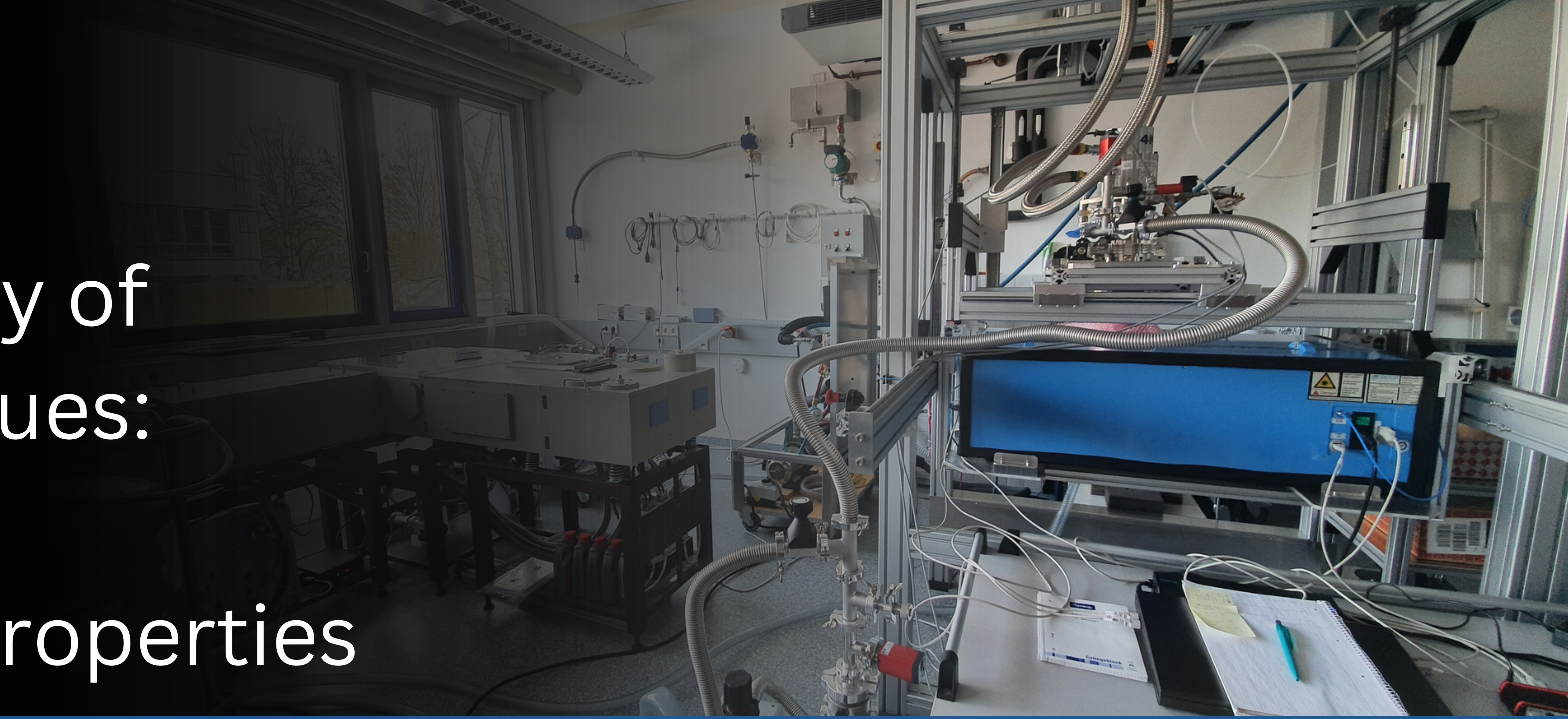
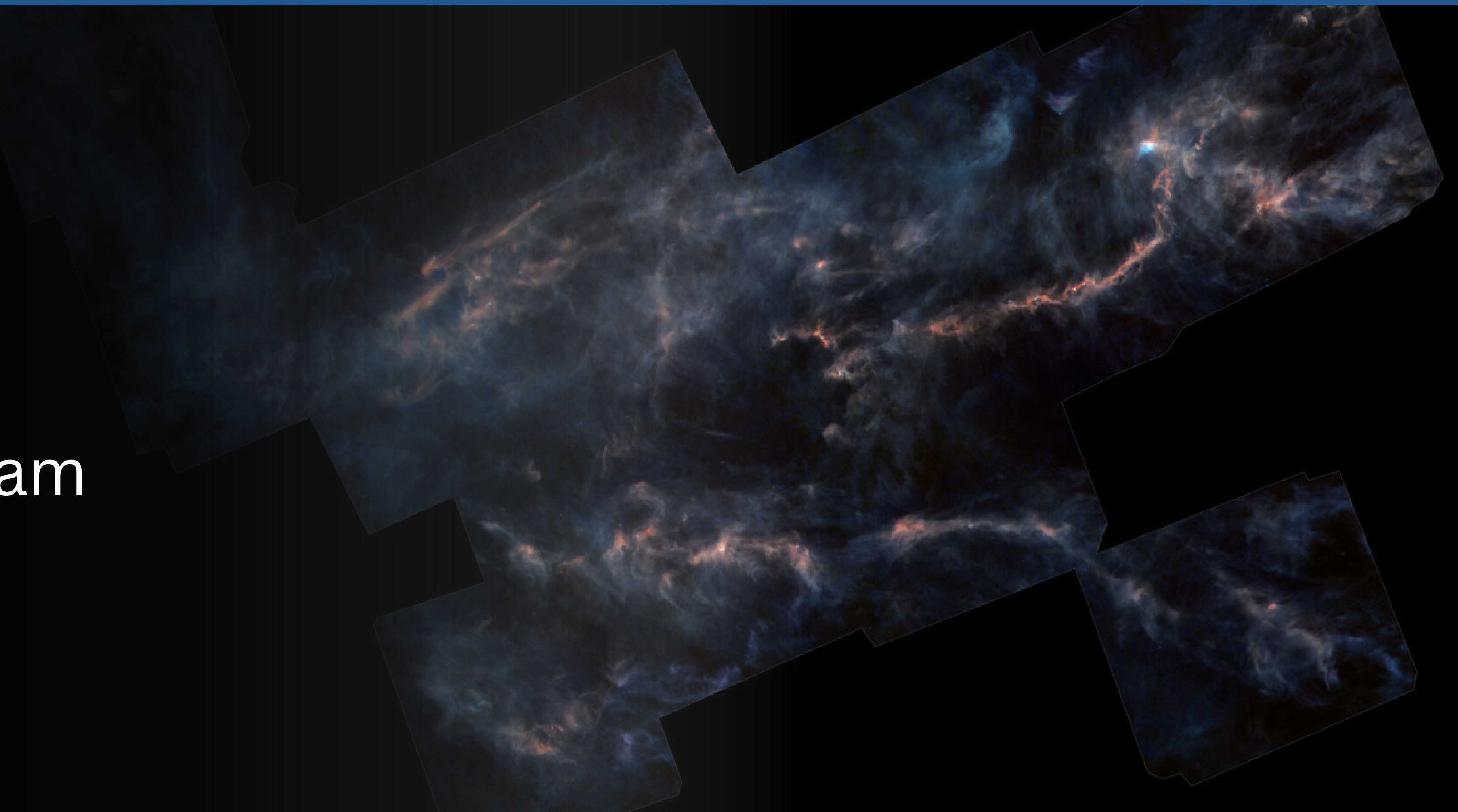


Broadband spectroscopy of astrophysical ice analogues: reconstruction of CO and CO_2 ice optical properties

Franciele KRUCZKIEWICZ
Laboratoire d'Astrophysique de Marseille - LAM
Max-Planck Institute for Extraterrestrial Physics – MPE
Astro-chemical Origins (ACO) ITN H2020 ESR

P. Theulé, A. Ivlev, B.M. Giuliano, P. Caselli & ACO team



ACO
EU H2020 Innovative Training Network
Astro-Chemical Origins

MPE
Max-Planck-Institut für extraterrestrische Physik

LAM
LABORATOIRE D'ASTROPHYSIQUE DE MARSEILLE

Image credit: Taurus Molecular Cloud observed in the FIR by ESA's Herschel observatory

ICE OPACITIES

...and how to access information hidden in cold regions of the ISM

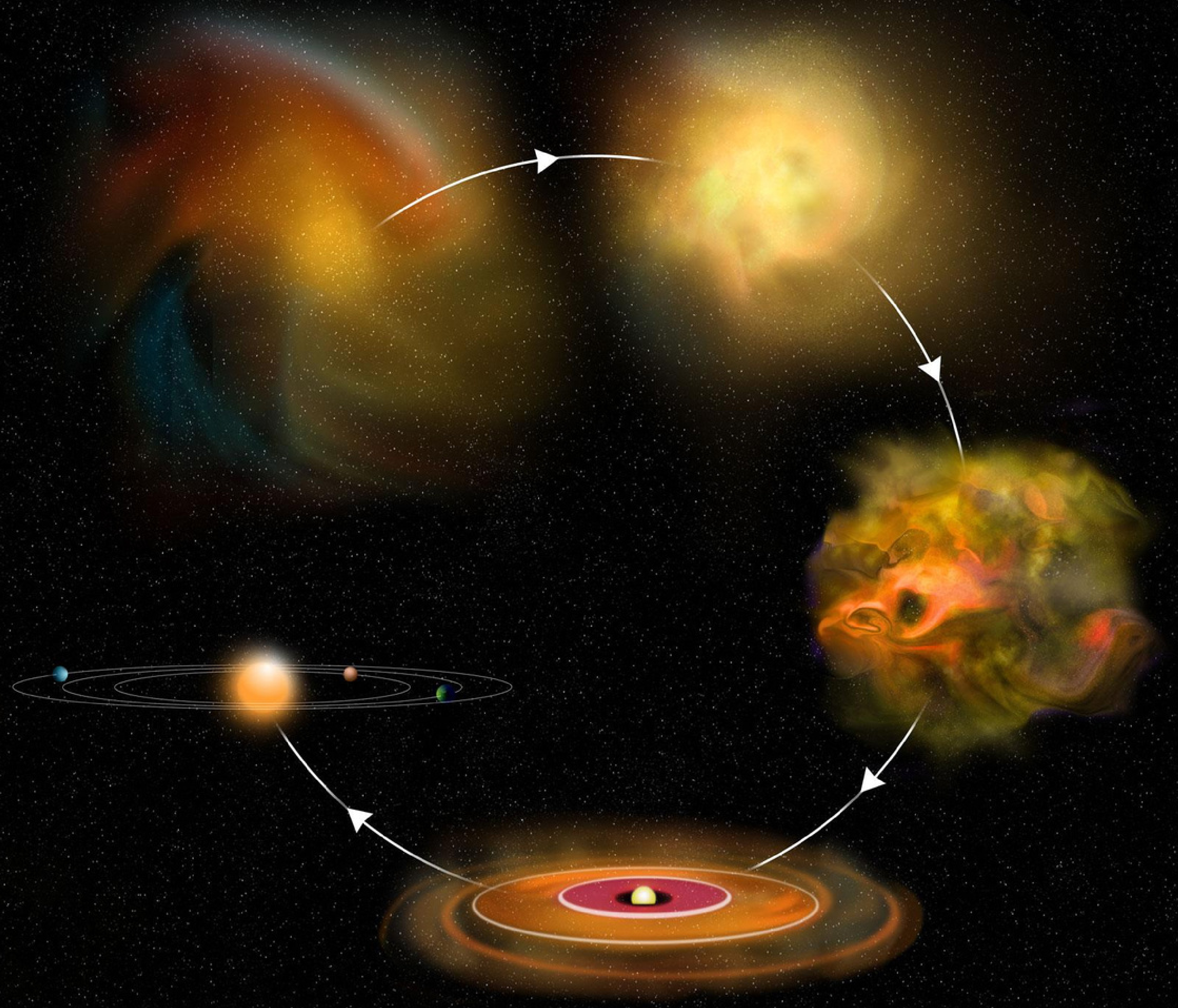


Image credit: Bill Saxton, NRAO/AUI/NSF

Molecular composition is
a tool to reveal the structure,
evolution and dynamics of
star- and planet-forming regions

