HOW LABORATORY ICE EXPERIMENTS ENABLE OBSERVATIONAL ANALYSIS OF STAR AND PLANET FORMATION

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Ices form in molecular clouds
& evolve during star formation.
(Pre-)stellar core
T ~ 20 K
T ~ 10 K
Protostar
T ≳100 K
Dense molecular cloud
Protoplanetary disk
Solar System
T ~ 10-10,000 K
Are ices inherited
or totally reset?
Image credits: NASA (L), Bill Saxton, NRAO, L. I. Cleeves (R)
Diffuse ISM

Goals of laboratory experiments

Ice identification & optical properties

- Abundant ices & rarer complex organic molecules (COMS)
- Determination of optical constants for modeling

Ice physical structure

- Measuring grain sizes & porosity

Ice chemical environment

- Efficiency of formation pathways
- Measuring reaction rates

Ice processing

- Thermal & irradiation evolution
- Mass loss rates
- Desorption temperatures

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Outline of talk

Historical ice experiments

- Growing astrophysical ice analogs
- Techniques for characterizing ices
- Common experimental sequences

Applications to JWST data

- Physical structure
- Chemical environment
- Thermal processing

Future laboratory ice needs

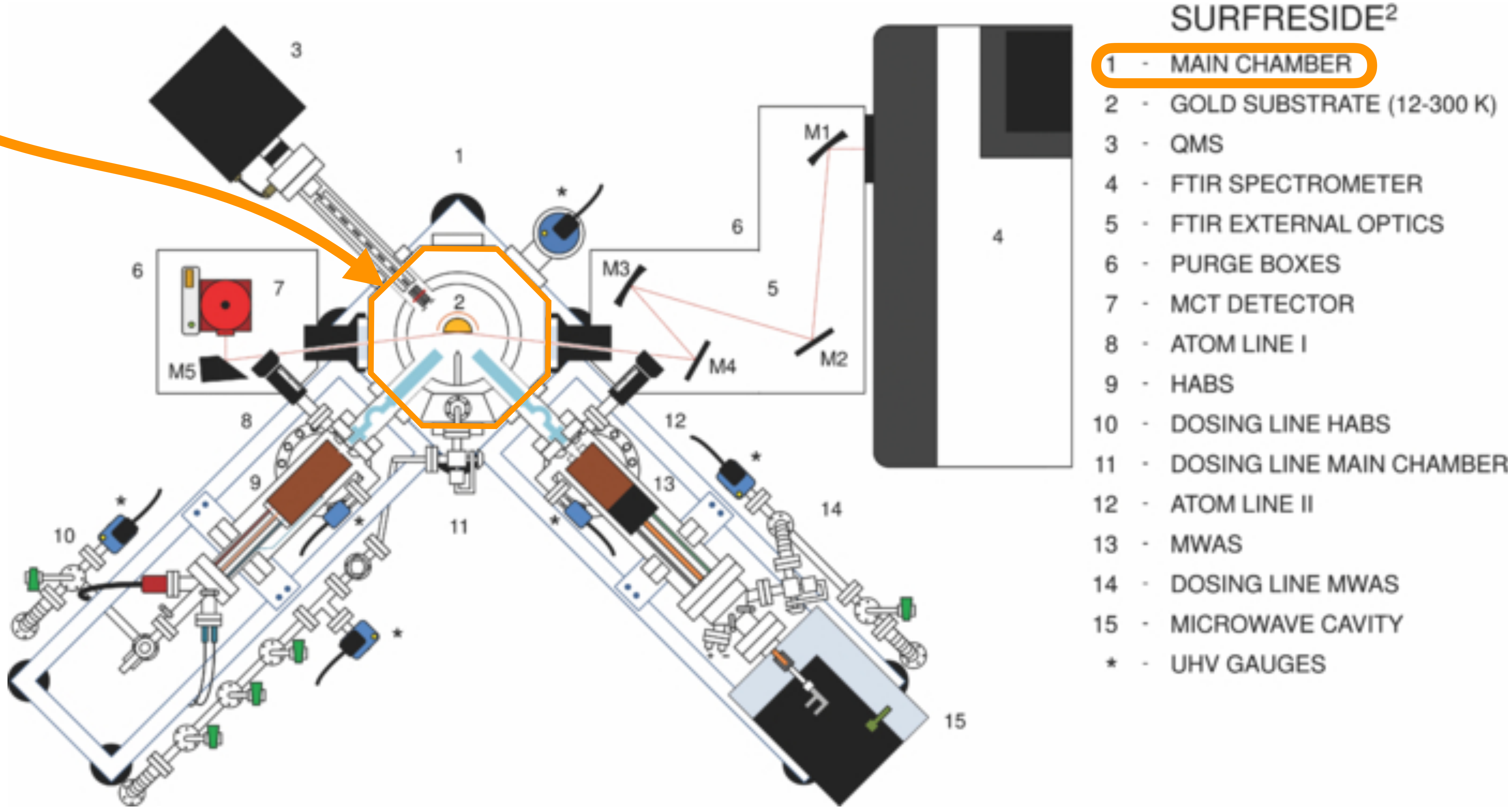
- Exploration of thermal cycling
- Trapping with larger molecular sizes
- Interactions with silicates

Growing astrophysical ice analogs (SURFRESIDE*)

*SURFace REaction SImulation DEvice

Ultra-high vacuum chamber

P~10^{-10} mbar



Ioppolo et al. (2013)

Growing astrophysical ice analogs (SURFRESIDE)

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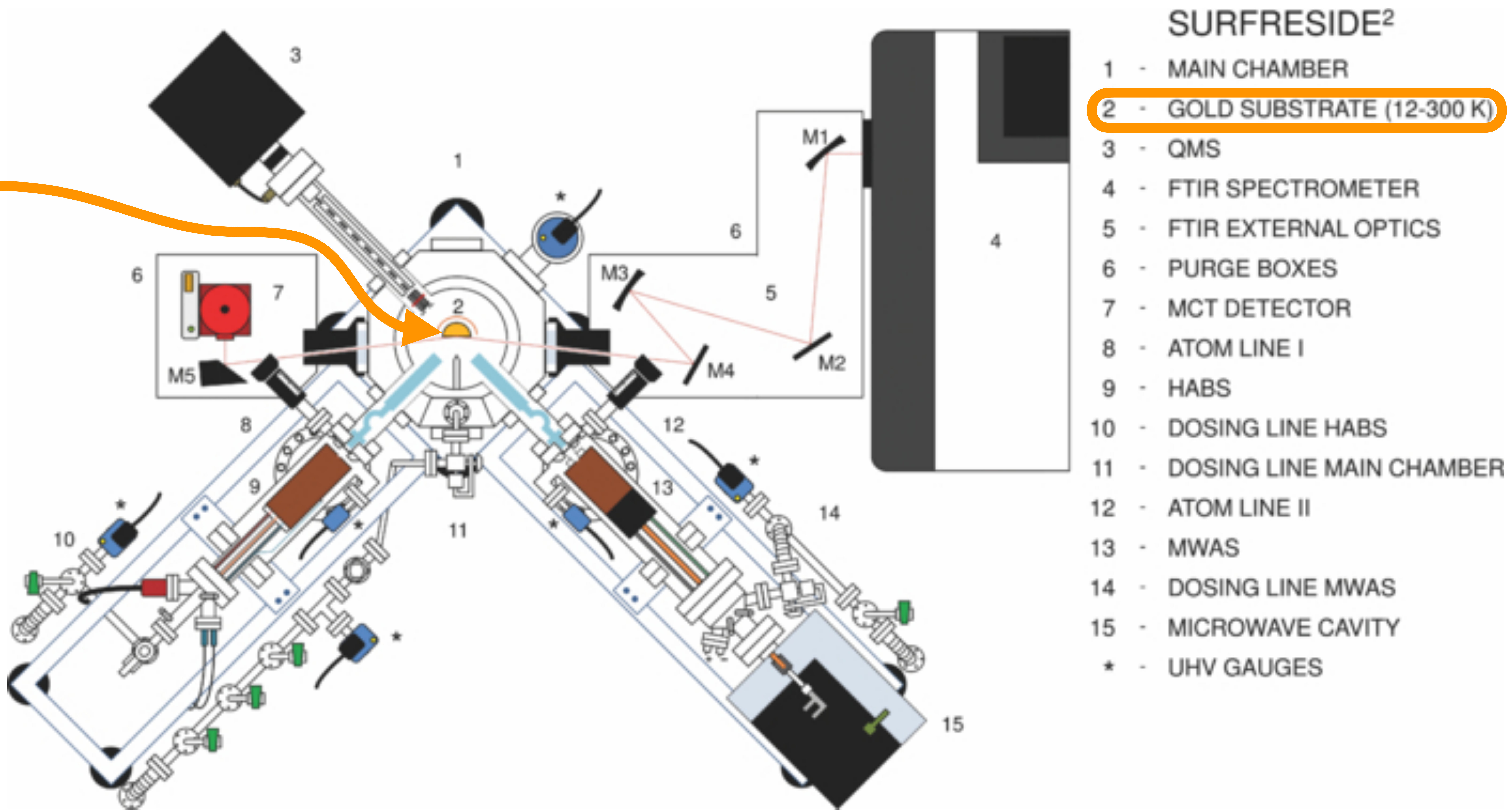
Ultra-high vacuum chamber

P~10^{-10} mbar

Cryogenically cooled substrate

T = 10 K (cloud) -160 K (disks)



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Growing astrophysical ice analogs (SURFRESIDE)

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Ultra-high vacuum chamber

P~10^{-10} mbar

Cryogenically cooled substrate

T = 10 K (cloud) -160 K (disks)

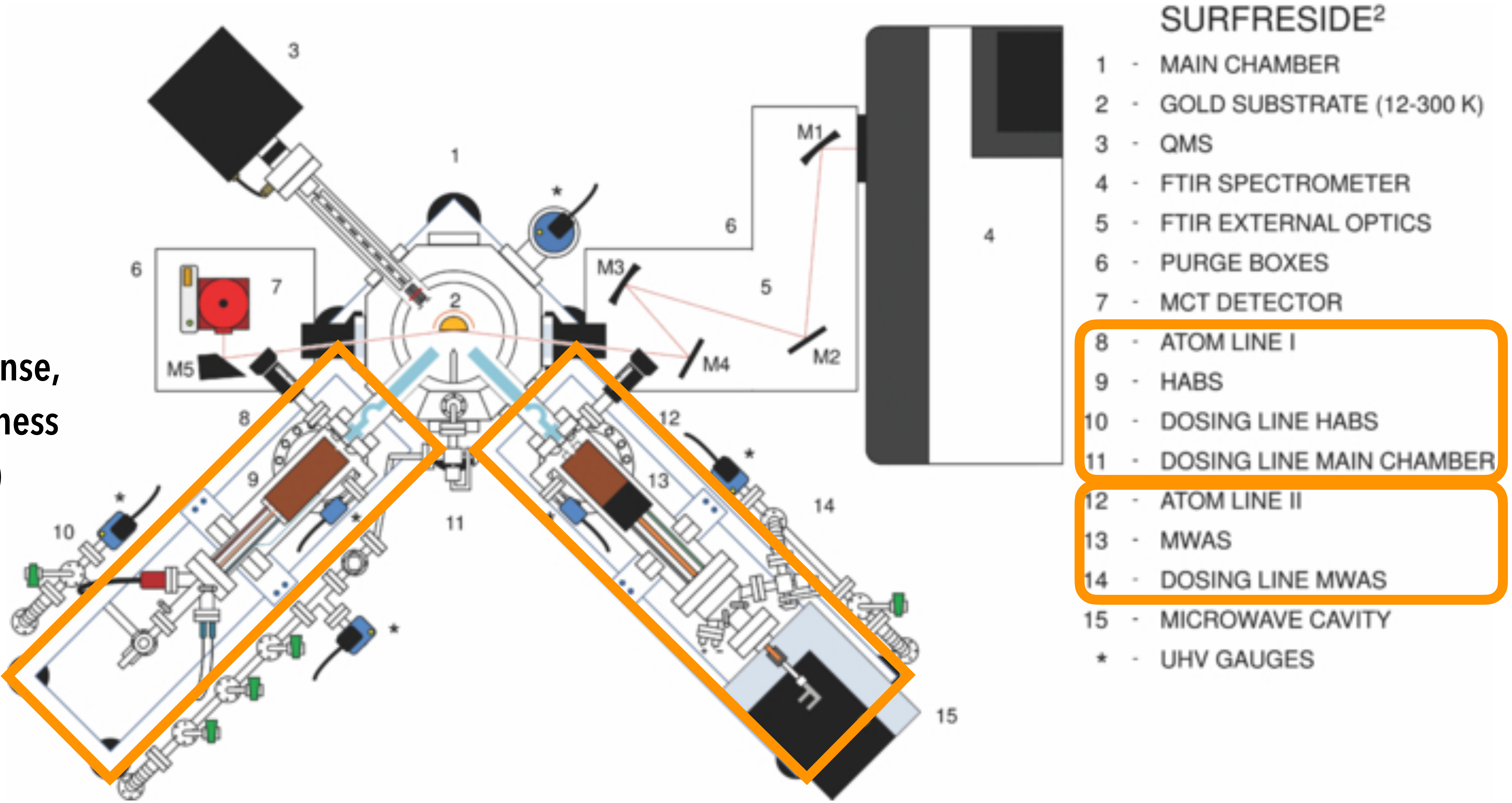
Gas dosing lines

Deposit gas on substrate to condense, strict dosing to control layer thickness

thin layer ≡ <20 monolayers (ML)

typical layer ~4000 ML

Note: Sometimes use laser to measure ice layer thickness, to make optical constants

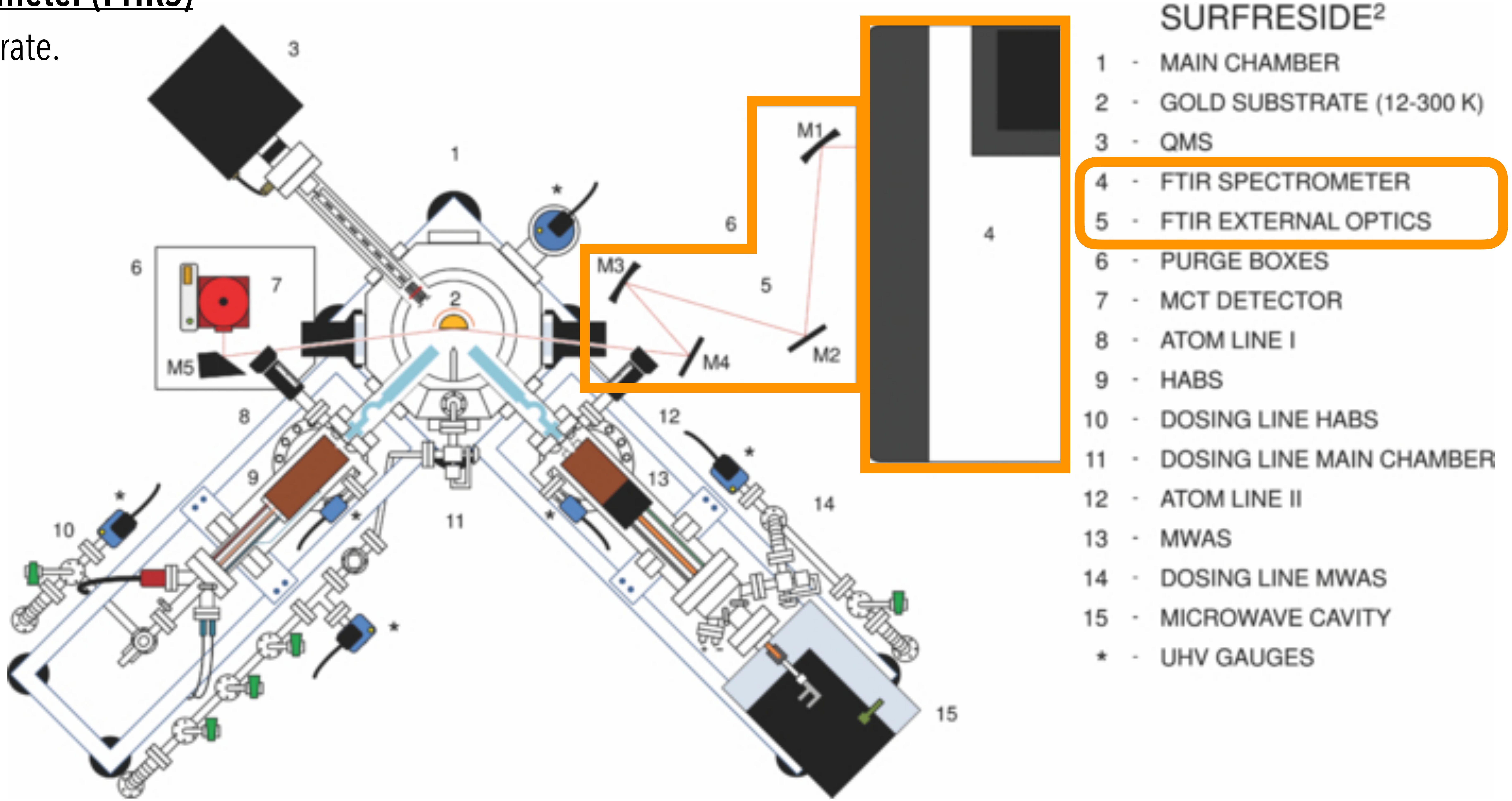


Ioppolo et al. (2013)

Techniques to analyze astrophysical ice analogs

Fourier-Transform InfraRed Spectrometer (FTIRS)

Measures spectra of ice layer on substrate.



Ioppolo et al. (2013)

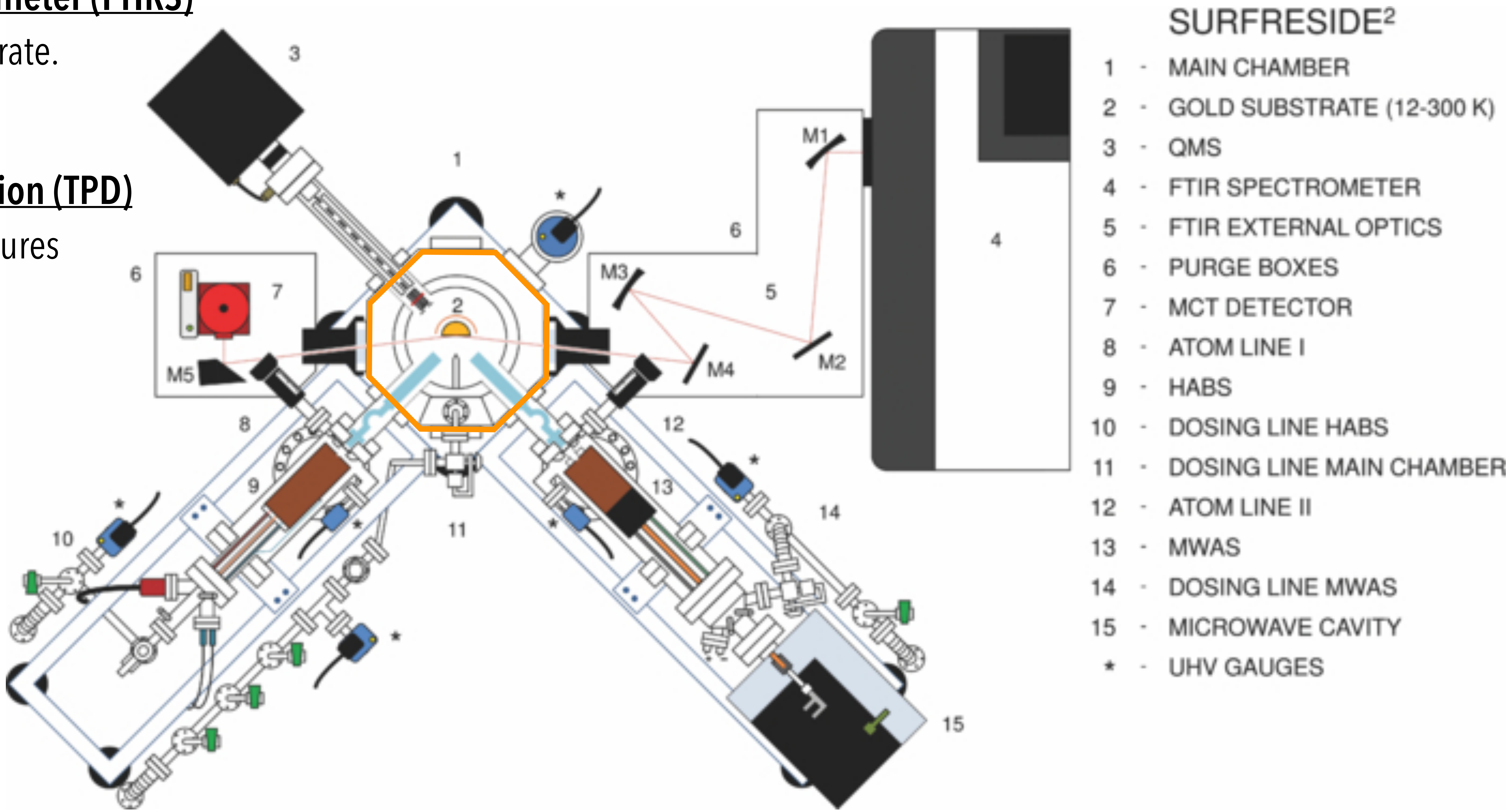
Techniques to analyze astrophysical ice analogs

Fourier-Transform InfraRed Spectrometer (FTIRS)

Measures spectra of ice layer on substrate.

