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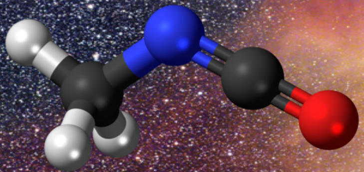
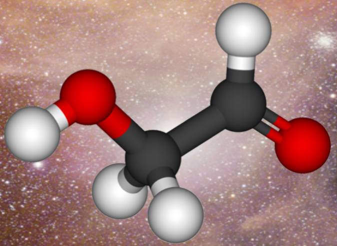
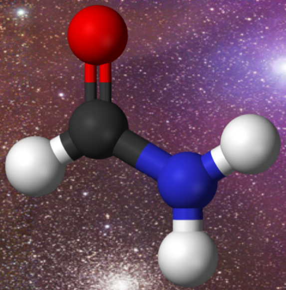
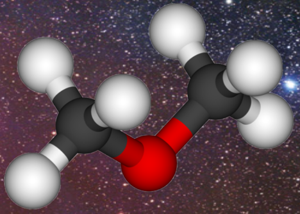
Queen Mary University of London

Influence of the cosmic ray ionisation rate on complex organic molecules chemistry









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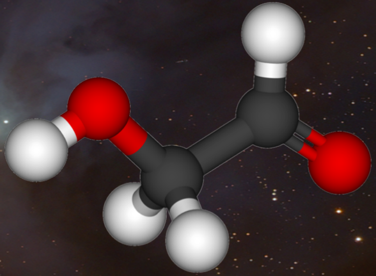
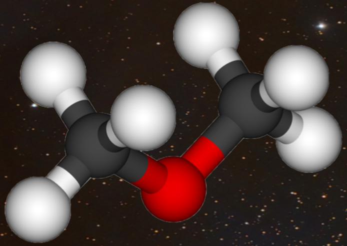
Complex Organic Molecules (COMs)

COMs are carbon-based compounds with >6 atoms

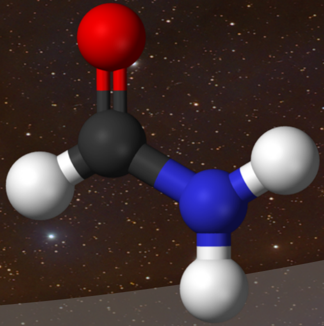
(Herbst & van Dishoeck 2009)

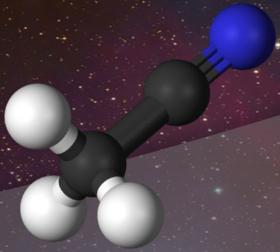
O-bearing COMs:
Glycolaldehyde
Dimethyl Ether





N-bearing COMs:
Formamide
Acetonitrile





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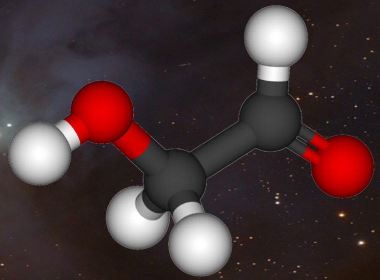
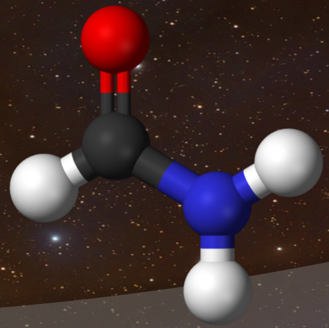
Glycolaldehyde



Simplest member of the monosaccharide sugars

Formamide



Peptide-like bond
Precursor of amino acids?

(Saladino et al. 2012)

Complex Organic Molecules (COMs)

Methylamine NH_2CH_3	Cyanamide NH_2CN	Aminoacetonitrile NH_2CH_2CN
Dimethyl Ether CH_3OCH_3	Methyl Formate $HCOOCH_3$	Acetic Acid CH_3COOH
Hydroxylamine NH_2OH	Acetamide NH_2COCH_3	Formamide NH_2CHO
N-Methyl Formamide $N\text{-}CH_3NHCHO$	Isocyanic Acid $HNCO$	Methyl Isocyanate CH_3NCO

➔ Understand the origin of the molecular complexity in star-forming regions and how far it can go.

Complex Organic Molecules (COMs)

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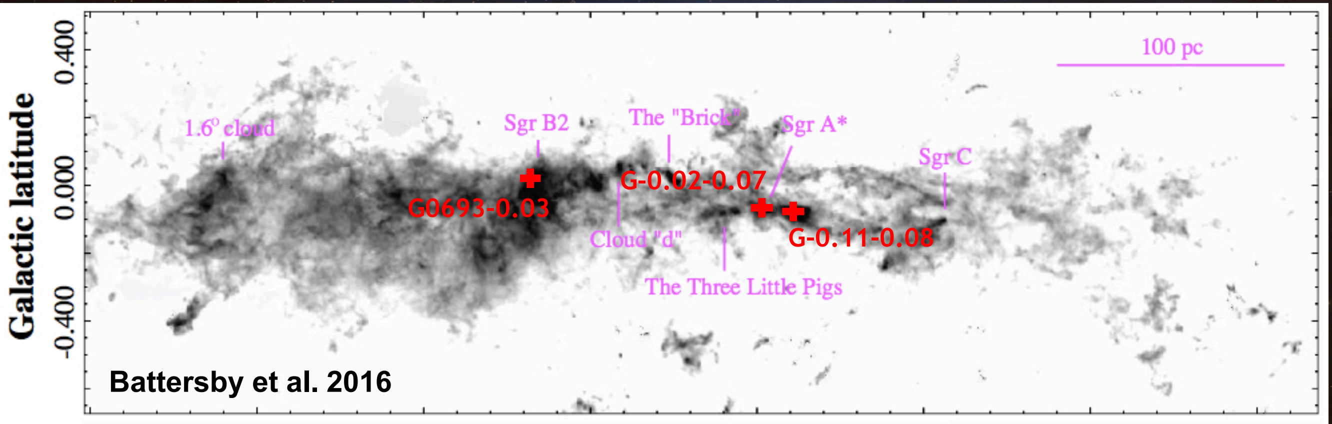
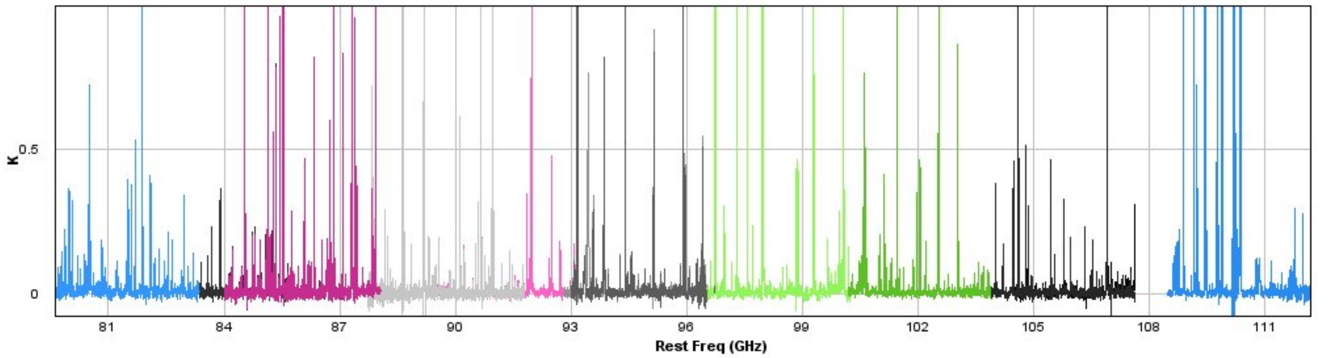
→ Understand the origin of the molecular complexity in star-forming regions and how far it can go.