ICE OPACITIES

...and how to access information hidden in cold regions of the ISM

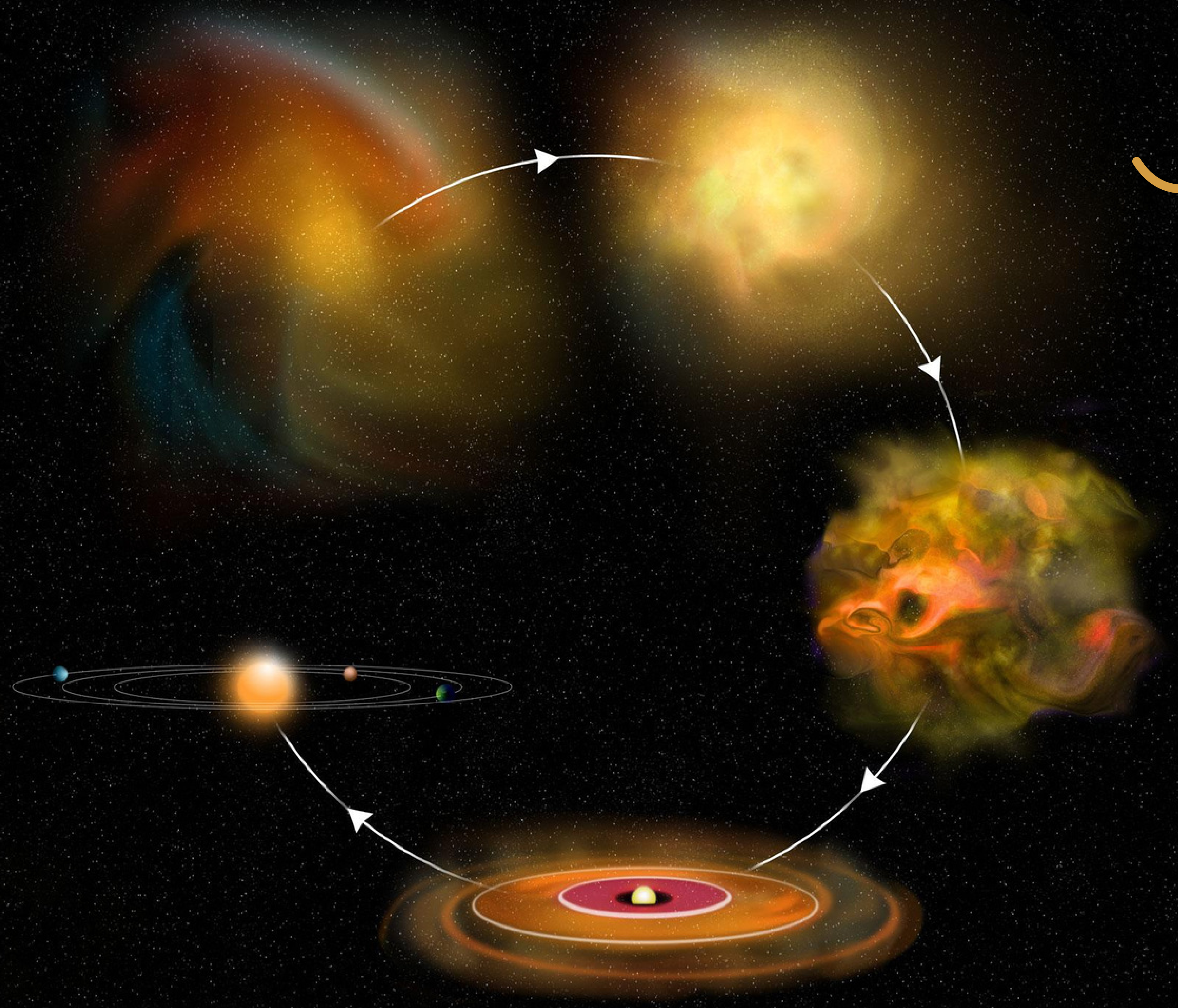


Image credit: Bill Saxton, NRAO/AUI/NSF

MOLECULAR DETECTION

gas

about 270 molecules

mostly by radioastronomy

ICE OPACITIES

…and how to access information hidden in cold regions of the ISM

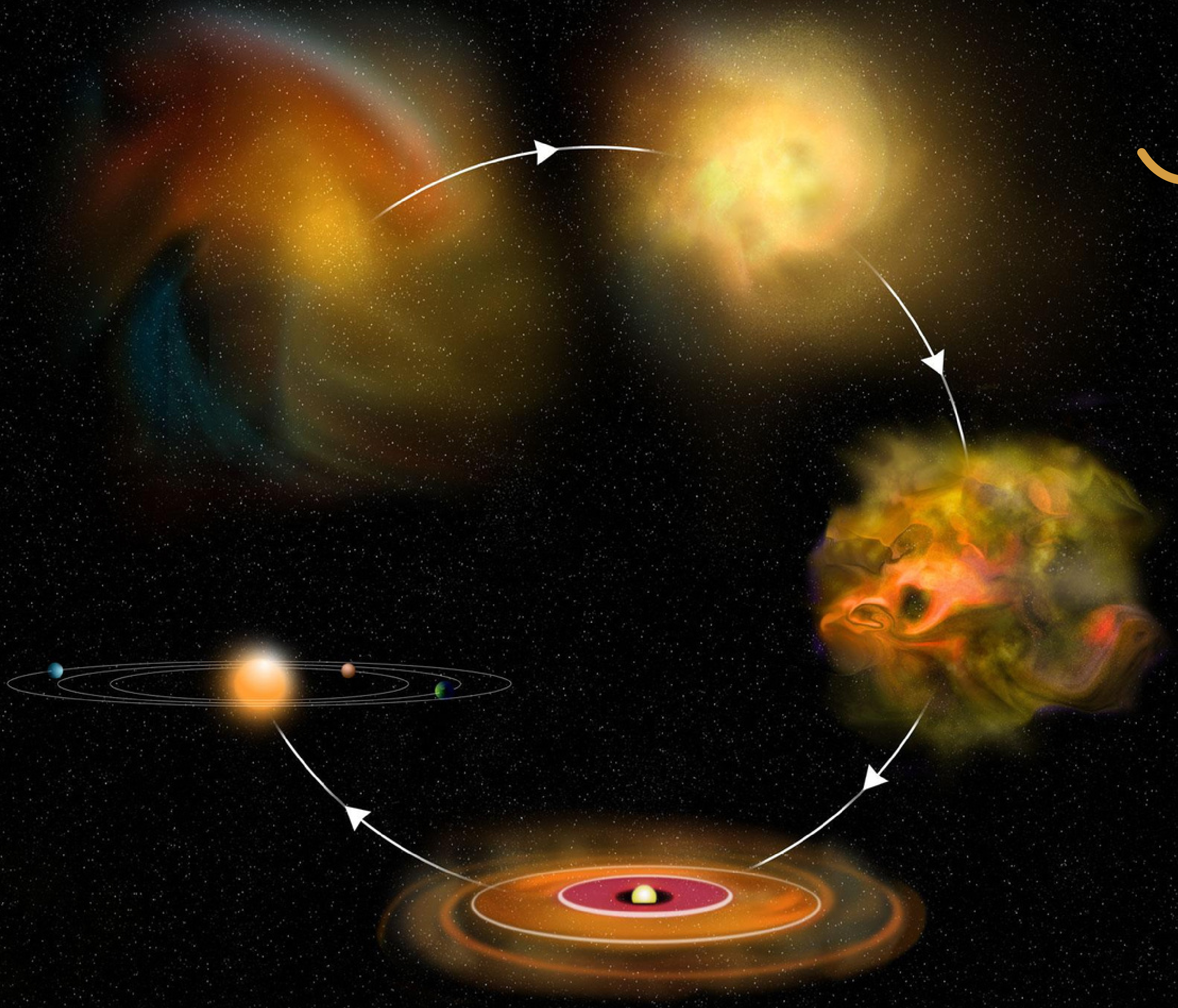


Image credit: Bill Saxton, NRAO/AUI/NSF

MOLECULAR DETECTION

gas → about 270 molecules → mostly by radioastronomy

grain → core (silicate and carbonaceous matter) + ice mantle → Infrared astronomy

ICE OPACITIES

...and how to access information hidden in cold regions of the ISM

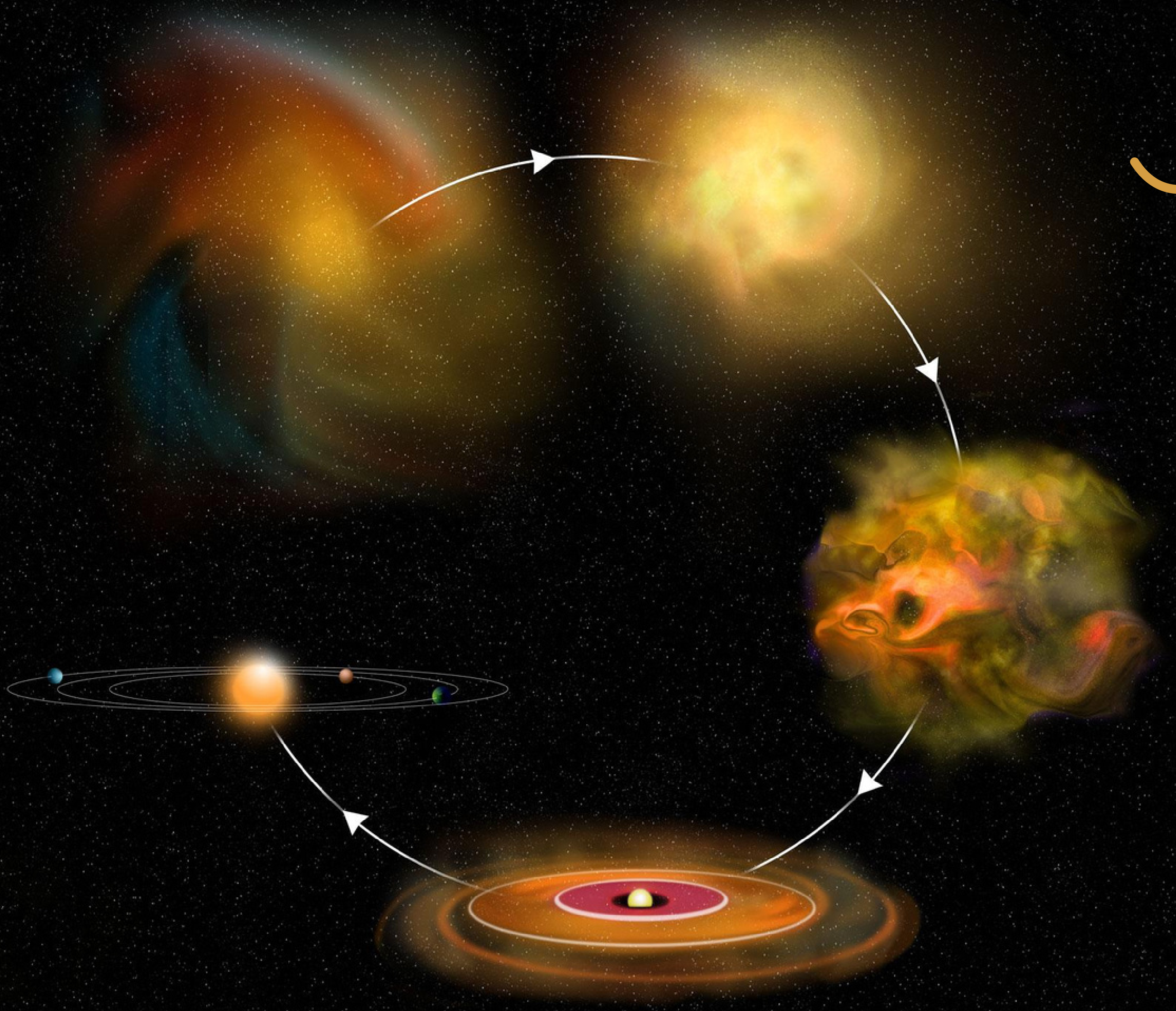


Image credit: Bill Saxton, NRAO/AUI/NSF

MOLECULAR DETECTION

grain

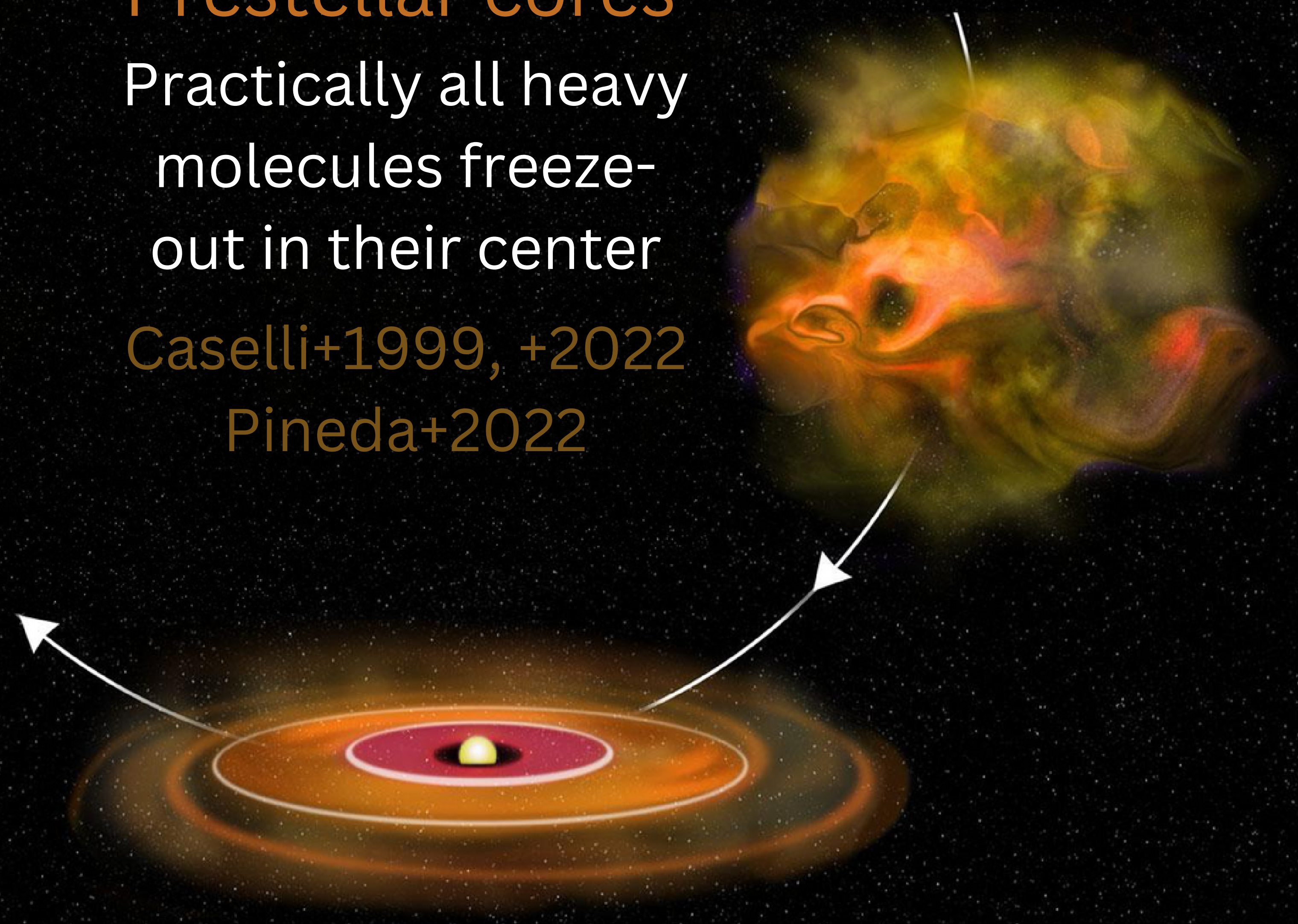
core
(silicate and
carbonaceous matter)
+ ice mantle

