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SPECFY - an important tool of the Leiden Ice Database for Astrochemistry in the era of the James Webb Space Telescope

W. R. M. Rocha[1,2], M. G. Rachid[1], B. Olsthoorn[3], E. F. van Dishoeck[2], M. K. McClure[2], K. Slavicinska[1] and H. Linnartz[1]

[1]Laboratory for Astrophysics, Leiden Observatory, Leiden University, P.O. Box 9513, NL 2300 RA Leiden, The Netherlands
email: rocha@strw.leidenuniv.nl

[2]Leiden Observatory, Leiden University, P.O. Box 9513, NL 2300 RA Leiden, The Netherlands

[3]Nordita, KTH Royal Institute of Technology and Stockholm University, Hannes Alfvéns väg 12, SE-114 21 Stockholm, Sweden

Abstract. Molecular data obtained from laboratory studies are crucial for deriving chemical abundances in astrophysical environments. The Leiden Ice Database for Astrochemistry (LIDA; https://icedb.strw.leidenuniv.nl/) has supported these studies for years in the context of astrophysical ices. For the era of the James Webb Space Telescope - JWST, LIDA hosts more than 1100 infrared spectra of pure and mixed ices that mimic different astrophysical conditions and UV-vis optical constants of water ice. Additionally, LIDA has an online tool - SPECFY, that allows the creation of protostar synthetic spectra. In this paper, we create a synthetic spectrum including OCS ice to check the detection feasibility of this molecule with a 3σ significance using JWST. The calculations are made with the exposure time calculator (ETC). LIDA is a prime deliverable of Ice Age, an Early Release Science JWST program. The collected data and online tools are also accessible for other programs collecting ice data.

Keywords. standards, molecular data, astronomical data bases: miscellaneous, methods: laboratory, methods: data analysis

1. Introduction

Molecules, frozen onto icy dust grains have been used to investigate star-forming regions and starless cores in the interstellar medium (ISM). Past ground- and space-based telescopes allowed us to quantitatively estimate abundances of volatile ice species to better understand the chemistry and physics of regions where stars and planets are formed. Extending on this, the *James Webb* Space Telescope (JWST), is being used to see farther with instruments such as NIRSpec (Near Infrared Spectrograph) and MIRI (Mid-Infrared Instrument). Particularly, JWST provides an improvement in sensitivity by several orders of magnitude compared to previous space telescopes. Moreover, its high spatial resolution allows zooming-in, discriminating, for example, signals from different regions in a proto-planetary disk.

The study of frozen molecules in space is carried out via IR spectroscopy, where the shape of the absorption ice bands is used as a diagnostic tool to further specify the physical and chemical conditions. It is, therefore, crucial that a large amount of IR ice spectra are publicly available to aid JWST data interpretation.

Precise measurements of ices have been made in different laboratories around the world. In the laboratory for astrophysics at Leiden Observatory, many IR spectra of simple and complex organic molecules (COMs), pure and mixed, have been measured for different temperatures and high-resolution spectra are available from the Leiden Ice Database for Astrochemistry (LIDA [Rocha *et al.* (2022)]). This database contains more than 1000 IR ice spectra of species already identified in space or expected to be present. The database also provides the optical constants of ices (e.g., H_2O) in the range of 0.25−20 μm. Among the interesting aspects of LIDA, the database contains an online tool - `SPECFY` - to create combined synthetic spectra of ices simulating spectra as observed toward protostars. `SPECFY` is available at `https://icedb.strw.leidenuniv.nl/Synt_Spec`.

In this proceeding, we explore `SPECFY` to show how to use LIDA and the JWST exposure time calculator (ETC) to check the feasibility of an ice molecule detection with JWST. In particular, we focus on the carbonyl sulfide (OCS) molecule, which may lock an important fraction of sulfur in the ISM. OCS was observed before by Palumbo *et al.* (1997), although at low resolution, and by Boogert *et al.* (2022) toward high-mass protostars using the Infrared Telescope Facility (IRTF). The presence of this molecule towards low-mass protostars is still under debate. Therefore, we assess the capability of JWST to detect OCS in such sources with a significance of 3σ.

