PROSPECTS:
Prebiotic mOlecules from SPacE to ComeTS

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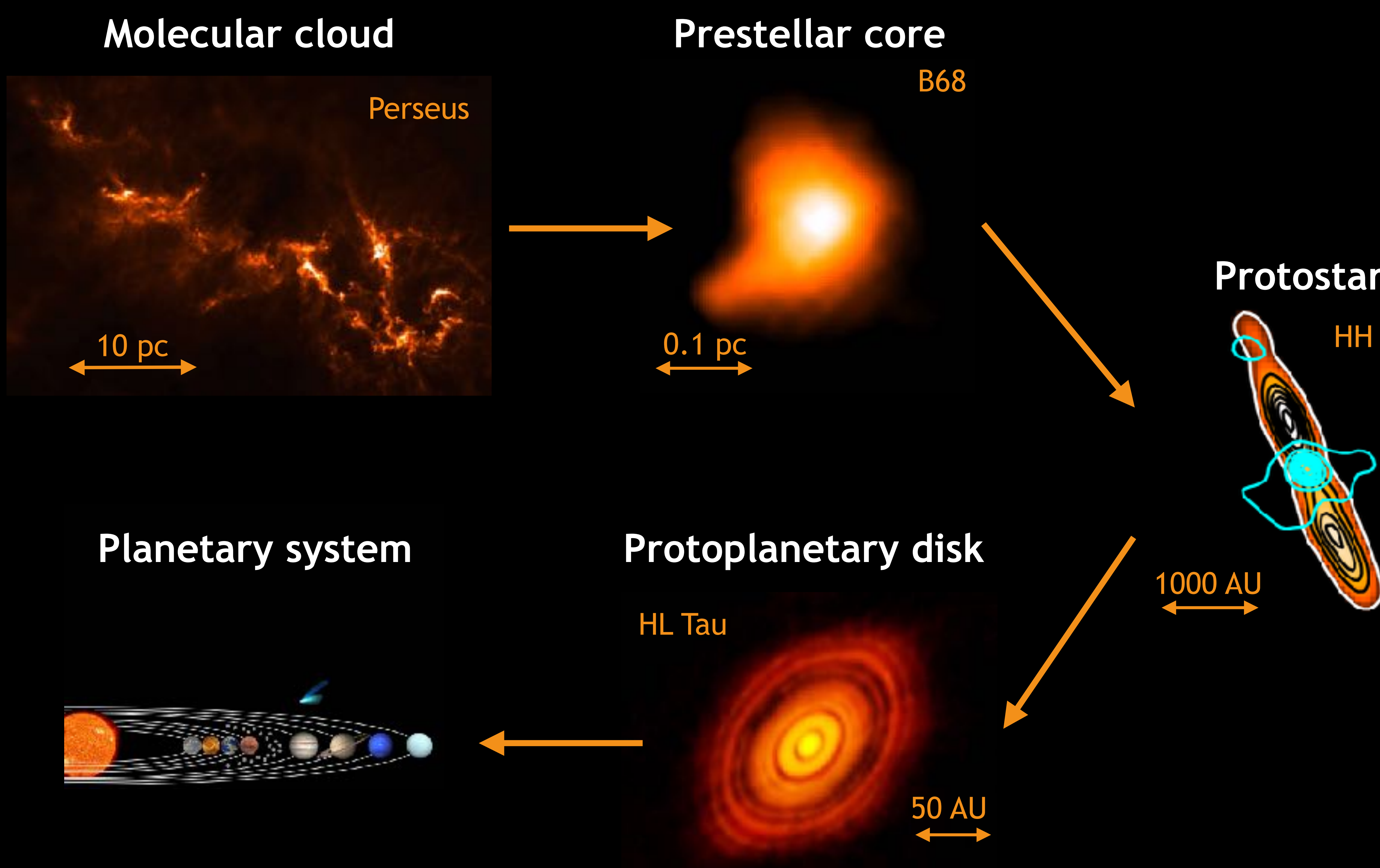
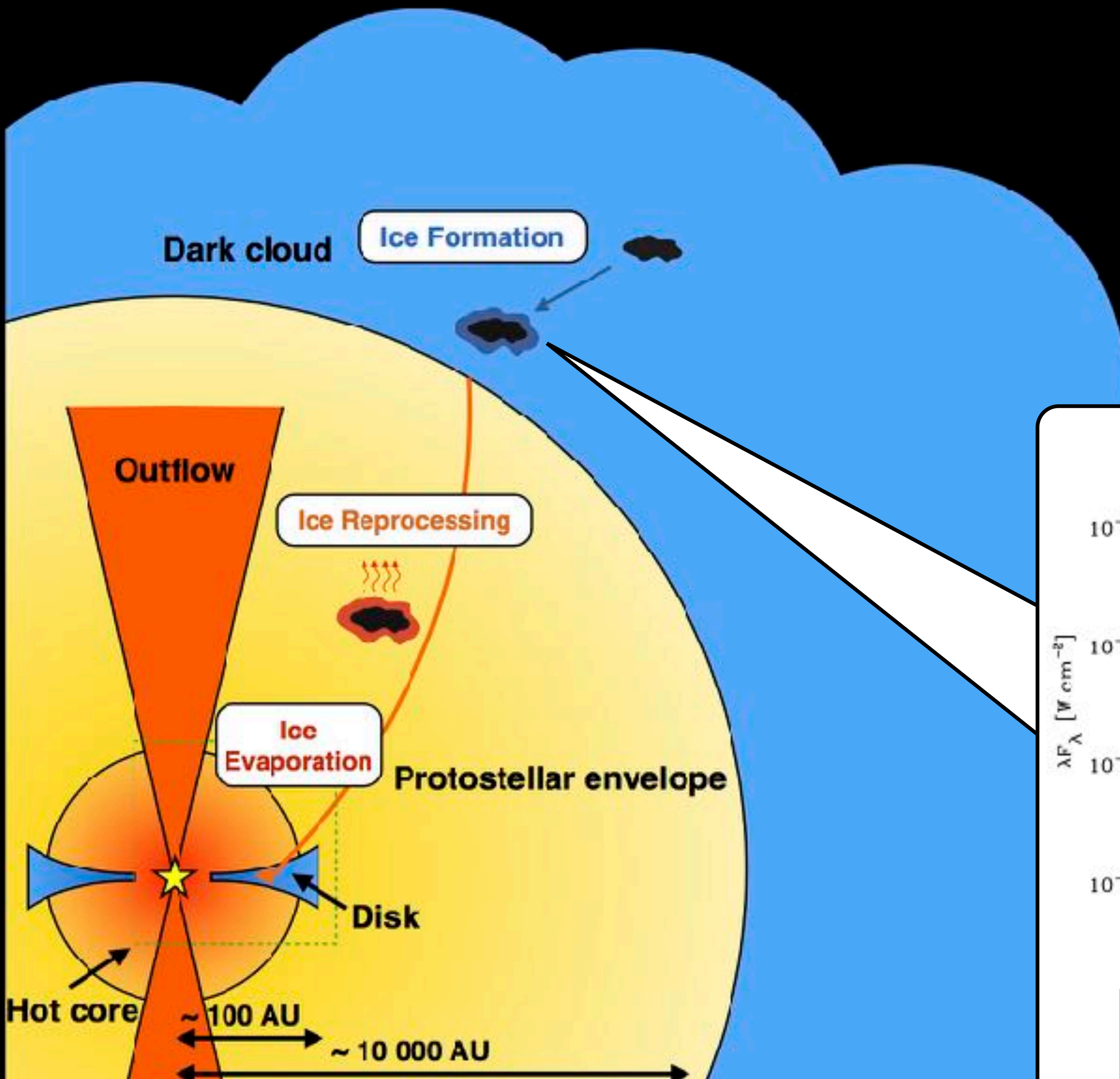
The formation of low-mass stars

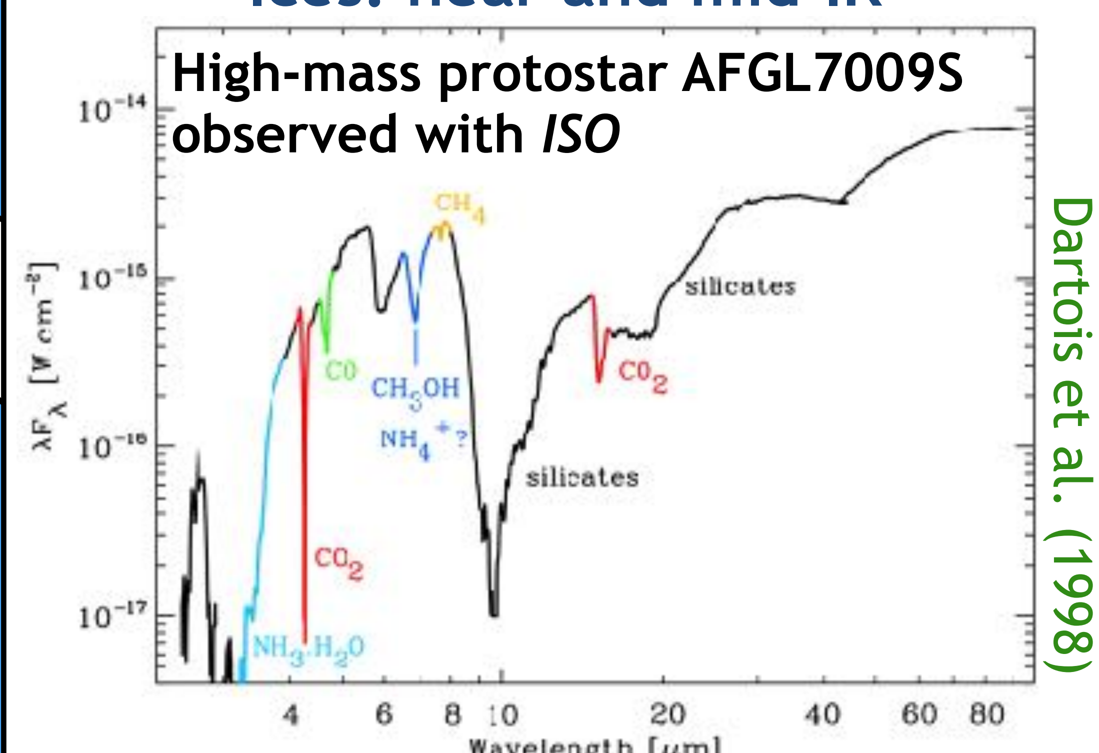


Zari et al. (2016), Roy et al. (2014),
Codella et al. (2014), ALMA et al. (2015)

How to observe molecules in star-forming regions ?

1. Infrared spectroscopy in absorption to study interstellar ices

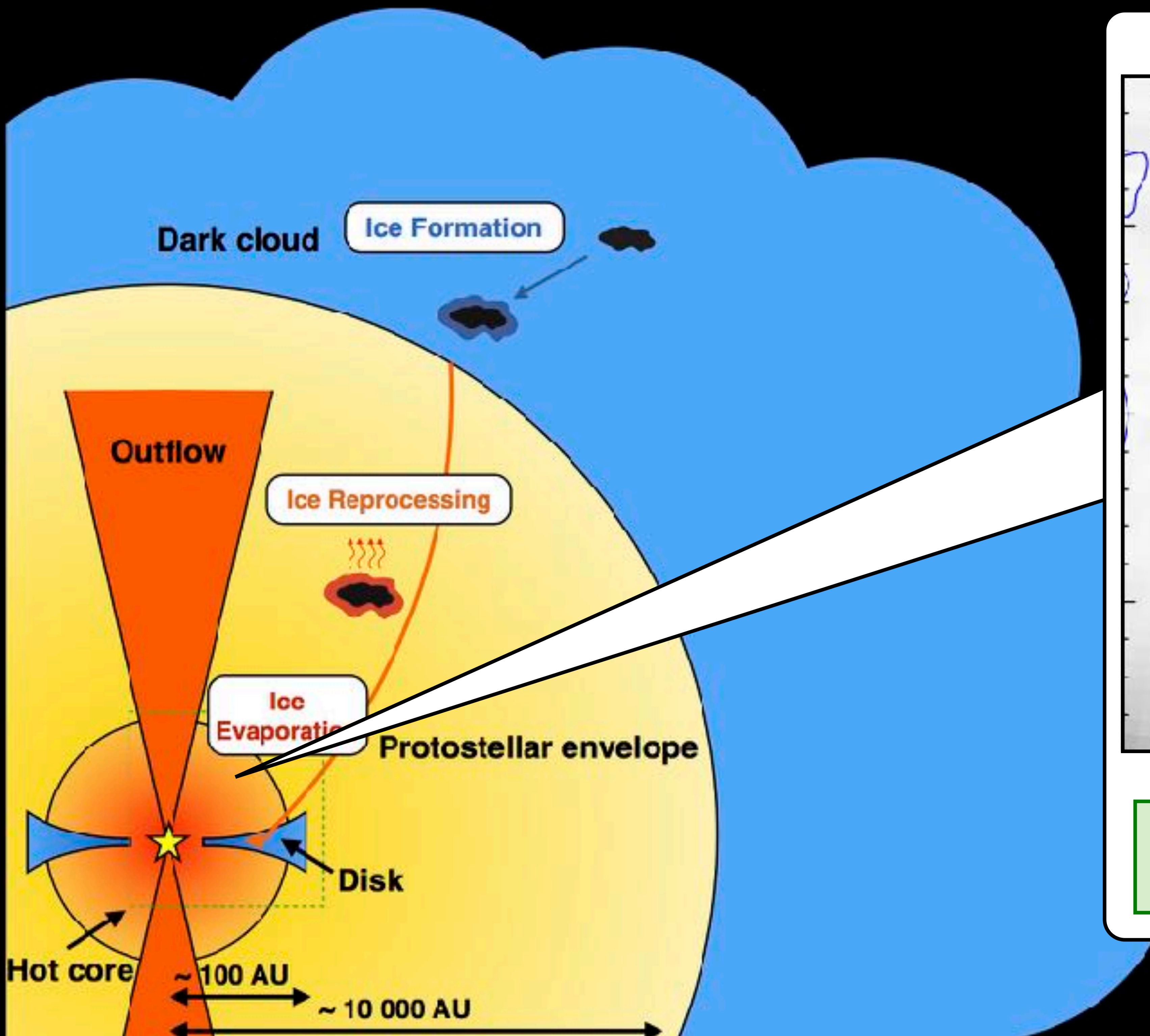




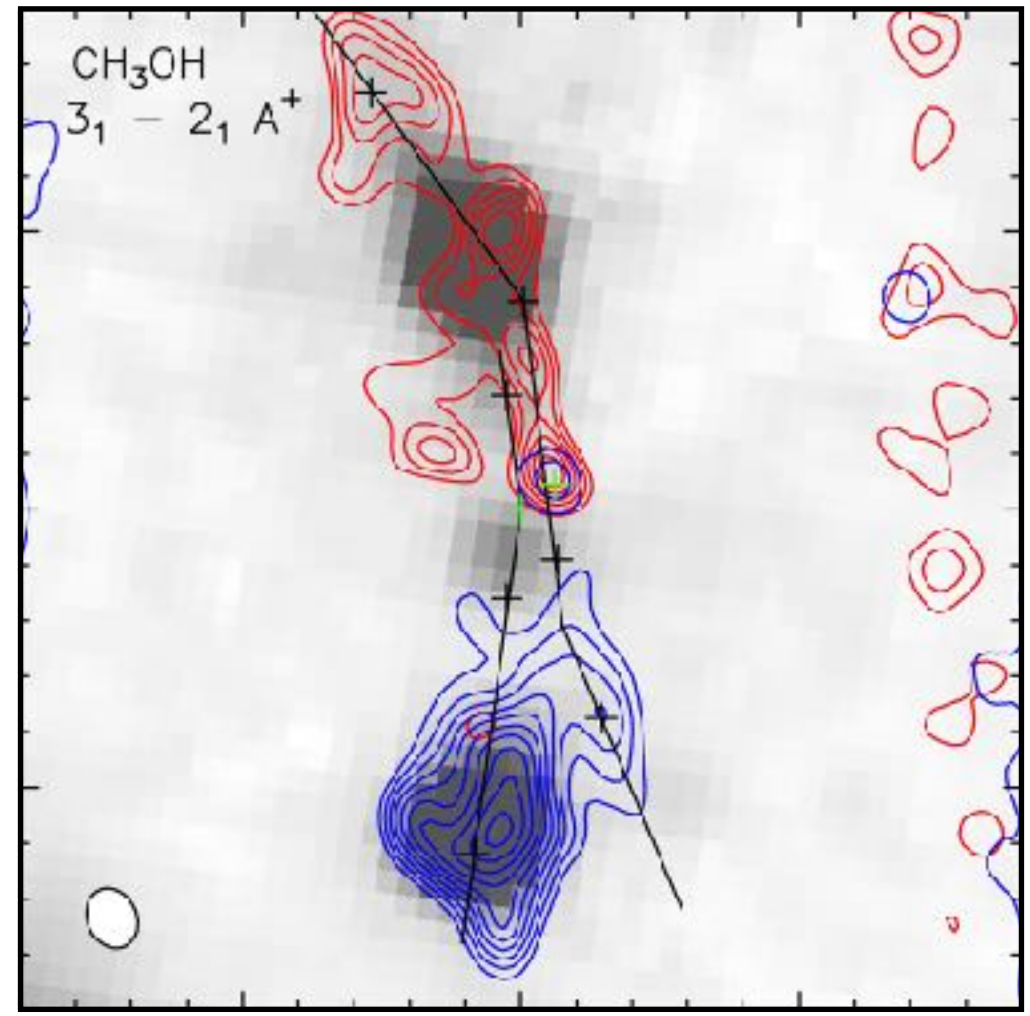
New observatories:
JWST, E-ELT, SPHEREx

How to observe molecules in star-forming regions ?

