

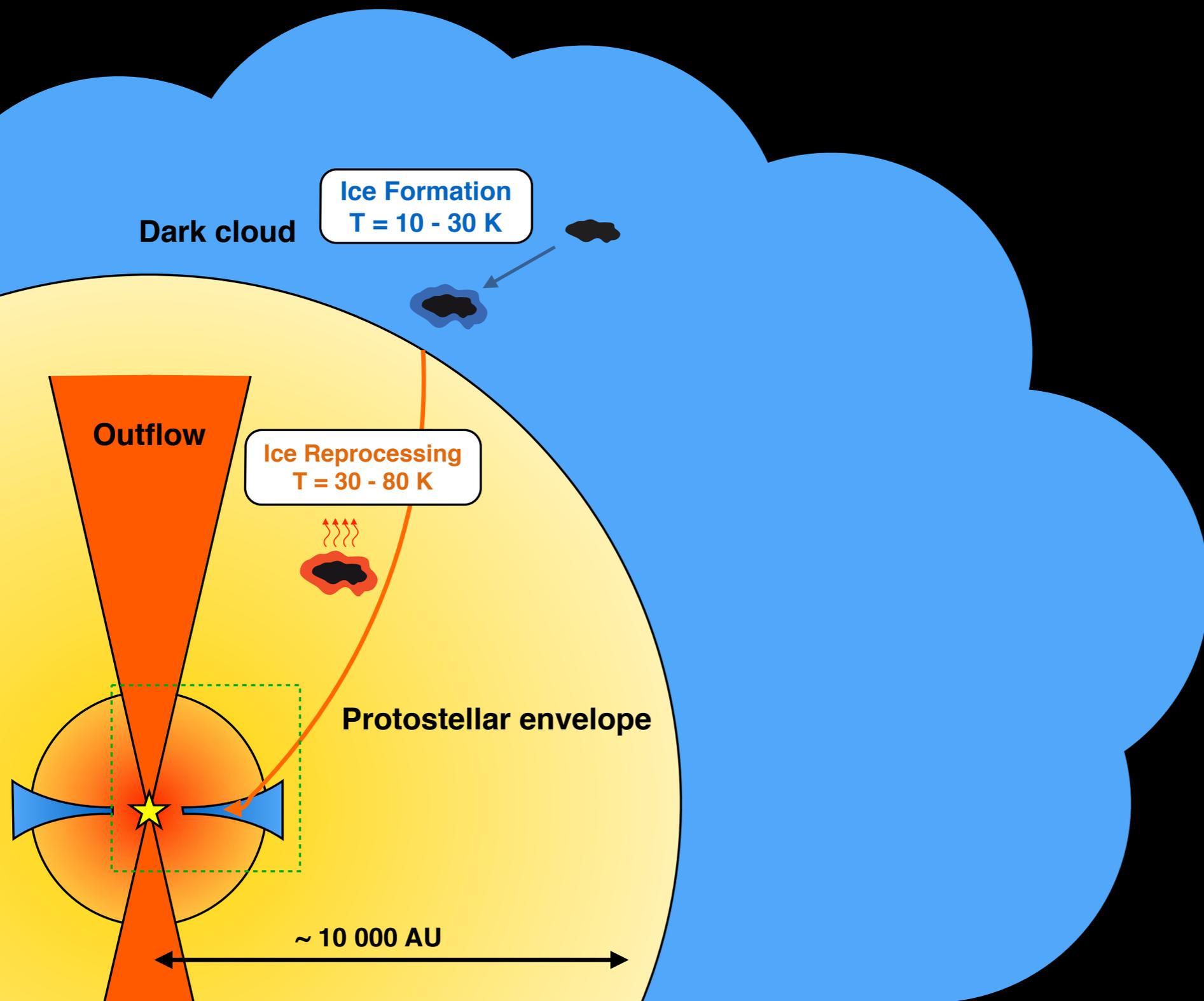
Tracing the chemical evolution of organic molecules from dark clouds to planetary systems

Vianney Taquet

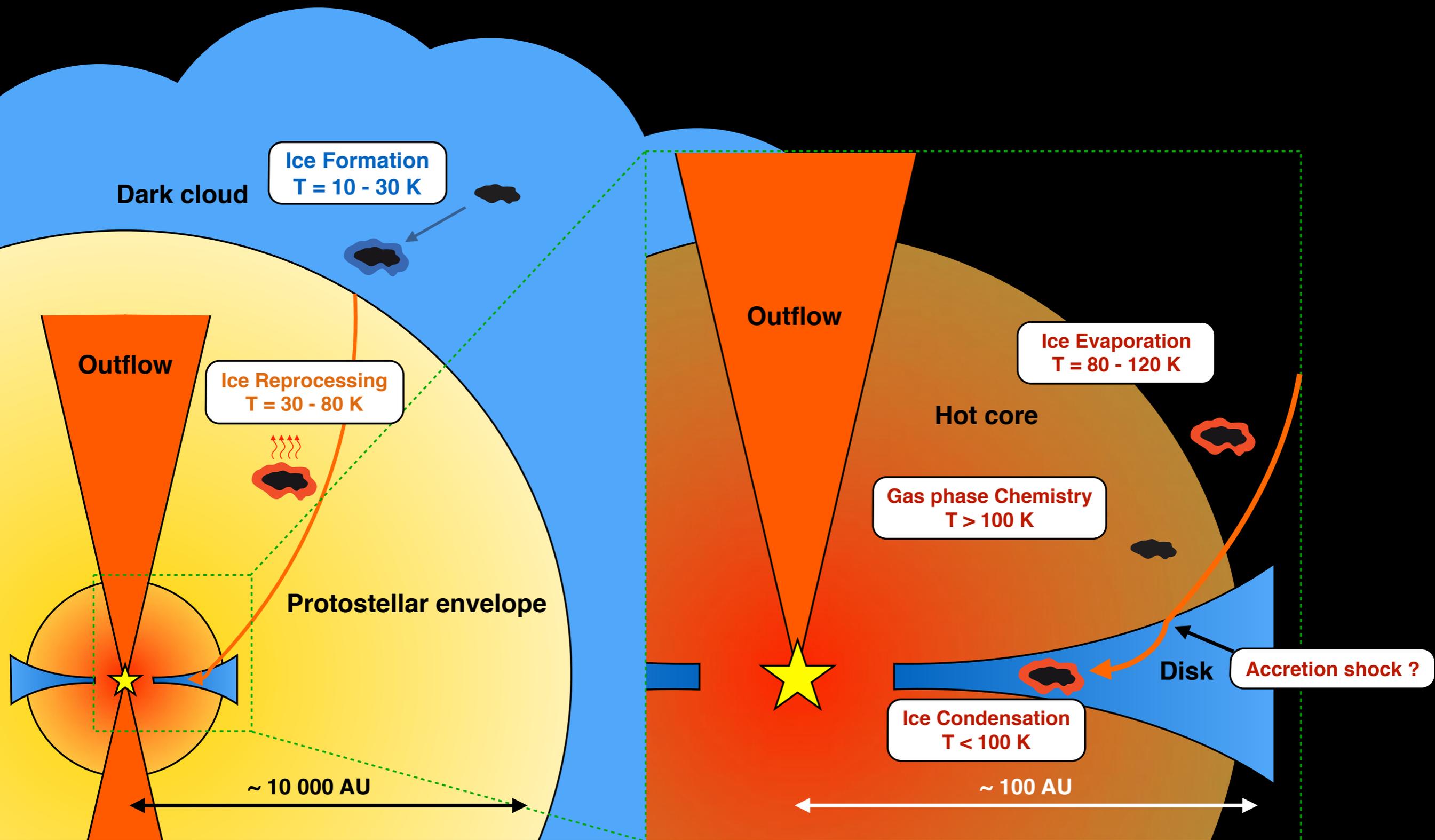
Osservatorio Astrofisico di Arcetri - INAF
AstroFlt 2 Fellowship



Chemical evolution from dark clouds to planetary systems



Chemical evolution from dark clouds to planetary systems



Interstellar complex organic molecules

Star formation is accompanied by a chemical complexity process

- 60 of the 175 detected interstellar species are complex organic molecules (COMs)

(molecules with ≥ 6 atoms based on carbon; Herbst & van Dishoeck 2009)

- Most of them detected towards massive star-forming regions, $\approx 30\%$ detected towards low-mass protostars

- Some of them could be at the origin of the formation of amino- and hydroxy-acids observed in meteorites (Pizzarello et al. 2006)

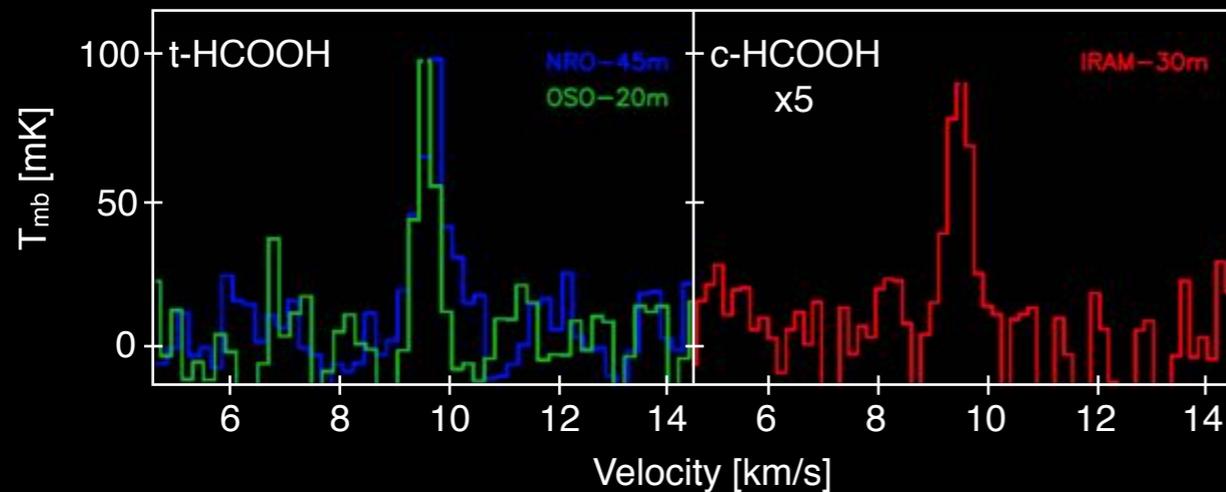
6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	>12 atoms
C_6H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N	<i>o</i> - $C_6H_6^*$	$HC_{11}N?$
i - H_2C_4	CH_2CHCN	$HC(O)OCH_3$	CH_3CH_2CN	$(CH_3)_2CO$	CH_3C_6H	<i>n</i> - C_7H_7CN	C_{60}^*
$C_2H_4^+$	CH_3C_2H	CH_3COCH	$(CH_3)_2O$	$(CH_2OH)_2$	C_2H_5OCHO	<i>i</i> - C_7H_7CN	C_{70}^*
CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO	$CH_3OC(O)CH_3$	$C_2H_5OCH_3?$	C_{60}^{**}
CH_3NC	CH_3CHO	C_6H_2	HC_7N	CH_3CHCH_2O 2018			
CH_3OH	CH_3NH_2	CH_2OHCHO	C_6H				
CH_3SH	<i>o</i> - C_2H_4O	<i>i</i> - HC_6H^*	$CH_3C(O)NH_2$				
HC_3NH^+	H_2CCHOH	CH_2CHCHO (?)	C_6H^+				
HC_2CHO	C_6H^-	CH_2CCHCN	C_7H_6				
NH_2CHO	CH_3NCO 2015	H_2NCH_2CN	CH_3CH_2SH (?)				
C_3N		CH_3CHNH					
i - HC_4H^+							
i - HC_4N							
<i>o</i> - H_2C_3D							
H_2CCNH (?)							
C_5N^-							
$HNCHCN$							