Near and Mid-IR
depends on
lines-of-sight

Infrared
astronomy

ICE OPACITIES

...and how to access information hidden in cold regions of the ISM



Prestellar cores

Practically all heavy molecules freeze-out in their center

Caselli+1999, +2022
Pineda+2022

Protoplanetary disks mid-planes

Catastrophic CO freeze out

Dutrey+1998
van Dishoeck2014
Boogert+2015

Challenge to obtain information in the cold and dense regions of ISM

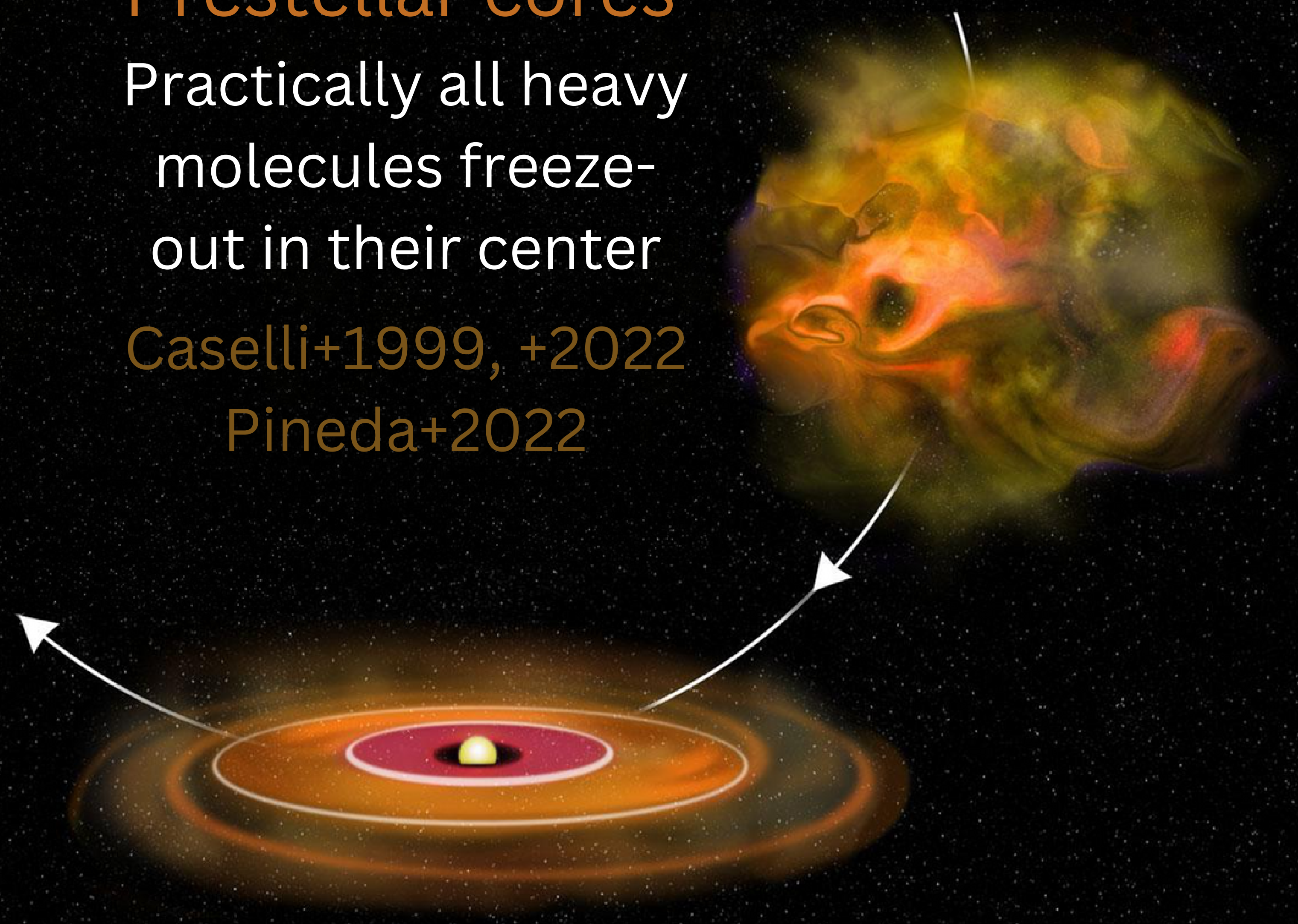
ICE OPACITIES

...and how to access information hidden in cold regions of the ISM

Prestellar cores

Practically all heavy molecules freeze-out in their center

Caselli+1999, +2022
Pineda+2022



Protoplanetary disks mid-planes

Catastrophic CO freeze out

Dutrey+1998
van Dishoeck2014
Boogert+2015

Challenge to obtain information in the cold and dense regions of ISM

↓

Use continuum emission in the FIR/THz

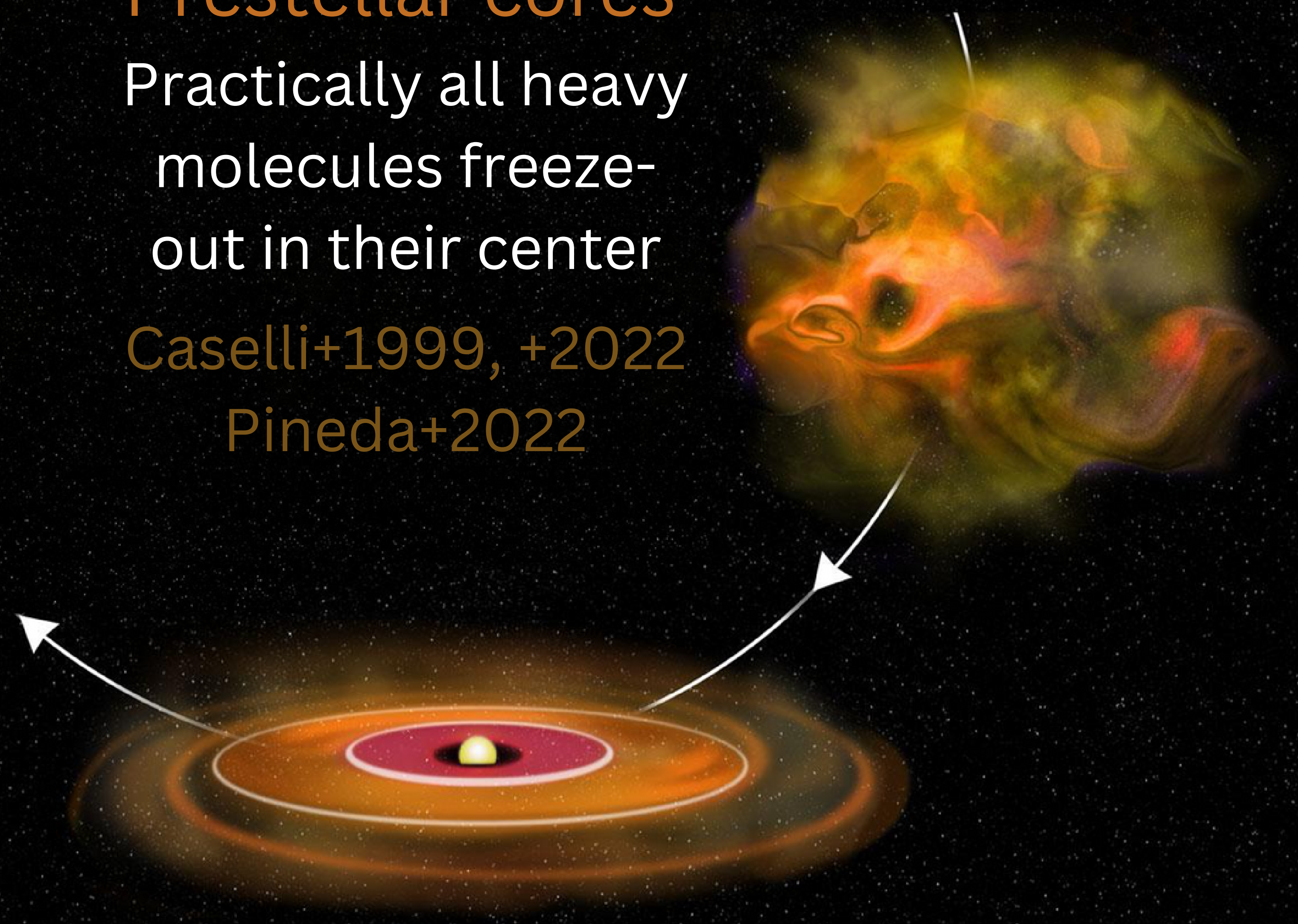
ICE OPACITIES

...and how to access information hidden in cold regions of the ISM

Prestellar cores

Practically all heavy molecules freeze-out in their center

Caselli+1999, +2022
Pineda+2022



Protoplanetary disks mid-planes

Catastrophic CO freeze out

Dutrey+1998
van Dishoeck2014
Boogert+2015

OUR GOAL

Use THz-Time Domain Spectroscopy to obtain directly measurements on the optical properties of ices in the Mid- and FIR

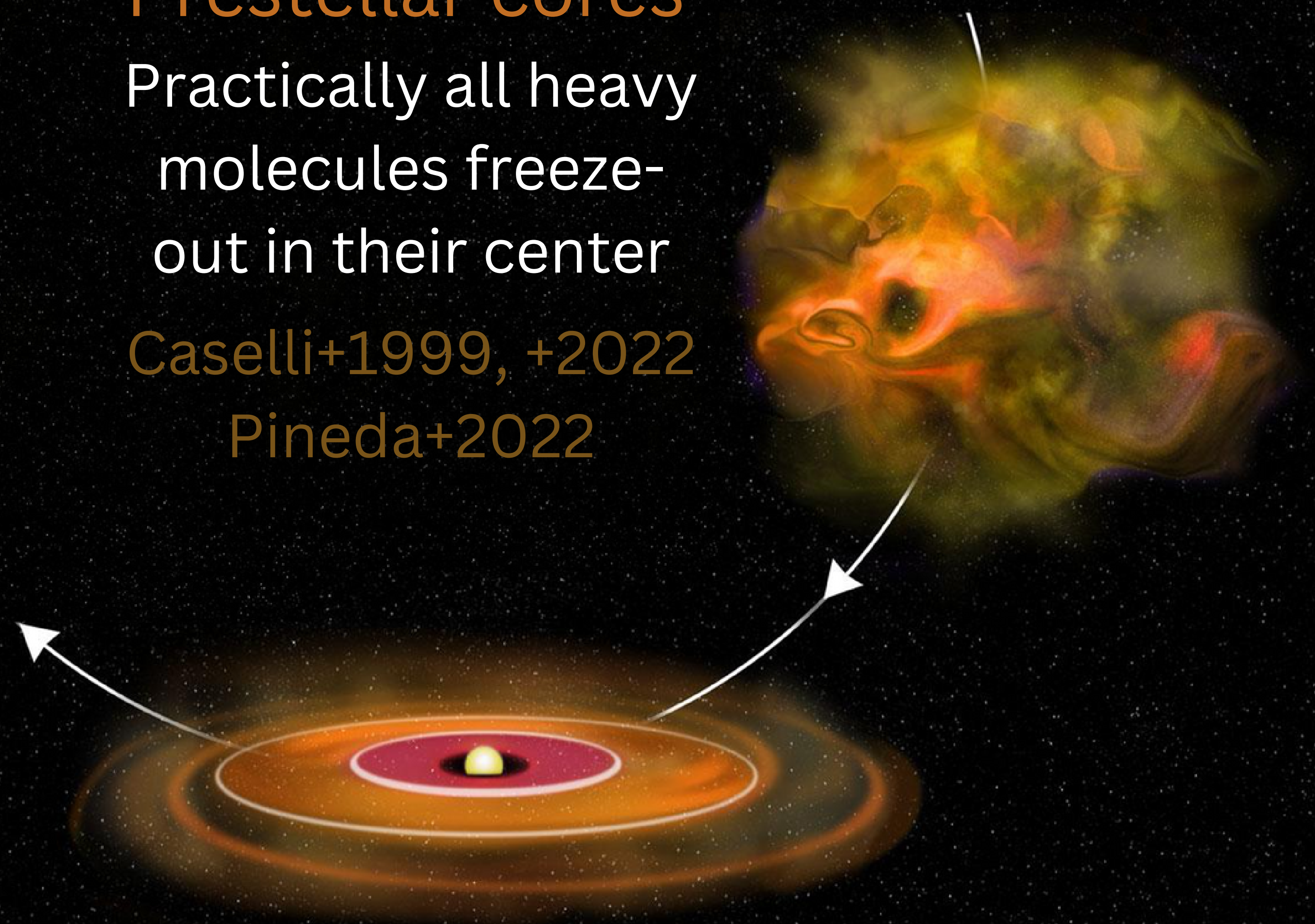
ICE OPACITIES

...and how to access information hidden in cold regions of the ISM

Prestellar cores

Practically all heavy molecules freeze-out in their center

Caselli+1999, +2022
Pineda+2022



Protoplanetary disks mid-planes

Catastrophic CO freeze out

Dutrey+1998
van Dishoeck2014
Boogert+2015

OUR GOAL

Use THz-Time Domain Spectroscopy to obtain directly measurements on the optical properties of ices in the Mid- and FIR

Dust opacities
K. Demyk talk!

OPTICAL CONSTANTS

…and how Time-Domain Spectroscopy can avoid long calculations

Optical constants *m* describe how the electromagnetic radiation interacts with a material

refractive index

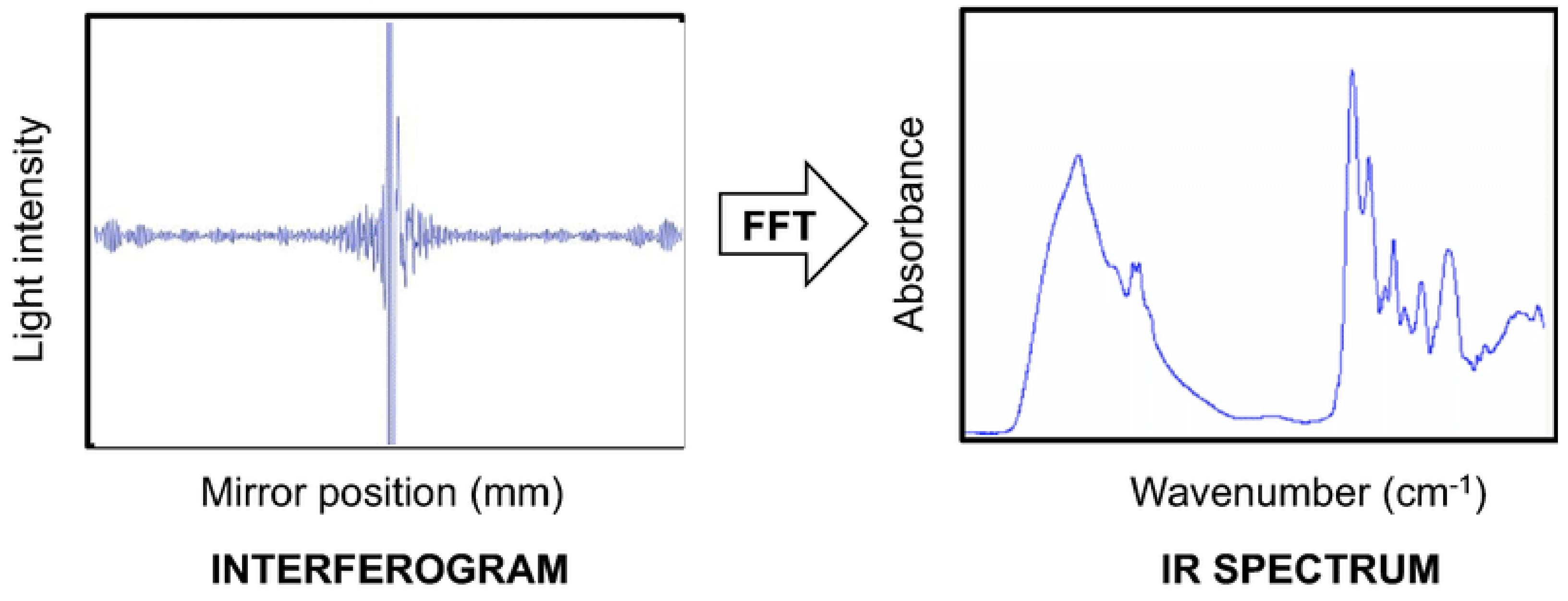
$$m = n + ik = \sqrt{\varepsilon}$$

absorption coefficient

OPTICAL CONSTANTS

…and how Time-Domain Spectroscopy can avoid long calculations

Experimentally FTIR spectroscopy is used to obtain them



It contains only the amplitude information, and thus the complex dielectric permittivity cannot be directly reconstructed

Optical constants *m* describe how the electromagnetic radiation interacts with a material

refractive index

$$m = n + ik = \sqrt{\varepsilon}$$

absorption coefficient

OPTICAL CONSTANTS

…and how Time-Domain Spectroscopy can avoid long calculations

Optical constants *m* describe how the electromagnetic radiation interacts with a material

Kramers-Kronig relations are used to relate the real and imaginary portions of the refractive index

$$n(\nu) = n(\infty) + \frac{2}{\pi} P \int_{o}^{\infty} \frac{\nu' \kappa(\nu')}{\nu'^2 - \nu^2} d\nu'$$

$$k(\nu) = -\frac{2}{\pi} P \int_{o}^{\infty} \frac{n(\nu')}{\nu'^2 - \nu^2} d\nu'$$

refractive index

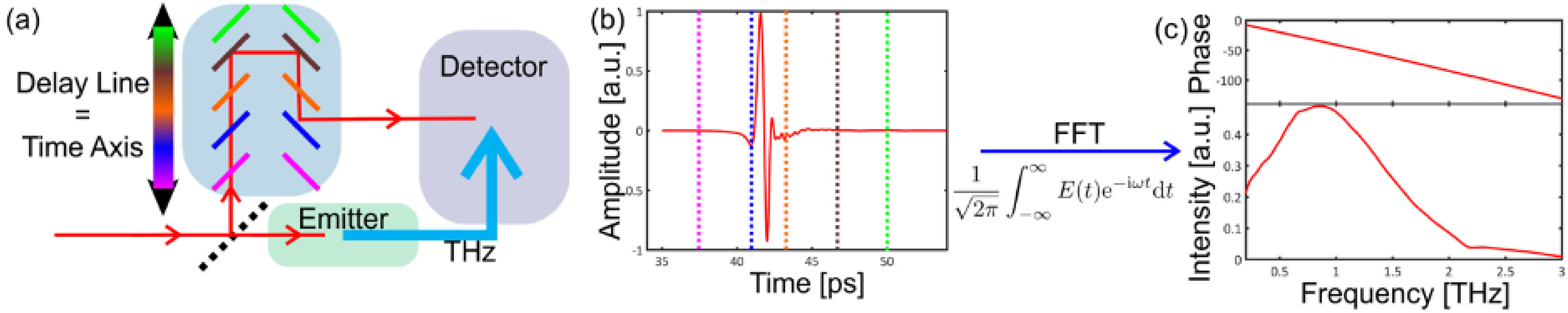
$$m = n + ik = \sqrt{\varepsilon}$$

absorption coefficient

OPTICAL CONSTANTS

…and how Time-Domain Spectroscopy can avoid long calculations

Time-Domain Spectroscopy (TDS) gives amplitude and phase information about the transmitted pulse

