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UNVEILING ICE CHEMISTRY WITH SYNTHICESPEC - SOLID CO_2 AS A DUST THERMOMETER AND CH_3CN DETECTABILITY IN COLD CORES

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Abstract. In molecular clouds, as density increases and visual extinction is high enough ($A_V > 2$), atoms and molecules will start to deplete onto the dust grains, forming an ice mantle. The *James Webb Space Telescope* (JWST) has opened a new window for the solid-phase observations with its incredibly high sensitivity. However, these observations probe all the material along the line-of-sight, entangling ices, minerals, grain scattering and blackbody emission from the background source in a single spectrum. To support the analysis of the incoming data, modellers and experimentalists are providing new chemical models and laboratory spectra to help observers. We present a public code, SynthIceSpec, able to produce synthetic ice spectra based on laboratory data at the JWST instrument parameters (wavelength and spectra resolution). Additional observational effects can be added (silicates spectrum, continuum, extinction...) on the produced ice absorption spectrum. We provide examples of how the code can be used as chemical model post-processing, studying CO_2 formation and how it can be used to identify new species in the ices, like CH_3CN.

Keywords: ISM: molecules , infrared , astrochemistry , Instrumentation and Methods for Astrophysics

1 Introduction

As the JWST is now collecting thousands of spectra towards background sources in the interstellar medium, from diffuse cloud to young stellar objects, astronomers are dealing with laborious data analysis. Indeed, solid-phase observations are probing the entire material toward a line-of-sight, with photons emitted by the background source experiencing scattering from the grain and ice-mantle. We provide a tool which main objective is to help observers to support the interpretation of JWST observations. We present two possible uses of SynthIceSpec.

2 Synthetic ice spectra generator

SynthIceSpec, short for "synthetic ice spectra generator", is a tool designed to produce ice spectra from laboratory data. The tool is available online*. It is based on a simple approximation: any vibration mode can be represented by a Gaussian described by a band strength, a line width, and a position on the IR spectrum. The input is the ice composition from column densities, chosen by the user or as predicted by chemical models. The resulting ice spectra is calibrated over the wavelength coverage and spectral resolutions of the JWST spectroscopy instruments. To simulate a realistic observation, the following components can be added to each spectrum: the contribution of the silicate component of the grains, different sources of continuum (stellar photospheric spectra, black body), instrumental noise and extinction. A spectral database is available for the pure spectra of many solid species, which is expanding, notably with the addition of certain ice mixtures (which impact the spectral parameters). To this day, the spectral database counts more than 25 species.

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*`https://forge.oasu.u-bordeaux.fr/LAB/astrochem-tools/synthicespec`

3 Use cases

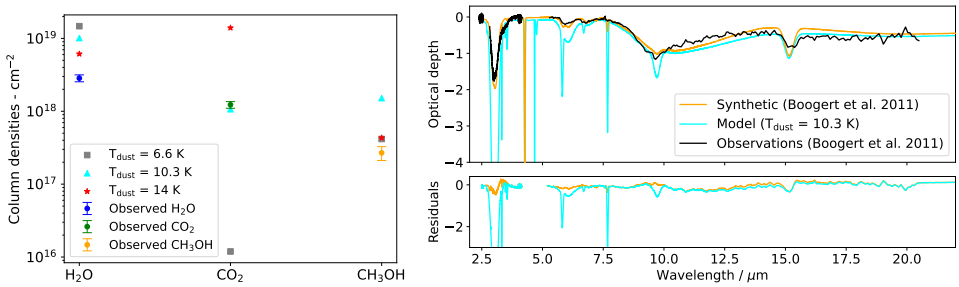

Fig. 1. Left: Predicted column densities of solid H_2O, CO_2 and CH_3OH from three models with T_{dust} = 6.6 K, 10.3 K and 14 K respectively. The observed column densities as derived in Boogert et al. (2011) towards the background star 2MASS J18170957-0814136, are plotted with their uncertainties in blue, green and yellow. **Right:** Top: Optical depth derived from the observation towards 2MASS J18170957-0814136 (black) with, overlapping, the synthetic optical depth spectrum using the column densities derived by the authors (orange) and the resulting optical depth spectrum from the model outputs T_{dust} = 10.3 K (cyan). Bottom: the residuals between the observations and the synthetic spectra.

As mentioned, SynthIceSpec can take as inputs the column densities predicted by a chemical model. We ran Nautilus (Ruaud et al. 2016; Wakelam et al. 2024) with the same physical parameters as the ones we derived in Taillard et al. (2023) to reproduce the ice observations of the cold core L429-C (Boogert et al. 2011). Since CO_2 formation is deeply impacted by the dust temperature, we ran three different models with T_{dust} = 6.6 K, 10.3 K and 14 K respectively named cold, intermediate and warm models. In Figure. 1, we plot the predicted ice column densities of H_2O, CO_2 and CH_3OH compared with the observations. T Using the best model to reproduce CO_2 (intermediate, in cyan), we compare the synthetic spectrum with the IRTF/Spitzer observation (black). We have high residuals for H_2O, H_2CO and CH_4 features as the chemical model overproduces them, combined to the fact that pure spectrum is not accurate as mixing is expected and impacts the shape of absorption bands. However, CO_2 is a great match, that could be used in models as a good constraint on the dust temperature.

SynthIceSpec can also be used to prepare observations and test the detectability of certain species, as we have showed extensively in Taillard et al. (2025). Here, se explore the detectability of CH_3CN in cold core through the identification of its feature at 4.4 μm. We estimated its 5σ detection thresholds using fiducial noise and showed that it could be detected at a low column densities (1×10^{16} to 2.6×10^{17} cm^{-2} for flux varying between 1 and 0.04 mJy). However, adding photospheric absorption strongly hinder its detection, with very few effective temperature allowing the detection. We demonstrate that the detection of the CH_3CN feature at 4.4 μm is strongly dependant on the background source type.

4 Conclusions

With SynthIceSpec, we hope to provide to the community a useful tool to help supporting the analysis effort of the JWST observations in the incoming years. We will include future updates to make it closer to observations and extend the spectral database with new species.

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