Organic molecules in prestellar cores

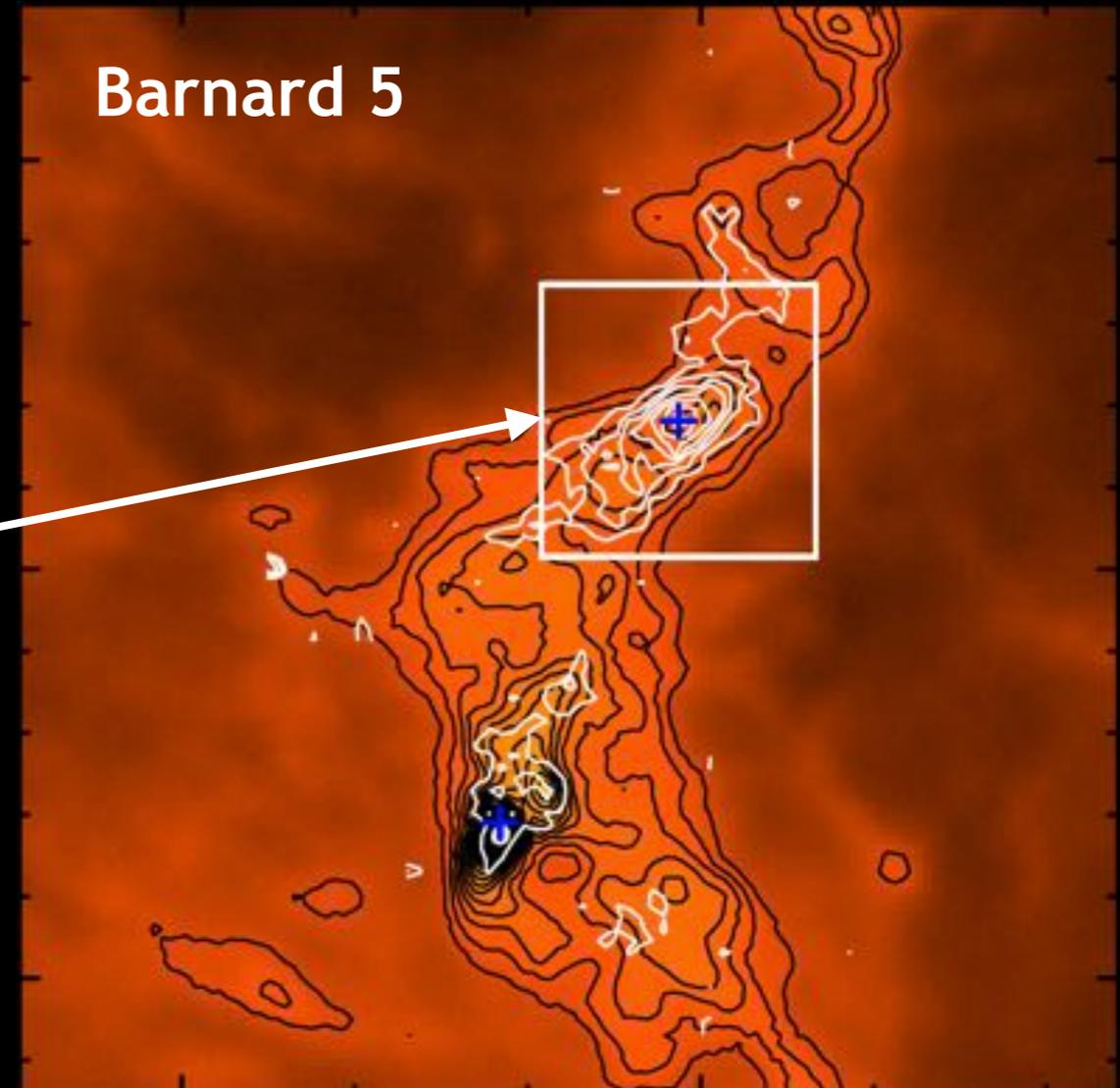
Recent detection of a handful of O-bearing organic molecules with millimetric single dish telescopes towards a few prestellar cores

Example: Detection of the usual complex organics (CH_3CHO , CH_3OCHO , CH_3OCH_3 , HCOOH) with the IRAM 30m, NRO 45m, and OSO 20m towards the the Barnard 5 dark cloud

Acid formic HCOOH in its two conformers



Taquet et al. (2017)

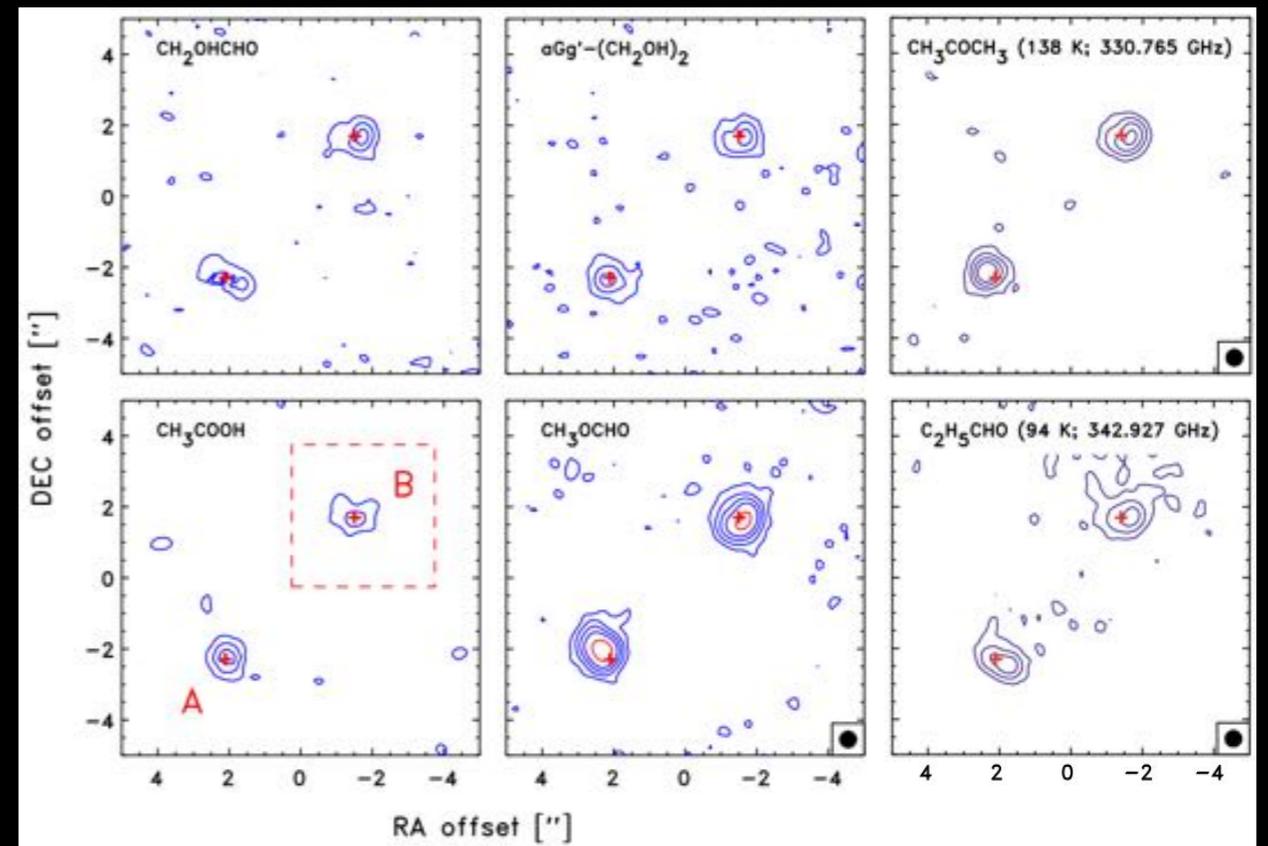
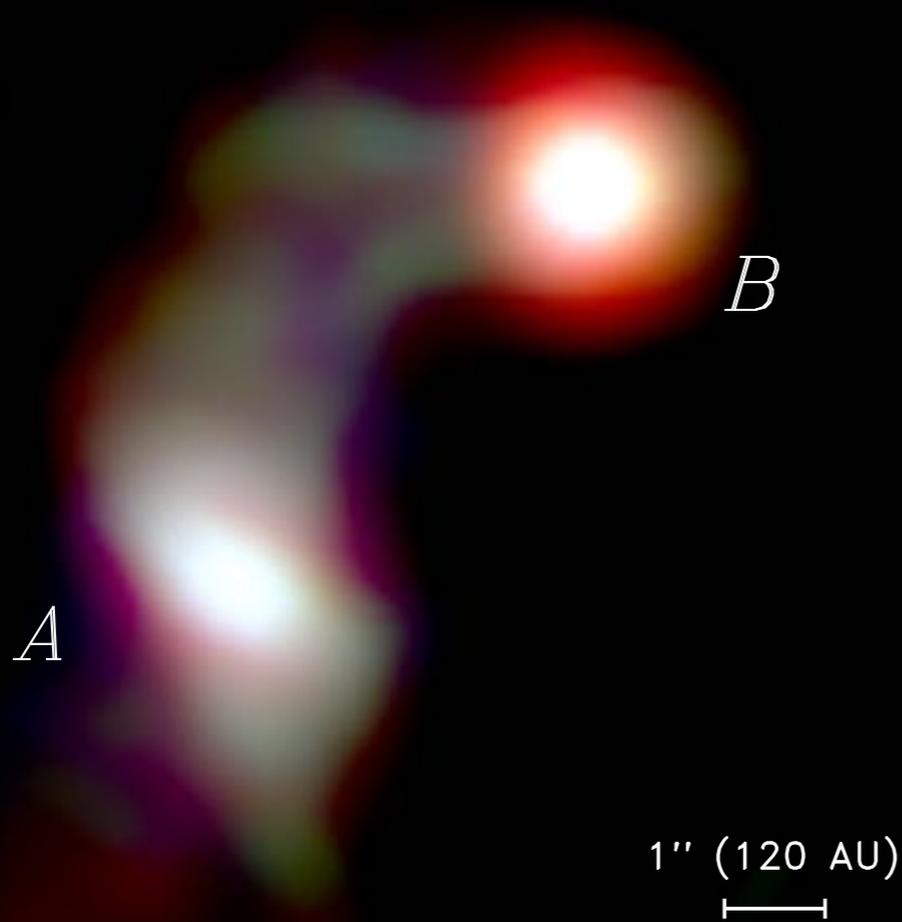