Temperature Programmed Desorption (TPD)

Heats ice to pre-determined temperatures until it desorbs into gas phase.



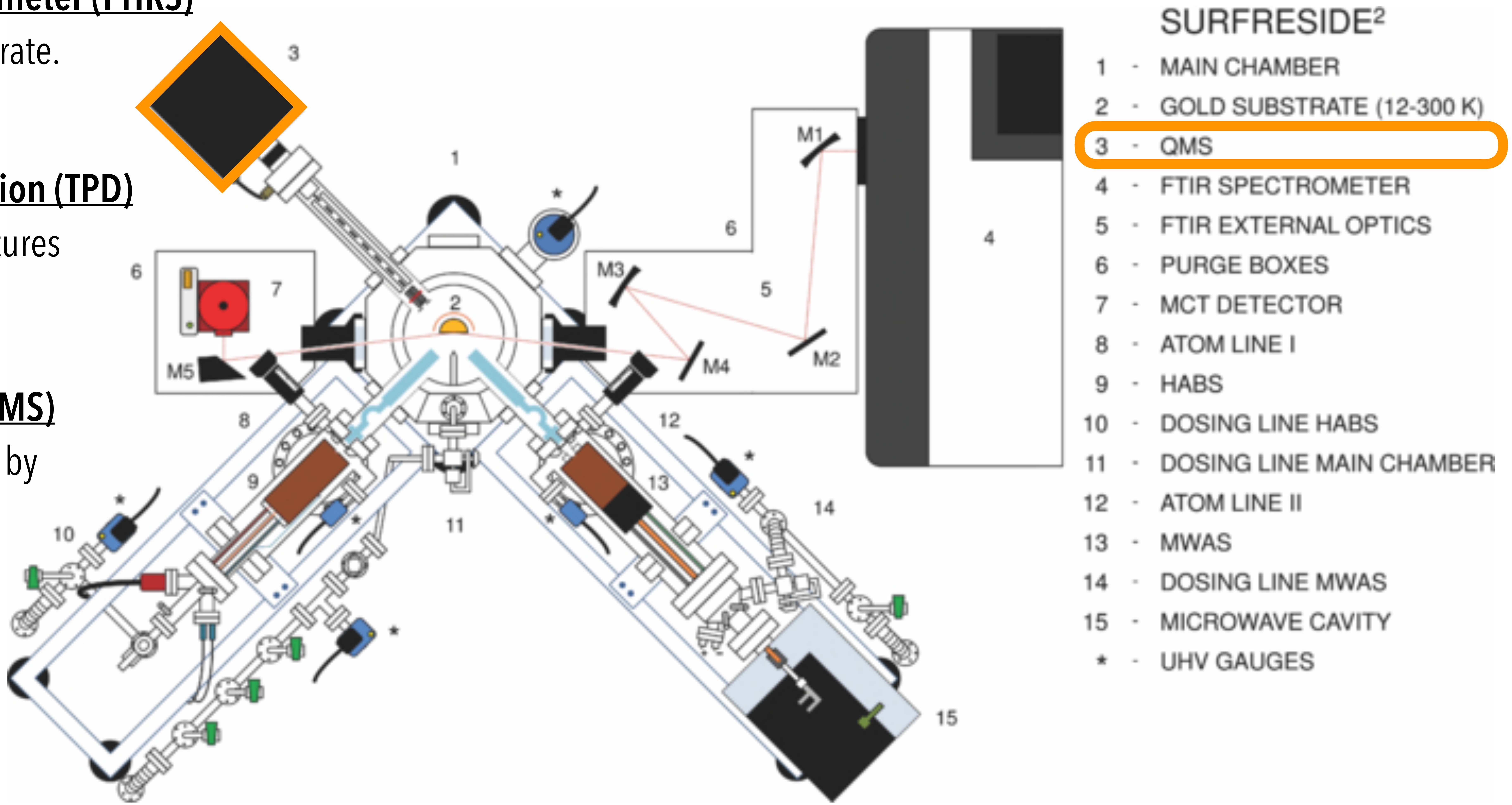
Ioppolo et al. (2013)

Techniques to analyze astrophysical ice analogs

Fourier-Transform InfraRed Spectrometer (FTIRS)
Measures spectra of ice layer on substrate.

Temperature Programmed Desorption (TPD)
Heats ice to pre-determined temperatures until it desorbs into gas phase.

Quadrupole Mass Spectrometer (QMS)
Identified molecules in desorbed gas by mass-to-charge ratio.



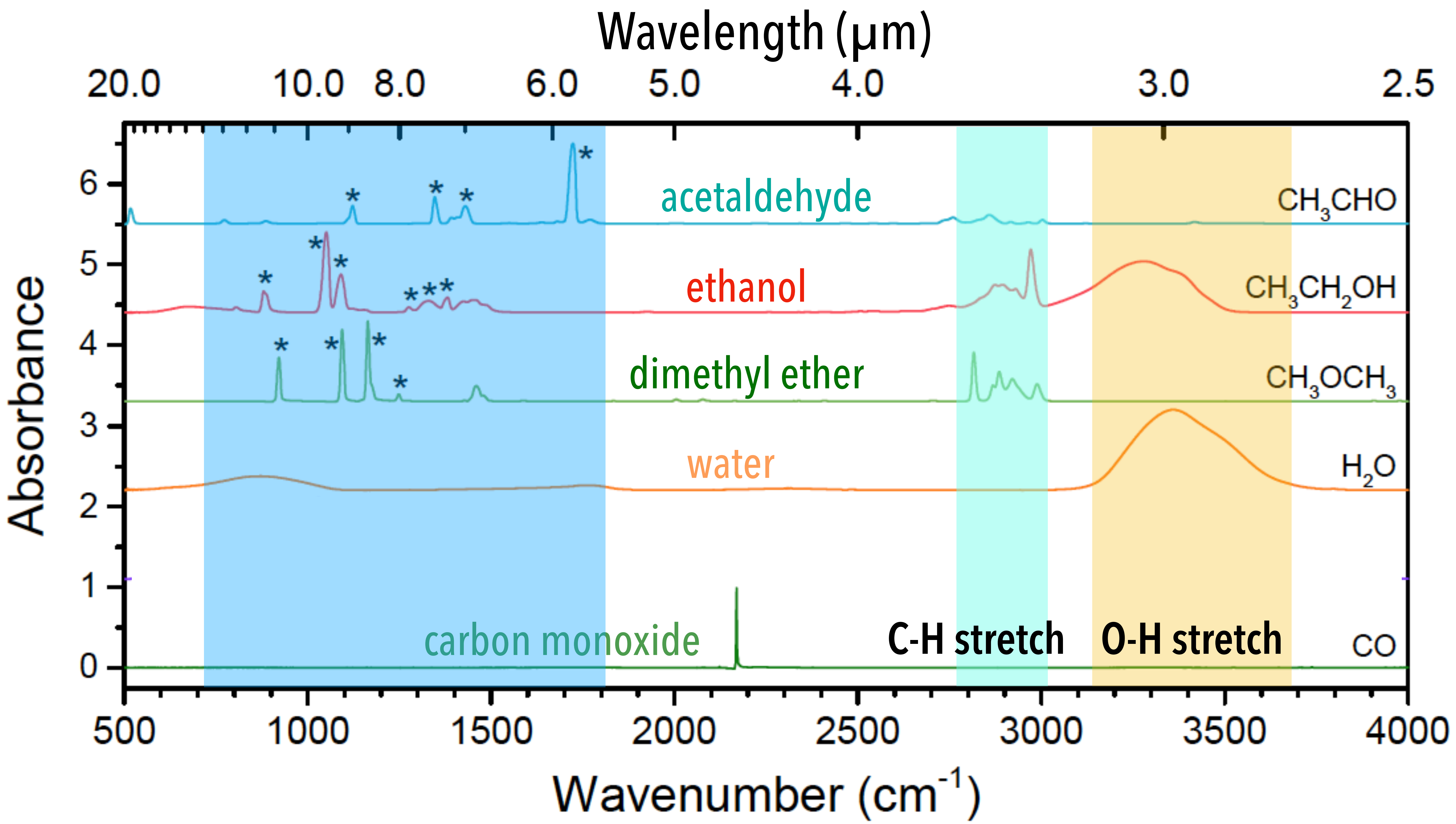
Ioppolo et al. (2013)

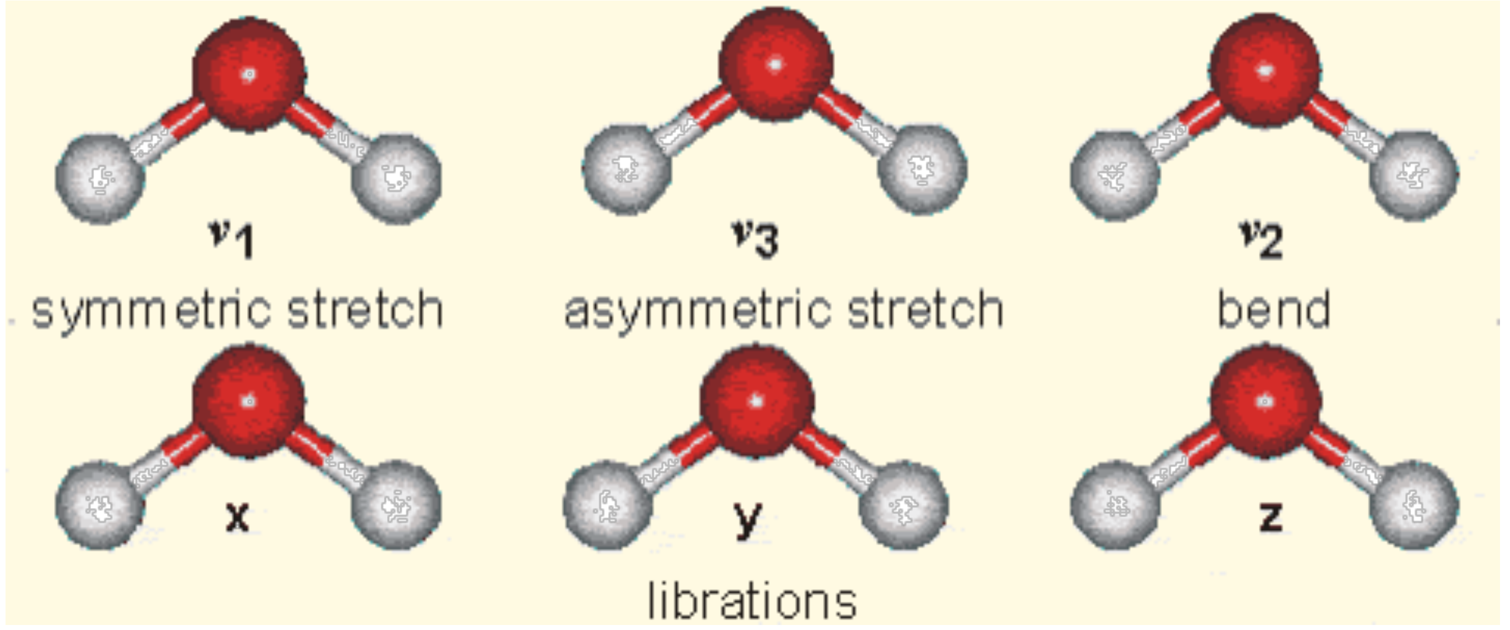
Typical experimental sequences

1. Ice identification

1. Ice identification. Simple ices & complex organic molecules (COMs)

FTIRS





Column density

Absorbance

$$N_X = \frac{\int A_\nu \mathrm{d}\nu}{S_X} [\mathrm{cm}^{-2}]$$

Band strengths

- Atomic motion (e.g. stretches) produce ***"functional groups"*** at similar wavelengths
- Line ratios between all functional groups can identify ices

Terwisscha van Scheltinga et al. (2018), Animation credit: http://www1.lsbu.ac.uk/water/water_vibrational_spectrum.html

Typical experimental sequences

1. Ice identification

2. Ice chemical & physical structure

2. Ice chemical environment. Some ices form faster within H_2O-rich ice matrix.

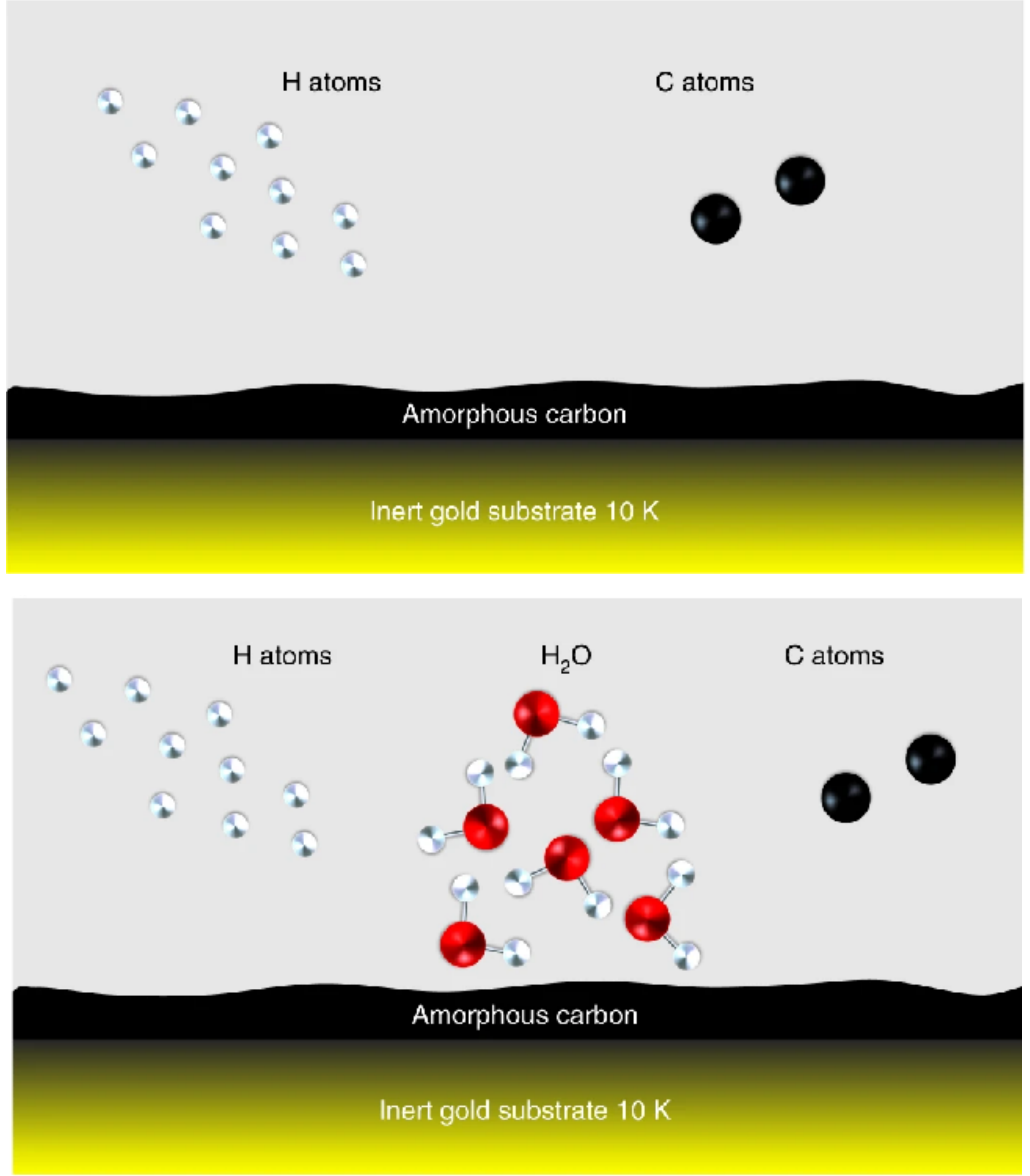
RAIRS + FTIRS

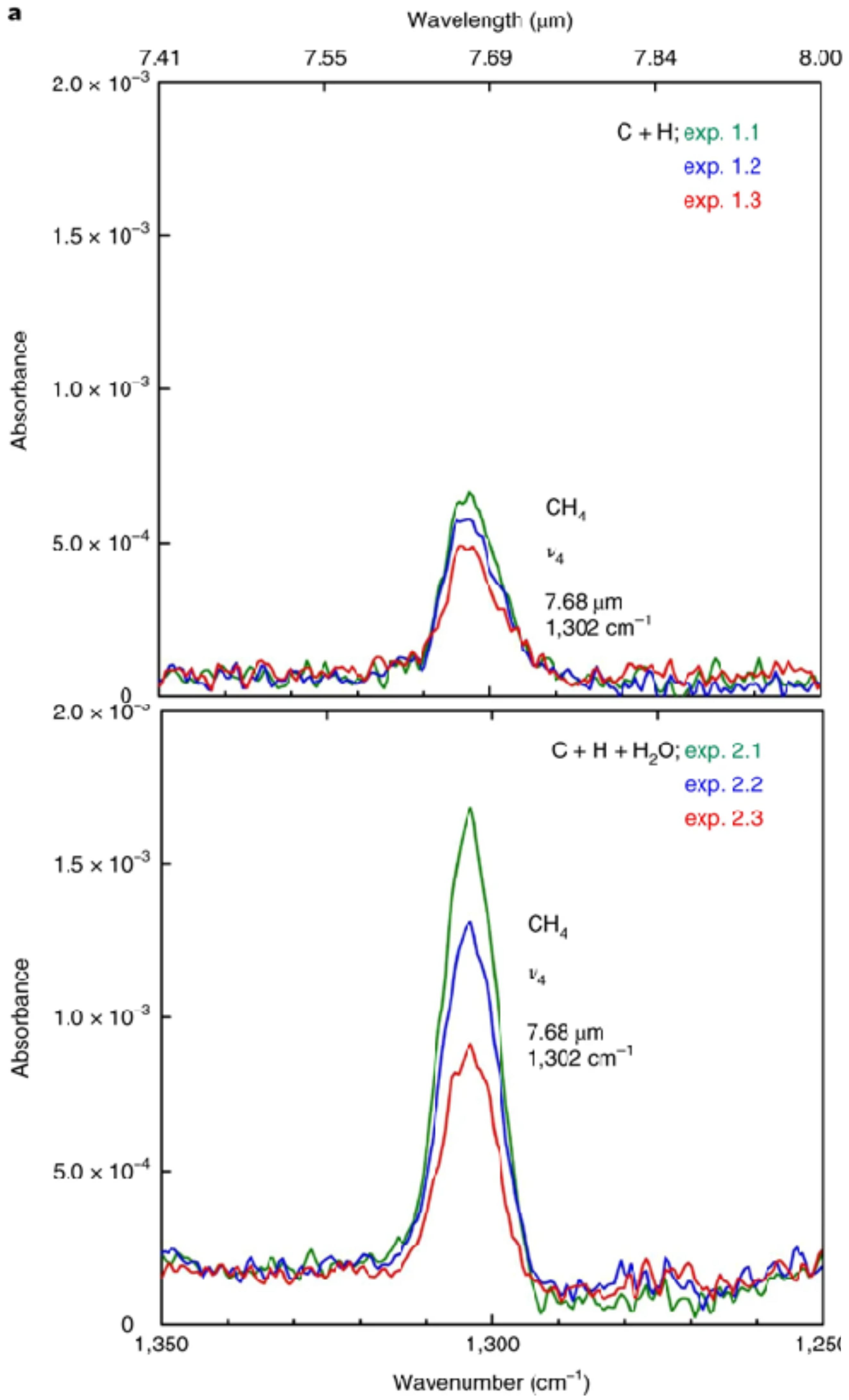
Methane formation pathway #1

$$C + H \longrightarrow \mathbf{CH_4}$$

Methane formation pathway #2

$$C + H + H_2O \longrightarrow \mathbf{CH_4}$$



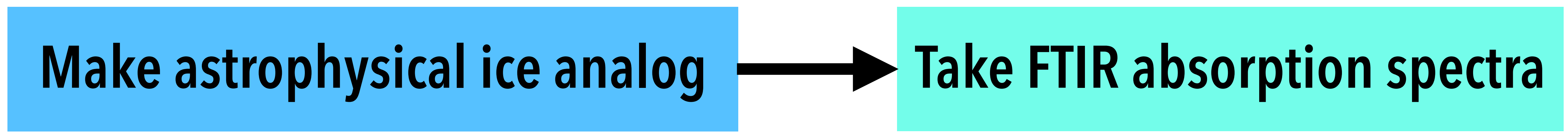


Qasim et al. (2020) *Nature Astronomy*

Yields reaction rates for chemical models.

