

Ice inventory towards the protostar Ced 110 IRS4 observed with the James Webb Space Telescope

Results from the Early Release Science Ice Age program

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ABSTRACT

Context. Protostars contain icy ingredients necessary for the formation of potential habitable worlds, therefore, it is crucial to understand their chemical and physical environments. This work is focused on the ice features towards the binary protostellar system Ced 110 IRS4A and IRS4B, separated by 250 au and observed with *James Webb* Space Telescope (JWST) as part of the Early Release Science (ERS) Ice Age collaboration.

Aims. This study is aimed at exploring the JWST observations of the binary protostellar system Ced 110 IRS4A and IRS4B primarily to unveil and quantify the ice inventories towards these sources. Finally, we compare the ice abundances with those found for the same molecular cloud.

Methods. We used data from multiple JWST instruments (NIRSpec, NIRCam, and MIRI) to identify and quantify ice species in the Ced 110 IRS4 system. The analysis was performed by fitting or comparing the laboratory infrared spectra of ices to the observations. Spectral fits are carried out with the ENIIGMA fitting tool that searches for the best fit out of a large number of solutions. The degeneracies of the fits are also addressed and the ice column densities are calculated. In cases where the full nature of the absorption features is not yet known, we explore different laboratory ice spectra to compare them with the observations.

Results. We provide a list of securely and tentatively detected ice species towards the primary and the companion sources. For Ced 110 IRS4B, we detected the major ice species H₂O, CO, CO₂, and NH₃. All species are found in a mixture except for CO and CO₂, which have both mixed and pure ice components. In the case of Ced 110 IRS4A, we detected the same major species as in Ced 110 IRS4B, as well as the following minor species: CH₄, SO₂, CH₃OH, OCN[−], NH₄⁺, and HCOOH. A tentative detection of N₂O ice (7.75 μm), forsterite dust (11.2 μm), and CH₃ gas emission (7.18 μm) in the primary source was also made. Compared with the two lines of sight towards background stars in the Chameleon I molecular cloud, the protostar exhibits similar ice abundances, except in the case of the ions that are higher in IRS4A. The most clear differences are the absence of the 7.2 and 7.4 μm absorption features due to HCOO[−] and icy complex organic molecules in IRS4A. There is also evidence of thermal processing in both IRS4A and IRS4B, as probed by the CO₂ ice features.

Conclusions. We conclude that the binary protostellar system Ced 110 IRS4A and IRS4B has a large inventory of icy species. The similar ice abundances in comparison to the starless regions in the same molecular cloud suggests that the chemical conditions of the protostar were set at earlier stages in the molecular cloud. It is also possible that the source inclination and complex geometry cause a low column density along the line of sight, which hides the bands at 7.2 and 7.4 μm. Finally, we highlight that a comprehensive analysis using radiative transfer modelling is needed to disentangle the spectral energy distributions of these sources.

Key words. astrochemistry – solid state: volatile – ISM: molecules

1. Introduction

The astrochemical investigation of low-mass young stellar objects (LYSOs) with the James Webb Space Telescope (JWST) has provided astronomers with a unique vantage point to explore the intricate interplay between physics and chemistry during the early stages of star formation. For example, recent JWST observations resulted in the detection of shallow absorption features due to minor solid-phase molecular species, which are still crucial for understanding the chemical composition of those

ices (Yang et al. 2022; Rocha et al. 2024b; Brunken et al. 2024a,b; Nazari et al. 2024a; Chen et al. 2024; Tyagi et al. 2024; Slavicinska et al. 2024, 2025).

In this context, the Director's Discretionary-Early Release Science (DD-ERS) program “Ice Age: Chemical evolution of ices during star formation” (ID 1309, PIs: Melissa McClure, Adwin Boogert, Harold Linnartz - in memoriam) aims to trace the chemical evolution of ices within regions at different evolutionary stages. For example, observations of two background stars, NIR38 and J110621, by McClure et al. (2023) have shown that the molecular cloud Chameleon I hosts the major ice

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species (H_2O , CO , CO_2 , NH_3 , CH_4 , and CH_3OH), minor species (OCN^- , OCS , $^{13}\text{CO}_2$, and ^{13}CO), and likely complex organic molecules (COMs) in ices. Furthermore, [Dartois et al. \(2024\)](#) and [Noble et al. \(2024\)](#) found evidence of grain growth and the OH dangling feature, respectively, in the Chameleon I molecular cloud. In the later stage of evolution, the protoplanetary disk phase, [Sturm et al. \(2023\)](#) demonstrated that, except for the COMs and ^{13}CO , the same features were observed in the protoplanetary disk HH48. Our work aims to compare the ice inventory and abundances found towards NIR38 and J110621 in the Chameleon I molecular cloud and those in the protostar Cederblad 110 IRS4 (hereafter, Ced 110 IRS4). Additionally, we searched for evidence of ice thermal processing, which is not present in the molecular cloud, as also found in previous works ([Boogert et al. 2011, 2013](#)).