See also Bacmann, Taquet et al. (2012), Cernicharo et al. (2012), Vastel et al. (2014), Jimenez-Serra et al. (2016)

Organic molecules in low-mass protostars

Organic molecules of increasing complexity are detected in the inner regions of low-mass protostars with large millimetric interferometers (ALMA, NOEMA)

Example: IRAS 16293 observed with the ALMA-PILS survey



Jørgensen et al. (2016), Lykke et al. (2017)

See also Cazaux et al. (2003), Bottinelli et al. (2004, 2007), Caux et al. (2011), Taquet et al. (2015), Santangelo et al. (2015), Lopez-Sepulcre et al. (2017)

Organic molecules in low-mass protostars

Organic molecules of increasing complexity are detected in the inner regions of low-mass protostars with large millimetric interferometers (ALMA, NOEMA)

Water H₂O

CO₂ (in interstellar ices)

Alcohol: Ethanol CH₃CH₂OH

Sugar: Glycol aldehyde HCOCH₂OH

Acid: Acetic acid CH₃COOH

Organic molecules in low-mass protostars

Organic molecules of increasing complexity are detected in the inner regions of low-mass protostars with large millimetric interferometers (ALMA, NOEMA)

Water H_2O

CO_2 (in interstellar ices)

Alcohol: Ethanol $\text{CH}_3\text{CH}_2\text{OH}$

Sugar: Glycol aldehyde HCOCH_2OH

Acid: Acetic acid CH_3COOH

Interstellar mojito !

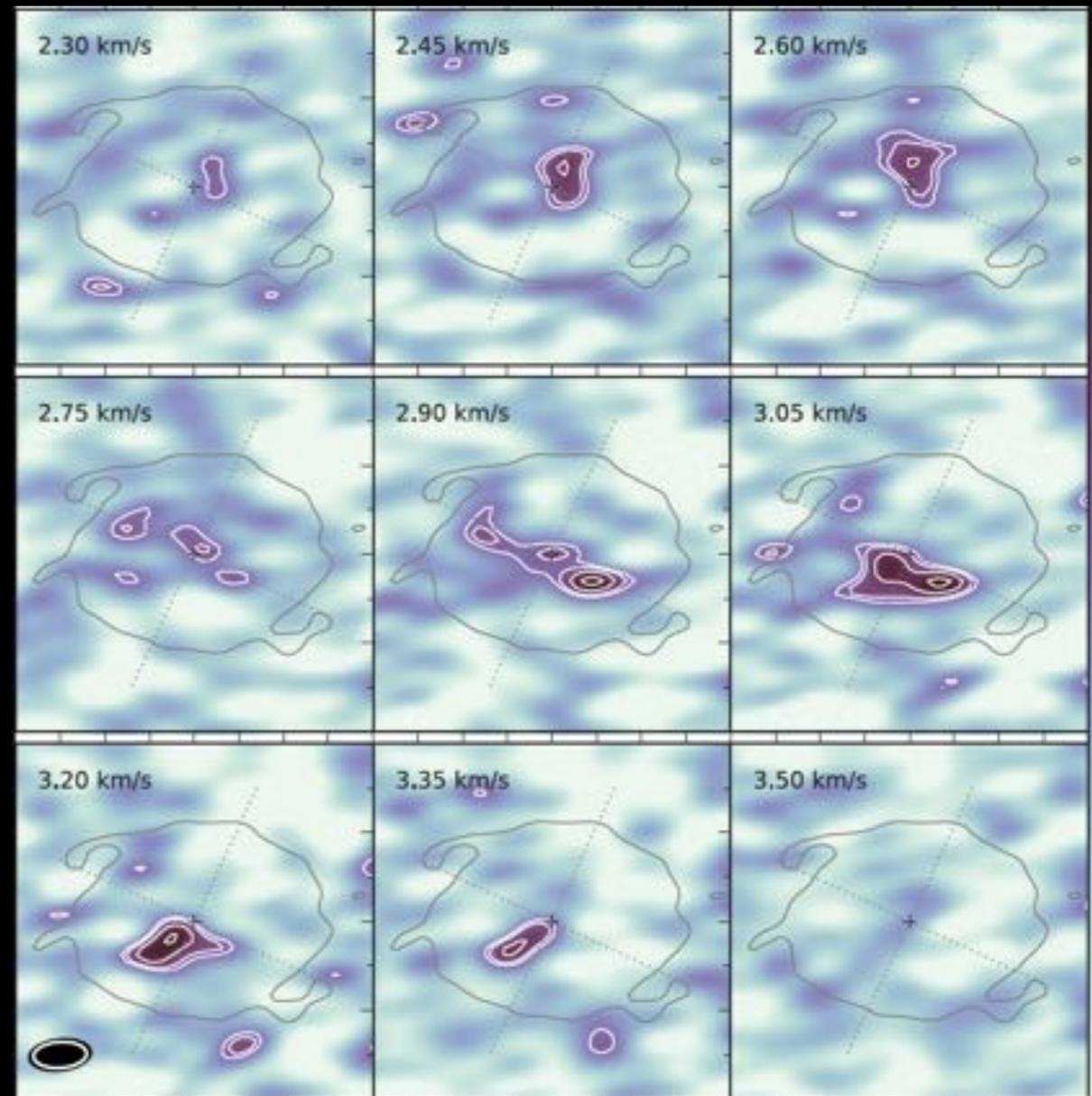
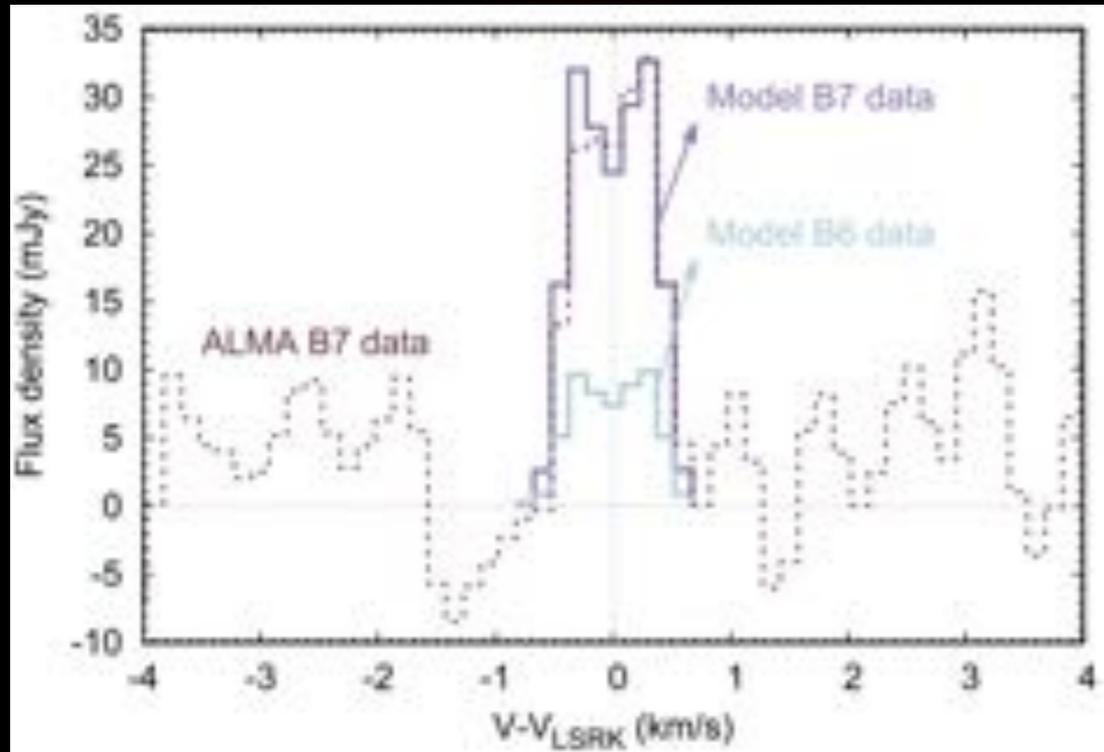
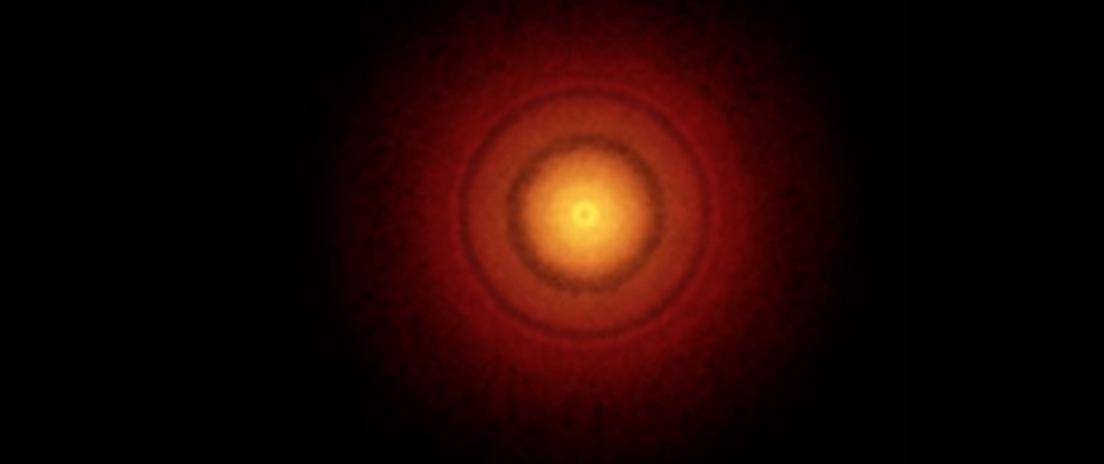


Mint is still missing though...