2. Millimetric spectroscopy in emission to study the molecular gas



Gas: sub-mm/mm

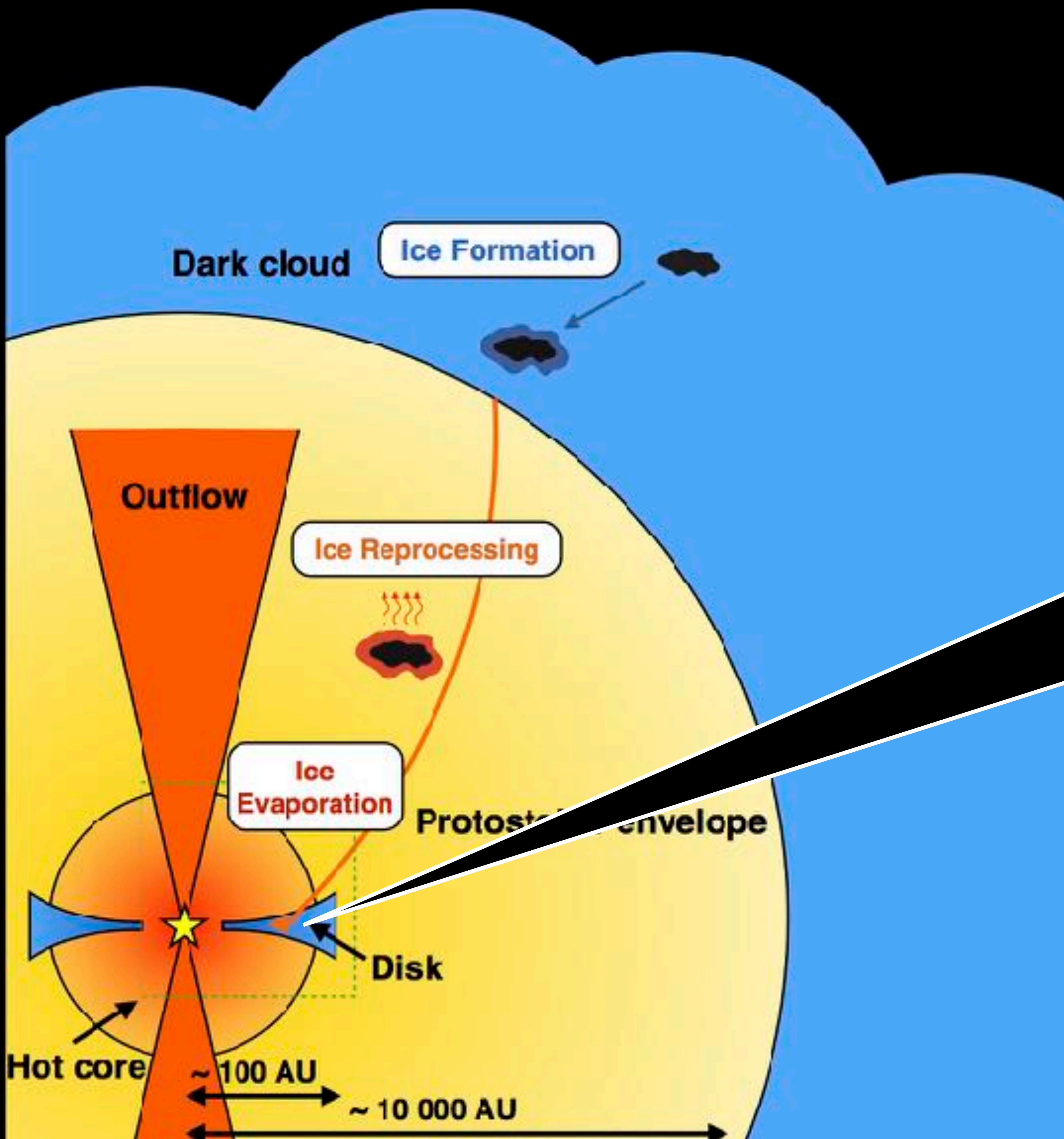


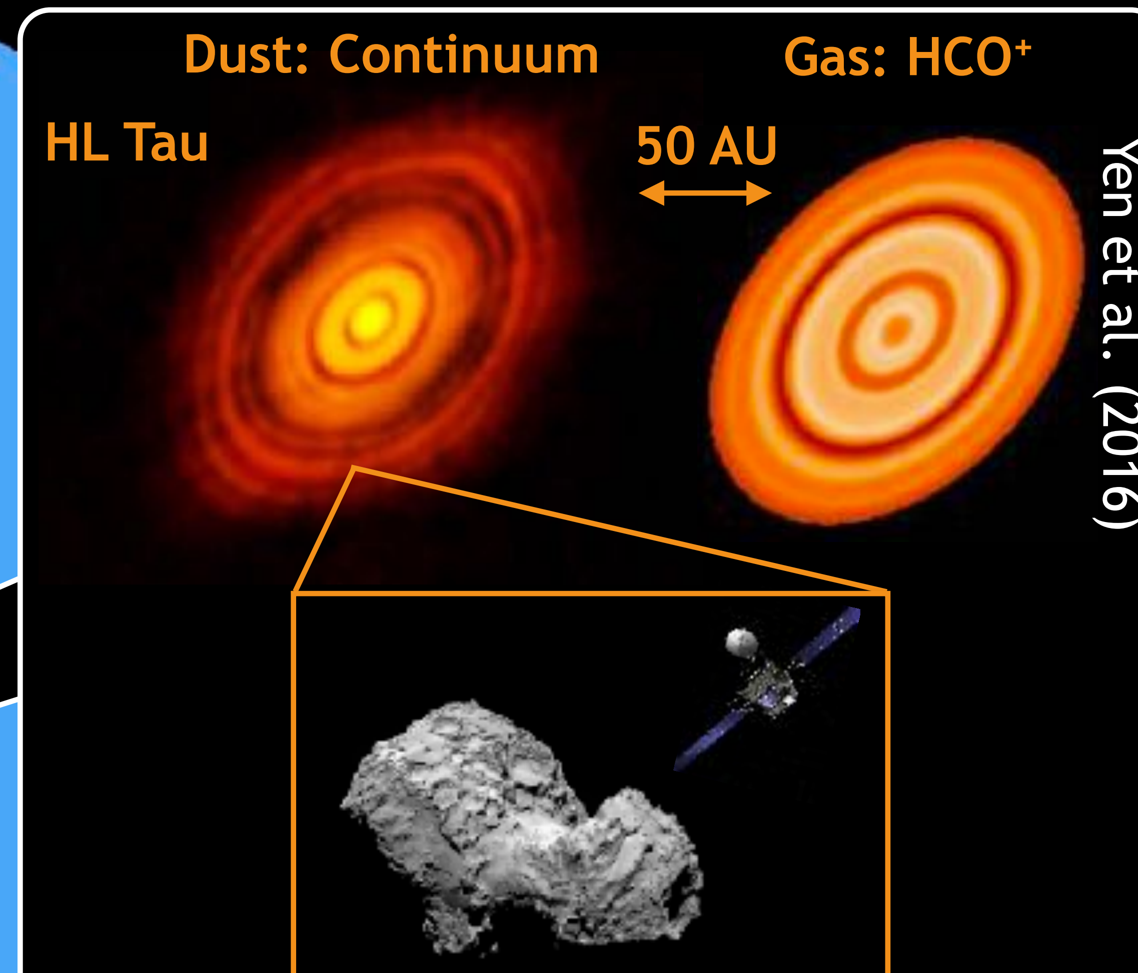
Taquet et al. (in prep.)

New observatories:
NOEMA, ALMA, ngVLA ?

How to observe molecules in star-forming regions ?

3. Space missions: final composition of the Solar Nebula

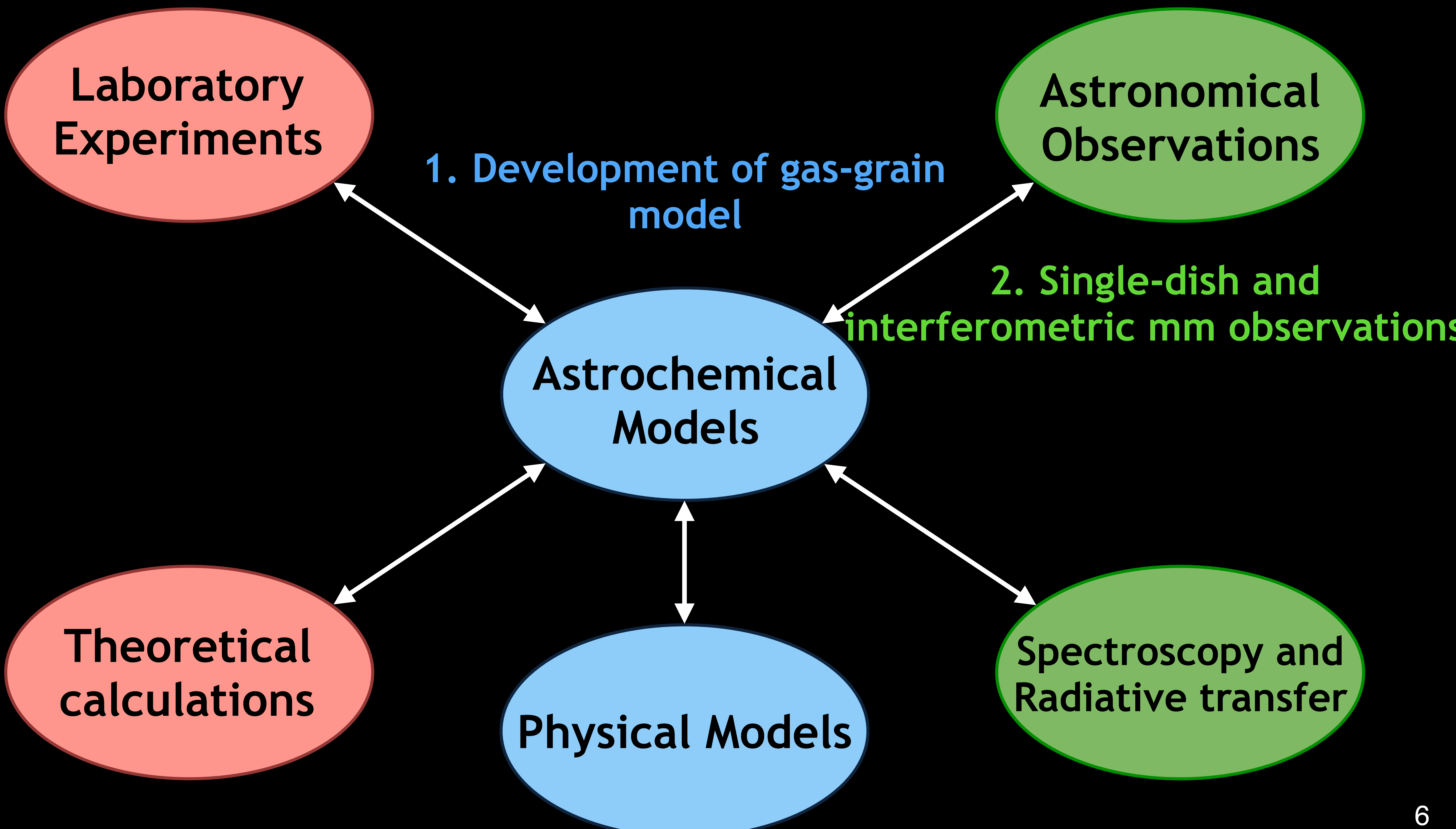




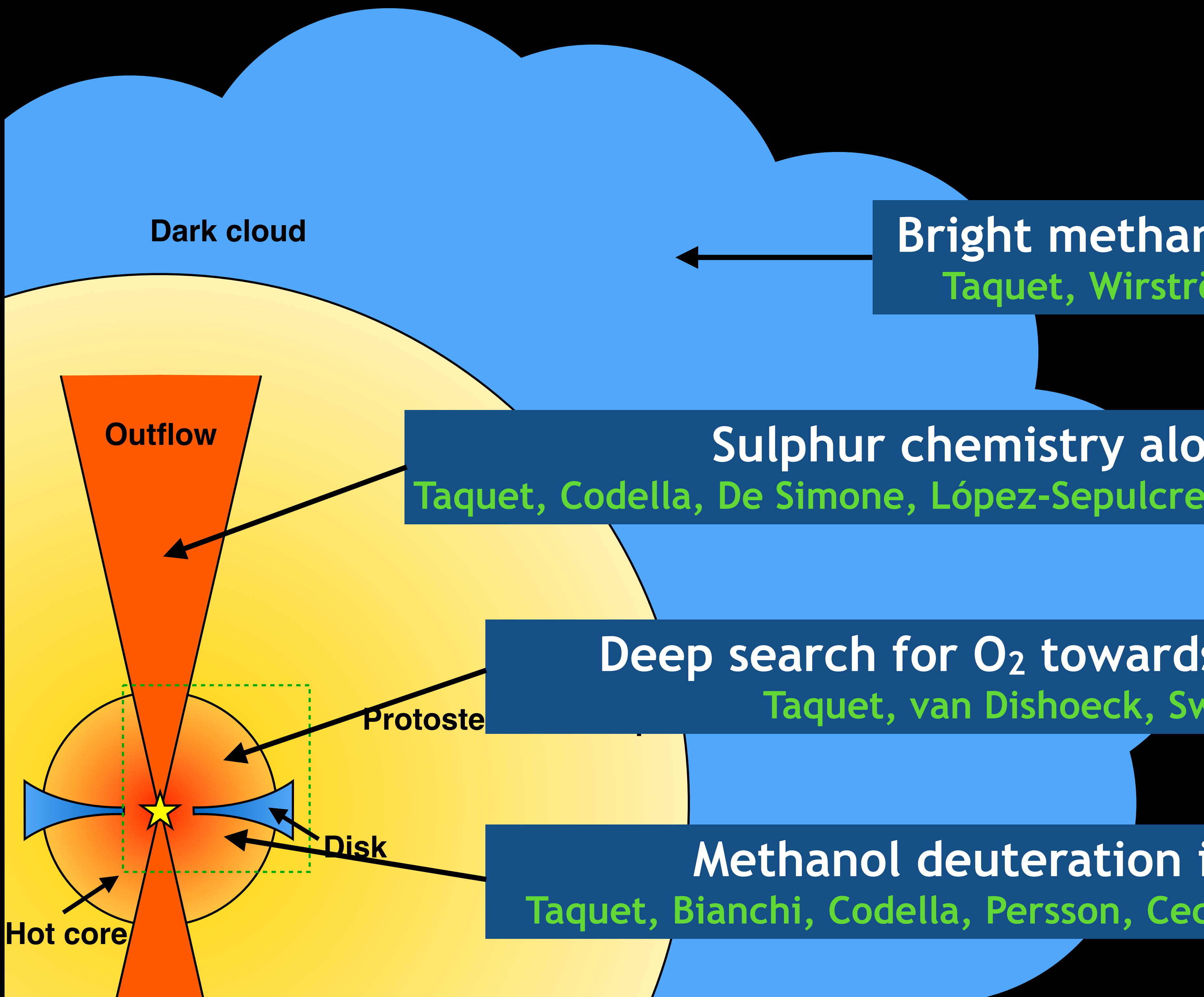
Rosetta - Comet 67P

Expertises in Astrochemistry

Theoretical and experimental chemistry | **Modelling** | **Observations**



Main projects during ASTROFIT2 program



Bright methanol in a cold dark cloud
Taquet, Wirström, Charnley et al. (In prep.)