The Galactic Centre: G+0.693-0.027





G0693-0.03 - 3mm survey

Located at ~8 kpc in the Central Molecular Zone

T_{gas} = 70 - 140 K

T_{dust} ~ 20 K

$n_H = [3 - 4] \times 10^4\ cm^{-3}$

$\zeta = [1 - 10] \times 10^{-15}\ s^{-1}$

➔ More details in Zeng et al. (2018) (accepted in MNRAS)

Image courtesy of S. Zeng

Chemical modelling in G+0.693-0.027

3-steps chemical modelling

Grid: cosmic ray ionisation rate ζ = 1, 10, 100, 1000 x ζ_{std} (= 1.3×10^{-17} s^{-1})

Phase 0

➔ Diffuse cloud step with n_H = 100 cm^{-3} and T=20 K.

➔ Evolution of the chemistry for a few millions years.

➔ Low A_V: no icy mantle formation but gas phase chemistry.

Phase 1

➔ Collapse phase to n_H = [3 - 4] x 10^4 cm^{-3} with T=10 K.

Phase 2

➔ Warm-up phase to T_{gas} = 70-105-140 K with T_{dust} = 20 K

➔ **Rich gas-phase chemistry at warm T_{gas}**

➔ **Small impact of grain surface chemistry because of low T_{dust}!**

Chemical code

UCLCHEM (Viti et al. 2004; Holdship et al. 2017) ➔ https://uclchem.github.io/

Gas-phase + dust grain chemical code (372 species; 3514 reactions)

➔ Modelling of the chemistry in G+0.693-0.027

N-bearing chemistry: CH_3NCO

UCLCHEM (Viti et al. 2004; Holdship et al. 2017) ➔ https://uclchem.github.io/

Gas-phase + dust grain chemical code (372 species; 3514 reactions)
➔ Modelling of the chemistry in G+0.693-0.027

Recently proposed gas-phase/grain-surface reactions for CH_3NCO (+ isomers)

= grain surface

Quénard et al., (2018)

Methyl Isocyanate – CH_3NCO	
$HNCO + CH_3 \longrightarrow CH_3NCO + H$	Halfen et al. (2015)
$\#CH_3 + \#OCN \longrightarrow \#CH_3NCO$	Belloche et al. (2017) ; Ligterink et al. (2017)
$\#CH_3 + \#HNCO \longrightarrow \#CH_3NCO + \#H$	Ligterink et al. (2017)
$\#CH_3 + \#HNCO \longrightarrow \#CH_4 + \#OCN$	Ligterink et al. (2017)
$\#CH_3NCO + \#H \longrightarrow \#CH_3NH + \#CO$	Ligterink et al., private communication

N-bearing chemistry: CH_3NCO

New theoretical calculations from Majumdar et al. (2018)

Reaction		α	β	γ
$HNCO + CH_3$	$\rightarrow CH_3NCO + H$	1.00×10^{-10}	0	8.04×10^{3}
$CH_3NCO + H_3{}^+$	$\rightarrow CH_3NCOH^+ + H_2$	1.00×10^{-9}	-0.5	0
$CH_3NCO + HCO^+$	$\rightarrow CH_3NCOH^+ + CO$	1.09×10^{-9}	-0.5	0
$CH_3NCO + H^+$	$\rightarrow CH_3NCO^+ + H$	1.00×10^{-9}	-0.5	0
$CH_3NCO + CO^+$	$\rightarrow CH_3NCO^+ + CO$	1.00×10^{-9}	-0.5	0
$CH_3NCO + He^+$	$\rightarrow CH_3NCO^+ + He$	1.00×10^{-9}	-0.5	0
$CH_3NCO^+ + e^-$	$\rightarrow CH_3 + OCN$	1.50×10^{-7}	-0.5	0
$CH_3NCOH^+ + e^-$	$\rightarrow CH_3NCO + H$	3.00×10^{-7}	-0.5	0
CH_3NCO + CRP	$\rightarrow CH_3 + OCN$	4.00×10^{3}	0	0
CH_3NCO + Photon	$\rightarrow CH_3 + OCN$	5.00×10^{-10}	0.0	0
HCN + s-CO	→ s-HCN...CO	1	0	0
s-HCN...CO + s-H	→ s-H_2CNCO	1	0	2.40×10^{3}
s-H_2CNCO + s-H	→ s-CH_3NCO	1	0	0
s-CH_3 + s-HNCO	→ s-CH_3NCO	1	0	8.04×10^{3}
s-CH_3 + s-OCN	→ s-CH_3NCO	1	0	0
s-CH_3 + s-OCN^-	→ s-CH_3NCO + e^-	0	0	0
s-N + s-CH_3CO	→ s-CH_3NCO	1	0	0