Ced 110 IRS4 is nestled within the Chameleon I Molecular Cloud (RA $11^{\text{h}}06^{\text{m}}46.3682^{\text{s}}$ and Dec $-77^{\circ}22'32.882''$). The distances between Ced 110 IRS4 and NIR38 and J110621 are 81 and $114''$, respectively. This region is bright in the near and mid-infrared (IR), and four other names exist for the same target in the literature, namely, NIR76, IRAS 11051–7706 and 2MASS J11064638–7722287, [PMG2001] NIR 72. [Zinnecker et al. \(1999\)](#) observed this source in the near-IR with the Infrared Spectrometer And Array Camera (ISAAC) camera mounted on the Very Large Telescope (VLT). It is described as a bisected reflection nebula with a dark lane and a highly reddened central source. A later work by [Persi et al. \(2001\)](#) used ESO-SOFI, a sub-arcsecond resolution near-IR camera, to study the Ced 110 region, and derived an average extinction of $A_V = 30$ mag. Ced 110 IRS4 is classified as Class I source ([Lehtinen et al. 2001](#)), which implies the presence of a large envelope and a young disk. However, a Class 0 designation was attributed to this source based on the bolometric temperature derived from the Photodetector Array Camera and Spectrometer (PACS) data from Herschel ($T_{\text{bol}} = 56$ K; [Kristensen et al. 2012](#)). The same classification (Class 0, $T_{\text{bol}} = 68$ K) is reported by [Ohashi et al. \(2023\)](#), which is derived from a complete spectral energy distribution (SED) of the source, that includes data between 2 and $1000\ \mu\text{m}$. Another important discovery about Ced 110 IRS4 was recently made by the “Early Planet Formation in Embedded Disks (eDisk)” large program (PI: Nagayoshi Ohashi), using observations from the Atacama Large Millimeter/submillimeter Array (ALMA). It revealed that Ced 110 IRS4 is actually a binary system ([Sai et al. 2023](#)) with a separation of 250 au, thus being renamed as Ced 110 IRS4A (same coordinates as above) and IRS4B (RA $11^{\text{h}}06^{\text{m}}46.8194^{\text{s}}$ and Dec $-77^{\circ}22'32.505''$). This pair presents disk-like structures where the primary and secondary sources have a dust disks with estimated radii of 91.7 ± 0.2 and 33.6 ± 0.6 au, respectively.

Gas-phase observations of the Ced 110 IRS4A system have shown molecular (H_2 , H_2O , CO , HCO^+ ; e.g. [Hiramatsu et al. 2007](#); [van Kempen et al. 2009](#); [Kristensen et al. 2012](#); [Sai et al. 2023](#)) and atomic (Fe II; e.g. [Lahuis et al. 2010](#)) emissions. Based on C^{18}O lines, [van Kempen et al. \(2009\)](#) concluded that no foreground cloud is present along the line of sight towards this source, but there is warm gas, which is related to an outflow from IRS4A ([Belloche et al. 2006](#)). Non-detections towards IRS4A include CH_3OH and SiO , known as shock tracers, based on Atacama Submillimeter Telescope Experiment (ASTE) observations ([Hiramatsu et al. 2007](#)). [van Gelder \(2022\)](#) further confirmed that no CH_3OH gas detection is present at Ced 110 IRS4 system. On the other hand, SO , another shock tracer, was detected by [Sai et al. \(2023\)](#) and shows an arc-like structure on the north side of the system. Solid-phase species,

such as H_2O , CO_2 and silicates were identified towards this source based on the Infrared Spectrograph (IRS) onboard the *Spitzer* Space Telescope ([Manoj et al. 2011](#)). Regarding larger species, so far no complex organic molecules (COMs) has been reported towards this source in either in the solid or gas phases.

The solid-phase nature of the Chameleon I dense cloud where Ced 110 IRS4 is located was recently addressed in two papers from the Ice Age collaboration, [McClure et al. \(2023\)](#), [Dartois et al. \(2024\)](#) and [Noble et al. \(2024\)](#), who provided an important comparison to the protostellar environment. For example, the two background stars, NIR38 and J110621228, which were targeted in [McClure et al. \(2023\)](#), reveal the presence of many ice species, including H_2O , CO , CO_2 , NH_3 and OCS , as well as CH_3OH , which highlights the complex ice chemistry already occurring prior to protostellar formation. Additionally, [Noble et al. \(2024\)](#) shows the presence of the elusive OH dangling bond at $2.7\ \mu\text{m}$. Regarding grain sizes, [Dartois et al. \(2024\)](#) show that grain growth occurs in the Chameleon I cloud by accretion and aggregation given the presence of icy grains of a larger radius ($0.9\ \mu\text{m}$) in comparison to the interstellar medium (ISM, $0.25\ \mu\text{m}$; [Mathis et al. 1977](#)).

In this work, we analyze the spectrum of Ced 110 IRS4A and IRS4B using multiple JWST instruments and covering the critical spectral ranges for tracing thermal processing (CO_2 ; 4.27 and $15.2\ \mu\text{m}$) and COMs ($7\text{--}9\ \mu\text{m}$). It is important to mention that, for the first time, we present an ice study of the companion protostar, IRS4B, recently discovered by [Sai et al. \(2023\)](#). This work primarily focuses on the ice features and although we point out a few gas-phase lines, a detailed study of gaseous species will be deferred to a future paper. The structure of this work is as follows. Section 2 presents the JWST observations and the data reduction process, and the ice laboratory data used for spectral fitting and comparison is presented in Section 3. The methodology with the different approaches adopted in this manuscript is presented in Section 4. We describe the analysis and results in Section 5. Our discussion is presented in Section 6 and our conclusions are outlined in Section 7.

2. Observations

In this section we describe the steps performed for data reduction of the JWST data from multiple instruments. In Figure 1 we present a flowchart with key procedures with specific highlights of the data analysis described in Section 4.

