

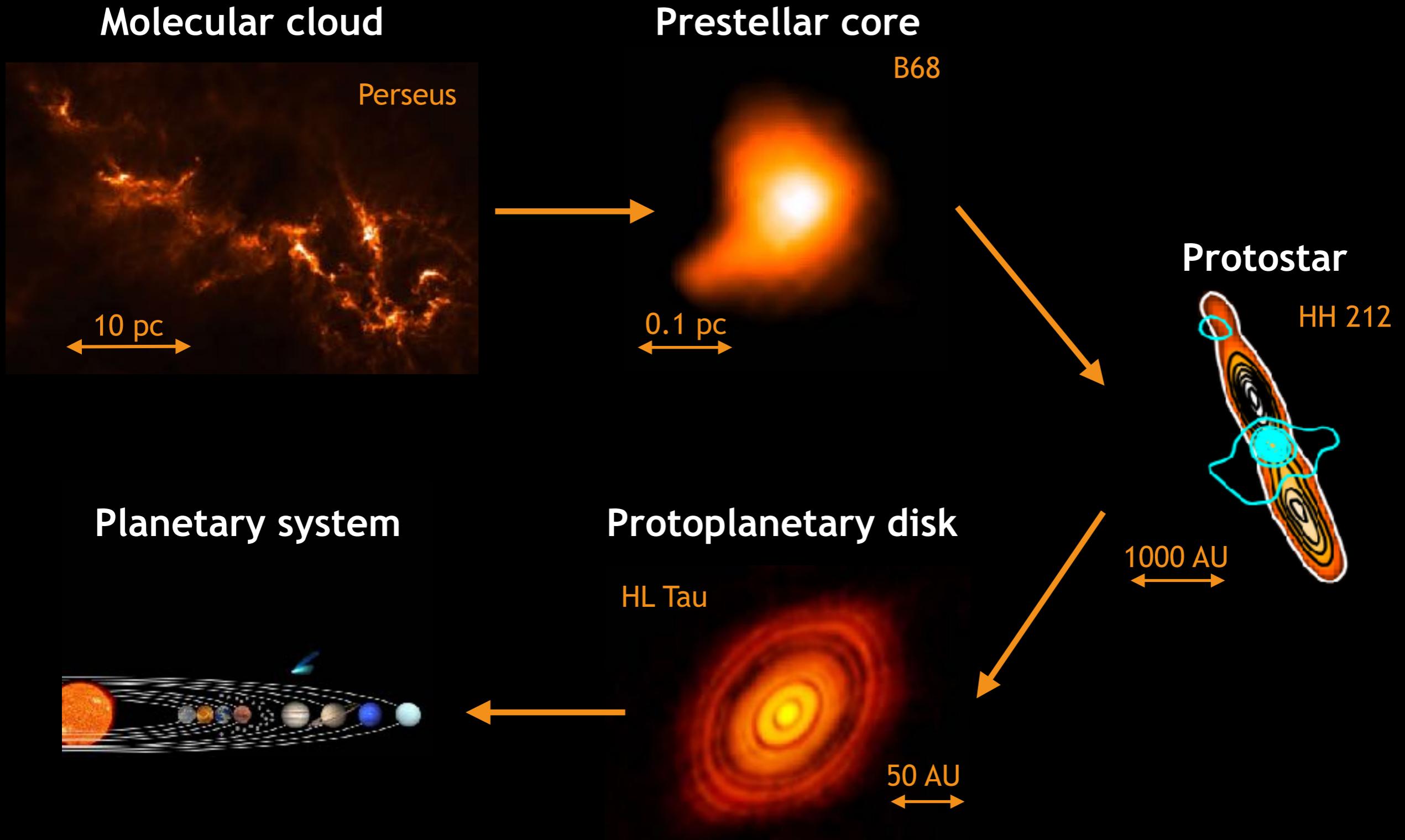
# PROSPECTS: Prebiotic mOlecules from SPacE to ComeTS

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Osservatorio Astrofisico di Arcetri - INAF  
AstroFlt 2 Fellowship



# The formation of low-mass stars

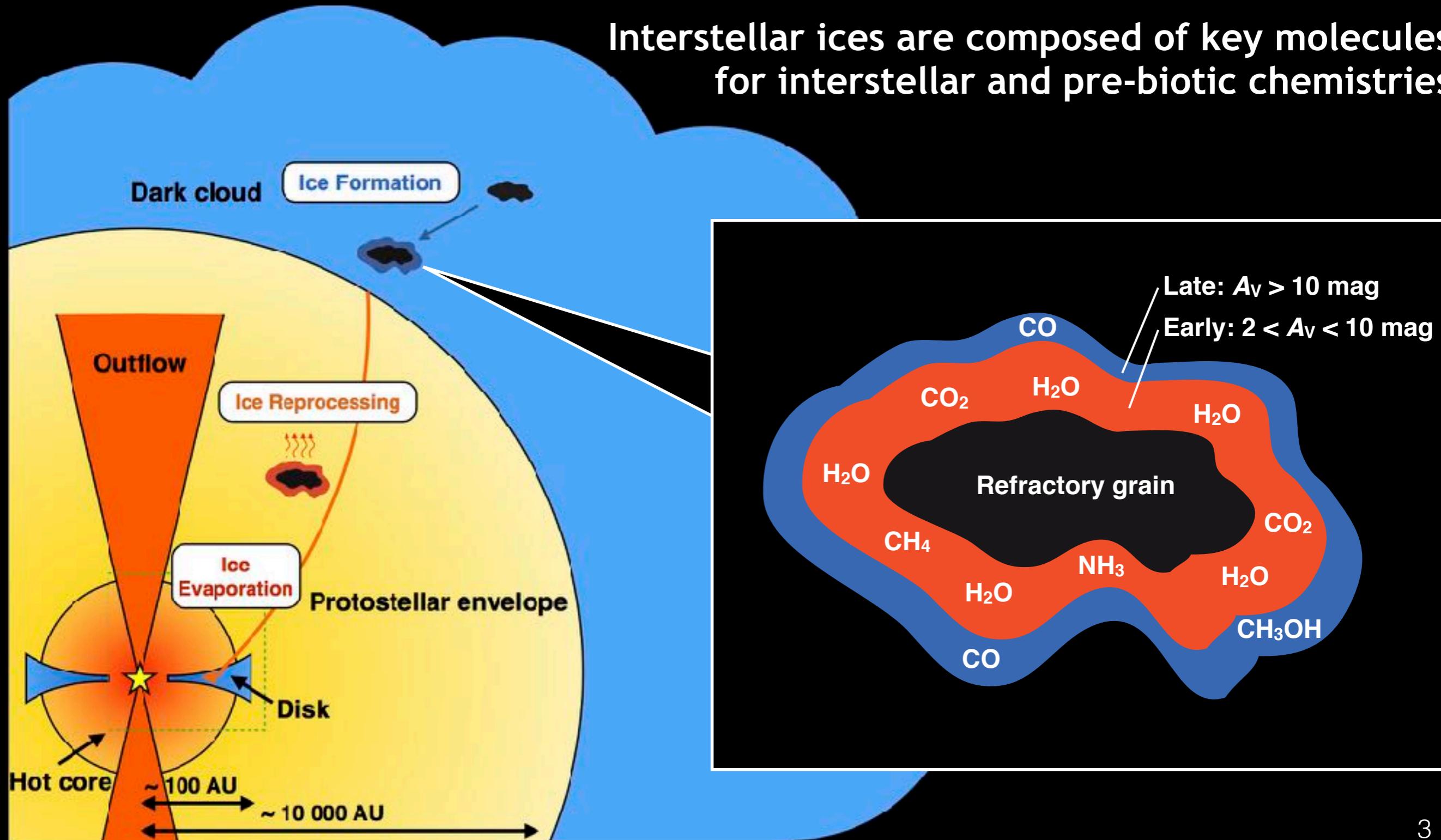


Zari et al. (2016), Roy et al. (2014),  
Codella et al. (2014), ALMA et al. (2015)