N-bearing chemistry: CH_3NCO

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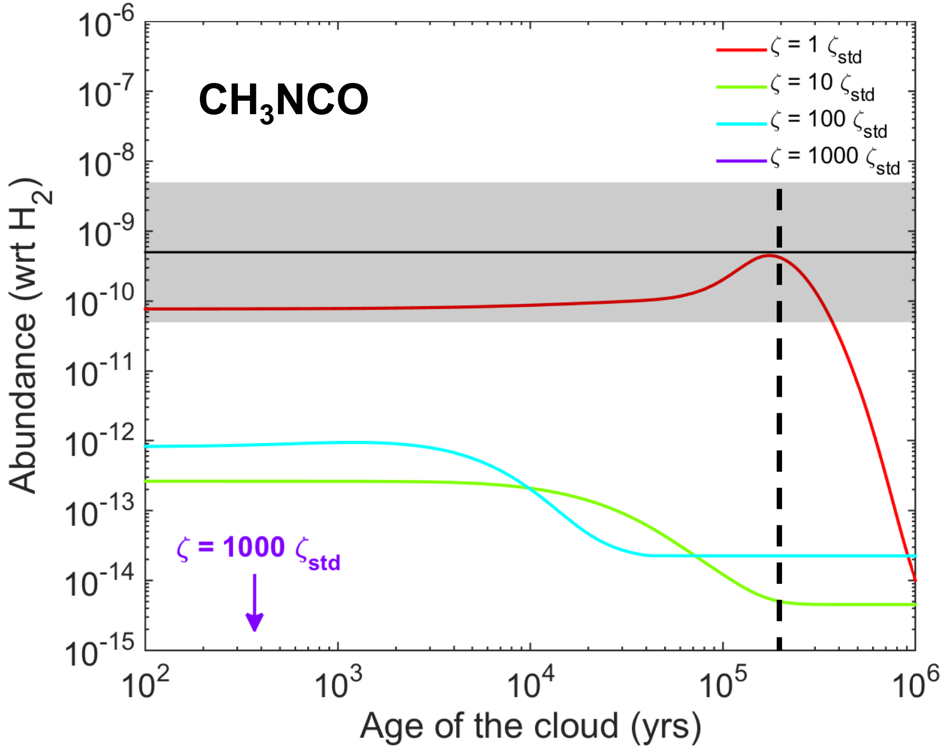
s-CH_3 + s-OCN	$\rightarrow$ s-CH_3NCO	1	0	0
s-CH_3 + s-OCN^-	$\rightarrow$ s-CH_3NCO + e^-	0	0	0
s-N + s-CH_3CO	$\rightarrow$ s-CH_3NCO	1	0	0

