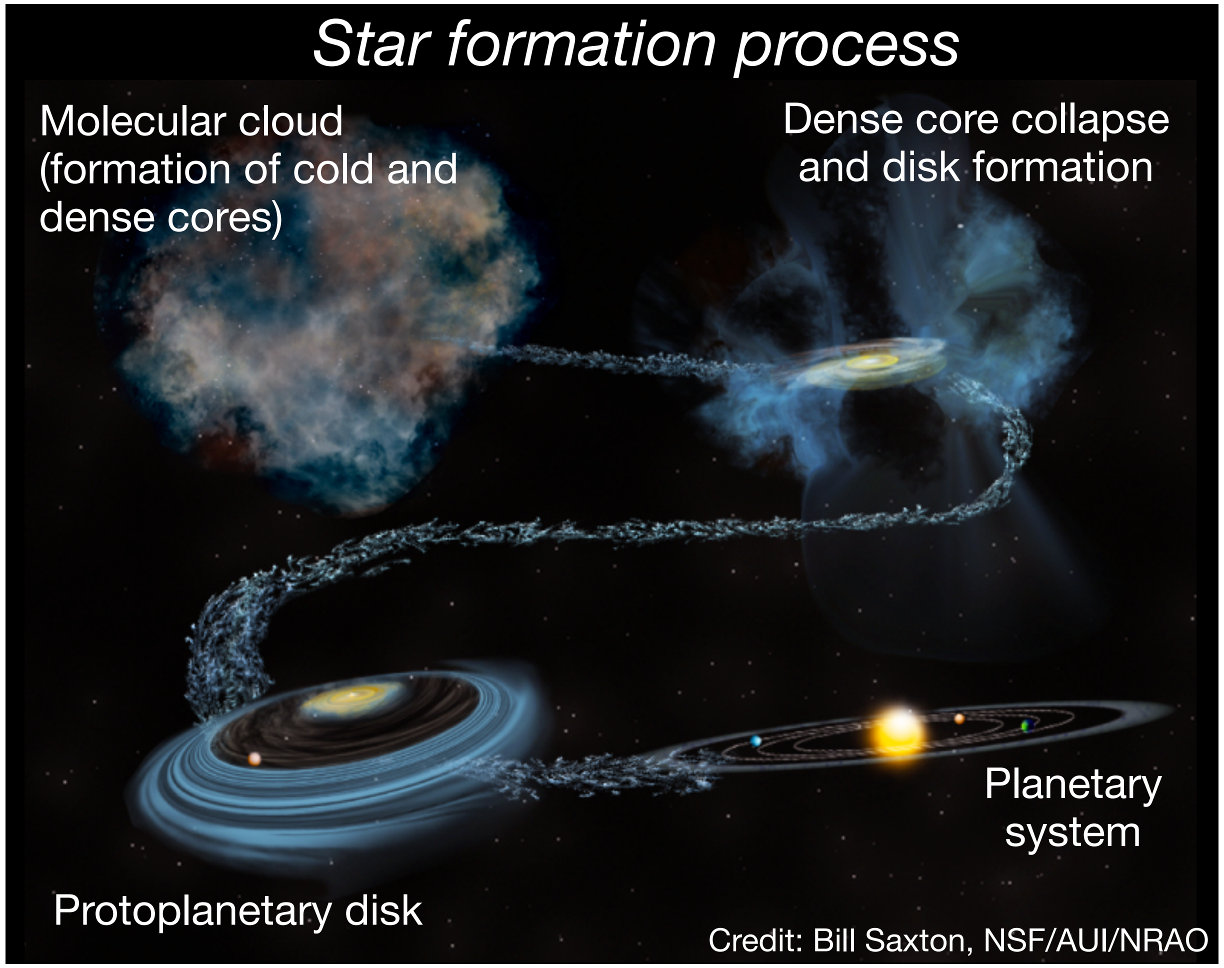
Chemical evolution during the formation of a protoplanetary disk

A. Coutens (LAB), B. Commerçon (CRAL) & V. Wakelam (LAB)



QUESTIONS

- ✻ How does the chemical content evolve during the star formation process ?
- ✻ What is the chemical composition of protoplanetary disks (in which planets are expected to form) ?
- ✻ Does the disk inherit the chemical composition of the cold and dense core or does the physical changes during the collapse play a major role on the disk composition ?

