Broadband spectroscopy of astrophysical ice analogues: reconstruction of CO and CO$_2$ ice optical properties

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Astro-chemical Origins (ACO) ITN H2020 ESR

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

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

Image credit: Bill Saxton, NRAO/AUI/NSF

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ICE OPACITIES

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

MOLECULAR DETECTION

gas

about 270 molecules

mostly by radioastronomy

Image credit: Bill Saxton, NRAO/AUI/NSF
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gas

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grain

core (silicate and carbonaceous matter) + ice mantle

Infrared astronomy

Image credit: Bill Saxton, NRAO/AUI/NSF
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MOLECULAR DETECTION

grain

core
(silicate and carbonaceous matter)

+ ice mantle

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

Infrared astronomy

Image credit: Bill Saxton, NRAO/AUI/NSF
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**ICE OPACITIES**

**Prestellar cores**
Practically all heavy molecules freeze-out in their center
- Caselli+1999, +2022
- Pineda+2022

**Protoplanetary disks**
mid-planes
- Dutrey+1998
- van Dishoeck2014
- Boogert+2015

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

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Protoplanetary disks
mid-planes
Catastrophic CO freeze out
Dutrey+1998
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Boogert+2015

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

Use continuum emission in the FIR/THz
ICE OPACITIES

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**OUR GOAL**

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

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Dust opacities
K. Demyk talk!
Optical constants $m$ describe how the electromagnetic radiation interacts with a material

$$m = n + ik = \sqrt{\varepsilon}$$
Experimentally FTIR spectroscopy is used to obtain them.

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

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

It contains only the amplitude information, and thus the complex dielectric permittivity cannot be directly reconstructed.
Kramers-Kronig relations are used to relate the real and imaginary portions of the refractive index

\[ n(\nu) = n(\infty) + \frac{2}{\pi} P \int_{\infty}^{\nu} \frac{\nu'k(\nu')}{\nu'^2 - \nu^2} d\nu' \]

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

Optical constants \( m \) describe how the electromagnetic radiation interacts with a material

\[ m = n + ik = \sqrt{\varepsilon} \]

refractive index

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

\[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} E(t)e^{-i\omega t} dt \]

Neu & Schmuttenmaer, 2018
Time-Domain Spectroscopy (TDS) gives amplitude and phase information about the transmitted pulse.

New algorithm that reconstructs the real and imaginary part of the optical constants without having to use Kramers-Kronig relations (Giuliano+2019)
Time-Domain Spectroscopy (TDS) gives amplitude and phase information about the transmitted pulse.

Narrow frequency range
0.1 – 4.0 THz

Neu & Schmuttenmaer, 2018
Time-Domain Spectroscopy (TDS) gives amplitude and phase information about the transmitted pulse.

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

Gavsdush & Kruczkiewicz+2022

Narrow frequency range 0.1 – 4.0 THz
Check our virtual lab tour on:
https://discussions.astrochem.net/videos

CASICE LAB

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

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BROADBAND SPECTROSCOPY MEASUREMENTS

FTIR 0.1 – 12 THz

Gavsdush & Kruczkiewicz+2022

Arsenii GAVDUSH
Prokhorov General Physics Institute
BROADBAND SPECTROSCOPY MEASUREMENTS

...and how we merge the data

FTIR 0.1 – 12 THz

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

Merge the transmission spectra

- FTIR phase must be reconstructed
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Combine TDS + FTIR data

TDS: thickness, amplitude and phase  
FTIR: amplitude, phase from KK and correct with TDS data
Merge the transmission spectra

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ICE OPACITY

...and how our data compares with the literature

Opacity model from Ossenkopf & Henning 94 (OH94)

H₂O:CH₃OH:CO:NH₃
100 : 10 : 1 : 1

volume ratio can vary

\{ V = 0 \text{ bare grain} \\
V = 4.5 \text{ thick ice} \}

OH94

AC + Si

grain size distribution

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...and how our data compares with the literature

Opacity model from Ossenkopf & Henning 94 (OH94)

H₂O:CH₃OH:CO:NH₃
100 : 10 : 1 : 1

pure CO or CO₂ ice

This work

OH94

AC + Si

grain size distribution

AC + Si

grain size distribution

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ICE OPACITY

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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
...and how our data compares with the literature

Gavsdush & Kruczkiewicz+2022
ICE OPACITY

...and how our data compares with the literature
...and how the temperature affect the ice optical properties

FTIR spectra of CO
FTIR spectra of CO

Annealing at 35 K affects the band at 8 THz
...and how the temperature affect the ice optical properties

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)
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