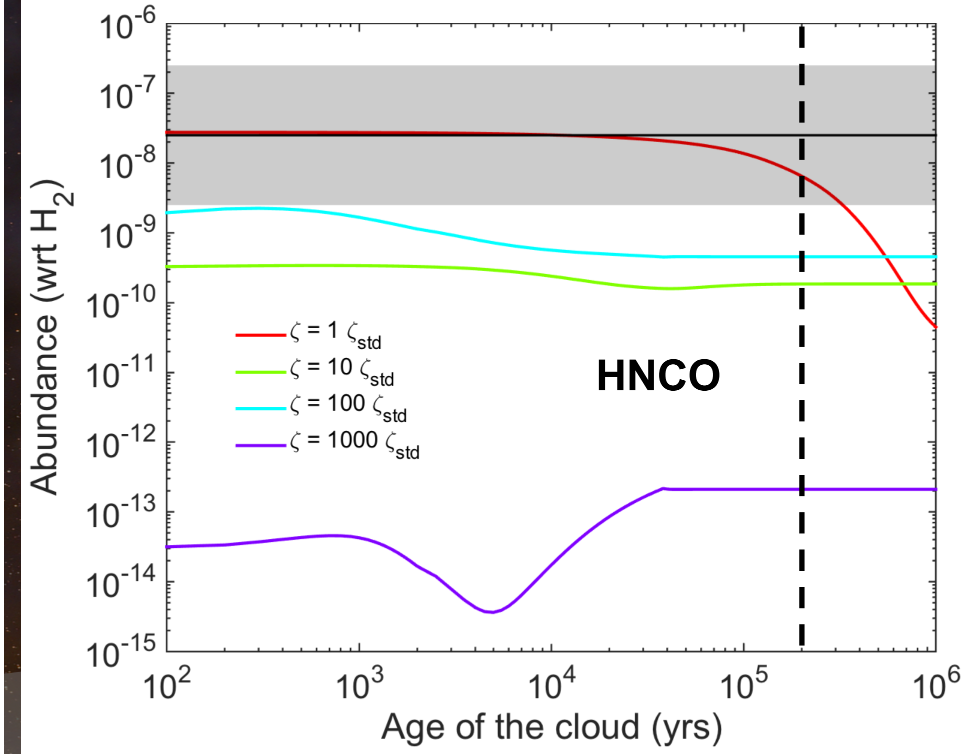
N-bearing chemistry: CH_3NCO

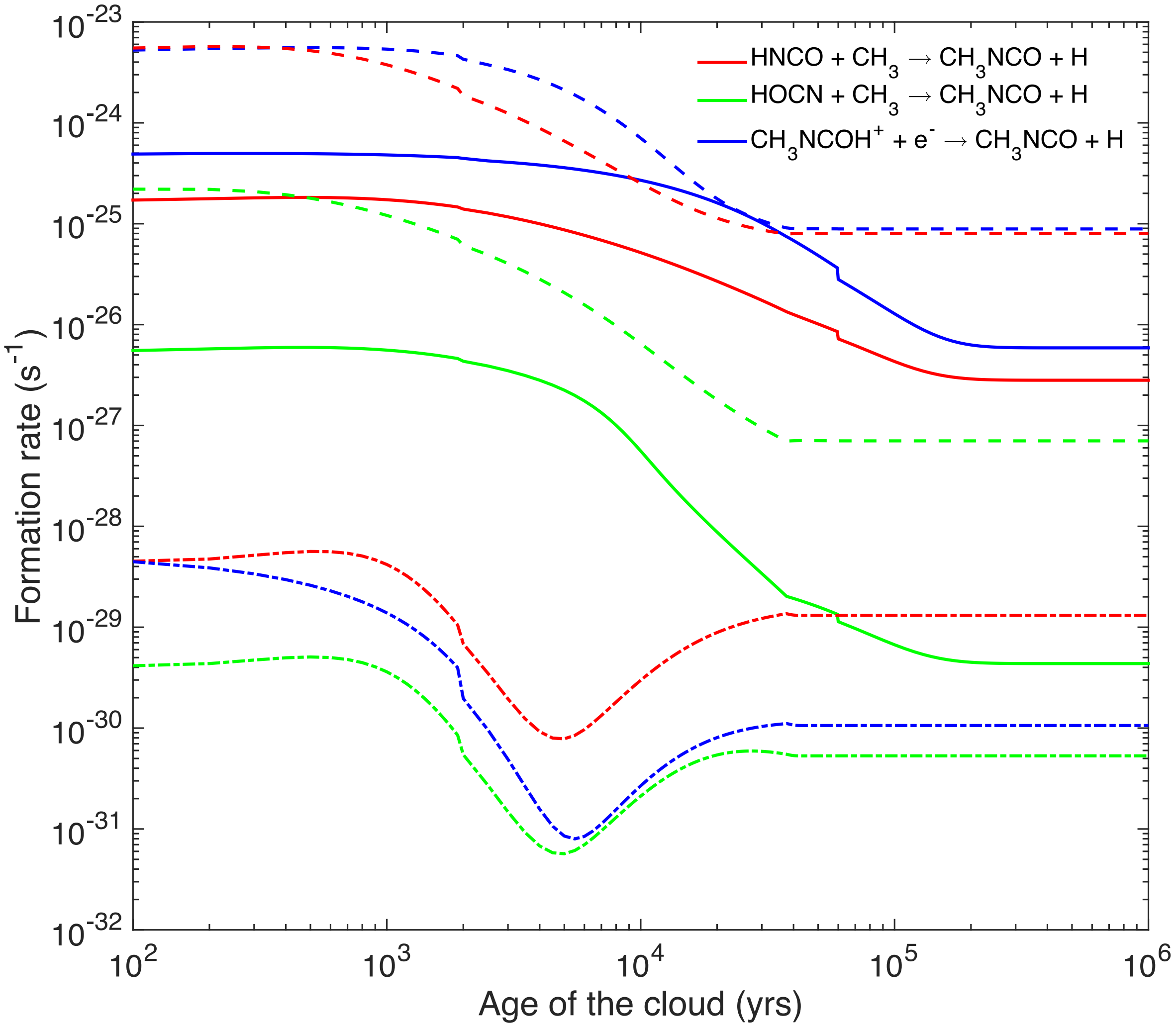
WORK IN PROGRESS

Higher cosmic-ray ionisation rates efficiently destroys HNCO and CH_3NCO

Higher abundance for x100 than x10 for both molecules!







N-bearing chemistry: CH_3NCO

Full lines: x10
Dashed: x100
Dash-dotted: x1000

Production rate of CH_3NCO higher at x100 than at x10 or x1000

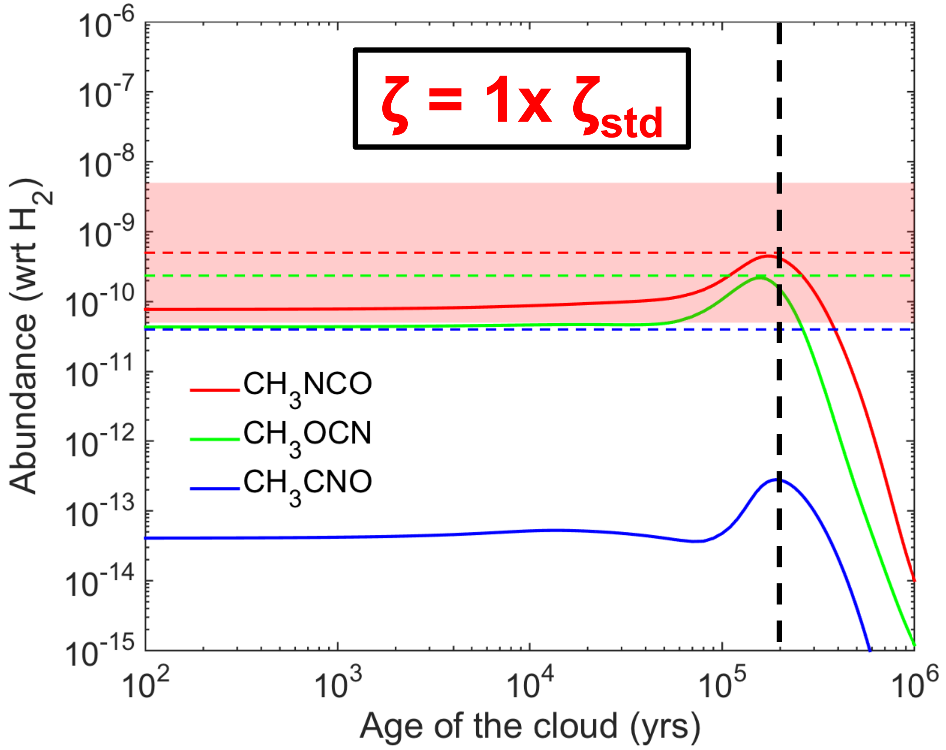
➔ Cosmic-rays can activate the chemistry!