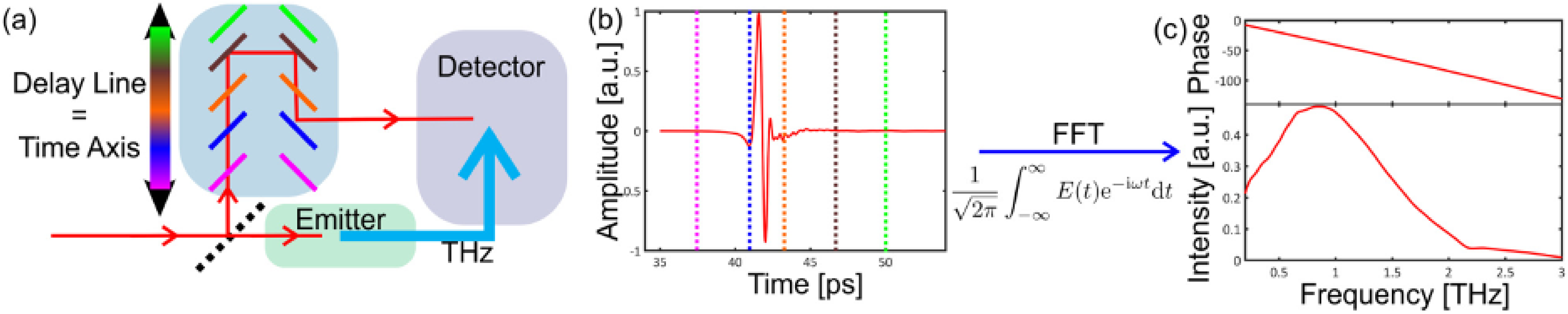


Neu & Schmuttenmaer, 2018

OPTICAL CONSTANTS

…and how Time-Domain Spectroscopy can avoid long calculations

Time-Domain Spectroscopy (TDS) gives amplitude and phase information about the transmitted pulse



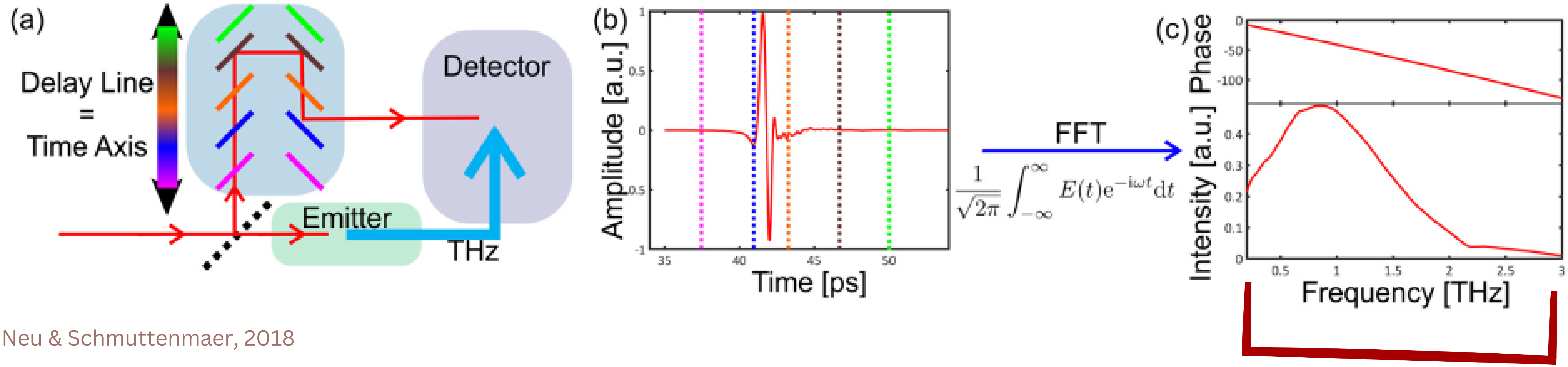
Neu & Schmuttenmaer, 2018

New algorithm that reconstructs the real and imaginary part of the optical constants without having to use Kramers-Kronig relations (Giuliano+2019)

OPTICAL CONSTANTS

…and how Time-Domain Spectroscopy can avoid long calculations

Time-Domain Spectroscopy (TDS) gives amplitude and phase information about the transmitted pulse



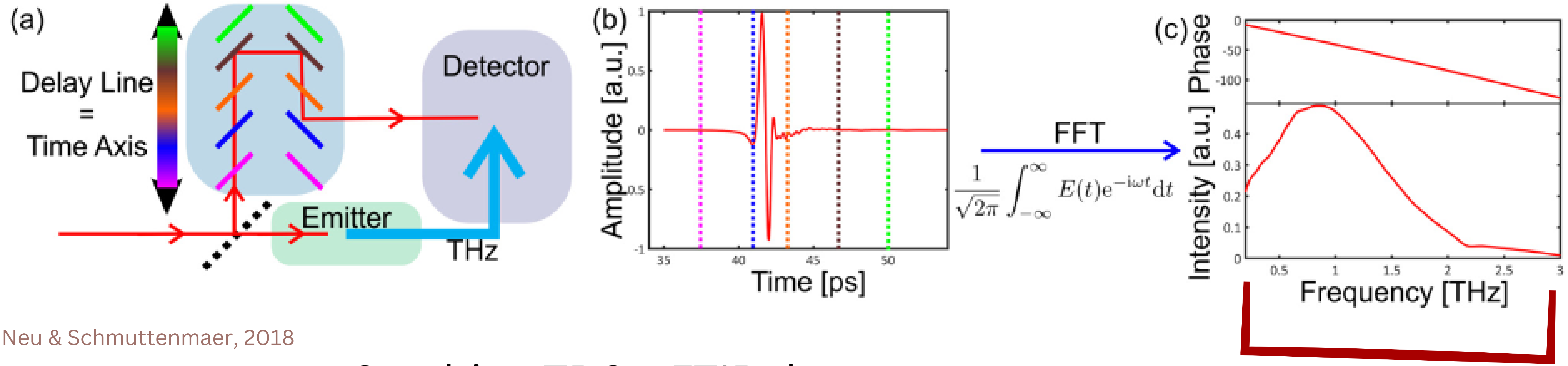
Neu & Schmuttenmaer, 2018

Narrow frequency range
0.1 – 4.0 THz

OPTICAL CONSTANTS

…and how Time-Domain Spectroscopy can avoid long calculations

Time-Domain Spectroscopy (TDS) gives amplitude and phase information about the transmitted pulse



Neu & Schmuttenmaer, 2018

Combine TDS + FTIR data to directly reconstruct optical constants in a broad range of wavelenghts

