**Title:** Modeling ices and infrared spectra in the JWST era

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**Abstract:**

In molecular clouds, where the visual extinction is high enough (Av > 2), atoms will gradually be incorporated into the dust grains, forming an ice mantle that will keep growing as the cloud evolves toward a dense core and later phases. Before the launch of the James Webb Space Telescope (JWST), ice observations were only limited to a few line-of-sights per cloud. It has now reached a milestone thanks to the JWST's incredible sensitivity, spectral and spatial resolution. Ice mapping is now possible, even within highly extinguished regions, allowing us to uncover the complexity of the solid-phase chemistry, the interplay between dust grain and gas and detect never-seen-before molecules. However, ice observations are tedious and hard to untangle, as they are mixed with material along the line-of-sight, affected by the size and shape of the grains, polluted by the blackbody emission of the background source… The conjoint effort of laboratory experimentalists to identify the solid species and provide priceless data and modelers to understand the surface chemistry is needed to help observers.

We present our recent advances on modelling ices, may it be from gas-grain chemical models or with a public code aiming to help with the preparation of JWST data. The latter, SynthIceSpec, can produce synthetic ice spectra, based on laboratory data and on the simple approximation that each vibrational band can be represented by a Gaussian or sum of Gaussians. It recreates the JWST instruments parameters (wavelength and spectral resolution), to where synthetic noise can be added, as well as silicates spectrum, continuum, photospheric absorption bands and an extinction law. We show how the code works and can be used for post-processing of chemical models, the identification and determination of detection thresholds for species possibly present in the ices. In parallel, we will present the recent additions to the Nautilus gas-grain model, to which the grain size distribution is the main goal of our project.