (CH₃CH₂CHO)

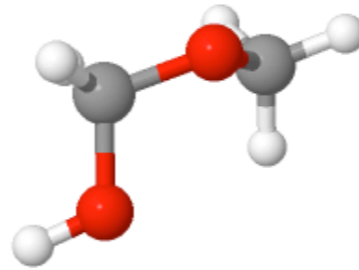
Lykke et al. (2017)

Propylene
(C₃H₆)

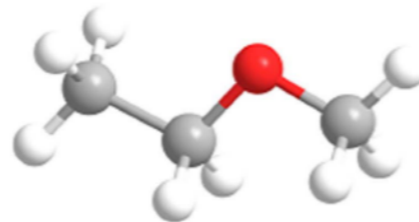


Methyl isocyanate (CH₃NCO)

Ligterink et al. 2017
Martin-Domenech et al. 2017

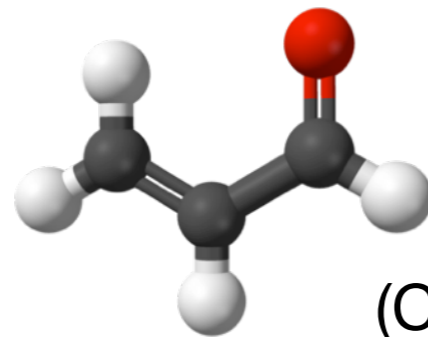


Methoxymethanol (CH₃OCH₂OH)



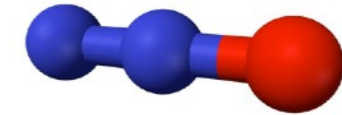
Trans-ethyl methyl ether (t-C₂H₅OCH₃)

Manigand et al. 2020



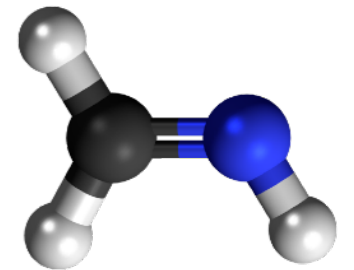
Propenal (CH₂CHCHO)

Manigand et al. 2021

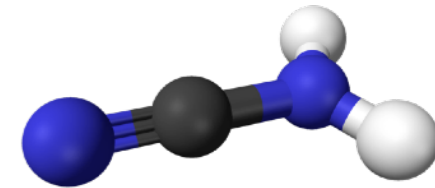


Nitrous oxide (N₂O)

Methanimine
(CH₂NH)

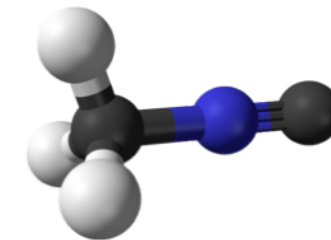


Ligterink et al. 2018

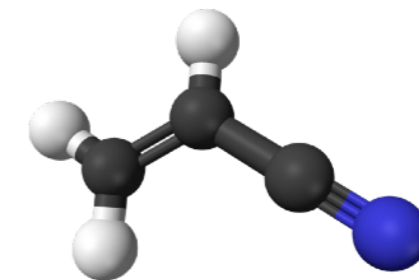


Cyanamide (NH₂CN)

Coutens et al. 2018



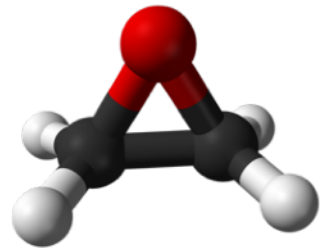
Methyl
isocyanide
(CH₃NC)



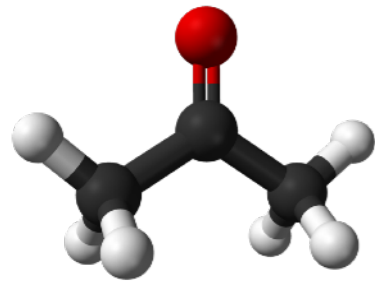
Vinyl
cyanide
(CH₂CHCN)

Calcutt et al. 2018

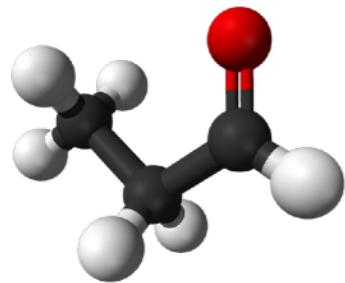
First detections in solar-type protostars



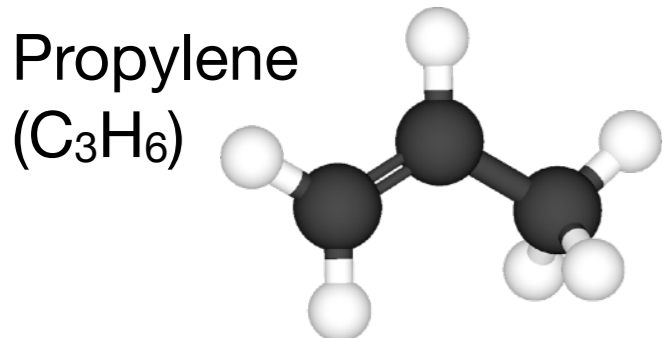
Ethylene oxide (c-C₂H₄O)



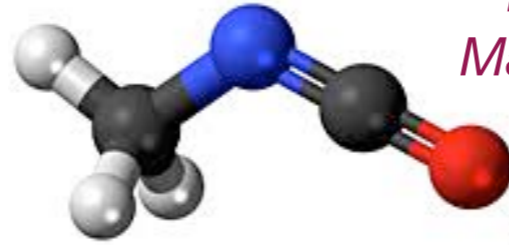
Acetone (CH₃COCH₃)



Propanal (CH₃CH₂CHO)
Lykke et al. (2017)

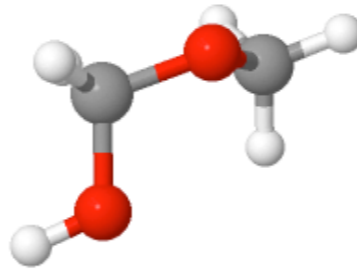


Propylene
(C₃H₆)

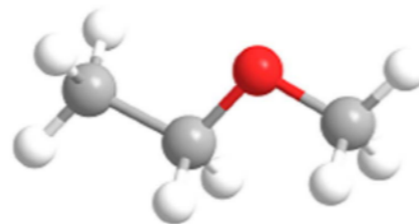


Ligterink et al. 2017
Martin-Domenech et al. 2017

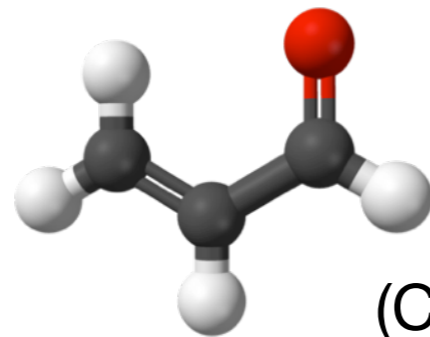
Methyl isocyanate (CH₃NCO)



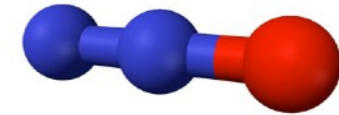
Methoxymethanol (CH₃OCH₂OH)



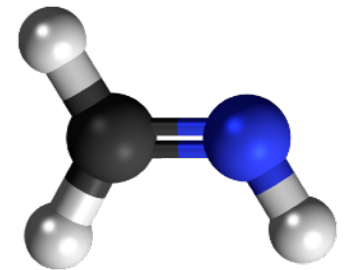
Trans-ethyl methyl ether (t-C₂H₅OCH₃)
Manigand et al. 2020



Propenal (CH₂CHCHO)
Manigand et al. 2021

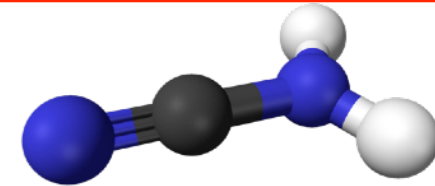


Nitrous oxide (N₂O)

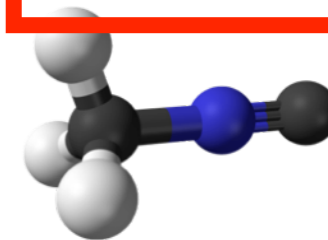


Methanimine
(CH₂NH)

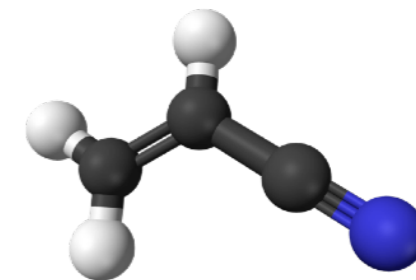
Ligterink et al. 2018



Cyanamide (NH₂CN)
Coutens et al. 2018



Methyl
isocyanide
(CH₃NC)

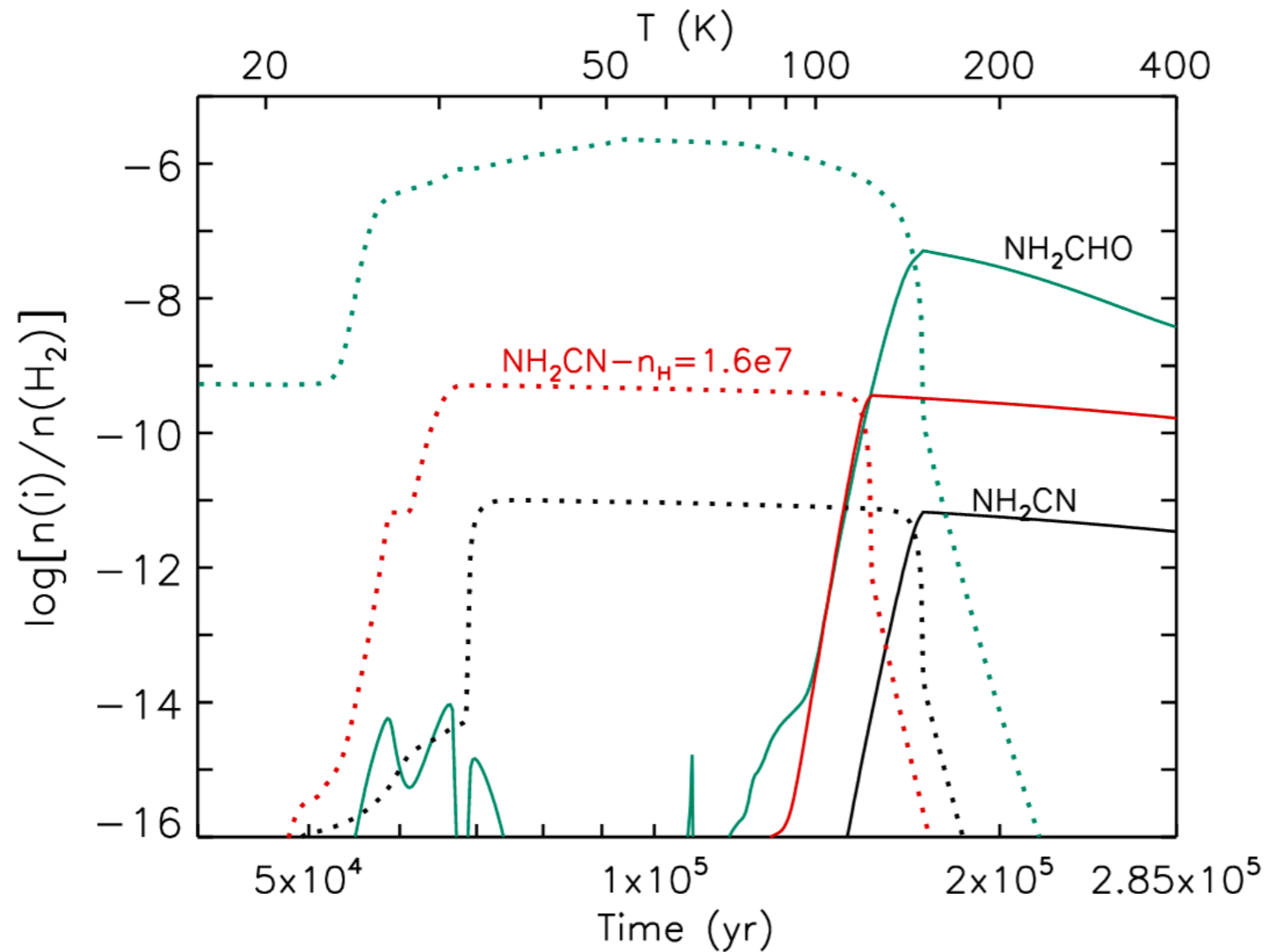


Vinyl
cyanide
(CH₂CHCN)