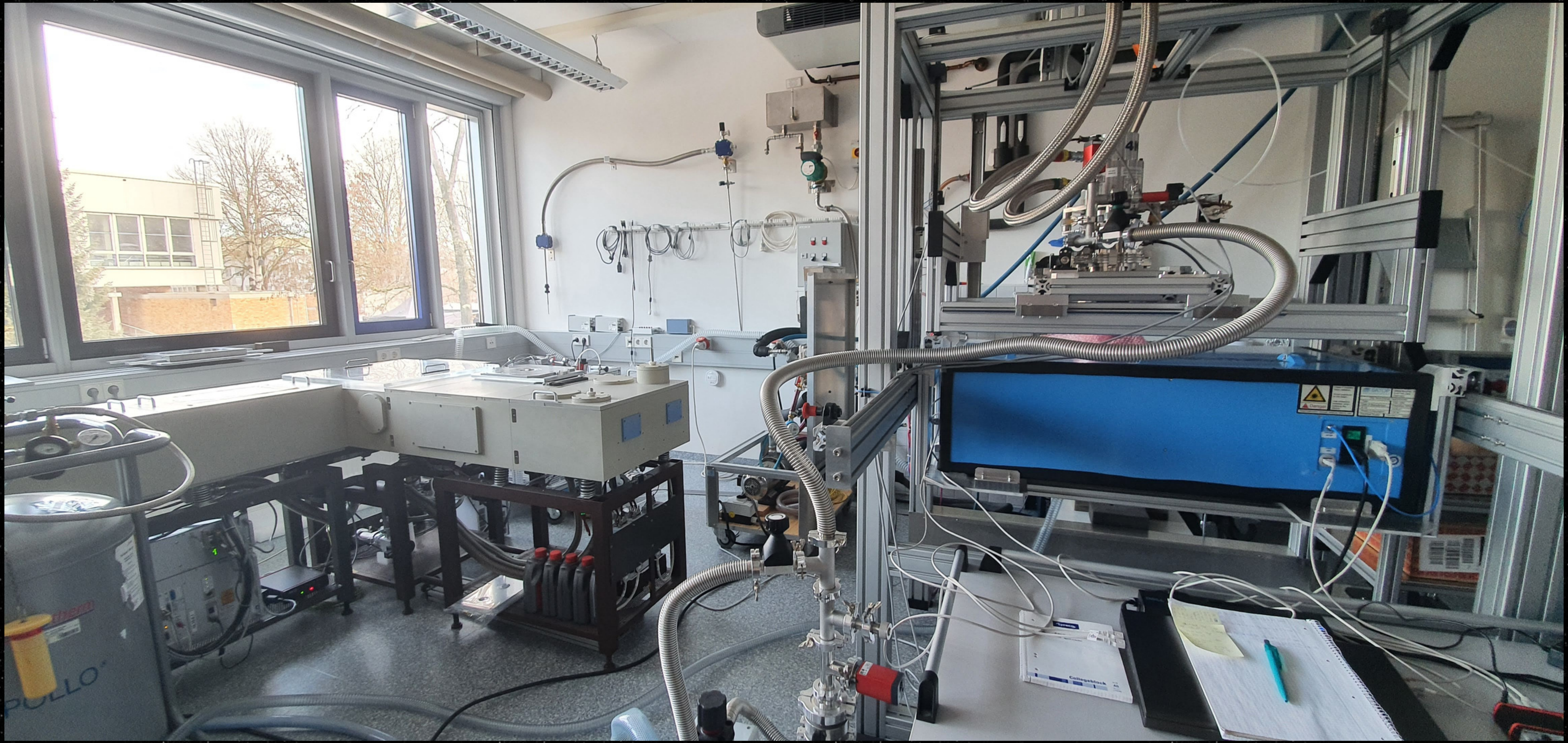
Gavsdush & Kruczkiewicz+2022

← Narrow frequency range 0.1 – 4.0 THz

Check our virtual lab tour on:
https://discussions.astrochem.net/videos

CASICE LAB

Max-Planck-Institut für
extraterrestrische Physik



FTIR spectrometer // THz Time-Domain spectrometer

TIME-DOMAIN AND FTIR SPECTROSCOPY

...and how the experiments are done

CASICE set-ups

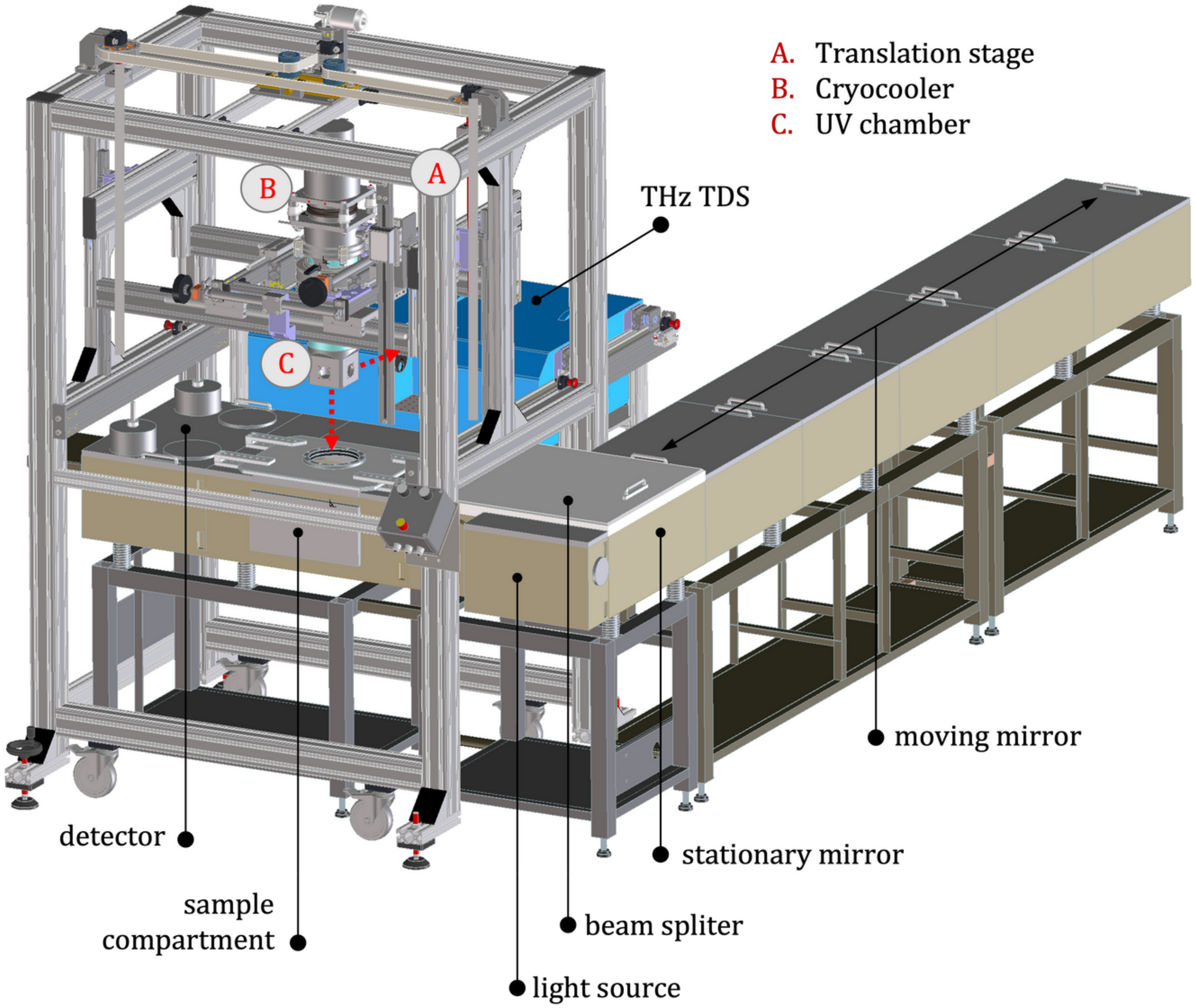
- THz-TDS
- FTIR

Mutual experimental chamber

- Moved using translation stage
- Cryostat designed to avoid vibrations

Ice deposition

- Pbase = 10-7 mbar
- T = 10 K
- Ices are too thick for laser interferometry



TIME-DOMAIN AND FTIR SPECTROSCOPY

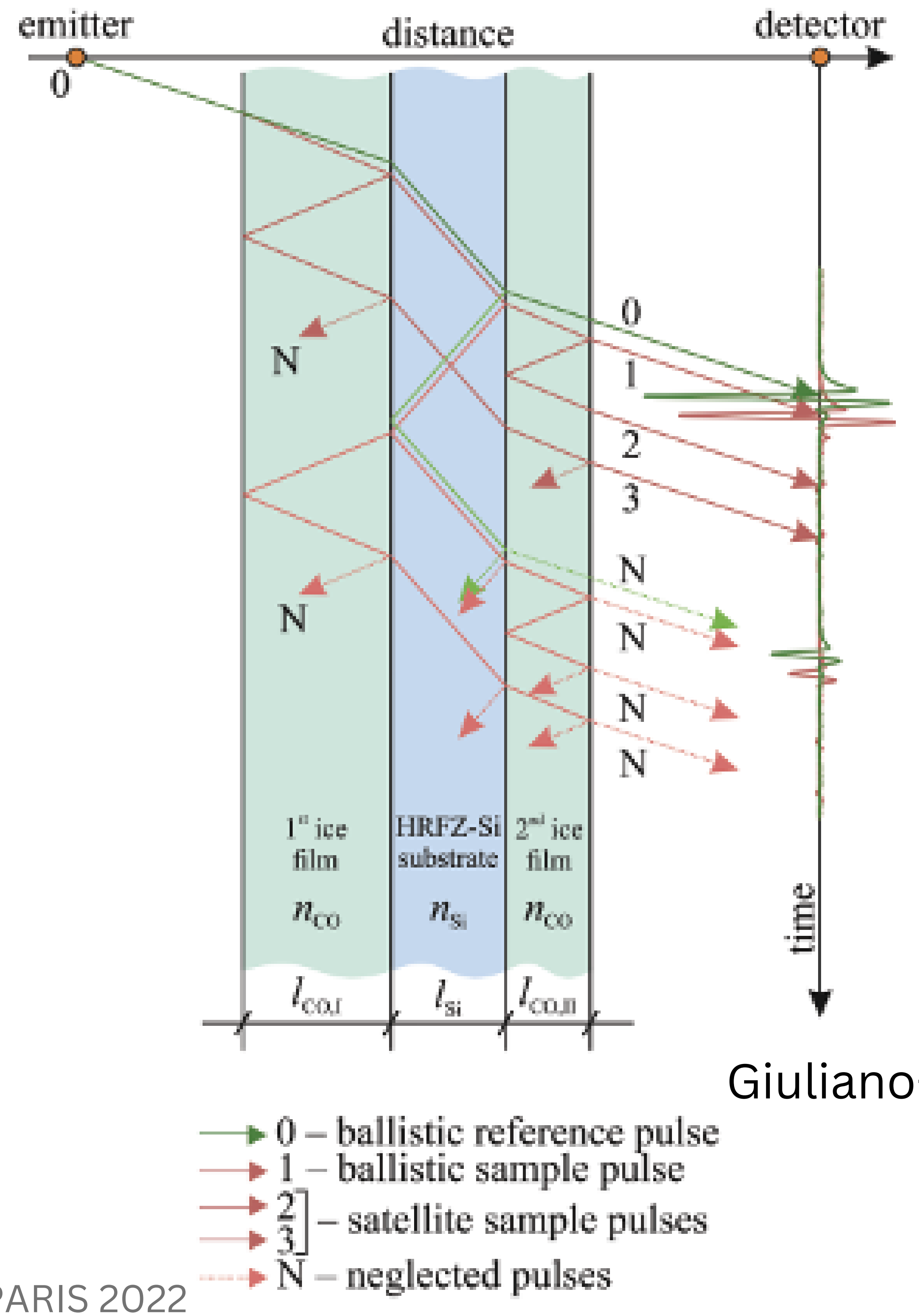
...and how the experiments are done

CASICE set-ups
- THz-TDS
- FTIR

Mutual experimental chamber
- Moved using translation stage
- Cryostat designed to avoid vibrations

Ice deposition
- Pbase = 10-7 mbar
- T = 10 K
- Ices are too thick for laser interferometry

model the sample waveforms to obtain the ice thickness

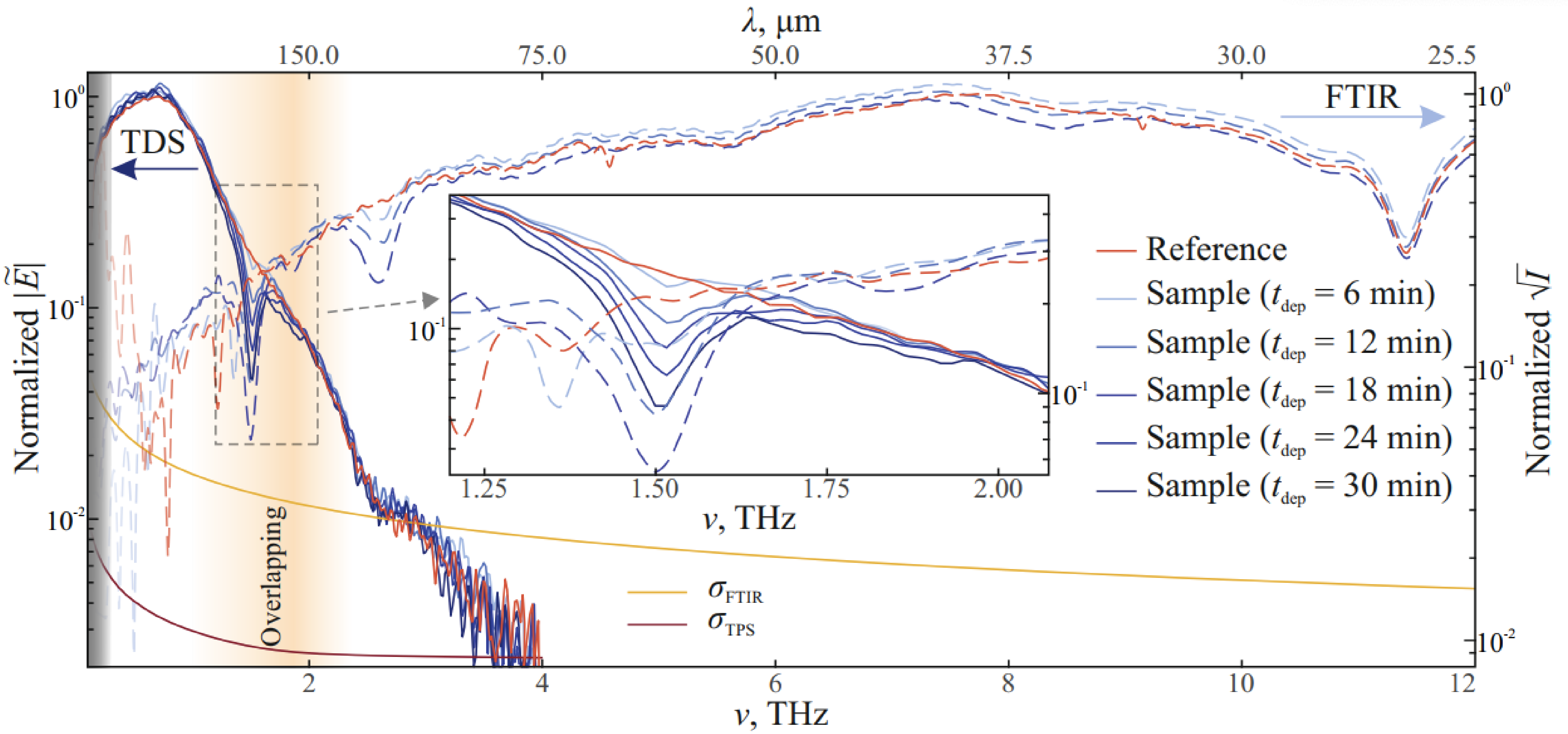


Giuliano+2019

BROADBAND SPECTROSCOPY MEASUREMENTS

...and how we merge the data

FTIR 0.1 – 12 THz



Gavsdush & Kruczkiewicz+2022

Arsenii GAVDUSH

Prokhorov General Physics Institute

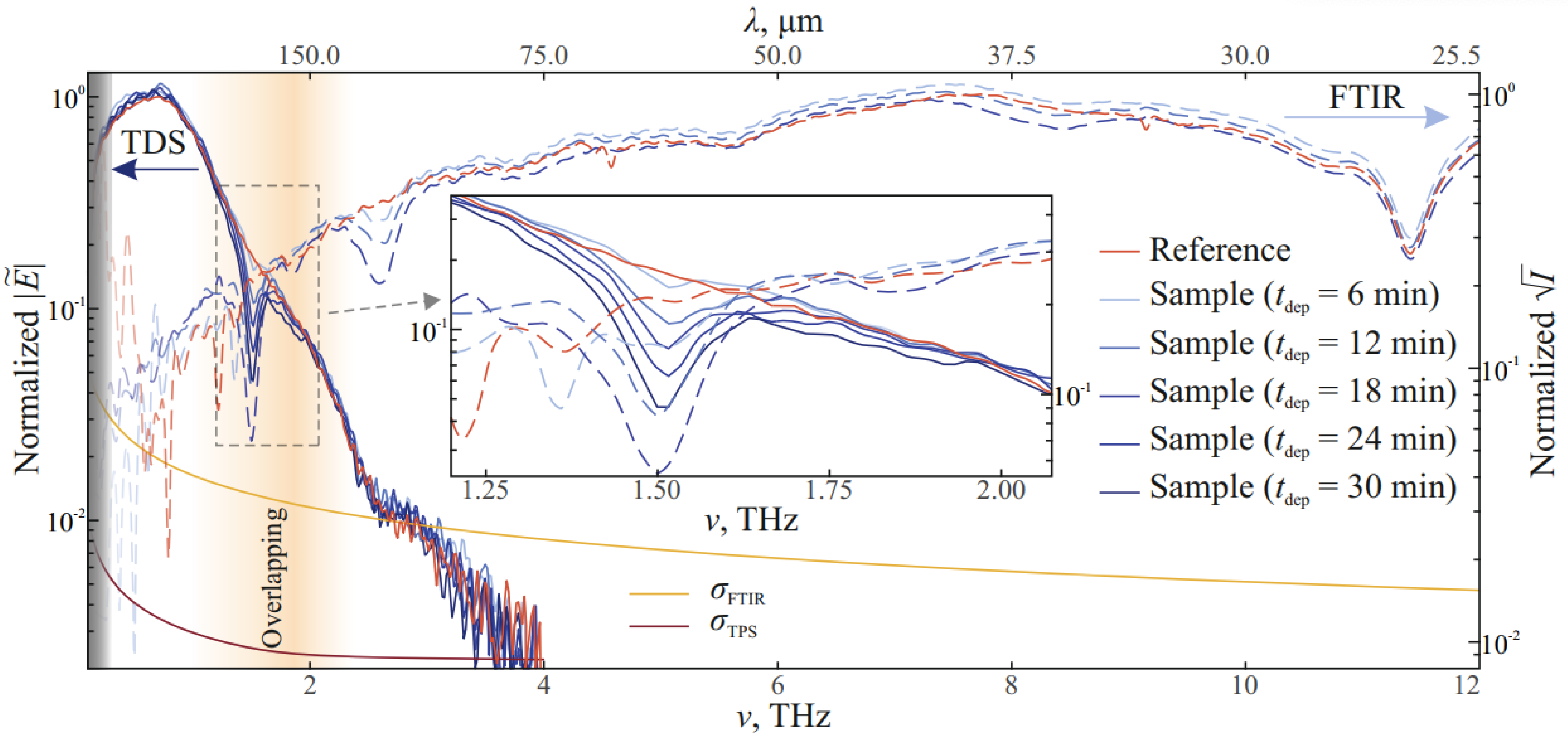
TDS

0.1 – 4.0 THz

BROADBAND SPECTROSCOPY MEASUREMENTS

...and how we merge the data

FTIR 0.1 – 12 THz



Gavsdush & Kruczkiewicz+2022

TDS

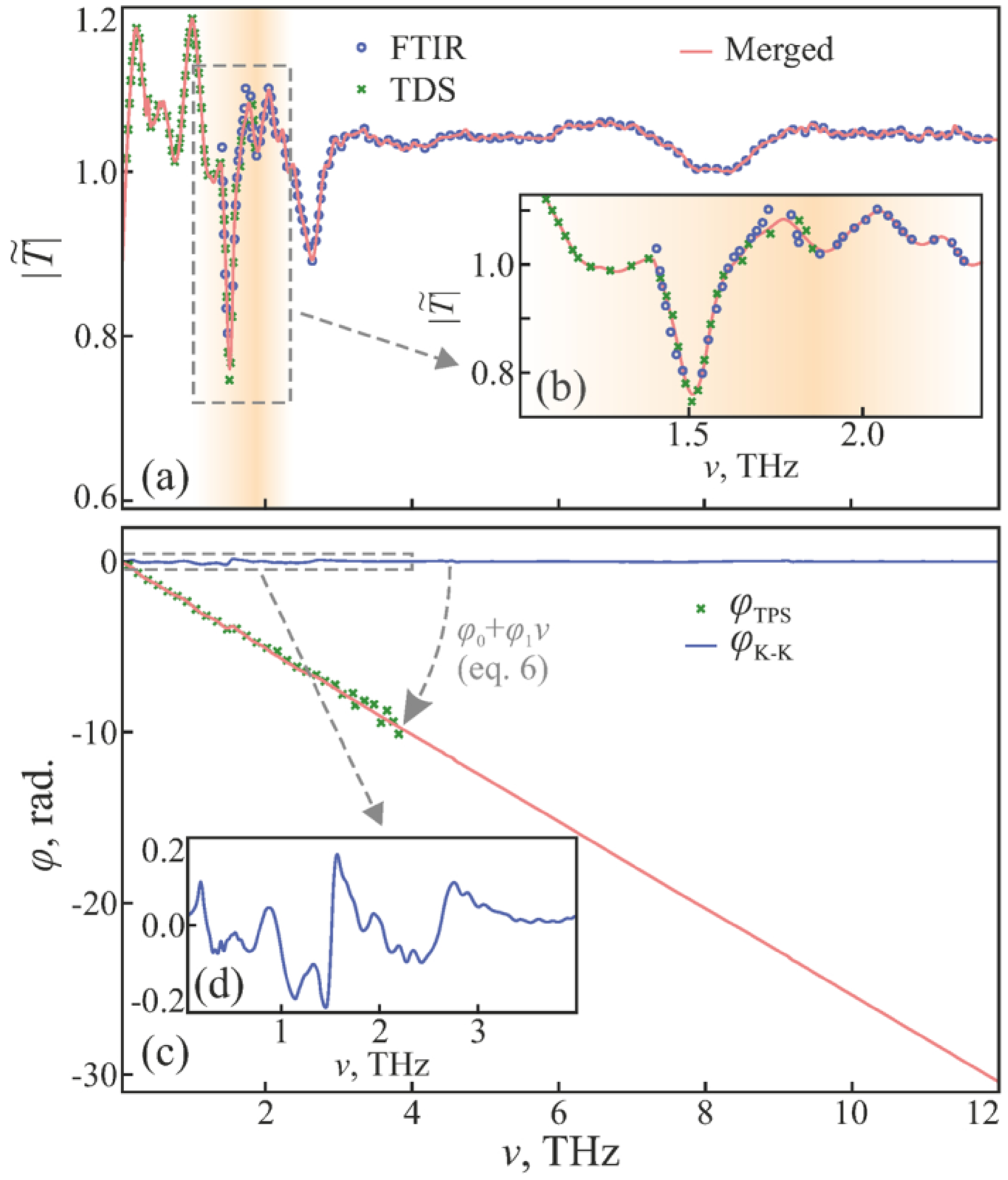
0.1 – 4.0 THz

Merge the transmission spectra

- FTIR phase must be reconstructed
- TDS and FTIR amplitudes and phases must be matched

