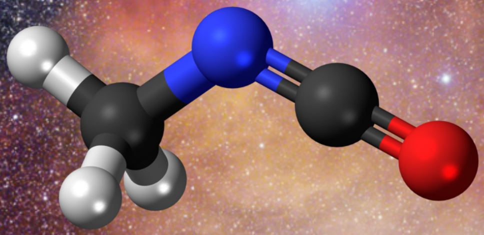
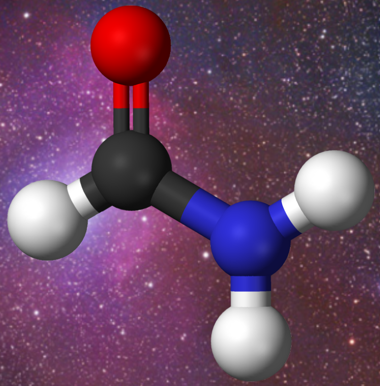
Chemical modelling of formamide and methyl isocyanate in star-forming regions





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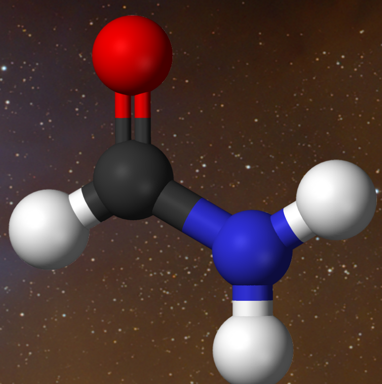
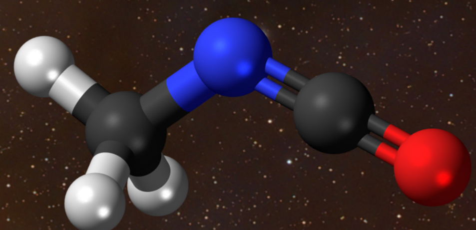
The search for pre-biotic species

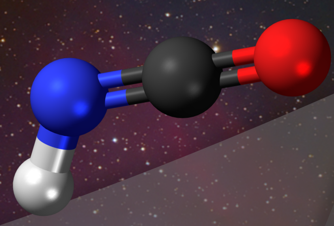
The peptide bond: CO-NH

Important bond in biochemistry (link between two amino-acid)

Several species detected with a peptide-like bond (e.g. NH_2CHO, CH_3NCO) or a peptide bond (HNCO)







The search for pre-biotic species

Glycine
(NH_2CH_2COOH)

Methylamine NH_2CH_3	**Cyanamide** NH_2CN	**Aminoacetonitrile** NH_2CH_2CN
Glycolaldehyde $HOCH_2CHO$	**Methyl Formate** $HCOOCH_3$	**Acetic Acid** CH_3COOH
Hydroxylamine NH_2OH	**Acetamide** NH_2COCH_3	**Formamide** NH_2CHO
N-Methyl Formamide N-CH_3NHCHO	**Isocyanic Acid (+isomers)** HNCO/HCNO/HOCN	**Methyl Isocyanate** CH_3NCO (+isomers)

➔ Understand the chemistry of glycine precursors and COM-related species.

The search for pre-biotic species

Glycine
(NH_2CH_2COOH)

Methylamine NH_2CH_3	Cyanamide NH_2CN	Aminoacetonitrile NH_2CH_2CN
Glycolaldehyde $HOCH_2CHO$	Methyl Formate $HCOOCH_3$	Acetic Acid CH_3COOH
Hydroxylamine NH_2OH	Acetamide NH_2COCH_3	Formamide NH_2CHO
N-Methyl Formamide N-CH_3NHCHO	Isocyanic Acid (+isomers) HNCO/HCNO/HOCN	Methyl Isocyanate CH_3NCO (+isomers)

➔ **Understand the chemistry of glycine precursors and COM-related species.**

Modelling of NH_2CHO, CH_3NCO, HNCO (& isomers)

UCL_CHEM (Viti et al. 2004; Holdship et al. 2017)

https://uclchem.github.io/

Gas-phase + dust grain chemical code (364 species; 3446 reactions)

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

= grain surface

Reactions	Reference
Isocyanic Acid – HNCO/HOCN/HCNO	
Complex gas/grain network	Quan et al. (2010)
#NH + #CO $\longrightarrow$ #HNCO	Fedoseev et al. (2015)
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

Quénard et al., submitted

Modelling of NH_2CHO, CH_3NCO, HNCO (& isomers)

Recently proposed gas-phase/grain-surface reactions for NH_2CHO

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., submitted

COMs in the pre-stellar core L1544

O-bearing and N-bearing COMS are **more abundant at r~4000 AU** (methanol peak position) (Jiménez-Serra et al. 2016)

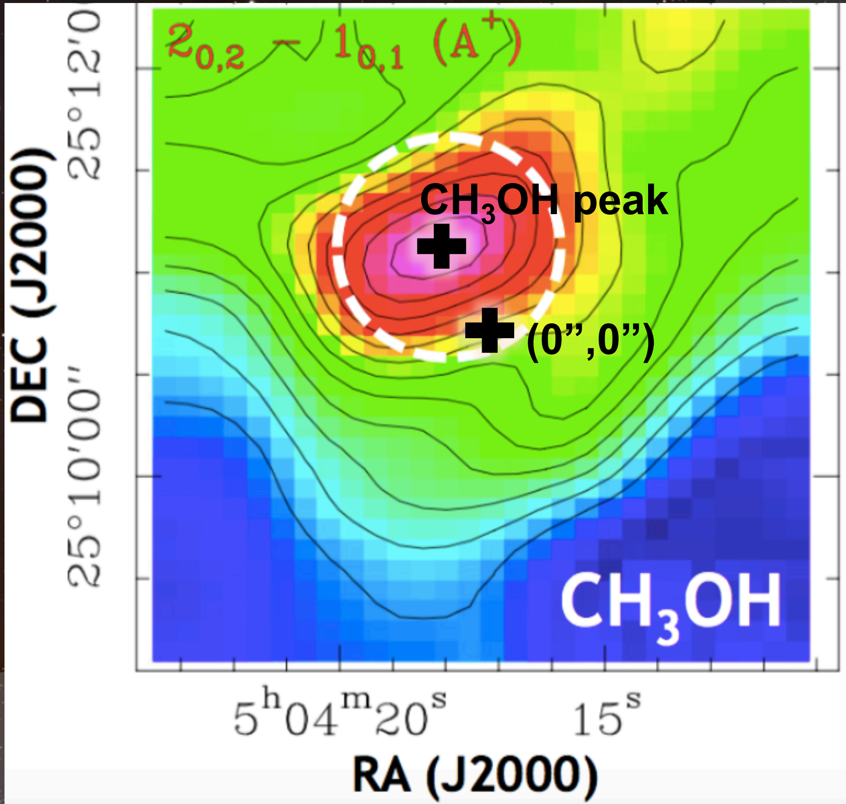
Important non-detections:

Core centre	Methanol peak
X [NH_2CHO] < 2.4×10^{-13}	X [NH_2CHO] < 6.7×10^{-13}
X [CH_3NCO] < 2.0×10^{-12}	X [CH_3NCO] < 6.0×10^{-12}

Chemical modelling by Vasyunin et al. (2017)

- Gas-phase + dust grain model of Vasyunin & Herbst (2013)
- Focused on the O-bearing COMs chemical modelling