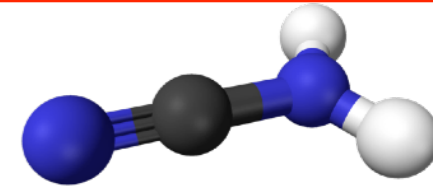
Calcutt et al. 2018

First detections in solar-type protostars

- Gas-grain chemistry model
- Possible formation of NH_2CN through the $\text{NH}_2 + \text{CN}$ reaction on grains



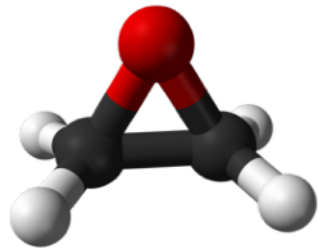
Coutens et al. 2018



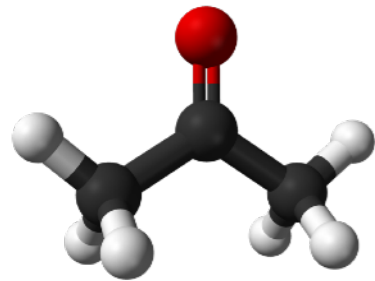
Cyanamide (NH_2CN)

Coutens et al. 2018

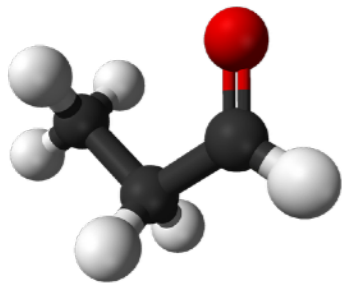
First detections in solar-type protostars



Ethylene oxide (c-C₂H₄O)



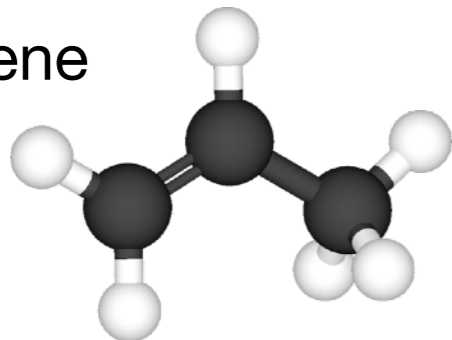
Acetone (CH₃COCH₃)



Propanal (CH₃CH₂CHO)

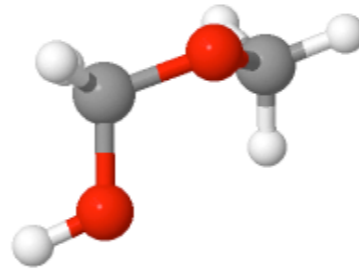
Lykke et al. (2017)

Propylene
(C₃H₆)

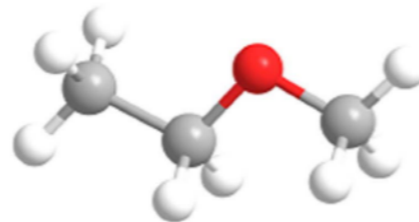


Methyl isocyanate (CH₃NCO)

Ligterink et al. 2017
Martin-Domenech et al. 2017

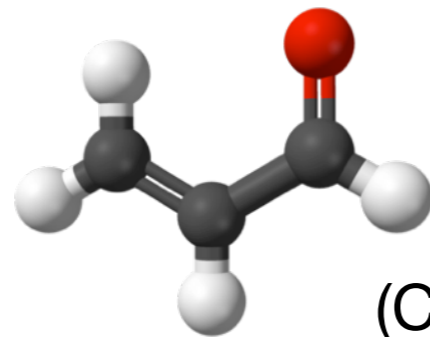


Methoxymethanol (CH₃OCH₂OH)



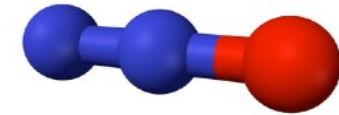
Trans-ethyl methyl ether (t-C₂H₅OCH₃)

Manigand et al. 2020



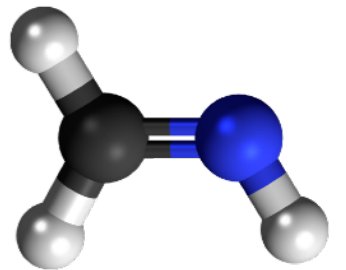
Propenal (CH₂CHCHO)

Manigand et al. 2021

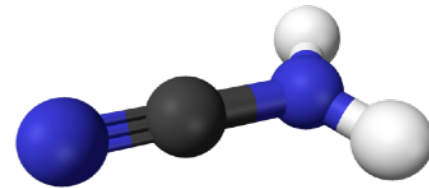


Nitrous oxide (N₂O)

Methanimine
(CH₂NH)

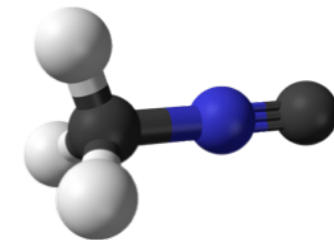


Ligterink et al. 2018

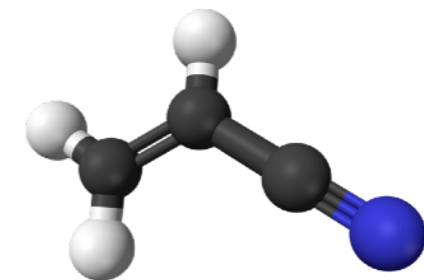


Cyanamide (NH₂CN)

Coutens et al. 2018



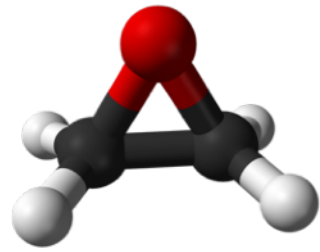
Methyl
isocyanide
(CH₃NC)



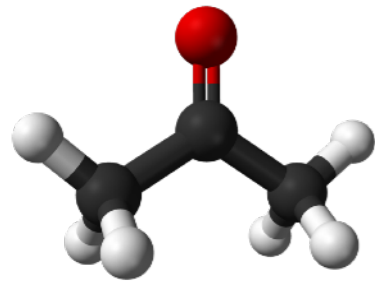
Vinyl
cyanide
(CH₂CHCN)

Calcutt et al. 2018

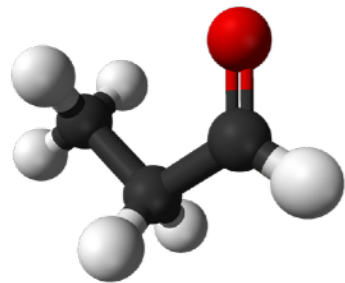
First detections in solar-type protostars



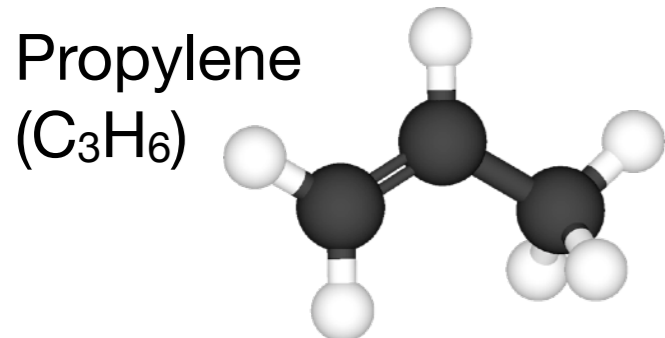
Ethylene oxide (c-C₂H₄O)



Acetone (CH₃COCH₃)



Propanal (CH₃CH₂CHO)
Lykke et al. (2017)

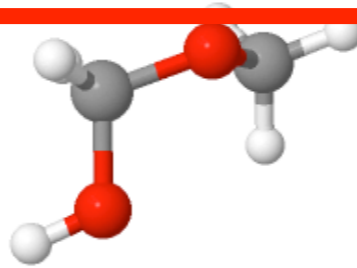


Propylene
(C₃H₆)

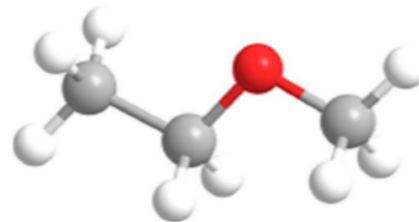


Methyl isocyanate (CH₃NCO)

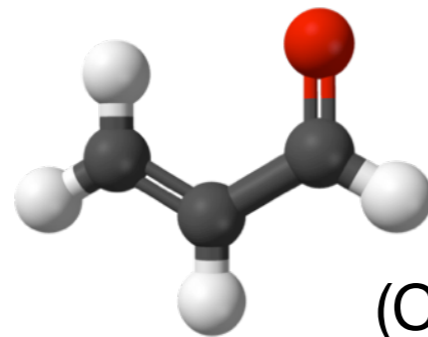
Ligterink et al. 2017
Martin-Domenech et al. 2017



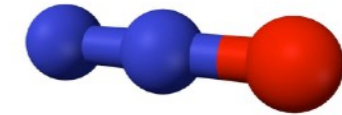
Methoxymethanol (CH₃OCH₂OH)



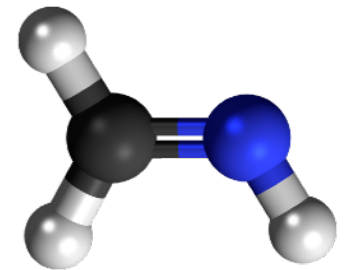
Trans-ethyl methyl ether (t-C₂H₅OCH₃)
Manigand et al. 2020



Propenal (CH₂CHCHO)
Manigand et al. 2021

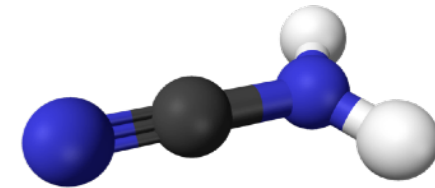


Nitrous oxide (N₂O)

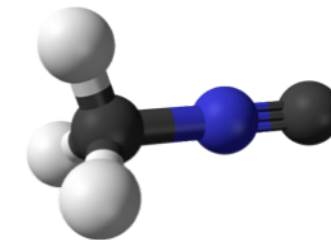


Methanimine
(CH₂NH)

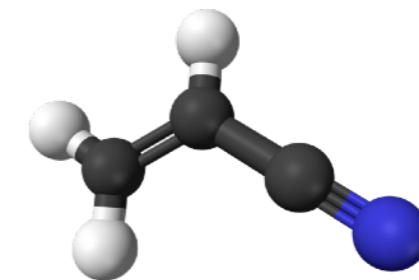
Ligterink et al. 2018



Cyanamide (NH₂CN)
Coutens et al. 2018



Methyl
isocyanide
(CH₃NC)



Vinyl
cyanide
(CH₂CHCN)