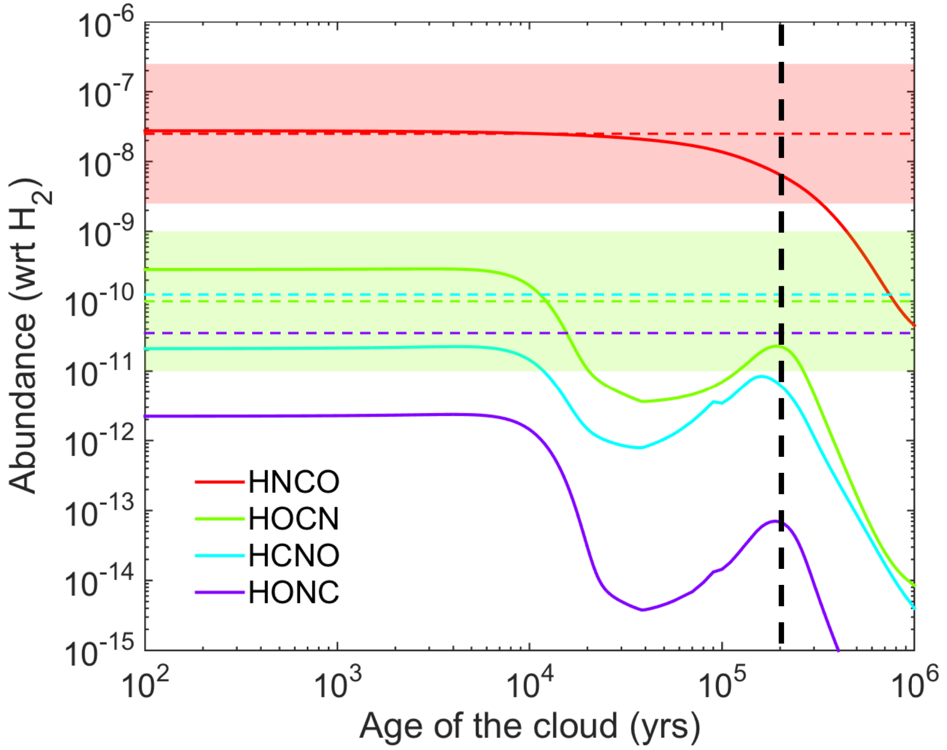
Same conclusions apply for HNCO

N-bearing chemistry: CH_3NCO

Good agreement for CH_3OCN and CH_3CNO and **within a factor of 10 for** CH_3NCO

Very good agreement for HNCO and its isomers: HOCN, HCNO and HONC





N-bearing chemistry: NH_2CHO

Calculations

Experiments

Guessed

Reactions	Reference
Formamide – NH_2CHO	
$NH_2 + H_2CO \longrightarrow NH_2CHO + H$	Skouteris et al. (2017)
$\#HNCO + \#H \longrightarrow \#NH_2 + \#CO$	Song & Kästner (2016)
$\#HNCO + \#H \longrightarrow \#H_2NCO$	Song & Kästner (2016)
$\#H_2NCO + \#H \longrightarrow \#NH_2CHO$	Song & Kästner (2016)
$\#H_2NCO + \#H \longrightarrow \#HNCO + \#H_2$	Noble et al. (2016)
$\#NH_2 + \#HCO \longrightarrow \#NH_2CHO$	Fedoseev et al. (2016)
$\#NH_2 + \#HCO \longrightarrow \#NH_3 + CO$	Fedoseev et al. (2016)
$\#NH_2 + \#H_2CO \longrightarrow \#NH_2CHO + \#H$	Fedoseev et al. (2016)
$\#NH_2 + \#H_2CO \longrightarrow \#NH_3 + \#HCO$	Fedoseev et al. (2016)
$\#H_2NCO + \#CH_3 \longrightarrow \#CH_3CONH_2$	Belloche et al. (2017)
$\#NH_2CHO + \#OH \longrightarrow \#H_2NCO + \#H_2O$	Belloche et al. (2017)
$\#NH_2CHO + \#CH_2 \longrightarrow \#CH_3CONH_2$	Belloche et al. (2017)

Quénard et al., (2018)

N-bearing chemistry: NH_2CHO

Calculations

Experiments

Guessed

Reactions	Reference
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$\#H_2NCO + \#H \longrightarrow \#HNCO + \#H_2$	Noble et al. (2016)
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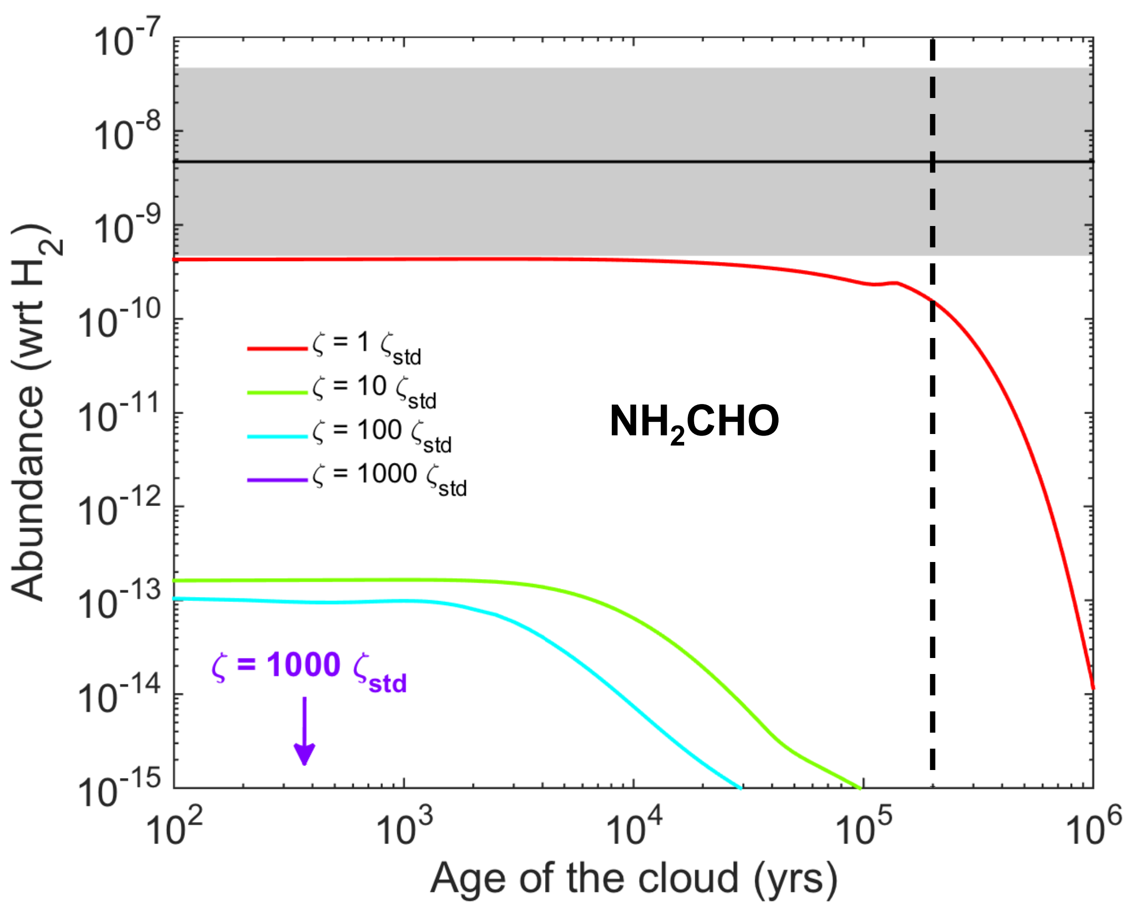
$\#H_2NCO + \#CH_3 \longrightarrow \#CH_3CONH_2$	Belloche et al. (2017)
$\#NH_2CHO + \#OH \longrightarrow \#H_2NCO + \#H_2O$	Belloche et al. (2017)
$\#NH_2CHO + \#CH_2 \longrightarrow \#CH_3CONH_2$	Belloche et al. (2017)

Quénard et al., (2018)

N-bearing chemistry: NH_2CHO



Not enough NH_2CHO!