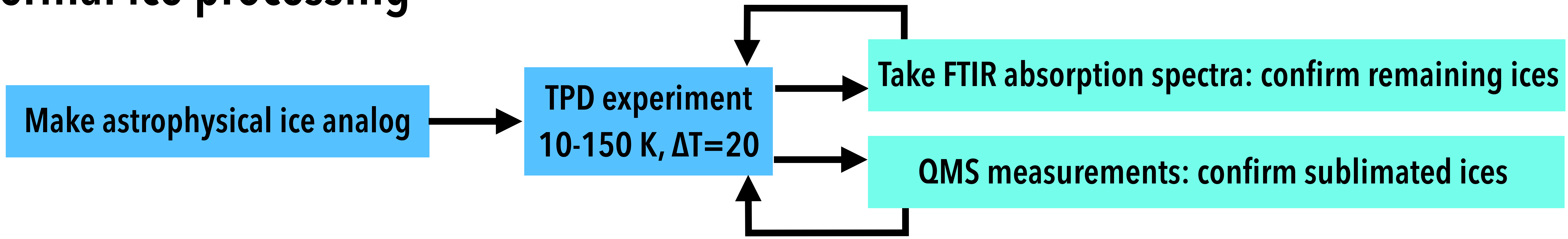
Typical experimental sequences

1. Ice identification



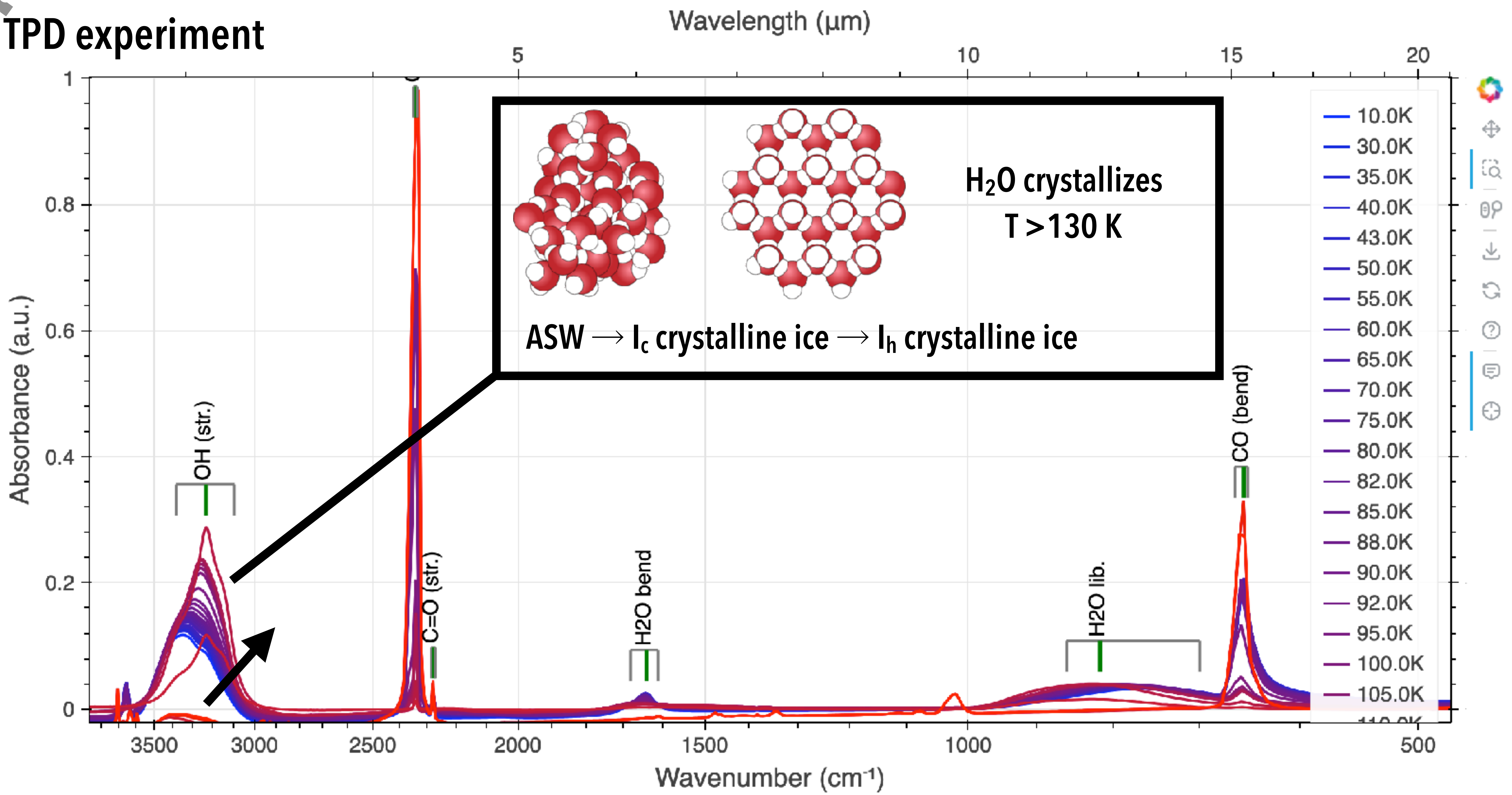
2. Ice chemical & physical structure

3. Thermal ice processing



3. Ice thermal processing. Heating ices shifts profile & reduces amplitude.

TPD experiment



Leiden Ice Database entry for Ehrenfreund et al. (1999): CO_2:H_2O (1:1) ratio, T=10 K - 187 K, Credit: Christopher AuYeung

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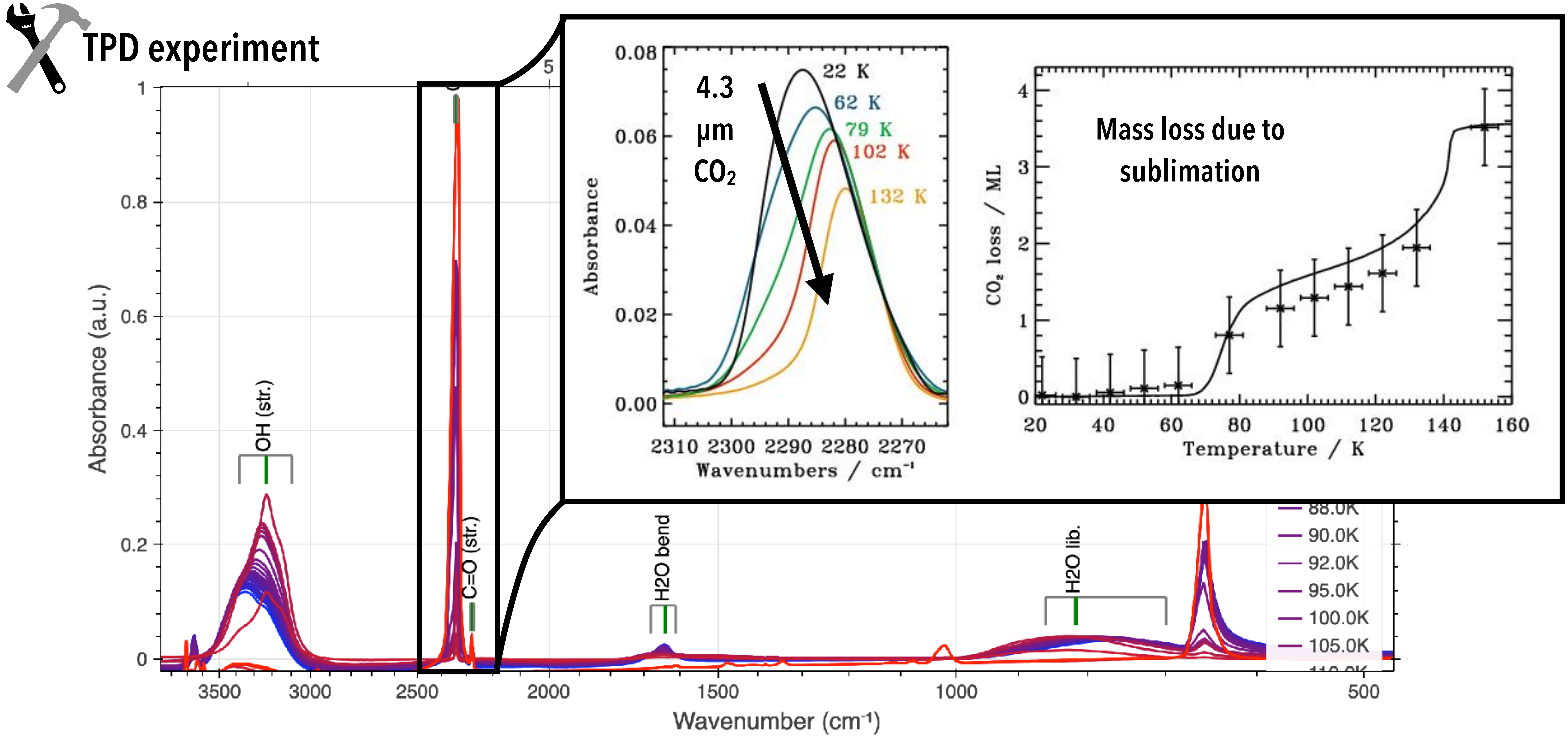
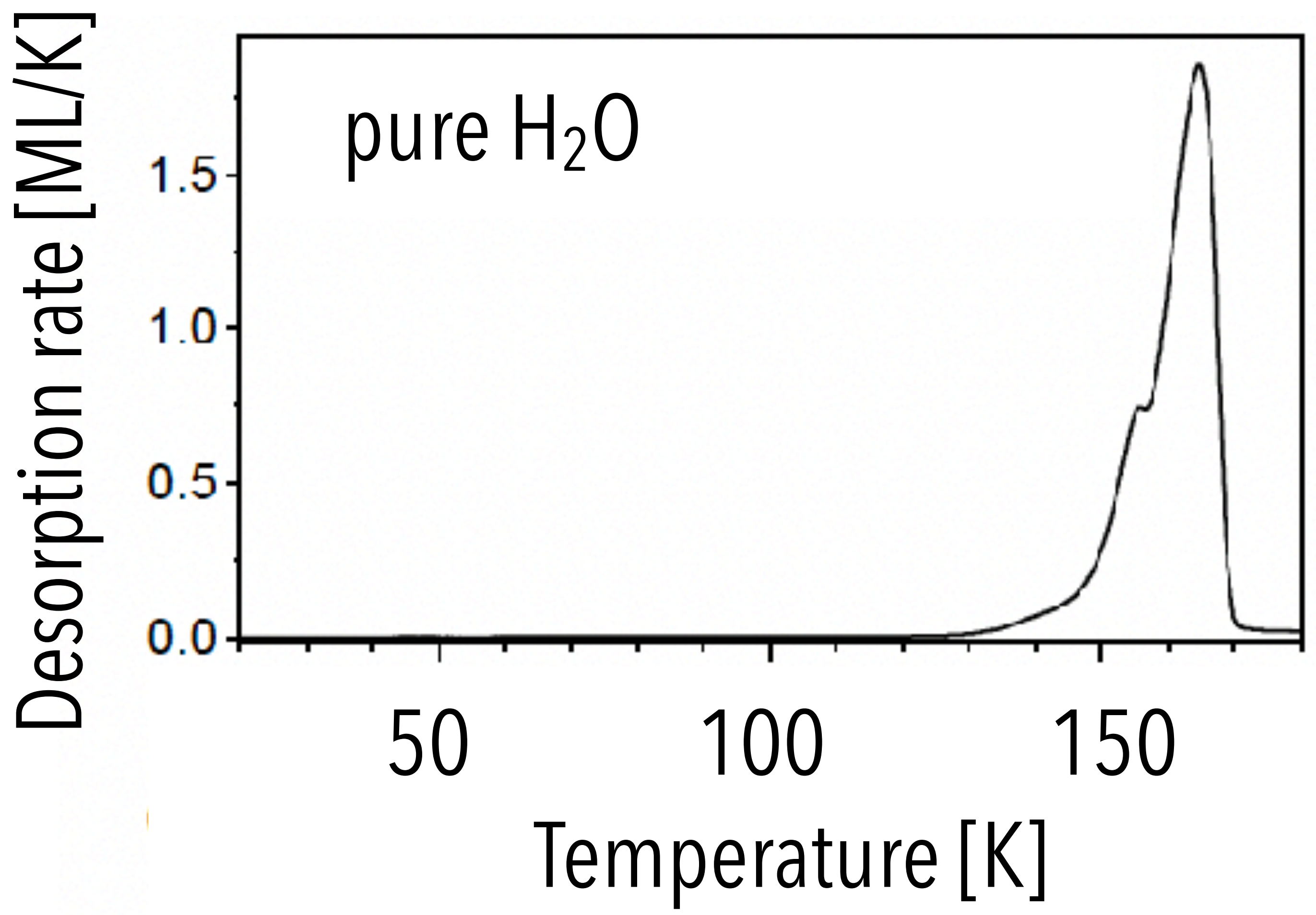
TPD experiment



Leiden Ice Database entry for Ehrenfreund et al. (1999): CO_2:H_2O (1:1) ratio, T=10 K - 187 K, **Fig. 2 Fayolle et al. (2011)**

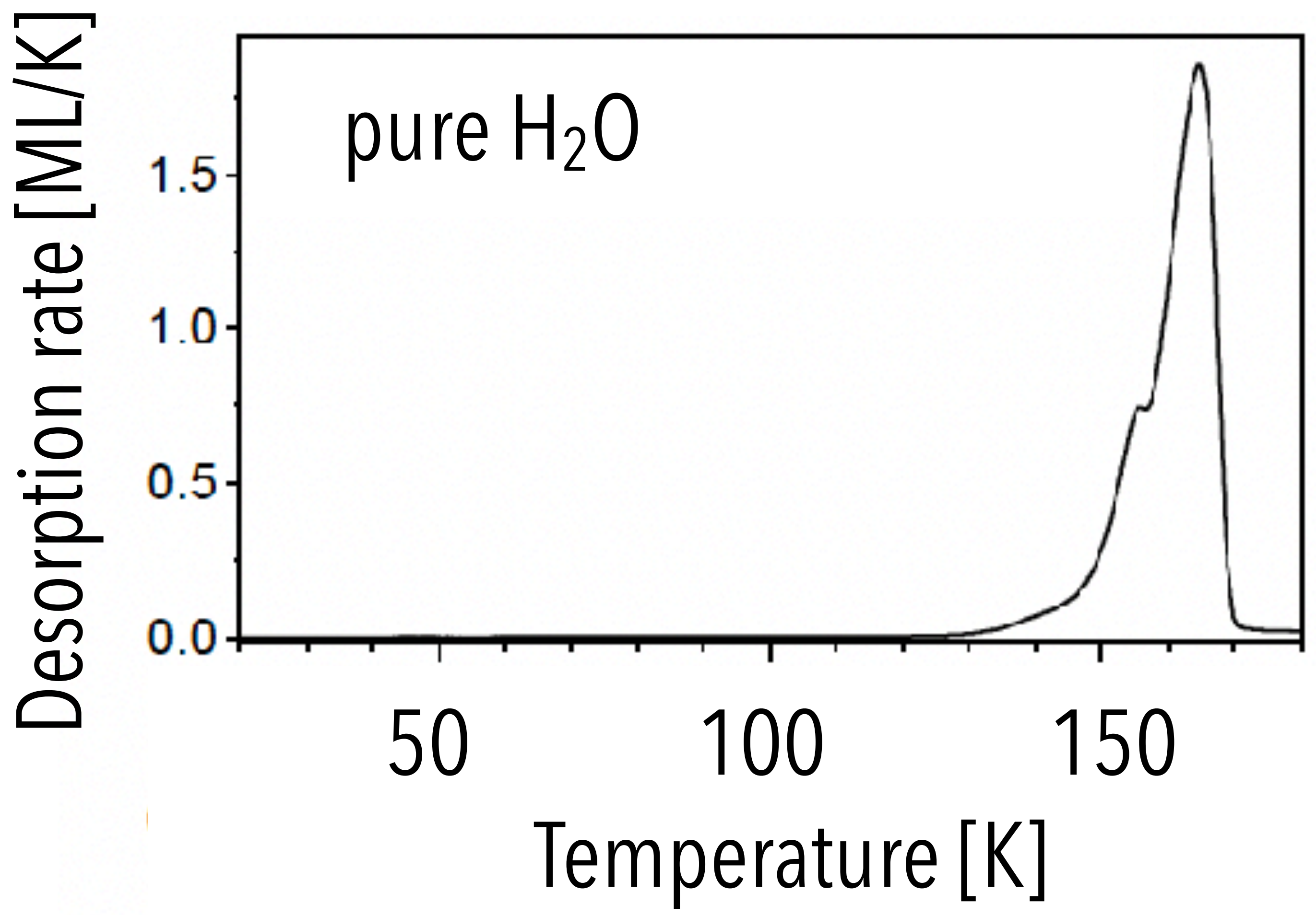
3. Ice thermal processing. Desorption temperatures in pure vs mixed ices.