METHODS

Physical modeling

- ✻ 3D dense core collapse magneto-hydrodynamic (MHD) calculations with the RAMSES code (adaptative-mesh refinement)
- ✻ 10^6 initial particles
- ✻ $M = 1\ M_\odot$
- ✻ Resistive MHD

Chemical modeling

- ✻ 3-phase chemistry code NAUTILUS
- ✻ Chemical network :
  - 589 gas phase species
  - 540 grain species
  - 13,384 reactions

Initial abundances

- ✻ 2 sets of initial abundances (A and B) that correspond to 2 cold cores with different history
- ✻ SPH simulations of dense core formation (Ruaud et al. 2018)
- ✻ Different reservoirs for O, C, N, S, Si, and P

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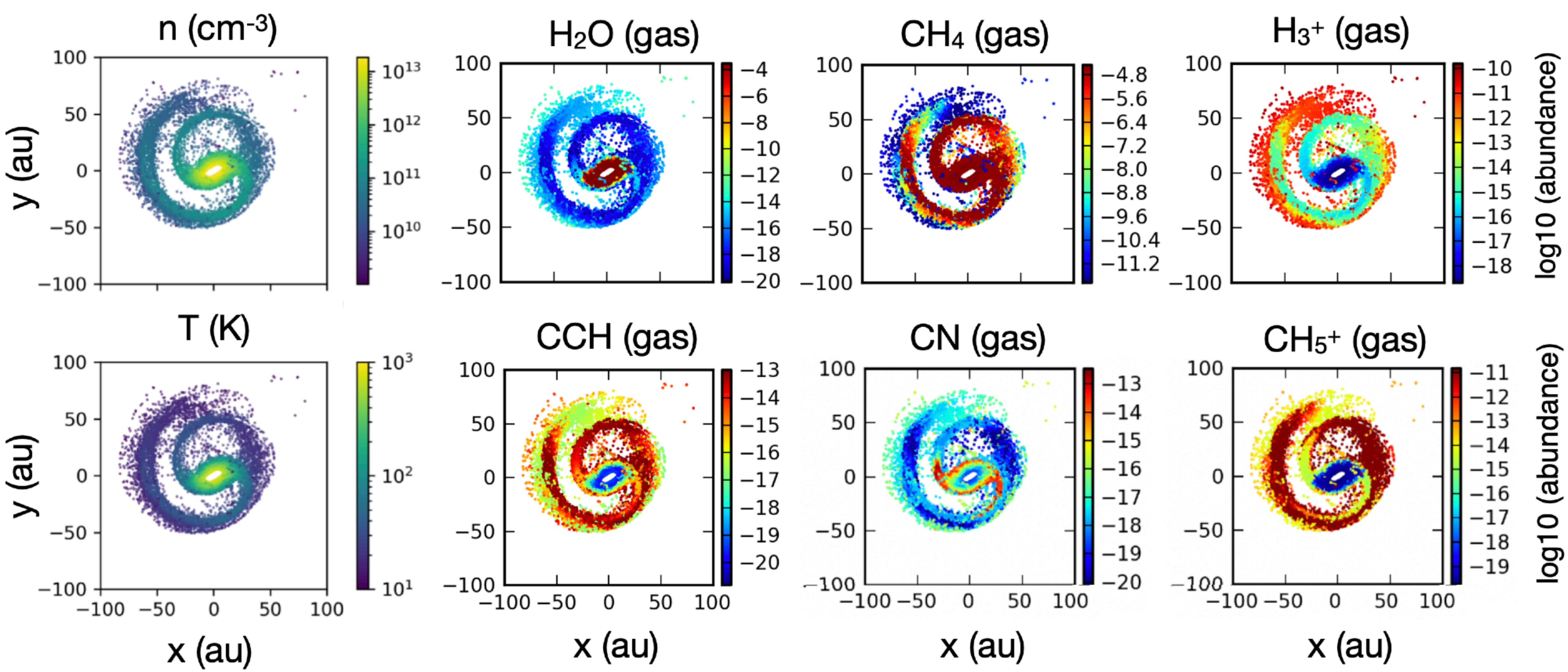
RESULTS

- ✻ 15,000 particles end in the disk at the final time of the simulations (5.8 x 10^4 yrs)
- ✻ First hydrostatic core stage = 5.0 x 10^4 yrs

1. Spatial distribution

- ✻ Different spatial distribution according to the species
- ✻ Sensitivity of molecules to temperature and density distribution
- ✻ Same spatial distributions for different initial abundances (except for HCO, HNO, OH, SO, SO_2, CH_3)
- ✻ Similar distribution for water and complex organic molecules (COMs)



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2. Final reservoirs

- The main carriers of the chemical elements in the disk are usually the same ones as in the cold core
- No change for N, Si, Cl, F
- For O and C, the contributions of HCO and CH_2OH decrease significantly (cloud B)
- For S, H_2S_3 becomes a major carrier instead of HS (clouds A and B)
- For P, the contributions of PO, HCP, and CP increase (cloud B)
- Even if the reservoirs are similar, important changes are seen for less abundant species