2. Creating a synthetic ice spectrum

Ices toward protostars are observed against the stellar continuum. Often, this continuum is subtracted to allow a direct comparison of the protostar spectrum with experimental data measured using a transmission technique. The ice spectra available in LIDA are provided in "absorbance" units, which is defined as:

$$Abs_\nu = -\log_{10}\frac{I_\nu}{I_{0,\nu}}, \tag{2.1}$$

where $I_{0,\nu}$ and I_ν are the frequency-dependent (ν) light intensities before and after reaching the ice sample. Equation 2.1 is also used to derive the column density of the molecules in the ice:

$$N_{\rm ice} = \frac{1}{\mathcal{A}}\int_{\nu_1}^{\nu_2} \tau_\nu^{\rm lab} d\nu, \tag{2.2}$$

where $\mathcal{A}$ is the band strength of a specific vibrational mode, and $\tau_\nu^{\rm lab} = \ln 10 \cdot {\rm Abs}_\nu$.

<u>*Optical depth spectrum:*</u> The first step in `SPECFY` is the creation of a combined ice spectrum in optical depth scale. The optical depth is calculated from the absorbance data, and the combined spectrum is given by:

$$\tau_\nu^{\rm tot} = \sum_{i=0}^{n} w_i \tau_{\nu,{\rm i}}^{\rm lab}, \tag{2.3}$$

where w_i is a scaling factor to increase or decrease the intensity of the ice bands, based on the ice column density (Equation 2.2), which is given by:

$$w_i = \frac{N_{\rm ice}^{\rm inp}}{N_{\rm ice}^{\rm lab}}, \tag{2.4}$$

where $N_{\rm ice}^{inp}$ is the ice column density indicated by the user, and $N_{\rm ice}^{lab}$ is the experimental ice column density. The top panel of Figure 1 shows a combined spectrum including the OCS band at 4.9 μm (CO stretching), chosen to have an abundance of 1% with respect to H_2O ice. We do not focus on other OCS bands because they are much weaker compared to the 4.9 μm band. Table 1 specifies the experimental data used in the values for $N_{\rm ice}^{inp}$.

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Table 1. Ice spectra used to construct a synthetic protostar spectrum in optical depth scale.

Analog	T (K)	N_{ice}^{inp} (cm^{-2})	Reference
Pure H_2O	15	1.4×10^{17}	Öberg *et al.* (2007)
H_2O:CO_2 (10:1)	10	2.5×10^{18}	Ehrenfreund *et al.* (1997)
CO:CO_2 (2:1)	15	7.0×10^{17}	van Broekhuizen *et al.* (2006)
OCS	17.5	2.6×10^{16}	Slavicinska *et al.* (in prep.)

Spectrum in flux scale - Jansky: The second step in SPECFY is the conversion of the optical depth spectrum to a flux scale in units of Jansky. This conversion is possible when the continuum spectrum of the protostar is known, and it can be expressed as:

$$F_\lambda^{\mathrm{synth}} = F_\lambda^{\mathrm{cont}} \exp(-\tau_\lambda^{\mathrm{tot}}), \tag{2.5}$$

where $F_\lambda^{\mathrm{cont}}$ is the continuum spectrum of the protostar. For this reason, the continuum spectra of a few protostars are compiled from the literature and used by SPECFY. For the purpose of this paper, we adopt the continuum spectrum of the protostar CRBR 2422.8-3423 because it has a lower flux density around the OCS band (0.16 Jy) in the list from LIDA. The result is shown in the bottom panel of Figure 1. The data generated with SPECFY can be downloaded to be used by external tools.