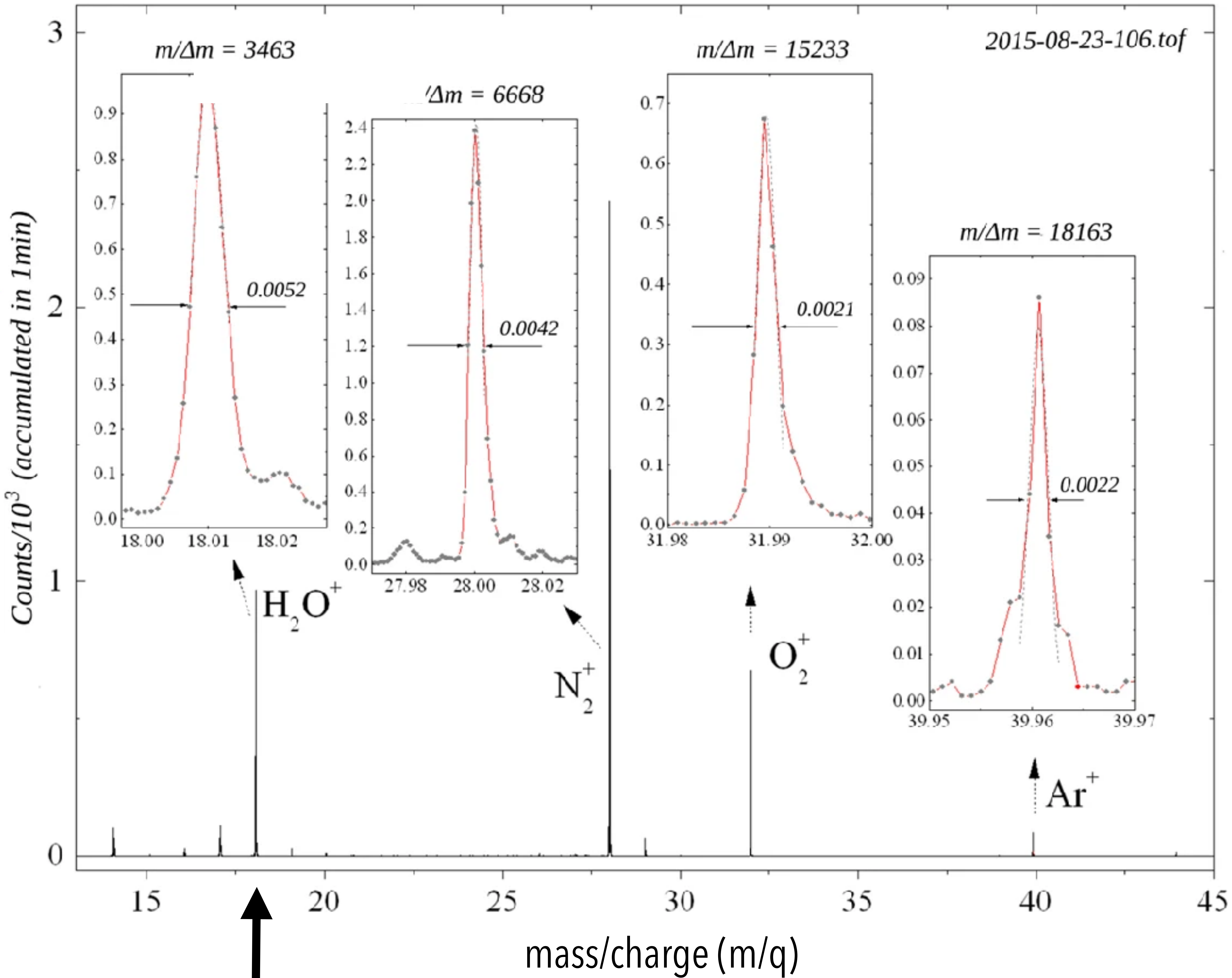


TPD curve

Figs. 2, 4, 5 from Kruczkiewicz et al. (2021), Fayolle et al. (2011), Lauk et al. (2015), Simon et al. (2019)

3. Ice thermal processing. ID'ing sublimated ices using mass and charge.



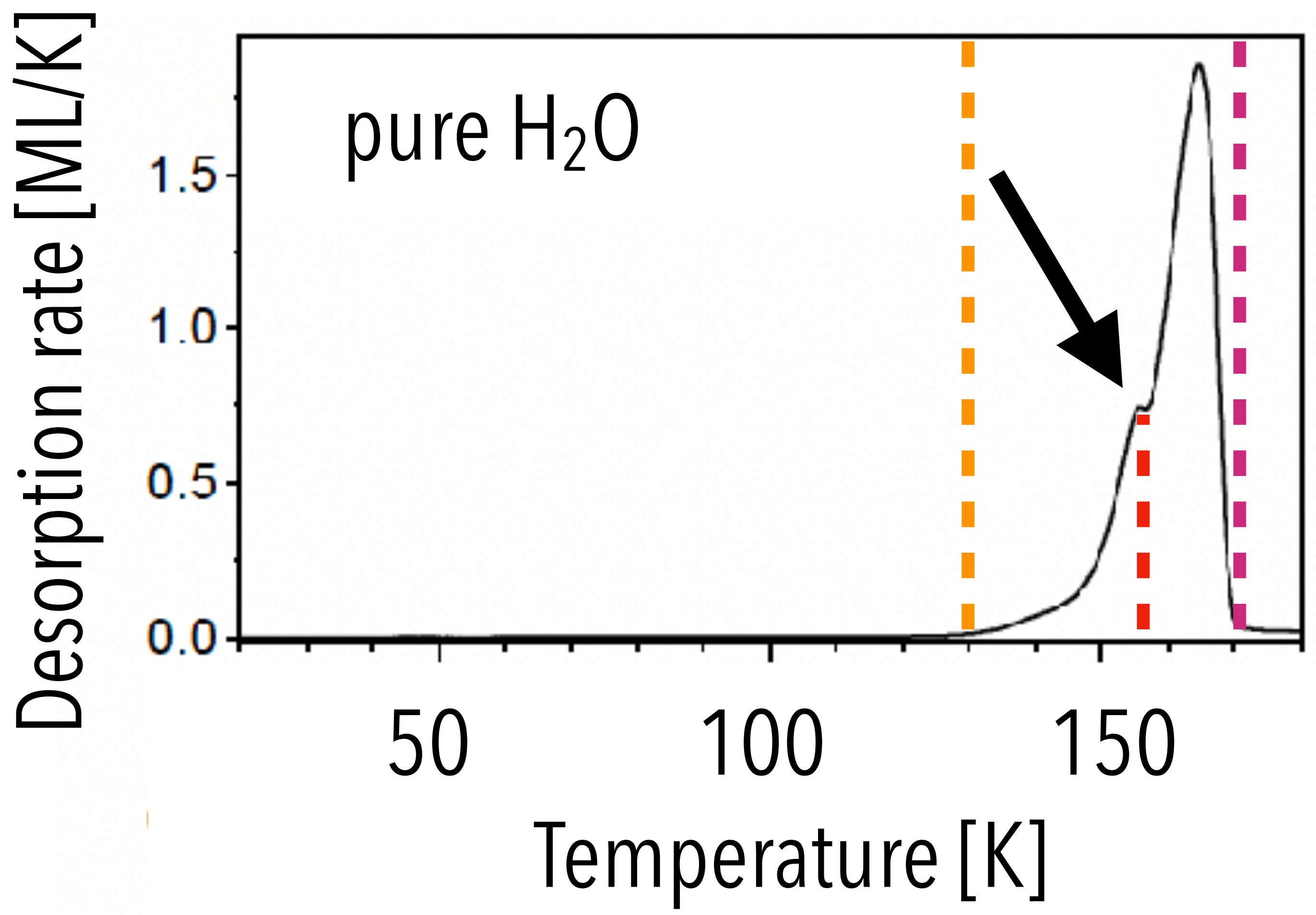


QMS

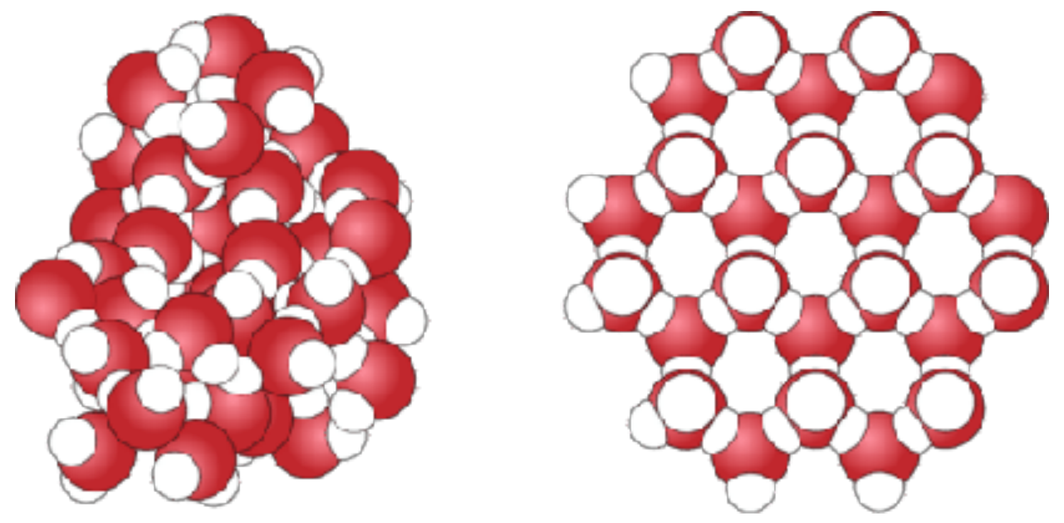
Peaks indicate specific molecules

Figs. 2, 4, 5 from Kruczkiewicz et al. (2021), Fayolle et al. (2011), Lauk et al. (2015), Simon et al. (2019),Fig. 3, Simcic et al. (2021)

3. Ice thermal processing. Desorption temperatures in pure vs mixed ices.



TPD curve



Phase transformation

H_2O crystallizes @ T >130 K,

irreversible @ T >154 K,

total desorption @ T>170 K

ASW ⟶ I_c crystalline ice ⟶ I_h crystalline ice

Figs. 2, 4, 5 from Kruczkiewicz et al. (2021), Fayolle et al. (2011), Lauk et al. (2015), Simon et al. (2019)

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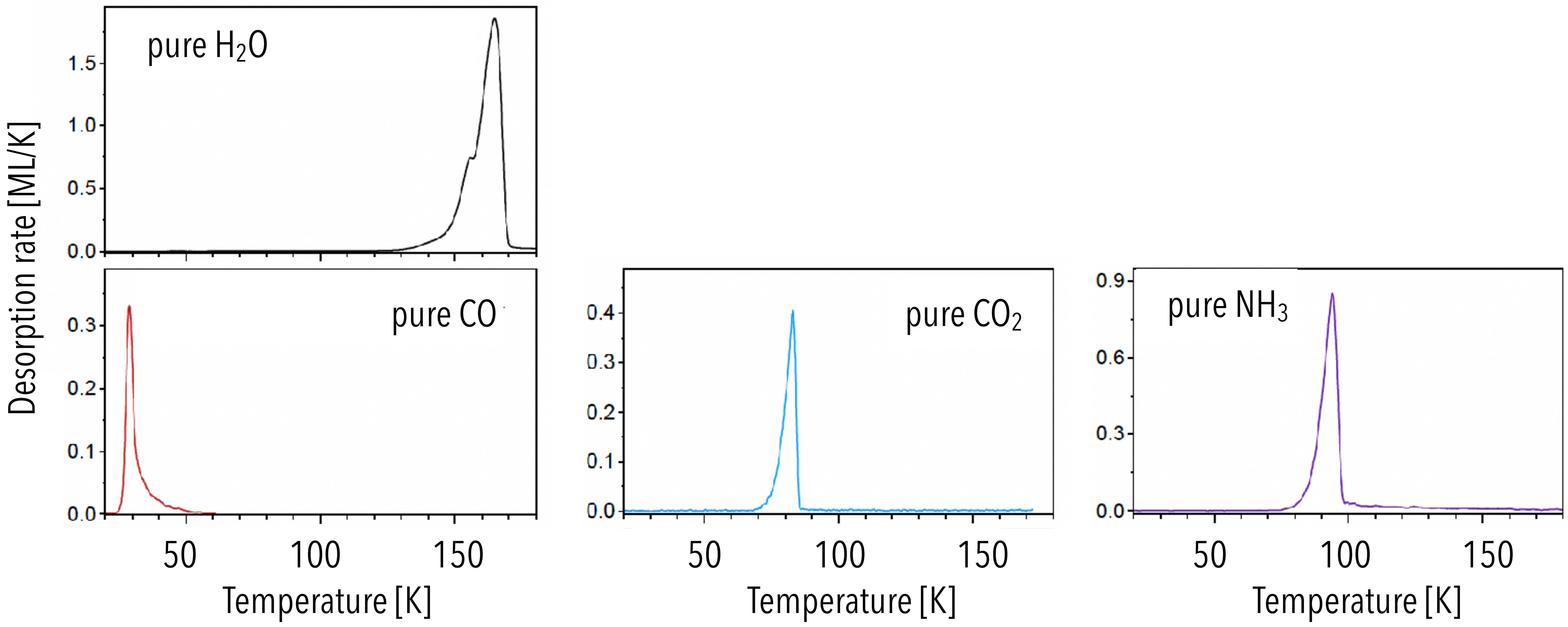
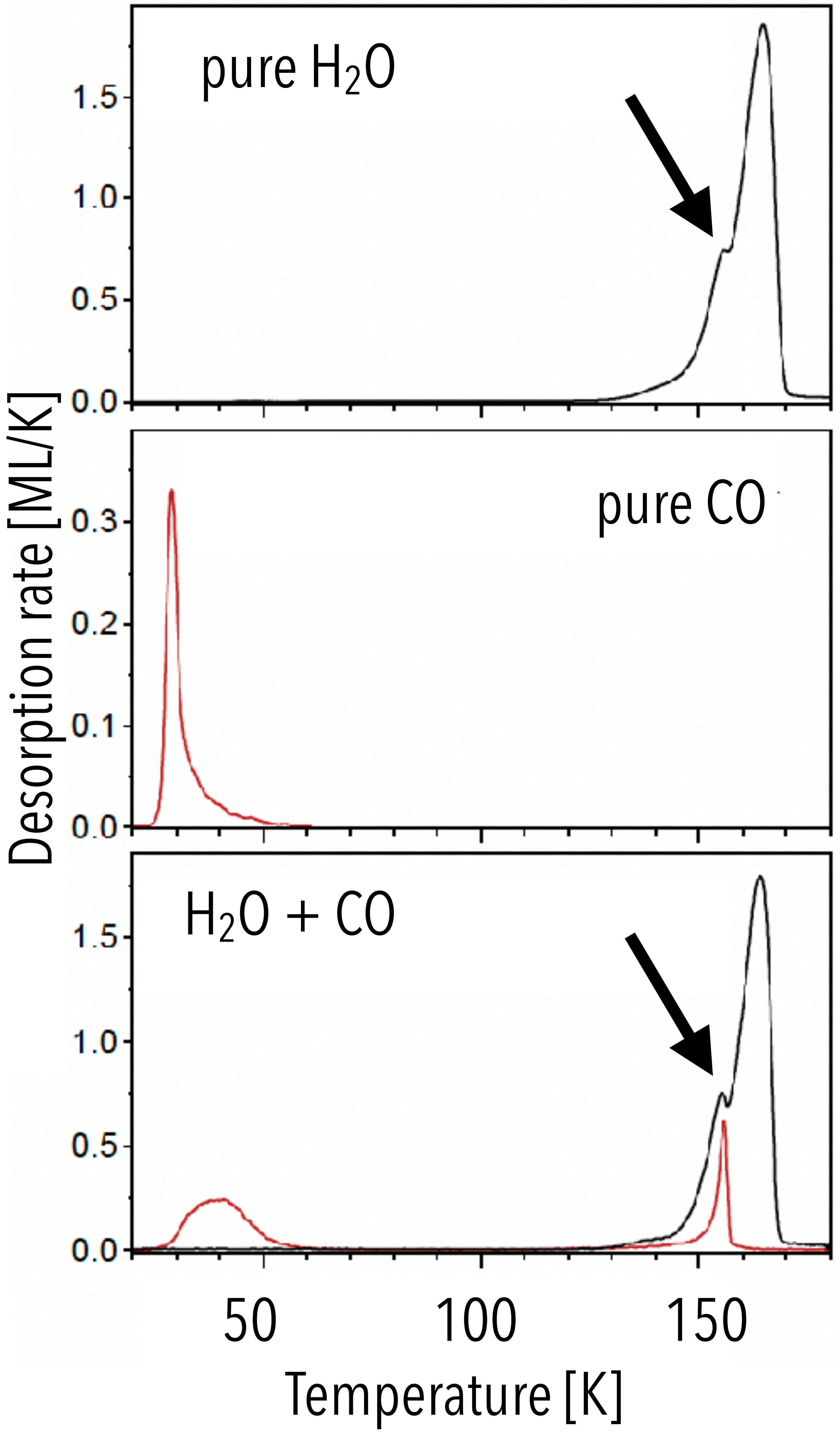


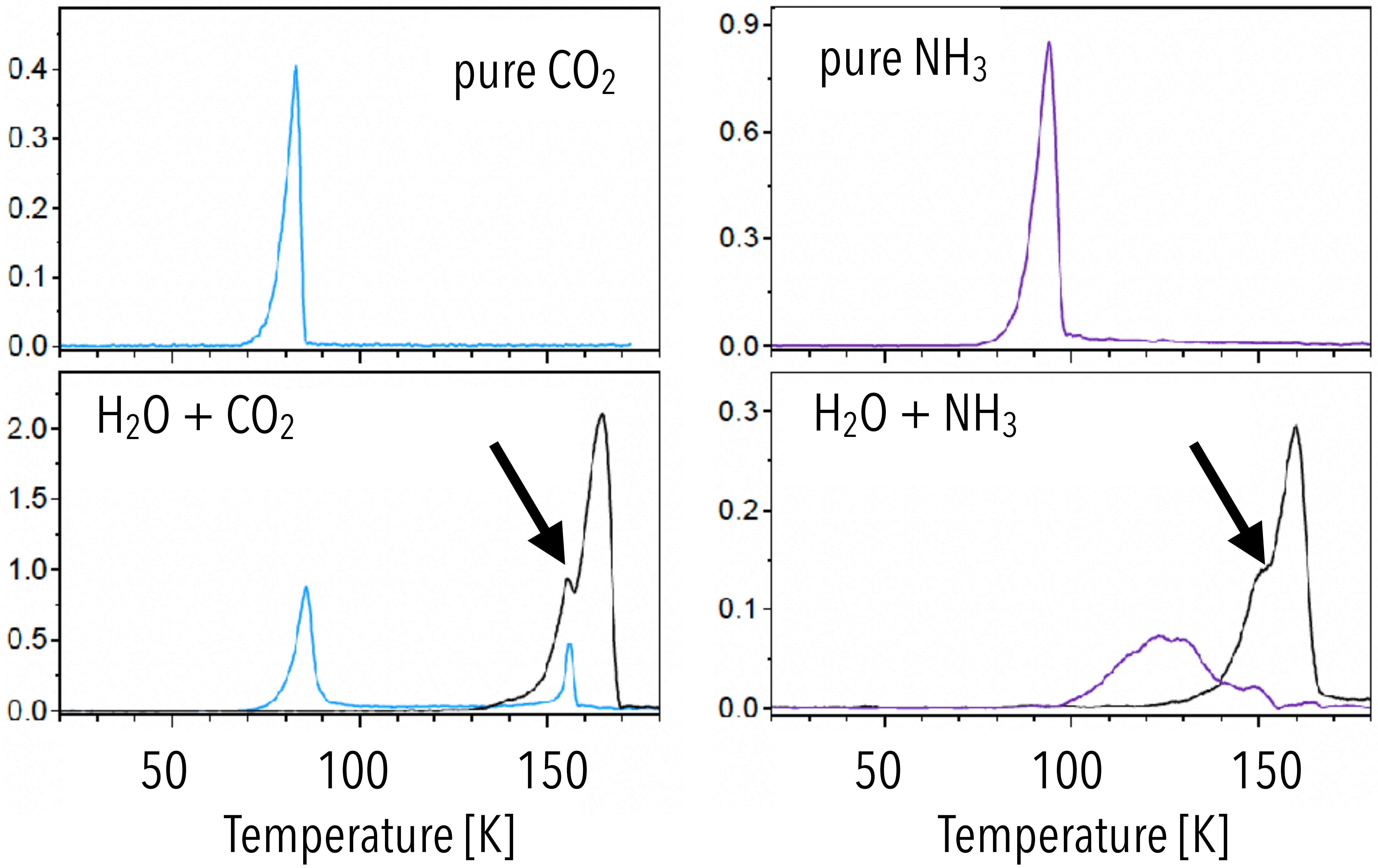
Figs. 2, 4, 5 from Kruczkiewicz et al. (2021), Fayolle et al. (2011), Lauk et al. (2015), Simon et al. (2019)