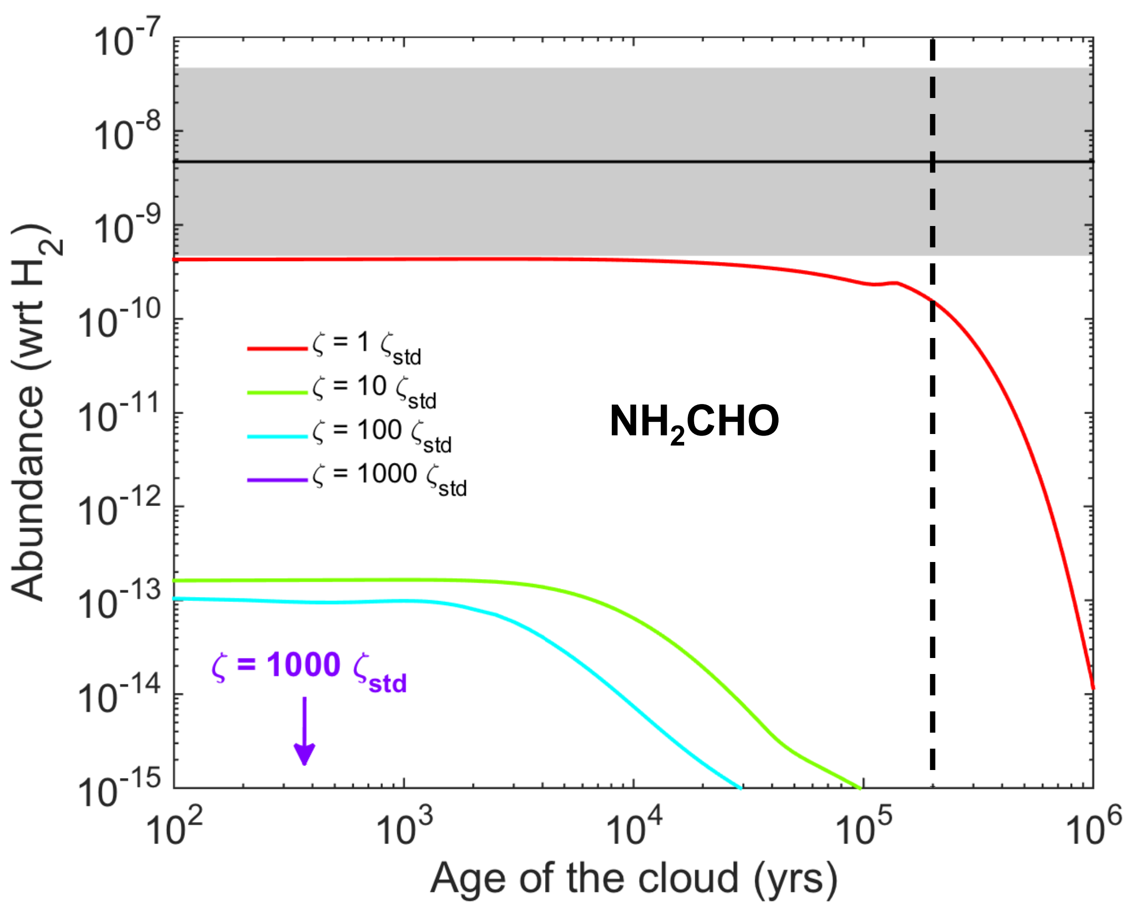
How to produce more?

➔ CR-induced reactions on grain surface to form NH_2CHO

➔ Energetic processing of ices
Kanuchová et al. (2016)

See Poster 13 by Christopher Shingledecker

N-bearing chemistry: NH_2CHO



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➔ CR-induced reactions on grain surface to form NH_2CHO

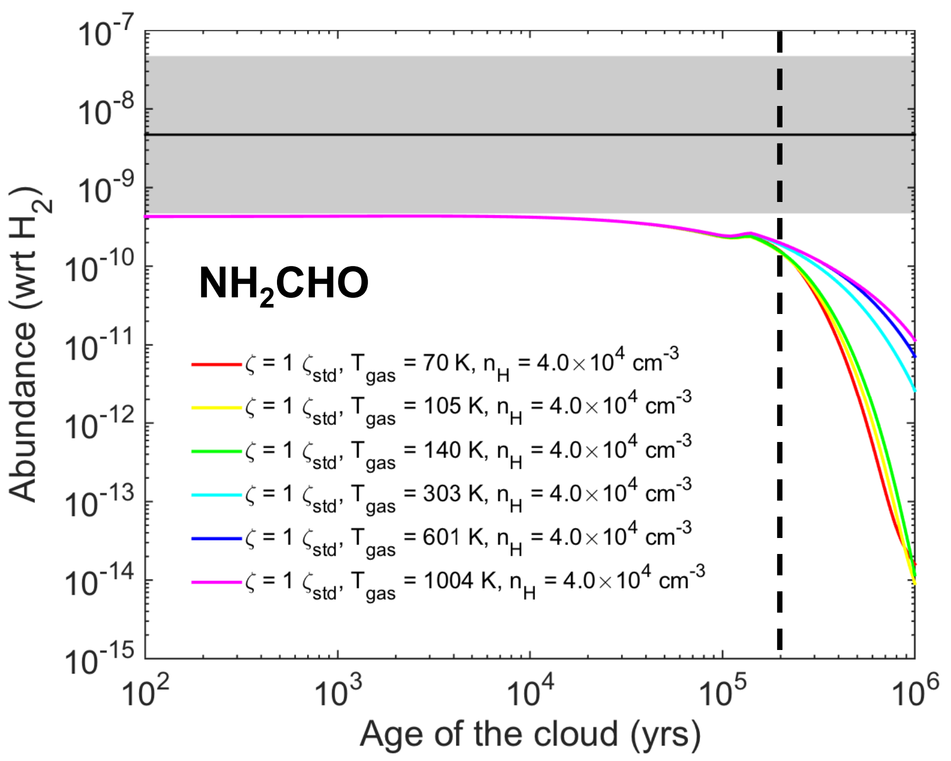
➔ Energetic processing of ices
Kanuchová et al. (2016)