Large discrepancy found for NH_2CHO: ~100 times higher

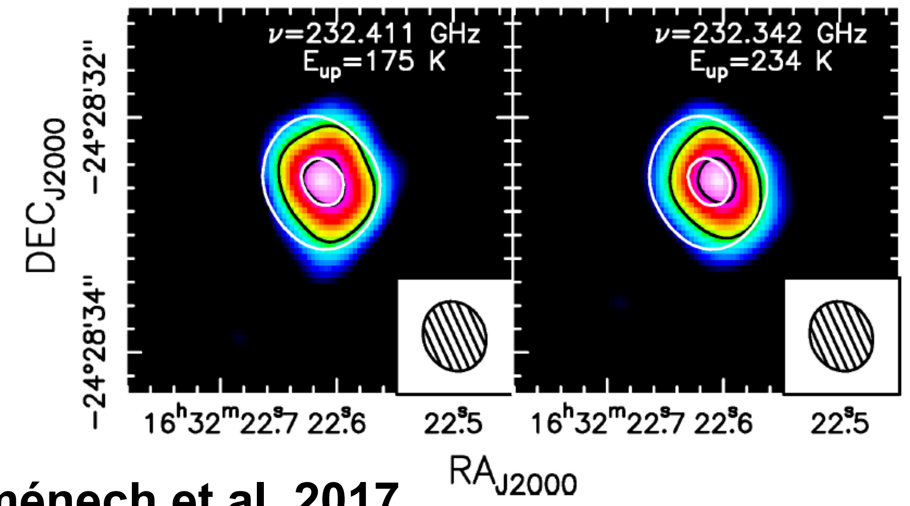


Bizzocchi et al. (2014)

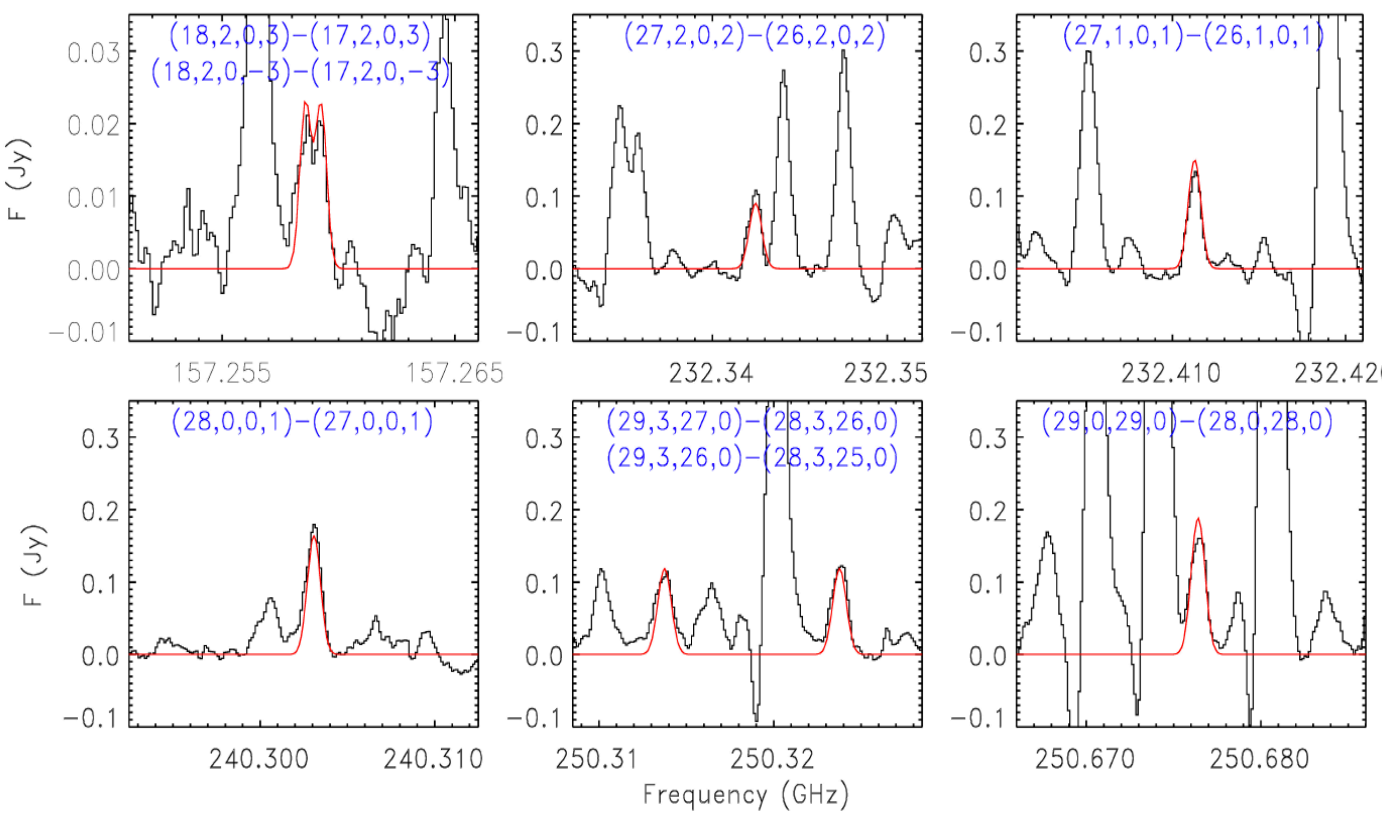
CH_3NCO in IRAS16293

Detection of CH_3NCO towards source B!

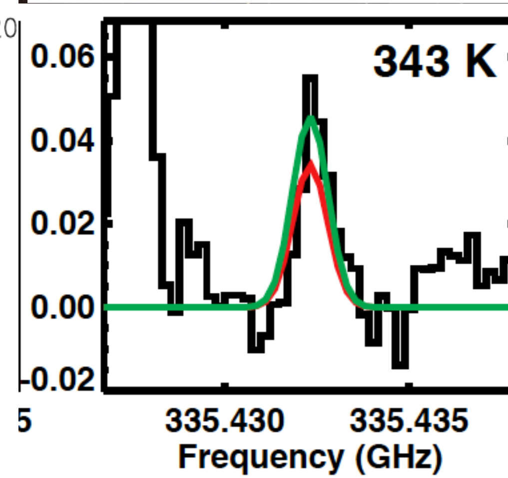
(Martín-Doménech et al. 2017, Ligterink et al. 2017)



Martín-Doménech et al. 2017



Ligterink et al. 2017



N-bearing COMs chemical modelling in L1544

2-steps chemical modelling

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 = $5x10^6$ cm^{-3} (core centre) and n_H = $4x10^5$ cm^{-3} (methanol peak) with T=10 K.
➔ Depletion of species onto grain surface

N-bearing COMs chemical modelling in IRAS16293

3-steps chemical modelling

Phase 0

➔ Same as for L1544 (diffuse cloud phase)