BROADBAND SPECTROSCOPY MEASUREMENTS

...and how we merge the data



Gavsdush & Kruczkiewicz+2022

Merge the transmission spectra

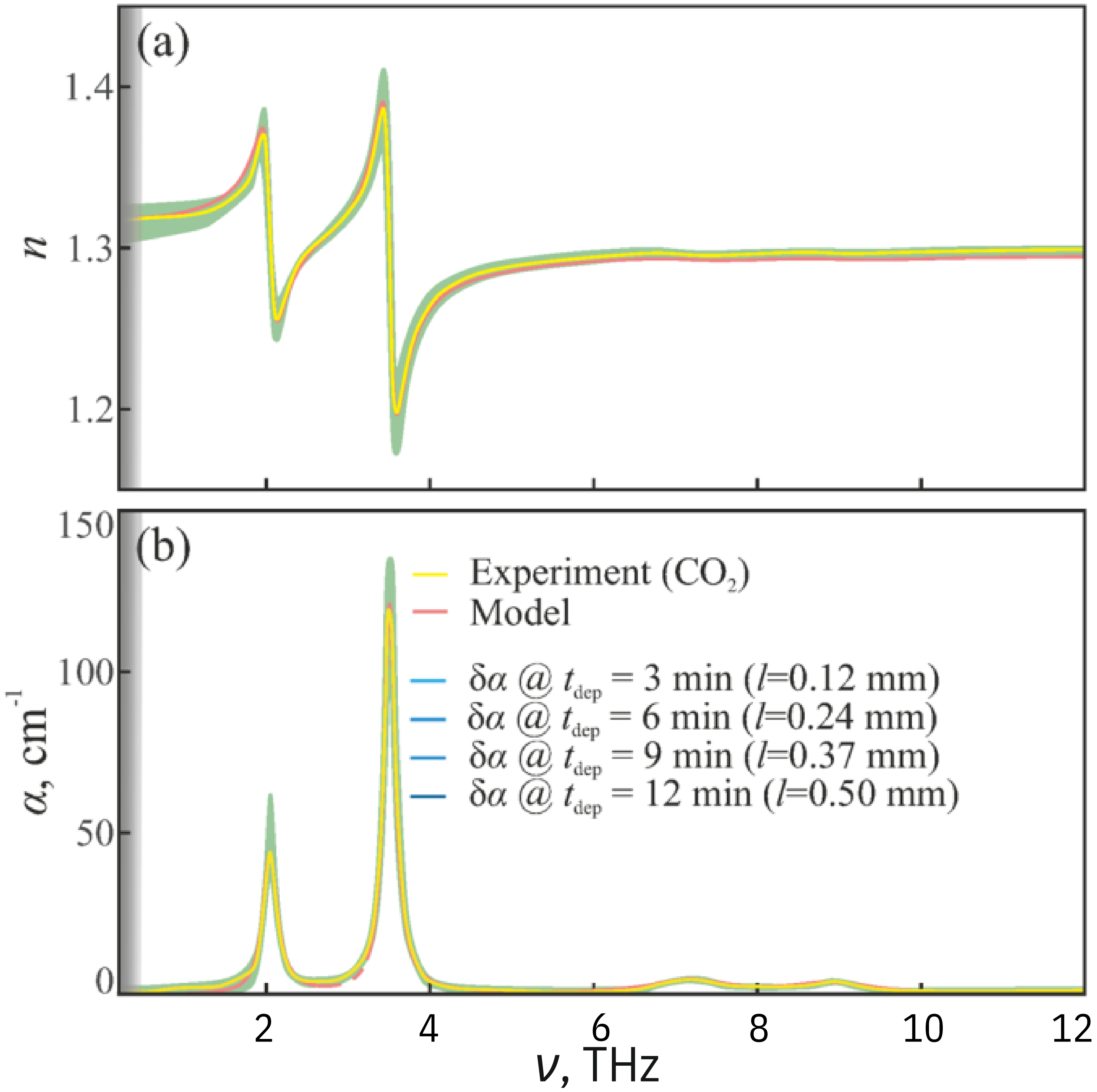
- FTIR phase must be reconstructed
- TDS and FTIR amplitudes and phases must be matched

Combine TDS + FTIR data

TDS: thickness, amplitude and phase
FTIR: amplitude, phase from KK
and correct with TDS data

BROADBAND SPECTROSCOPY MEASUREMENTS

...and finally the optical constants



Gavsdush & Kruczkiewicz+2022

Merge the transmission spectra

- FTIR phase must be reconstructed
- TDS and FTIR amplitudes and phases must be matched

Combine TDS + FTIR data

TDS: thickness, amplitude and phase
FTIR: amplitude, phase from KK
and correct with TDS data

ICE OPACITY

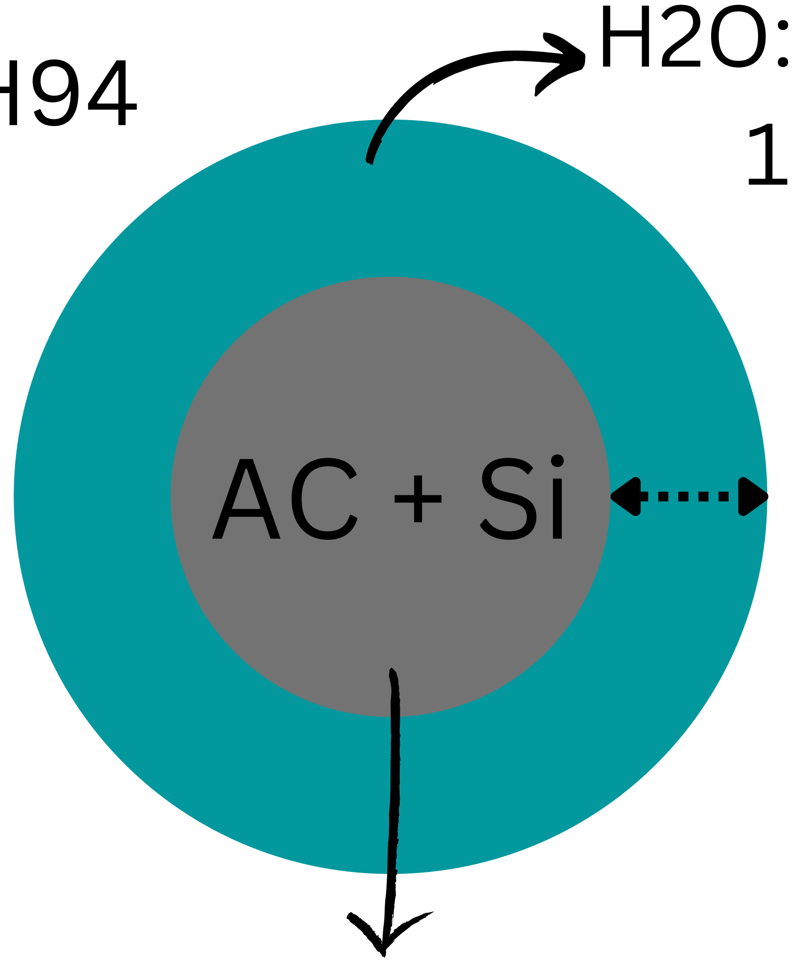
...and how our data compares with the literature

Opacity model from Ossenkopf & Henning 94 (OH94)

OH94

$H_2O:CH_3OH:CO:NH_3$

100 : 10 : 1 : 1



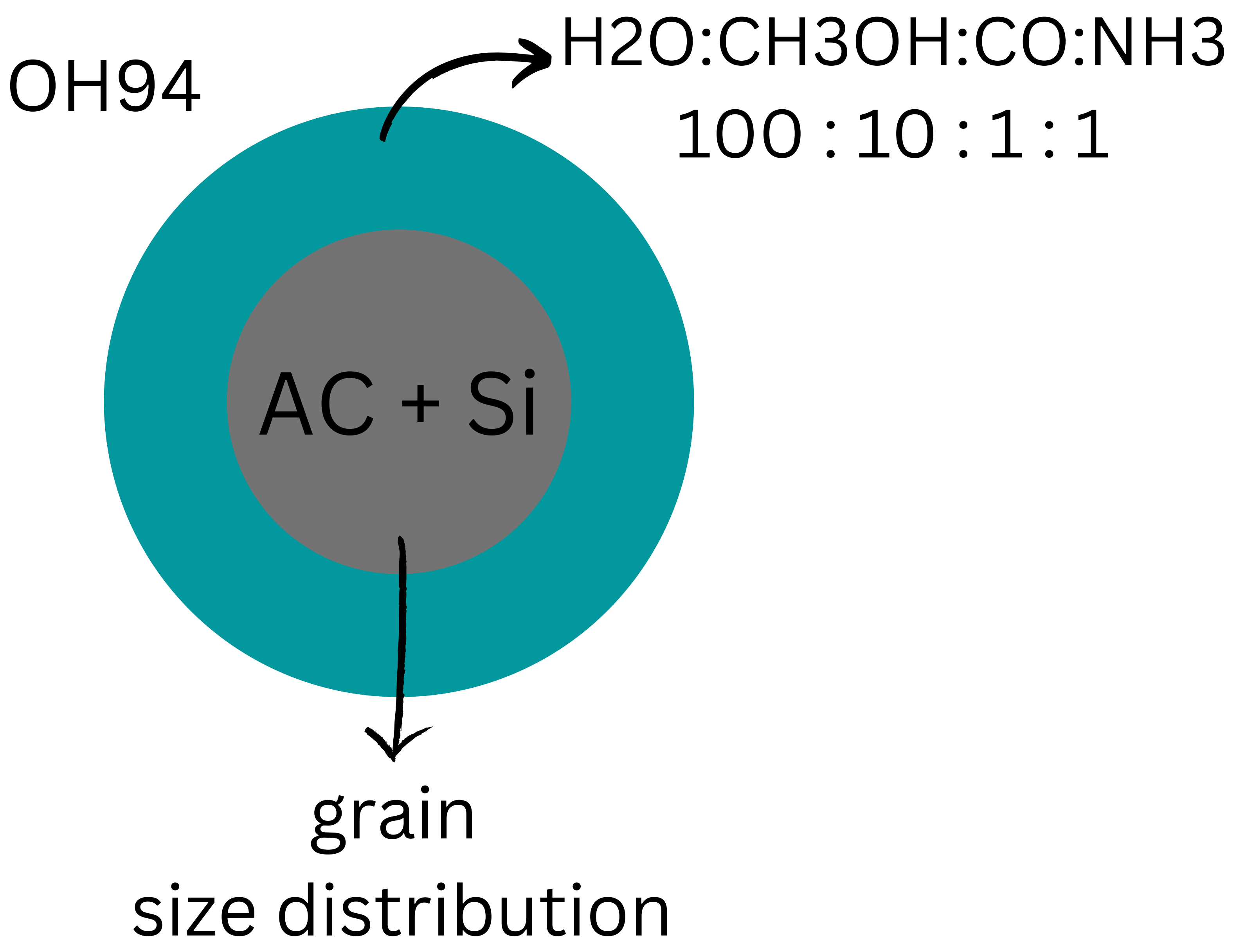
volume ratio can vary } V = 0 bare grain; V = 4.5 thick ice

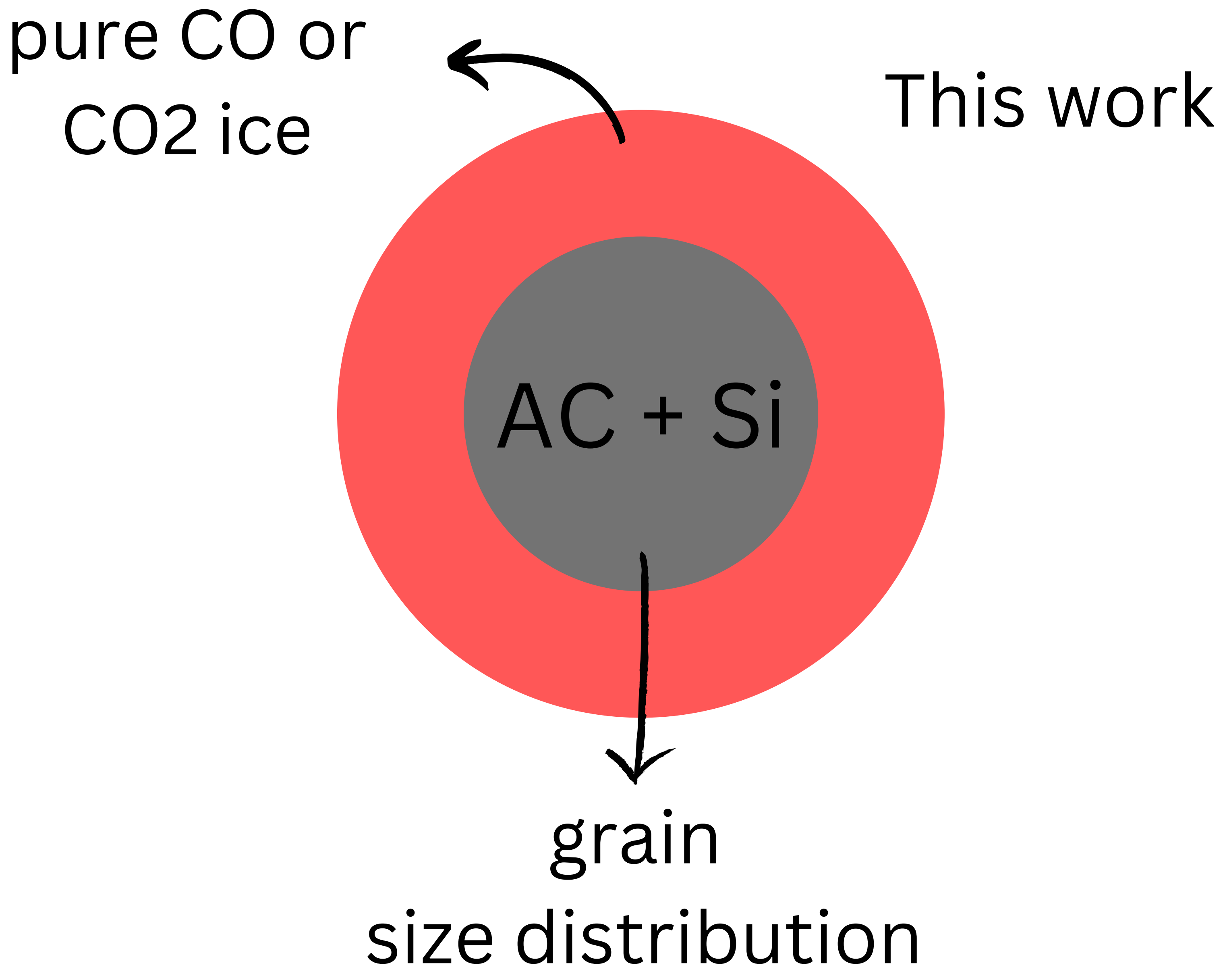
grain size distribution

ICE OPACITY

…and how our data compares with the literature

Opacity model from Ossenkopf & Henning 94 (OH94)