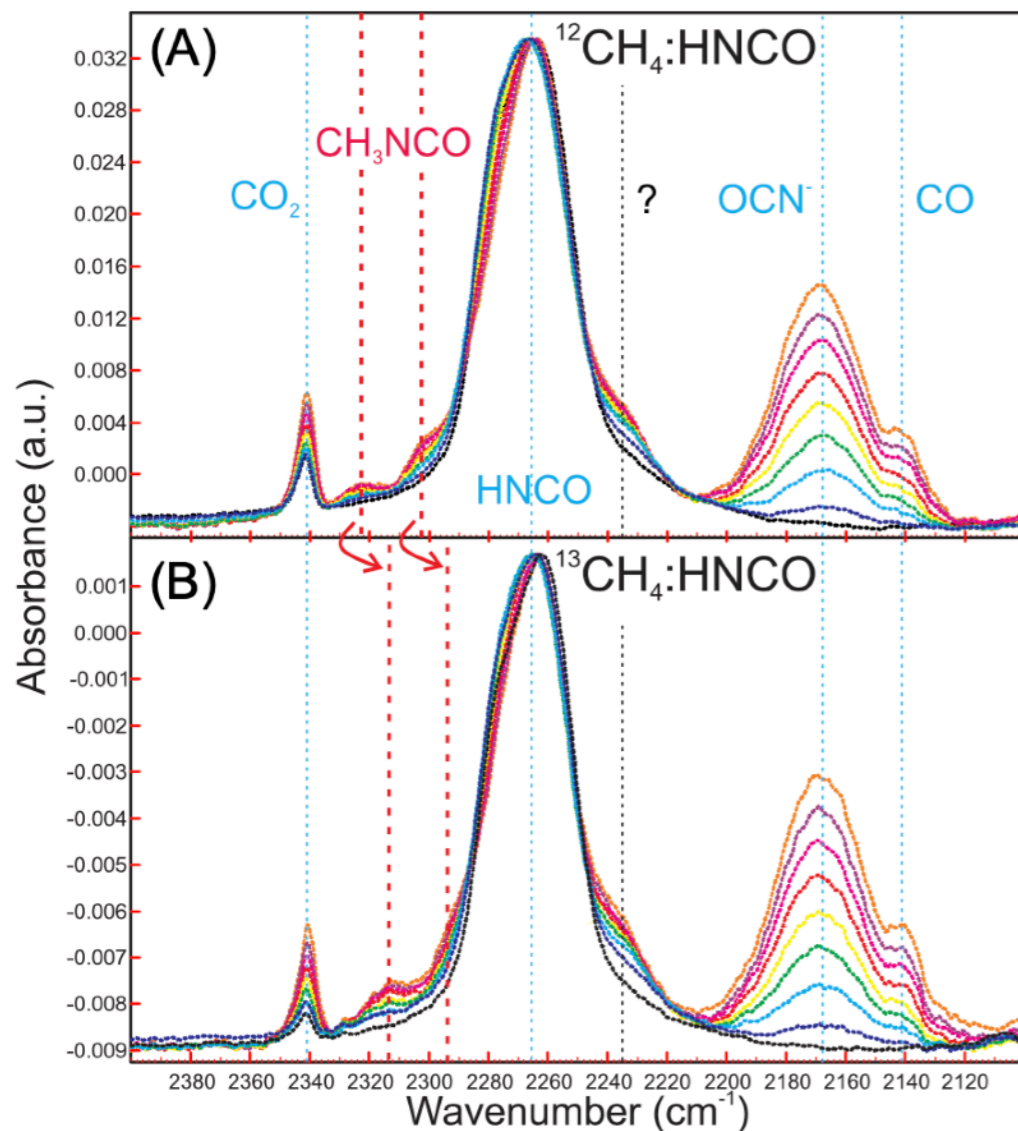
Calcutt et al. 2018

First detections in solar-type protostars



Ligterink et al. 2017
Martin-Domenech et al. 2017

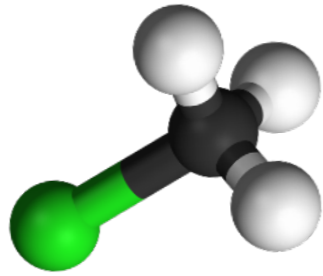
Methyl isocyanate (CH_3NCO)



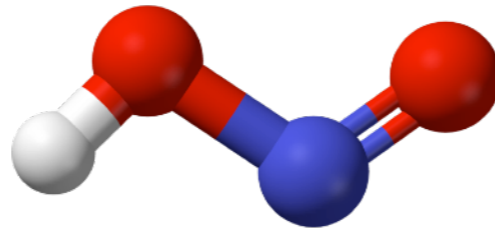
- Laboratory experiments
- VUV irradiation of $\text{CH}_4\text{:HNCO}$ mixtures at 20 K
- Formation on grains through CH_3 and (H)NCO recombinations

Ligterink et al. 2017

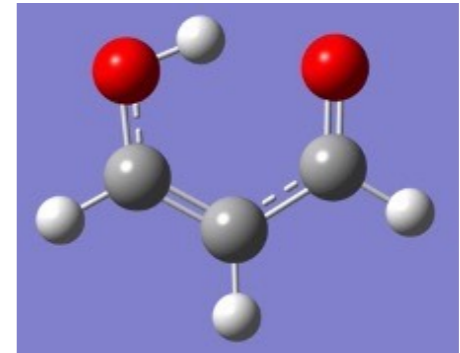
First detections in the ISM



Methyl chloride (CH₃Cl)
Fayolle et al. 2017



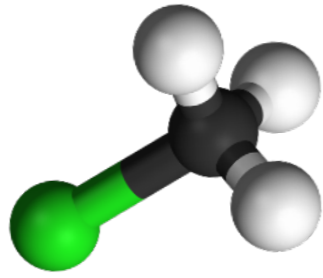
Nitrous acid (HONO)
Coutens et al. 2019



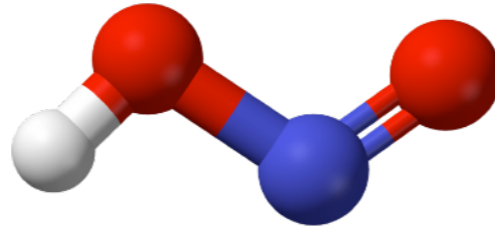
3-hydroxypropenal (HOCHCHCHO)
Coutens et al. 2022

+ a lot of isotopologues !

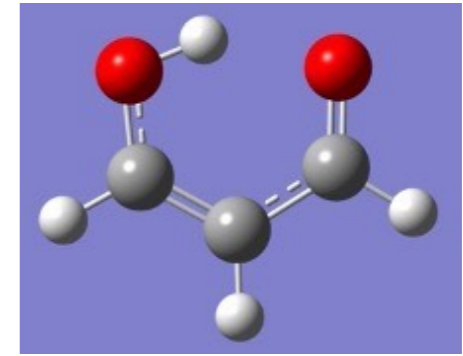
First detections in the ISM



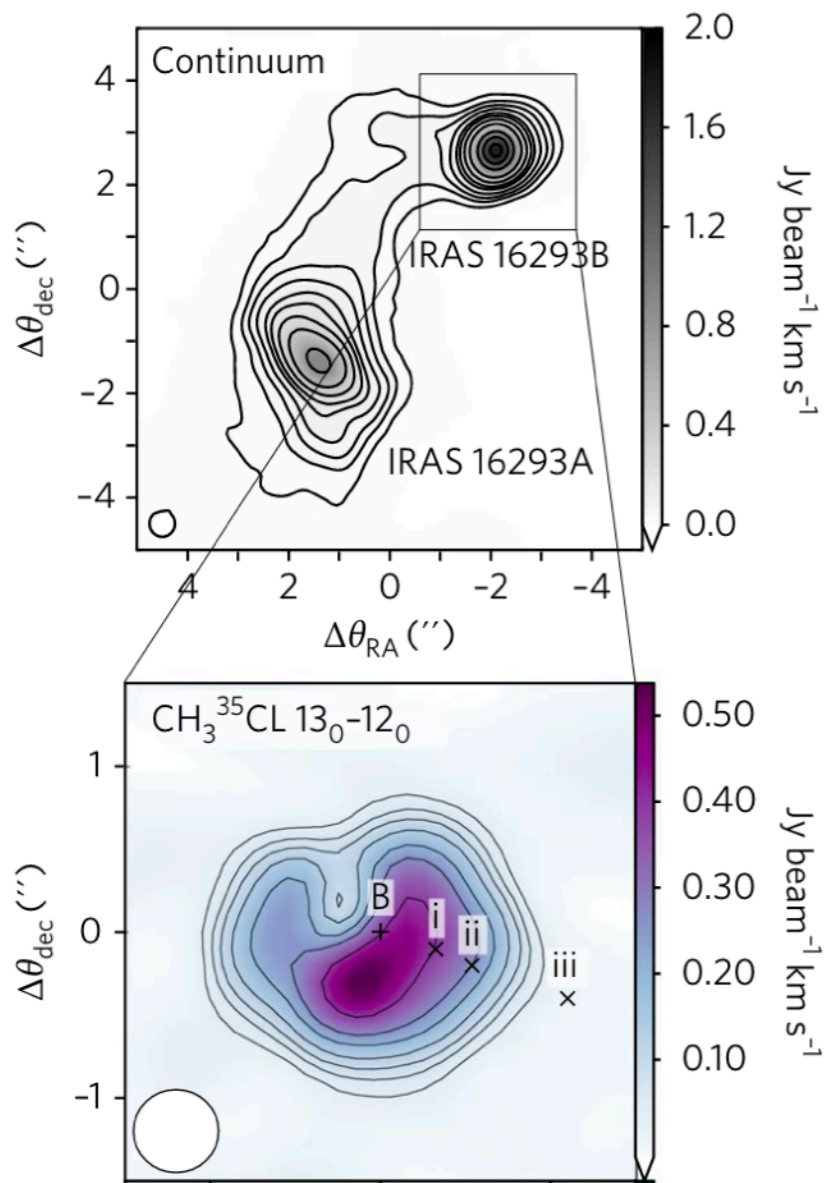
Methyl chloride (CH₃Cl)
Fayolle et al. 2017



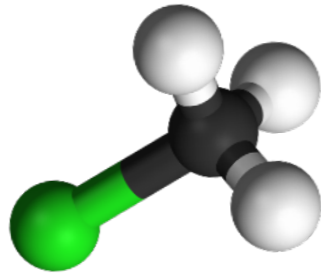
Nitrous acid (HONO)
Coutens et al. 2019



3-hydroxypropenal (HOCHCHCHO)
Coutens et al. 2022

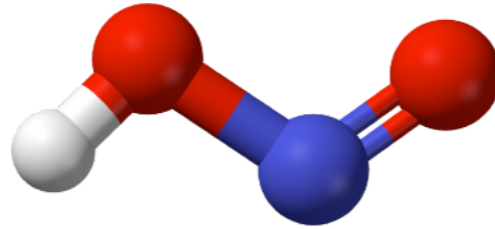


First detections in the ISM



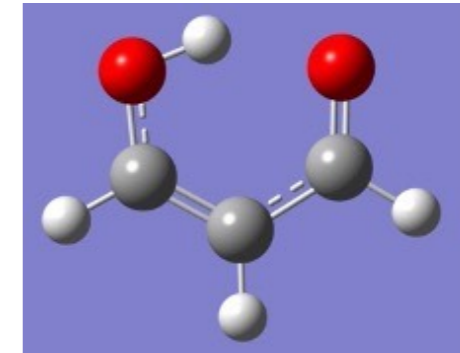
Methyl chloride (CH_3Cl)

Fayolle et al. 2017



Nitrous acid (HONO)

Coutens et al. 2019



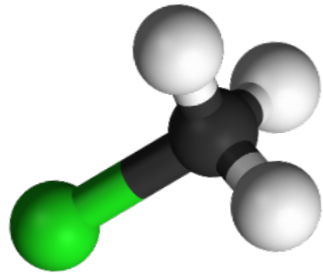
3-hydroxypropenal (HOCHCHCHO)

Coutens et al. 2022

Molecule	Formula	N_{tot}^{\dagger} (cm^{-2})	T_{ex} (K)
Nitrous acid	HONO	$(9 \pm 5) \times 10^{14}$	100
Nitric oxide [‡]	NO	$(2.0 \pm 0.5) \times 10^{16}$	40–150
Nitrous oxide [‡]	N_2O	$\geq 4.0 \times 10^{16}$	25–350
Hydroxylamine [‡]	NH_2OH	$\leq 4 \times 10^{14}$	[100]
Nitrosyl hydride	HNO	$\leq 3 \times 10^{14}$	[100]
Nitrogen dioxide	NO_2	$\leq 2 \times 10^{16}$	[100]
Nitrosyl cation	NO^+	$\leq 2 \times 10^{14}$	[100]
Nitric acid	HNO_3	$\leq 5 \times 10^{14}$	[100]

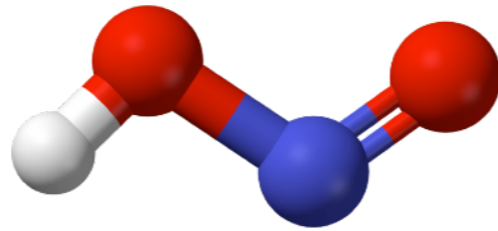
- Production on grains through s-O + s-HNO, s-H + s- NO_2 , and s-OH + s-NO surface reactions

First detections in the ISM



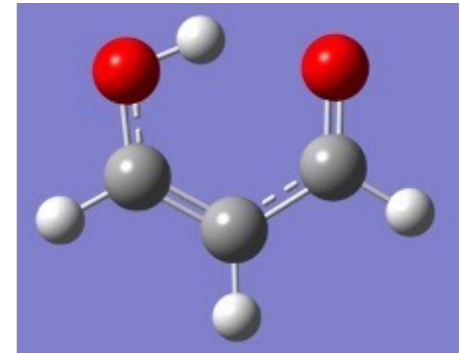
Methyl chloride (CH₃Cl)