3. Ice thermal processing. Desorption temperatures in pure vs mixed ices.

Volcano peak

H_2O crystallizes irreversibly @ T > 154 K,
Forces out less volatile ices trapped inside its matrix





Figs. 2, 4, 5 from Kruczkiewicz et al. (2021), Fayolle et al. (2011), Lauk et al. (2015), Simon et al. (2019)

Typical experimental sequences

1. Ice identification

Make astrophysical ice analog → Take

2. Ice chemical & physical structure

Make astrophysical ice analog (Pathway #1 vs Pathway #2) → Refl

Alternative: Irradiate ices instead of TPD

(with similar FTIR & QMS measurements)

See poster by Chun-Yi Lee

"Carbon Chain and CO_2 Formation Induced by EUV Irradiation"

3. Thermal ice processing

Make astrophysical ice analog → TPD experiment 10-150 K, ΔT=20

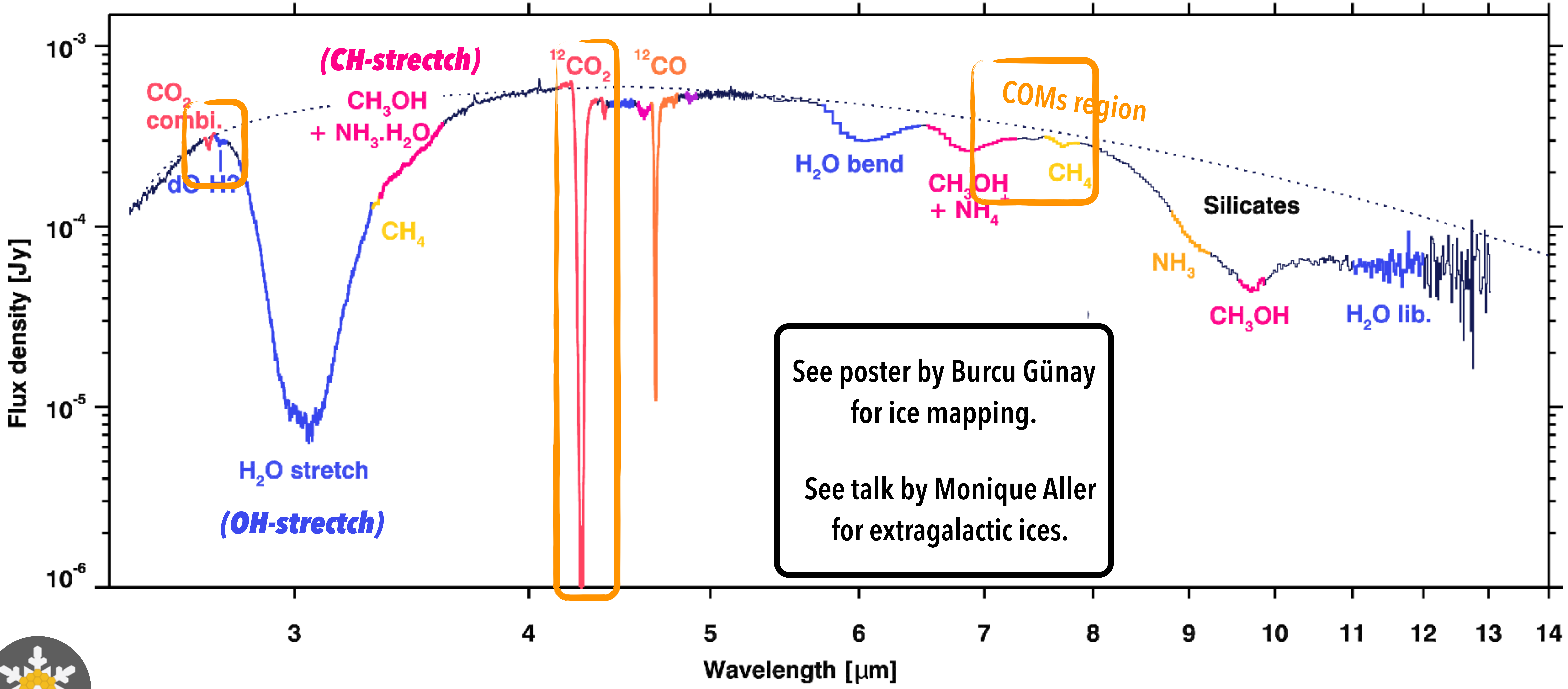
→ Take FTIR absorption spectra: confirm remaining ices

→ QMS measurements: confirm sublimated ices

Ex. Ice Age ERS (PI McClure): Darkest ices detected within molecular clouds

Credit: NASA, ESA, CSA, M. Zamani (ESA/Webb), **Fengwu Sun** (Steward Observatory), **Zak Smith** (The Open University + Leiden)

Laboratory spectra enabled ID and column densities for darkest cloud ices

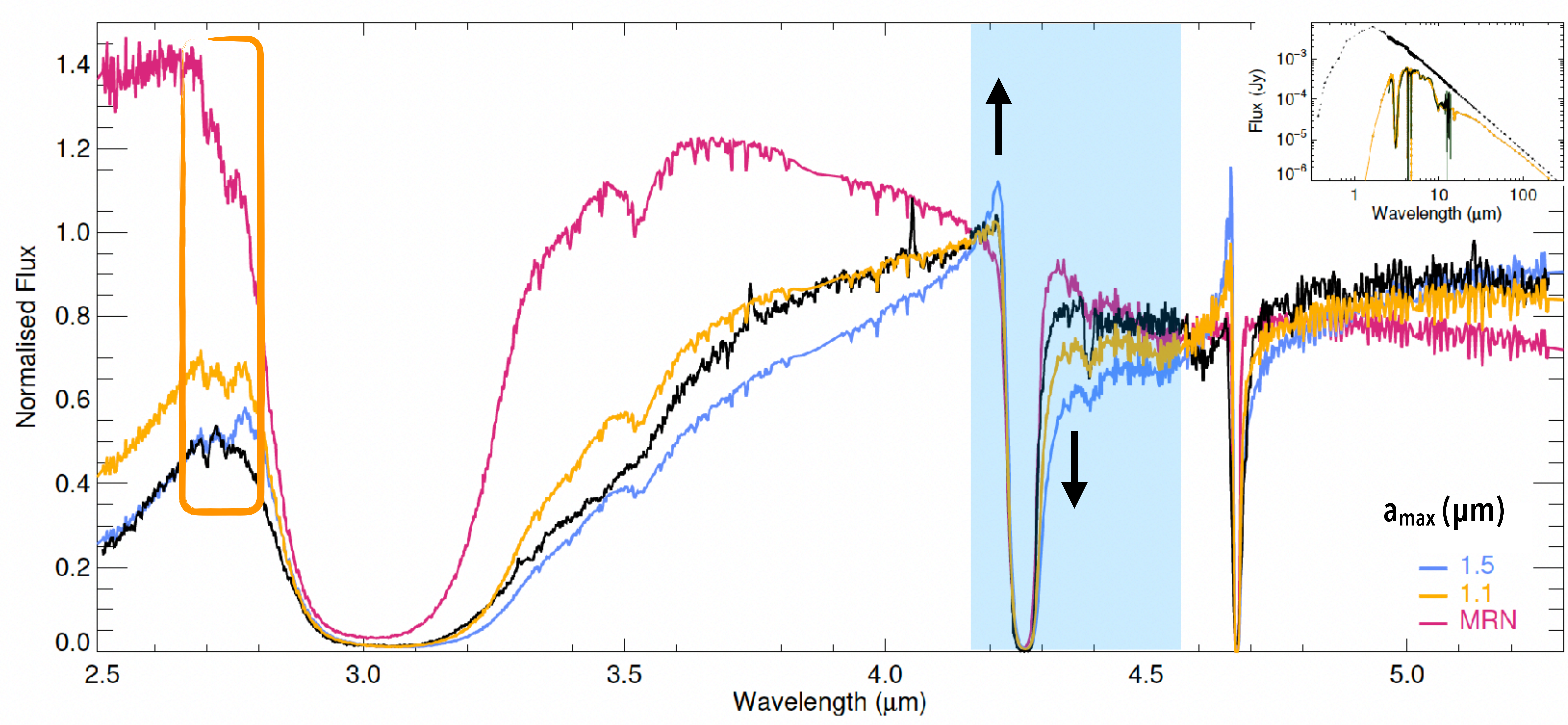


See poster by Burcu Günay for ice mapping.

See talk by Monique Aller for extragalactic ices.

McClure et al. (2023) ***Nature Astronomy***, Smith et al. (2025) *Nature Astronomy*

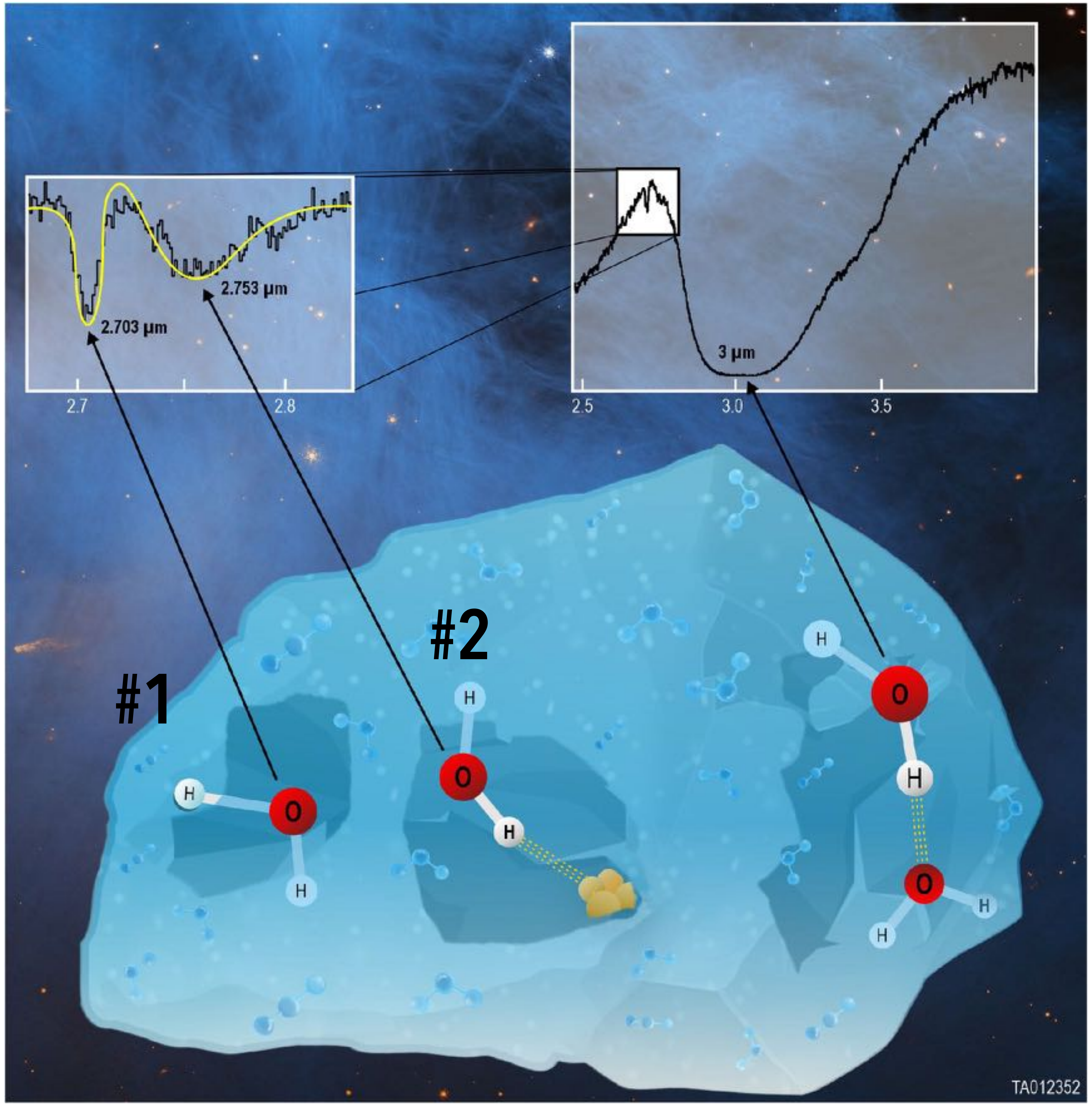
Lab-derived optical constants permit derivation of physical structure from RT modeling.



Scattering distortions indicate grain growth to 1 µm!

Dartois, Noble, et al. (2024), Dartois et al. (2022)

Lab ices match dangling OH, suggest that cloud ices are porous and mixed.



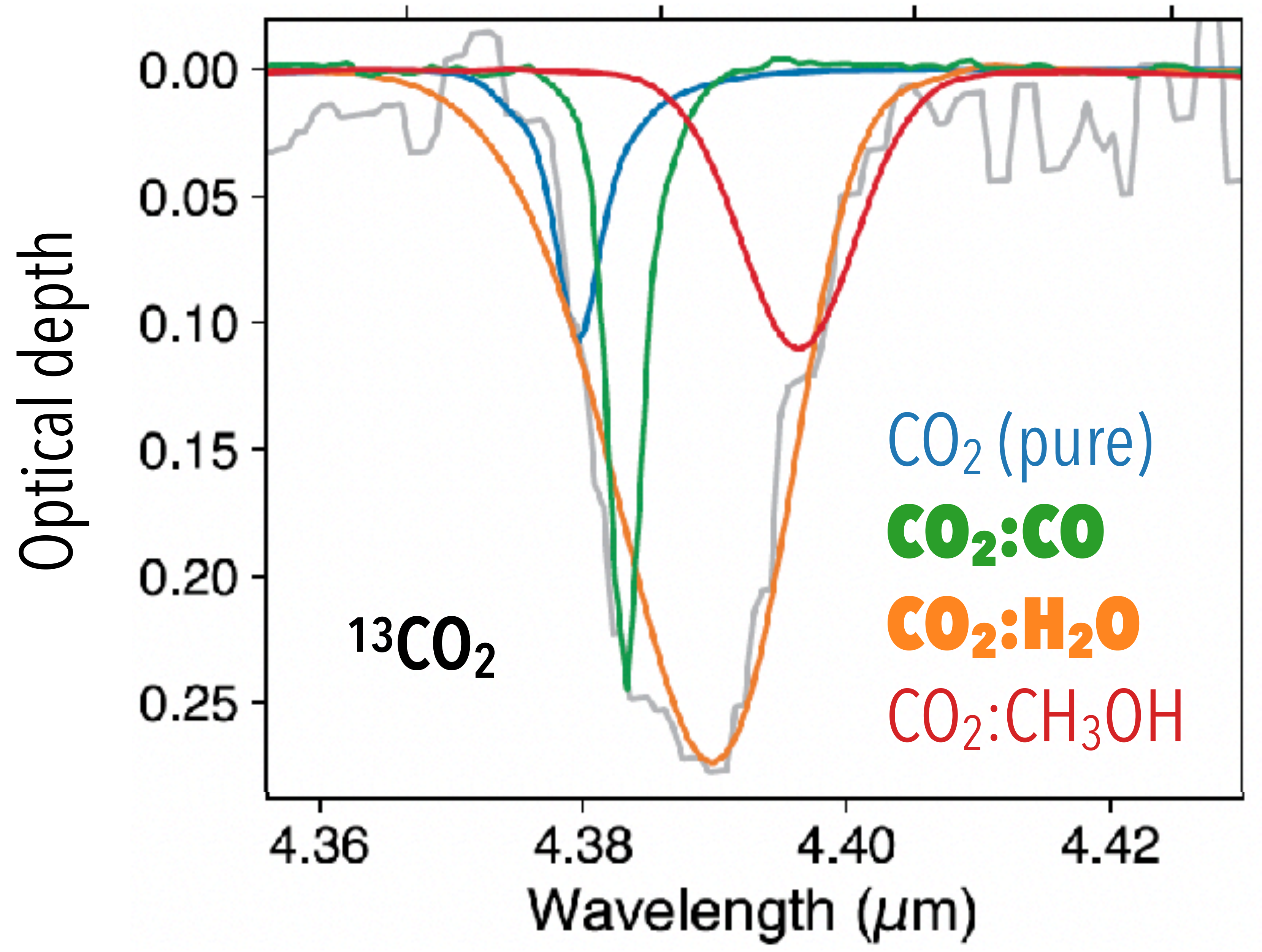
O-H stretch at 3 µm caused well-bonded water.

Option 1: d-OH suggests water ice has porous structure

Option 2: d-OH implies mixture of other ices in water ice matrix.

Noble et al. (2024) ***Nature Astronomy***

Pathway experiments & absorption spectroscopy confirm ice mixing in H_2O.



$T_{sub, CH4}$ & $T_{sub, CO2}$ << $T_{sub, H2O}$

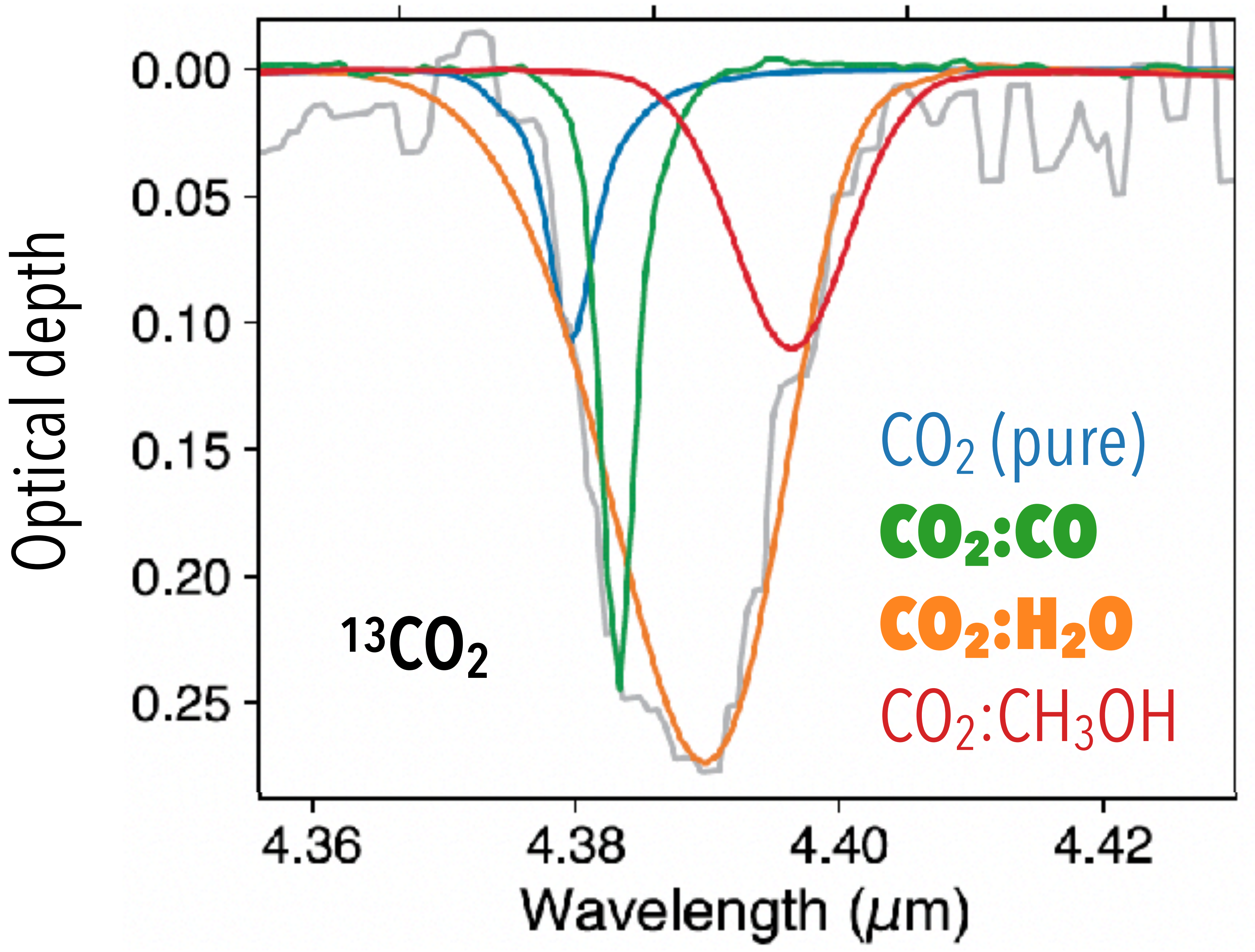
(more volatile ice mixed in less volatile ice.)