2.1. NIRCam data reduction

The JWST/NIRCam Wide-Field Slitless Spectroscopy (WFSS) observations of Ced 110 IRS4 were taken over two observing periods on August 11th and August 12th 2022 as part of the Ice Age program ([McClure et al. 2017](#)). These two observation sets used the F322W2 filter with the Grism R dispersion direction for the spectral observations and F150W, F410M and F140M for the direct imaging observations, though we only discuss the F150W images in this study. These observations each used a dither setup of four sub-pixel and three primary dither positions with a mosaic pattern of 1 row \times 2 columns, leading to Ced 110 IRS4A and IRS4B being observed within 24 F322W2 spectral images. Ced 110 IRS4A and IRS4B were placed within NIRCam’s module B during these observations, resulting in a $\sim 25\%$ sensitivity decrease compared to module A. This was because Ced 110 IRS4 was not the primary target of the IceAge NIRCam WFSS observations. The full IceAge NIRCam WFSS observing programme, image processing and spectral extraction and reduction

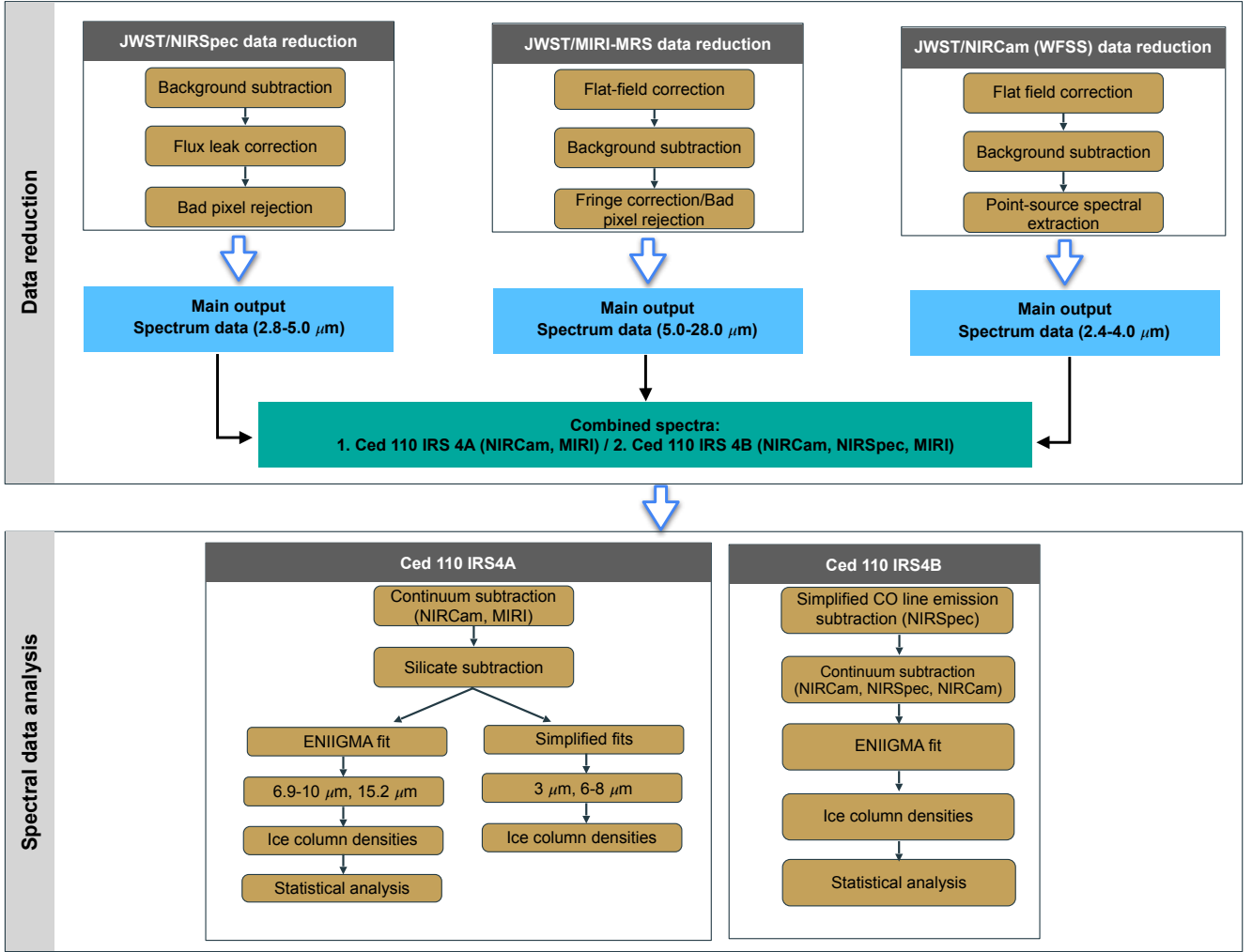


Fig 1. Summary of steps performed in the data reduction and data analysis of Ced 110 IRS4A and IRS4B.

are described in McClure et al. (2023), Noble et al. (2024), and Smith et al. (2024). The data reduction steps are described again here.

Direct image processing of the F150W images is the first stage of data reduction, where the techniques outlined in Sun et al. (2022) are used. This is performed by combining the data outputs from up to and including stage 2 of the JWST NIRCam direct imaging standard pipeline. Following this, members of the NIRCam calibration team performed additional reduction steps, as described in Sun et al. (2023), where the F150W images were cleaned, astrometry corrected to Gaia stars in the field of view, cross-matched to each other, and mosaicked together.