Organic molecules in protoplanetary disks

Only two complex organics (CH_3CN and CH_3OH) detected in protoplanetary disks so far, partly because of small size and weak brightness of disks

TW Hydrae observed with ALMA: need to stack several CH_3OH transitions

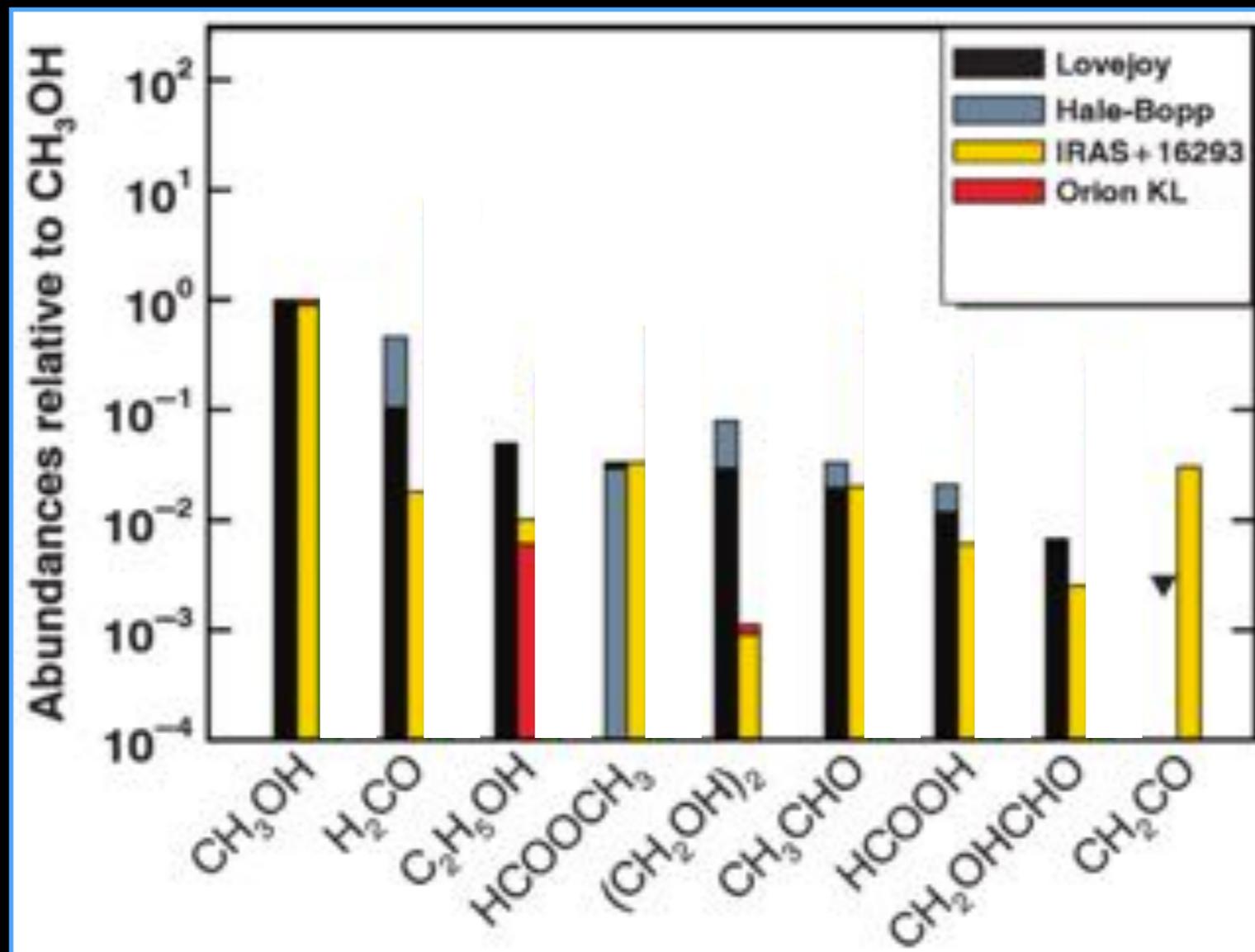


Organic molecules in comets

Remote sensing and in-situ analysis revealed the chemical richness of comets and meteorites

Similar organic molecules detected in protostars in comets with millimetric observatories, with similar abundances

See Bockelée-Morvan et al. (2000),
Biver et al. (2015)



And comet 67P/C-G analysed by *Rosetta*...

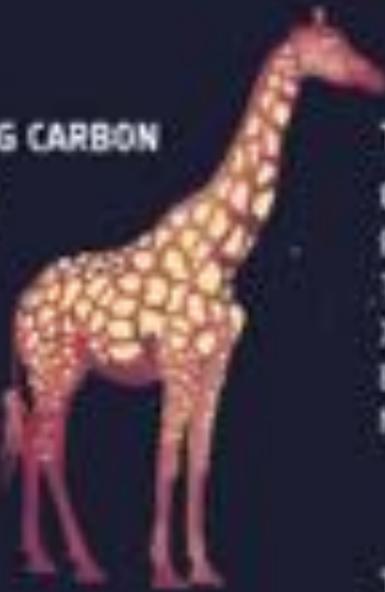
The Rosetta/ROSINA zoo



→ THE COMETARY ZOO: GASES DETECTED BY ROSETTA

THE LONG CARBON CHAINS

- Methane
- Ethane
- Propane
- Butane
- Pentane
- Hexane
- Heptane



THE AROMATIC RING COMPOUNDS

- Benzene
- Toluene
- Xylene
- Benzoic acid
- Naphtalene



THE KING OF THE ZOO Glycine (amino acid)



THE "MANURE SMELL" MOLECULES

- Ammonia
- Methylamine
- Ethylamine



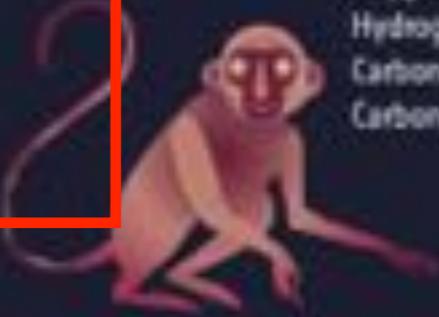
THE "POISONOUS" MOLECULES

- Acetylene
- Hydrogen cyanide
- Acetonitrile
- Formaldehyde



THE ALCOHOLS

- Methanol
- Ethanol
- Propanol
- Butanol
- Pentanol



THE VOLATILES

- Nitrogen
- Oxygen
- Hydrogen peroxide
- Carbon monoxide
- Carbon dioxide



THE "SMELLY" MOLECULES

- Hydrogensulphide
- Carbonylsulphide
- Sulphur monoxide
- Sulphur dioxide
- Carbon disulphide



THE "SMELLY AND COLOURFUL" MOLECULES

- Sulphur
- Disulphur
- Trisulphur
- Tetrasulphur
- Methanethiol
- Ethanethiol
- Thioformaldehyde



THE TREASURES WITH A HARD CRUST

- Sodium
- Potassium
- Silicon
- Magnesium



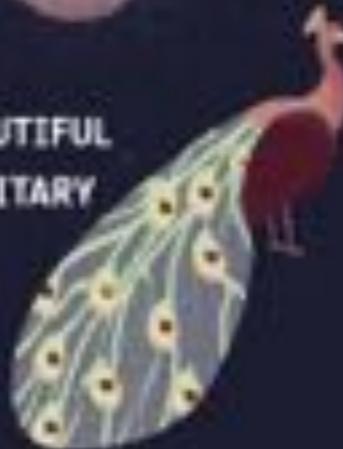
THE "SALTY" BEASTS

- Hydrogen fluoride
- Hydrogen chloride
- Hydrogen bromide
- Phosphorus
- Chloromethane



THE BEAUTIFUL AND SOLITARY

- Argon
- Krypton
- Xenon



THE "EXOTIC" MOLECULES

- Formic acid
- Acetic acid
- Acetaldehyde
- Ethylenglycol
- Propylenglycol
- Butanamide



THE MOLECULE IN DISGUISE

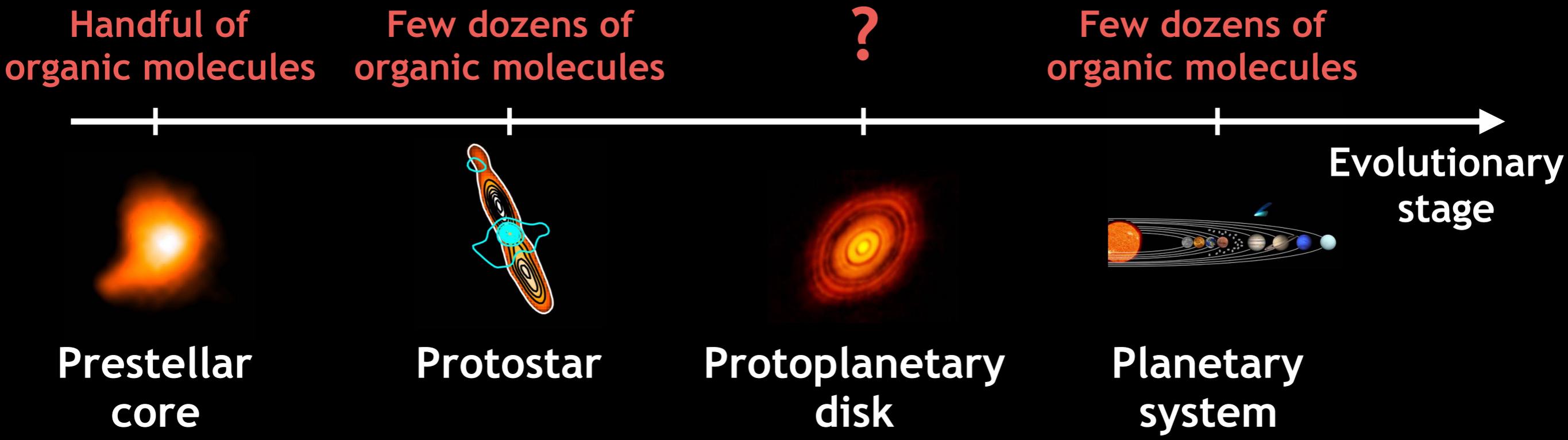
- Cyanogen



Questions

How to interpret the observed chemical complexity?