Sulphur chemistry along molecular outflows
Taquet, Codella, De Simone, López-Sepulcre, Pineda et al. (to be subm.)

Deep search for O_2 towards a low-mass protostar
Taquet, van Dishoeck, Swayne, Harsono et al. (2018)

Methanol deuteration in low-mass protostars
Taquet, Bianchi, Codella, Persson, Ceccarelli et al. (A&A, in press)

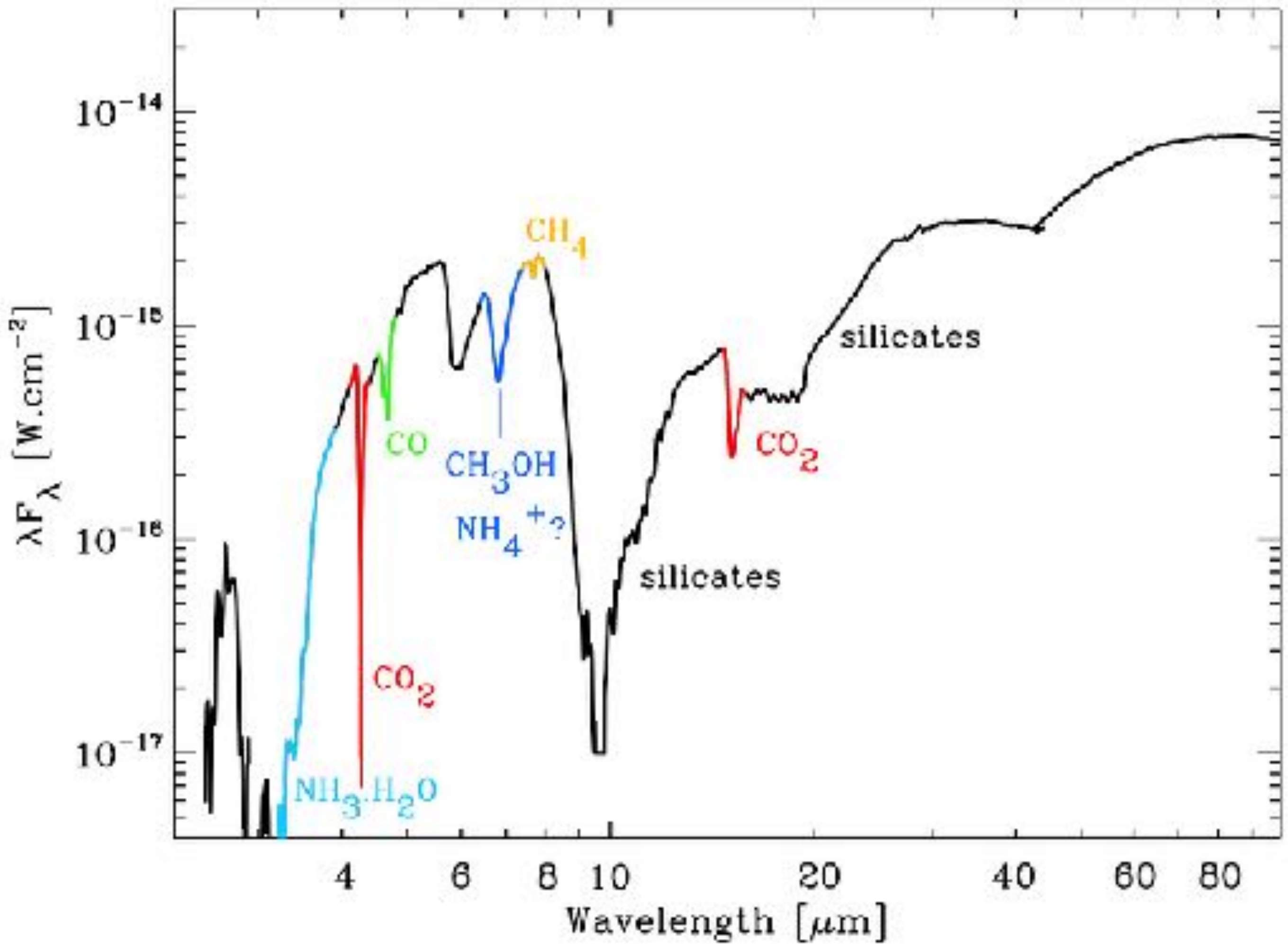
Bright cold methanol emission in Barnard 5

Taquet, Wirström, Charnley et al. (In prep.)

Methanol: a key molecule for organic chemistry

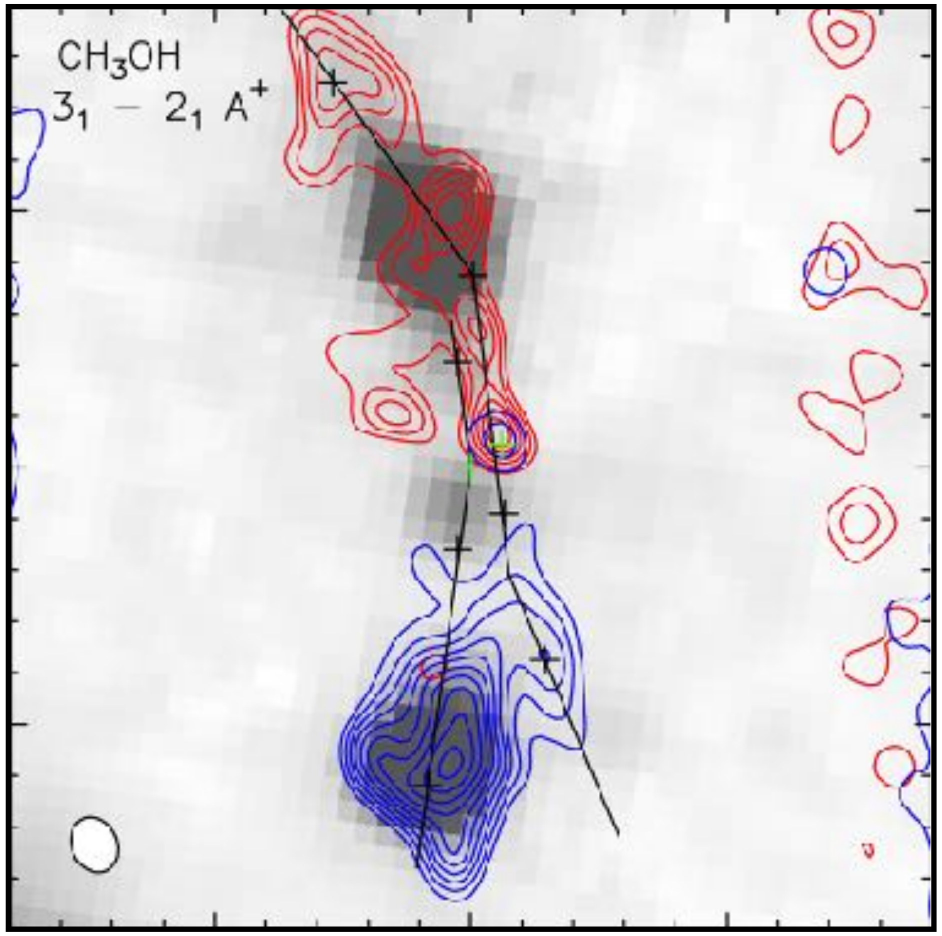
High methanol abundances both in interstellar ices and gas

High-mass protostar AFGL7009S observed with *ISO*



Dartois et al. (1998), Boogert et al. (2015)

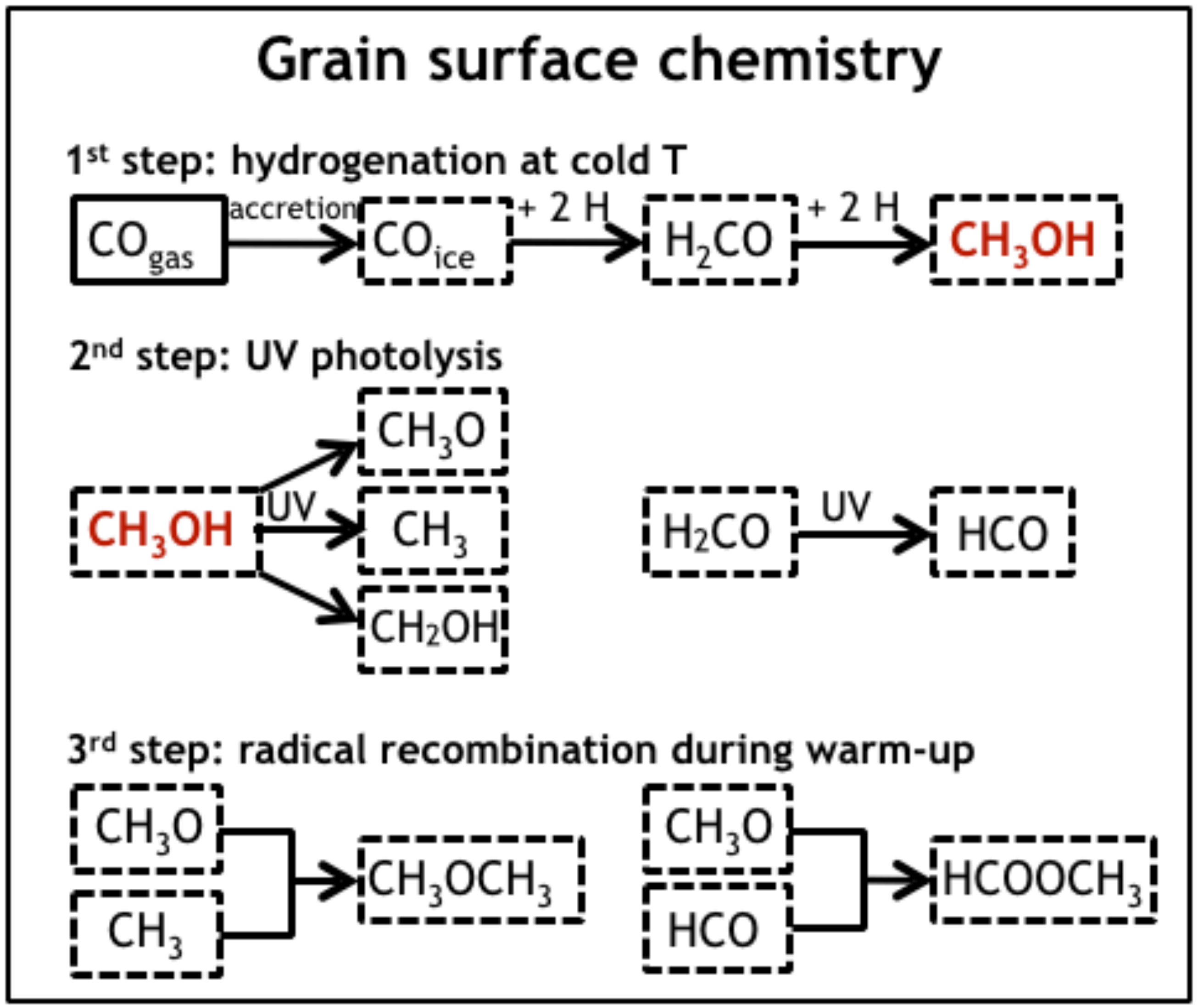
Low-mass protostar IRAS4A observed with NOEMA

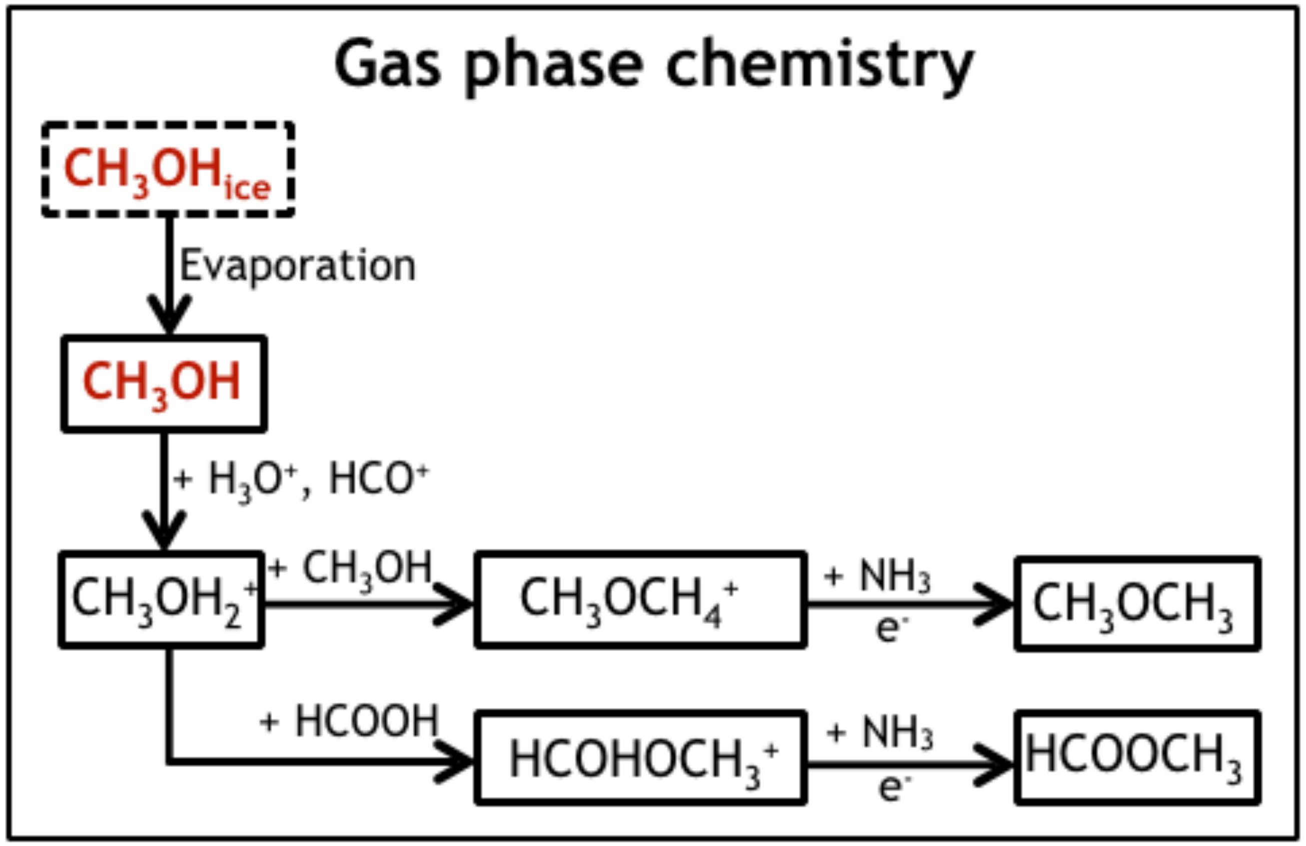


De Simone et al., Taquet et al. (in prep.)