To obtain the spectral data presented in this study, each individual grism spectroscopic image frame was reduced using the standard JWST calibration pipeline v1.6.2 up to and including stage 2a, using the default CRDS set-up with JWST’s operational pipeline, OPS, and no modifications (CRDS context 0953). A flat-field correction was then applied using the imaging flat data obtained with the same filter (F322W2), followed by two-dimensional (2D) sky-background subtraction using sigma-clipped median images that were constructed for each individual spectral image in our dataset in which the Ced 110 IRS4 sources were found.

Due to the strong cloud emission and radiative transfer effects around Ced 110 IRS4 precluded almost any data from

around these sources being extracted via the original NIRCam spectral extraction in the IceAge programme. Therefore, we artificially placed sources across the two emission lobes extending vertically, and perpendicular to the disc shadow of IRS4A and 4B, as shown in Figure 2, to complement MIRI data for Ced 110IRS 4A and the NIRSpec and MIRI data for Ced 110IRS 4B. We then ran the bespoke NIRCam WFSS extraction code, as described Noble et al. (2024) and Smith et al. (2024), to successfully extract “point source” spectra at these positions.

Once the source positions were determined, a custom spectral extraction methodology developed by the IceAge ERS team, described in Noble et al. (2024) and Smith et al. (2024), was used to extract the presented spectra. This is because the standard JWST NIRCam WFSS spectral extraction pipeline is unsuited to extracting crowded and highly varying background fields like that surrounding IRS4. A brief outline is provided here. A spectrum was extracted at each source position from each of the 24 spectral images across wavelengths 2.4–4 μm . These extracted spectra were then wavelength and flux calibrated using the in-flight measurements obtained with JWST Commissioning Program #1076. We then took these individual spectral image spectra and used the SpectRes (Carnall 2017) Python package to regrid them all onto a common wavelength grid with 1.006 nm wavelength steps. This allows these spectra to be reliably recombined using the weighted median values of each spectral data

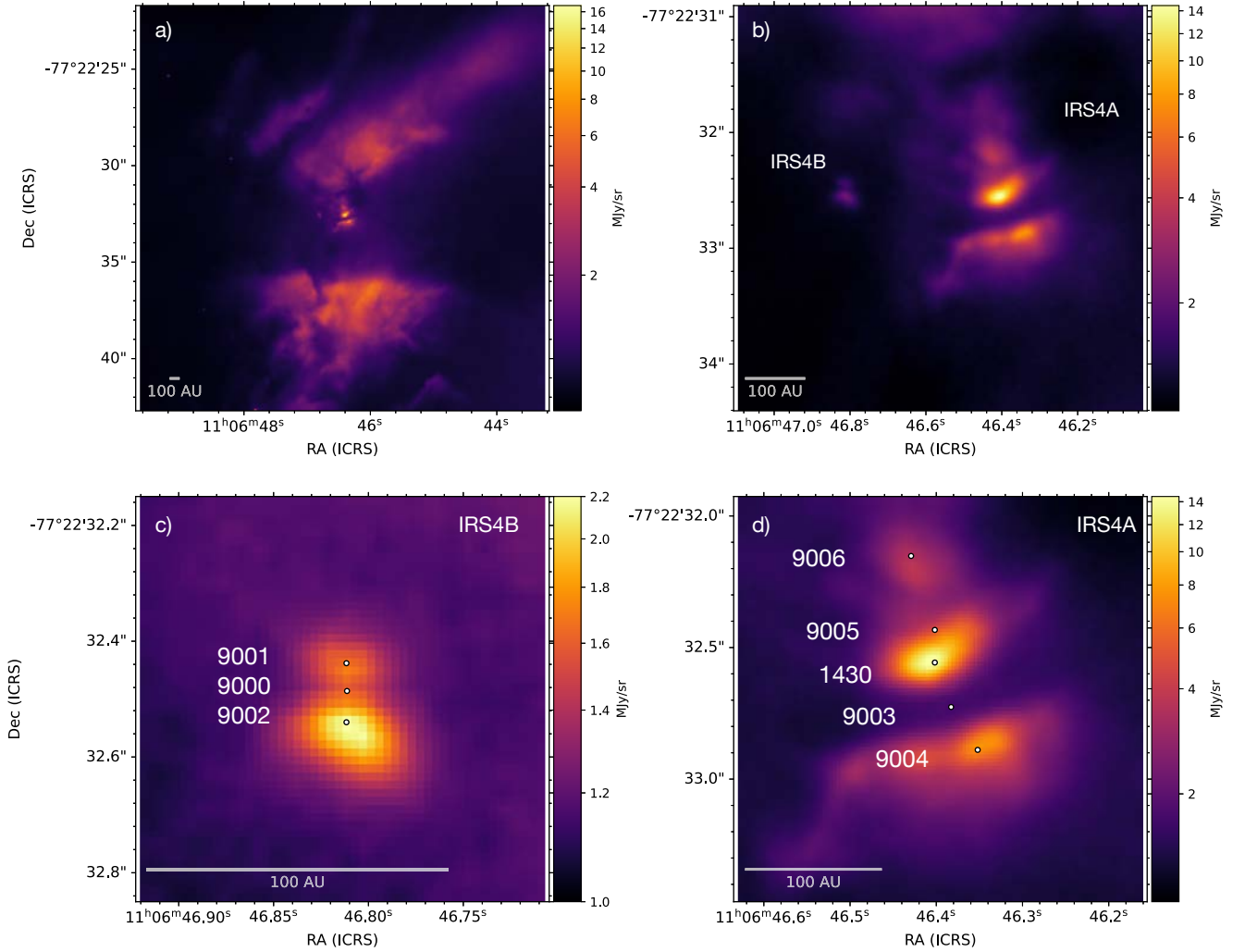


Fig 2. NIRCam image at $1.5\ \mu\text{m}$ of Ced 110 IRS4A and IRS4B. Panel a displays the large scale image of the Ced 110 IRS4 system and panel b shows a zoom in panel a. Panels c and d highlight the IRS4B and IRS4A source morphologies, respectively. The small white circles show the starting positions of the PSF extractions and the numbers are identifications of the individual spectra shown in Figure A.1.