Can interstellar molecules survive in disks?



Do cometary (and Solar System) organics have an interstellar origin?

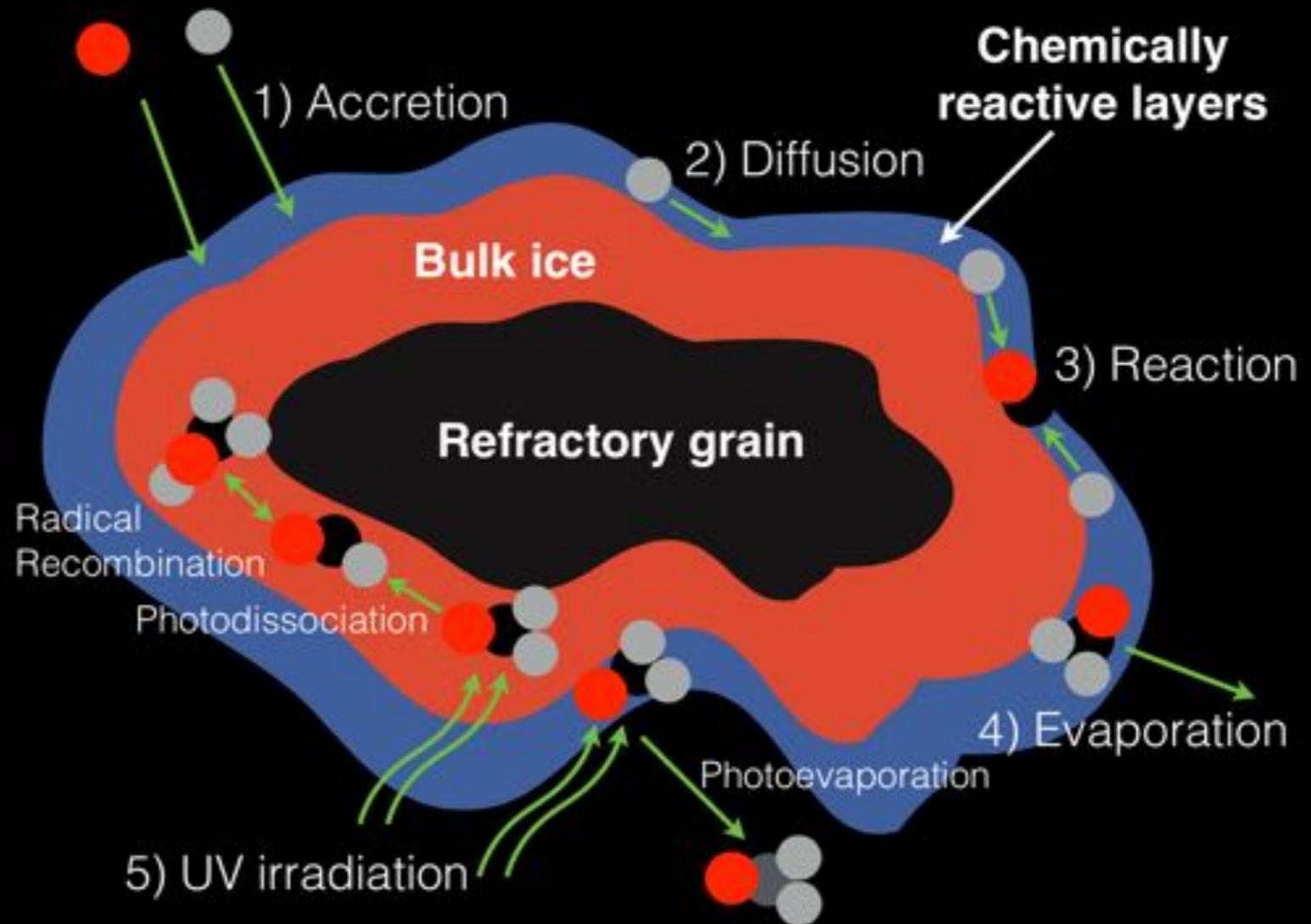
Chemical processes in the Interstellar Medium

Gas-grain astrochemical models have been developed for several decades to understand the presence in high quantities of these organics

Gas phase chemistry

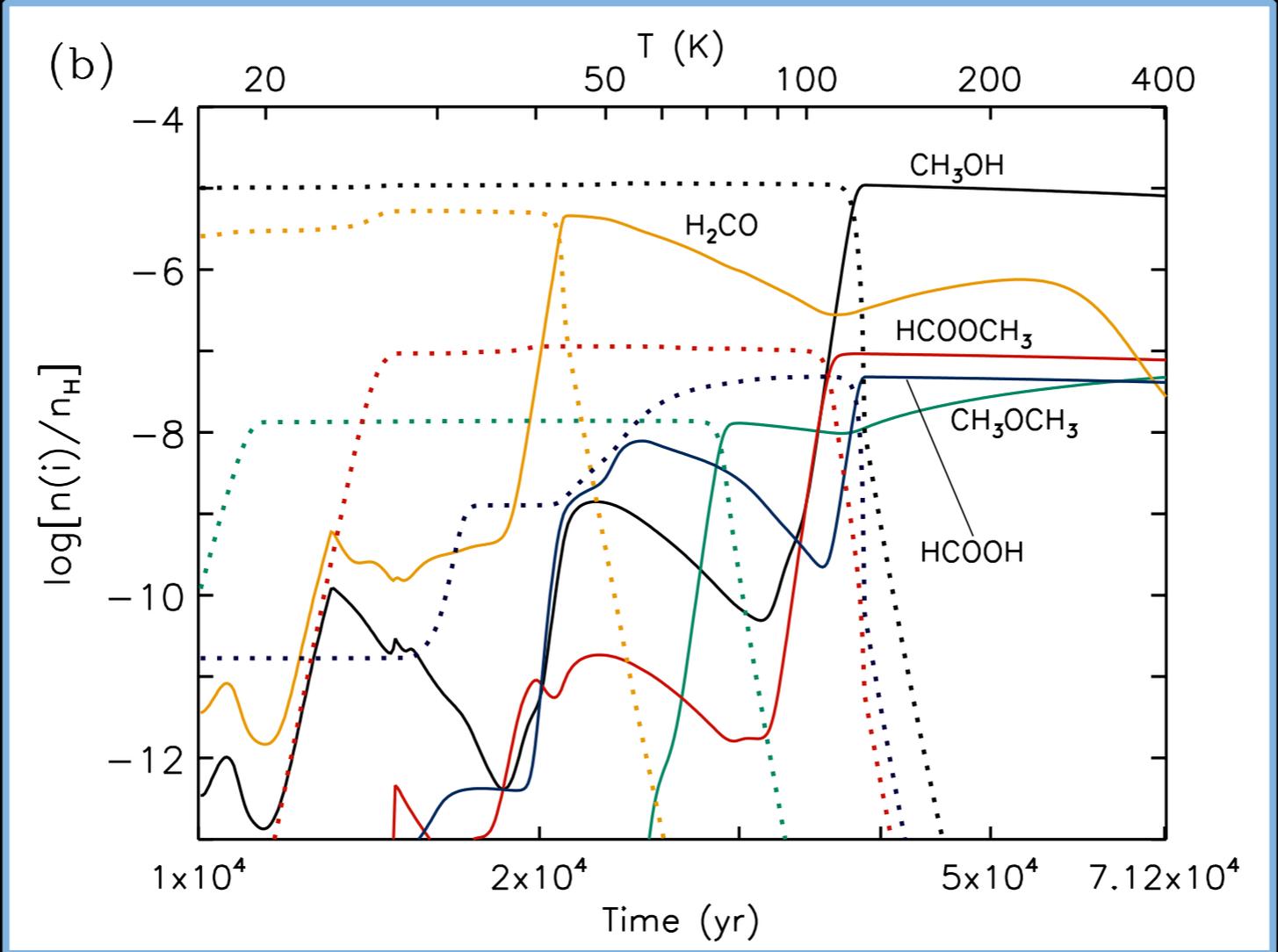
Dissociation, ionisation, ion-neutral, neutral-neutral reactions (KIDA, or UMIST chemical databases)

Gas-grain processes



Astrochemical model predictions

Observed organic molecules can be formed on interstellar ices and/or in the gas phase



Garrod (2013)