# How to observe molecules in star-forming regions ?

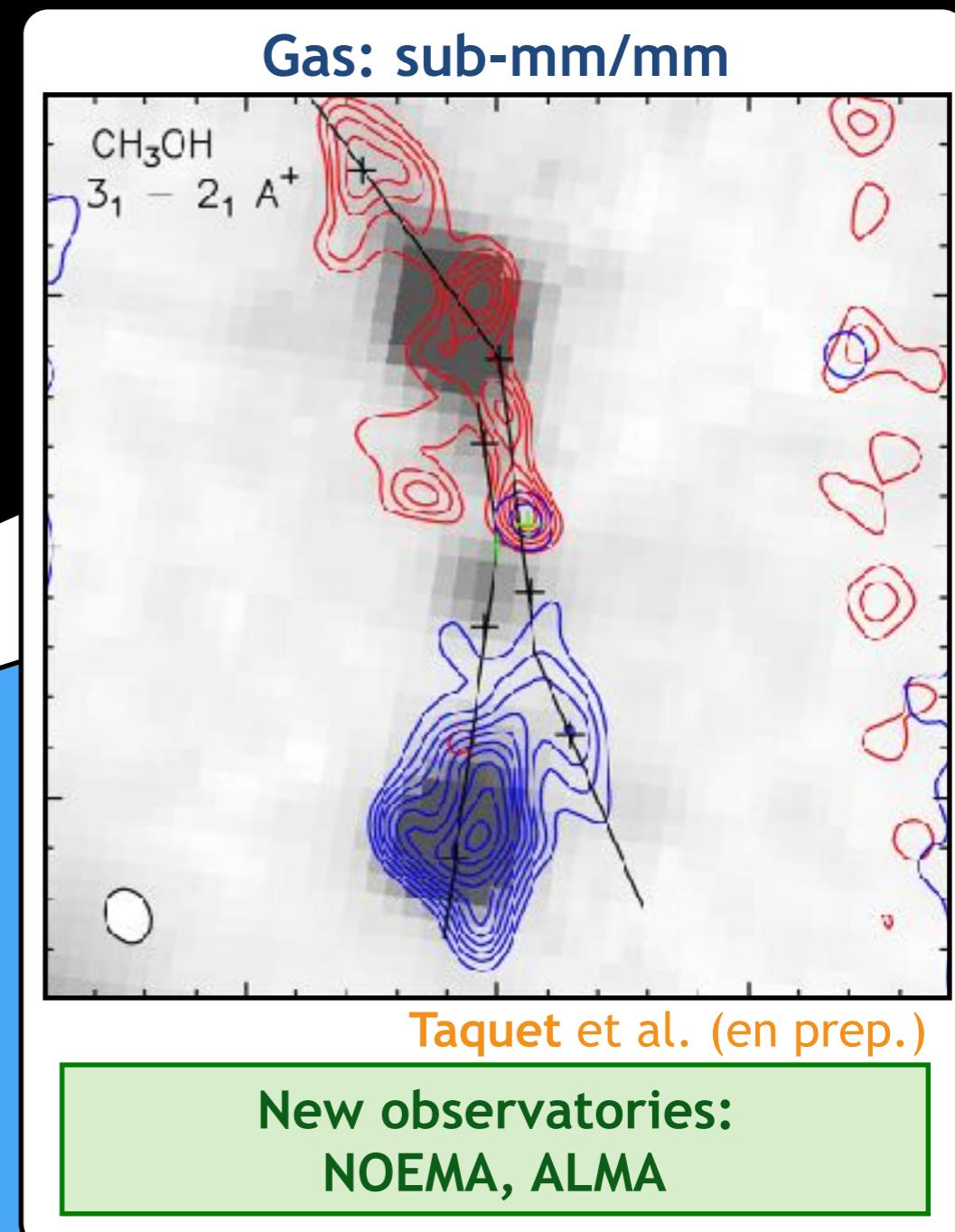
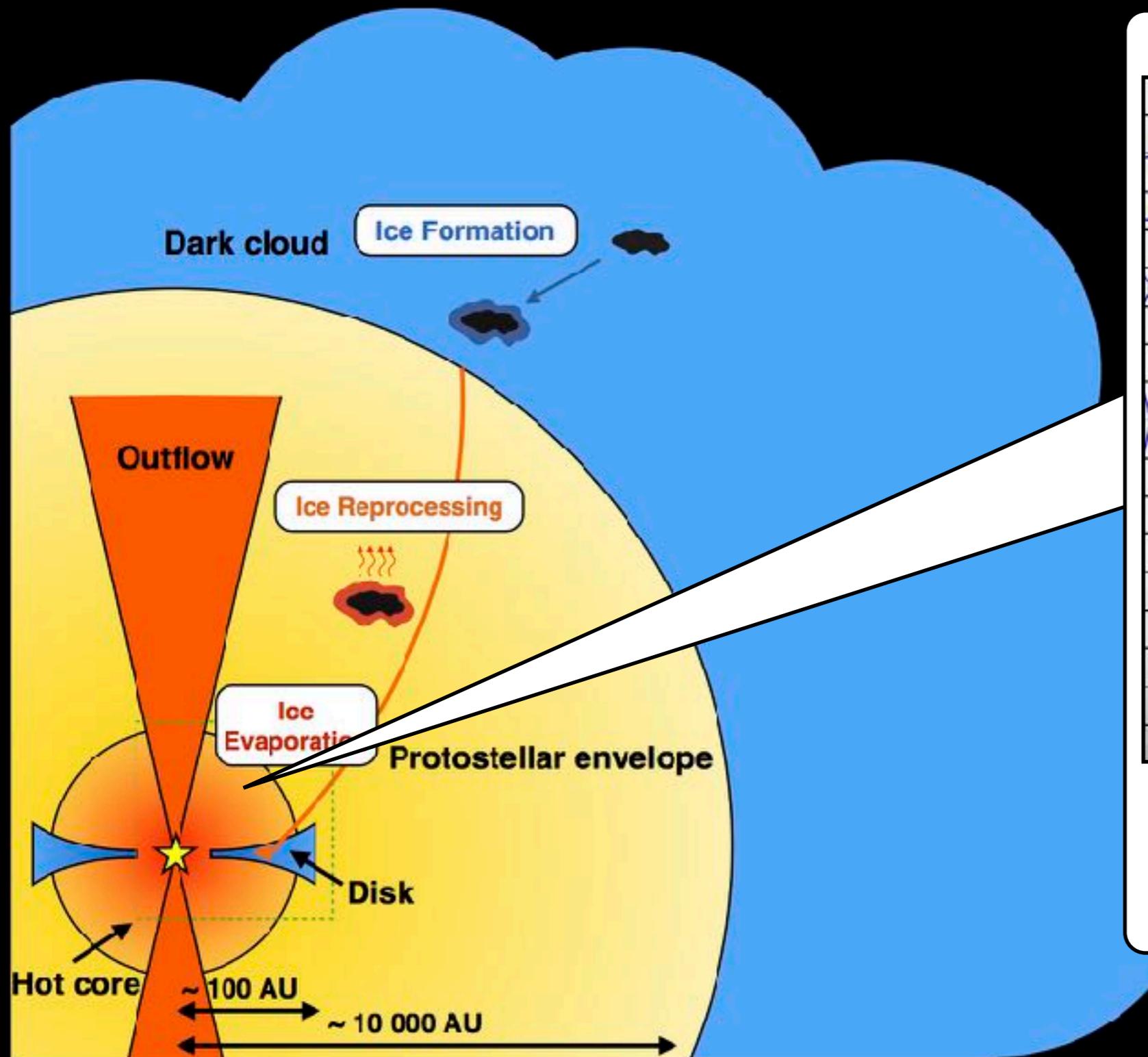
## 1. Infrared spectroscopy in absorption to study **interstellar ices**

Interstellar ices are composed of key molecules for interstellar and pre-biotic chemistries



# How to observe molecules in star-forming regions ?

## 2. Millimetric spectroscopy in emission to study the molecular gas



# How to observe molecules in star-forming regions ?

## 2. Millimetric spectroscopy in emission to study the molecular gas

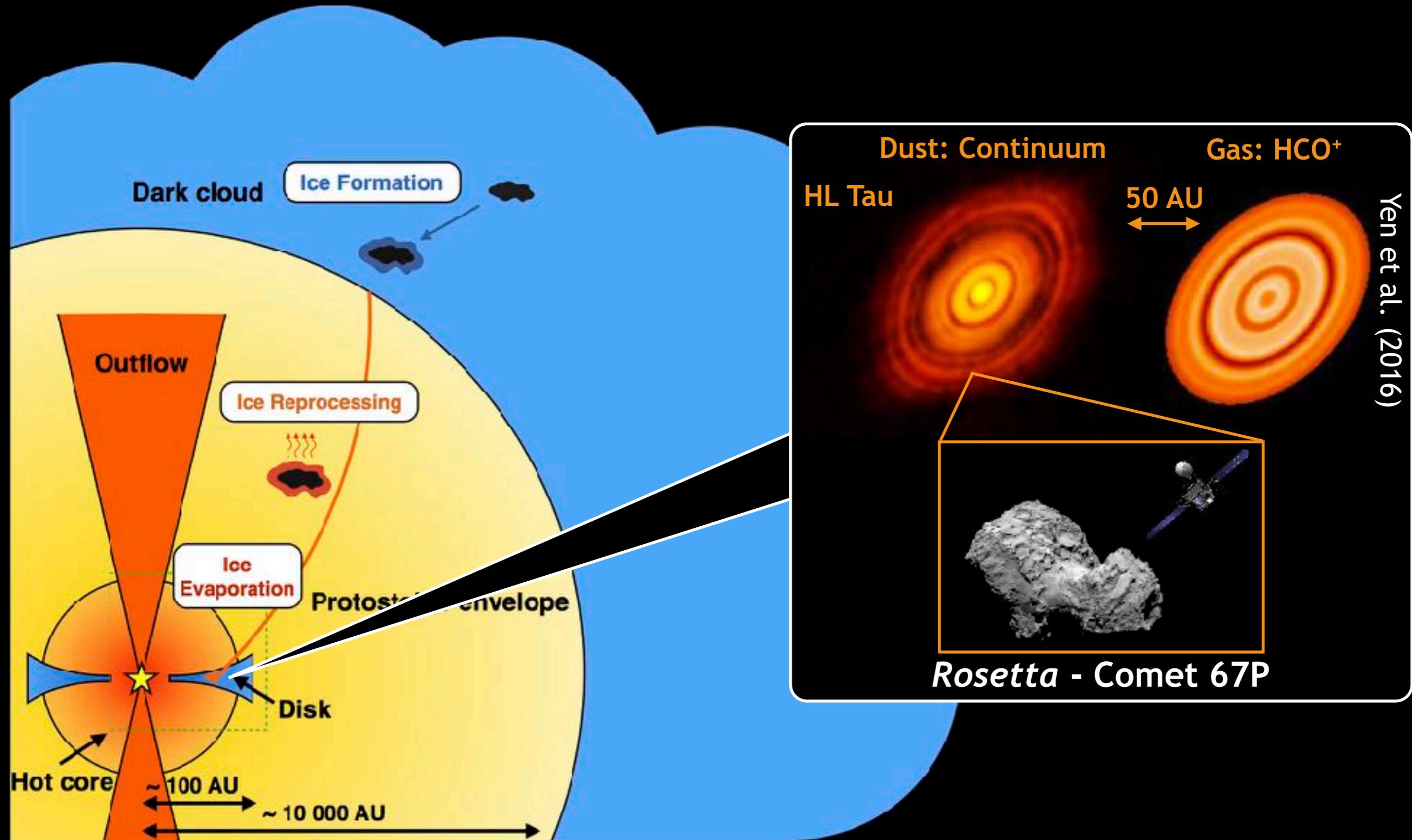
Star formation is accompanied by a chemical complexity process

- 60 of the 175 detected interstellar species are **complex organic molecules (COMs)**
- Importance for the **formation of amino- and hydroxy-acids** ?

6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	>12 atoms
C <sub>5</sub> H	C <sub>6</sub> H	CH <sub>3</sub> C <sub>3</sub> N	CH <sub>3</sub> C <sub>4</sub> H	CH <sub>3</sub> C <sub>5</sub> N	HC <sub>9</sub> N	c-C <sub>6</sub> H <sub>6</sub> *	HC <sub>11</sub> N?
i-H <sub>2</sub> C <sub>4</sub>	CH <sub>2</sub> CHCN	HC(O)OCH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> CN	(CH <sub>3</sub> ) <sub>2</sub> CO	CH <sub>3</sub> C <sub>6</sub> H	n-C <sub>3</sub> H <sub>7</sub> CN	C <sub>60</sub> *
C <sub>2</sub> H <sub>4</sub> *	CH <sub>3</sub> C <sub>2</sub> H	CH <sub>3</sub> COCH	(CH <sub>3</sub> ) <sub>2</sub> O	(CH <sub>2</sub> OH) <sub>2</sub>	C <sub>2</sub> H <sub>5</sub> OCHO	i-C <sub>3</sub> H <sub>7</sub> CN	C <sub>70</sub> *
CH <sub>3</sub> CN	HC <sub>5</sub> N	C <sub>7</sub> H	CH <sub>3</sub> CH <sub>2</sub> OH	CH <sub>3</sub> CH <sub>2</sub> CHO	CH <sub>3</sub> OC(O)CH <sub>3</sub>	C <sub>2</sub> H <sub>5</sub> OCH <sub>3</sub> ?	C <sub>60</sub> **
CH <sub>3</sub> NC	CH <sub>3</sub> CHO	C <sub>6</sub> H <sub>2</sub>		HC <sub>7</sub> N	CH <sub>3</sub> CHCH <sub>2</sub> O 2016		
CH <sub>3</sub> OH	CH <sub>3</sub> NH <sub>2</sub>	CH <sub>2</sub> OHCHO		C <sub>8</sub> H			
CH <sub>3</sub> SH	c-C <sub>2</sub> H <sub>4</sub> O	i-HC <sub>6</sub> H*		CH <sub>3</sub> C(O)NH <sub>2</sub>			
HC <sub>3</sub> NH <sup>+</sup>	H <sub>2</sub> CCCHOH	CH <sub>2</sub> CHCHO (?)	C <sub>8</sub> H-				
HC <sub>2</sub> CHO	C <sub>6</sub> H-	CH <sub>2</sub> CCHCN	C <sub>3</sub> H <sub>6</sub>				
NH <sub>2</sub> CHO	CH <sub>3</sub> NCO 2015	H <sub>2</sub> NCH <sub>2</sub> CN	CH <sub>3</sub> CH <sub>2</sub> SH (?)				
C <sub>5</sub> N		CH <sub>3</sub> CHNH					
i-HC <sub>1</sub> H*							
i-HC <sub>4</sub> N							
c-H <sub>2</sub> C <sub>3</sub> O							
H <sub>2</sub> CCNH (?)							
C <sub>5</sub> N-							
HNCHCN							