point from every individual dispersed frame spectra to produce the final spectrum for each source position in Figure 2. The recombination slightly decreases the spectrum length from 1670 to 1638 wavelength elements as expected from pre-flight measurements. This is a minor change that still results in an R value very close to the measured $R \sim 1600$ at $3.95\ \mu\text{m}$ and $R \sim 1150$ at $2.5\ \mu\text{m}$ from the JWST pre-flight measurements. Each source position’s final spectrum was then summed together to produce the final spectrum for Ced 110 IRS4A, where we show the individual source position and summed spectra in Appendix A.

2.2. NIRSpec data reduction

The protostar Ced 110 IRS4 was targeted for observations with the Near InfraRed Spectrograph (NIRSpec) onboard JWST on 2022 July 19th. The requested pointing was defined to be $11^{\text{h}}06^{\text{m}}47.1^{\text{s}}$, $-77^{\circ}22'34.0''$ (J2000), based on the resolved K band imaging in Persi et al. (2001). However, the Persi et al. coordinates of this source and many of the infrared sources in this field proved to be systematically offset with respect to the Spitzer IRAC coordinates. Because we did not perform a target acquisition, the NIRSpec observation was therefore mis-pointed by $2.4''$ and did not capture the image of Ced 110 IRS4.

Serendipitously, the NIRSpec observations did capture a companion protostar (IRS4B) at a separation of $1.3''$.

The spectroscopic data were taken with a standard four-point dither pattern for a total integration of 1225 s. The G395H/F290LP disperser/filter combination was used with NIRSpec, which covers wavelengths from $2.87\text{--}4.08\ \mu\text{m}$ and $4.19\text{--}5.25\ \mu\text{m}$ at a resolving power of $R \sim 2700$. Leaked exposures were acquired which observe the four-point dither pattern with the IFU aperture closed so that excess flux leaking through the finite contrast MSA shutters was effectively removed.

The data were processed through the November 2022 development version of the JWST NIRSpec pipeline (2022_2a; 1.8.3.dev26+g24aa9b1d). We used the calibration reference file database version 11.16.16, which includes the updated flight flat field and throughput calibrations for the absolute flux calibration accuracy estimate of the order of $\sim 6\text{--}8\%$. The standard steps in the JWST pipeline were carried out to process the data from the raw (uncal files) ramp format to the cosmic ray corrected slope image (rate files). Further processing of the 2D slope image for WCS, flat fielding, flux calibration, etc. was also carried out using standard steps in the “Level 2” data pipeline calwebb_spec2 (cal files). To build the calibrated 2D IFU slice images into the 3D datacube, the “Stage 3” pipeline

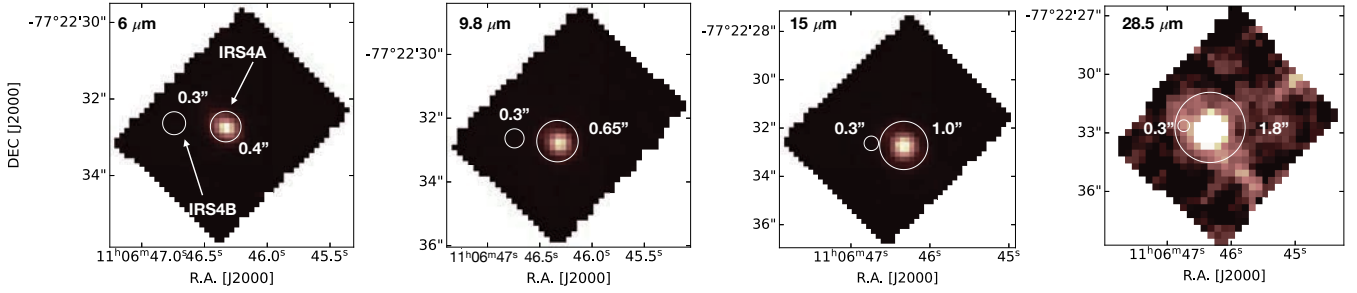


Fig 3 MIRI images from key spectral regions, namely, 6 μm : H₂O ice, 9.8 μm : silicate, 15.2 μm : CO₂ ice and 28.5 μm : continuum. The white circles show the regions used for spectral extraction. For IRS 4A we use an aperture size proportional to the size of the PSF, and for IRS 4B a constant size of 0.3'' is adopted.

was run step-wise and intermediate products were investigated for accuracy. The four dithers were combined using the “drizzle” algorithm with equal weighting and full pixel regions used. The final pipeline processed product presented here was built into 3D with the outlier bad pixel rejection step turned off, as running this over-corrected and removed target flux associated with the protostar.