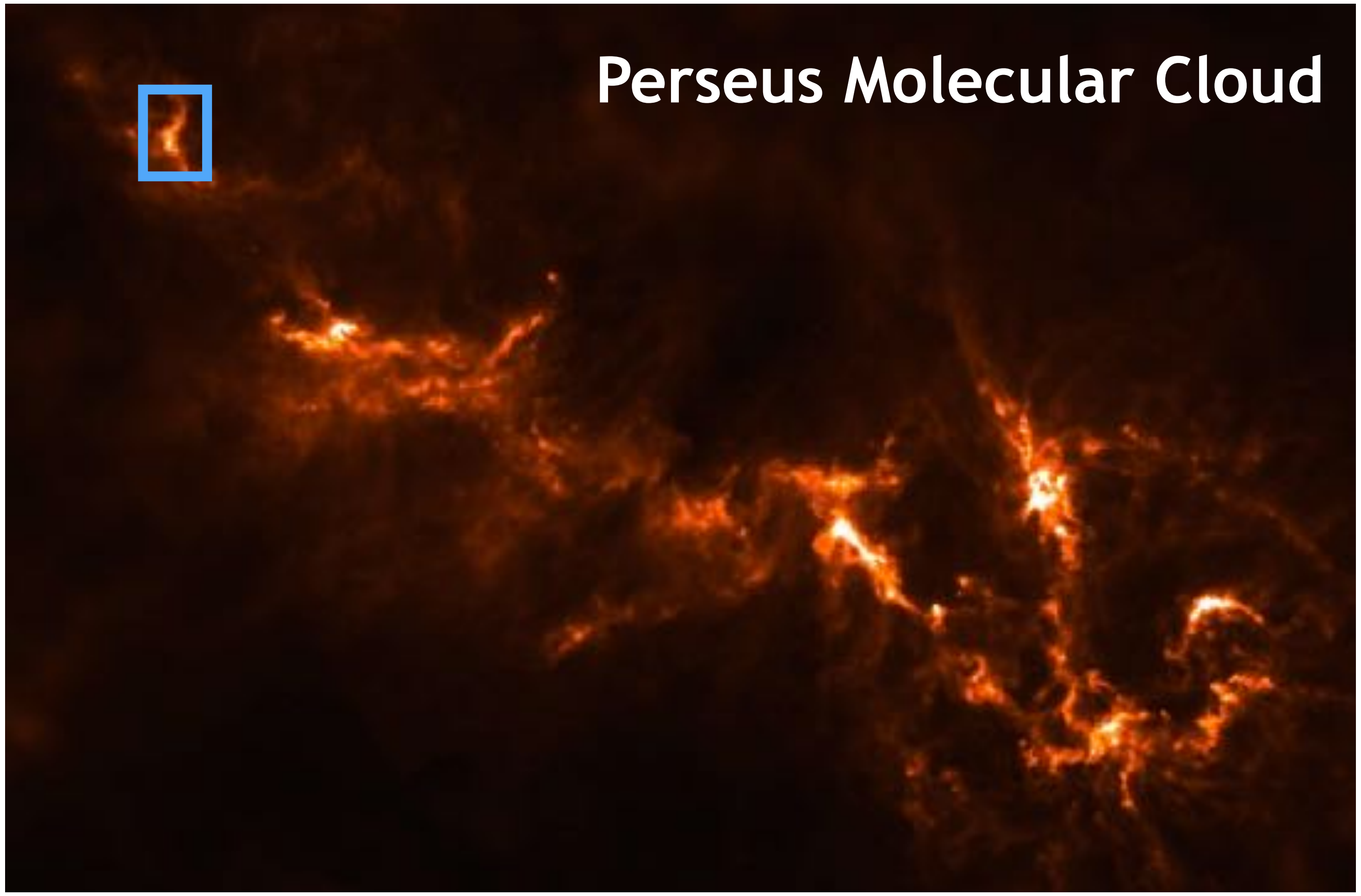
Methanol: a key molecule for organic chemistry

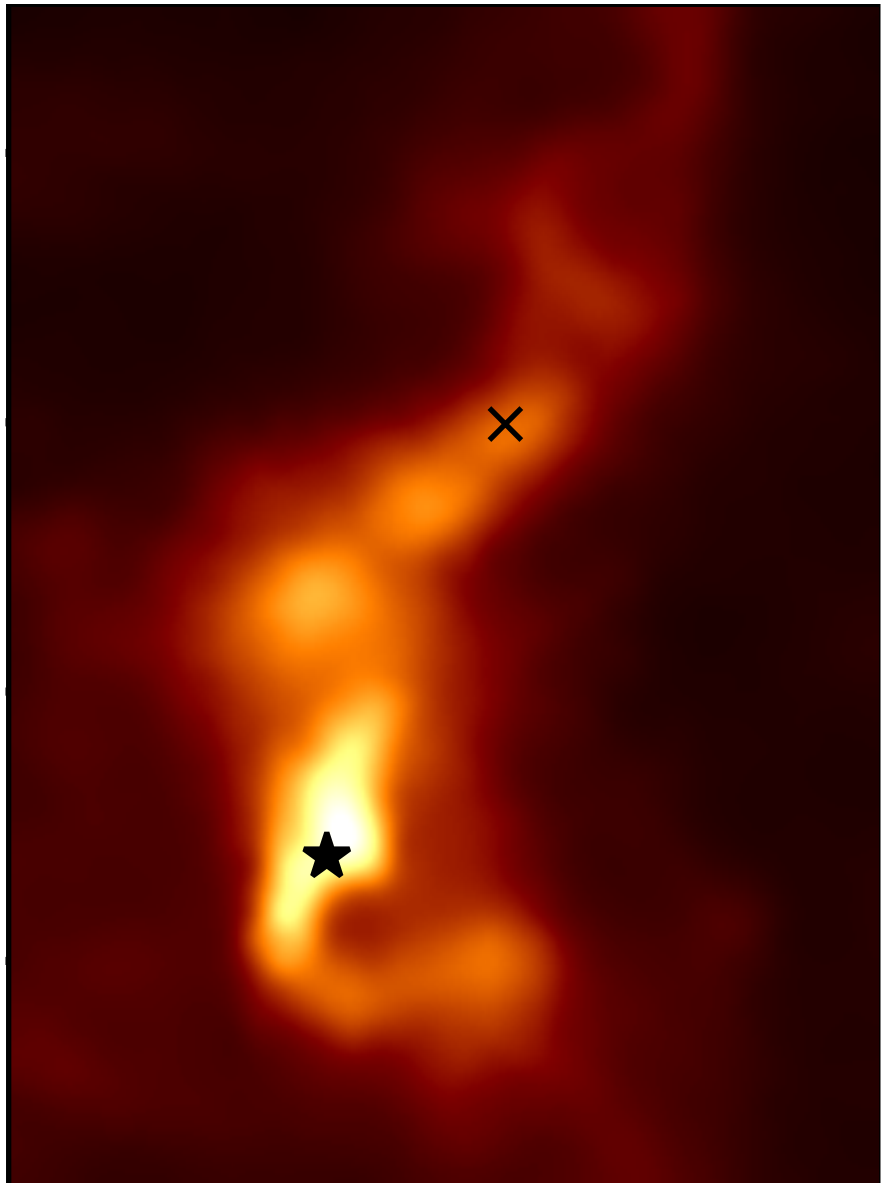
Methanol is likely the mother molecule of many interstellar Complex Organic Molecules





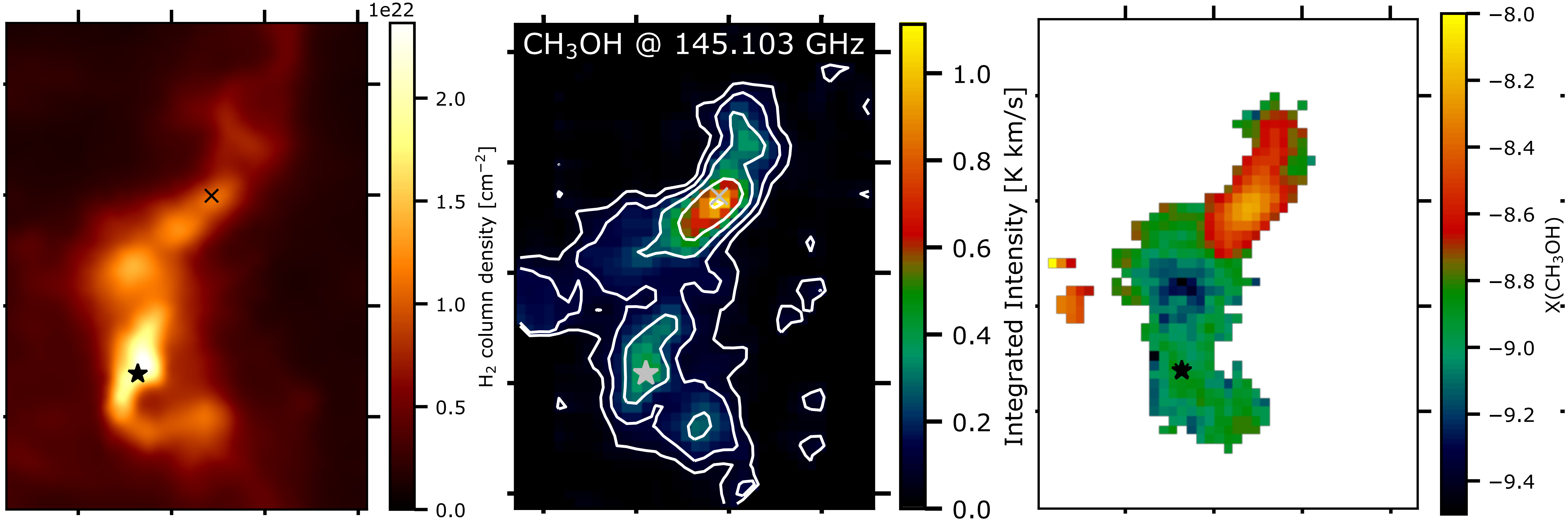
Molecular mapping of the Barnard 5 molecular cloud





Bright unexpected methanol emission in Barnard 5

Cold methanol is detected in a "secondary" part of the cloud with relatively high abundances



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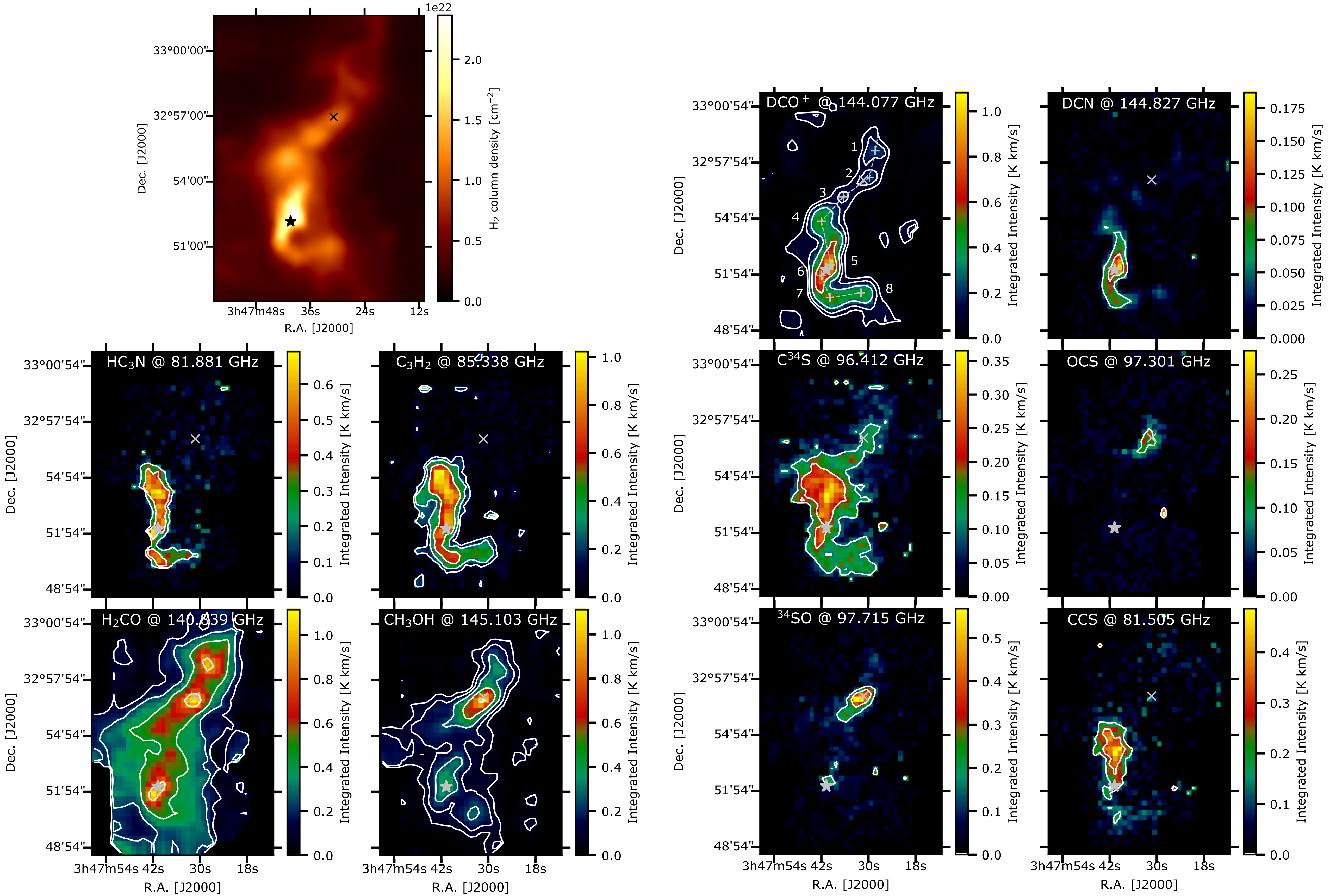
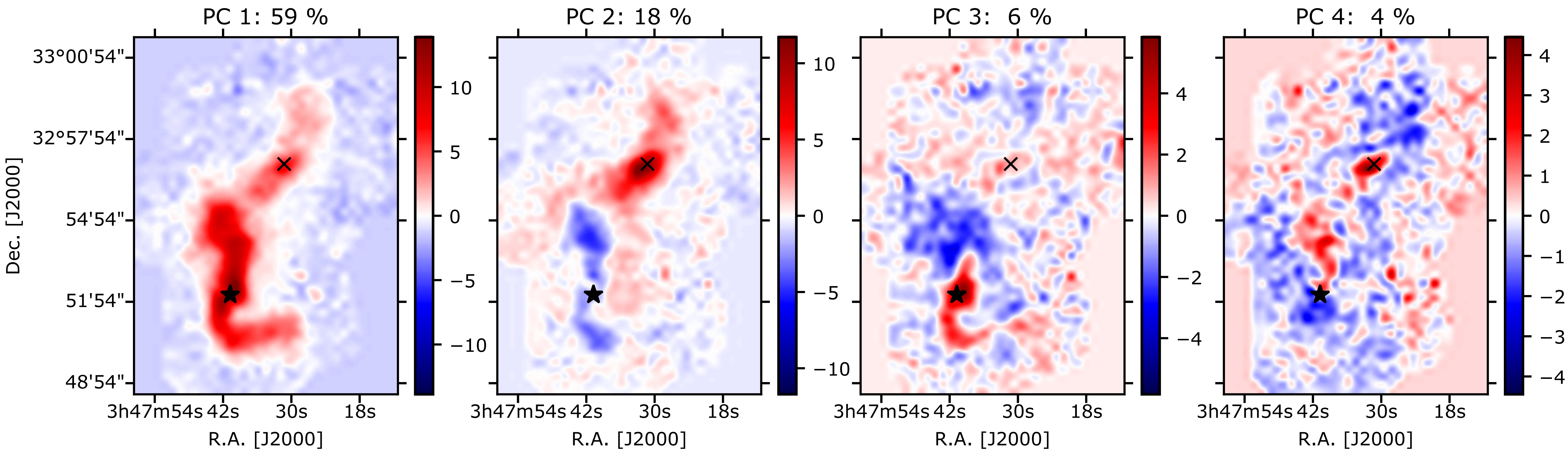


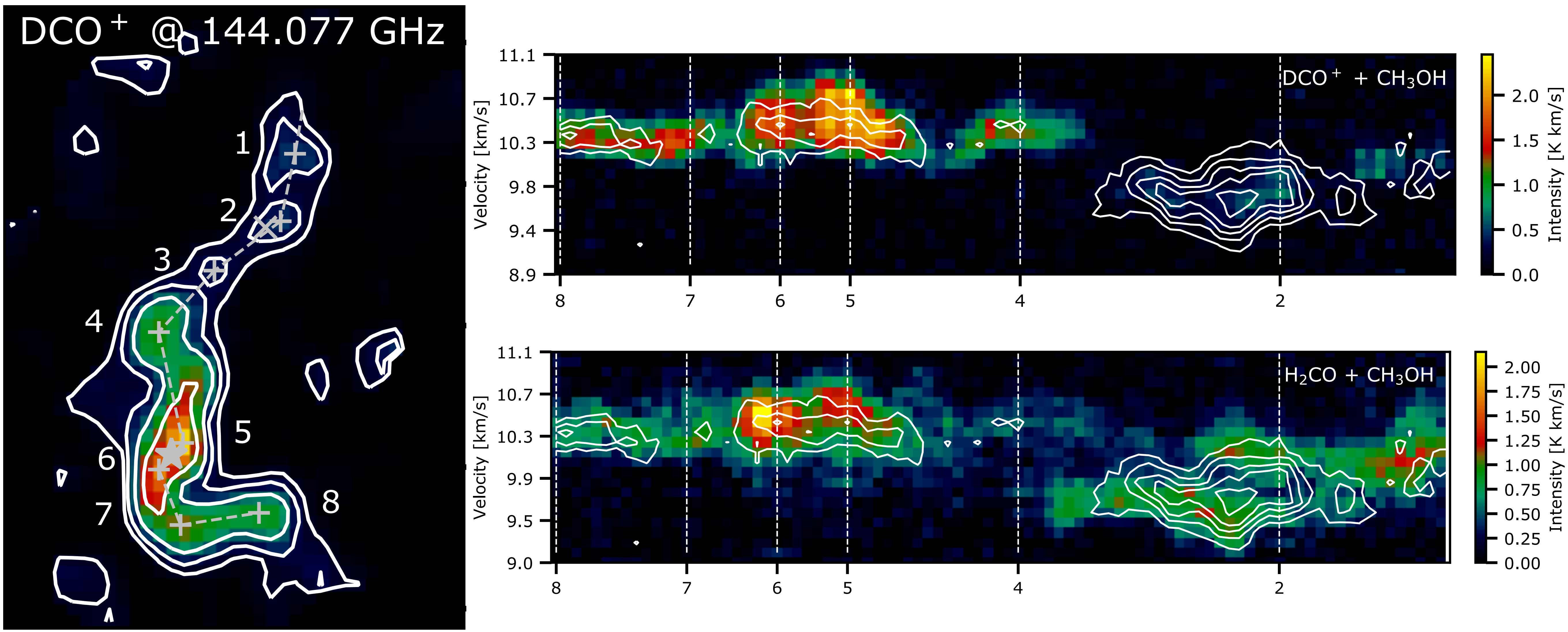
Multi-variate analysis of the molecular emission

Decomposition of initial dataset into principal components: orthogonal variables that maximise the observed variance



Methanol emission triggered by cloud-cloud emission ?