Fayolle et al. 2017



Nitrous acid (HONO)

Coutens et al. 2019



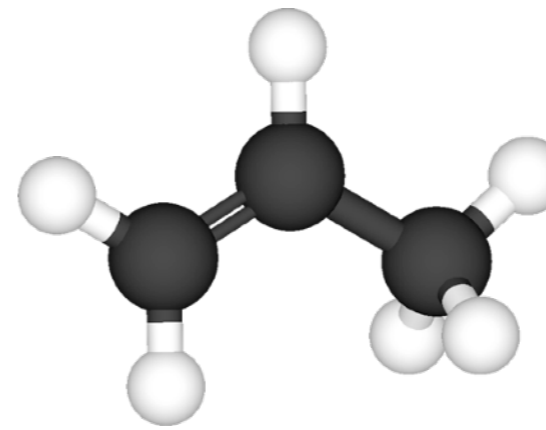
3-hydroxypropenal (HOCHCHCHO)

Coutens et al. 2022

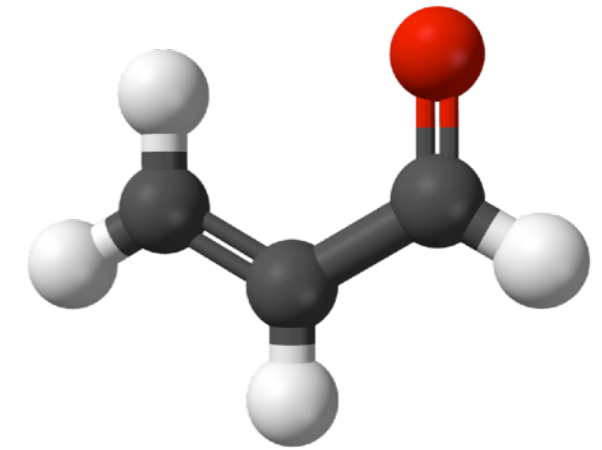
The chemistry of 3-carbon species

Unsaturated 3-carbon molecules

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



Propylene
(C₃H₆)

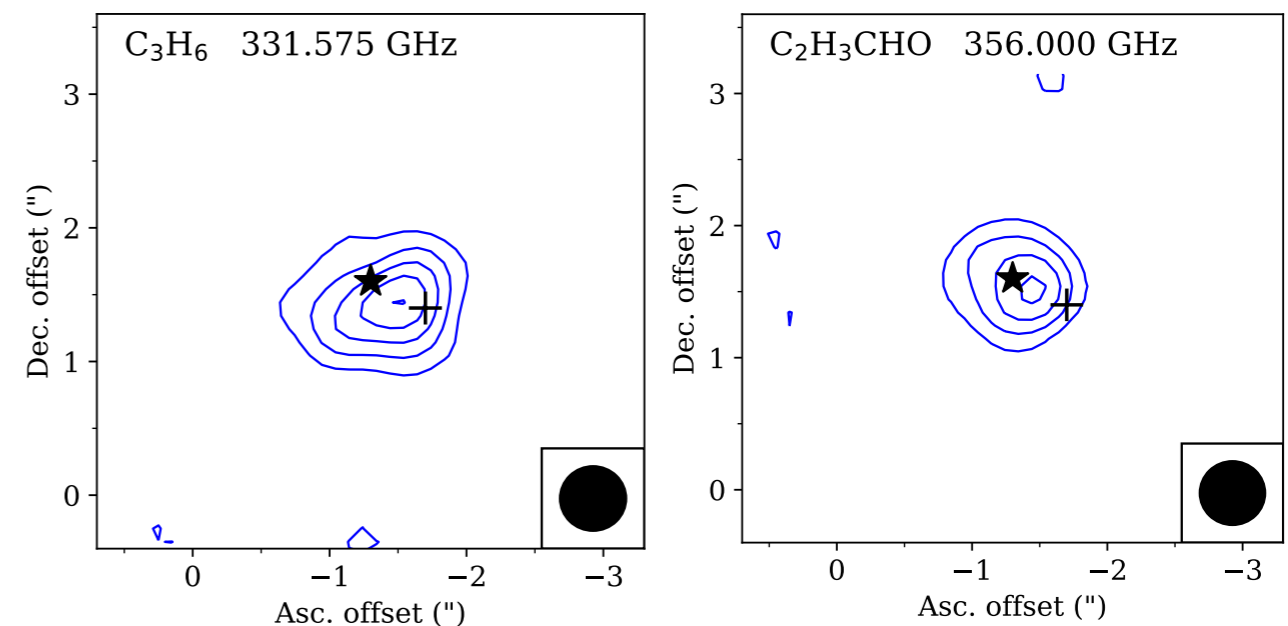


Propenal = Acrolein
(CH₂CHCHO)

Manigand et al. 2021, Lykke et al. 2017

Species	T_{ex} (K)	N_{tot} (cm ⁻²)
C ₂ H ₃ CHO	125 ± 25	3.4 ± 0.7 × 10 ¹⁴
C ₃ H ₆	75 ± 15	4.2 ± 0.8 × 10 ¹⁶
HCCCHO	100 ^(a)	<5.0 × 10 ¹⁴
<i>n</i> -C ₃ H ₇ OH	100 ^(a)	<3.0 × 10 ¹⁵
<i>i</i> -C ₃ H ₇ OH	100 ^(a)	<3.0 × 10 ¹⁵
C ₃ O	100 ^(a)	<2.0 × 10 ¹³
cis-HC(O)CHO	100 ^(a)	<5.0 × 10 ¹³
C ₃ H ₈	100 ^(a)	<8.0 × 10 ¹⁶
CH ₃ CCH	100 ± 20	1.1 ± 0.2 × 10 ¹⁶
C ₂ H ₅ CHO	125 ± 25	2.2 ± 1.1 × 10 ¹⁵ (†)
CH ₃ CHO	125 ± 25	7.0 ± 3.5 × 10 ¹⁶ (†)
CH ₃ COCH ₃	125 ± 25	1.7 ± 0.8 × 10 ¹⁶ (†)
C ₂ H ₅ OCH ₃	100 ± 20	1.8 ± 0.2 × 10 ¹⁶ (†)

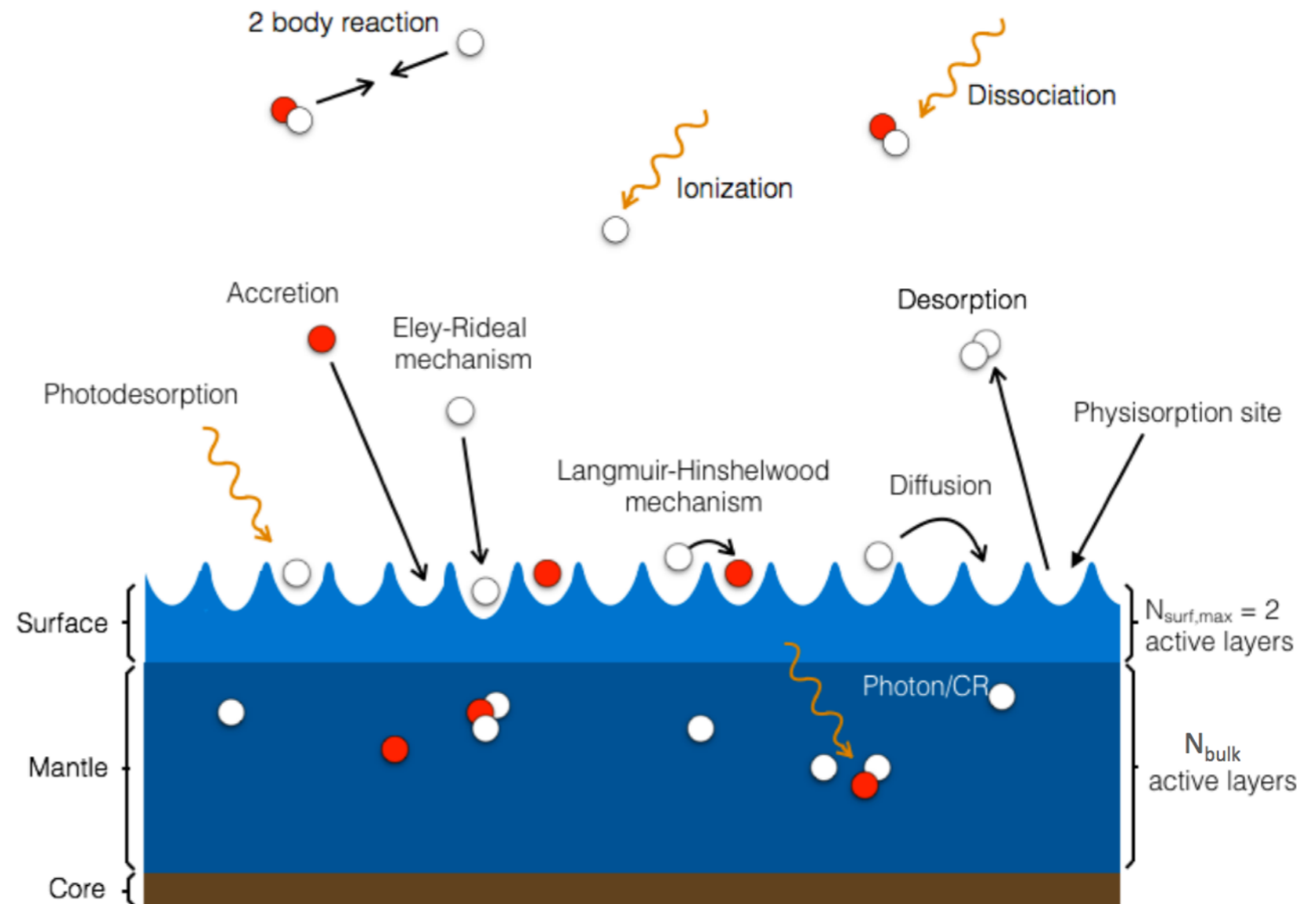
Detection towards IRAS 16293 B



Manigand et al. 2021

The chemistry of 3-carbon species

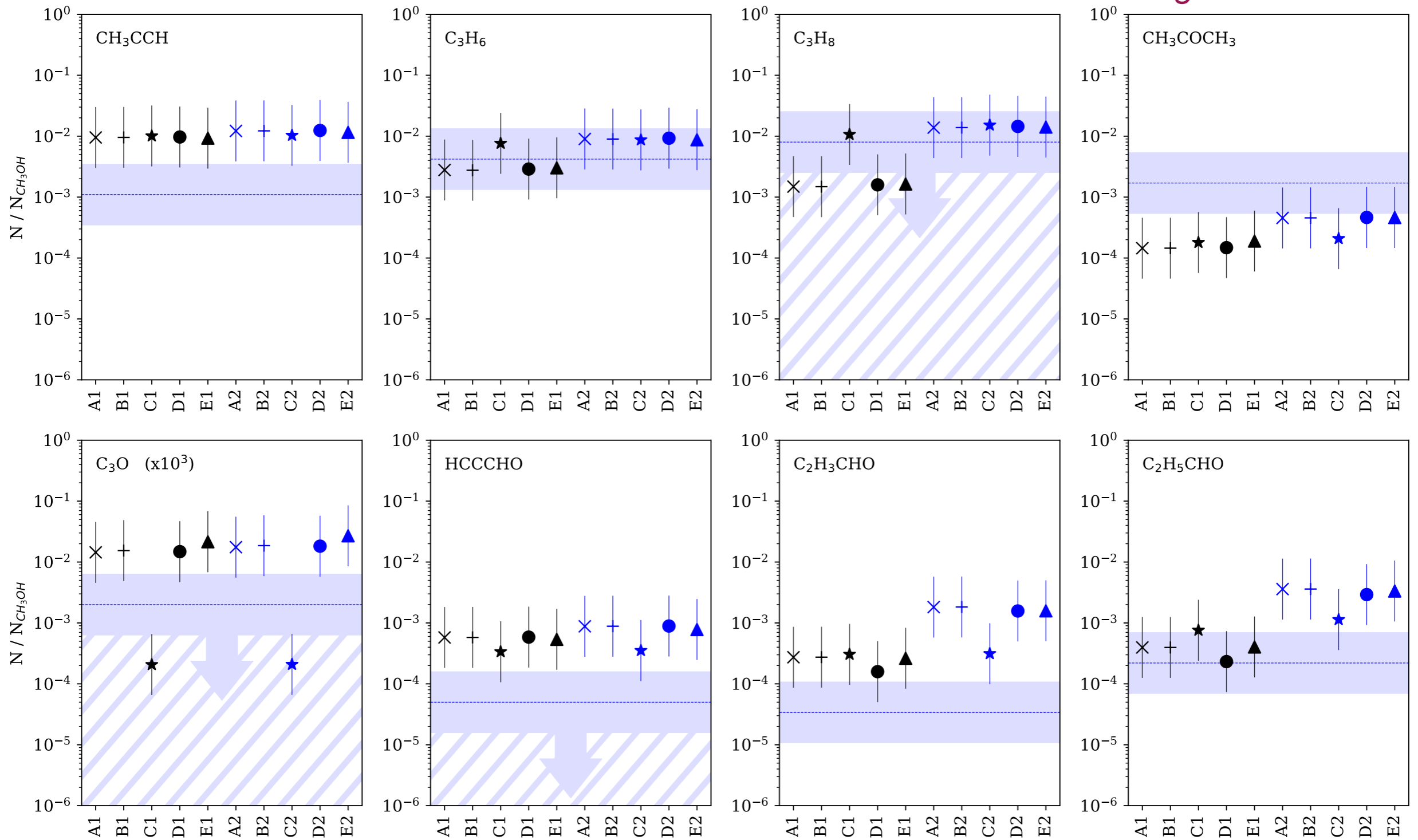
- Three-phase chemistry code Nautilus (PI: V. Wakelam)
- Prestellar phase followed by a 1D hydrodynamical collapse (*Masunaga & Inutsuka 2000*)
- Tests of different formation pathways (successive hydrogenation of C_3 and C_3O and radical-radical additions on grain surfaces) to assess which are the dominant formation mechanisms