2.3. MIRI data reduction

The JWST/MIRI observations of Ced 110 IRS4 were conducted on December 7, 2023. Spectroscopic measurements were acquired using a conventional 4-point dither scheme, totaling an integration time of 1665 s, with the telescope pointing set at 11^h06^m46.45^s, −77°22′32.93″. An additional observation was made on March 23, 2023, at 11^h04^m24.48^s −77°18′38.77″ to eliminate the background signal from the target flux. The data were processed using JWST pipeline version 1.11.4 (Bushouse et al. 2023), incorporating time-dependent corrections for channel 4 throughput. Calibration reference files from version 11.16.21 and jwst_1119.pmap were utilised, featuring updated onboard flat-field and throughput calibrations to achieve an absolute flux accuracy estimate of approximately 10%. Standard procedures within the JWST pipeline were executed to transform the data from the 3D ramp format to the cosmic ray corrected slope image. Subtraction of the scientific background occurred post the “Level 1” processing stage. Subsequent processing of the 2D slope image for WCS, flat fielding, and flux calibration was performed using the standard procedures in the “Level 2” data pipeline calwebb_spec2. The creation of the calibrated 2D IFU slice images into the 3D datacube involved the execution of the “Stage 3” pipeline. The final product generated by the pipeline was a 3D datacube, where the outlier bad pixel rejection step was disabled to prevent excessive correction and removal of target flux.

Spectral extraction for the primary source (IRS4A) was performed using an aperture size proportional to the PSF distribution (see Figure 3). The spectrum of the companion source (IRS4B) was extracted by assuming a constant aperture radius of 0.3 arcsec. As shown in Figure 3, at 6 and 9.8 μm , the two sources are well separated, whereas the PSF of the two sources are blended longwards of 15 μm . A comparison between the spectrum from MIRI/MRS and the *Spitzer*/Infrared Spectrograph (IRS) is presented in Appendix B.

2.4. Combined spectra

Figure 4 shows the combined spectra of Ced 110 IRS4A and IRS4B extracted from NIRCcam, NIRSpec and MIRI/MRS.

Apart from the spectral gaps already mentioned, no data is available between 3.8 and 5 μm for the primary source. The primary source is brighter than the companion by a factor of 50–100 across the spectrum and both sources show clear ice and silicate features which are labelled. The silicate features in both sources also have peculiar shapes. For example, in IRS4A, the peak of the absorption feature is at 9 μm instead of around 9.6 μm as commonly seen in protostars (e.g. Chiar & Tielens 2006). However, other protostars showing a similar absorption band at 9 μm have been reported in the literature (e.g. Furlan et al. 2008). In IRS4B, a flatter profile is visible, which is likely caused by polycyclic aromatic hydrocarbons (PAH) emission where features are also labelled. The silicate absorption at 18 μm is absent in both sources (See Section 4.2.1). In the next sections, we explore the full spectral range, with special focus on the ice features.

3. Ice laboratory data

The laboratory data considered in this paper are listed in Appendix C. These data were taken mainly from the Leiden Ice Database for Astrochemistry¹ (LIDA; Rocha et al. 2022) and from the Goddard NASA database². For this paper, this includes a list of 71 species, corresponding to pure and ice mixtures, and at different temperatures.

We highlight in this section the series of CO:CO₂ ice IR spectra because it plays an important role in the ice fits presented in Section 5.2. This dataset was characterised by van Broekhuizen et al. (2005), where several spectroscopic details are provided. In particular, warmer ices (>50 K) have a prominent blue shoulder at 4.25 μm , which is caused by ice trapping (e.g. Sandford et al. 1988). Although it is not mentioned in van Broekhuizen et al. (2005), these data are characterised by H₂O contamination that could also play a role in trapping molecules in the ice. For this reason, we relabelled this ice mixture at 70 K as H₂O:CO₂ (0.7:1) based on the H₂O ice column density and the non-presence of CO ice in the spectrum at that specific temperature. Further details about this spectrum are provided in Appendix D. We kept this data in our analysis for three reasons: (1) this dataset was characterised in detail by van Broekhuizen et al. (2005), (2) the presence of H₂O ice supports the trapping effect, and 3) the blue shoulder is visible in the H₂O:CO₂ (1:1) at 70 K from Ehrenfreund et al. (1999), and therefore it is consistent with the data from van Broekhuizen et al. (2005).