Methanol emission is detected where two H_2CO components collide:

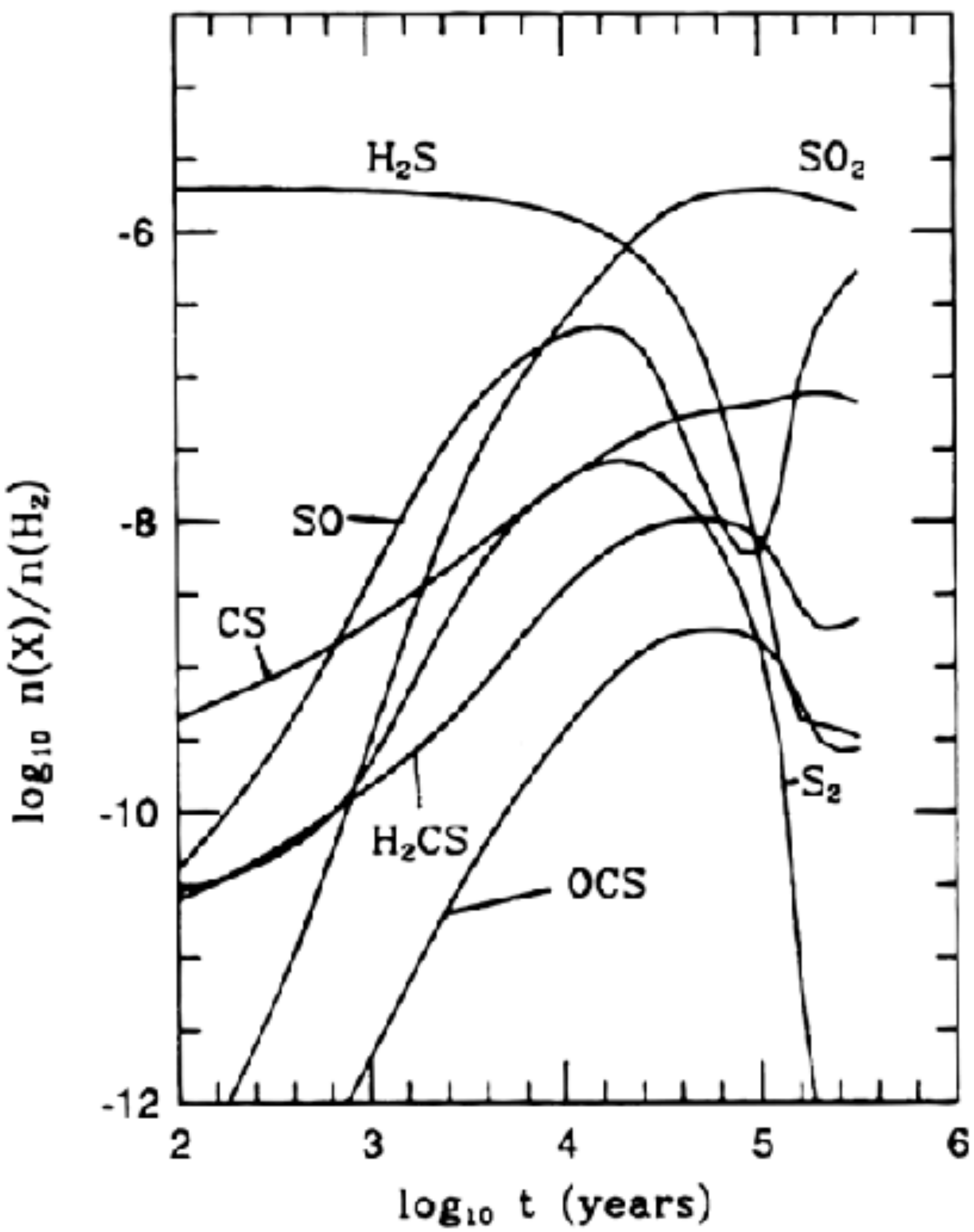


Sulphur chemistry along molecular outflows

Taquet, Codella, De Simone, López-Sepulcre, Pineda et al. (to be subm.)

Why sulfur chemistry ?

Potential chemical clock around protostars because abundances of "bright" species (i.e. CS, SO, H_2S, OCS, SO_2) are thought to evolve strongly with time



Charnley (1997)

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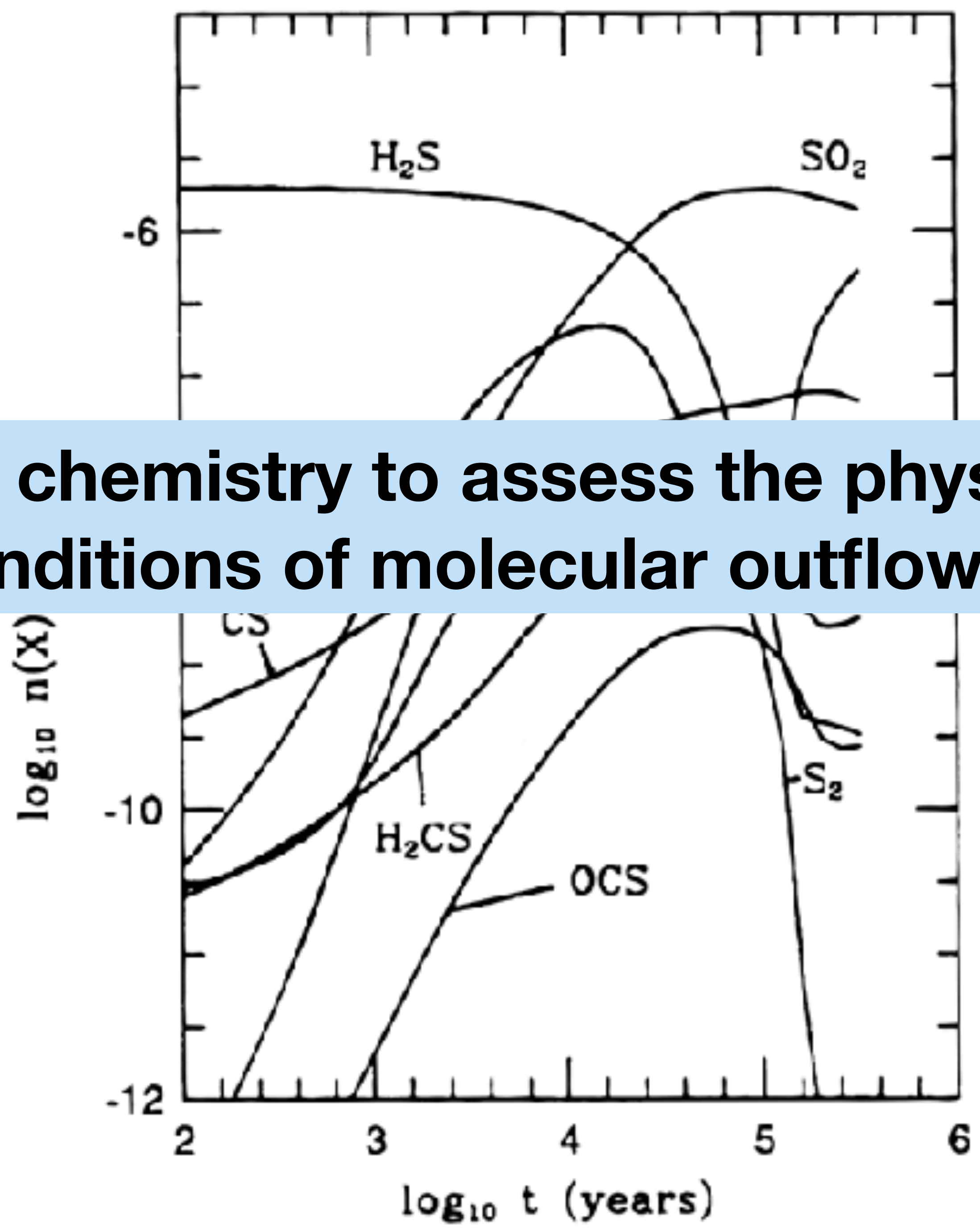
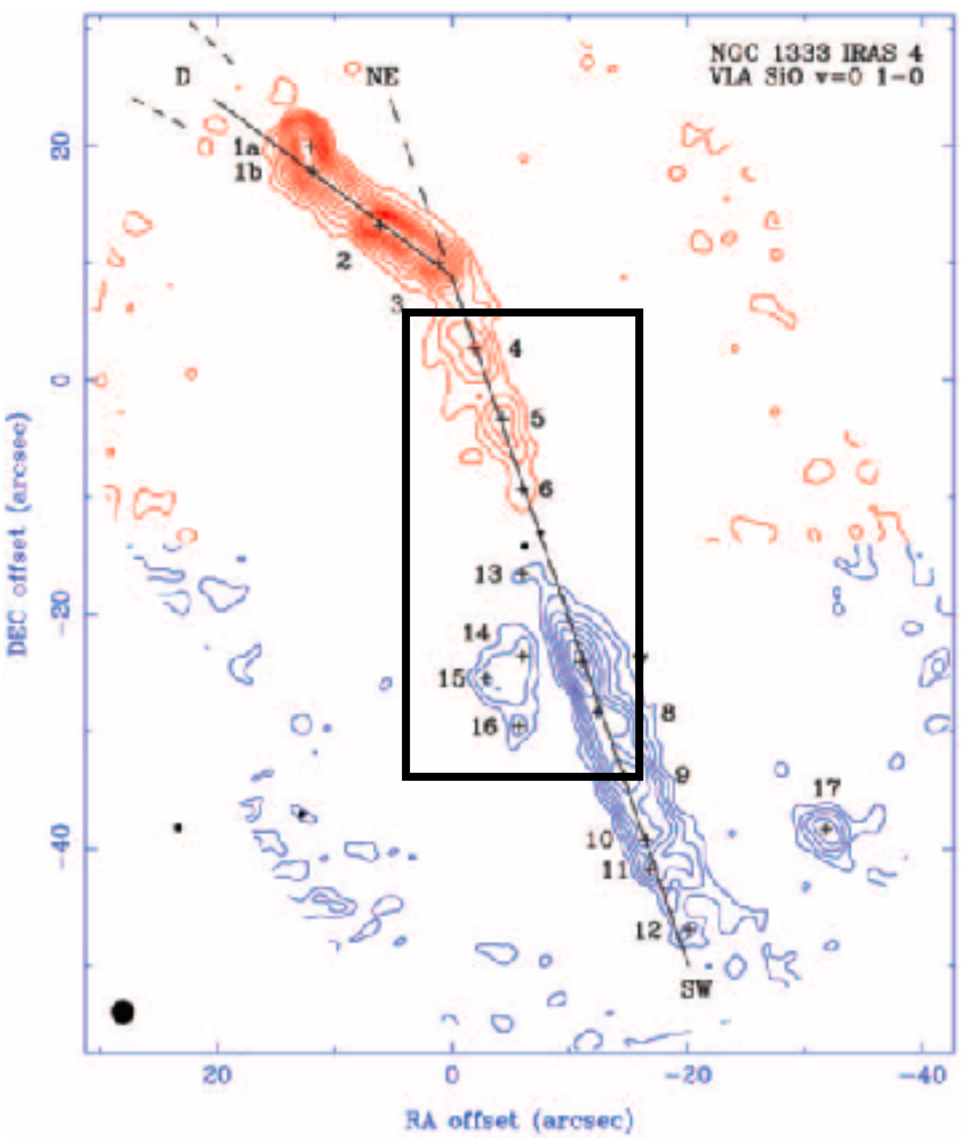


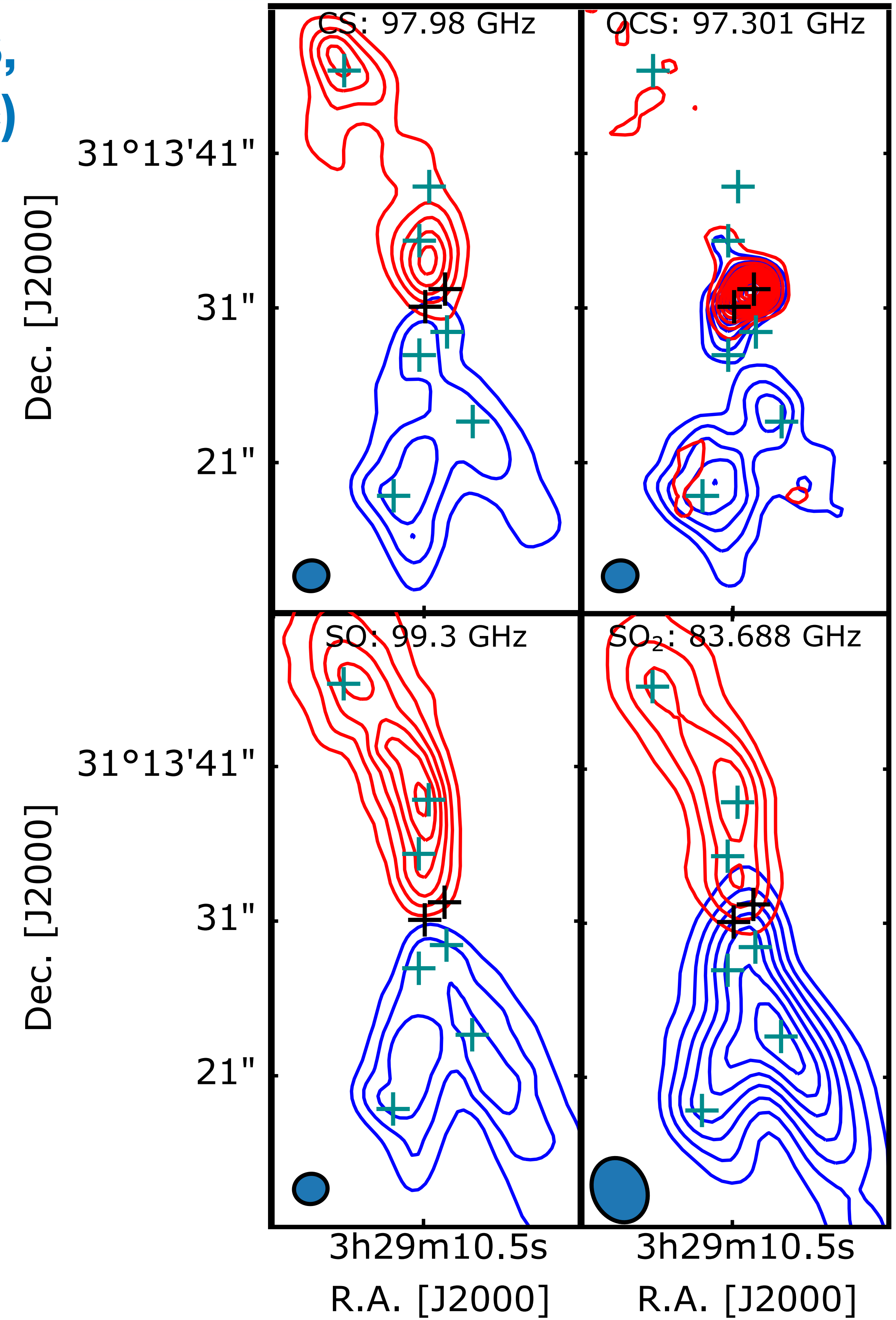
Can we use sulfur chemistry to assess the physical and chemical conditions of molecular outflows ?