Ruud et al. 2016

The chemistry of 3-carbon species

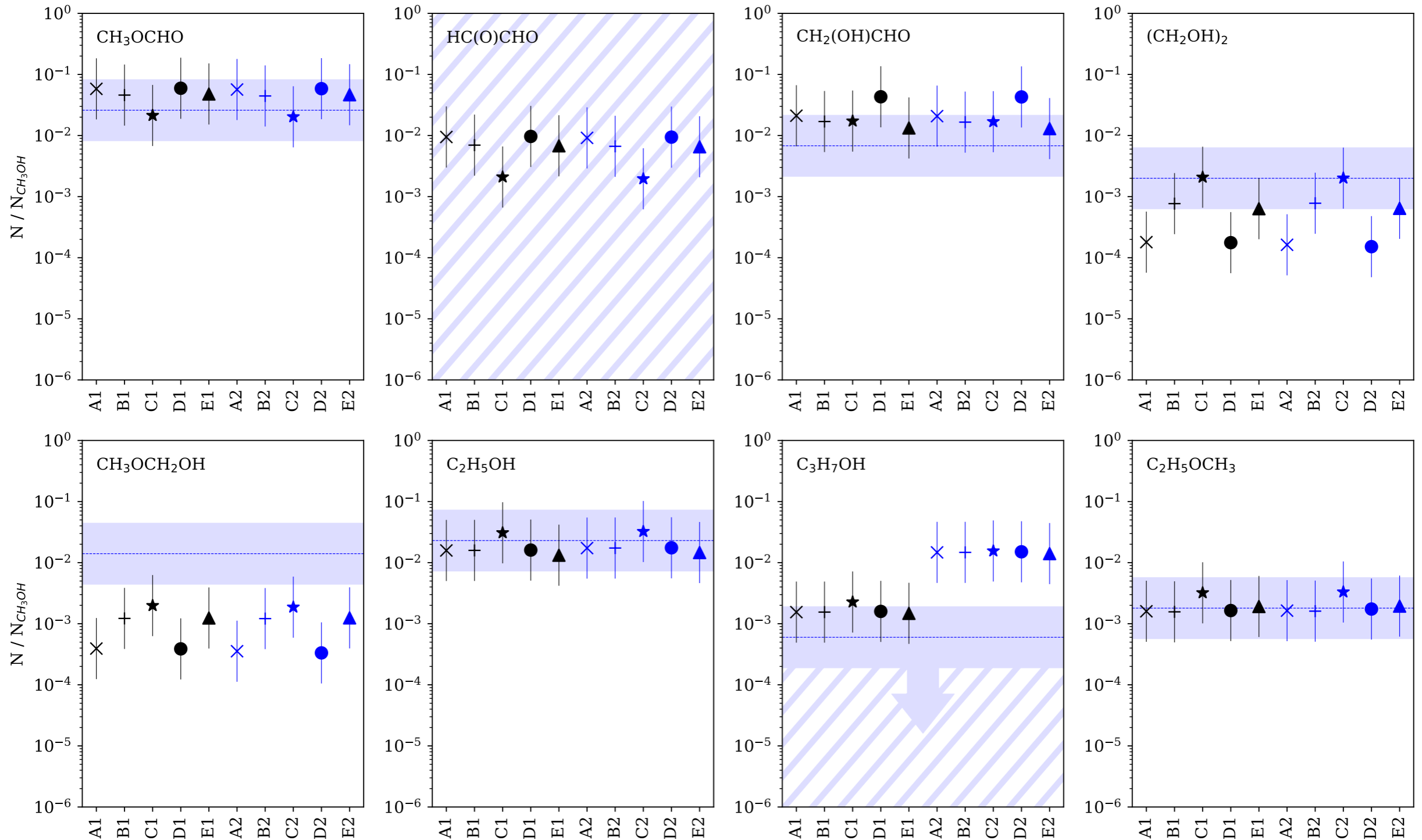
Manigand et al. 2021



The chemistry of 3-carbon species

+ comparison with 2C-species

Manigand et al. 2021

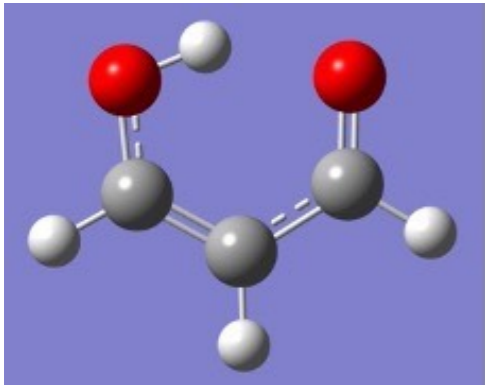


The chemistry of 3-carbon species

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_2H_3CHO and C_2H_5CHO through both :
 - ▶ successive hydrogenation reactions on ice surfaces of C_3O , with a formation of C_3O in the gas phase ($C_3 + OH \rightarrow C_3O + H$)
 - ▶ radical-radical additions of HCO and C_2H_3 or C_2H_5 on ice surfaces
- Rate of $10^{-12} \text{ cm}^3 \text{ s}^{-1}$ 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

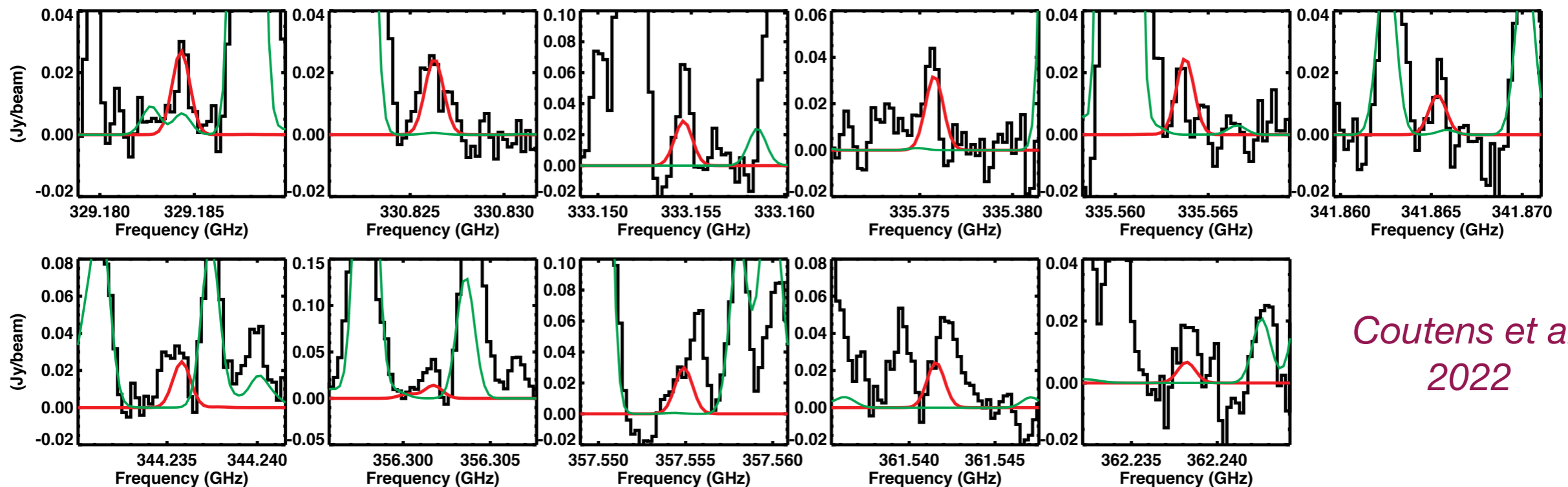


3-hydroxypropenal :
biomarker to
measure the level of
oxidative stress in
living organisms

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

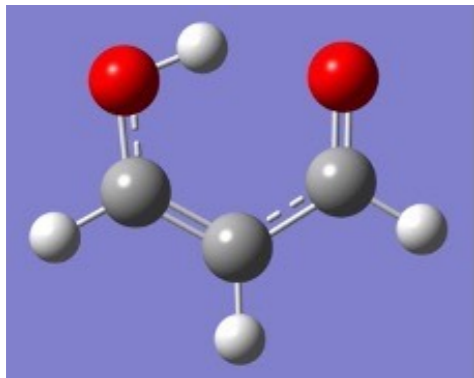


*Coutens et al.
2022*

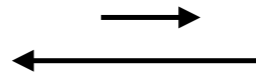
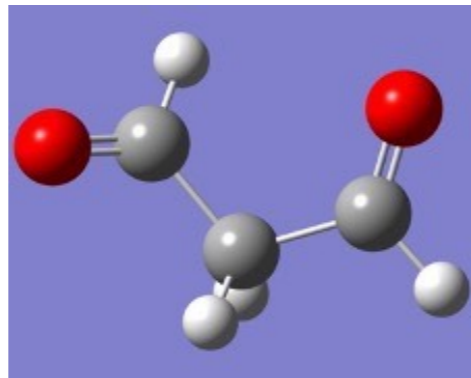
3-hydroxypropenal and isomers