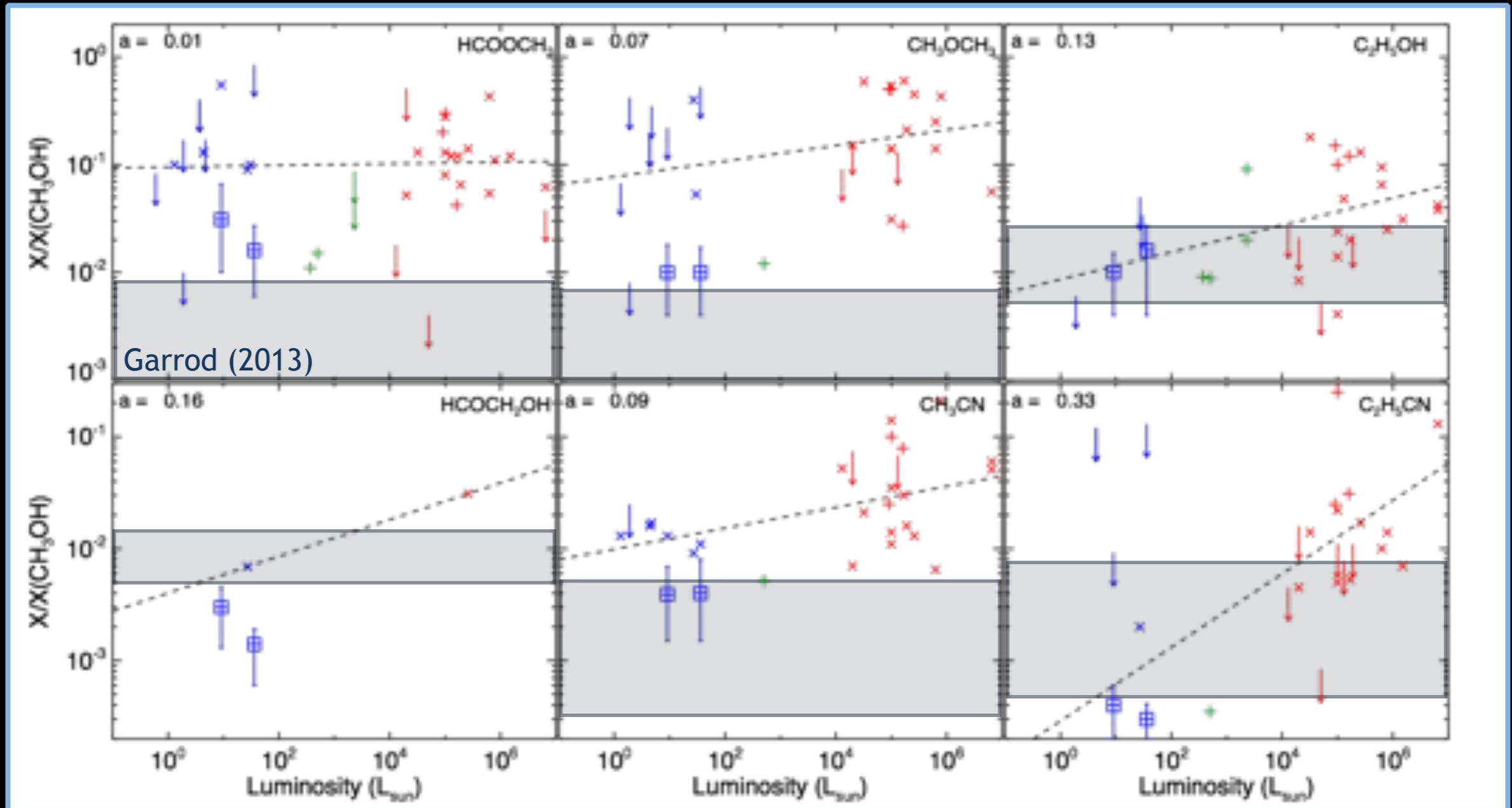
$T \sim 10 - 20 \text{ K}$
Ice formation

$20 < T < 100 \text{ K}$
Ice warm-up and reprocessing

$T > 100 \text{ K}$
Ice evaporation

Abundance underprediction of key molecules

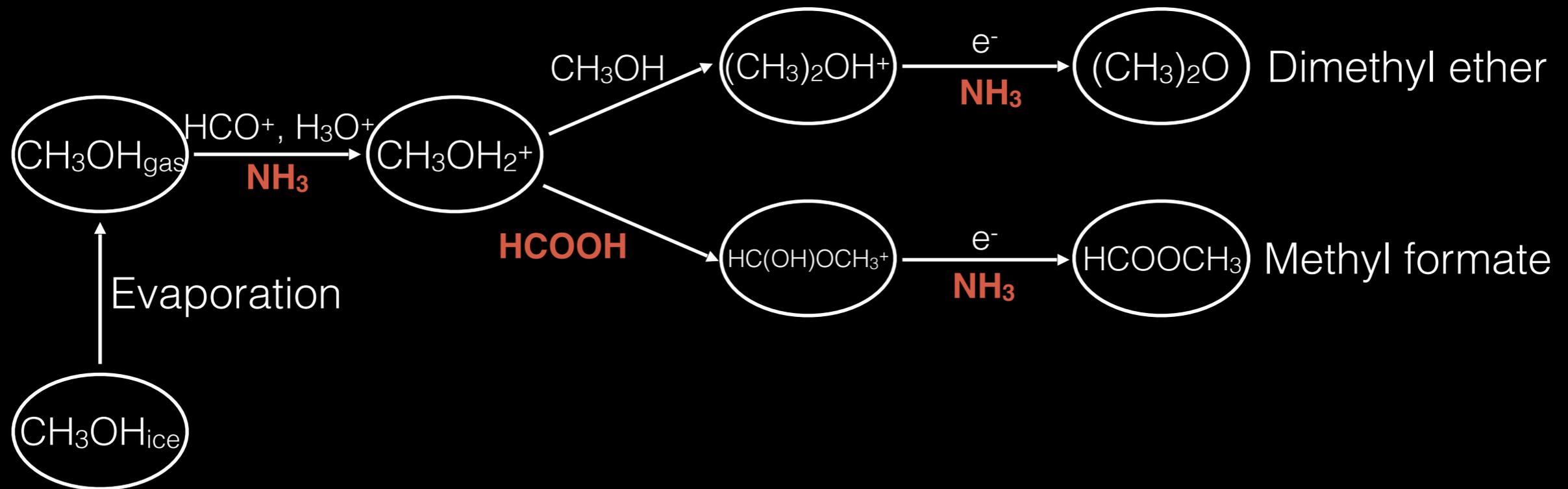
Abundance ratios of several bright organic molecules (HCOOCH_3 , CH_3OCH_3 , or CH_3CN) are still underpredicted by grain surface models



Data compiled in Taquet et al. (2015)

Impact of proton-transfer reactions

Proton-transfer reactions involving NH_3 increase gas-phase abundances of COMs by one-to-two orders of magnitude



- Highly exothermic proton transfer reactions between protonated COMs and NH_3 due to higher proton affinity of NH_3



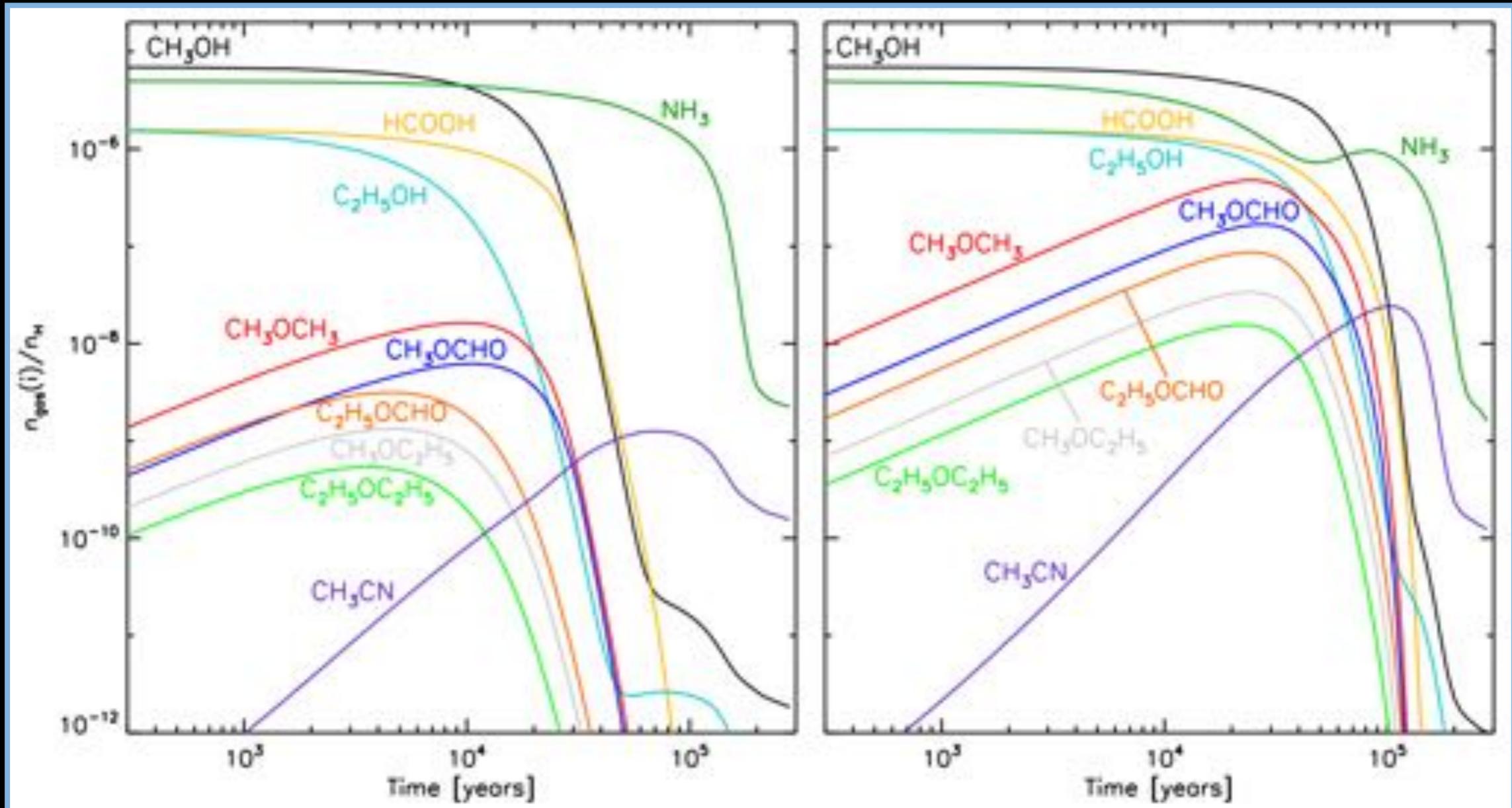
($k \approx 2 \times 10^{-9} \text{ cm}^3 \cdot \text{s}^{-1}$ for all studied reactions; see [Hemsworth et al. 1974](#))

Impact of proton-transfer reactions

Proton-transfer reactions involving NH_3 increase gas-phase abundances of COMs by one-to-two orders of magnitude

Without proton-transfer reactions

With proton-transfer reactions



$$n_{\text{H}} = 10^7 \text{ cm}^{-3}, T = 150 \text{ K}, \zeta = 3 \times 10^{-17} \text{ s}^{-1}$$

Perspectives: AstroFlt 2 project

1 - Chemical complexity pathways

What is the degree of chemical complexity reached in the ISM ?