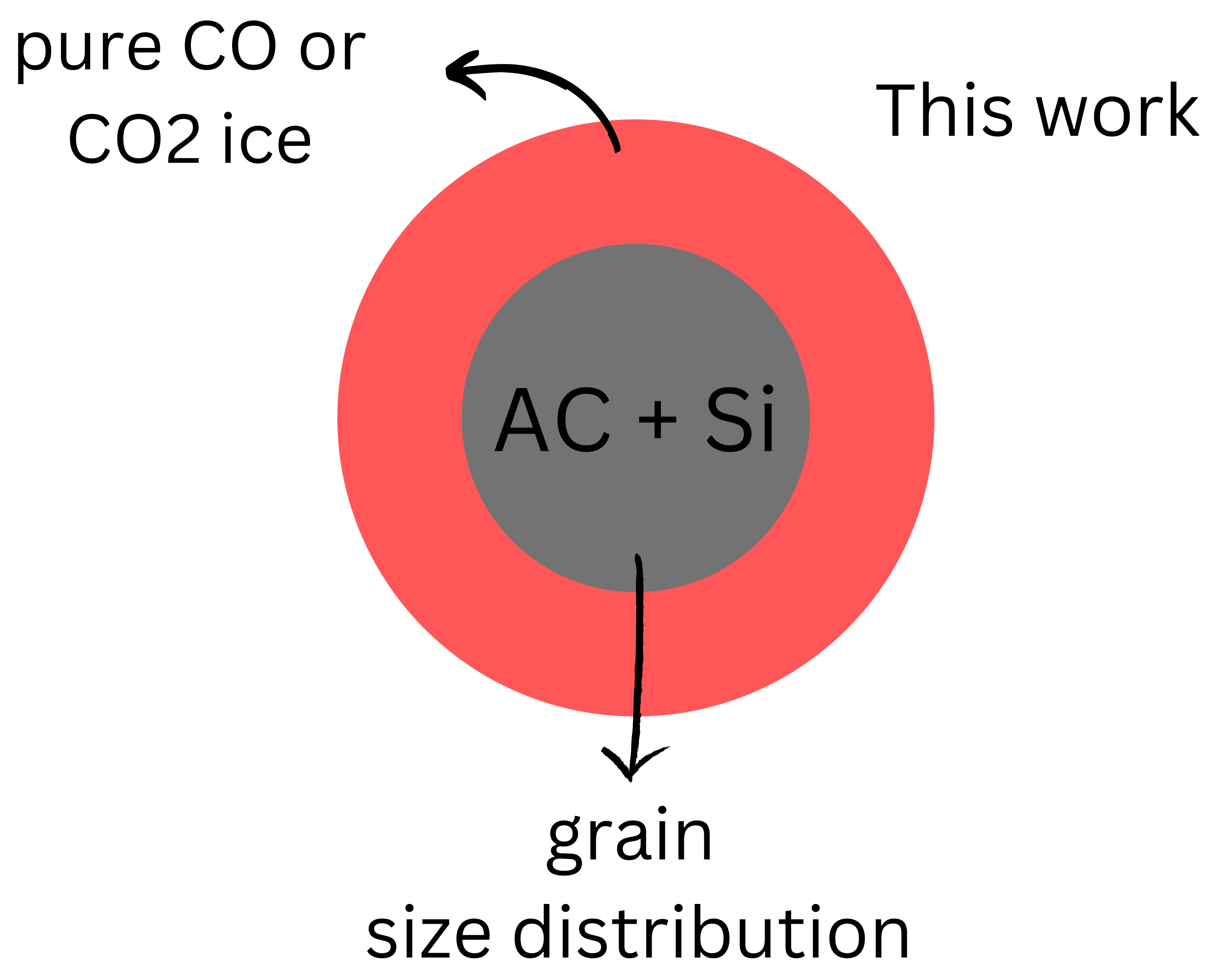


ICE OPACITY

…and how our data compares with the literature

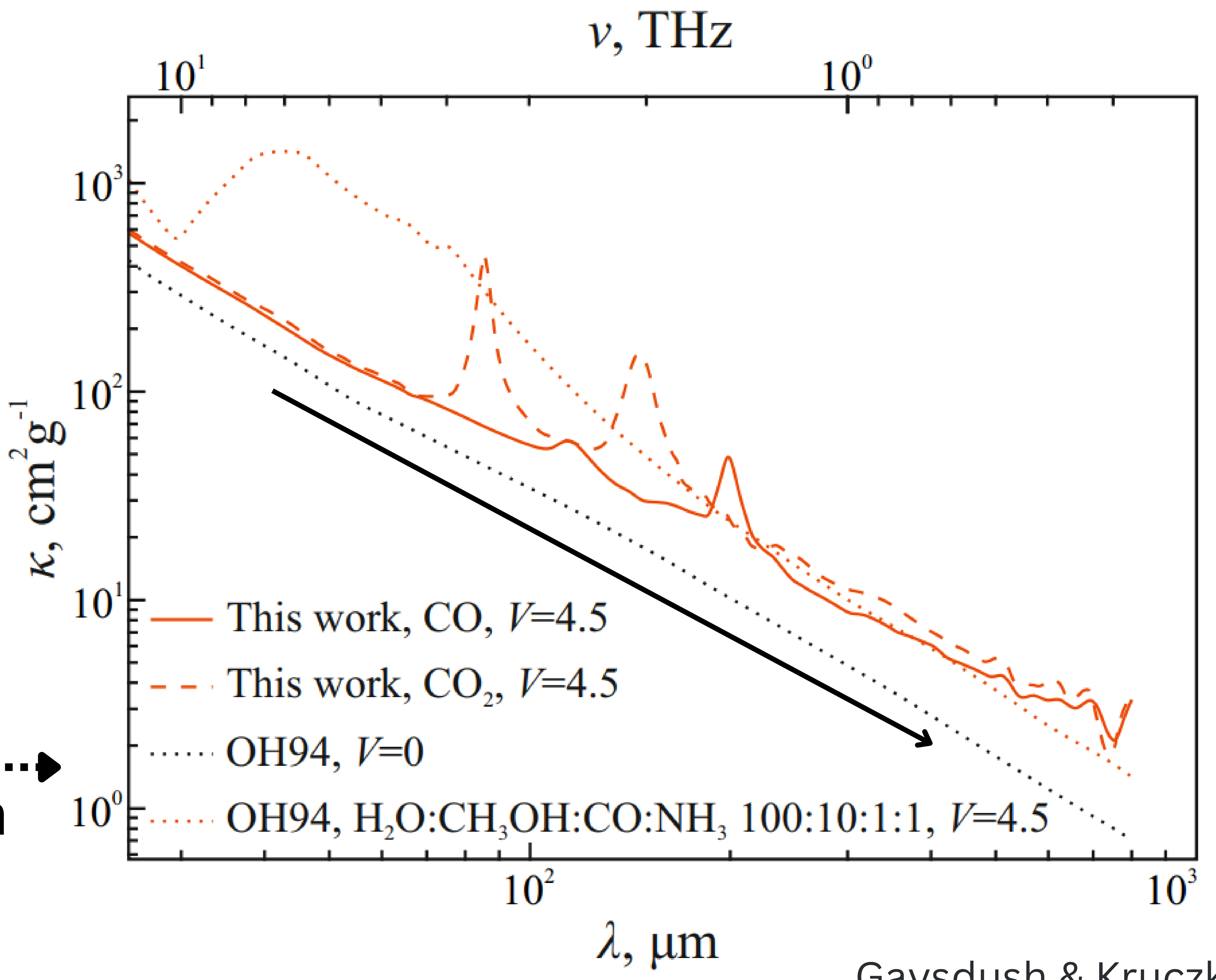
Opacity model from Ossenkopf & Henning 94 (OH94)

Our model accounts for drastic CO and CO2 freeze-out at the centre of pre-stellar cores or in protoplanetary disk mid-planes



ICE OPACITY

…and how our data compares with the literature

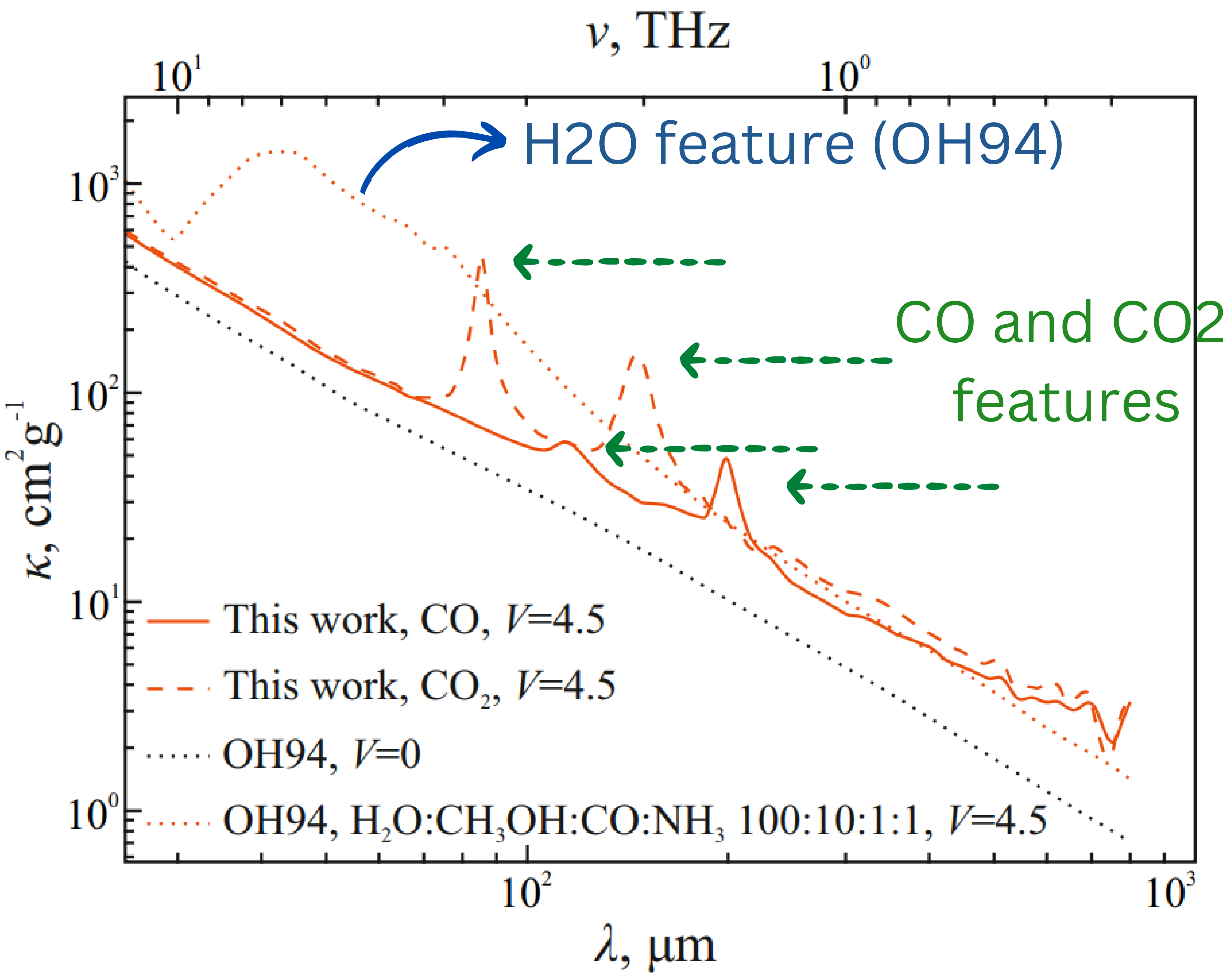


bare grain

Gavsdush & Kruczkiewicz+2022

ICE OPACITY

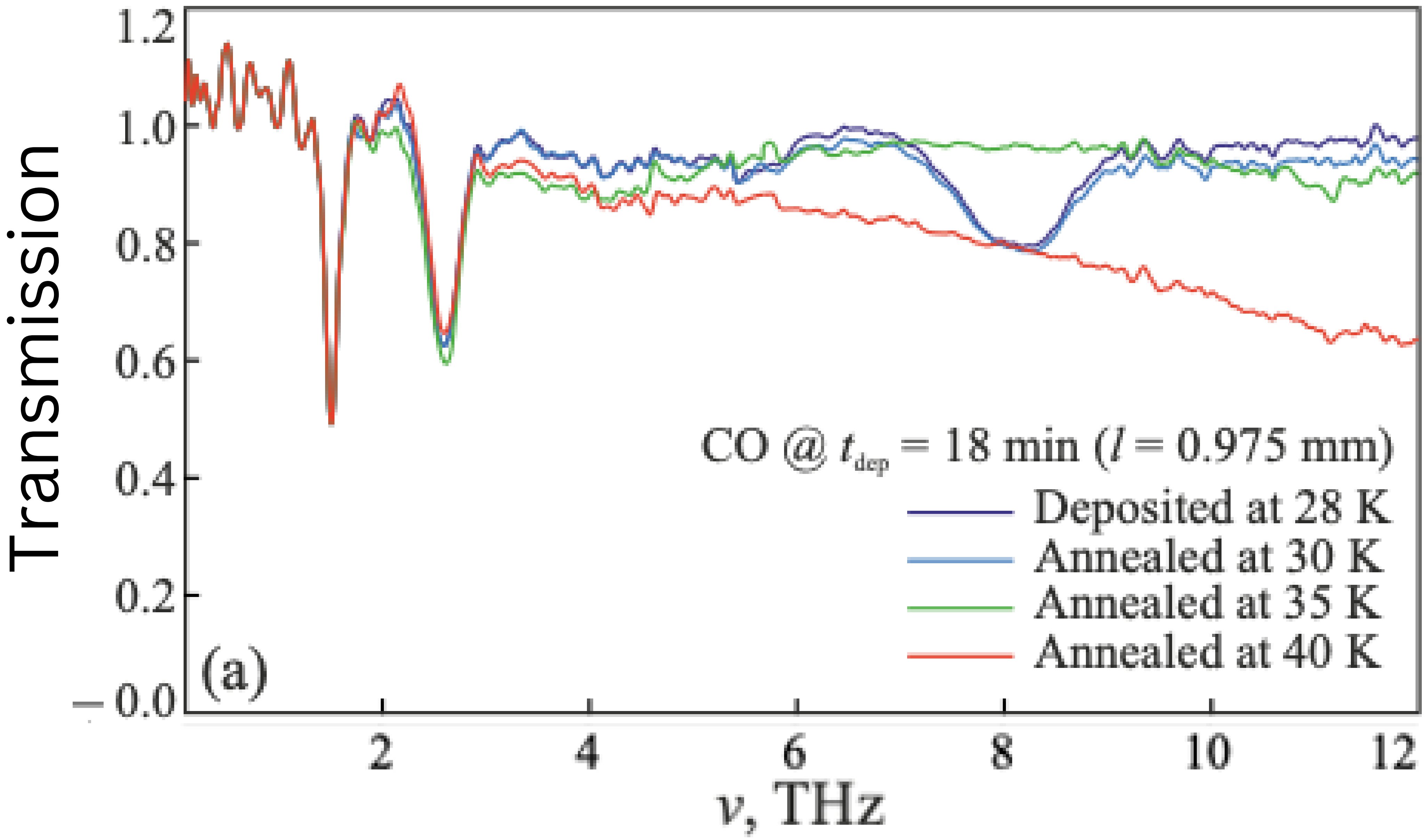
...and how our data compares with the literature