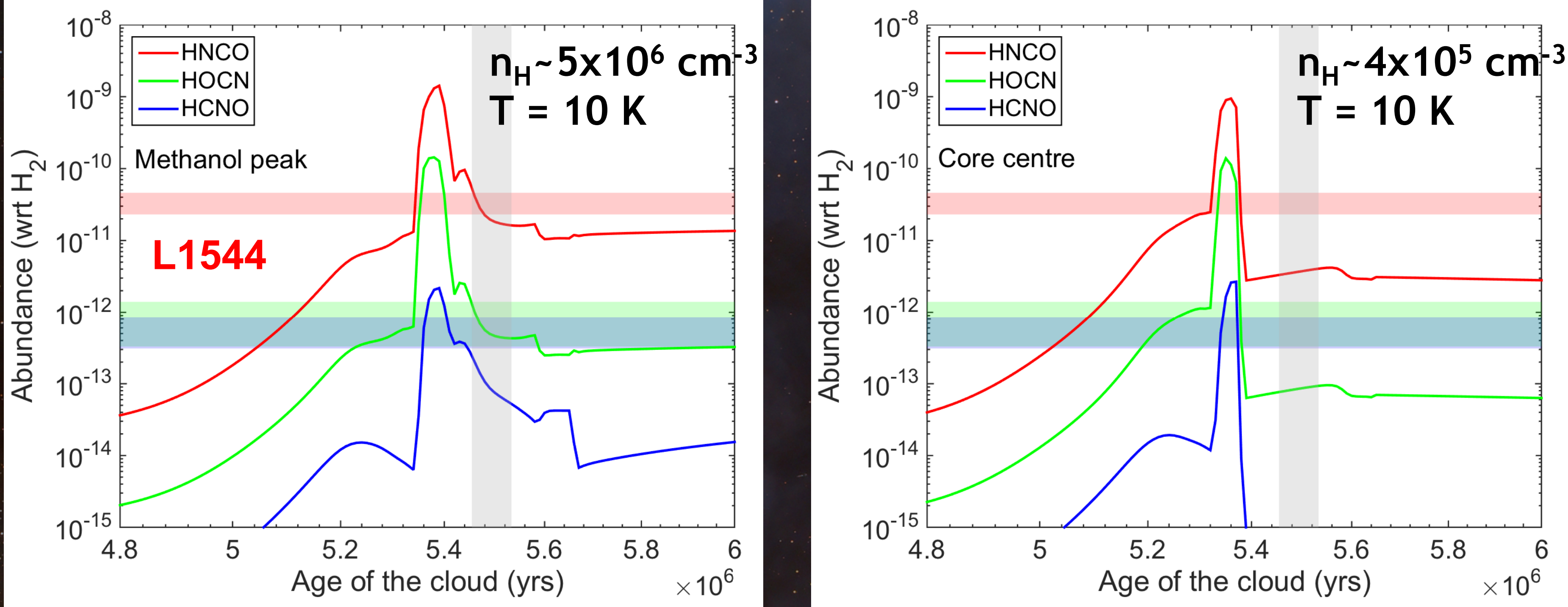
Phase 1

➔ Collapse phase to $n_H = 5x10^8$ cm^{-3} (hot corino) and $n_H = 2x10^6$ cm^{-3} (cold envelope) with T=10 K.

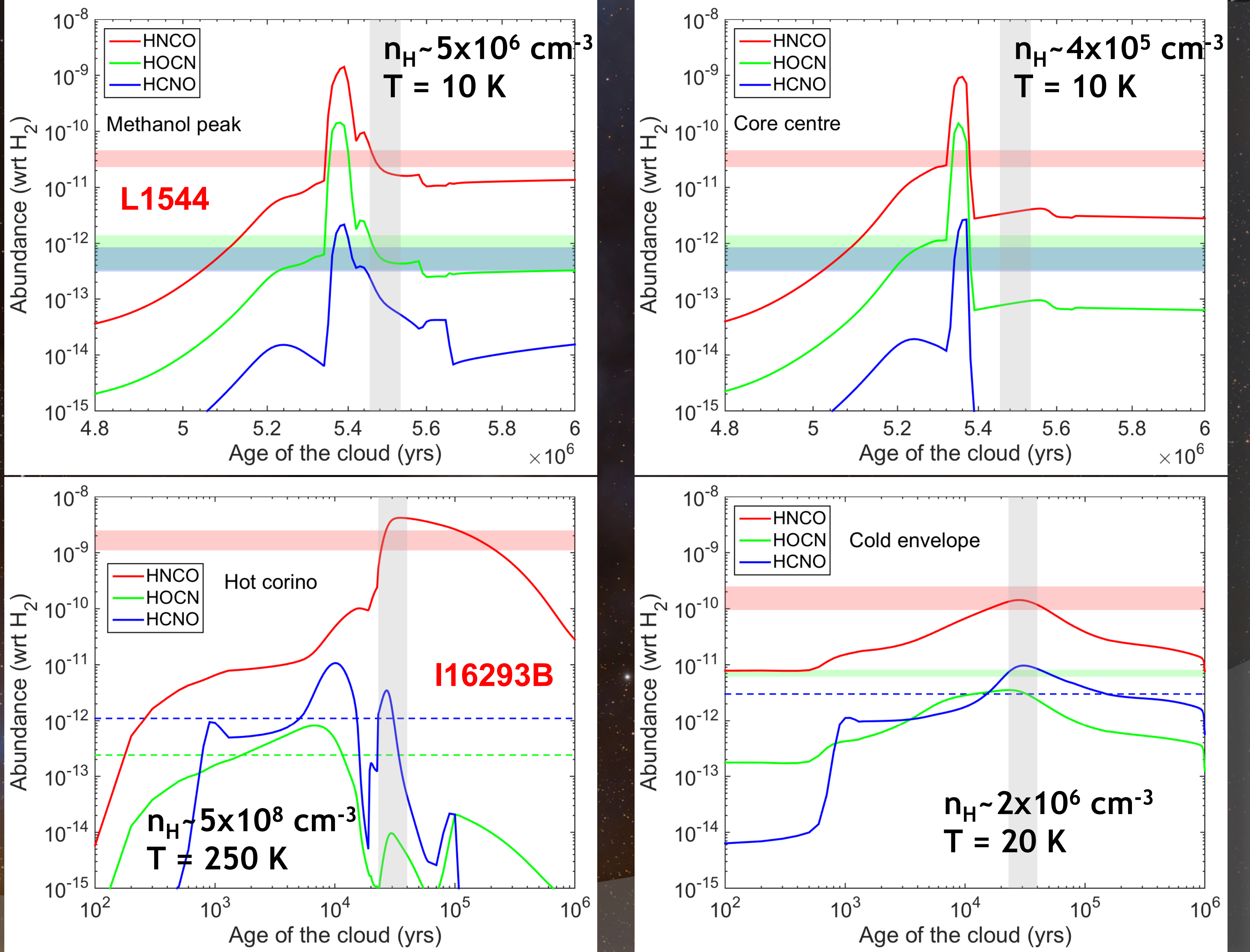
Phase 2

➔ Warm-up phase to 250 K (hot corino) and 20 K (cold envelope)