# How to observe molecules in star-forming regions ?

## 3. Space missions: final composition of the Solar Nebula



# How to observe molecules in star-forming regions ?

## Chemical census of a comet: → 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  
Naphthalene



THE KING OF THE ZOO  
Glycine [amino acid]



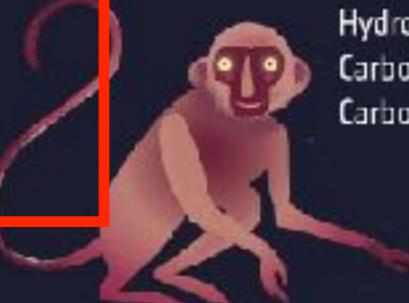
THE "MANURE SMELL" MOLECULES  
Ammonia  
Methylamine  
Ethylamine



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  
Hydrogen sulphide  
Carbonyl sulphide  
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



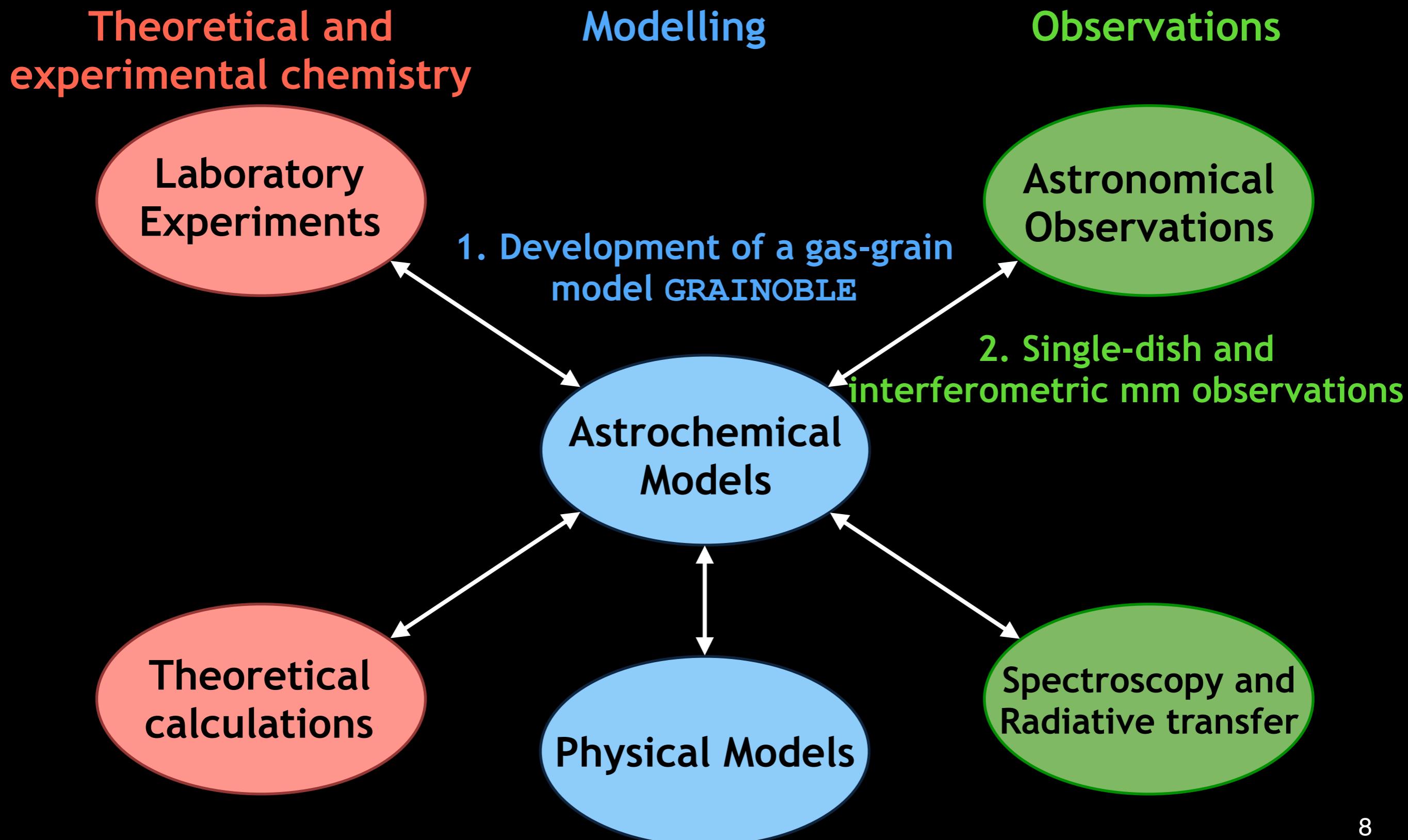
THE BEAUTIFUL AND SOLITARY  
Argon  
Krypton  
Xenon



THE "EXOTIC" MOLECULES  
Formic acid  
Acetic acid  
Acetaldehyde  
Ethylenglycol  
Propylenglycol  
Butanamide



# Expertises in Astrochemistry

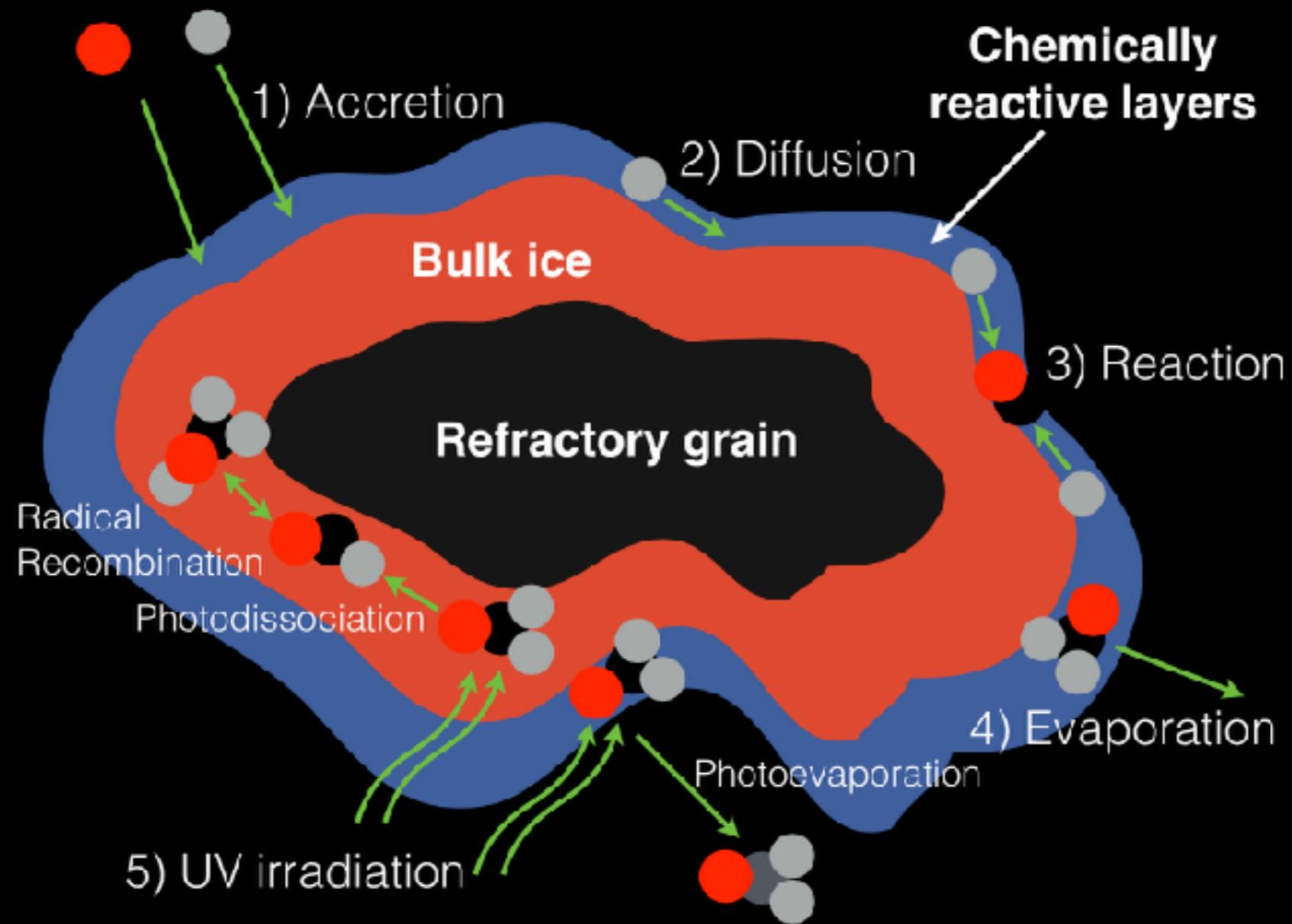


# Gas-grain astrochemical models

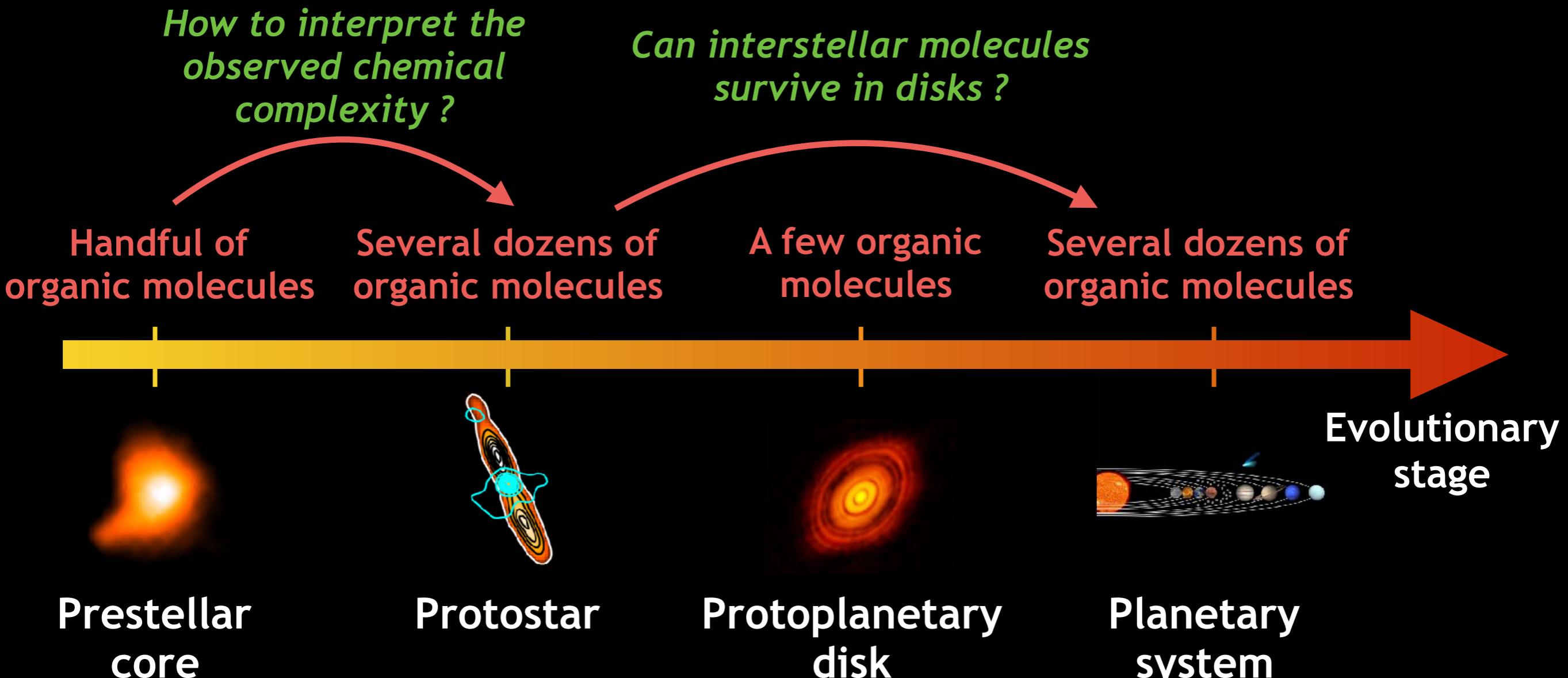
## Gas phase chemistry

Dissociation, ionisation, ion-neutral, neutral-neutral reactions  
(KIDA, or UMIST chemical databases)  
~ 10,000 reactions, 1,000 species