¹ <https://icedb.strw.leidenuniv.nl/>

² <https://science.gsfc.nasa.gov/691/cosmicice/spectra.html>

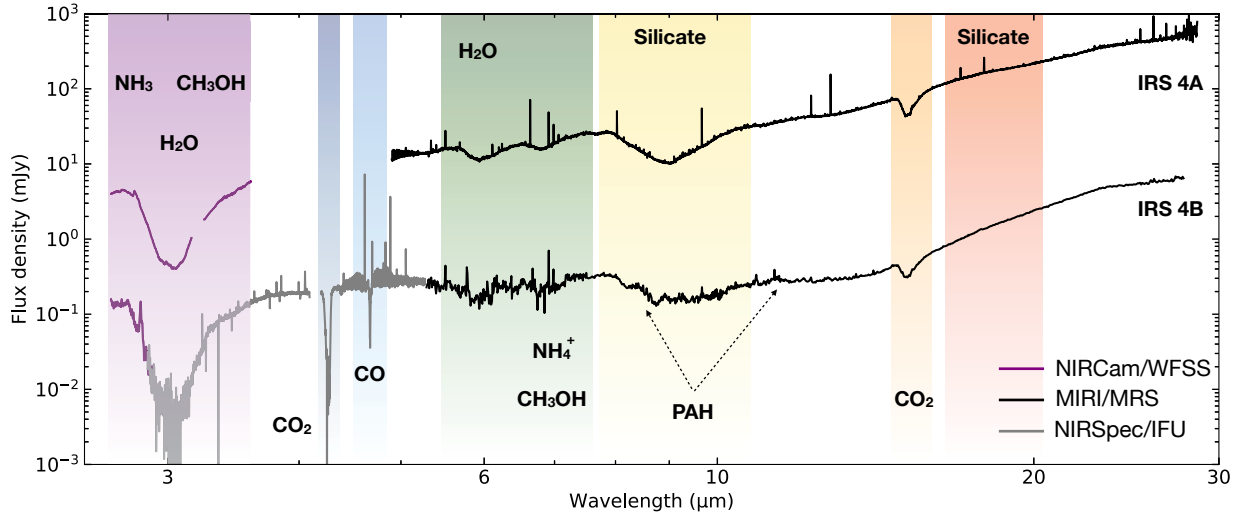


Fig 4 Spectra of Ced 110 IRS4A and IRS4B between 2.5–28 μm . These spectra use data from NIRSрec/IFU (grey), NIRCам/WFSS (purple) and MIRI/IFU (black). Major ice species and PAH features are indicated. The hatched areas highlight different spectral regions. Gas-phase line emissions are not masked or assigned in this figure. No offset is employed.

4. Methodology

This section describes the methods we used to perform global continuum subtraction covering both NIRSрec and MIRI ranges, as well as two approaches to subtract the silicate feature. The first approach is physically constrained with a SED empirical model, whereas the second method uses a polynomial function anchored at specific wavelengths. At the end of this section, we briefly describe the ENIIGMA spectral fitting methodology.

4.1. Continuum determination

To determine the baseline for the absorption features towards Ced 110 IRS4A and IRS4B, we used a low-order polynomial function as also adopted in previous works (e.g. Chiar & Tielens 2006; Boogert et al. 2008; Rocha et al. 2024b). Since the observations do not cover all wavelengths in the near-IR, we used different anchor points to trace the continuum. In addition, for IRS4A, we also considered photometry data from the Two Micron All Sky Survey (2MASS; Skrutskie et al. 2006)³ catalogue to further constrain the continuum determination below 2.8 μm . Similarly, in the MIRI range, different anchor data points are used to determine the continuum. Specifically, longwards of 15 μm , where there is PSF overlap of IRS4A with IRS4B, a larger spectral range is considered for IRS4B when tracing the continuum. This choice is made because it is no longer possible to constrain the long wavelength wing of the silicate bending mode at this range. The procedure does not affect the subsequent analysis of the IRS4B source that was limited to the NIRSрec range. Table 1 shows the spectral data used to determine the continuum for both Ced 110 IRS4A and IRS4B.

Once the global continuum is traced for each source, the spectrum is converted to an optical depth scale using the following equation:

$$\tau_{\lambda} = -\ln\left(\frac{F_{\lambda}^{\text{source}}}{F_{\lambda}^{\text{cont}}}\right), \quad (1)$$

where $F_{\lambda}^{\text{source}}$ is the observed spectrum and $F_{\lambda}^{\text{cont}}$ is the global continuum of the source.

³ <https://irsa.ipac.caltech.edu/Missions/2mass.html>

Figure 5 displays the continuum traced for Ced 110 IRS4A and IRS4B and the derived optical depth. We also highlight, that in the case of IRS4B, we first removed the CO emission lines between 4.3 and 5.0 μm before tracing the continuum. This procedure is presented in Appendix E. It is worth mentioning that PAH emission features are not seen towards the IRS4A source, whereas they are visible at 6.2, 8.6 and 11.2 μm towards the IRS4B protostar. For that source, no subtraction of the PAH features are performed because they would require a more detailed radiative transfer modelling that simulates the excitation of those PAHs. This is beyond the scope of this work. Since we do not perform the analysis of the absorption features in the MIRI range of IRS4B because of the low signal-to-noise ratio (S/N), the non subtraction of the PAH emission features does not compromise our analysis and results presented for that source.

4.2. Silicate subtraction

In order to analyze the ice bands, the strong silicate features at 10 and 20 μm must be removed. As demonstrated in the literature (e.g. Boogert et al. 2008; Bottinelli et al. 2010; Poteet et al. 2013), the standard approach is to subtract a scaled ice-free silicate profile from the Wolf-Rayet source GCS3 (Kemper et al. 2004). We first tried this methodology. However, Figure 6 shows an atypical silicate profile towards IRS4A compared with other protostars. While the 9.8 μm band of the low-mass protostars Elias 29 (Boogert et al. 2000b) and HH 46 (Noriega-Crespo et al. 2004) have a profile similar to GCS3, the spectrum of IRS4A is rather different given the strong absorption excess at the short-wavelength side of the observational feature around 9.8 μm . The small excess seen on the short-wavelength side of HH46 can be attributed to the composition of the silicate and ices and, in fact, was already discussed in the literature (e.g. Boogert et al. 2013; McClure et al. 2023; Rocha et al. 2024b). The silicate profile towards IRS4A seems rather strong to be attributed to only the composition of the dust and might also be affected by radiative transfer effects. Such an atypical profile was also observed previously in the literature (e.g. Furlan et al. 2008), but no explanation has been provided.

The complex environment of the Ced 110 IRS4 system suggests the presence of a disk surrounded by an envelope and

Table 1. List of wavelengths and flux densities used as anchor points to determine the continuum.