Element	Main reservoir, Case A	Main reservoir, Case B
O	H_2O (91%)	H_2O (49%), H_2CO (9%), CH_3OH (7%), HCOOH (2 × 6%)
C	HCN (28%), CH_4 (15%), CH_3OH (7%), C_3H_8 (3 × 5%)	H_2CO (16%), CH_3OH (13%), CH_4 (12%), HCOOH (12%), CO (7%), CO_2 (6%)
N	HCN (81%), NH_3 (6%), N_2 (2 × 6%)	NH_3 (58%), NH_2CH_2OH (10%), N_2 (2 × 7%), HCN (5%)
S	H_2S (35%), CH_3SH (11%), H_2S_3 (3 × 10%), CH_3S (5%)	H_2S (30%), H_2S_3 (3 × 11%), OCS (7%), NS (7%)
Si	SiH_4 (44%), SiC_8H (16%), SiC_6H (8%), SiC_4H (7%), HCSi (5%)	SiC_4H (27%), SiO (21%), SiH_4 (18%), SiC_6H (7%)
P	P (80%), CP (11%), HCP (7%)	P (40%), PO (26%), PN (14%), HCP (10%), CP (9%)
Cl	HCl (100%)	HCl (99%)
F	HF (100%)	HF (100%)

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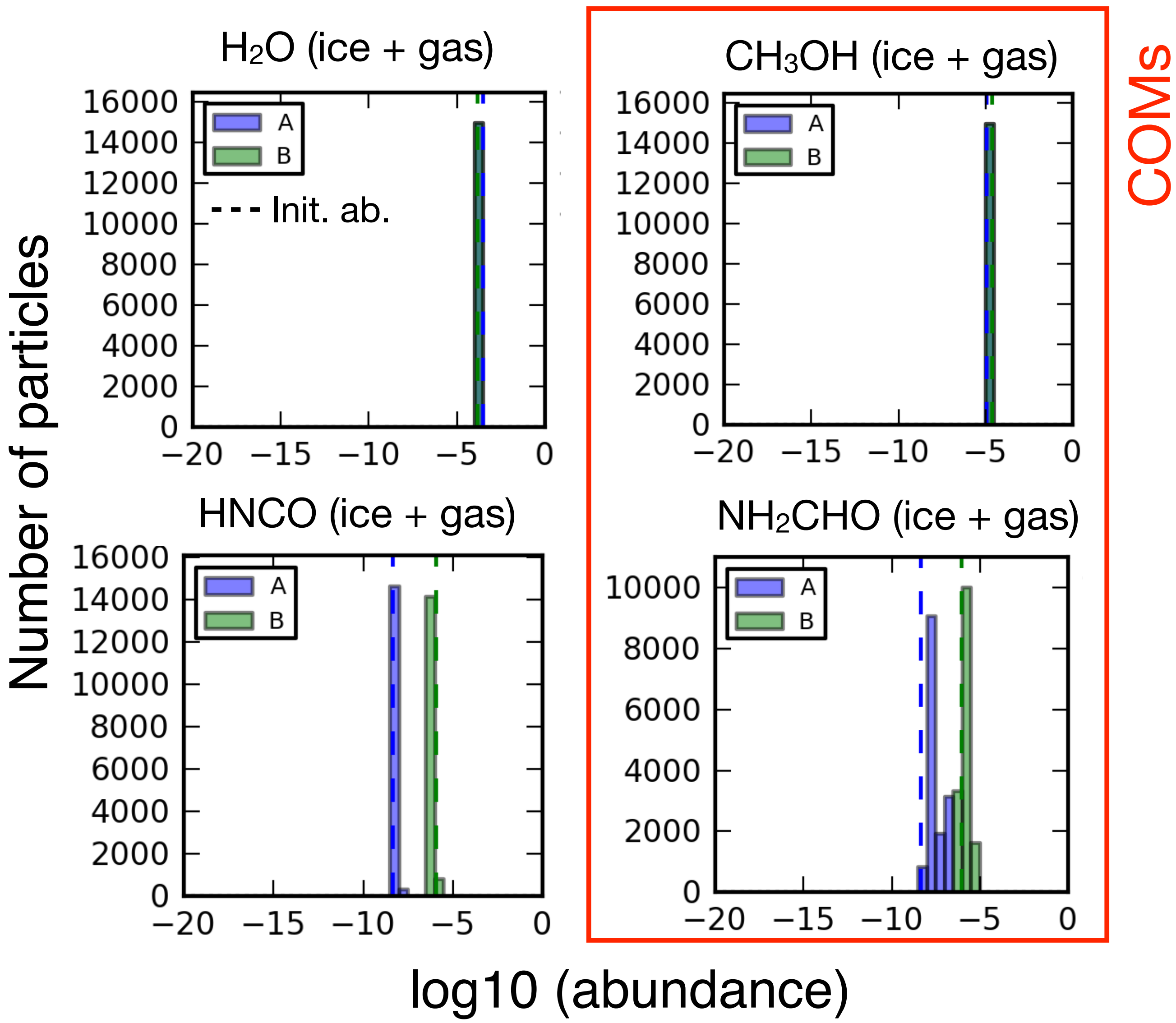
3. Chemical evolution