## Gas-grain processes



# Main objectives of the AstroFlt 2 project



*Have cometary (and Solar System) molecules an interstellar origin ?*

# Main objectives of the 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 **IN PROGRESS** (collaboration with F. Dulieu)
- B) Study the effect of new types of gas phase reactions  
**IN PROGRESS** (collaboration with S. Charnley)

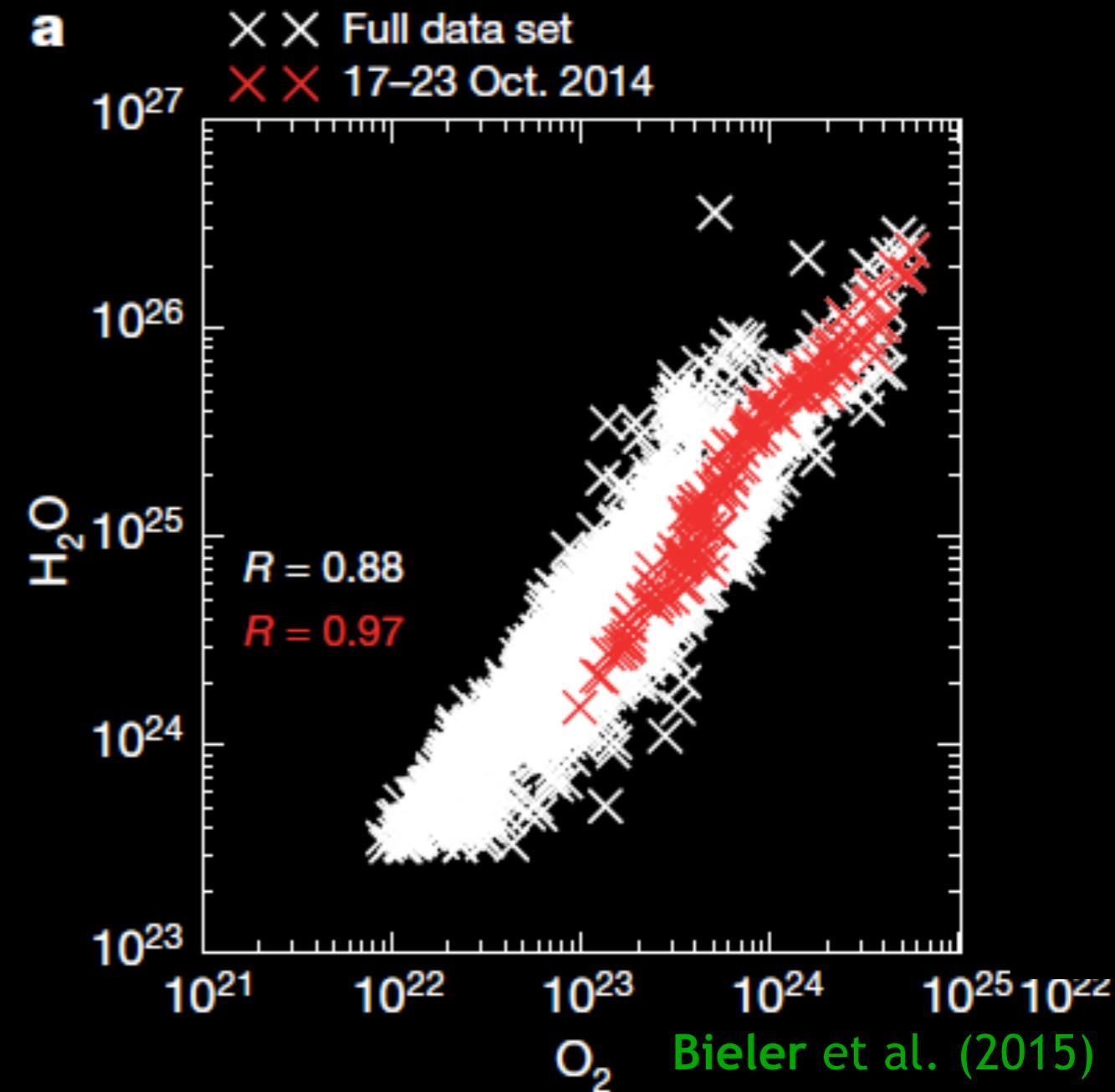
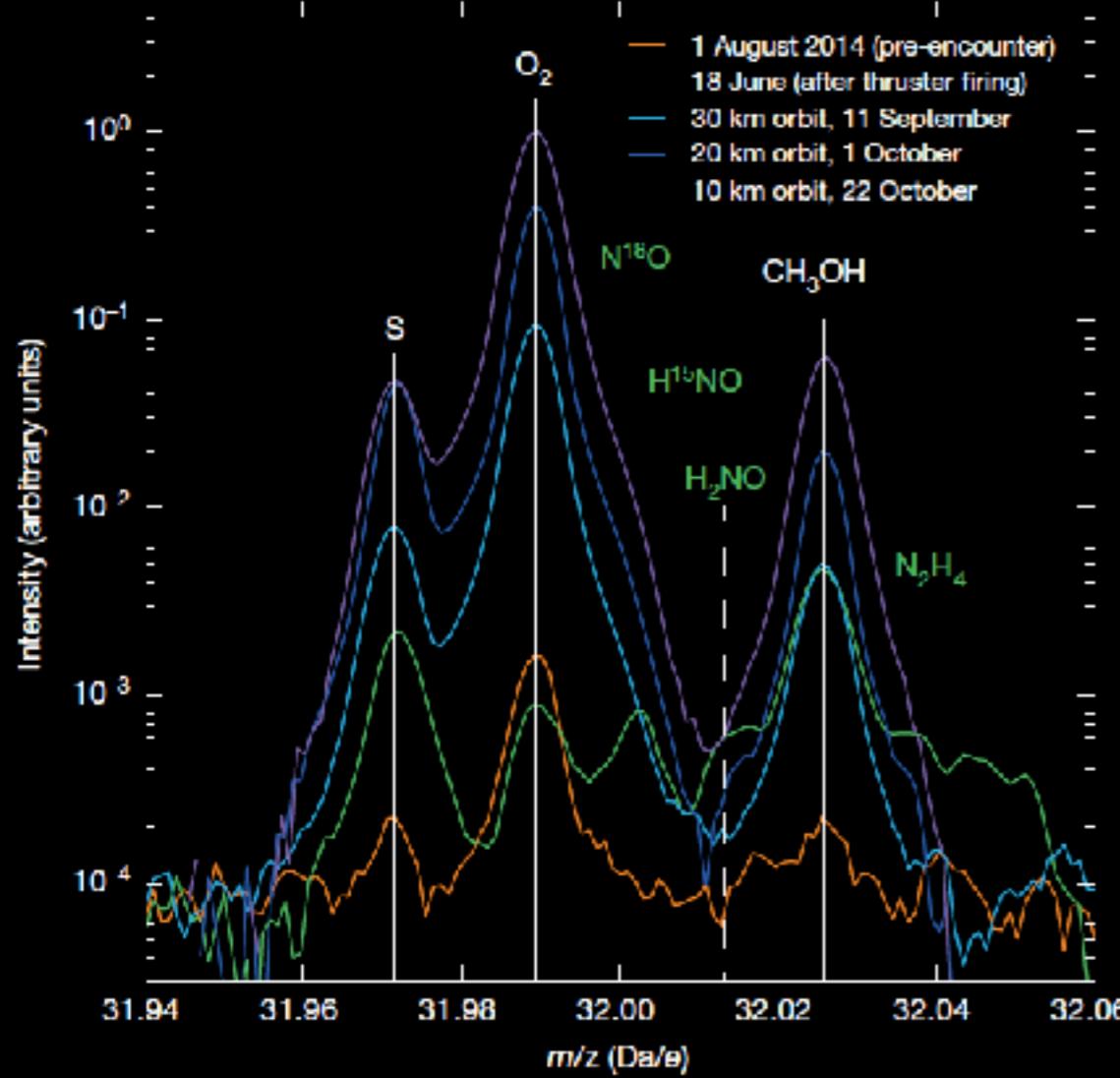
## 2 - Physical evolution and chemistry

*Have the cometary and meteoritic molecules an interstellar origin ?*

- A) Follow the chemical evolution from dark clouds to disks with dynamical models **TO BE STARTED** (collaboration with M. Padovani?)
- B) Interpret interferometric observations of star-forming regions  
**IN PROGRESS** (collaboration with C. Codella, C. Ceccarelli, ...)

# High abundance of O<sub>2</sub> in comets

First detection of O<sub>2</sub> in a comet by Rosetta:



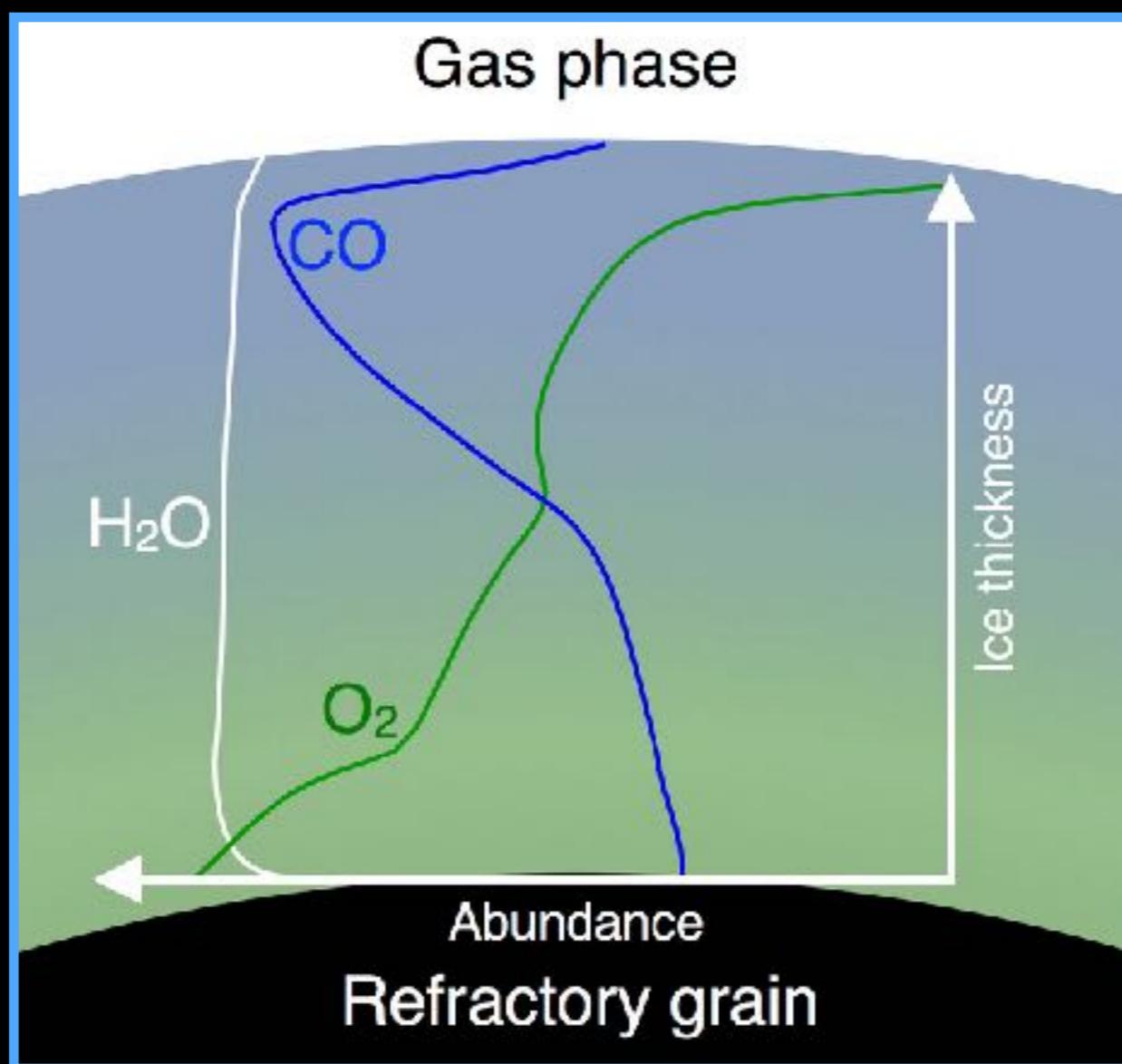
X(O<sub>2</sub>) / X(H<sub>2</sub>O) = 3.8 ± 0.9 % with strong correlation between O<sub>2</sub> and H<sub>2</sub>O