TRANSMISSION SPECTRA

...and how the temperature affect the ice optical properties

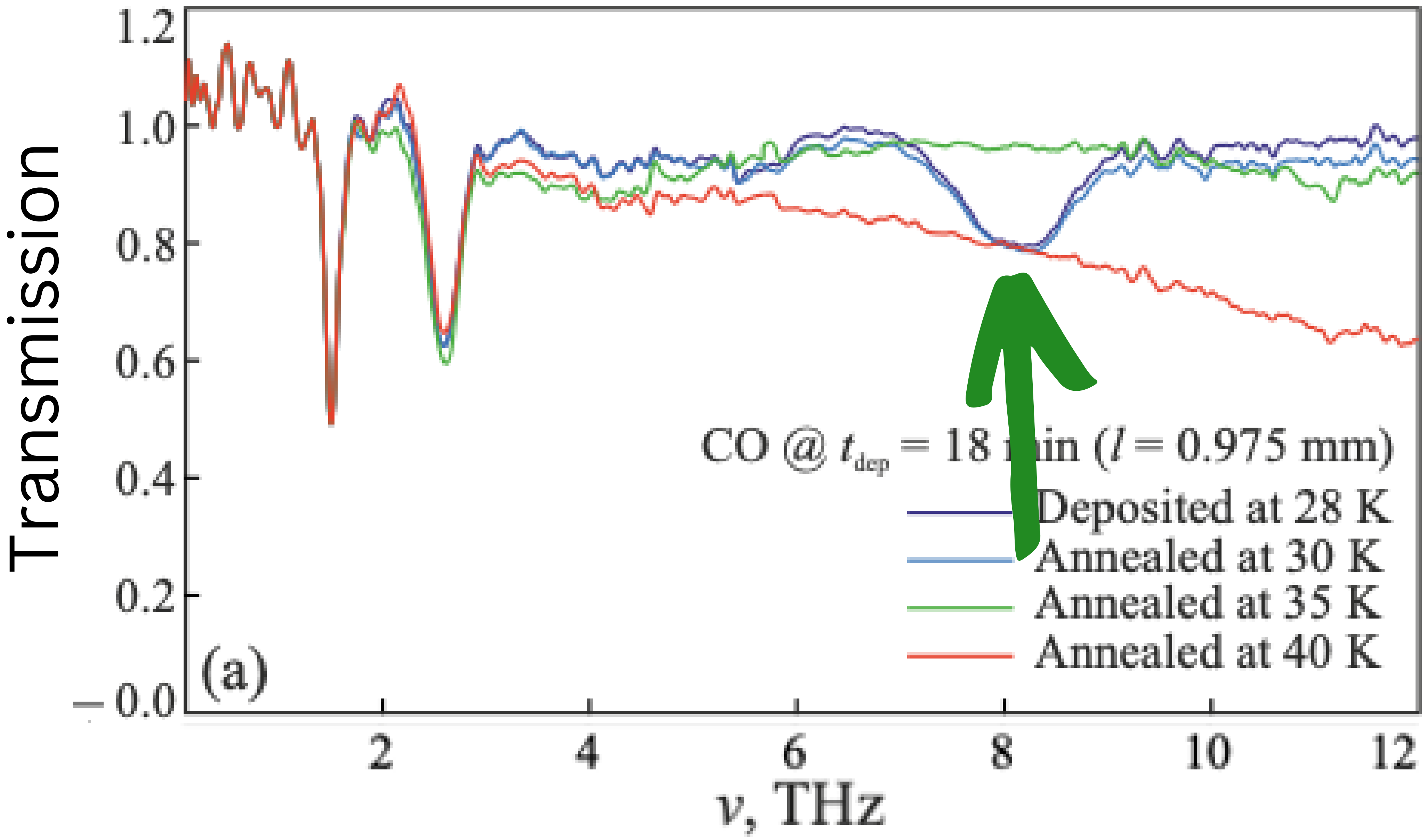
FTIR spectra of CO



TRANSMISSION SPECTRA

...and how the temperature affect the ice optical properties

FTIR spectra of CO

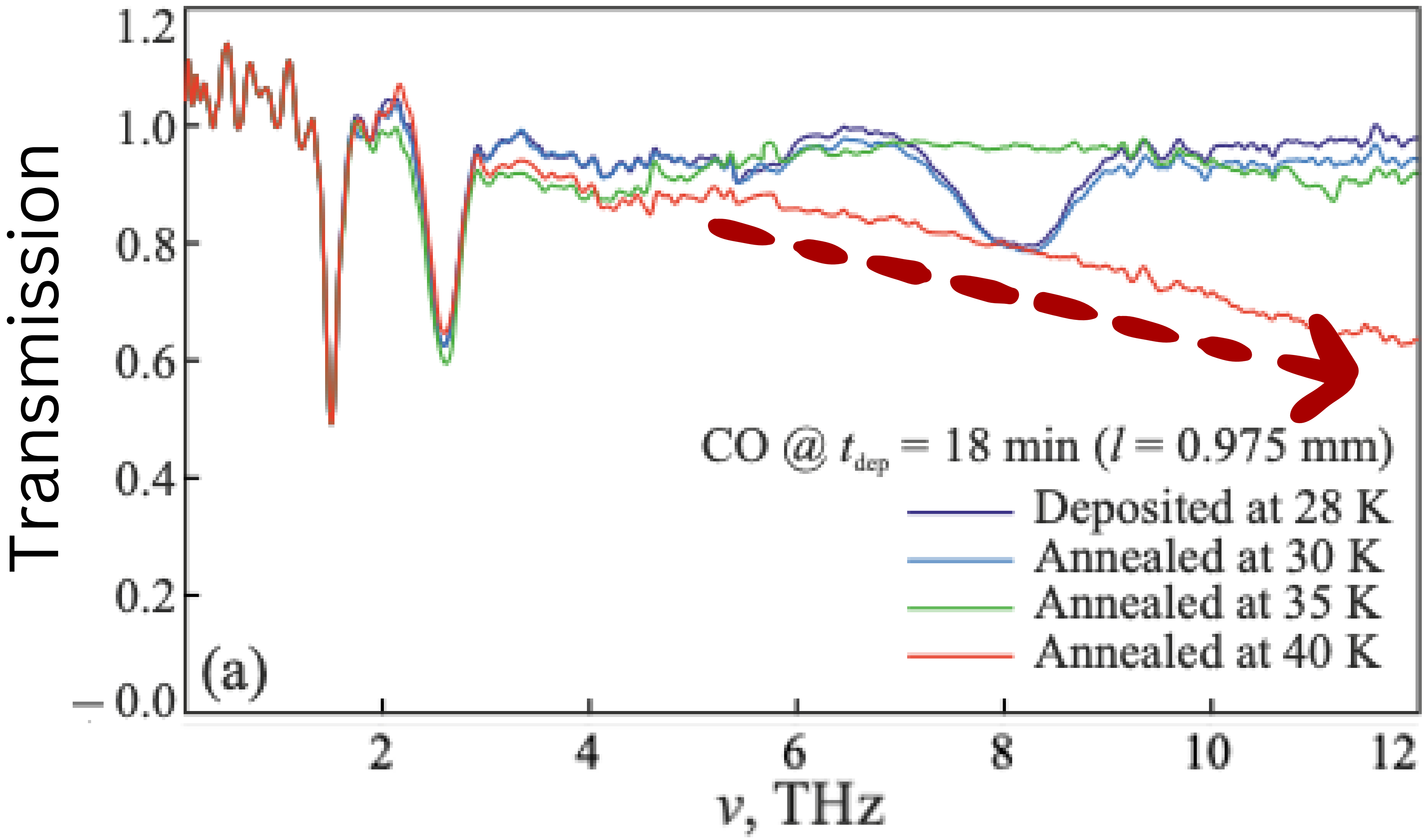


Annealing at 35 K affects the band at 8 THz

TRANSMISSION SPECTRA

...and how the temperature affect the ice optical properties

FTIR spectra of CO

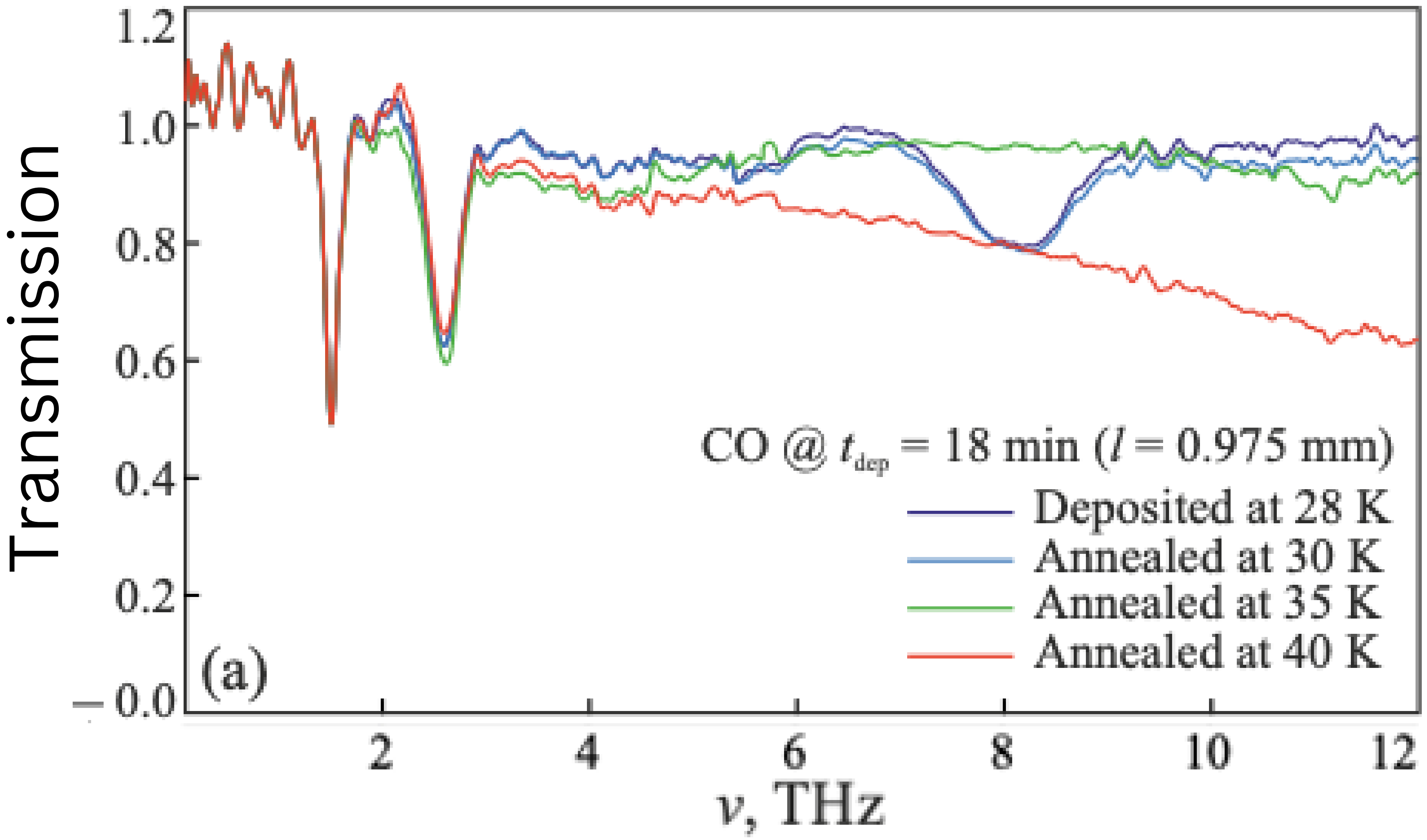


Annealing at 40 K causes imperfections in the ice that scatter light

TRANSMISSION SPECTRA

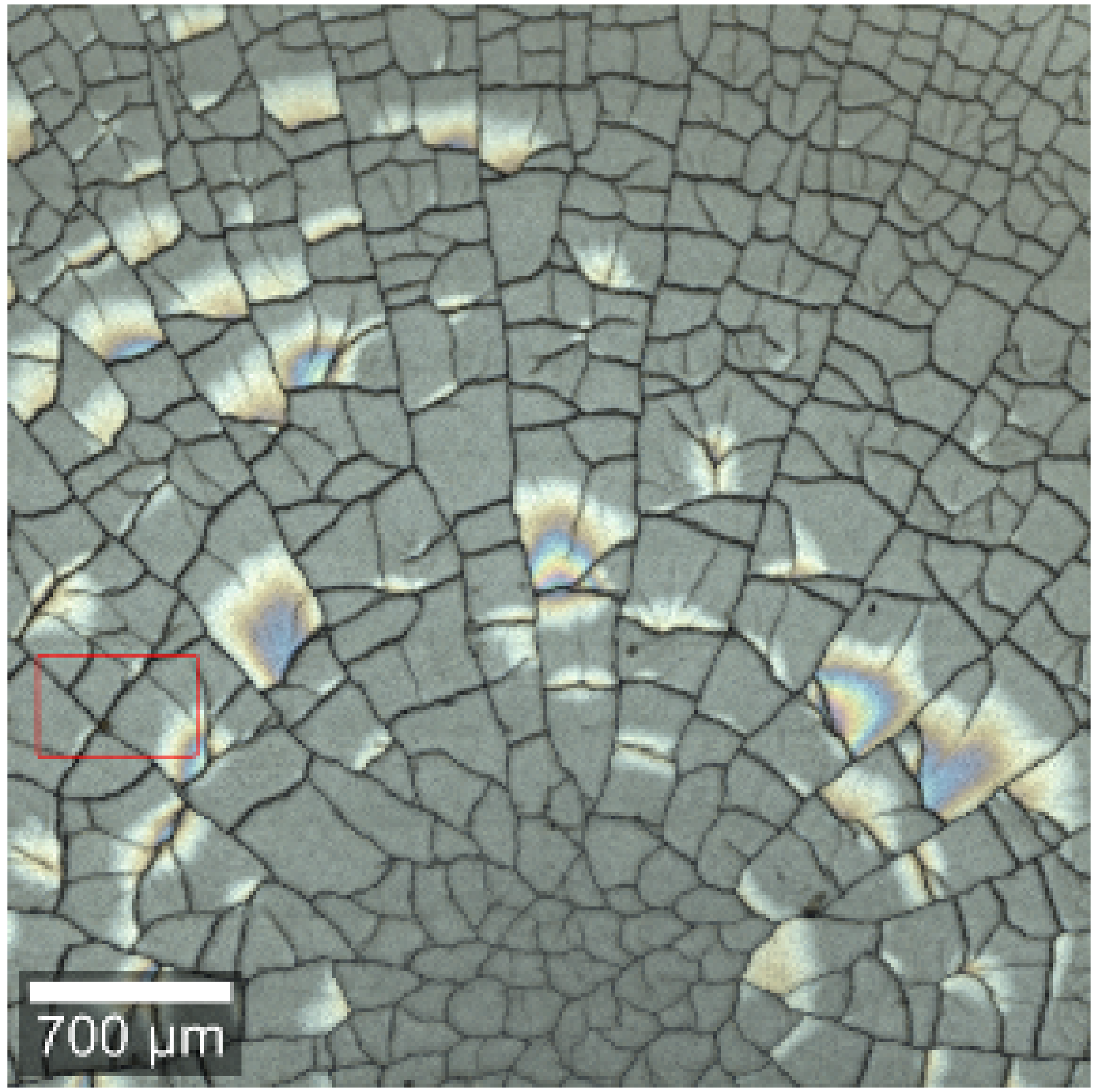
...and how the temperature affect the ice optical properties

FTIR spectra of CO



Annealing at 40 K causes imperfections in the ice that scatter light

Not the same ice, buuut...



Cracks in the surface of water ice seen by Raman microscopy

TAKE-AWAY MESSAGES

- Time-Domain Spectroscopy can be used to obtain directly measurements on the optical properties of ices Giuliano+2019

- We can extend the frequency range of measurements merging TDS + FTIR data Gavdush & Kruczkiewicz+2022

- Data of CO, CO2 published and N2 in prep

- Future plans: study pure H2O, start ice mixtures and obtain measurements in lower frequencies (< 0.1 THz)

ACKNOWLEDGEMENTS

A. A. Gavdush
B. M. Giuliano
A. V. Ivlev
T. Grassi
B. Müller
K. Zeytsev
P. Theulé
P. Caselli

ACO
EU H2020 Innovative Training Network
Astro-Chemical Origins

This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 811312

LAM
LABORATOIRE D'ASTROPHYSIQUE DE MARSEILLE

MPE
Max-Planck-Institut für extraterrestrische Physik

pcmi