Charnley (1997)

The NGCC1333-IRAS4A protostellar system

Chemical differentiation between OCS, CS, SO, and SO_2 at "low" (2-4 arcsec) resolution



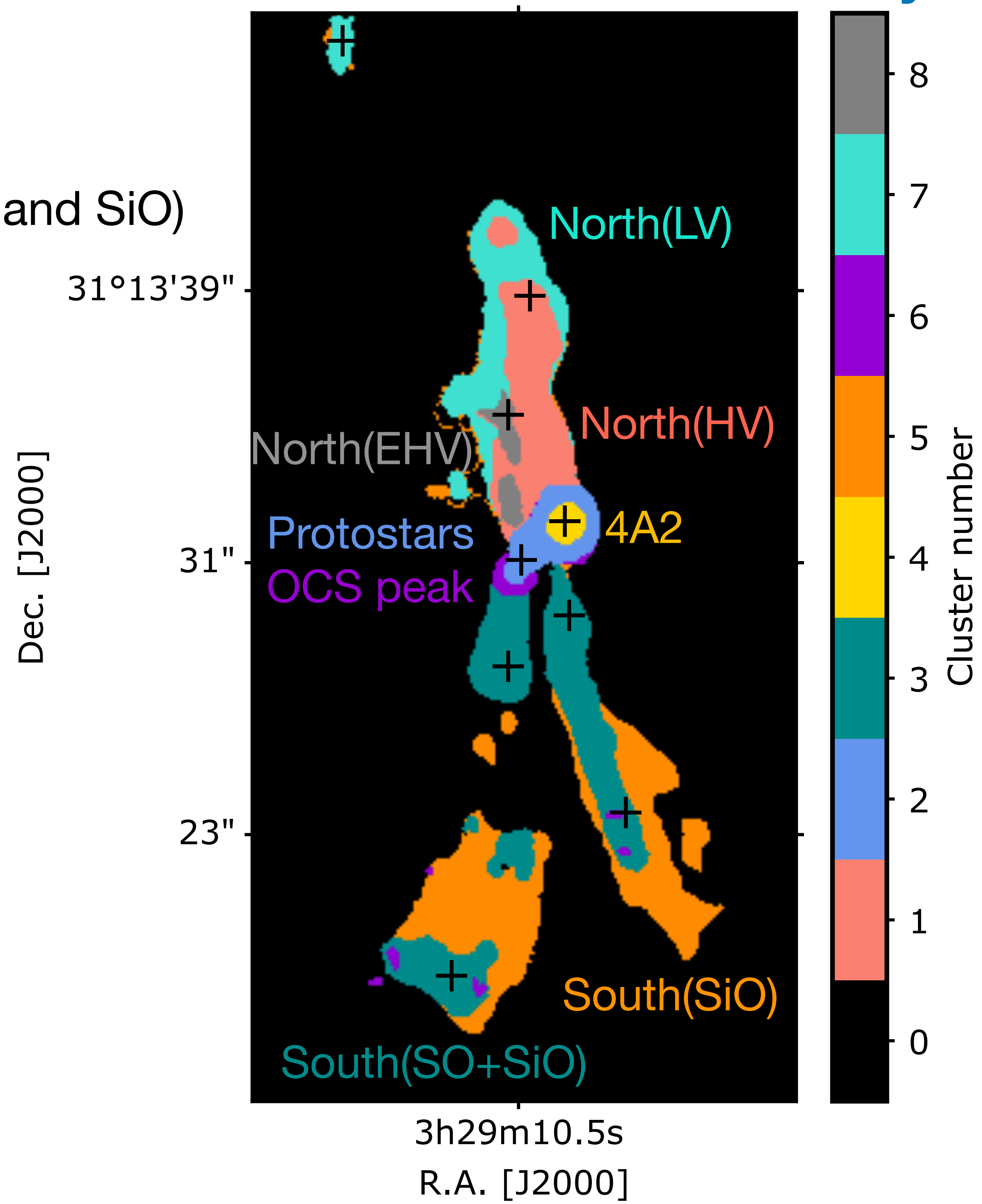


Choi (2005)

Dissecting the outflows with clustering methods

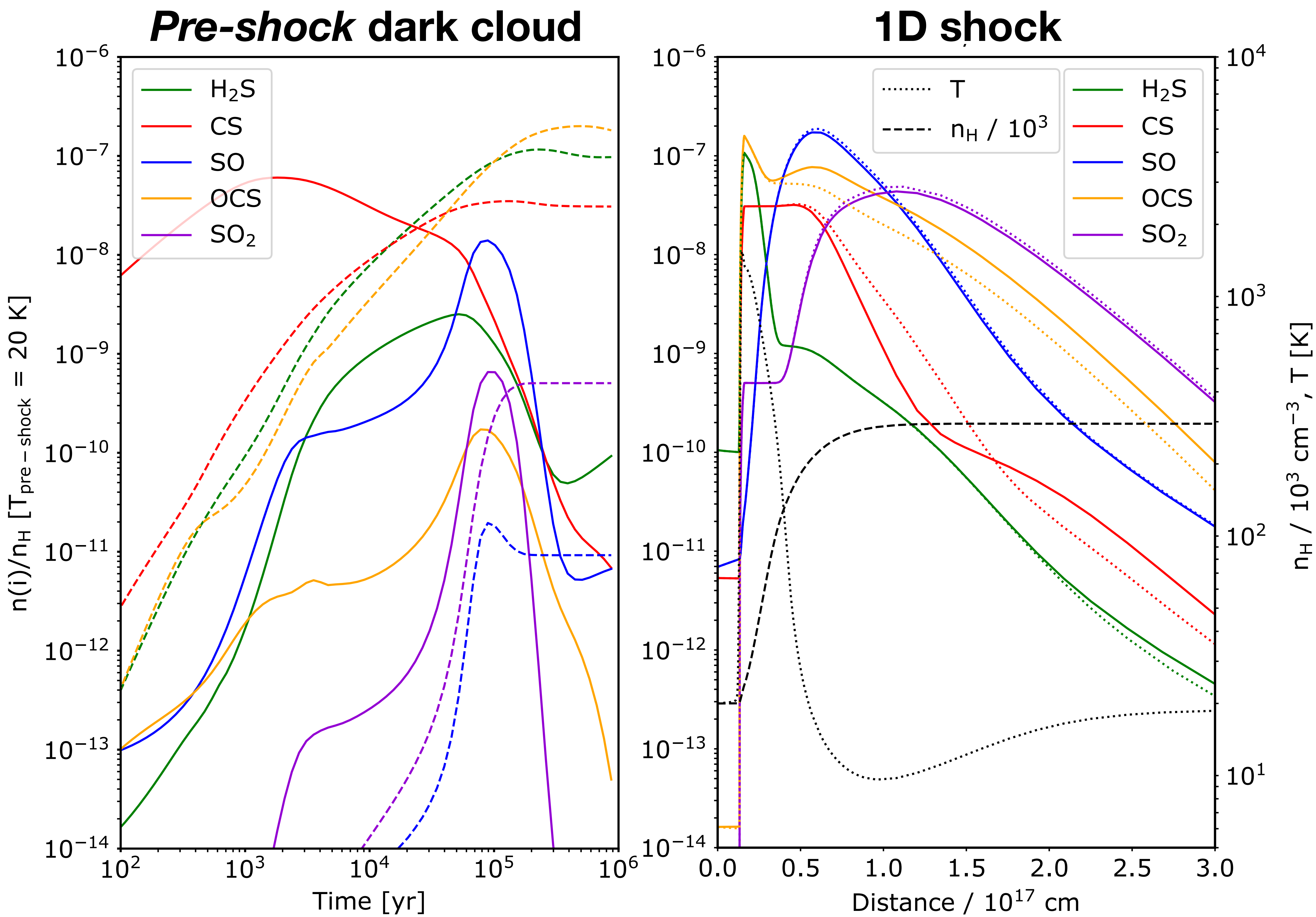
Decomposition of the outflows based on their molecular emission only:

- *K-Means* algorithm
- 9 *features* (mom. 0, 1, and 2 of OCS, SO, and SiO)
- Spatial information not used
- Number of *clusters K* as input



Chemical interpretation

OCS and H_2S should trace shock fronts whereas SO_2 more abundant in post-shock regions, SO and CS are present in and behind shock fronts



Methanol deuteration in low-mass protostars

Taquet, Bianchi, Codella, Persson, Ceccarelli et al. (A&A, in press)

Gas phase [D]/[H] in dark clouds

Methanol and water are formed through hydrogenation reactions on cold interstellar grains

→ their deuteration highly depends on atomic [D]/[H] in the gas

Key reaction for deuterium chemistry:

$$H_3^+ + HD \rightleftharpoons H_2D^+ + H_2 + \Delta E = 232\ K$$

Deuteration in the gas (and in ices) is governed by:

- Temperature
- CO abundance
- Ortho/para ratio of H_2
- Moment of formation

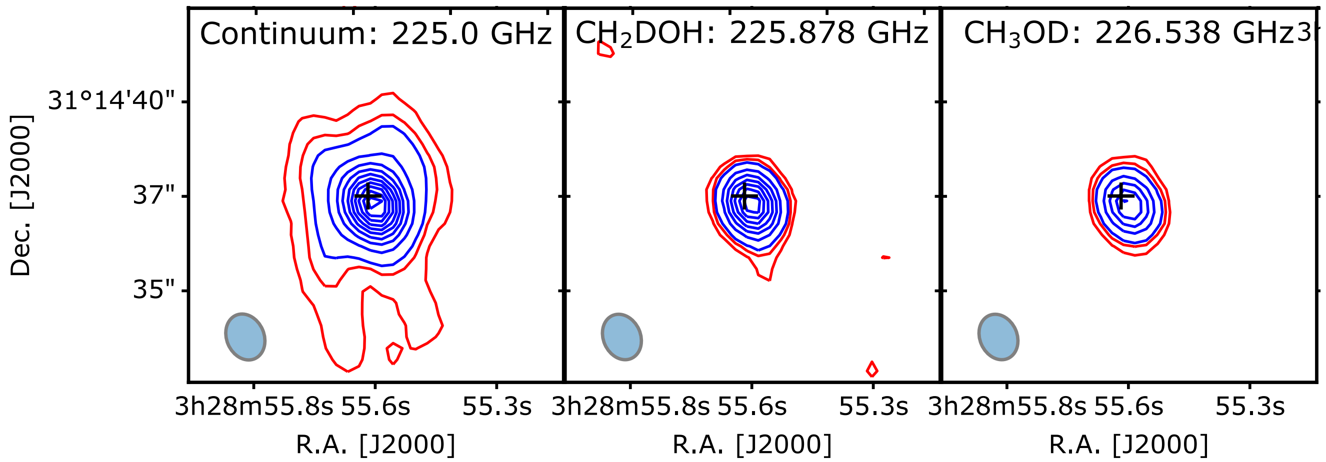
Deuteration: powerful chemical tracer !

See Pagani et al. (1992); Roberts et al. (2003, 2004); Flower et al. (2006); Hugo et al. (2009), …

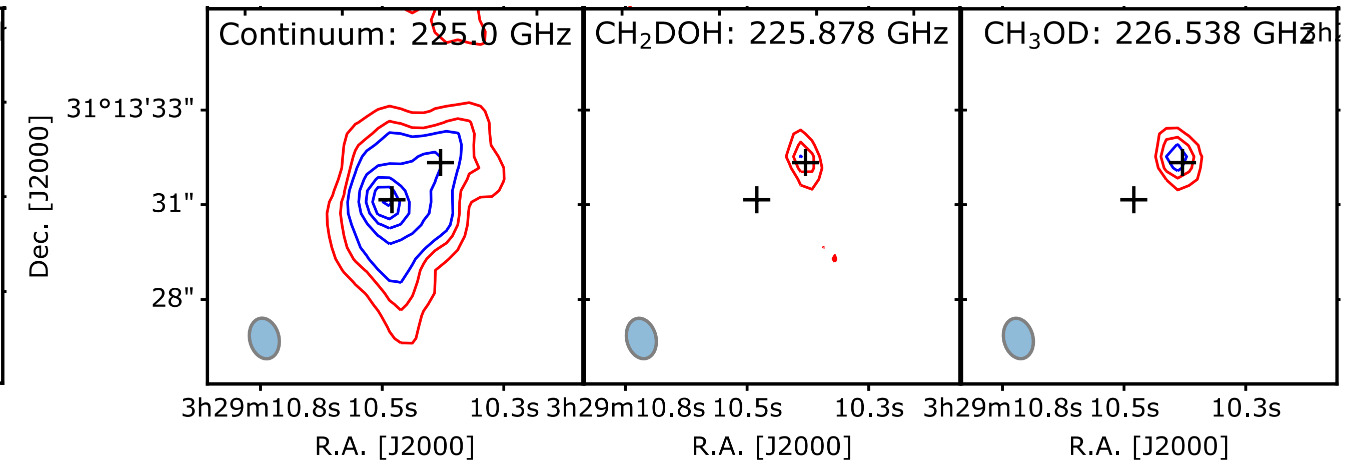
Warm deuterated methanol towards low-mass protostars

Analysis of NOEMA and ALMA observations towards four low-mass protostars in different molecular clouds: Perseus, Orion, Ophiuchus

IRAS2A (Perseus) with NOEMA

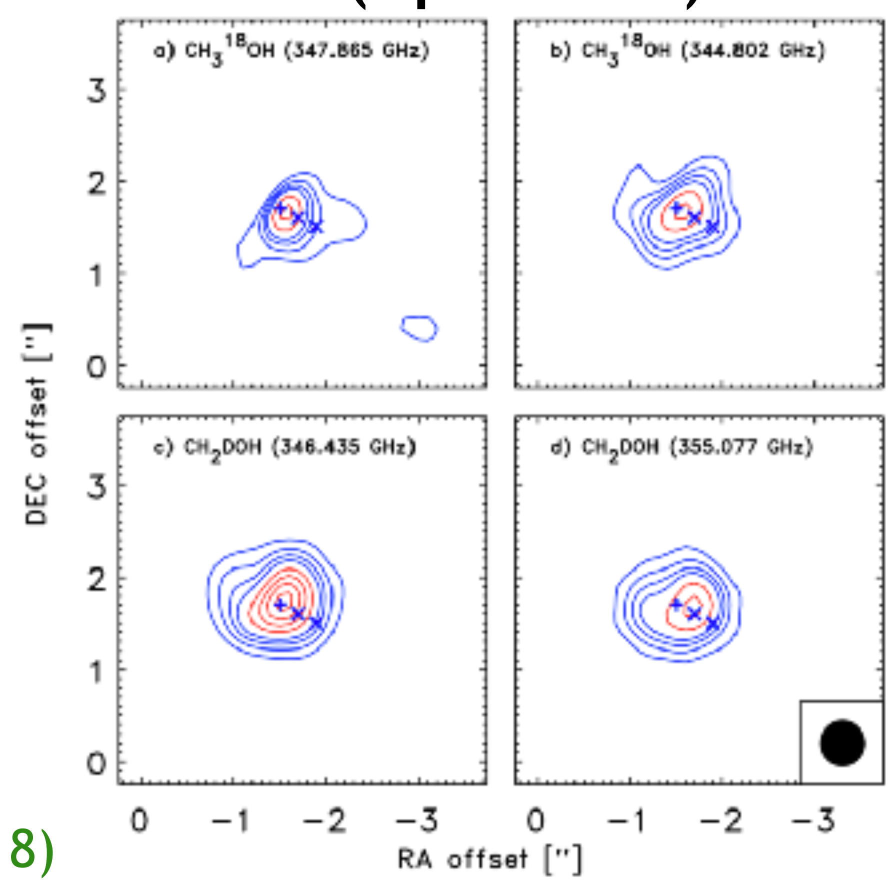


IRAS4A (Perseus) with NOEMA

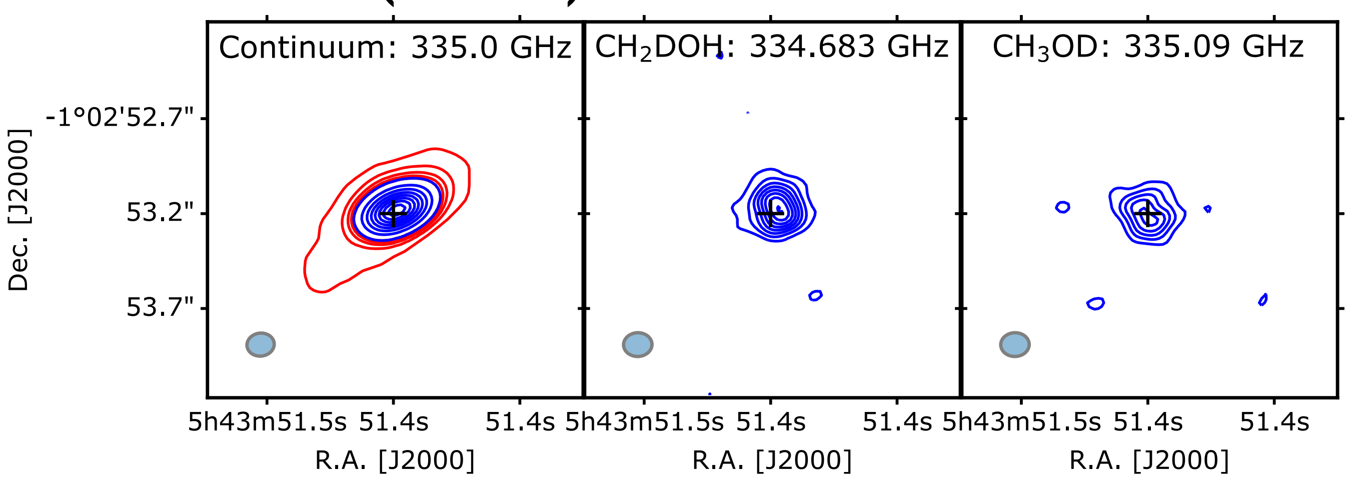


Taquet et al. (2019, in press)