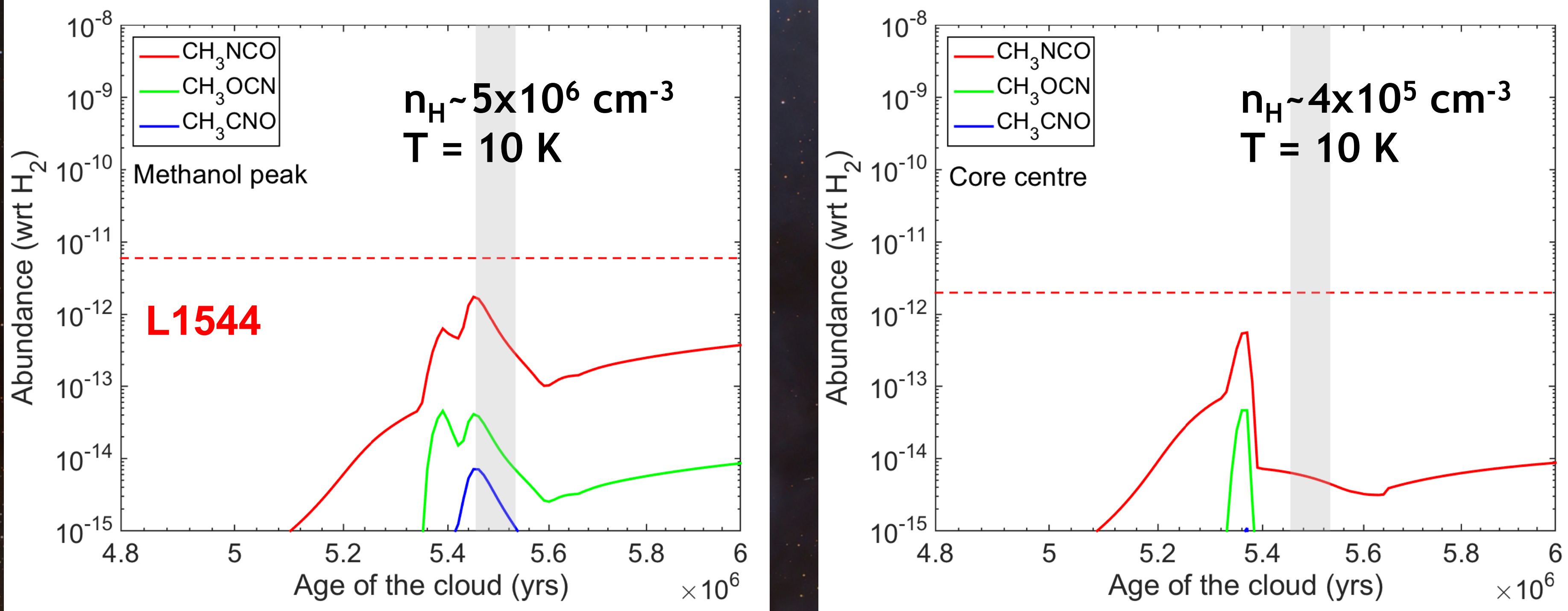
➔ Desorption of species from the grain mantle at high T !



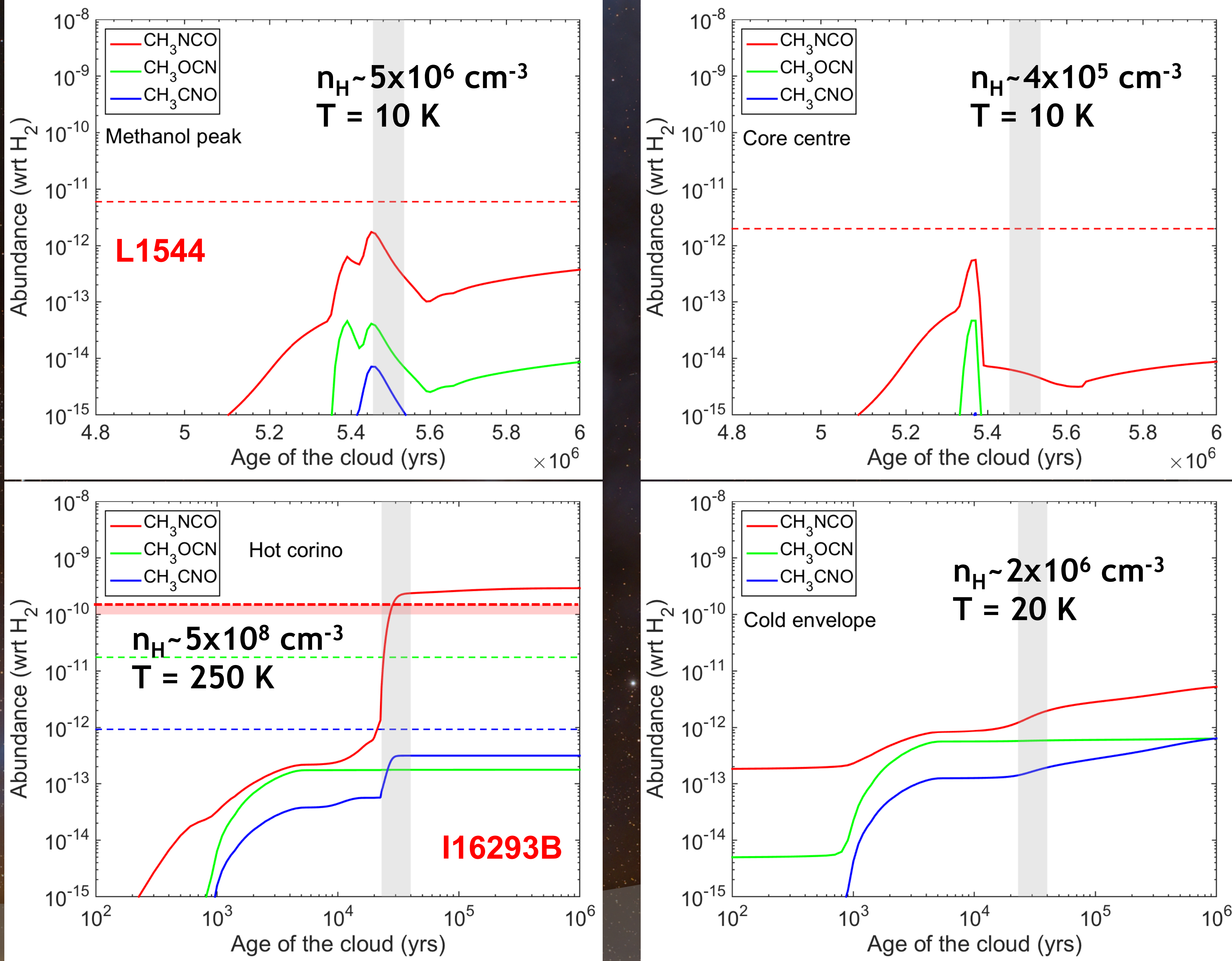
HNCO
HOCN
HCNO
n_H~5x10^6 cm^{-3}
T = 10 K
Methanol peak
L1544
Abundance (wrt H_2)
Age of the cloud (yrs)
×10^6
HNCO
HOCN
HCNO
n_H~4x10^5 cm^{-3}
T = 10 K
Core centre
Abundance (wrt H_2)
Age of the cloud (yrs)
×10^6