- A) Constrain the physical and chemical processes in ices with a modelling of laboratory experiments
- B) Study the effect of new types of gas phase reactions

2 - Physical evolution and chemistry

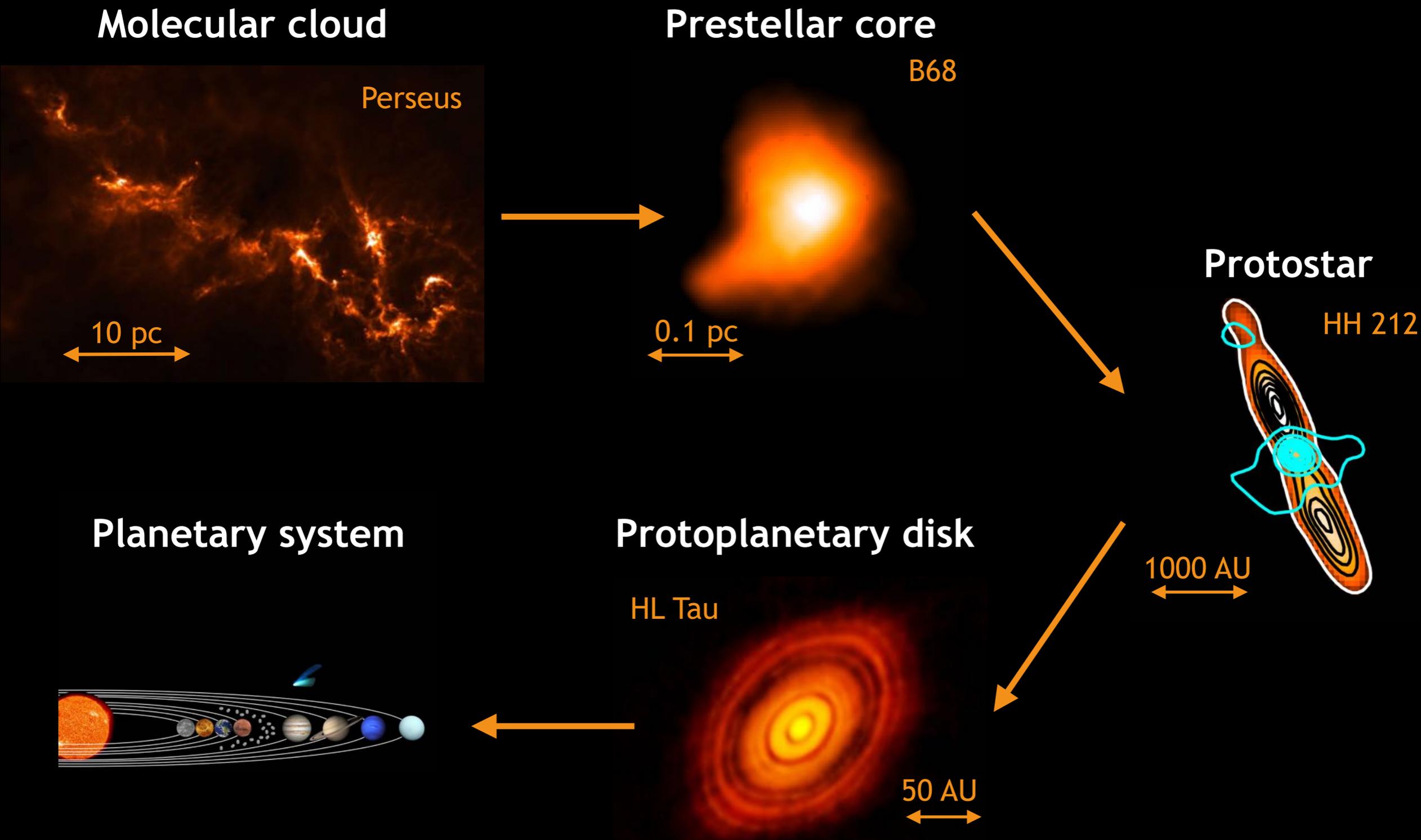
Have the cometary and meteoritic molecules an interstellar origin ?

- A) Follow the chemical evolution from dark clouds to disks with dynamical models
- B) Interpret interferometric observations of star-forming regions

Grazie !



The formation of low-mass stars



Zari et al. (2016), Roy et al. (2014),
Codella et al. (2014), ALMA et al. (2015)

Main objectives of the project

1) Chemical complexity pathways –

What is the degree of chemical complexity reached in the ISM ?

What are the chemical processes responsible for their formation and destruction ?

2) Physical evolution and chemistry –

Can interstellar molecules survive in the solar nebula / protoplanetary disk ?

Have the cometary and meteoritic molecules an interstellar origin ?

1) Chemical complexity pathways

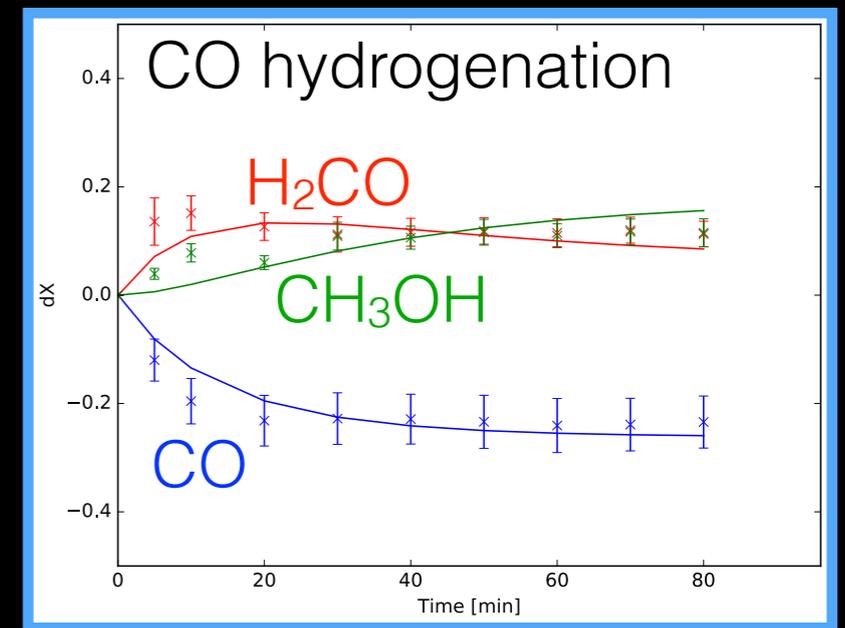
What is the degree of chemical complexity reached in the ISM ?

What are the chemical processes responsible for their formation and destruction ?

A) Constrain the physical and chemical processes in ices

→ study the results of laboratory experiments to constrain surface chemical models

Collaborations with F. Dulieu, P. Theulé, S. Ioppolo

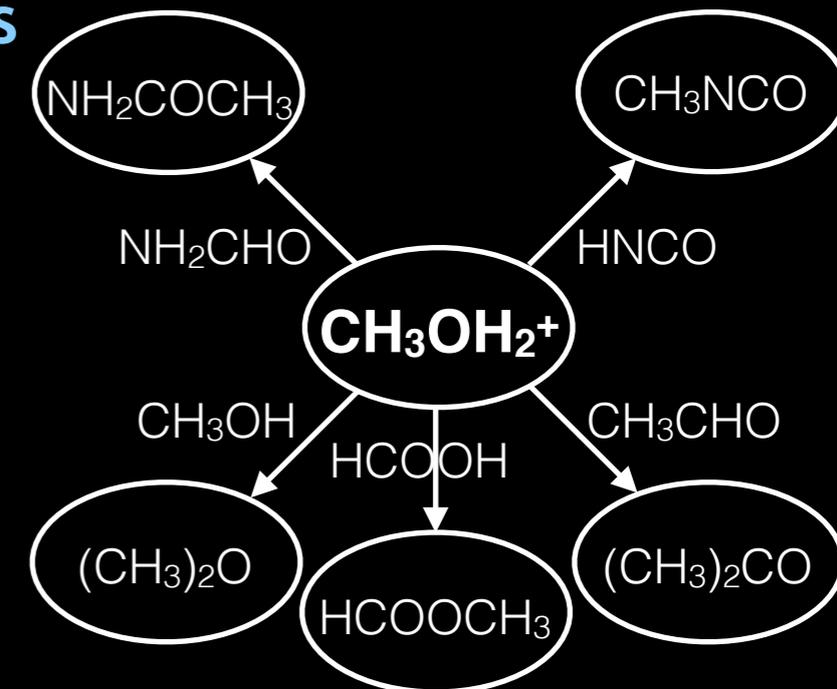


B) Study the effect of new types of gas phase reactions

→ include ion-neutral reactions in gas-phase chemical networks

→ investigate their importance for the formation of complex molecules

Collaborations with S. Charnley, N. Balucani, C. Ceccarelli



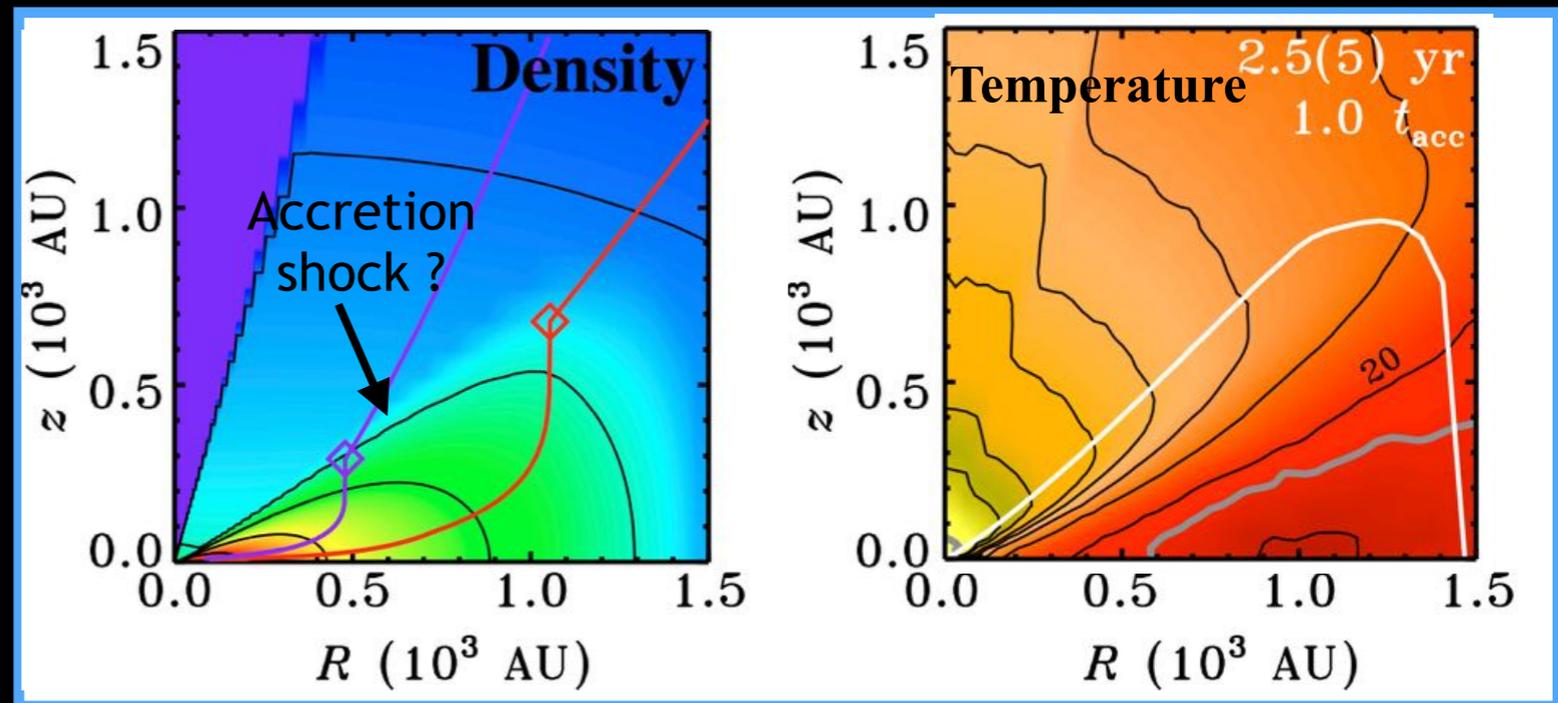
2) Physical evolution and chemistry

*Can interstellar molecules survive in the solar nebula / protoplanetary disk ?
Have the cometary and meteoritic molecules an interstellar origin ?*