O<sub>2</sub> is elusive in space, but can O<sub>2</sub> be detected around young stars ?

# A primordial origin for cometary O<sub>2</sub>

## 1) O<sub>2</sub> formation in molecular clouds ?

- High observed abundance reproduced for “dense” and “warm” physical conditions ( $n_H \sim 10^5 - 10^6 \text{ cm}^{-3}$ ;  $T \sim 20 \text{ K}$ )
- O<sub>2</sub> trapped in water ice → in agreement with *Rosetta* observations



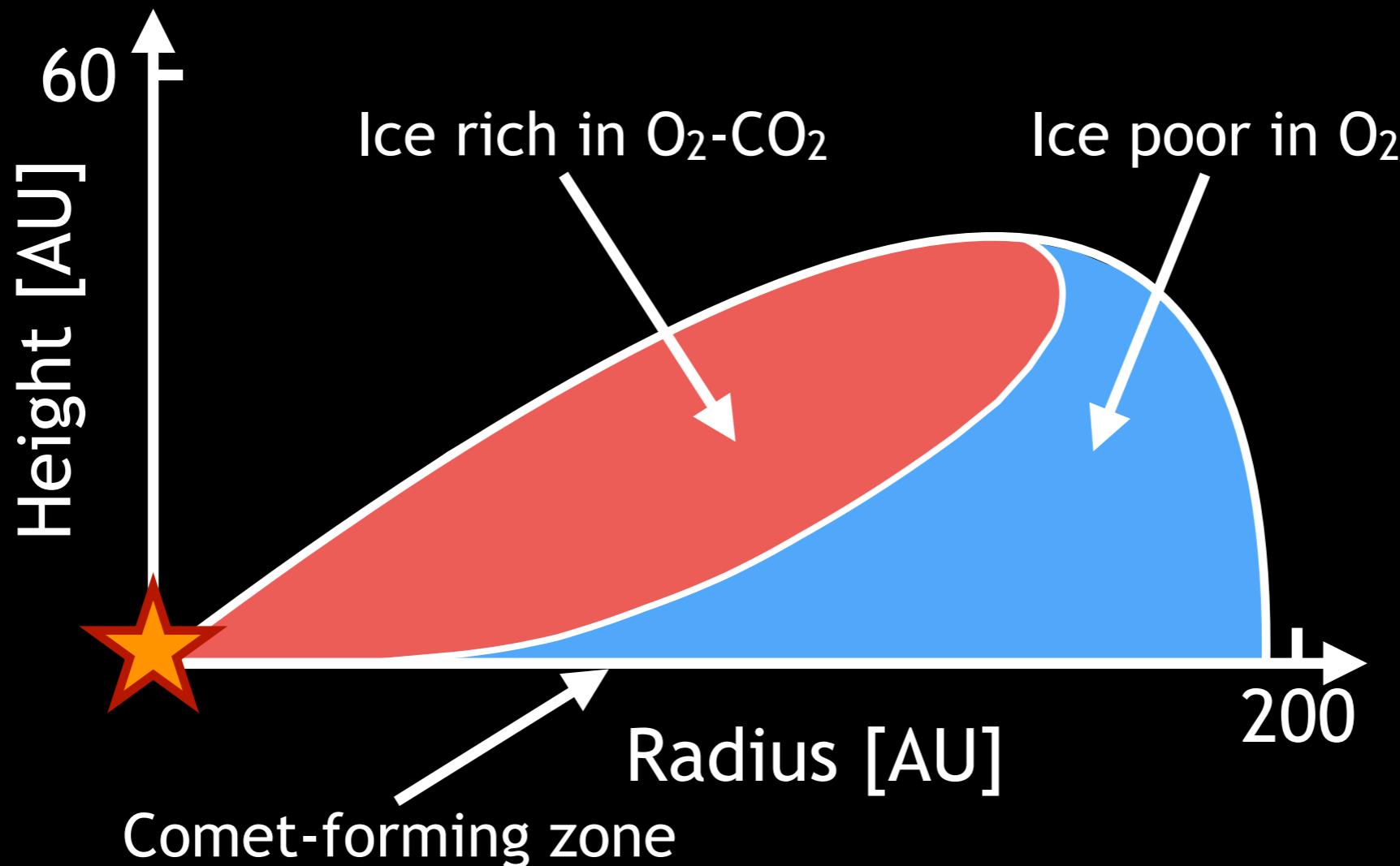
# A primordial origin for cometary O<sub>2</sub>

2) O<sub>2</sub> formation during protostellar collapse? NO

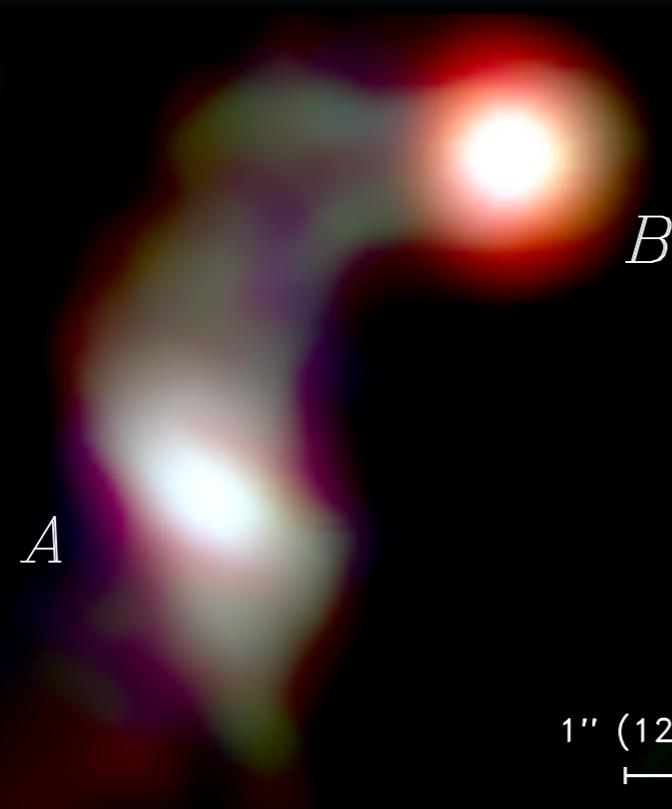
3) O<sub>2</sub> formation in protoplanetary disks? NO

- O<sub>2</sub> formation with CO<sub>2</sub> in external disk layers

→ **Non efficient formation in cometary formation zones**



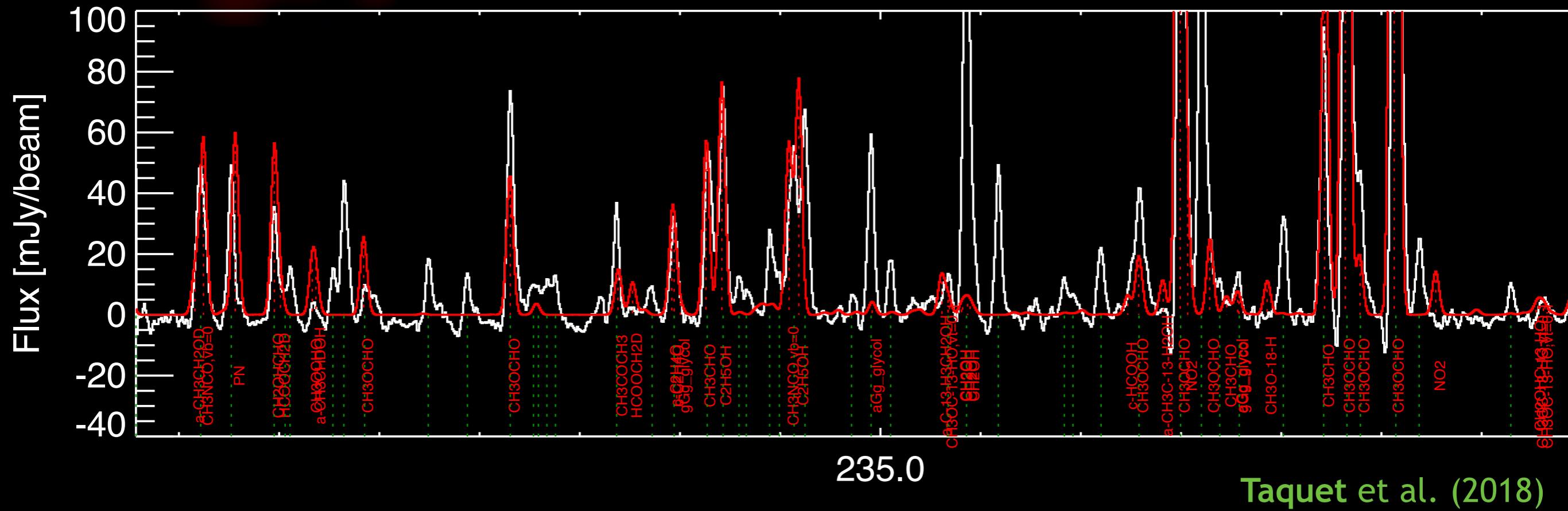
# A deep search of $^{16}\text{O}^{18}\text{O}$ towards IRAS 16293