Tautomers

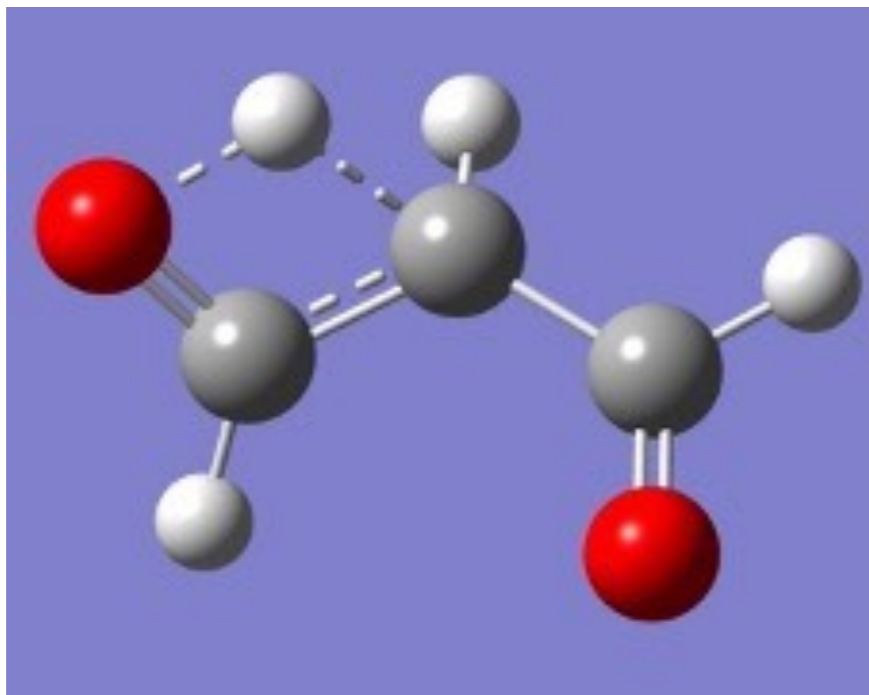
3-hydroxypropenal
enol



propanedial
dialdehyde

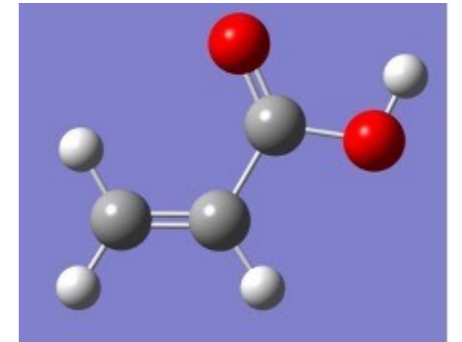


Tautomerization

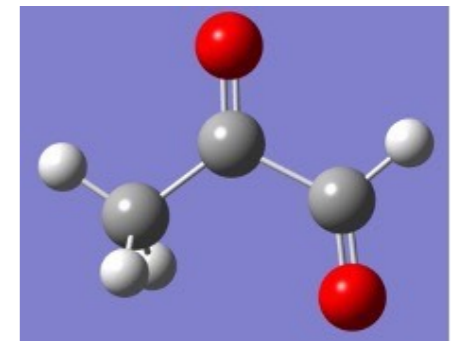


Isomers

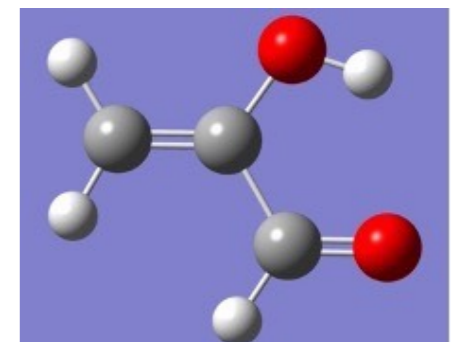
2-propenoic acid
(C_2H_3COOH)



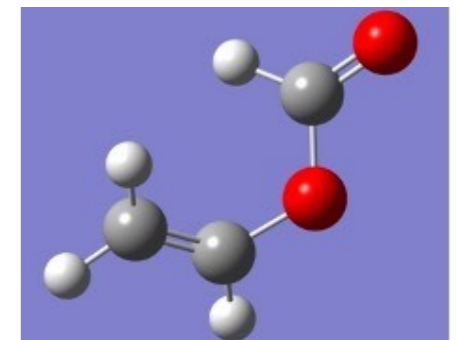
Methyl glyoxal
(CH_3COCHO)



2-hydroxypropenal
($CH_2COHCHO$)



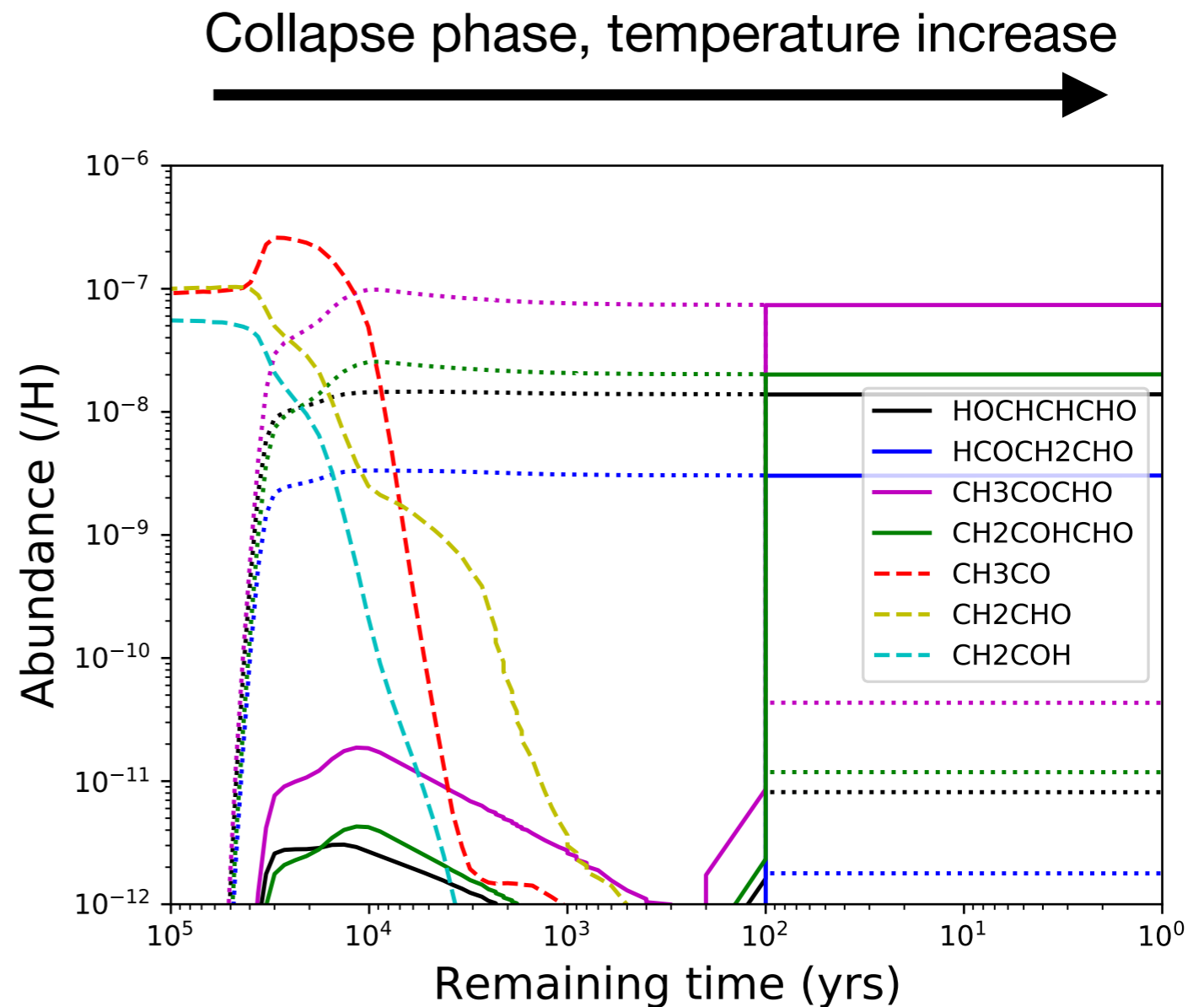
Vinyl formate
(C_2H_3OCHO)



Tautomers

Chemical modeling of the C₃H₄O₂ isomers

- Same physical model as in Manigand et al. 2021
- Update of the chemical network by including the reactions producing and consuming the C₃H₄O₂ isomers and some radical species linked to C₃H₄O₂
- Our model reproduces the abundance of HOCHCHCHO with respect to CH₃OH within the uncertainties (~10)
- $\text{CH}_2\text{CHO} + \text{HCO} \rightarrow \text{HCOCH}_2\text{CHO}$
 $\text{HCOCH}_2\text{CHO} \rightarrow \text{HOCHCHCHO}$



Coutens et al. 2022

Importance of spectroscopic studies

Isomer	Formula	Predicted abundance (/H)	Predicted abundance (/CH ₃ OH)	Observed abundance (/CH ₃ OH)
3-Hydroxypropenal	HOCHCHCHO	1.4×10^{-8}	4.6×10^{-4}	1.0×10^{-4}
Propanedial	HCOCH ₂ CHO	3.0×10^{-9}	9.9×10^{-5}	
Methyl glyoxal	CH ₃ COCHO	7.4×10^{-8}	2.4×10^{-3}	
2-Hydroxypropenal	CH ₂ COHCHO	2.0×10^{-8}	6.6×10^{-4}	
Vinyl formate	C ₂ H ₃ OCHO	8.4×10^{-10}	2.8×10^{-5}	$\leq 4 \times 10^{-4}$
2-Propenoic acid	C ₂ H ₃ COOH	2.2×10^{-13}	7.3×10^{-9}	$\leq 5 \times 10^{-4}$

- Upper limits in agreement for vinyl formate and 2-propenoic acid

Importance of spectroscopic studies

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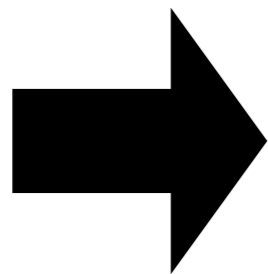
- Upper limits in agreement for vinyl formate and 2-propenoic acid
- Predictions of high abundances for propanedial, methyl glyoxal and 2-hydroxypropenal

Importance of spectroscopic studies

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- Upper limits in agreement for vinyl formate and 2-propenoic acid
- Predictions of high abundances for propanedial, methyl glyoxal and 2-hydroxypropenal

Spectroscopic studies are needed:



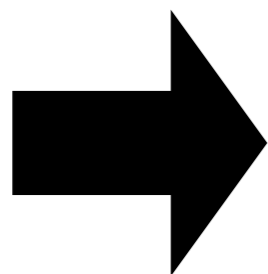
- to search for propanedial, methyl glyoxal and 2-hydroxyprop-2-enal in IRAS16293 and other sources
- to test the chemical network

2-hydroxyprop-2-enal

Isomer	Formula	Predicted abundance (/H)	Predicted abundance (/CH ₃ OH)	Observed abundance (/CH ₃ OH)
3-Hydroxypropenal	HOCHCHCHO	1.4×10^{-8}	4.6×10^{-4}	1.0×10^{-4}
Propanedial	HCOCH ₂ CHO	3.0×10^{-9}	9.9×10^{-5}	
Methyl glyoxal	CH ₃ COCHO	7.4×10^{-8}	2.4×10^{-3}	<i>Koucky, Kolesnikova et al. 2022</i>
2-Hydroxypropenal	CH ₂ COHCHO	2.0×10^{-8}	6.6×10^{-4}	< 2.4×10^{-4}
Vinyl formate	C ₂ H ₃ OCHO	8.4×10^{-10}	2.8×10^{-5}	$\leq 4 \times 10^{-4}$
2-Propenoic acid	C ₂ H ₃ COOH	2.2×10^{-13}	7.3×10^{-9}	$\leq 5 \times 10^{-4}$

- Upper limits in agreement for vinyl formate and 2-propenoic acid
- Predictions of high abundances for propanedial, methyl glyoxal and 2-hydroxypropenal

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

First detections of isotopologues in the ISM

Formamide

NH_2CDO
cis-NHDCHO
trans-NHDCHO

Isocyanic acid

DNCO

Cyanamide

NHDCN
 $\text{NH}_2^{13}\text{CN}$

Methyl cyanide

CHD_2CN

Glycolaldehyde

CHDOHCHO
 CH_2ODCHO
 CH_2OHCDO
 $^{13}\text{CH}_2\text{OHCHO}$
 $\text{CH}_2\text{OH}^{13}\text{CHO}$

Ethanol

a-a- $\text{CH}_2\text{DCH}_2\text{OH}$
a-s- $\text{CH}_2\text{DCH}_2\text{OH}$
 CH_3CHDOH