3. Linking LIDA and JWST/ETC

The detection feasibility of specific absorption features with JWST can be assessed by using the online exposure time calculator (ETC)†. Among the features of ETC, the user can also upload a spectrum to be used by the simulator. In this regard, we upload the synthetic spectrum created with LIDA (Fig. 1). Since our focus is on the OCS band, we simulate the use of the fixed slit mode of NIRSpec with a prism grating (Fig. 2). This simulation gives a total exposure time of 17 minutes and a signal-to-noise ratio of around 20 at 4.9 μm. The spectrum from ETC and LIDA are compared in Figure 3. In particular, the OCS band can be detected with a significance of 3σ at the selected column density. We also note that the bands of H_2O (3 μm), CO_2 (4.27 μm) and CO (4.67 μm) are saturated in this example. Moreover, the CO and CO2 bands are affected by the low spectral resolution when using the prism grating. Using another configuration to find the optimal spectrum without saturating any band is for now outside the purpose of this proceeding.

This example clearly shows how SPECFY can be helpful for the astrochemical community when submitting proposals for JWST in the upcoming cycles. Additionally, it highlights the need for different ice IR spectra to simulate various astrophysical conditions. This example also shows that SPECFY can help with deriving preliminary ice column densities toward protostars by comparing astronomical data in optical depth scale with the manually constructed combined spectrum from LIDA.

4. Summary

In the era of JWST, open-access experimental data and tools are crucial to maximize the scientific return of IR ice observations. In this context, LIDA provides a comprehensive list of molecules with IR spectra measured in different chemical environments and temperatures. Additionally, the online tool, SPECFY, is of utmost importance to assist scientists during the submission of proposals for JWST in the next cycles. Specifically, we demonstrate how SPECFY can be used to assess the detection feasibility of the OCS band using NIRSpec. According to those simulations, 3σ significance detection of the

† https://jwst.etc.stsci.edu/ - Pontoppidan *et al.* (2016)

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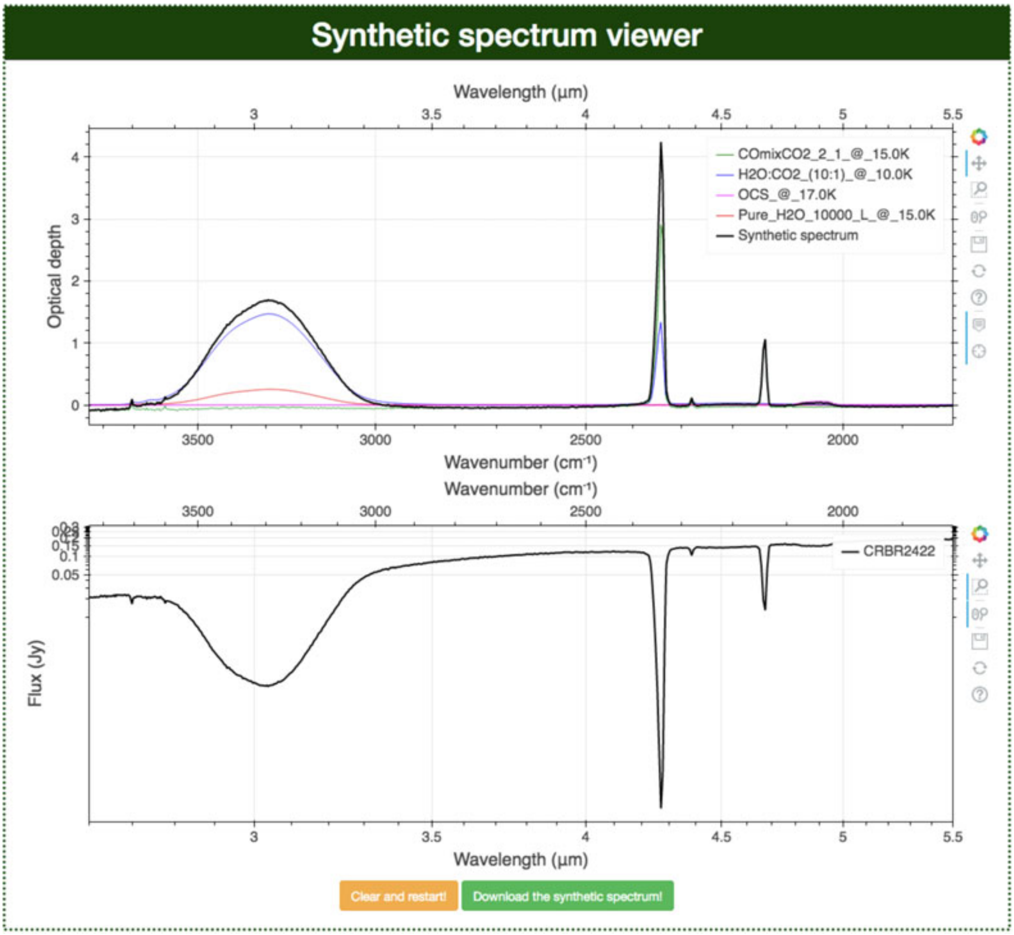