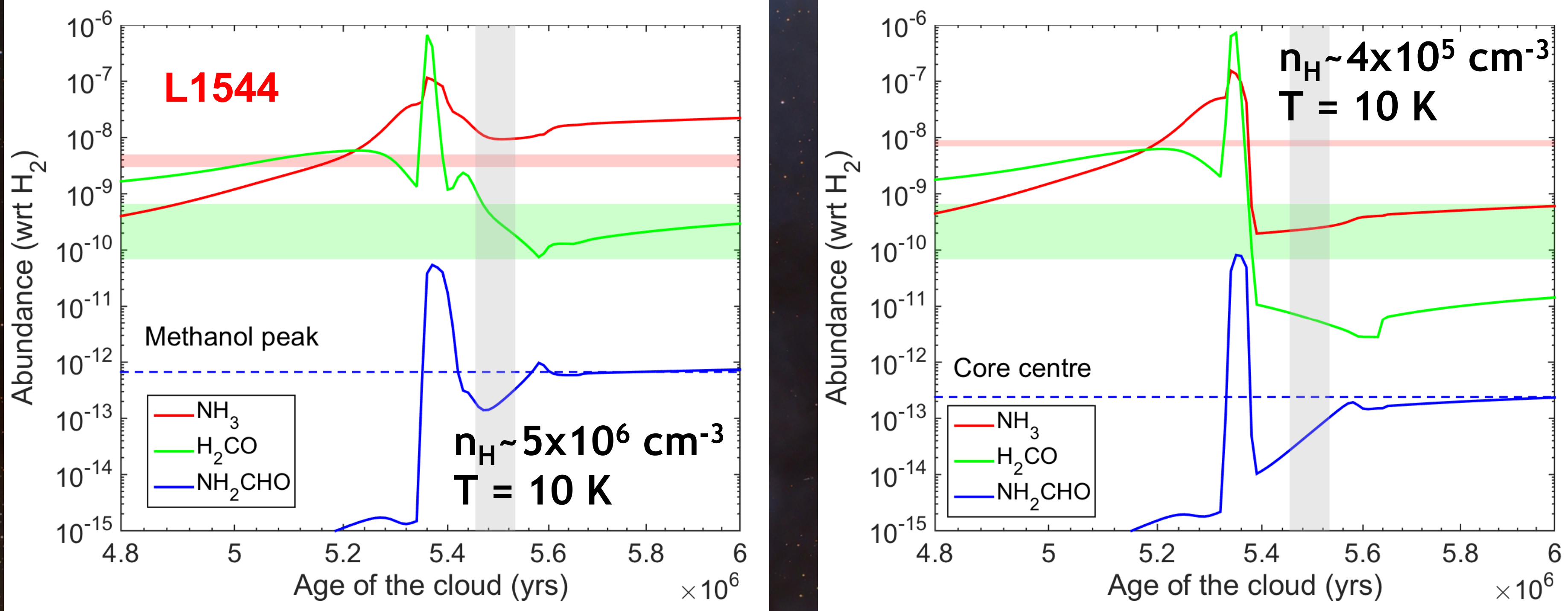
HNCO
HOCN
HCNO
$n_H \sim 5\times10^6$ cm^{-3}
T = 10 K
Methanol peak
L1544
Abundance (wrt H_2)
Age of the cloud (yrs)
$\times10^6$
$n_H \sim 4\times10^5$ cm^{-3}
T = 10 K
Core centre
Hot corino
I16293B
$n_H \sim 5\times10^8$ cm^{-3}
T = 250 K
Cold envelope
$n_H \sim 2\times10^6$ cm^{-3}
T = 20 K

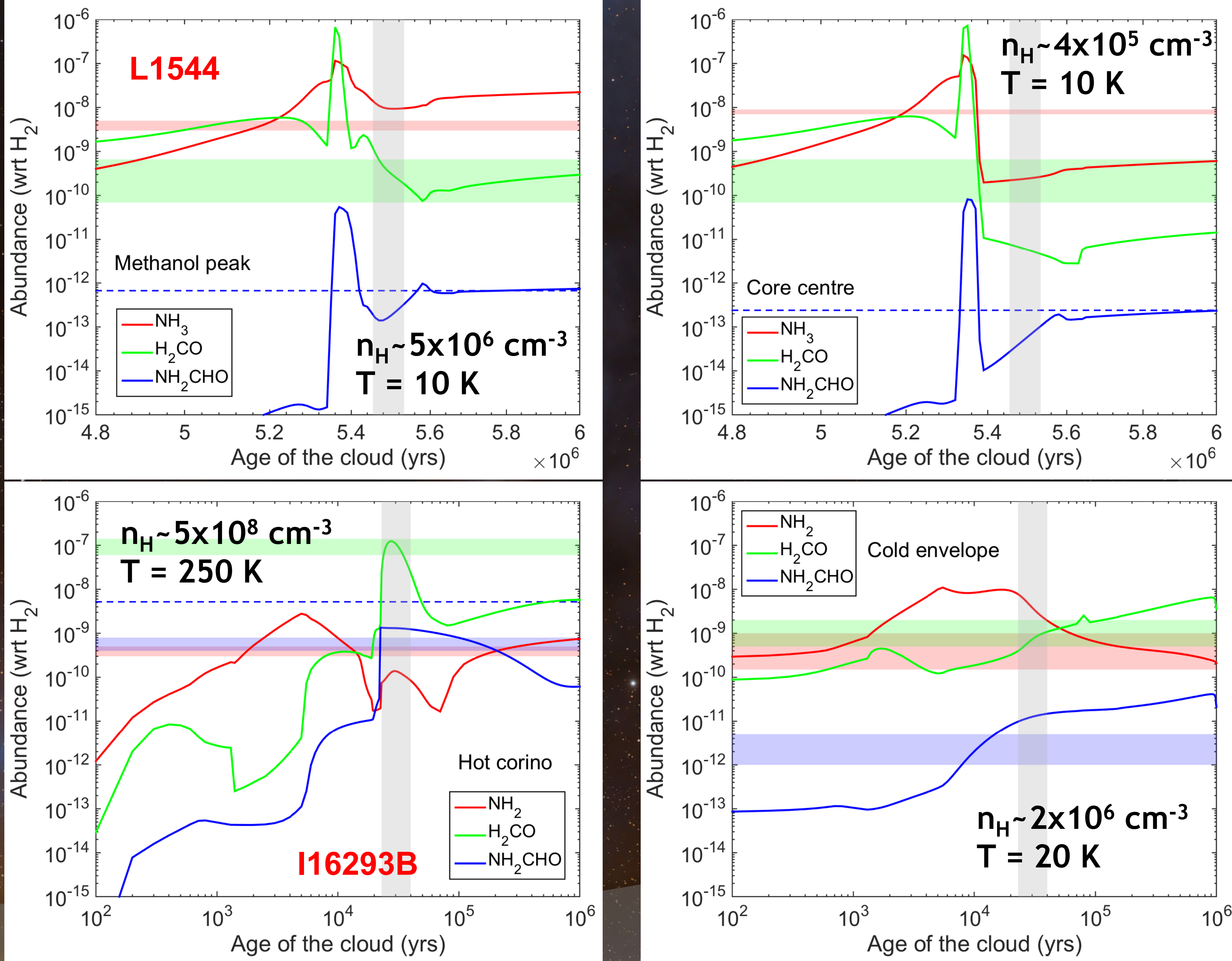


CH3NCO
CH3OCN
CH3CNO
Methanol peak
nH~5x10^6 cm^-3
T = 10 K
L1544
Abundance (wrt H2)
Age of the cloud (yrs)
×10^6
CH3NCO
CH3OCN
CH3CNO
Core centre
nH~4x10^5 cm^-3
T = 10 K
Abundance (wrt H2)
Age of the cloud (yrs)
×10^6