Methyl formate

HCOOCHD_2

Acetaldehyde

CH_3CDO
 $^{13}\text{CH}_3\text{CHO}$
 $\text{CH}_3^{13}\text{CHO}$

Oxyrane

c- $\text{C}_2\text{H}_3\text{DO}$

Dimethyl ether

CH_3OCHD_2

Formic acid

H^{13}COOH
t-D COOH
t-H COOD

Ketene

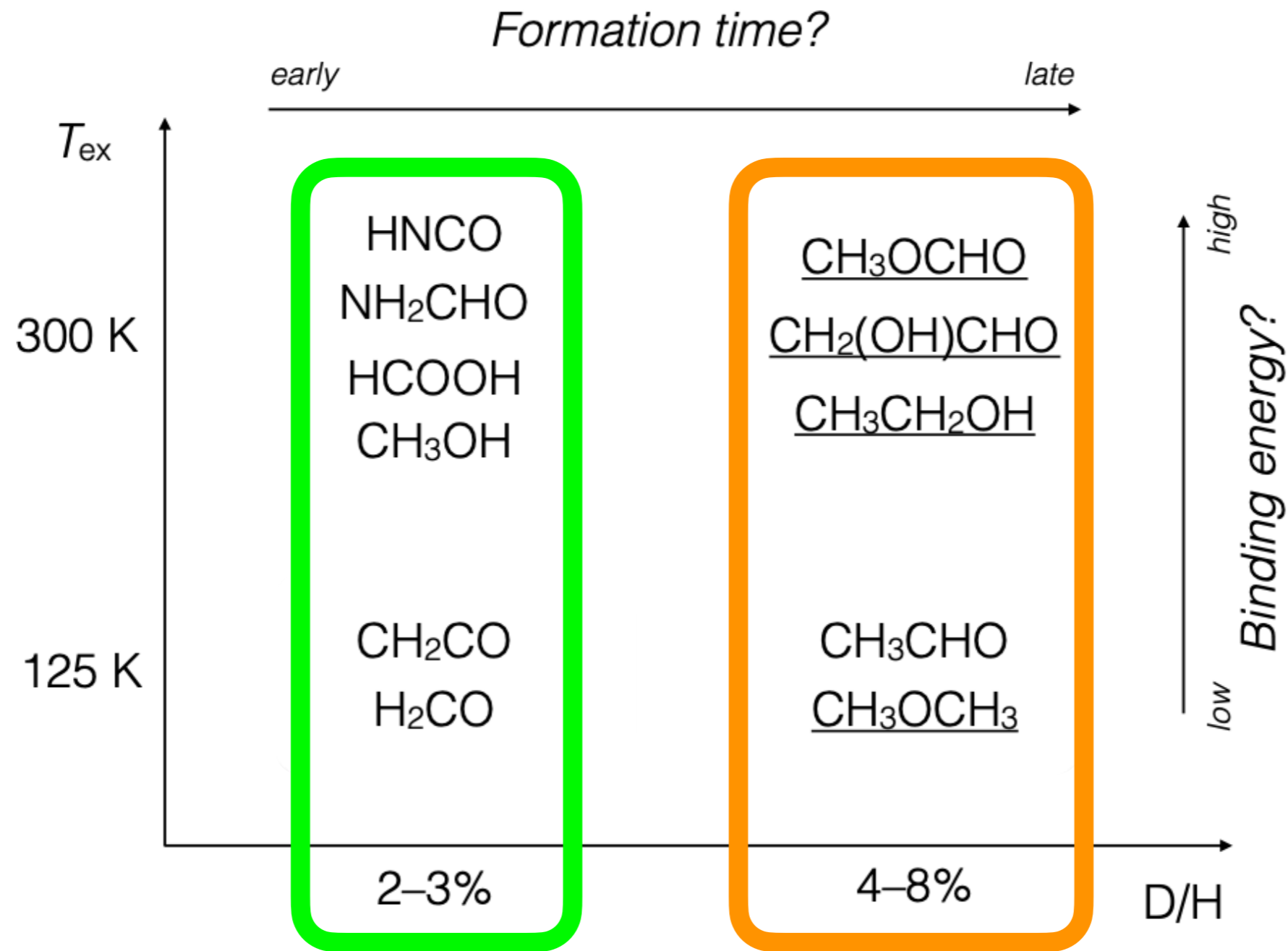
$^{13}\text{CH}_2\text{CO}$
 $\text{CH}_2^{13}\text{CO}$
CHDCO

Formaldehyde

$\text{H}_2\text{C}^{17}\text{O}$
 D_2^{13}CO

Coutens et al. 2016, 2018, Jørgensen et al. 2016, 2018, Persson et al. 2018, Calcutt et al. 2018, Manigand et al. 2019, Richard et al. 2021, Müller et al. 2022

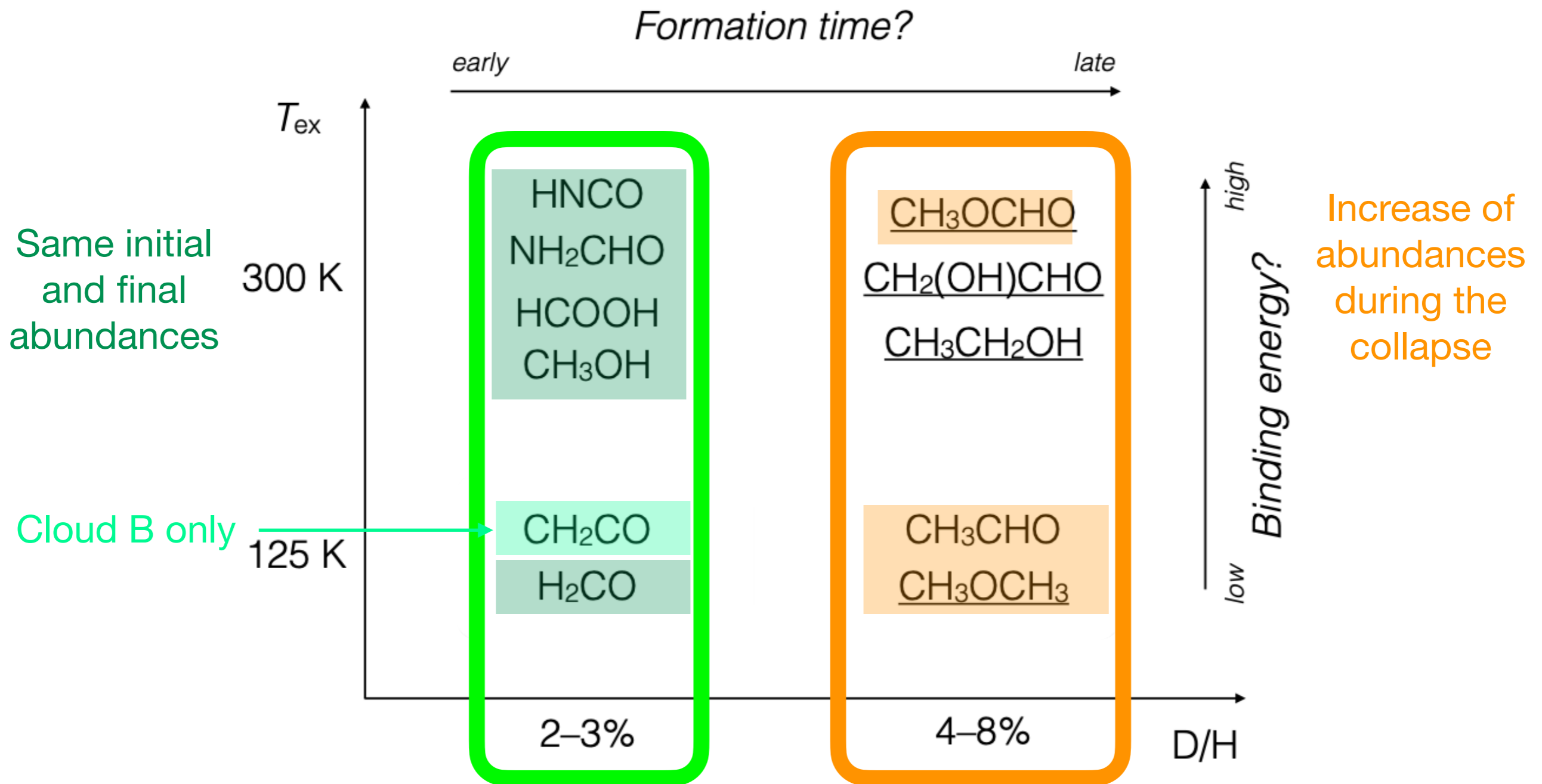
Deuteration of molecules



Jørgensen et al. 2018

Deuteration of molecules

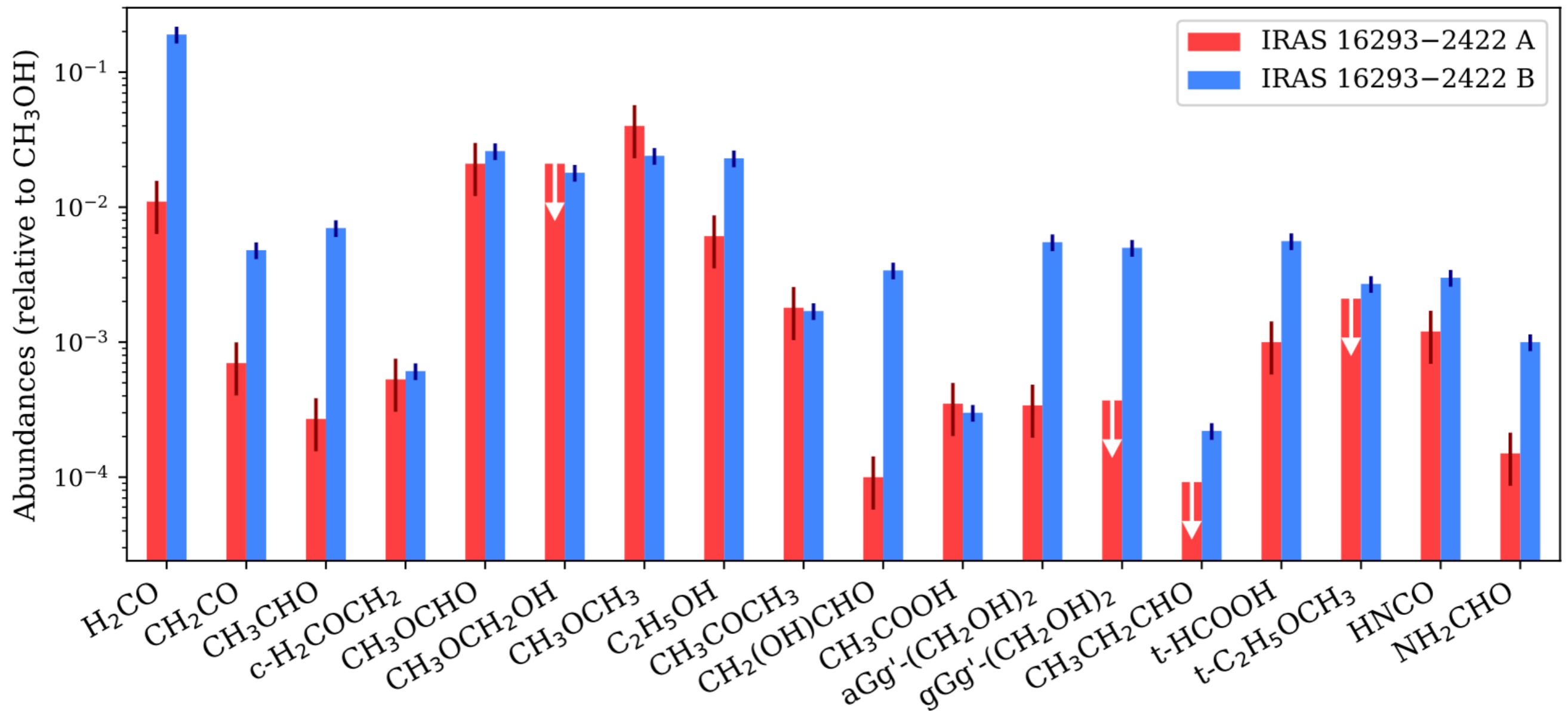
Comparison with 3D chemical modeling (*Coutens et al. 2020*)