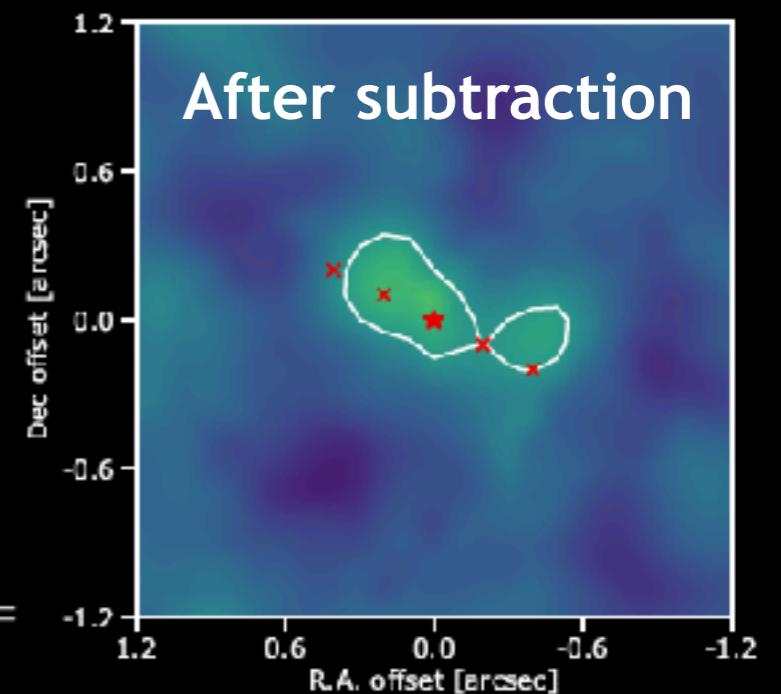
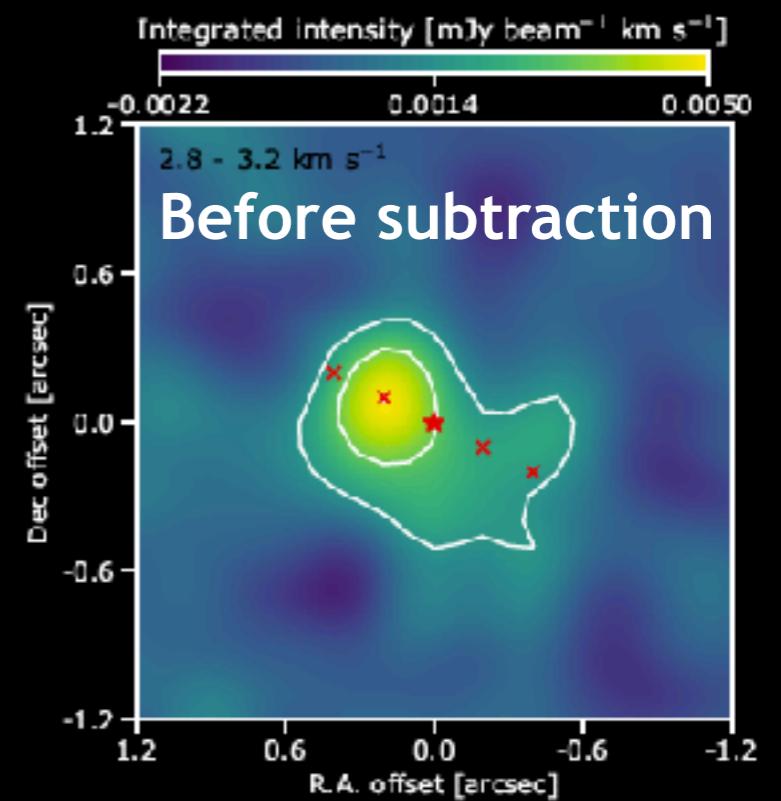
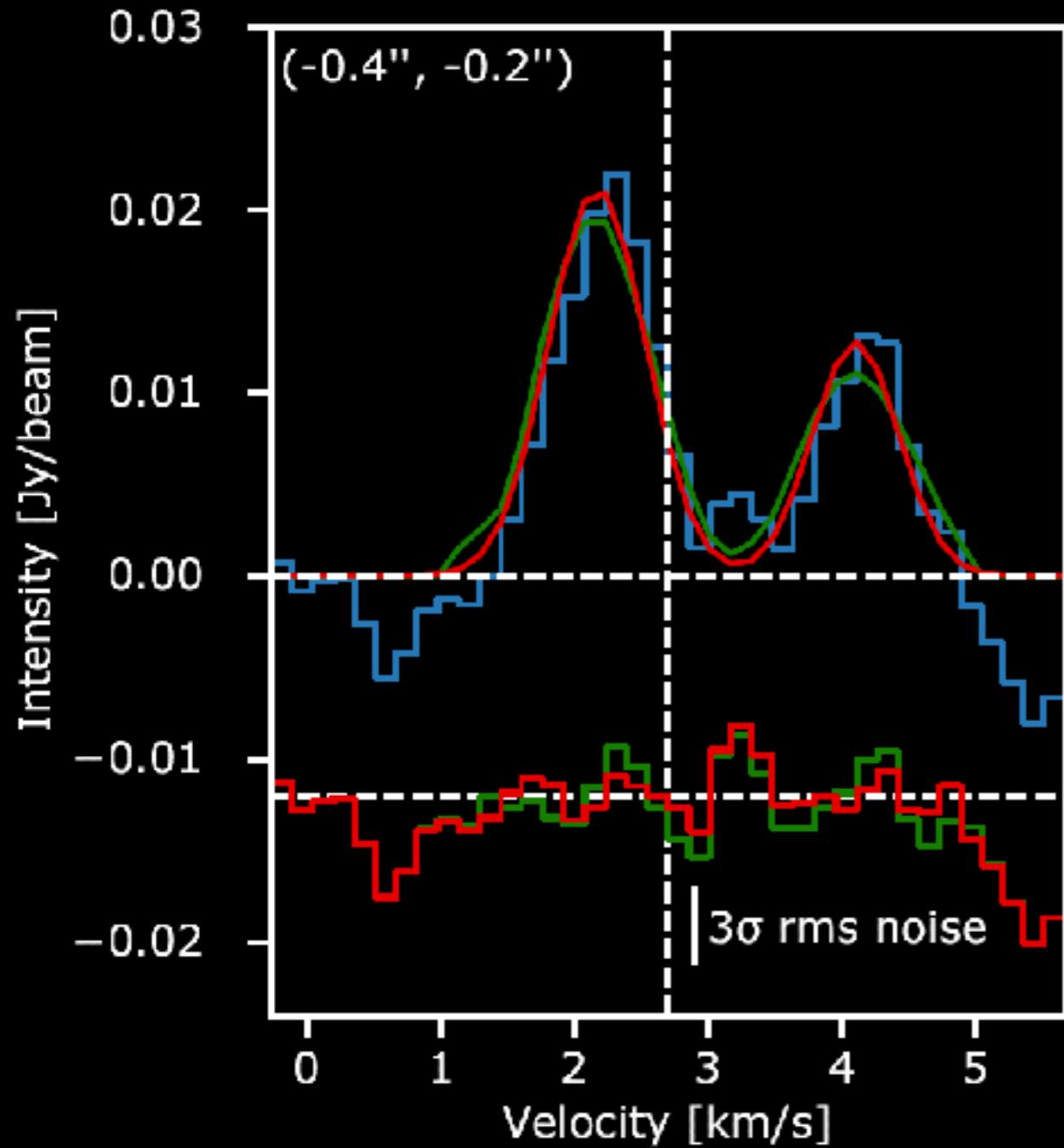
ALMA observations of the  $^{16}\text{O}^{18}\text{O}$  2<sub>1</sub>-0<sub>1</sub> transition at 233.946 GHz towards IRAS 16293 located in the Ophiuchus cloud:

1'' (120 AU)

Image credit: Jørgensen et al. (2016)



# Analysis of the $^{16}\text{O}^{18}\text{O}$ transition

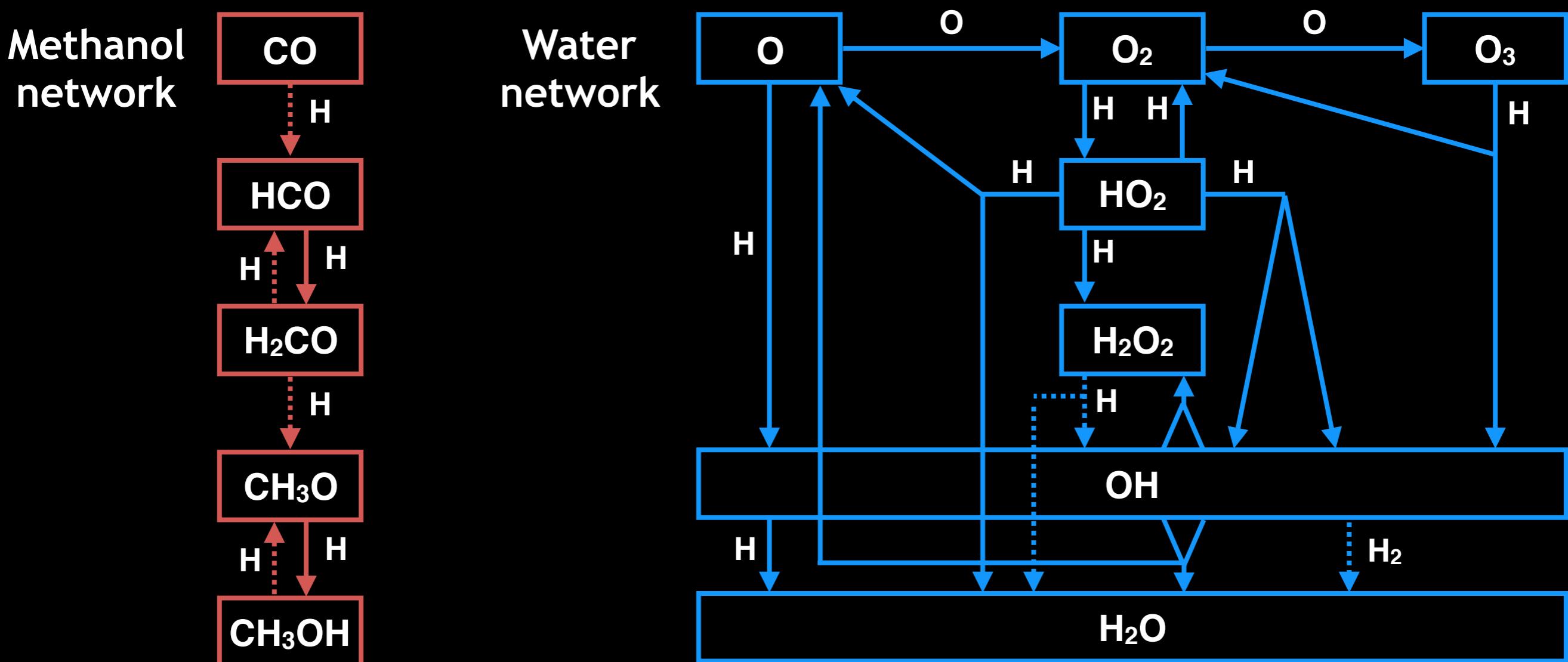


Molecule	$N$ (cm $^{-2}$ )	$N/N(\text{CH}_3\text{OH})$ (%)	Comet 67P/C-G <sup>c</sup>
	IRAS 16293		
$\text{O}_2$	$\leq (4.2 - 9.0) \times 10^{19}$ $(9.9 - 21) \times 10^{19}$	$\leq 2.1 - 4.5^{\text{a}}$ $5.0 - 10.5^{\text{b}}$	5 – 15 5 – 15

# Modelling of laboratory experiments

# Constrain the physical and chemical processes in ices with a modelling of laboratory experiments focusing on cold surface chemistry:

- Validate the formalism used in interstellar models with “in-situ” data
  - Constrain key physical and chemical parameters