Figure 1. Screenshot of the spectrum viewer in LIDA. The top panel shows the combined spectrum in optical depth scale, and the bottom panel shows the synthetic spectrum in units of Jy.

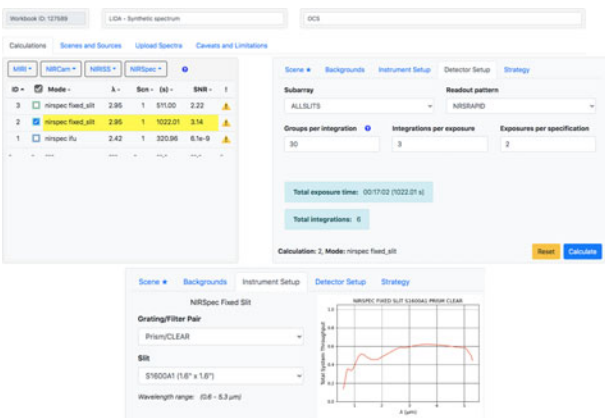

Figure 2. Screenshots of the JWST/ETC showing an example of the detector (top) and instrument (bottom) setup for calculating the exposure time using NIRSpec fixed slit mode.

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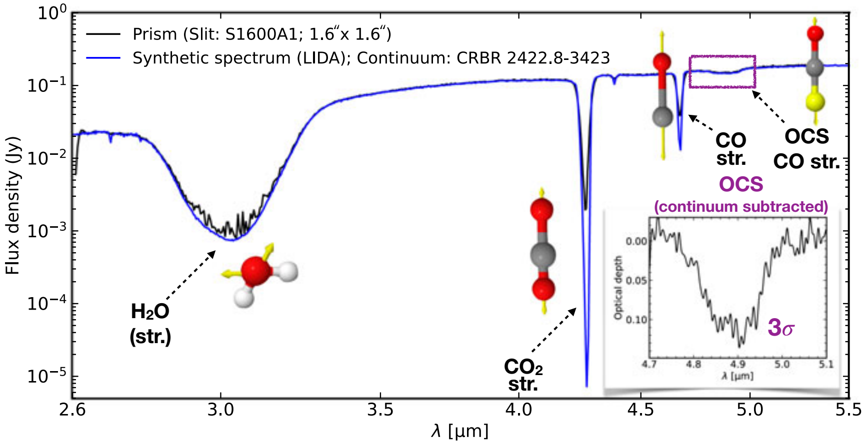

Figure 3. Comparison between the synthetic spectrum simulated with LIDA (blue) and from JWST/ETC (black). The inset shows the continuum subtracted profile of the OCS band with a detection level of 3σ. The absorption bands are indicated by the labels and the cartoon of the molecules. The yellow arrows point to the movement of the atoms during vibration. The mismatch at CO and CO_2 bands is due to the low spectral resolution prism grating used in this example.

OCS ice band with a column density of 2.6×10^{16} cm^{-2} is possible using the fixed slit spectroscopy mode in an exposure time of 17 minutes, without including overheads.

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