Unveiling ice chemistry with SynthIceSpec

Solid CO_2 as a dust thermometer and CH_3CN detectability in cold cores

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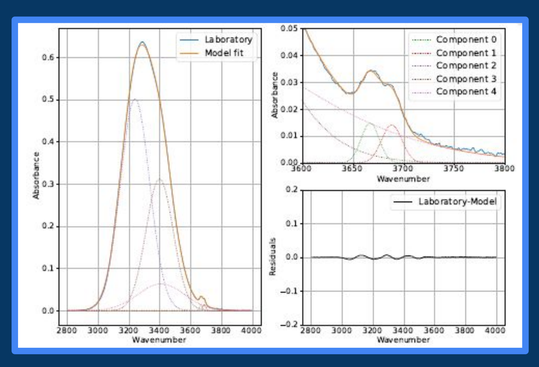
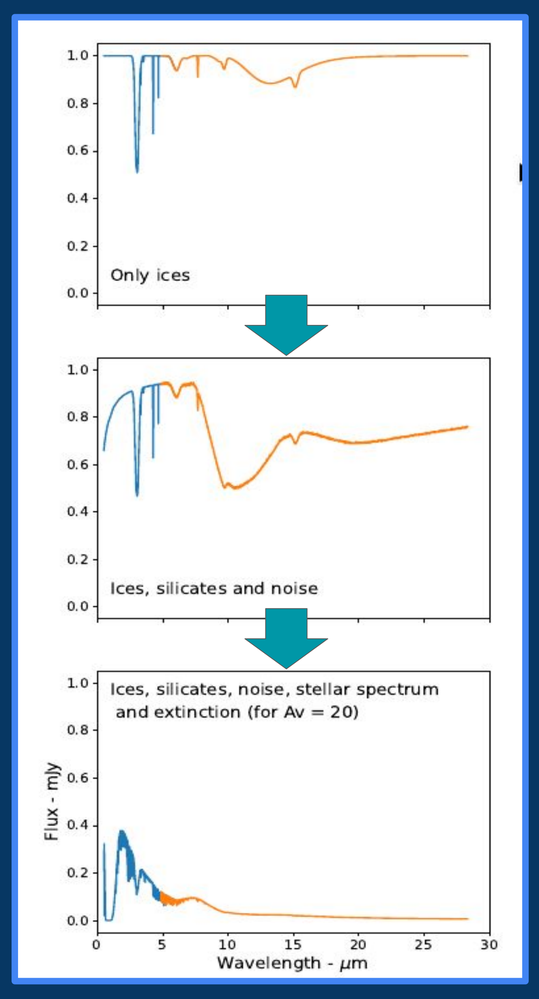
Aims

- **Main objective**: provide a flexible tool to help astrochemists to identify new species, interpret data and prepare JWST observations
- Test the detectability of solid CH_3CN with JWST in cold cores
- Using solid CO_2 as a probe to determine dust physical parameters

I. SynthIceSpec

- SynthIceSpec = produce ice spectra from laboratory data from an input ice composition
- Simple assumption: each functional group can be interpreted by a Gaussian or a series of Gaussians, characterised by their **width**, **band strength** and **peak position wave number**
- Based on the JWST instruments (resolving power and wavelength range)
- Input: column densities of the considered species
- Output: simple vibrational spectrum
- **Instrumental noise**, **stellar photospheres**, **extinction** and **modified black body continuum** can be added

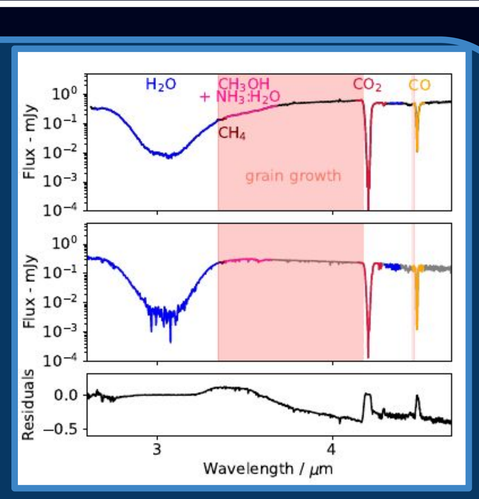




Public code and database*, easy to use in JWST Exposure Time Calculator for proposal purpose