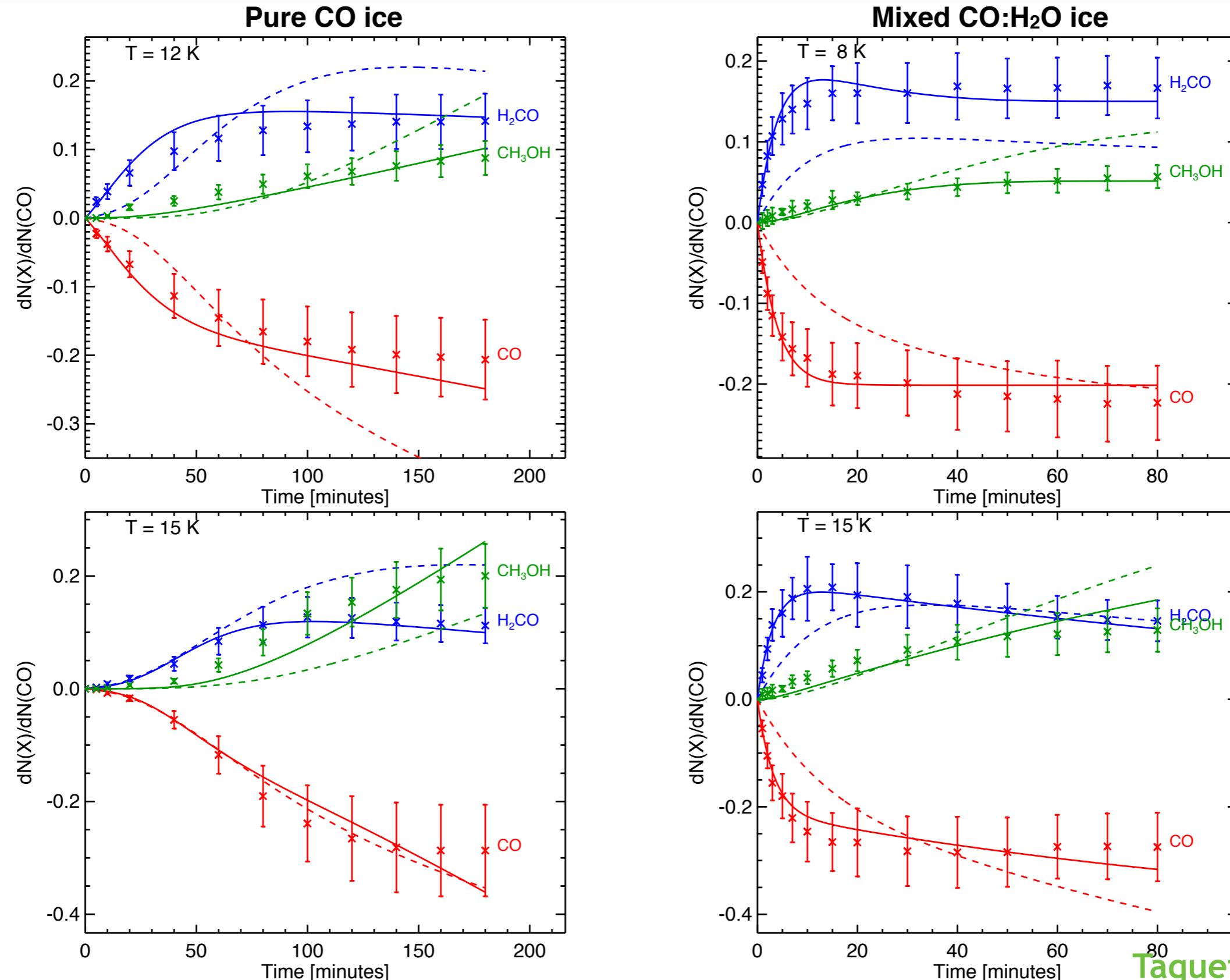


# Modelling of laboratory experiments

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Name	Experiment properties		Ice sample		Irradiation		Ref.
	Network	Temperature (K)	Species	Thickness (MLs)	Species	Flux (mol cm <sup>-2</sup> s <sup>-1</sup> )	
CO-1	CO+H	10	H <sub>2</sub> CO on H <sub>2</sub> O	1 on 10	H	1.0(+15)	H04
CO-2	CO+H	8-10-12	CO	10	H	5.0(+14)	W04
CO-3	CO+H	12-13.5-15-16.5	CO	8	H	5.0(+13)	F09
CO-4	CO+H	8-10-12-15-20	CO:H <sub>2</sub> O	6:24	H	5.0(+14)	W04
O <sub>2</sub> -1	O <sub>2</sub>	12-15-18-20-23-28	O <sub>2</sub>	30	H	5.0(+13)	I08
O <sub>2</sub> -2	O <sub>2</sub>	12-15-18-20-23-25-26-27	O <sub>2</sub>	35	H	2.5(+13)	I10
O <sub>2</sub> -3	O <sub>2</sub>	25	O <sub>2</sub>	1-3-5-8-12-25	H	2.5(+13)	I08
CO:O <sub>2</sub> -1	CO+O <sub>2</sub>	15-20	CO:O <sub>2</sub>	28:7	H	2.5(+13)	I11
CO:O <sub>2</sub> -2	CO+O <sub>2</sub>	15-20	CO:O <sub>2</sub>	14:14	H	2.5(+13)	I11
CO:O <sub>2</sub> -3	CO + O <sub>2</sub>	15-20	CO:O <sub>2</sub>	7:28	H	2.5(+13)	I11

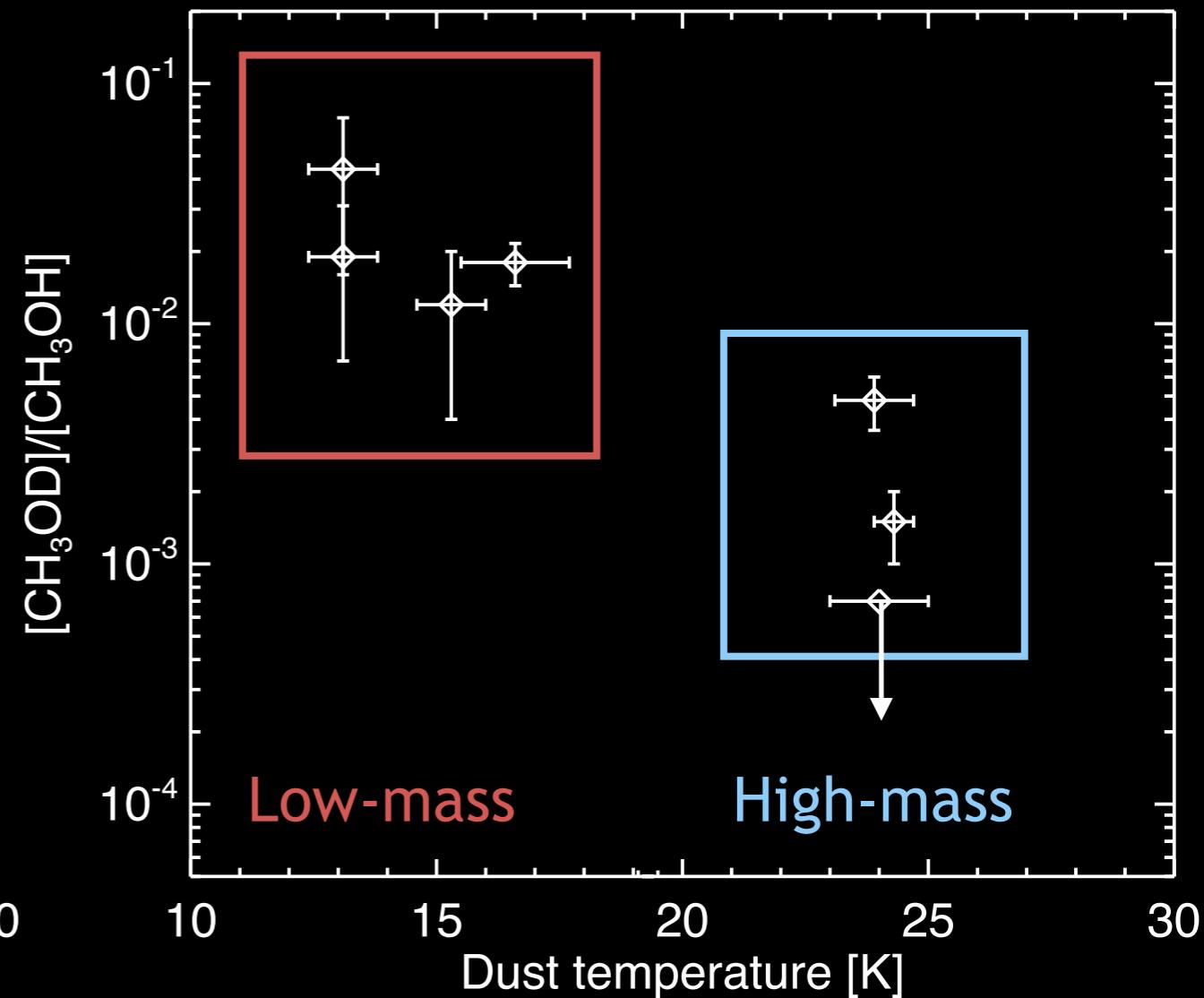
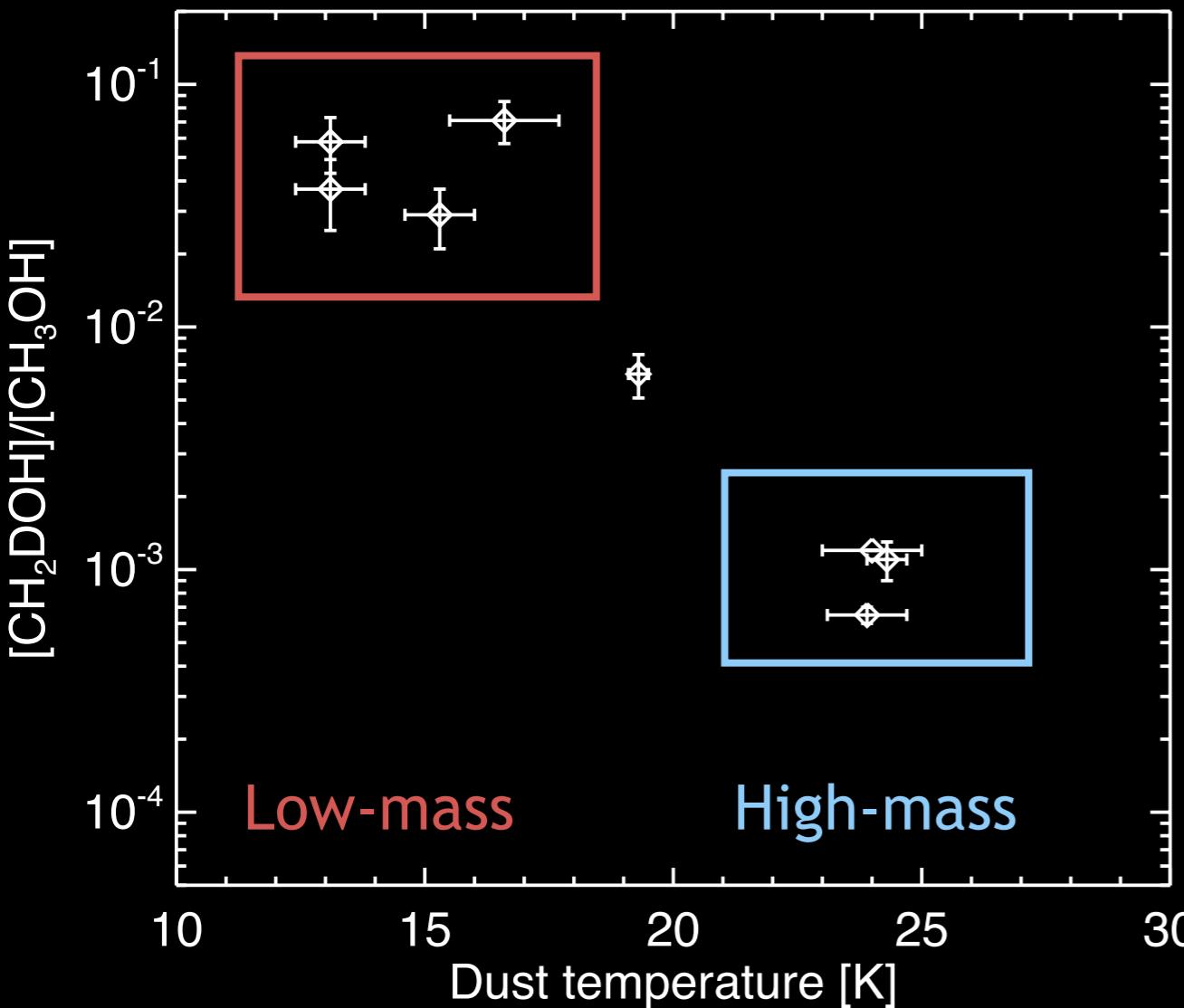
# Modelling of laboratory experiments