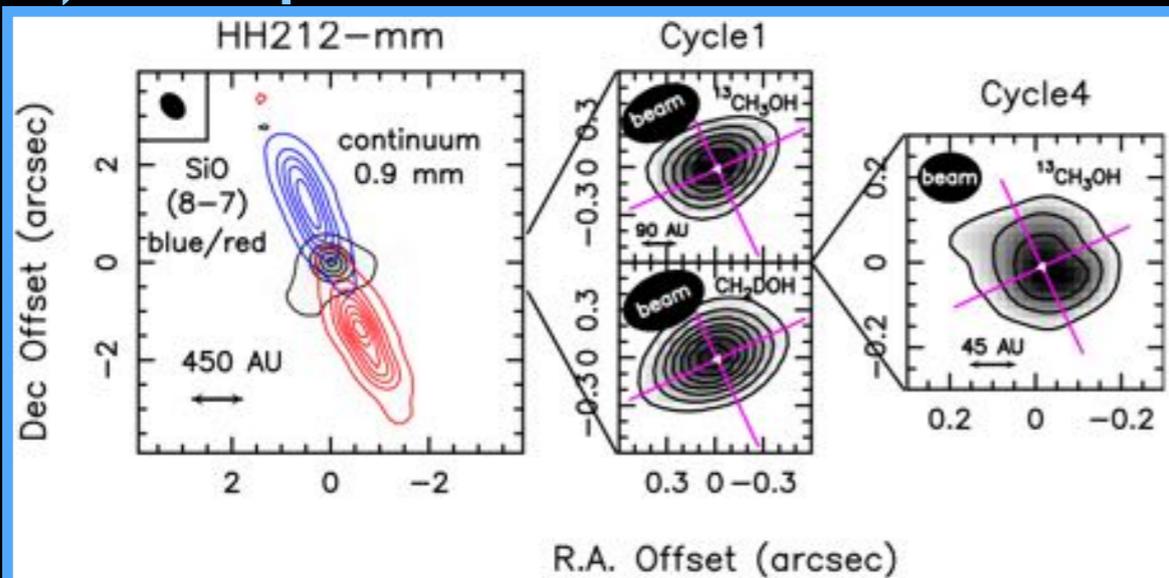
A) Follow the chemical evolution from dark clouds to disks

→ apply astrochemical model to 2D dynamic model and shock model

Collaborations with D. Harsono, A. Gusdorf, E. van Dishoeck



B) Interpret interferometric observations of star-forming regions



→ comparison with ALMA and NOEMA observations carried out in Arcetri

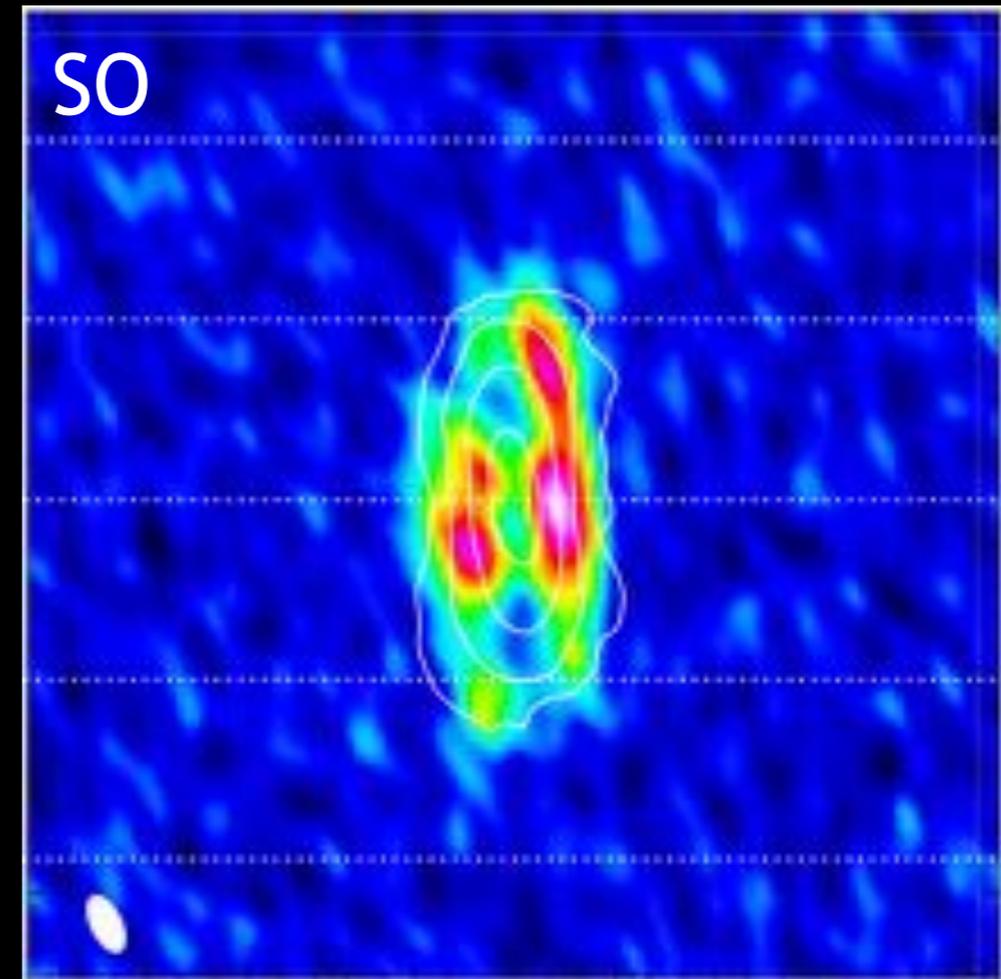
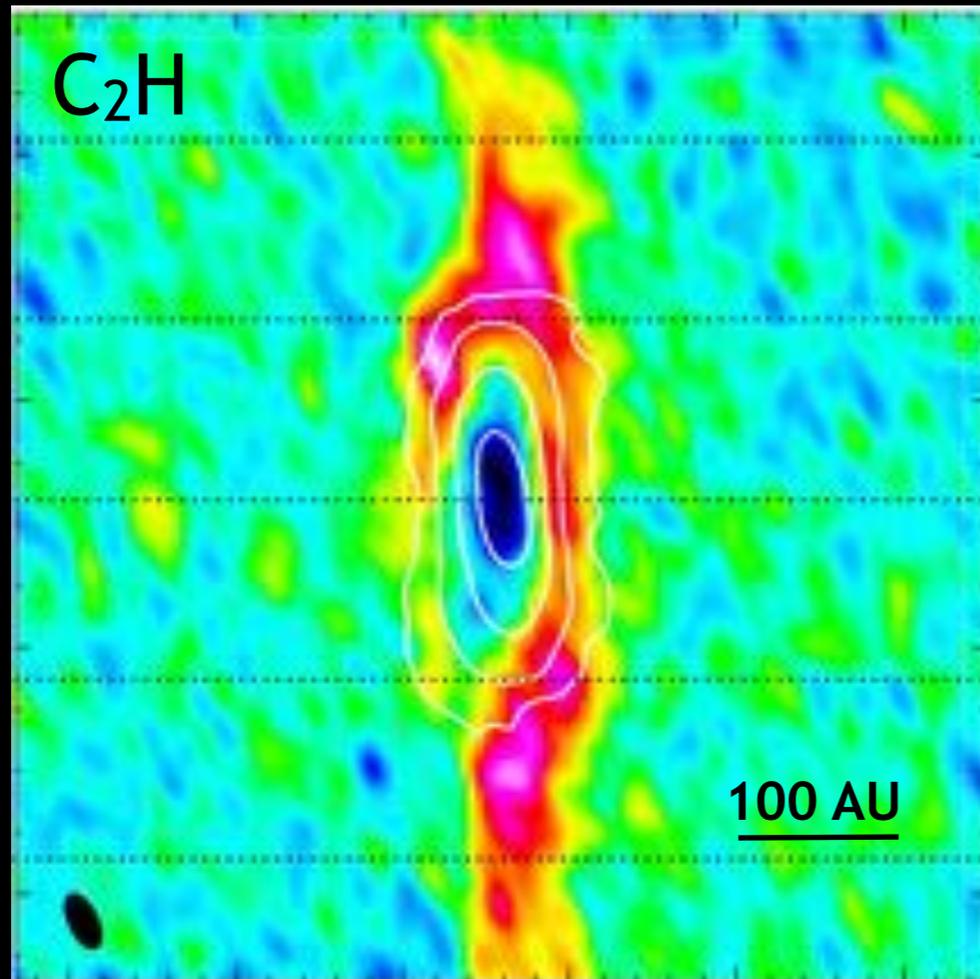
Collaborations with star formation group in Arcetri + C. Ceccarelli, E. van Dishoeck, ...

Bianchi et al. (2017, subm.)

Physical evolution and chemistry

ALMA now allows us to zoom in the inner 100 AU around protostars and show that the molecular emission strongly evolves near the protostar

→ evidence for powerful physical processes, such as accretion shock ?



Sakai et al. (2017)

GRAINOBLE: a multiphase astrochemical model

A multiphase model distinguish chemically active ice layers and more inert ice bulks has been developed since my PhD
(Taquet et al. 2012, 2013, 2014, 2016)