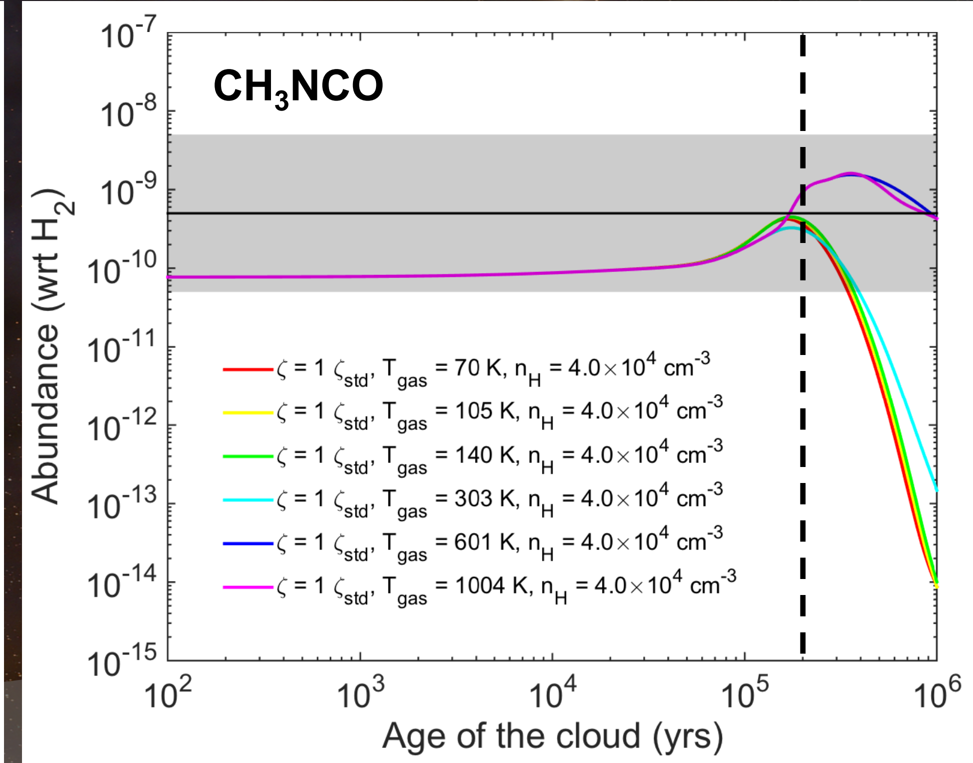
➔ Low velocity shocks at v~20 km/s?

N-bearing chemistry

Low velocity shocks at v~20 km/s might enhance the gas temperature (up to ~1000 K)

No enhancement of NH_2CHO at 300, 600, and 1000 K but slightly better for CH_3NCO



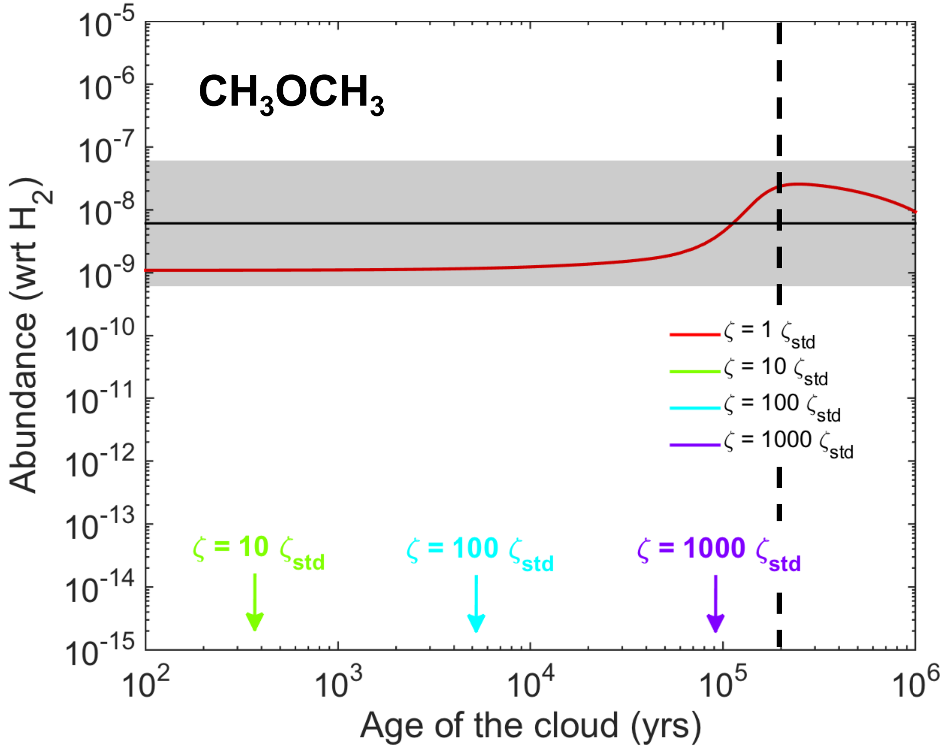


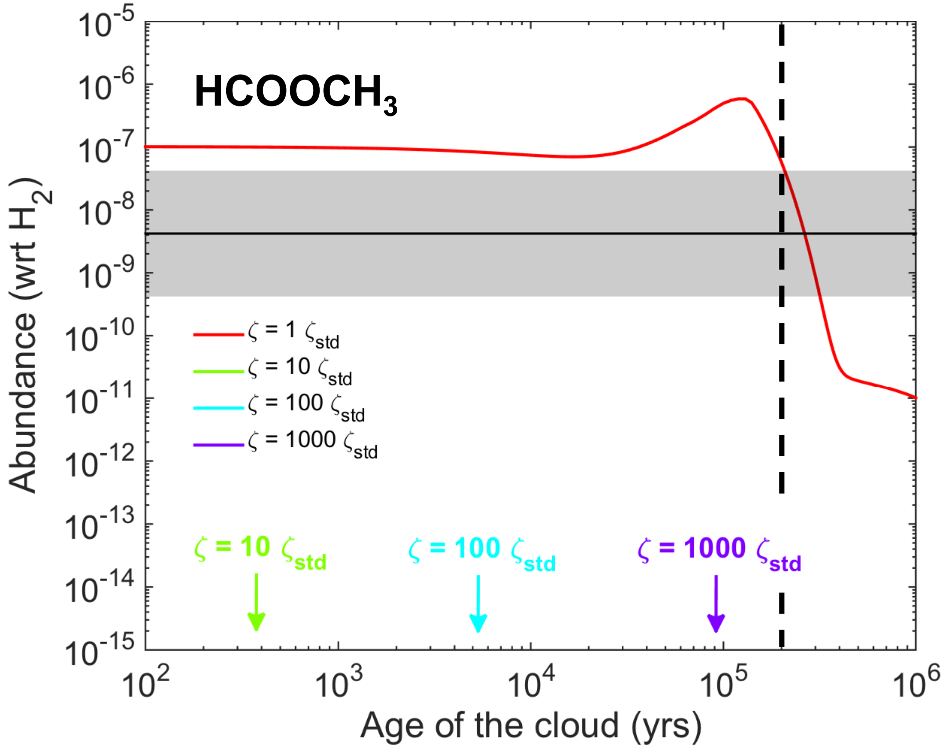
O-bearing chemistry

O-bearing COMs chemistry strongly influenced by cosmic ray ionisation rate!