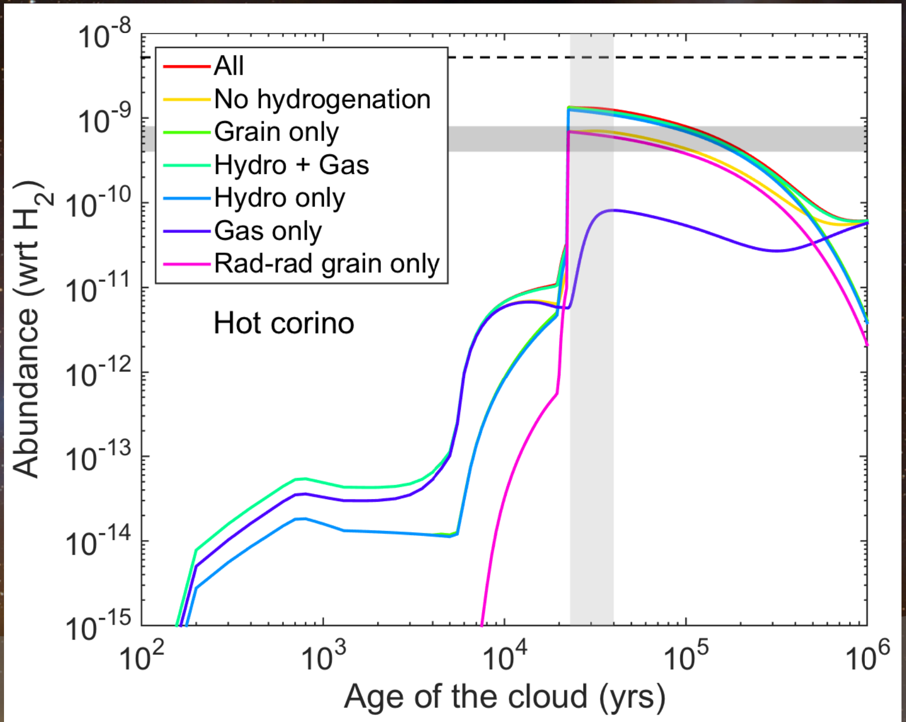
CH3NCO
CH3OCN
CH3CNO
Methanol peak
nH~5x10^6 cm^-3
T = 10 K
L1544
Abundance (wrt H2)
Age of the cloud (yrs)
×10^6
Core centre
nH~4x10^5 cm^-3
T = 10 K
Hot corino
nH~5x10^8 cm^-3
T = 250 K
I16293B
Cold envelope
nH~2x10^6 cm^-3
T = 20 K


L1544
Methanol peak
n_H~5x10^6 cm^{-3}
T = 10 K
NH$_3$
H$_2$CO
NH$_2$CHO
Abundance (wrt H$_2$)
Age of the cloud (yrs)
×10^6
Core centre
n_H~4x10^5 cm^{-3}
T = 10 K


L1544
Methanol peak
n_H~5x10^6 cm^{-3}
T = 10 K
n_H~4x10^5 cm^{-3}
T = 10 K
Core centre
n_H~5x10^8 cm^{-3}
T = 250 K
Hot corino
I16293B
Cold envelope
n_H~2x10^6 cm^{-3}
T = 20 K
NH3
H2CO
NH2CHO
NH2
Abundance (wrt H2)
Age of the cloud (yrs)

NH_2CHO chemistry

- **Gas phase** chemistry
- **Grain surface chemistry:**
  - **Radical-radical** reactions
  - **Hydrogenation**



NH_2CHO chemistry

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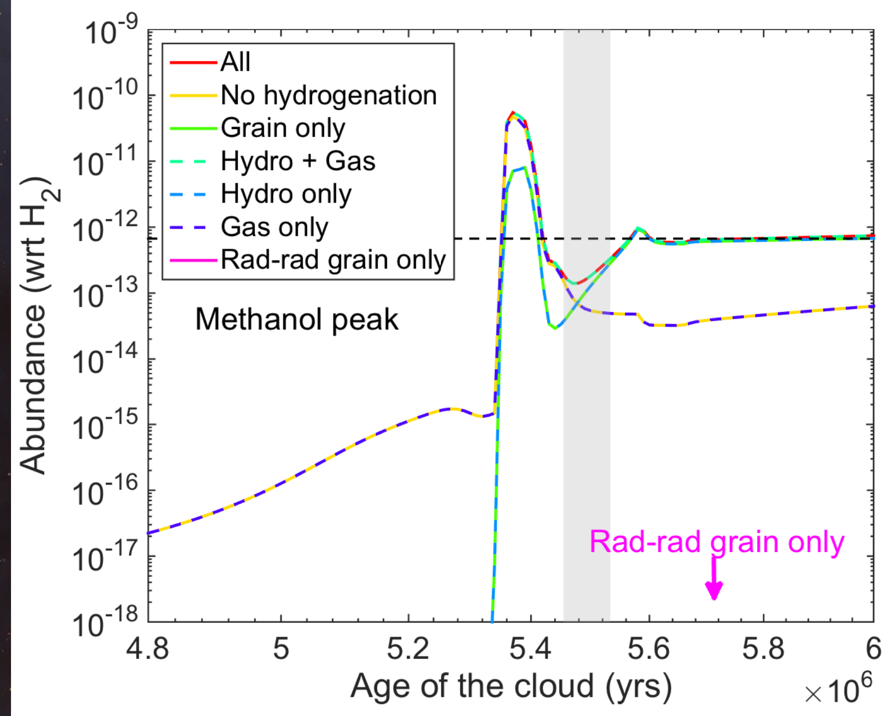
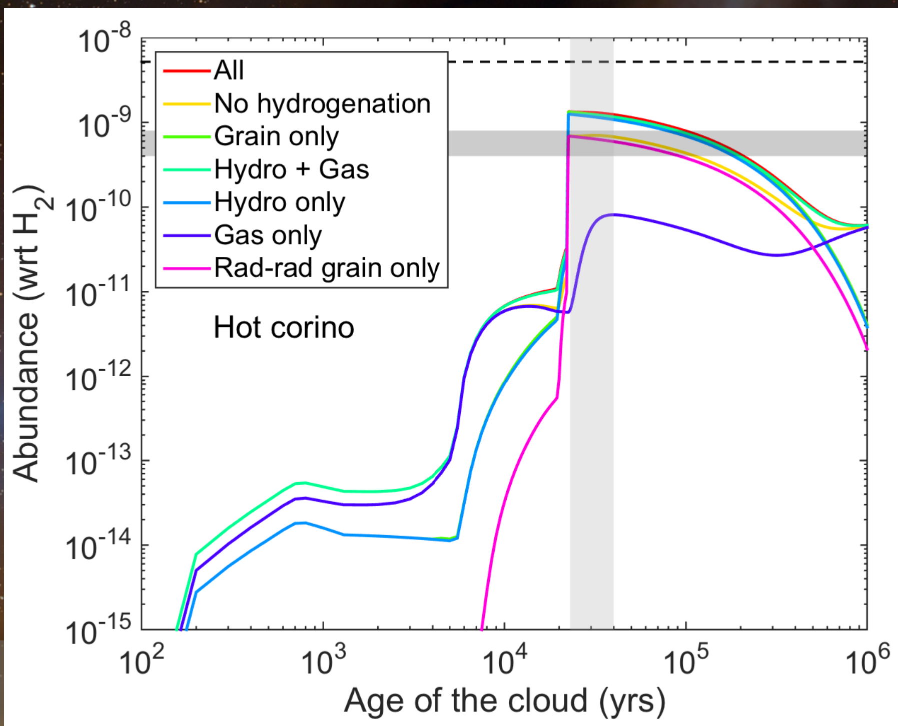
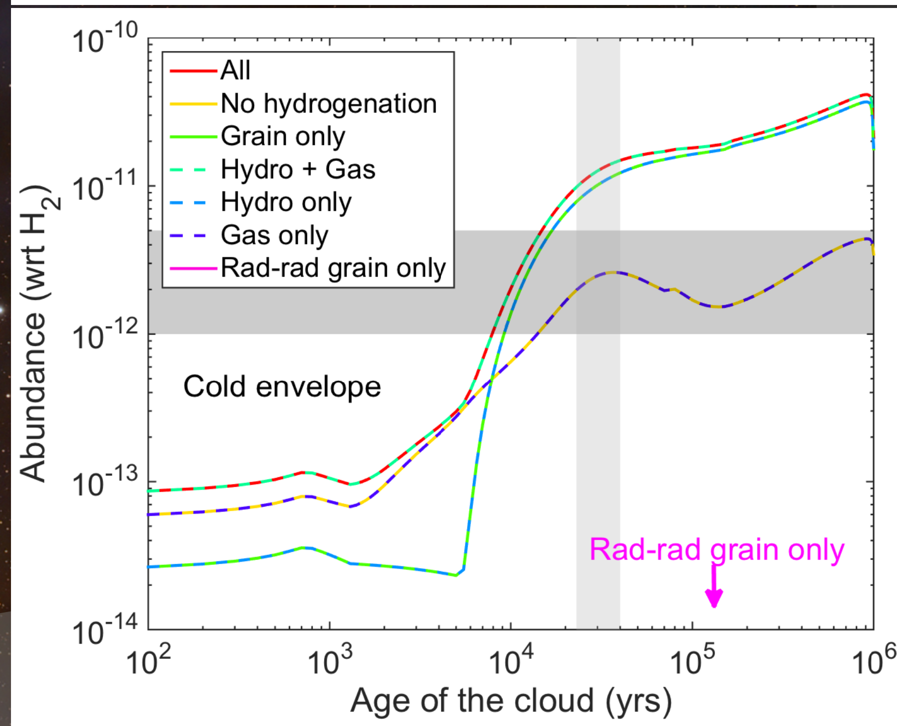