IRAS 16293-B (Ophiuchus) with ALMA



HH212 (Orion) with ALMA

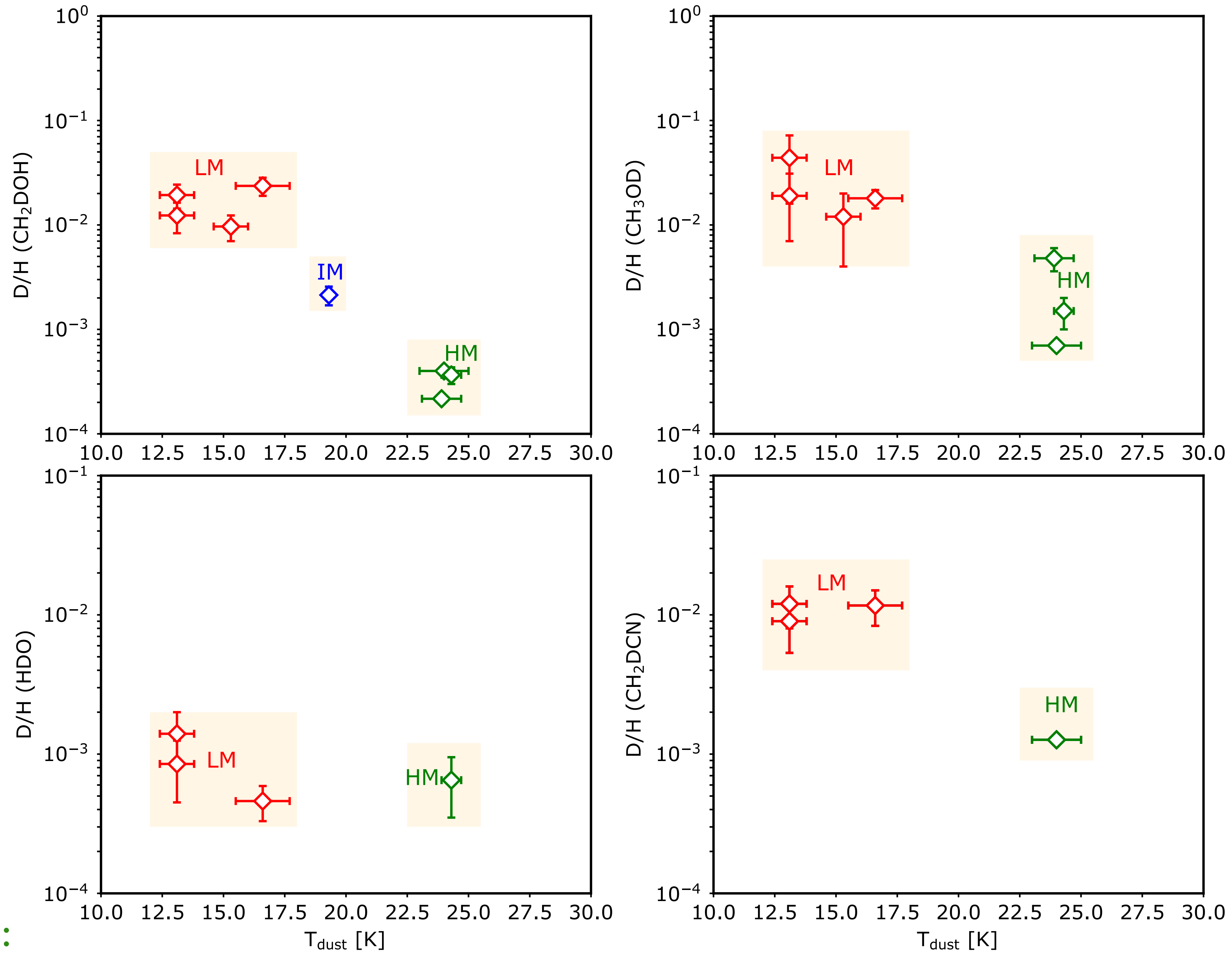


Bianchi et al. (2017),
Taquet et al. (2019, in press)

Jørgensen et al. (2018)

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 ?

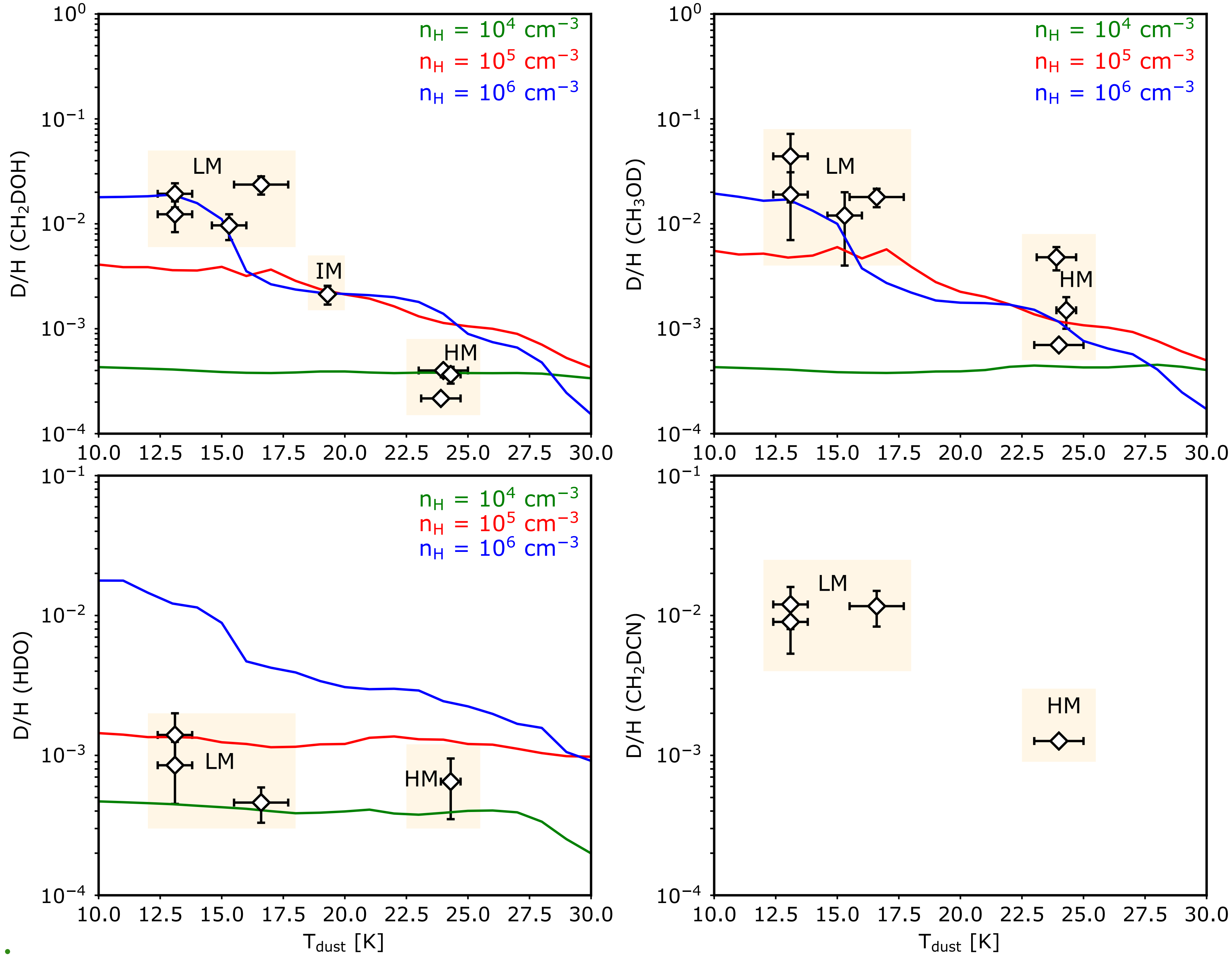


Taquet et al. (in press):
Observed data from **Peng**+ (2012, **OrionKL**), **Fuente**+ (2014, **NGC7129**), **Bianchi**+ (2017, **HH212**), **Belloche**+ (2016, **SgrB2**), **Bøgelund**+ (2018, **NGC6334**), **Jørgensen**+ (2018, **IRAS16293**)

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, warm ice or gas phase chemistry) at work ?



Taquet et al. (in prep.):
Predictions with the **Taquet**+ (2014) model but with constant physical conditions

MOMICE: MOdel for Multiphase Ice ChEmistry

Fortran90 code accompanied by Python scripts to run and analyse the simulations:

http://github.com/vtaquet/momice

Three networks:

- Network 1: H_2O, CO_2, and CH_3OH formation without gas phase chemistry
- Network 2: ice deuteration
- Network 3: extended surface + KIDA gas phase networks

Four options:

1) Invididual simulations with constant physical conditions
2) Spatial evolution with evolving physical conditions
3) Model grid to explore the impact of physical conditions on ice chemistry
4) Sensitivity analysis to evaluate the impact of surface and chemical parameter uncertainties on ice chemistry

"Astronomical" and "experimental" versions

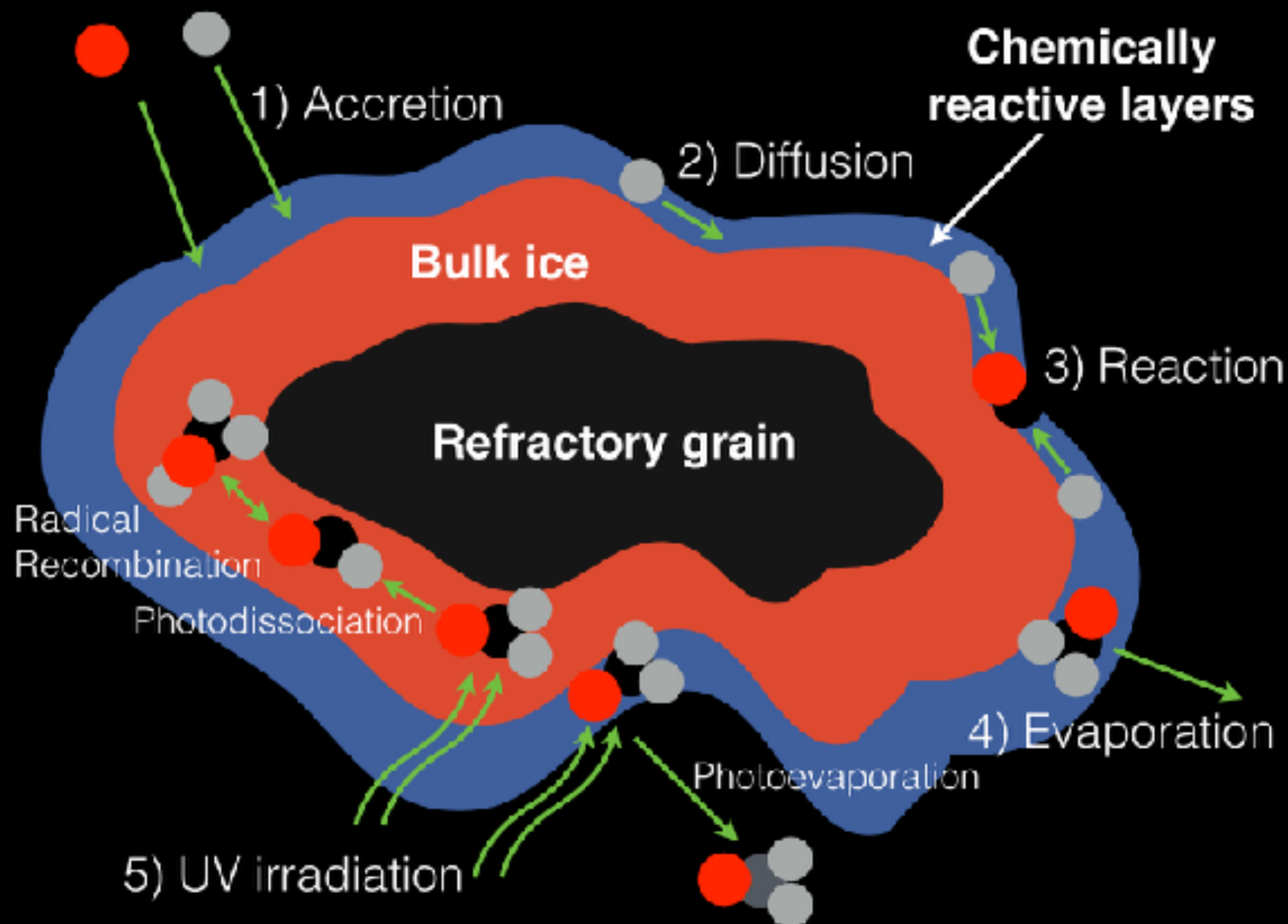
Processes included in the model

MOMICE multi-phase (bulk, surface, gas) astrochemical model

Taquet et al. (2012, 2013, 2014, 2016); Dulieu et al. (2018)

1) Gas phase chemical network **based on KIDA database**

2) Gas-grain processes



Constraining the models with experiments

Chemical modelling of laboratory experiments:

→ validation of the formalism **and** constraints on surface/chemical parameters

Example for CO hydrogenation (**Watanabe** et al. 2004 and **Fuchs** et al. 2009)