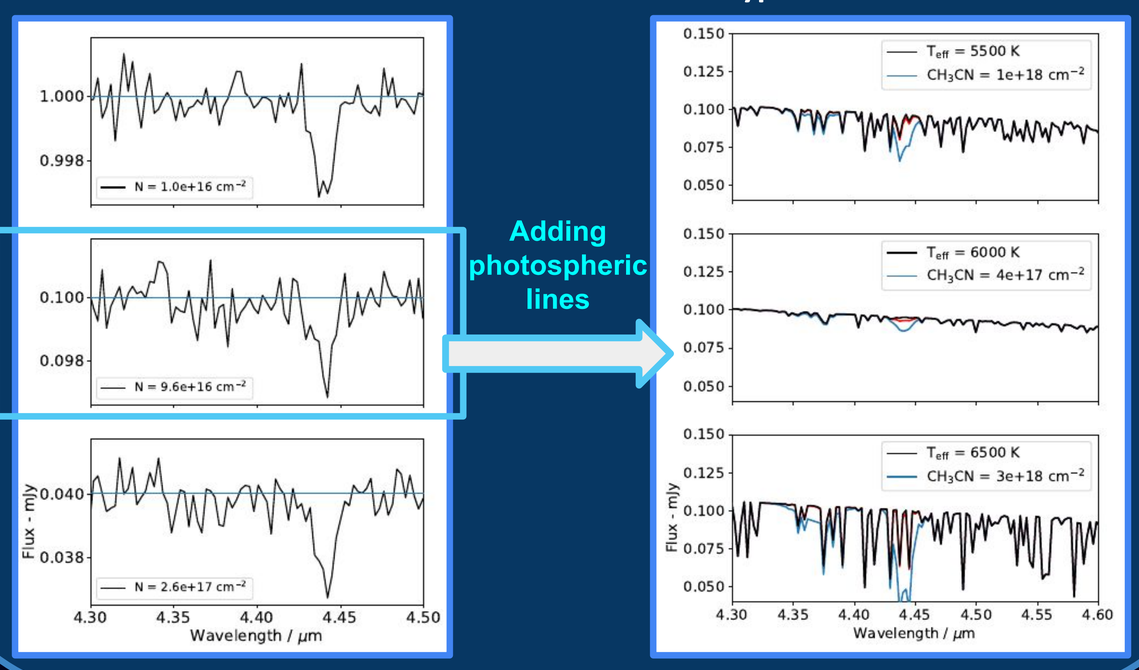
II. Benchmark

- As of now: Only based on "pure" species spectra, mixing is coming next (already experimented in Taillard et al. (2025a))
- Strong fitting of actual observations, physical parameters missing such as grain growth
- Easy to add new species in the database, as of now > 25 species present



III. Estimating the detectability of solid CH_3CN

- Narrow feature at 4.4 um, located in region free of other species expected in cold cores
- Estimating the 5σ detection threshold using fiducial flux and noise => **DETECTABLE** at low column densities
- Adding photospheric absorptions **strongly** hinder the detection
- Very **few** effective temperatures where detection possible
  => Highly dependant on **background source type**



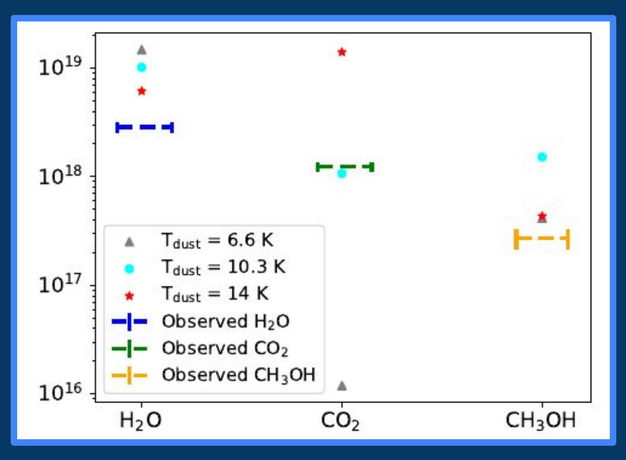
IV. Solid CO_2 as a dust thermometer

1 - Chemical modeling

- We test different T_{dust} to try to reproduce ice observations in the cold core L429-C (Boogert et al. 2011) with main focus on CO_2 using Nautilus gas-grain model
- Three models with strong impact on main ice constituents:
  - Cold: T_{dust} = 6.6 K ⟶ H_2O, CH_3OH, CO_2
  - Intermediate: T_{dust} = 10.3 K ⟶ H_2O, CH_3OH, CO_2
  - Warm: T_{dust} = 14 K ⟶ H_2O, CH_3OH, CO_2

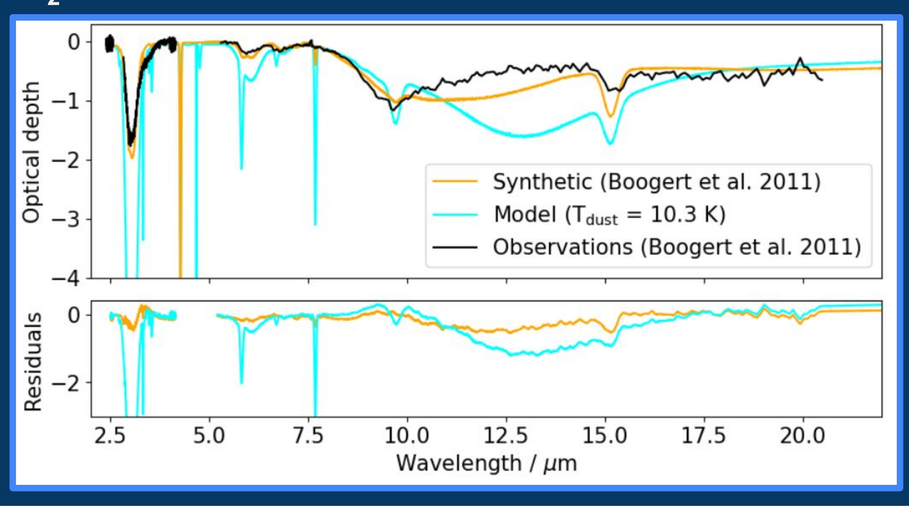
CO_2 ice strongly affected by T_{dust} in models

Although its chemistry could be better adjusted in Nautilus (sticking coeff, $E_{binding}$, diffusion mechanisms…)



2 - Comparison between observed and synthetic spectra

- Using best model to reproduce CO_2 ("intermediate" in cyan), we compare with the IRTF/Spitzer observation (black) and its derived column densities (orange)
  - High residuals for H_2O features by the chemical model overproduced and probably wrong type of spectrum used (mixing should help)
  - A few species overproduced (H_2CO, CH_4) but CO_2 feature well fitted
- **Solid CO_2 could be used as a constraint on model dust temperature!**



References
Taillard, A. et al. 2025, A&A, 694, A263
Boogert, A. C. A. et al. 2011, ApJ 729, 92

SynthIceSpec and its database available here !

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