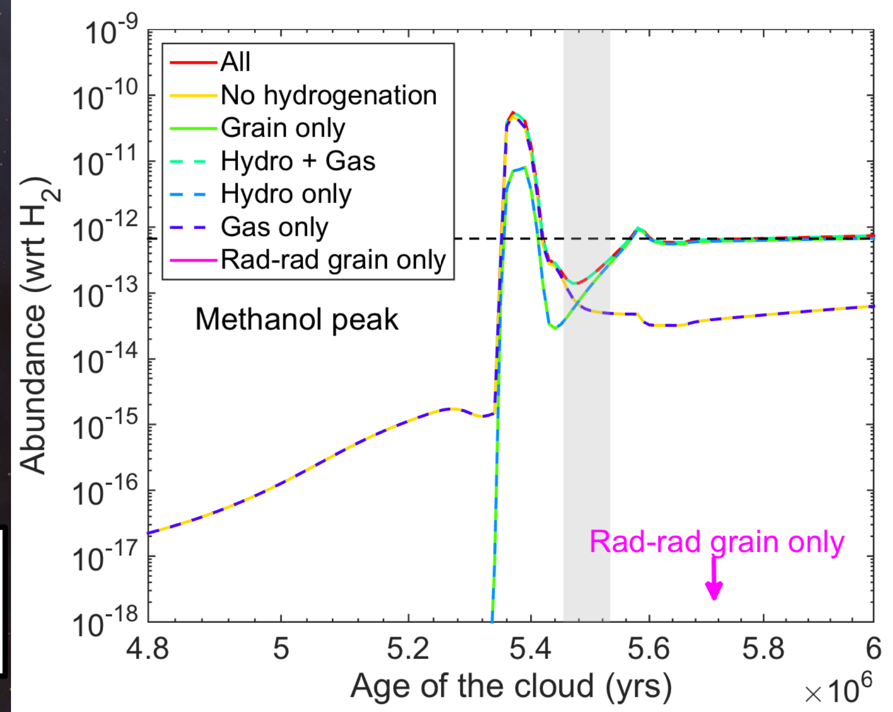


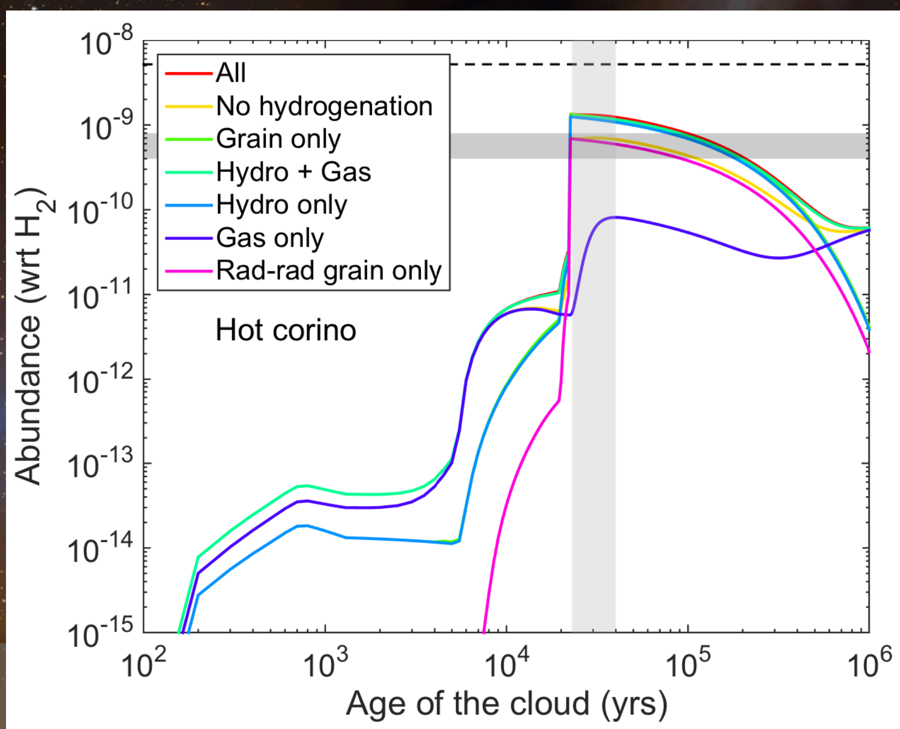


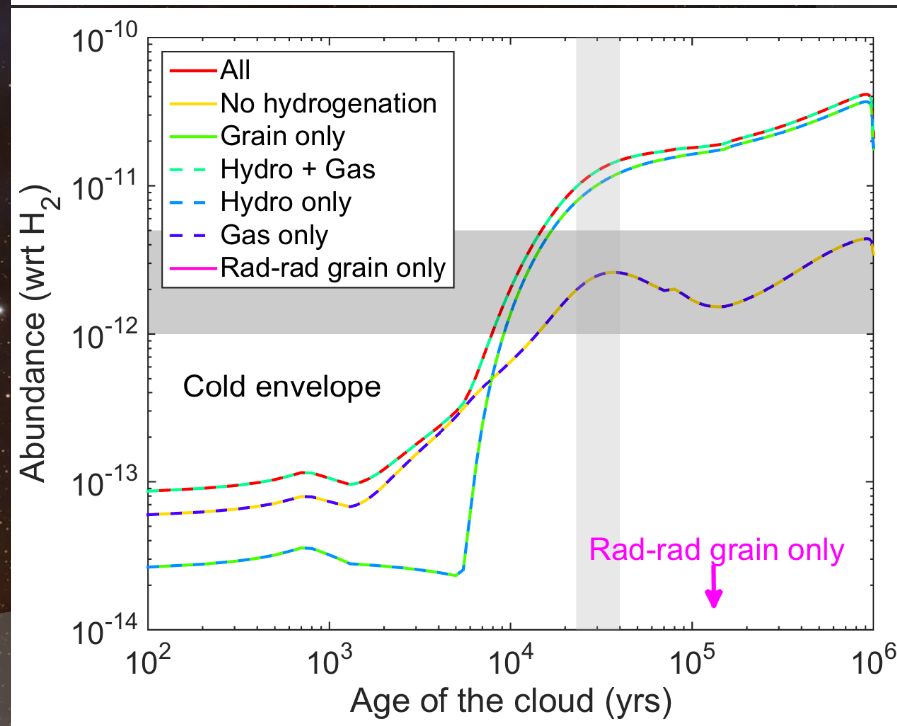
NH_2CHO chemistry

- **Gas phase** chemistry
- Grain surface chemistry:
  - **Radical-radical** reactions
  - **Hydrogenation**

Modelling different physical regimes help to constrain the chemistry !



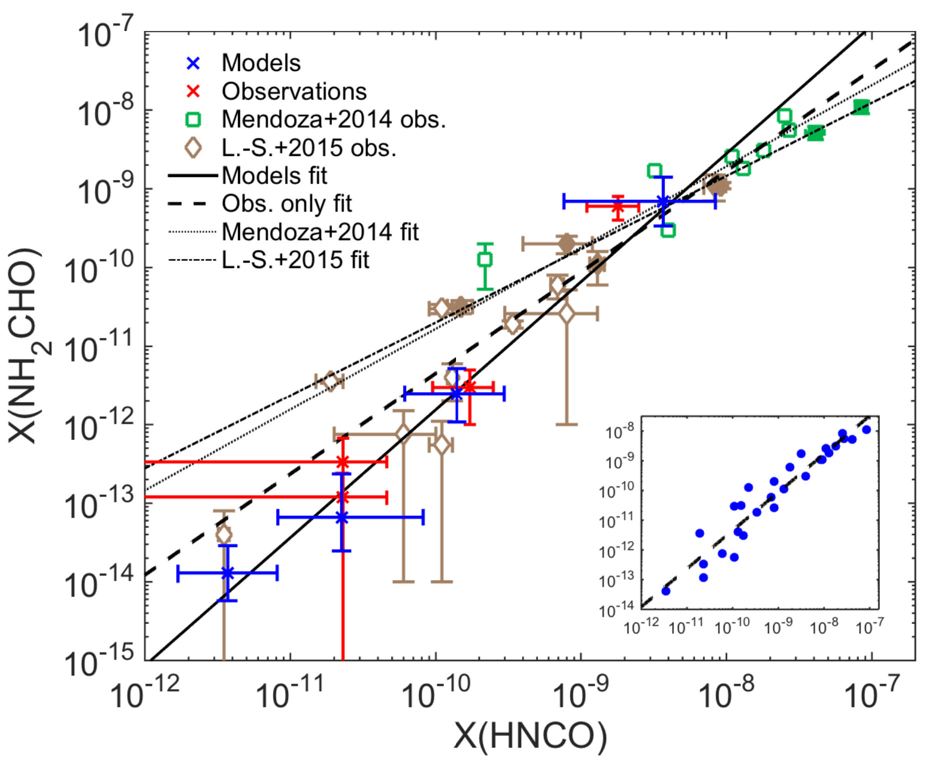


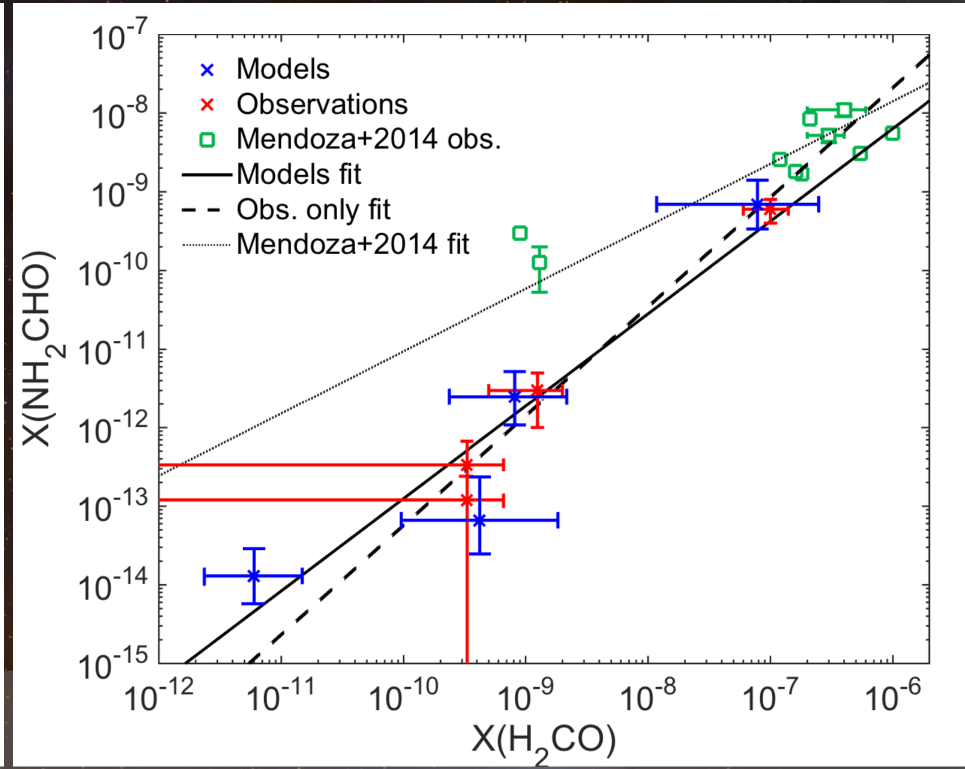


$HNCO$ & H_2CO vs NH_2CHO

Mendoza et al. (2014) and **Lopéz-Sepulcre et al. (2015)**:
Observational correlation ➔ **Chemical correlation** between the two?

Modelling of NH_2CHO (no hydrogenation from HNCO)
➔ **Physical (environmental) correlation** depending mainly on the **temperature** that triggers different **chemical processes.**





Conclusions

- Modelling of N-bearing COMs predicts abundances of NH_2CHO, CH_3NCO (and isomers), HNCO (and isomers) in L1544 and IRAS16293 B
  - L1544: core centre and methanol peak
  - IRAS16293 B: hot corino and cold envelope
- Both gas-phase and grain-phase chemistry are needed to explain the observed abundances of NH_2CHO
  - Hydrogenation of HNCO tend to overestimate the NH_2CHO abundance compared to radical-radical reactions
- The observed correlation between HNCO and NH_2CHO may come from an environmental correlation (temperature) rather than a chemical correlation