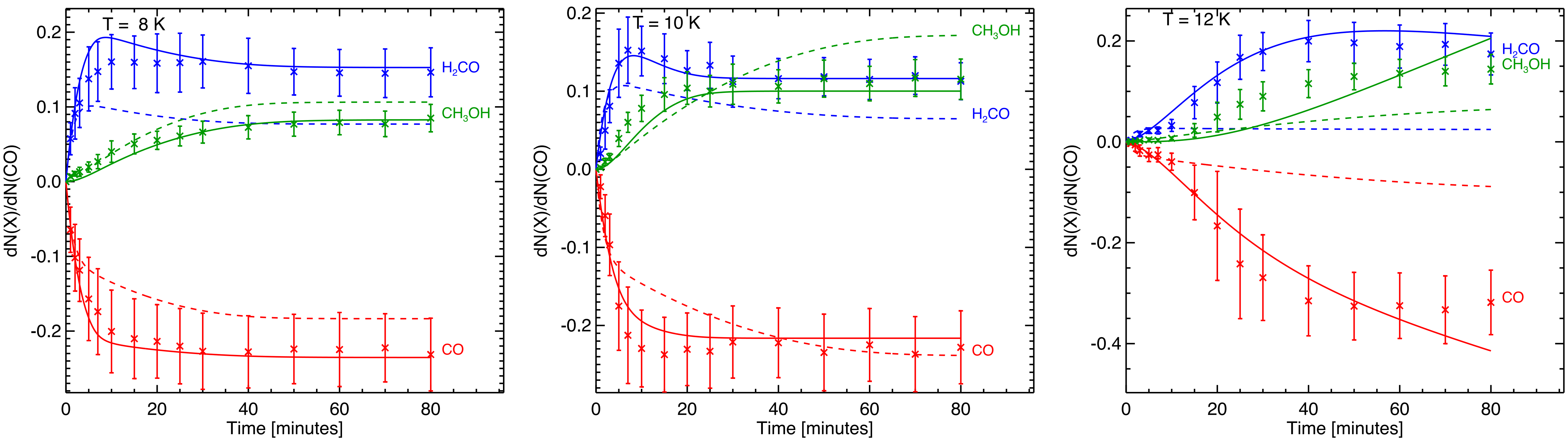
$E_d/E_b = 0.45 \pm 0.05$

$E_a(CO+H\text{->}HCO) = 4000 \pm 500$ K

$E_a(H_2CO+H\text{->}HCO+H_2) = 4000 \pm 250$ K

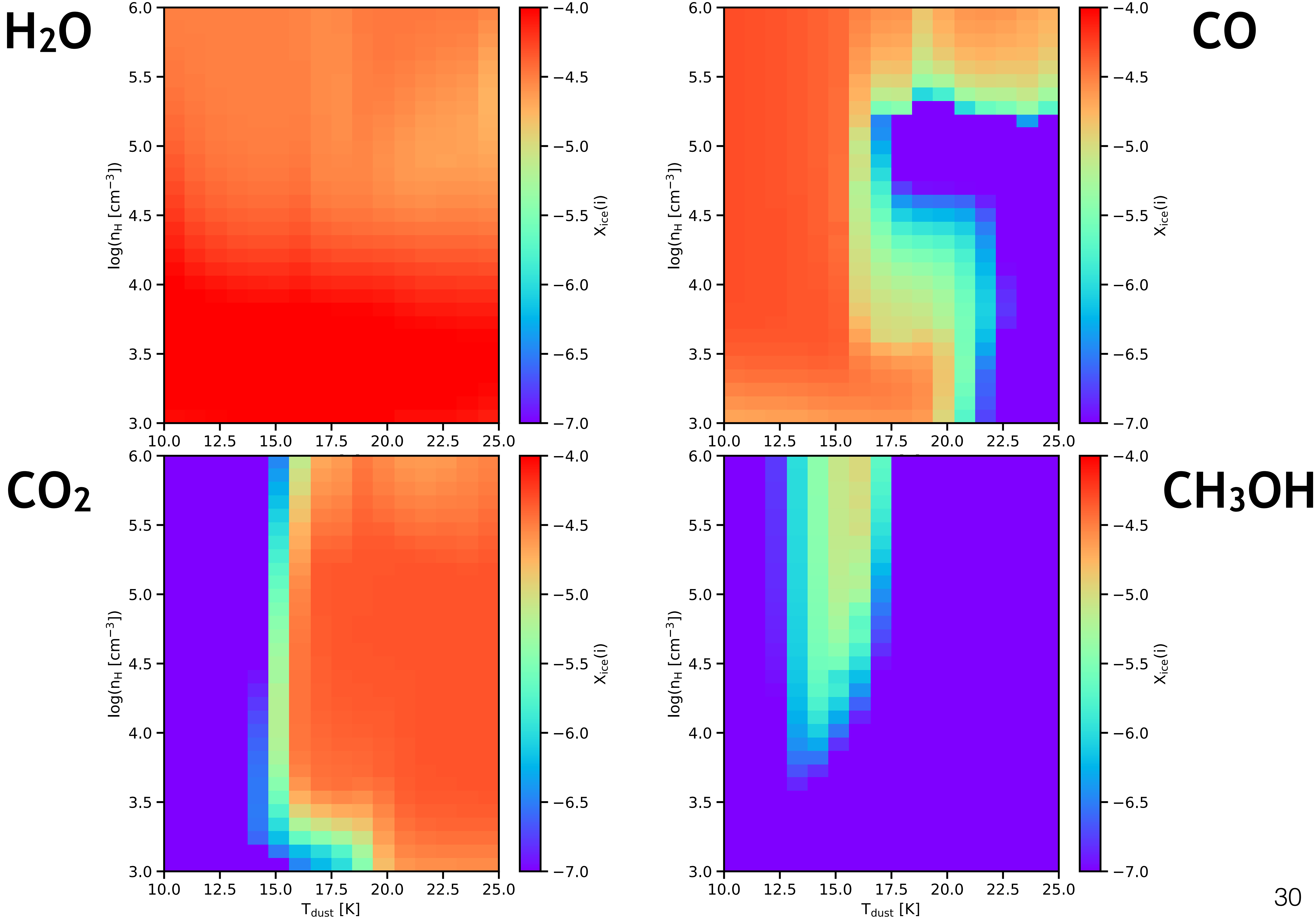
$E_a(H_2CO+H\text{->}CH_3O) = 4750 \pm 250$ K

Flux = 5×10^{14} cm^{-2} s^{-1}



Experiments from Watanabe et al. (2004)

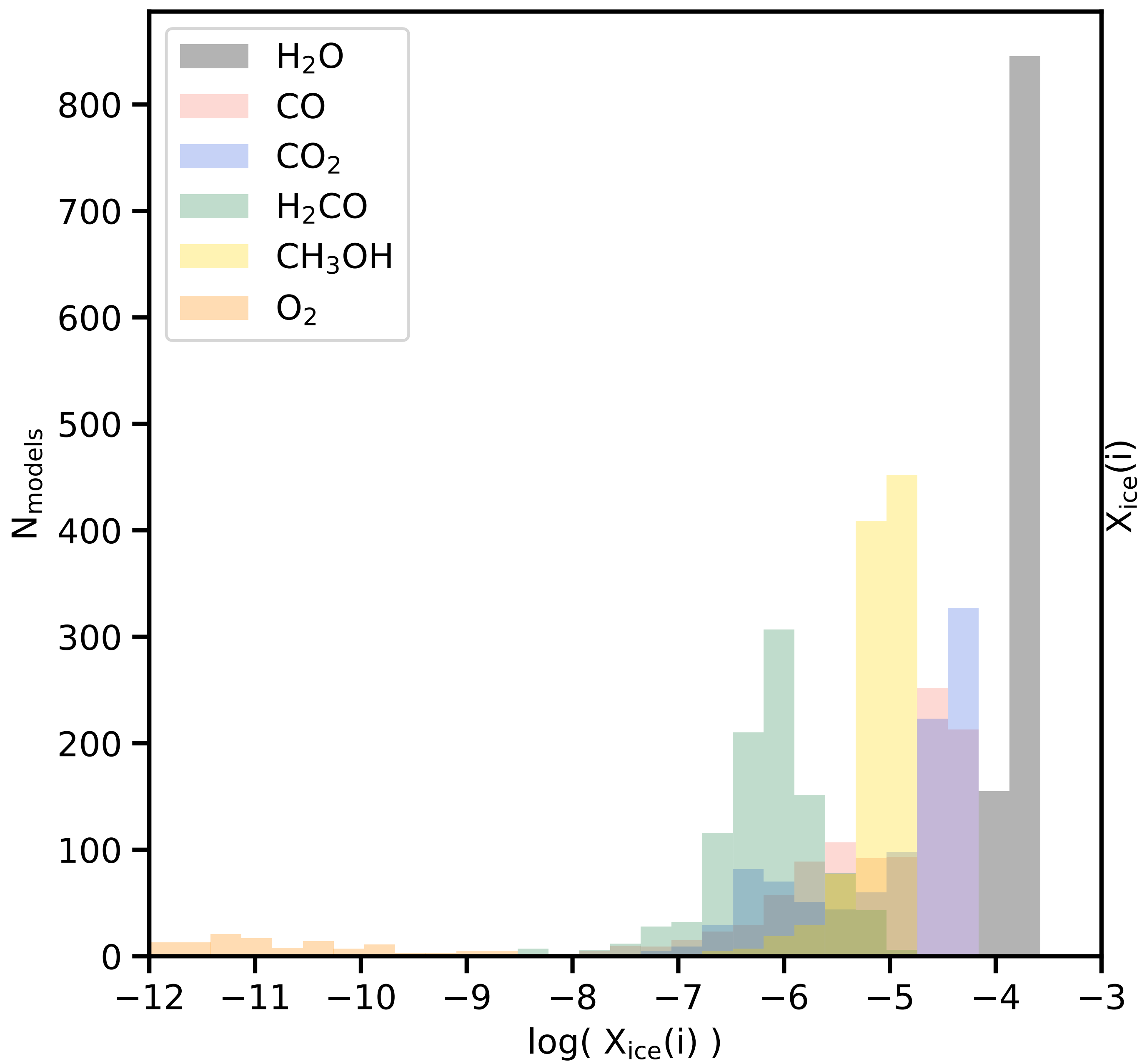
Impact of physical conditions on ice composition

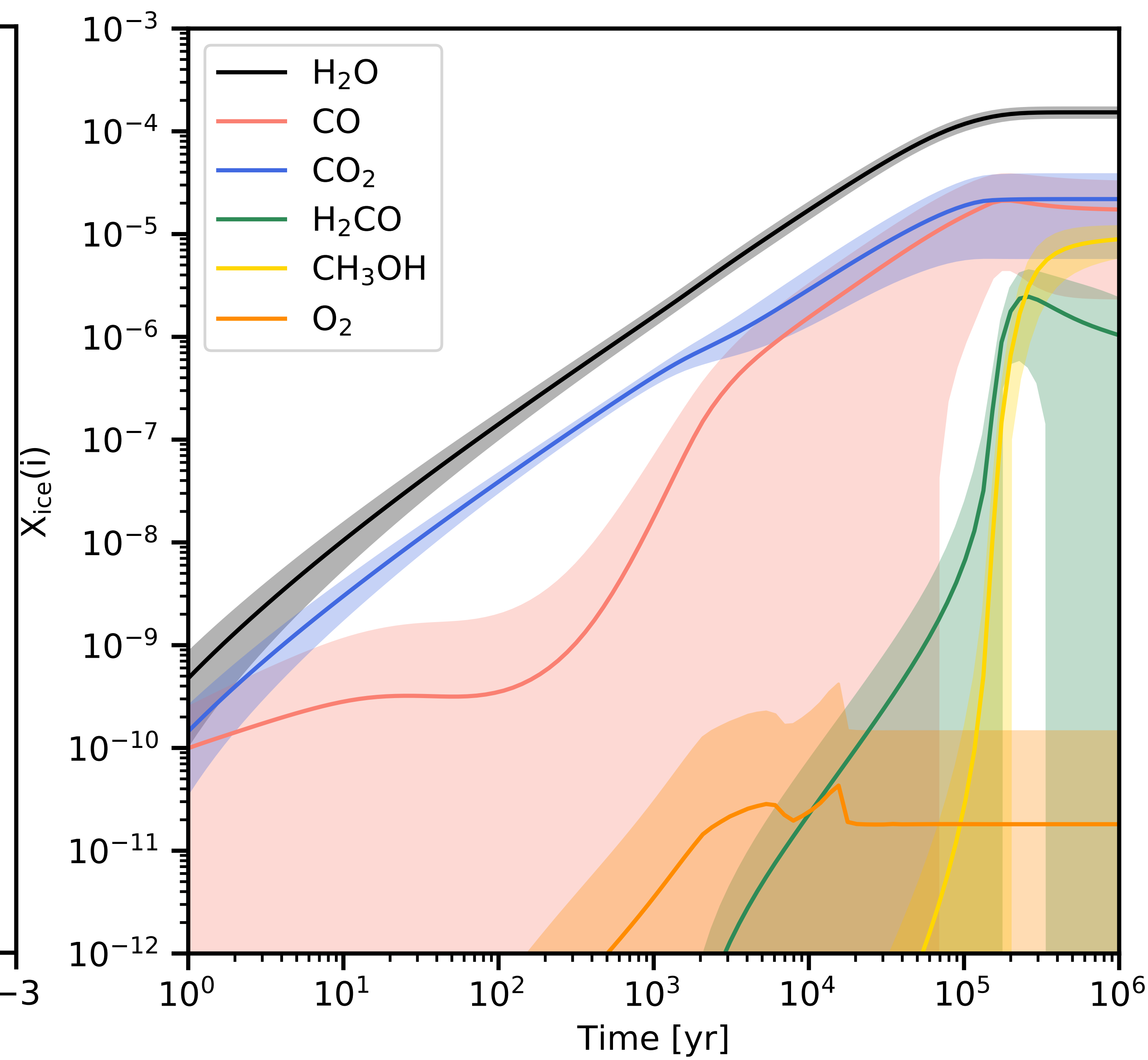


Impact of uncertainties on ice composition

10% uncertainty on binding energies, diffusion-to-binding energy ratio, and activation energies

$n_H = 2x10^4\ cm^{-3}$, T = 10 K





See recent works by Penteado et al. (2017), Holdship et al. (2018)

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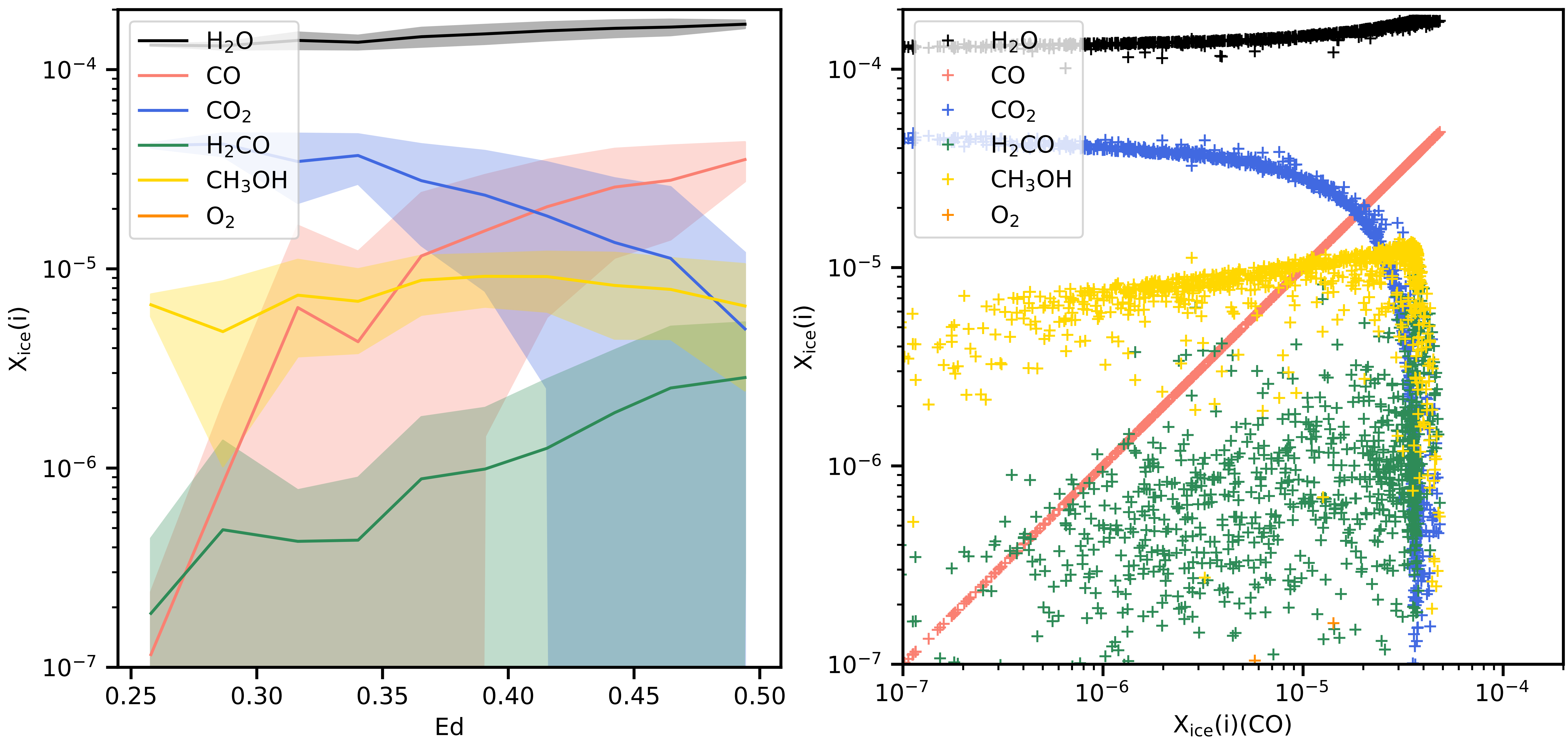

See recent works by Penteado et al. (2017), Holdship et al. (2018)

Main activities during the PROSPECTS project

- ~ 25 publications:
  - 4 first-author publications
  - 11 others with significant contributions

- Oral contributions:
  - 4 seminars
  - 5 invited talks

- Visits and collaborations:
  - Two visits at Paris Observatory (F. Dulieu)
  - Many visits at University of Grenoble (C. Ceccarelli)
  - Collaborations with Leiden Observatory, NASA Goddard