$CO + OH \longrightarrow CO_2$ (H_2O-rich environment)

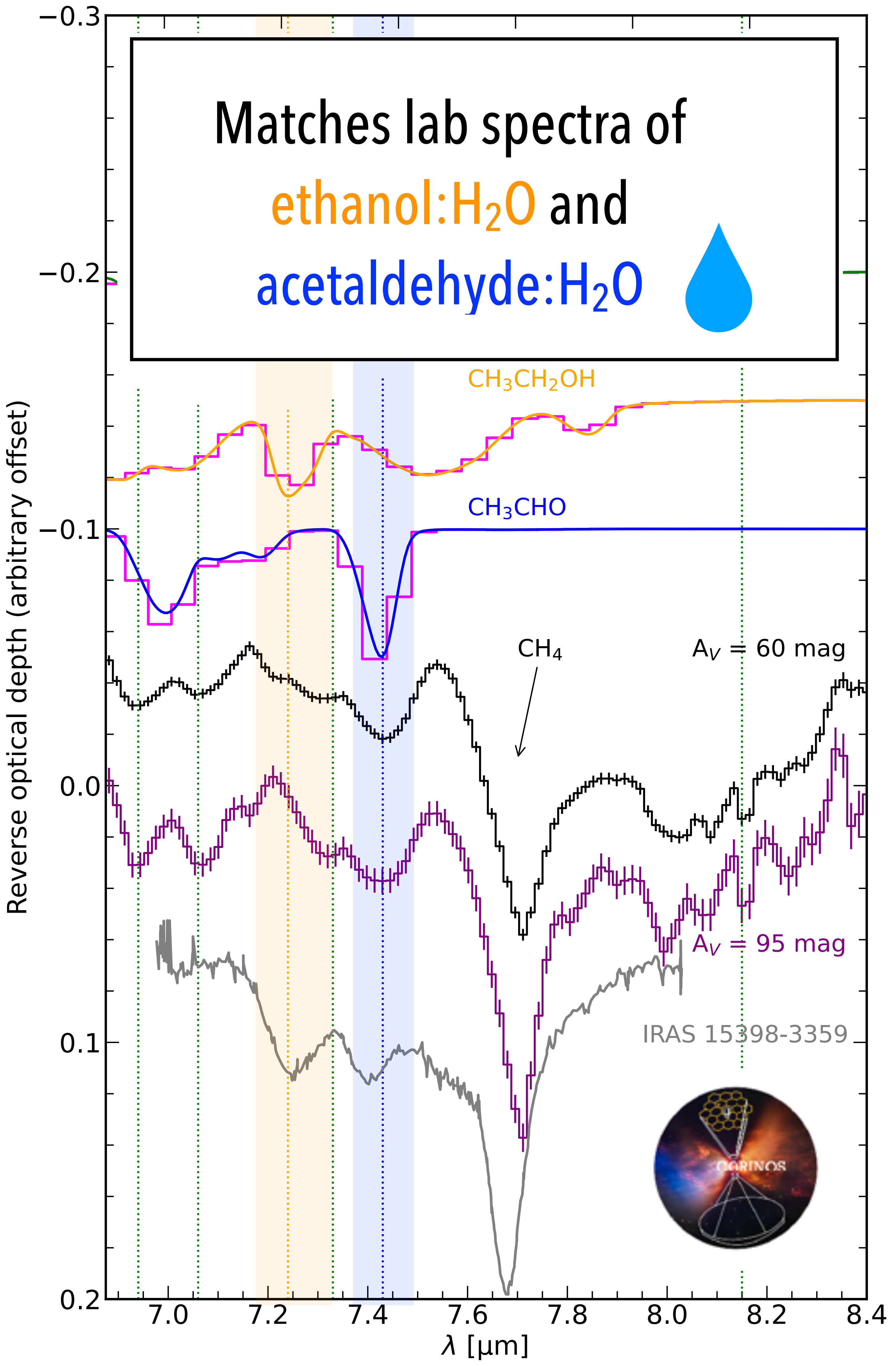
50% of CO_2 forms this way in chemical models.

Pontoppidan et al. (2003) for CO ice, **McClure et al. (2023), Jimenez-Serra et al. (2025)**

Pathway experiments & absorption spectroscopy confirm ice mixing in H_2O.



Early COM formation in H_2O ice in lab (Chuang et al. 2020) and in chemical models (Jin et al.'22, Garrod et al. '22)



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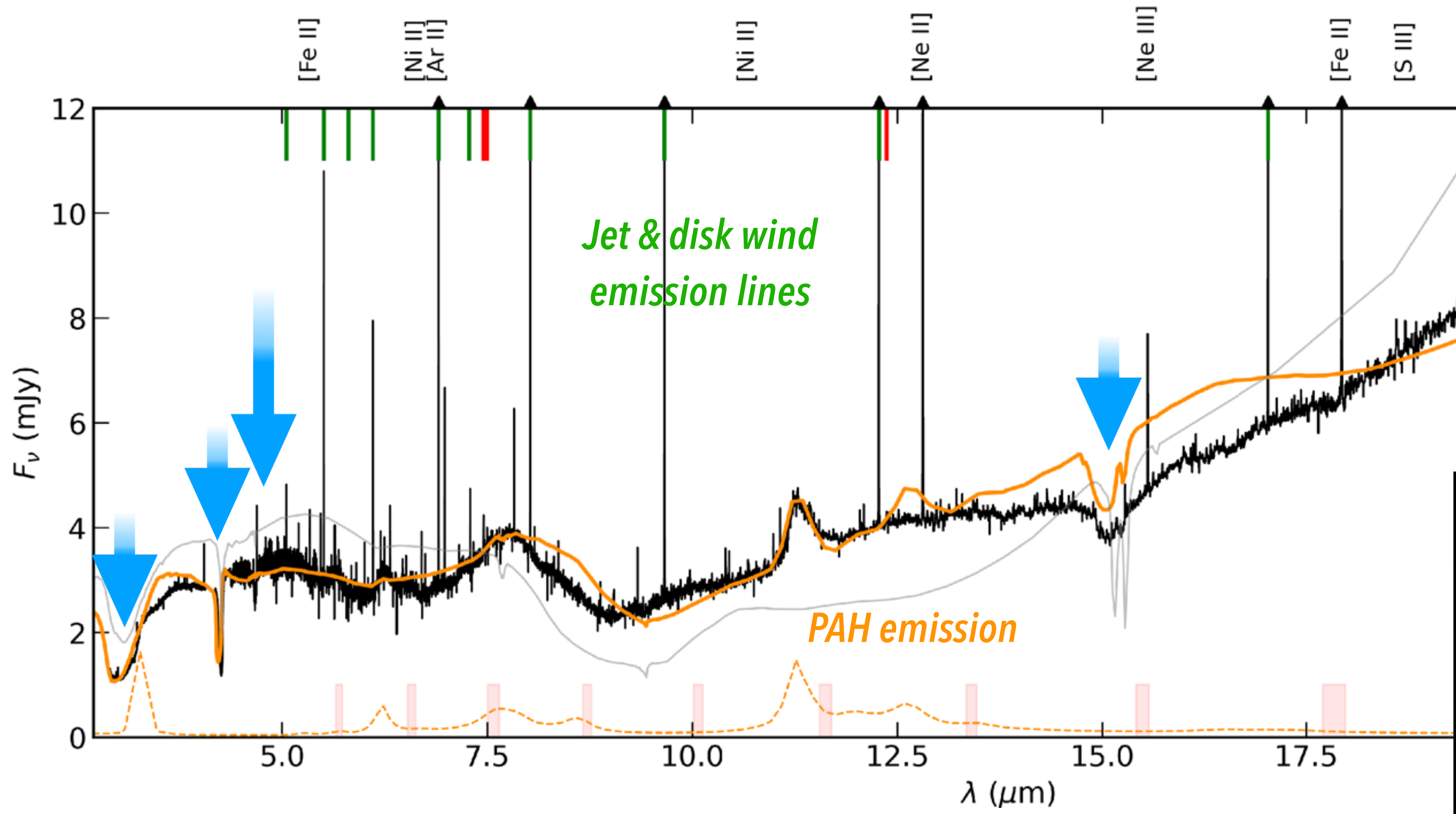
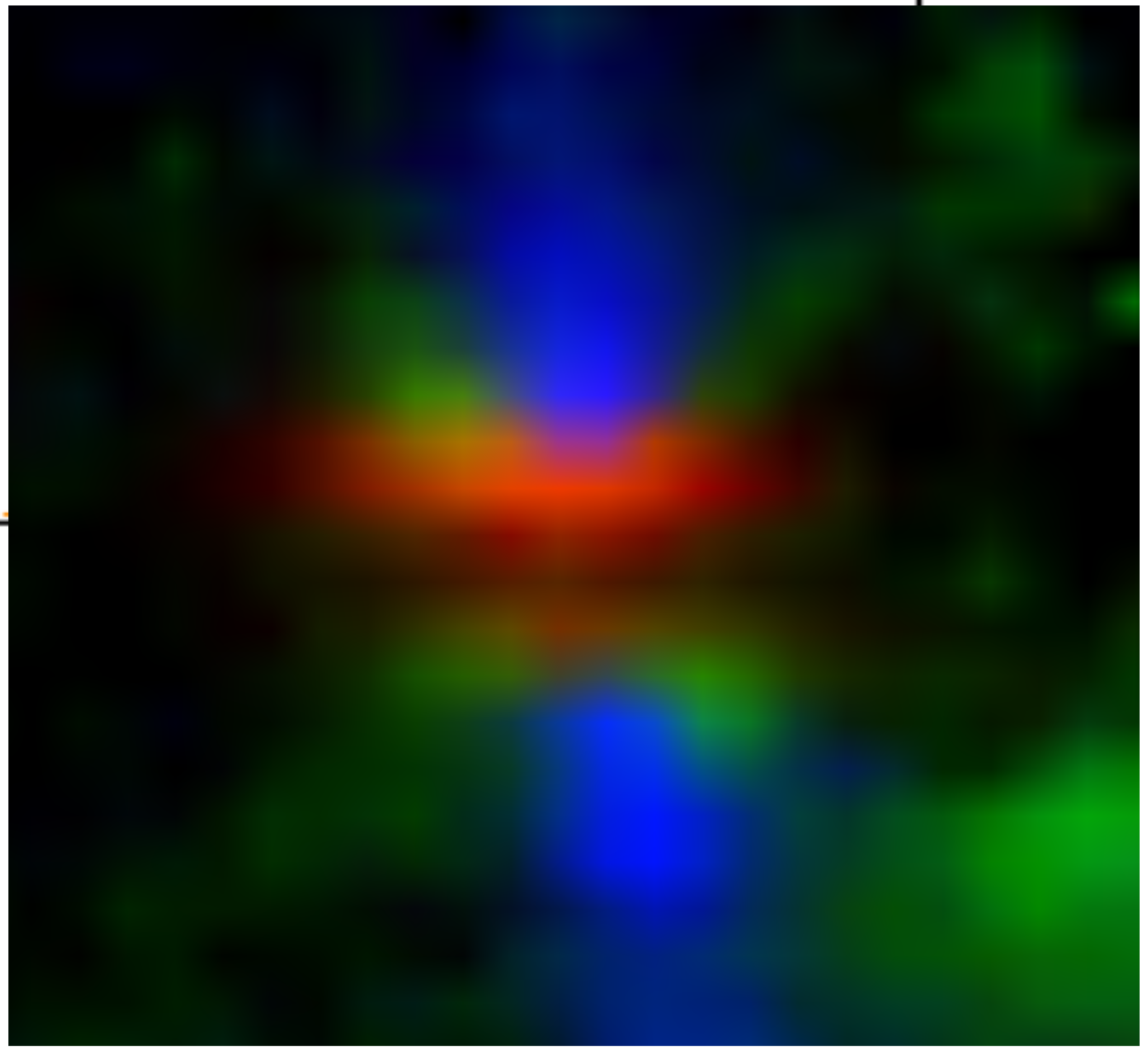
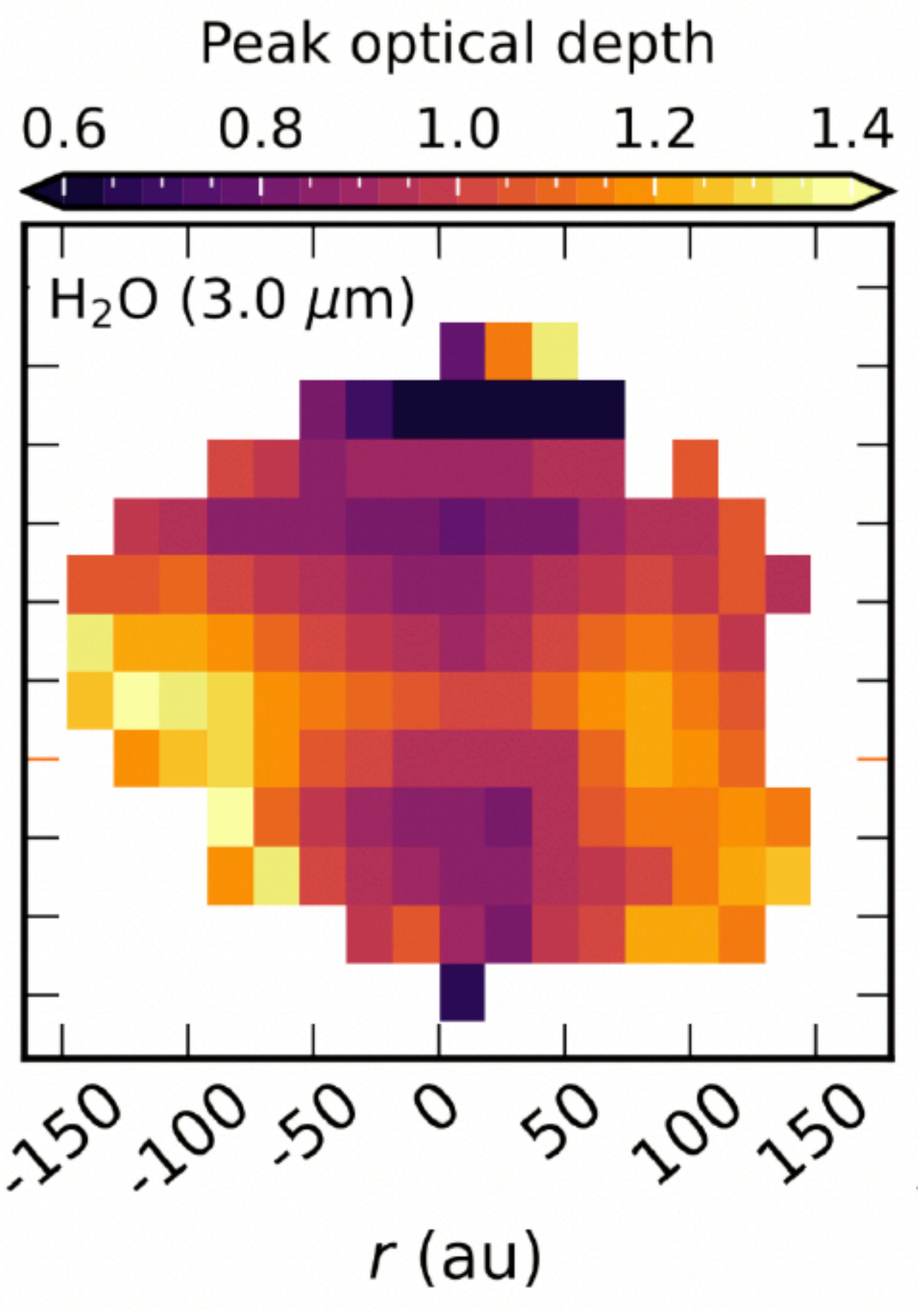
Do ices mixed into H_2O ice matrix become trapped? JWST disk observations prove it!

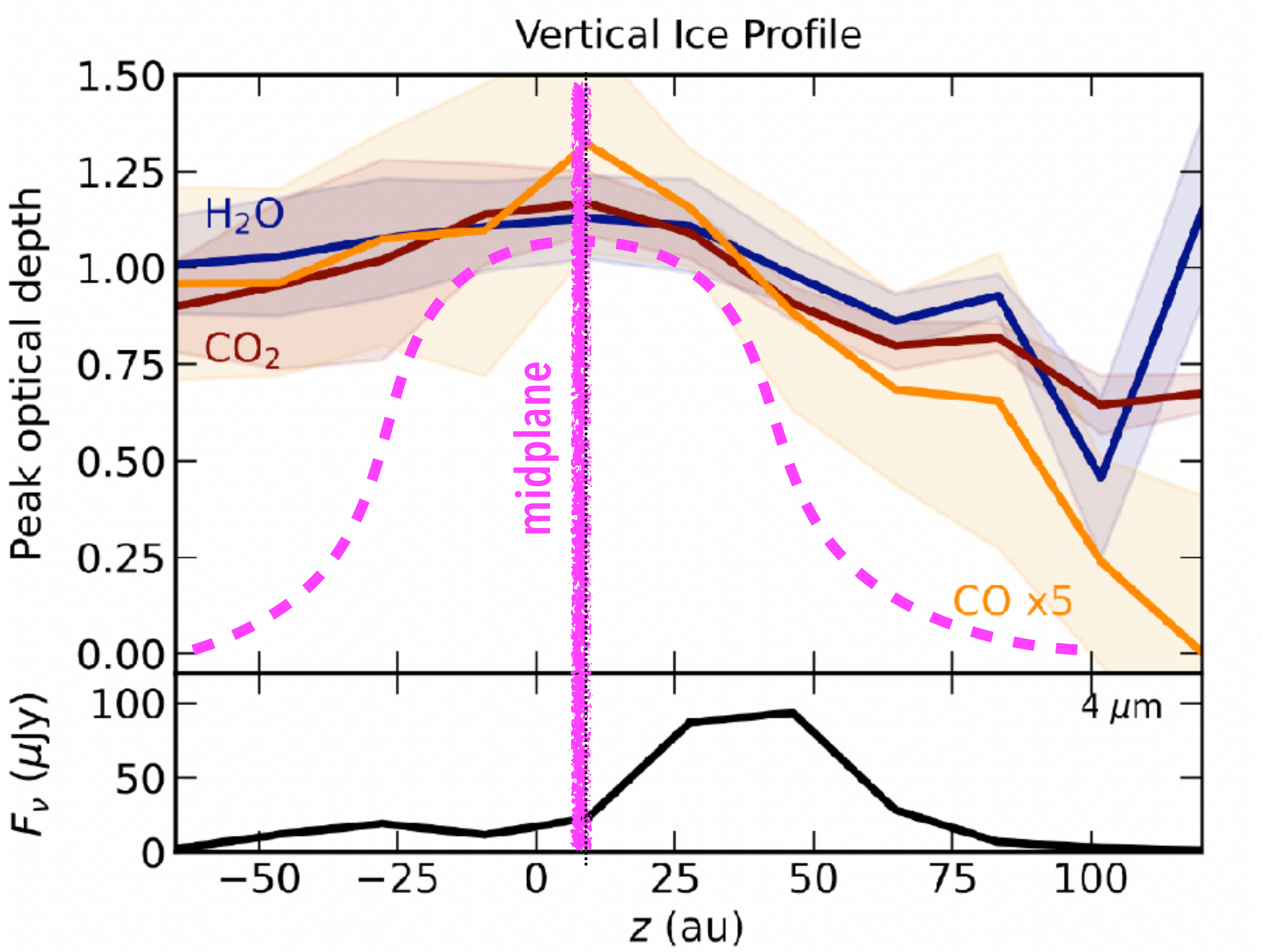




MIRI + model: Sturm, McClure et al. (2024);
NIRSpec: Sturm, McClure et al. (2023d)

CO ice should desorb just above midplane, if pure...but it does not!