Jørgensen et al. 2018

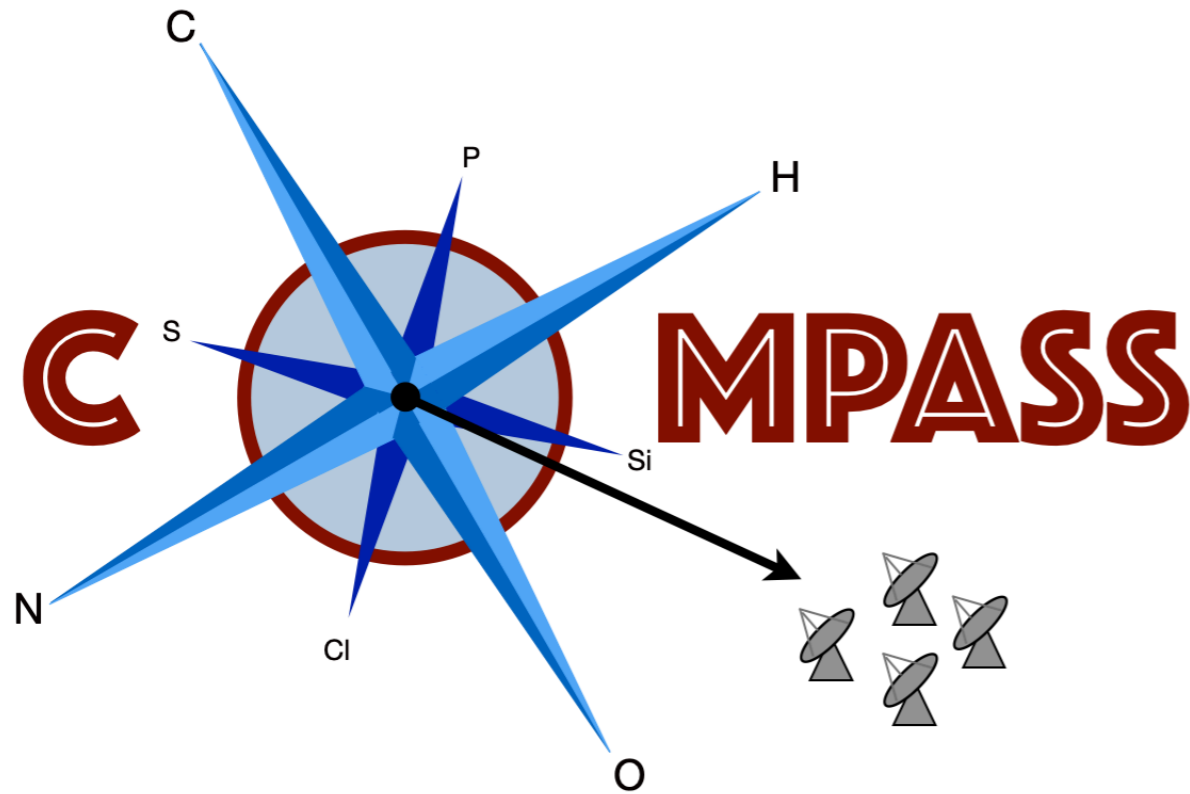
Comparison between IRAS16293 A and B

Manigand et al. 2020



- 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



Complex Organic Molecules in Protostars with ALMA Spectral Surveys

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

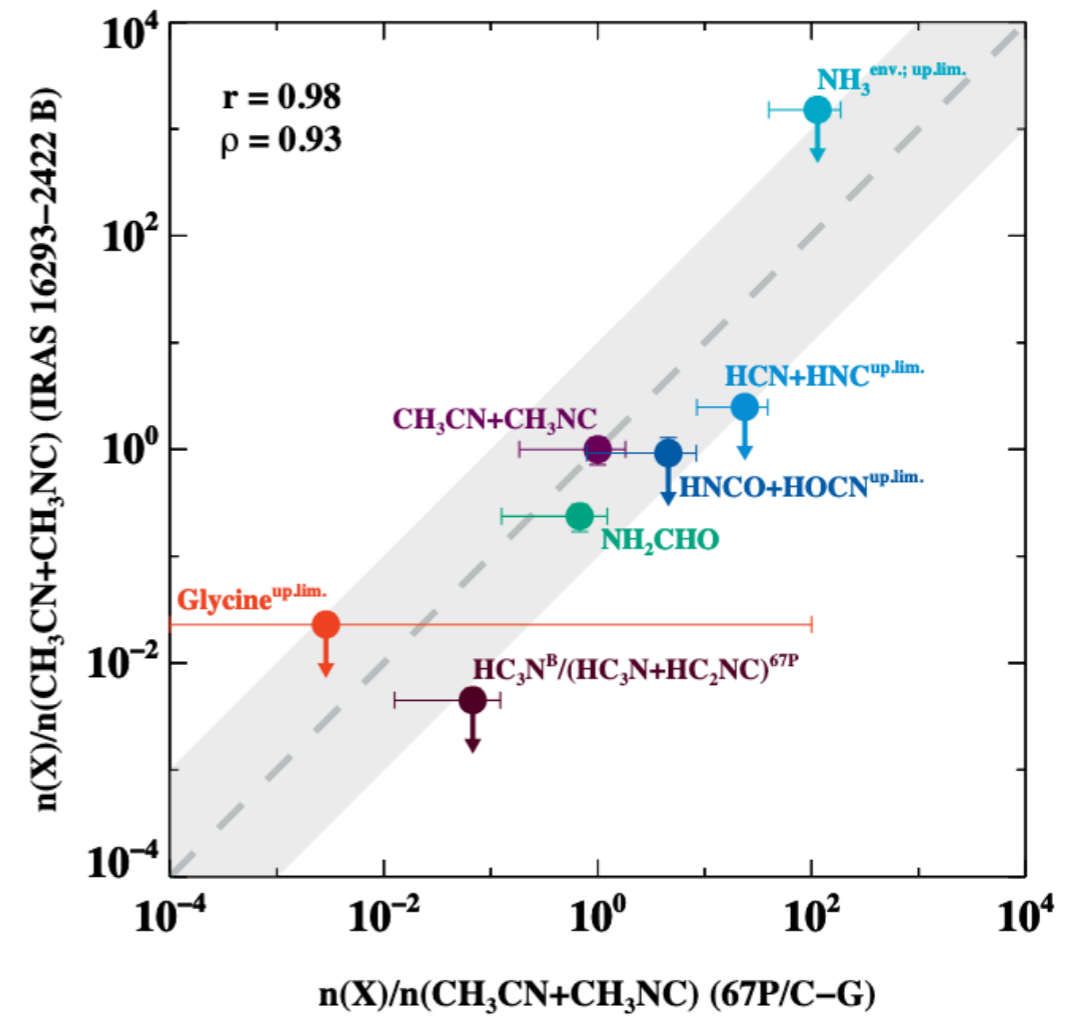
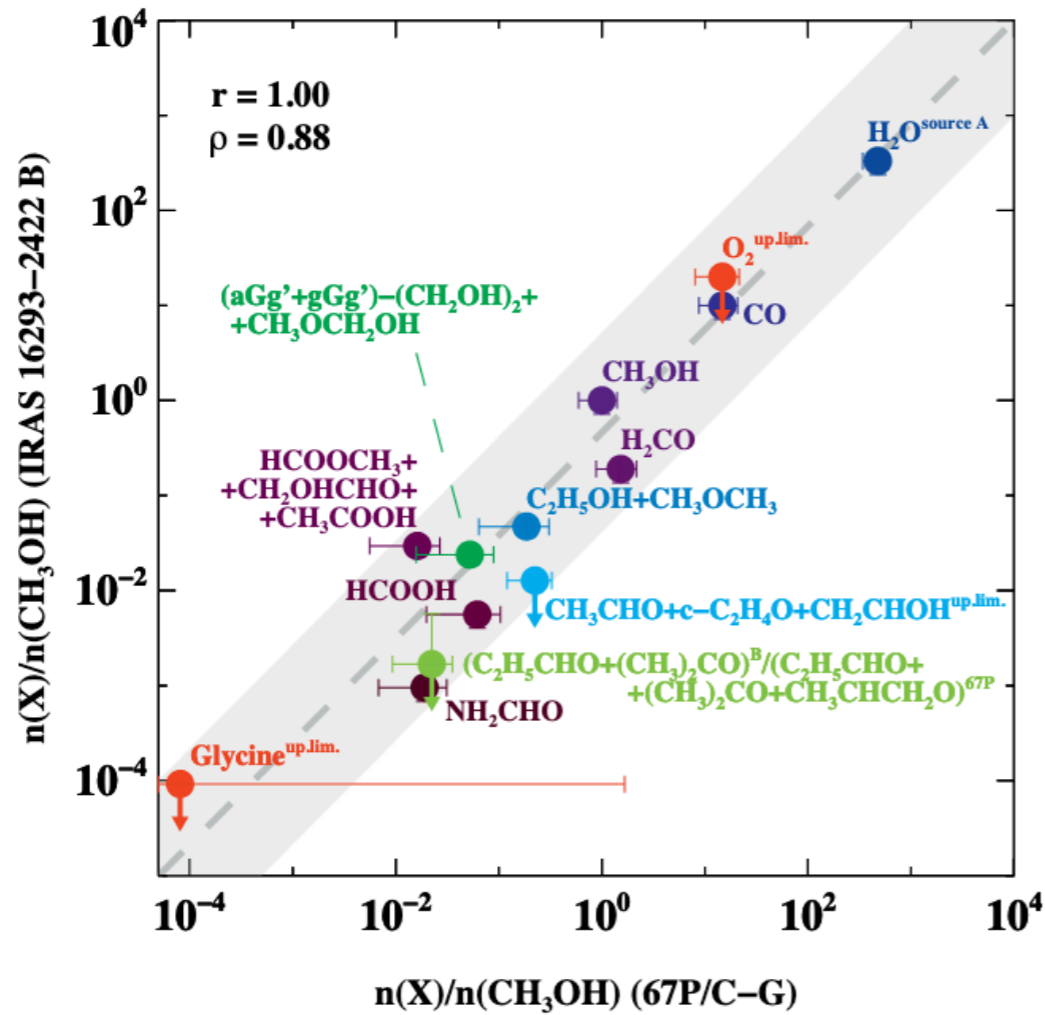
Merel van't Hoff

Yao-Lun Yang

- 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?*

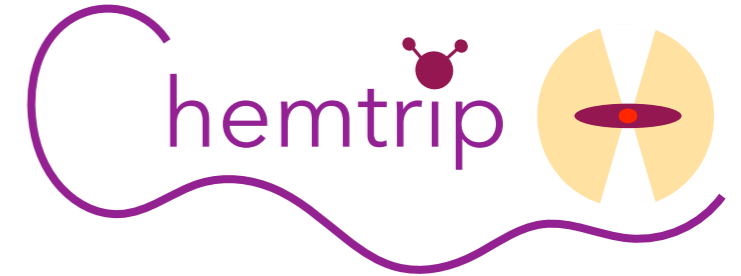
Comparison with comets



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

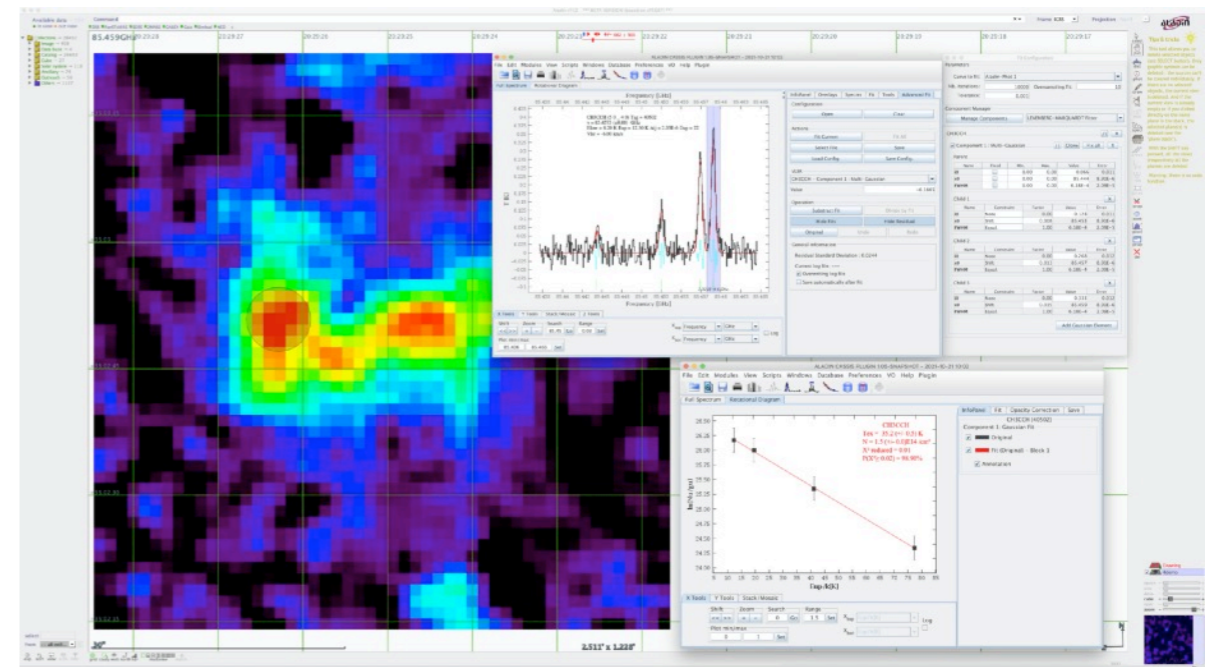


The CHEMical TRail In Protostars: From the deeply embedded phase to the planet-forming disk

- ◆ 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/>



Summary

- 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 !**