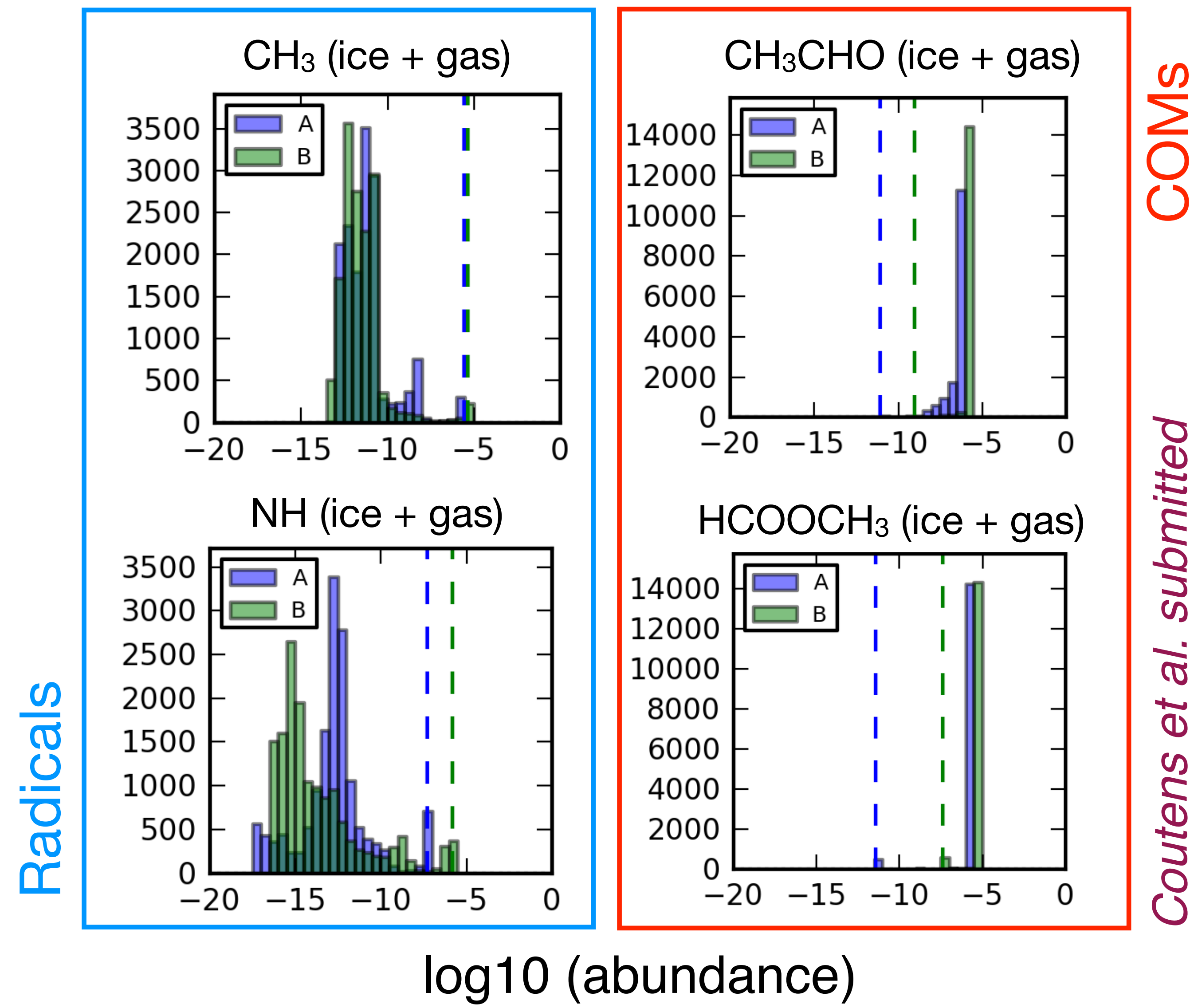
* Classification of more than 70 species according to their sensitivity to the initial abundances

Similar initial and final abundances : *H_2O, HNCO, H_2CO, CH_3OH, CH_3CN, NH_2CHO, HCOOH, …*



Inheritance from the cold and dense core

Different initial and final abundances : *CCH, HCO, CH_3O, CH_3CHO, $HCOOCH_3$, CH_3OCH_3, …*



The collapse plays a key role in the increase of the molecular complexity