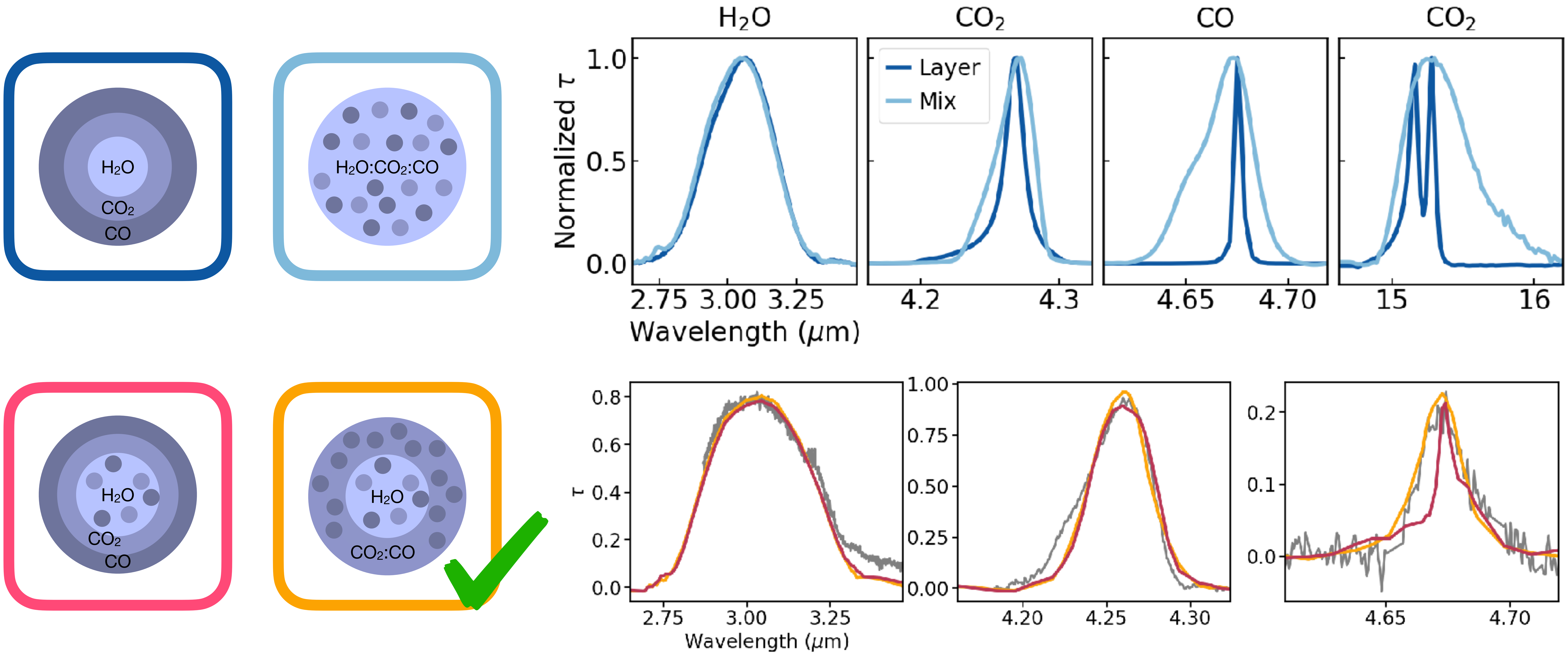




CO ice trapped in CO_2 or H_2O!

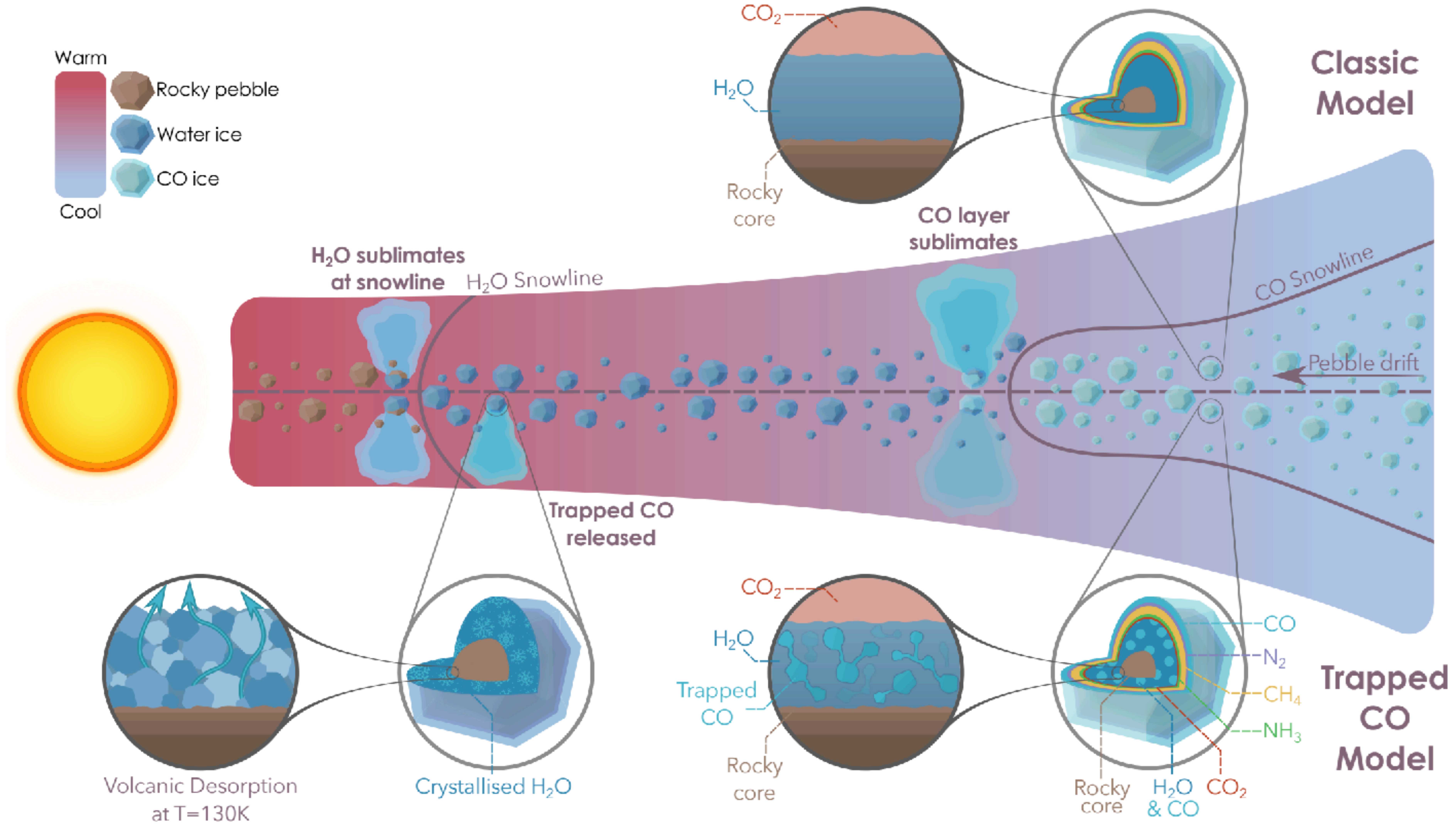
Sturm, McClure et al. (2023d),
Lab studies: Lauk et al. (2015), Simon et al. (2019)

Ice profiles fit by RT modeling using new laboratory optical constants confirm that the mixed cloud ices become trapped in H_2O matrix!



Bergner, Sturm, Piacentino, McClure et al. (2024)

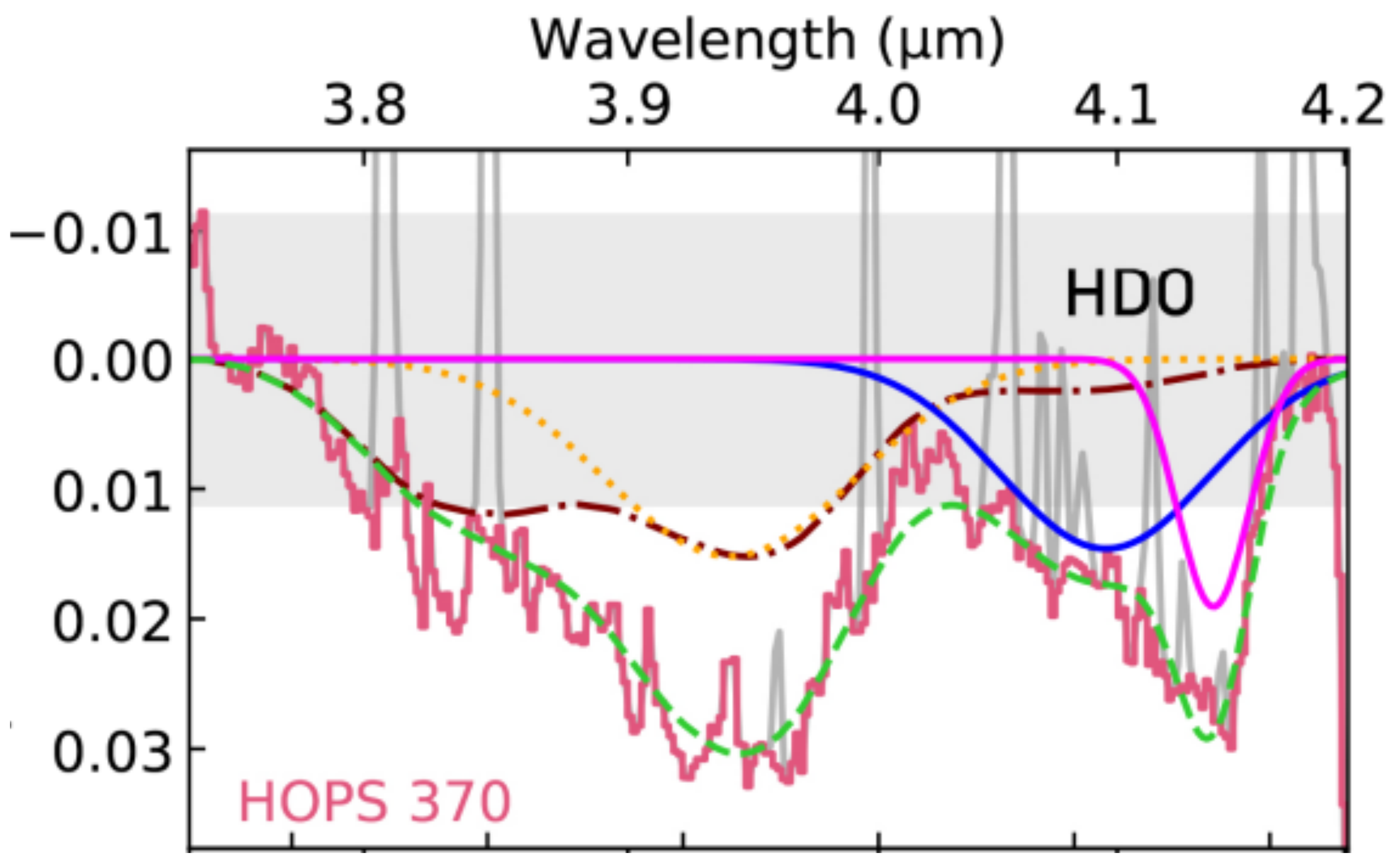
Trapped CO blurs CO, CO_2 snowlines, more C-rich solids in inner disk



Williams et al. (2025), Pebble radial drift models with(out) CO ice trapping

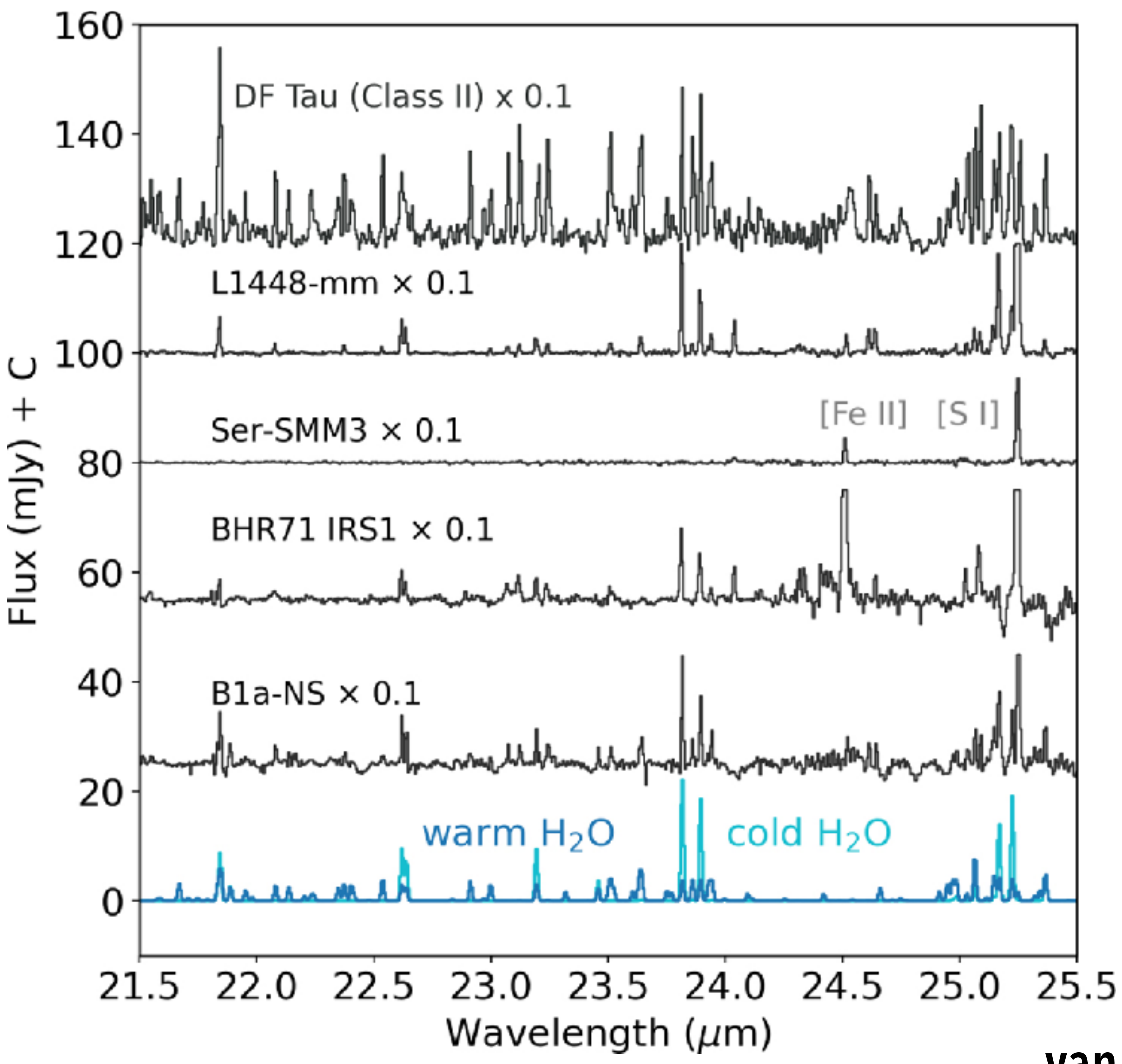
C-rich exoplanet composition...

See ice crystallization & sublimation in protostars, but no trapped ices (yet).



Detect both cold amorphous *and* hot crystalline **HDO ice** towards hot, massive protostars!

Slavicinska et al. 2024



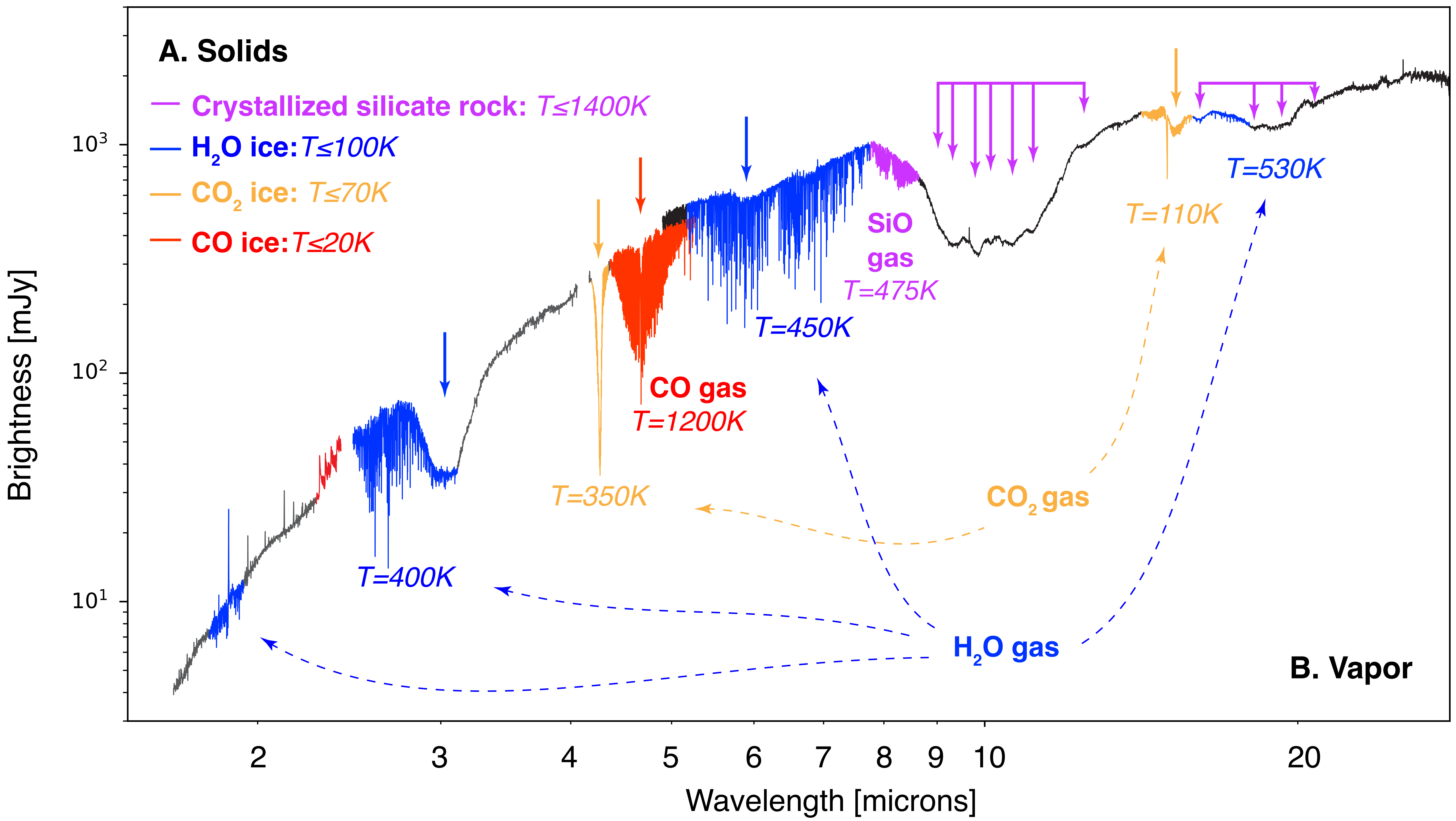
H_2O ice sublimation produces gas!

van Dishoeck et al. 2025

However, we have a good candidate!