# Methanol deuteration from low-mass to high-mass hot cores

Methanol deuteration observed towards hot cores mostly regulated by the temperature of the progenitor cloud

+ Other processes (time, gas phase chemistry) at work ?

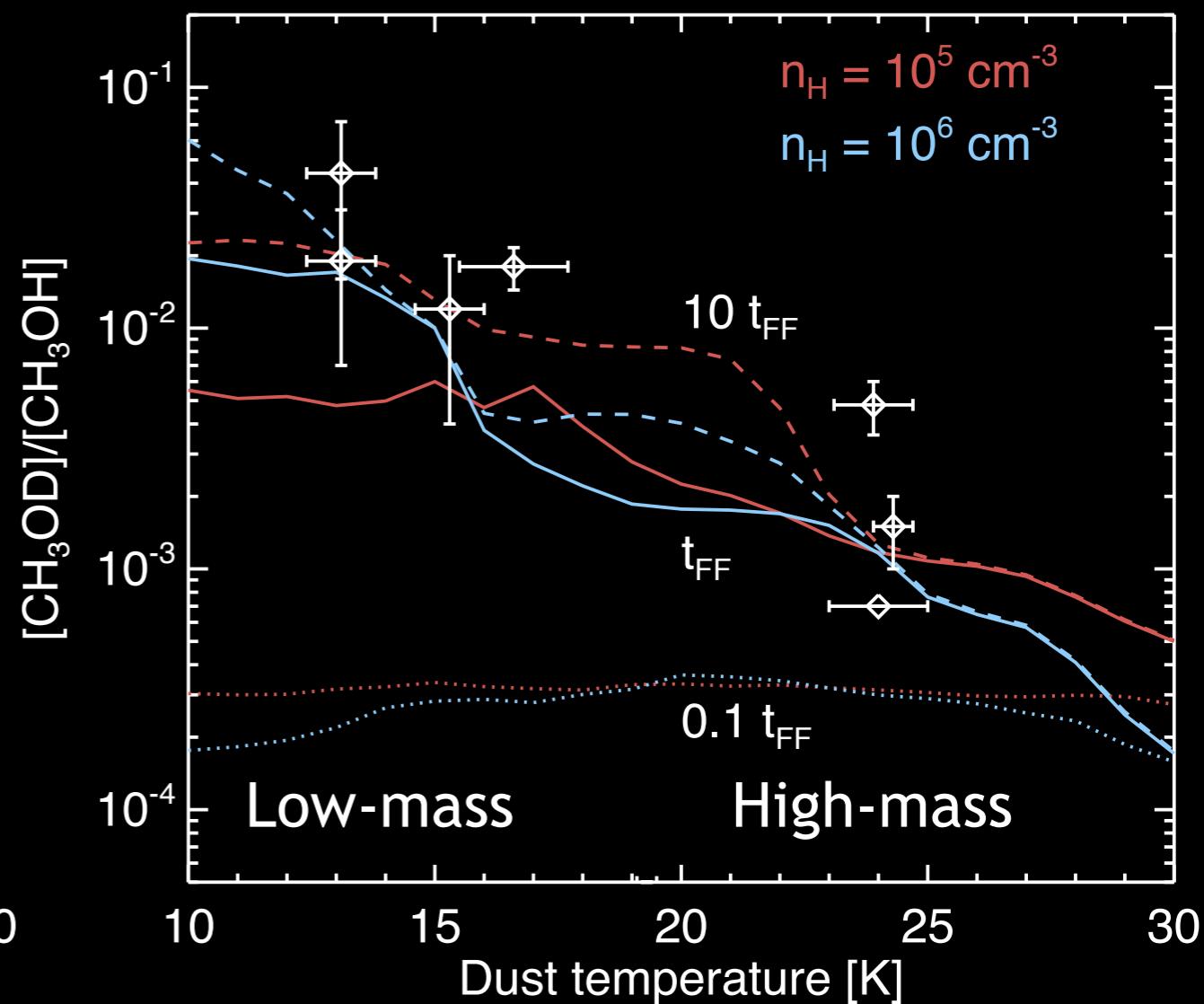
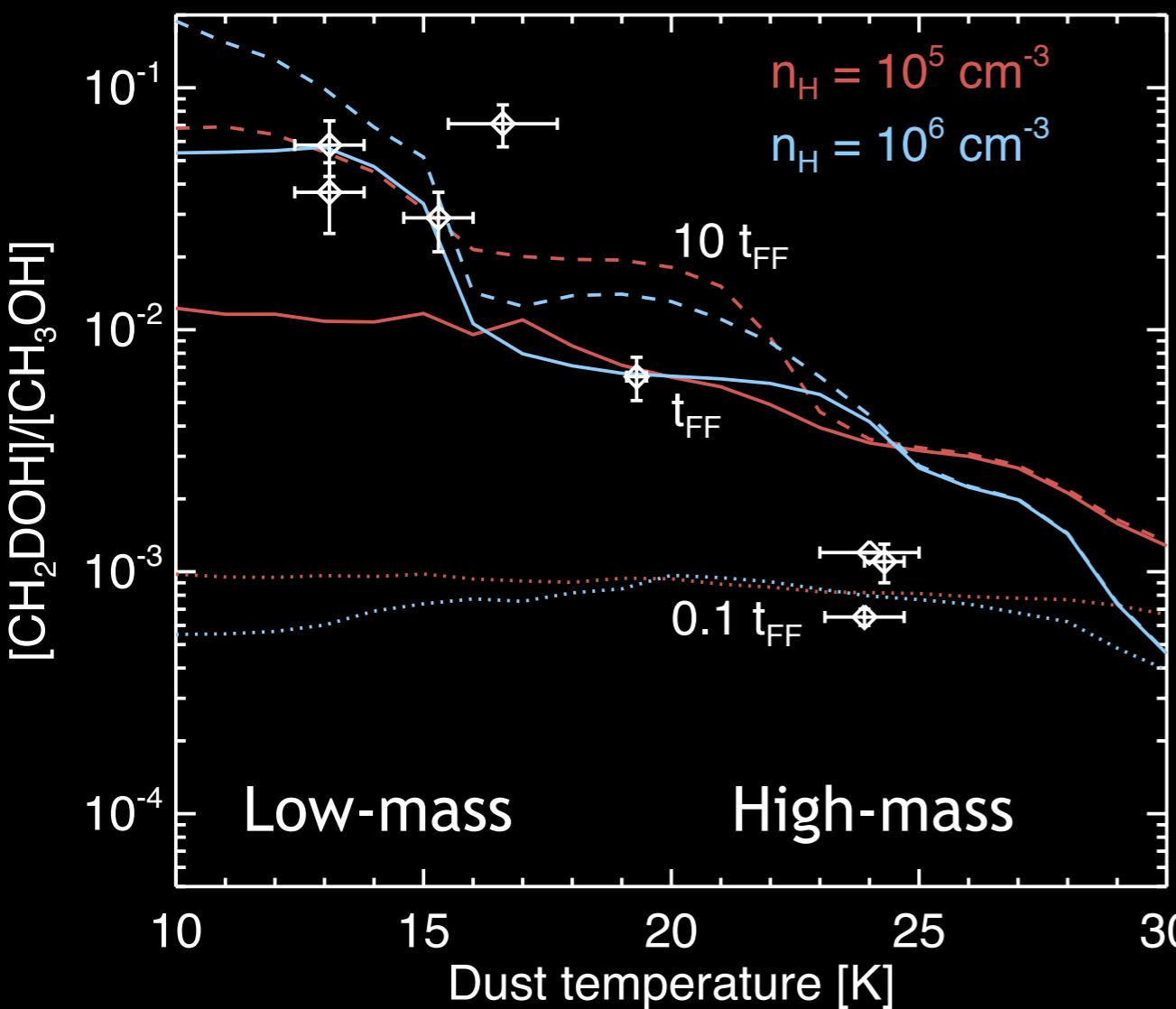


From Taquet et al. (2018, submitted); IRAS16293: Jørgensen et al. (2018), IRAS2A/IRAS4A: Taquet et al. (2018), HH212: Bianchi et al. (2017), NGC7129: Fuente et al. (2014), SgrB2(N2): Belloche et al. (2016), Orion KL: Peng et al. (2012), NNGC6334: Bøgelund et al. (2018)

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# Main activities

- 14 Publications:

## Models:

Ceccarelli, Viti, Balucani, **Taquet** 2018, *MNRAS*

## Observations:

**Taquet**, van Dishoeck, Swayne et al. 2018, *A&A*

**Taquet**, Bianchi, Codella et al. 2018, submitted to *A&A*

## Support to astronomers:

Bianchi, Codella, Ceccarelli, **Taquet** et al. 2017, *A&A*

Persson, ..., **Taquet** et al. 2017, *A&A*

Bøgelund, McGuire, Ligterink, **Taquet** et al. 2018, *A&A*

Jørgensen, ..., **Taquet** et al. 2018, *A&A*

Manigand, Calcutt, Jørgensen, **Taquet** et al. 2018, *A&A*

Van't Hoff, Persson, Harsono, **Taquet** et al. 2018, *A&A*

Bøgelund, Barr, **Taquet** et al. 2018, submitted to *A&A*

## Support to chemists:

Rimola, ..., **Taquet** et al. 2018, *Earth and Space Chemistry*

Ligterink, Terwisscha, **Taquet** et al. 2018, *MNRAS*

Dulieu, Nguyen, Congiu, Baouche, **Taquet** 2018, submitted to *MNRAS*

Qasim, Fedoseev, Chuang, **Taquet** et al. 2018, submitted to *MNRAS*

# Main activities

- **14 Publications:**  
2 first-author publications, 12 others with significant contributions
- **Two Invited talks since September 2017**  
Ciudad Real, “Gas phase cold chemistry of COMs”, December 2017  
Paris, “Oxygen in Space”, October 2018
- **Two visits at Paris Observatory with F. Dulieu’s group**

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- **One visit at the Ospedale !**