➔ More sensitive than than N-bearing COMs!

Good agreement for CH_3OCH_3 and $HCOOCH_3$ for $\zeta = 1x\ \zeta_{std}$

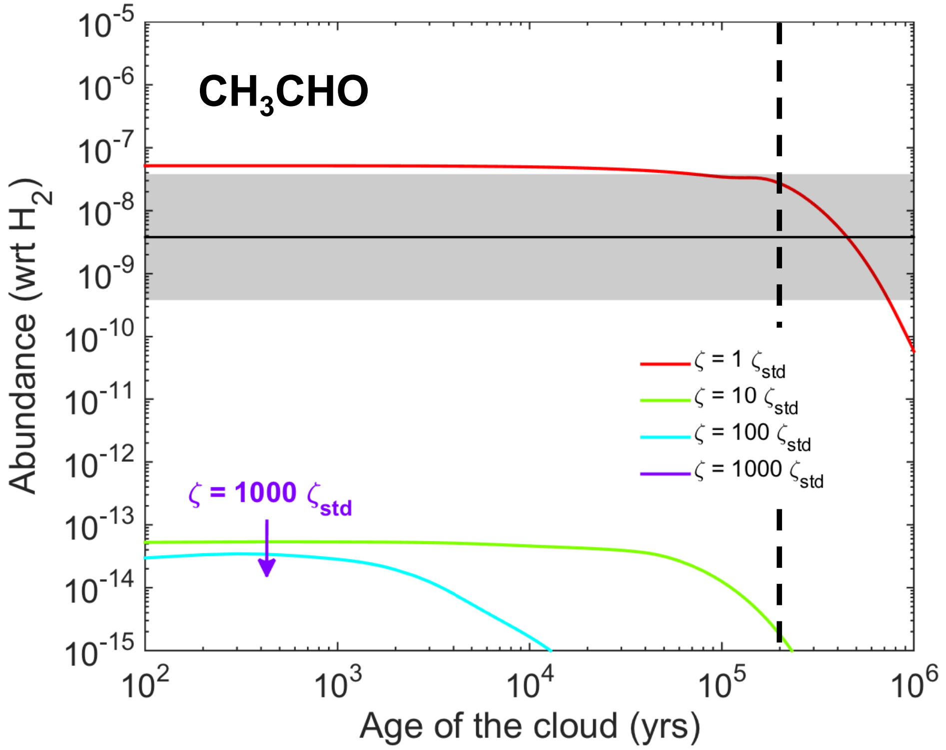


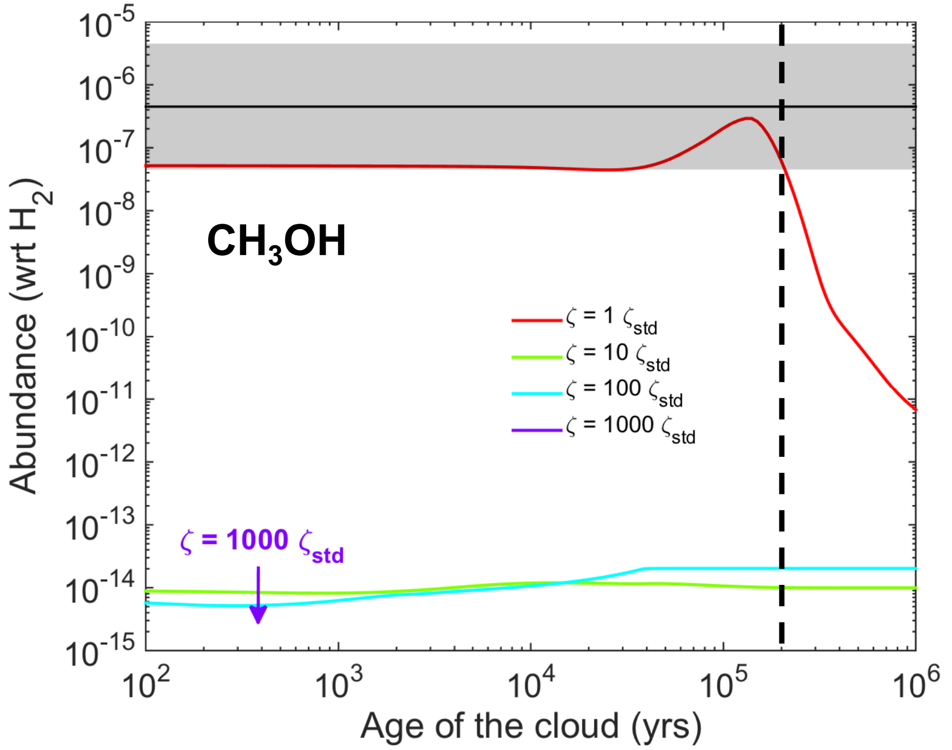


O-bearing chemistry

Good agreement for CH_3CHO and CH_3OH within a factor of 10

Less sensitive to cosmic-ray ionisation rate than bigger O-bearing COMs





Conclusions and perspectives

- N-bearing and O-bearing COMs chemistry strongly affected by cosmic-ray ionisation rate.

- N-bearing COMs less sensitive to higher CR rate than O-bearing COMs
  ➔ Higher value of CR rate may lead to higher abundances!

- G+0.693-0.027: CH3NCO (+ isomers) and HNCO (+ isomers) abundance OK but not enough NH_2CHO predicted by the models.

- Overall good agreement with observations for N-bearing and O-bearing COMs but for $\zeta = 1\text{x}\ \zeta_{std}$ (= $1.3 \times 10^{-17}\ s^{-1}$) ➔ different from observations!

- Adding CR-induced reactions on grain surface to mimic energetic processing of ice (Kanuchová et al. 2016) is needed to improve the NH_2CHO abundance predicted by the models.