Exceptional protostar with ***strong gas absorption***, including H_2O & SiO: Full interstellar dust reset?

Image credit: L. Calçada, for Nature



It's COMplicated
PI McClure

Fig. 2: McClure et al. (2025), Nature

It's COMplicated
PI McClure

Interstellar dust grains sublimate @ 1400 K, SiO gas cools

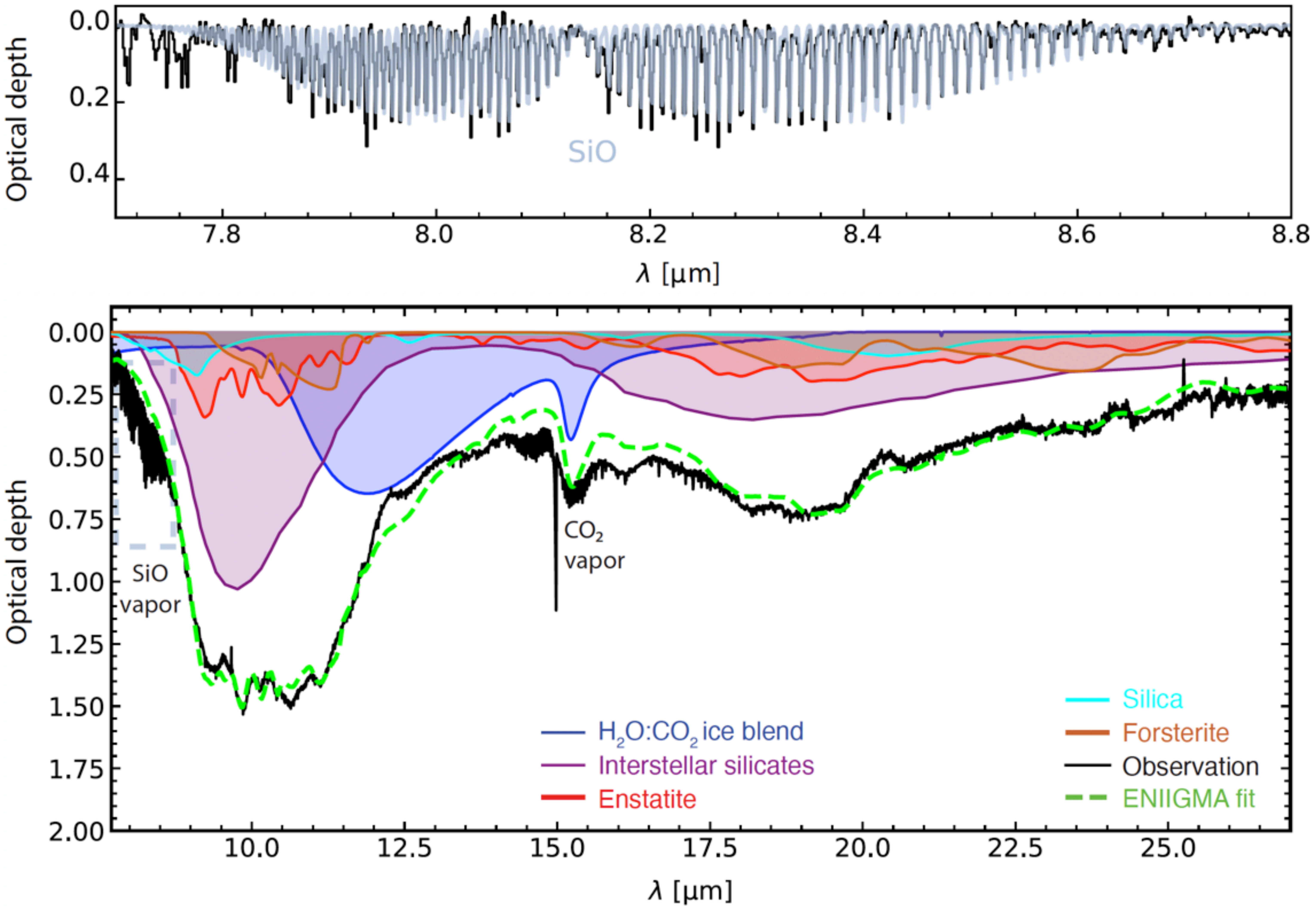


Fig. 3: McClure et al. (2025), Nature

500 K SiO gas, Δv_{SiO} (width) --> $\mathbf{R_{SiO}}$ **~ 1 AU**

SiO gas << 1400 K + specific minerals are consistent with **mineral re-condensation** from cooling SiO gas with **rapid condensate grain growth**.

CO_2 ice blended with H_2O @ 130 K.
Fitting ice profiles in NIRSpec,
Ballieux et al. in prep.

Seeing warm ice silhouetted against hot inner disk!

Stay tuned for ice analysis!

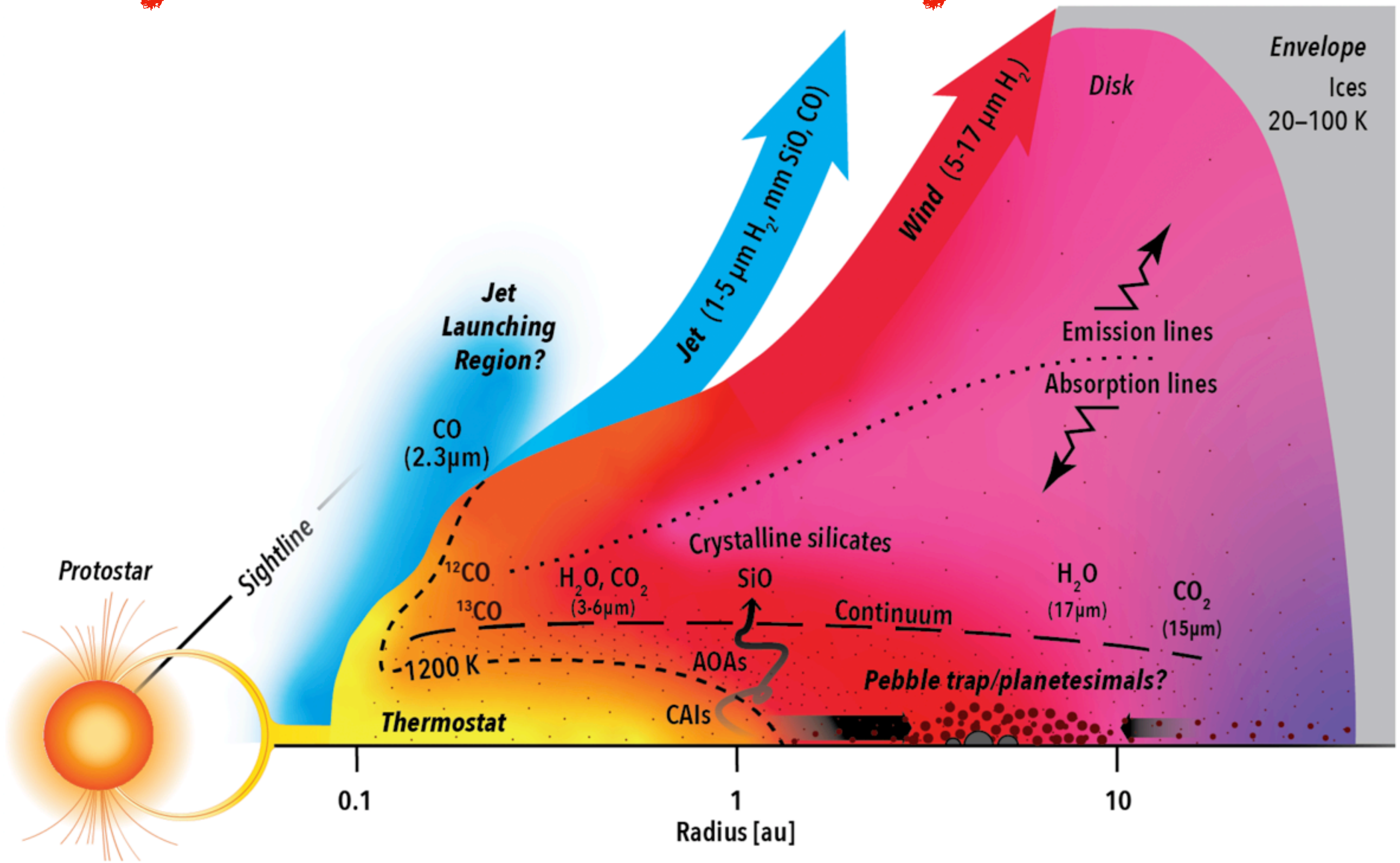
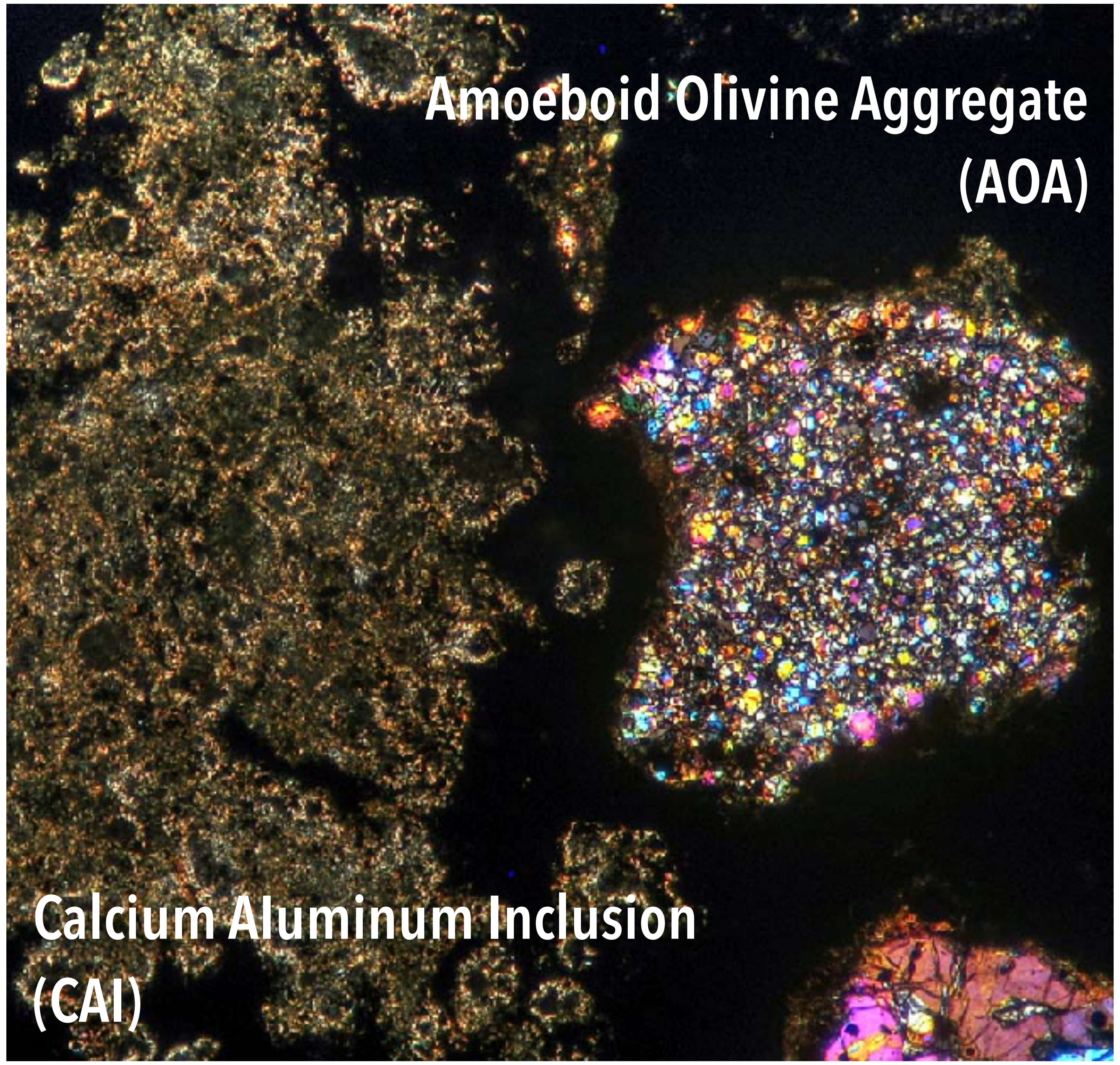
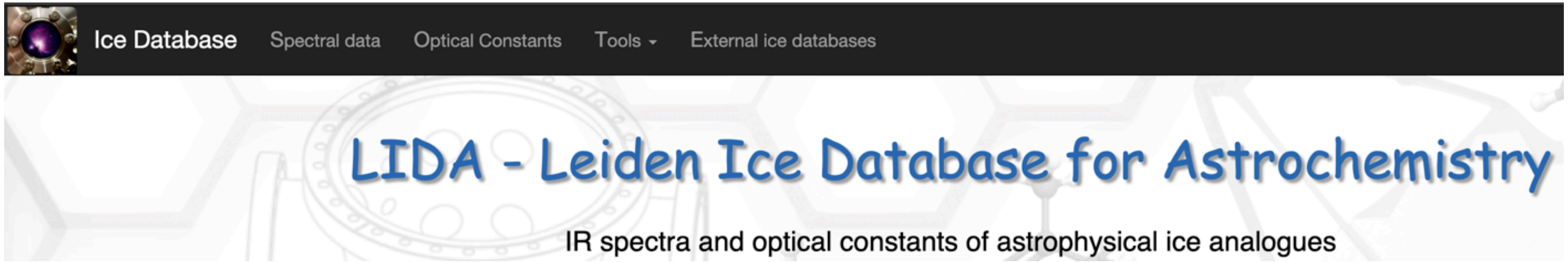


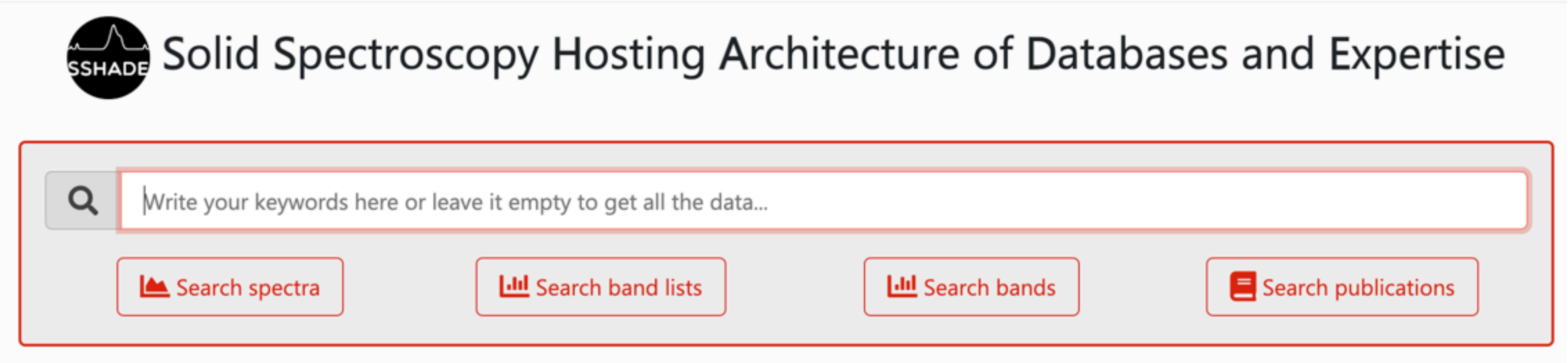
Fig. 1: McClure et al. (2025), Nature



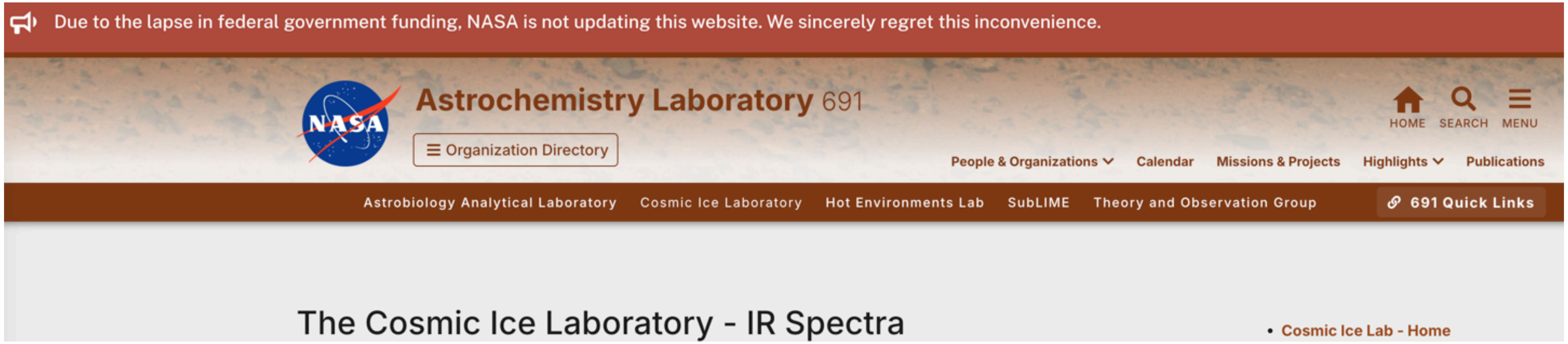
Crystalline silicates are analogs to 1st Solar System solids!

Where to find publicly available ice laboratory data used in these examples?





But do cite individual lab papers,
+ database paper!



Future directions for lab experiments

- **Simulate cyclic partial sublimation and re-condensation to study impact of ice trapping during protostellar outbursts?**

- **How does molecular size impact ice trapping?**
  - Larger ice molecules (e.g. CH_3SH) may "cork" the H_2O ice pores, enhancing trapping efficiency. **Narayanan et al. (2025)**

- **How do water ice and silicate substrate interact?**
  - Water ice can be trapped in silicates! **Monday talk by Tushar Suhasaria**
  - See **poster by Aki Takigawa** on silicate/water vapor interaction at low-temperatures.
  - Formation of phyllosilicates by water vapor chemisorption? **Thi et al. (2018)**

Summary: Lab experiments enable ice science!

Laboratory experiments allow us to:

- ☑ Identify ices
- ☑ Characterize their physical structure and chemical environment
- ☑ Measure reaction and desorption rates
- ☑ Interpret thermal history

Lab data allows inferences from JWST observations:

- → Ices form porous, grow to micron sizes in molecular cloud.
- → Volatile ices mixed with H_2O ice at every stage of star formation. Changes protoplanetary disk chemistry.
- → Protostellar ices are thermally processed and partially sublimated ($\leq$ 130 K) in protostellar environments.
- → See silicate analogs to oldest solids in Solar System planet formation timeline. Meteoritics right about early reset?

Future laboratory experiments will address:

Q1. Cyclical thermal processing on ice chemical environment

Q2. Impact of molecular size of ice trapping

Q3. Interaction between silicate substrate and water ice or vapor

Summary: Lab experiments enable ice science!

Laboratory experiments allow us to:

- ☑ Identify ices
- ☑ Characterize their physical structure and chemical environment
- ☑ Measure reaction and desorption rates
- ☑ Interpret thermal history

Lab data allows inferences from JWST observations:

→ Ices form porous, grow to micron sizes in molecular cloud.

→ Volatile ices mixed with H_2O ice at every stage of star formation. Changes protoplanetary disk chemistry.

→ Protostellar ices are thermally processed and partially sublimated ($\leq$ 130 K) in protostellar environments.

→ See silicate analogs to oldest solids in Solar System planet formation timeline. Meteoritics right about early reset?

Future laboratory experiments will address:

Q1. Cyclical thermal processing on ice chemical environment

Q2. Impact of molecular size of ice trapping

Q3. Interaction between silicate substrate and water ice or vapor

Thank you!