λ (μm)	Flux density ^(a) (mJy)
Ced 110 IRS4A	
J (1.23)	0.20±0.08
H (1.66)	1.21±0.51
K (2.16)	2.46±0.72
NIR (2.68, 2.71, 3.79)	4.31, 4.49, 8.43
MIR (5.45–5.57, 27.1–27.7)	15.84–16.46, 492.11–505.08
Ced 110 IRS4B	
J (1.23)	...
H (1.66)	...
K (2.16)	...
NIR (2.65–2.75, 4.0–4.1, 4.74, 4.95, 5.19)	0.13–0.14, 0.19–0.20, 0.23, 0.24, 0.25
MIR (5.45–5.57, 17.9–27.7)	0.25–0.26, 1.36–6.26

Notes. ^(a) Flux error is assumed to be 10% in both NIR and MIR.

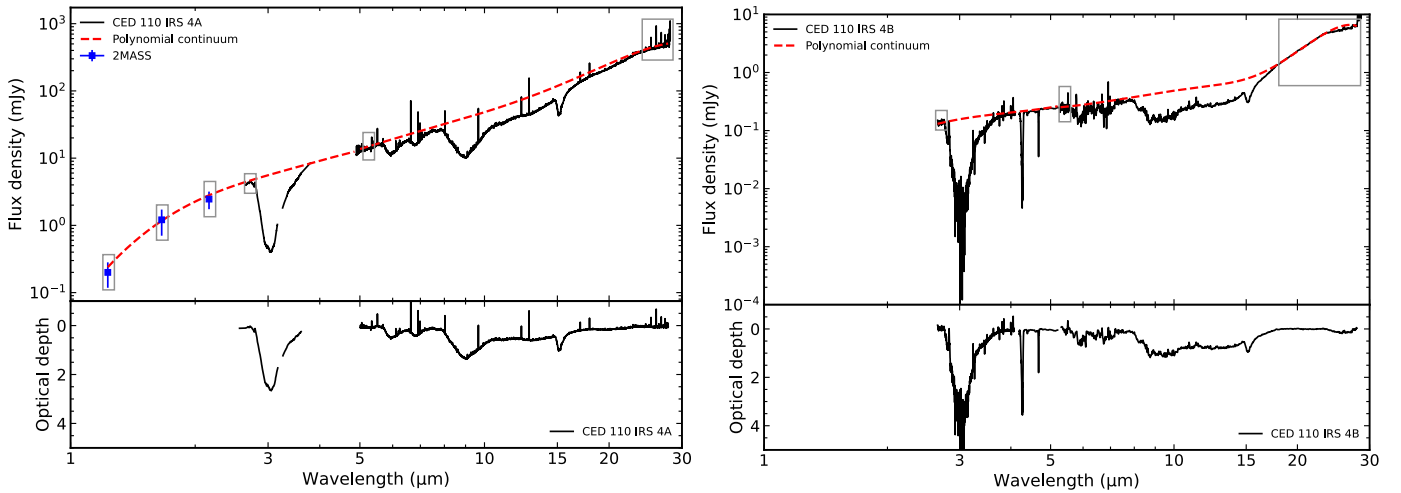


Fig. 5. Dust continuum profiles (top panels) and optical depth spectra (bottom panels) of Ced 110 IRS4A (left) and IRS4B (right). For IRS4A source, 2MASS data are used to trace the continuum below 2.5 μm . The red dashed line shows the continuum profile traced by a polynomial function and the grey boxes indicate the spectral regions used as anchor to guide the fit. The polynomials for IRS4A are 3rd order for NIRSpec and MIRI respectively. Similarly, for IRS4B, they are 2nd and 5th orders, respectively. The strong upward inflexion in the IRS4B source longwards of 15 μm is due to the PSF overlap in the MIRI range with the IRS4A source (see Figure 3).

may be the cause of the unusual silicate profile (Pontoppidan & Dullemond 2005). However, addressing this source geometry in detail or the dust mineralogy for the Ced 110 IRS4 system is beyond the scope of this paper. Therefore we used two alternative methodologies to perform the silicate subtraction for IRS4A, as described in Sections 4.2.1 and 4.2.2. No silicate analysis or subtraction is performed for the companion source, IRS4B. First, this data exhibit a low S/N, which hinders a profile analysis of the band. Second, this source has clear PAH emission features, which causes the flattened shape around 9.8 μm . A more refined model is needed for the silicate analysis of IRS4B.

4.2.1. SED empirical model

Given the nature of the unusual shape of the silicate profile towards IRS4A, we used a simplified model to perform continuum and silicate subtractions simultaneously as presented

below:

$$F_{\lambda}^{\text{source}} = F_{\lambda}^{\text{BB}} \exp\left(-\sum_i \tau_{i,\lambda}\right) + \sum_j \left\{ \frac{B_{\lambda}(T)}{\pi} [1 - \exp(-\tau_{j,\lambda})] \right\}, \quad (2)$$

where $F_{\lambda}^{\text{source}}$ is the received flux, F_{λ}^{BB} is the flux emitted from the source, which is simplified by a black-body function, τ is the dust grain optical depth, and $B_{\nu}(T)$ is the optically thick emission from the dust. The optical depth is calculated from the opacity data (κ), and is given by $\tau_{\lambda} = N \cdot \kappa_{\lambda}$, where N is the mass column density in units of g cm^{-2} . The first part of Equation (2) accounts for grain (dust and ice) absorption, whereas the second part accounts for dust emission (warm, cold). The indexes i and j indicate the kind of solid particle in the model. If the same material is in emission and absorption, then $i = j$.

To model the silicates in this approach, we calculated opacity models (κ) by assuming a power-law size distribution

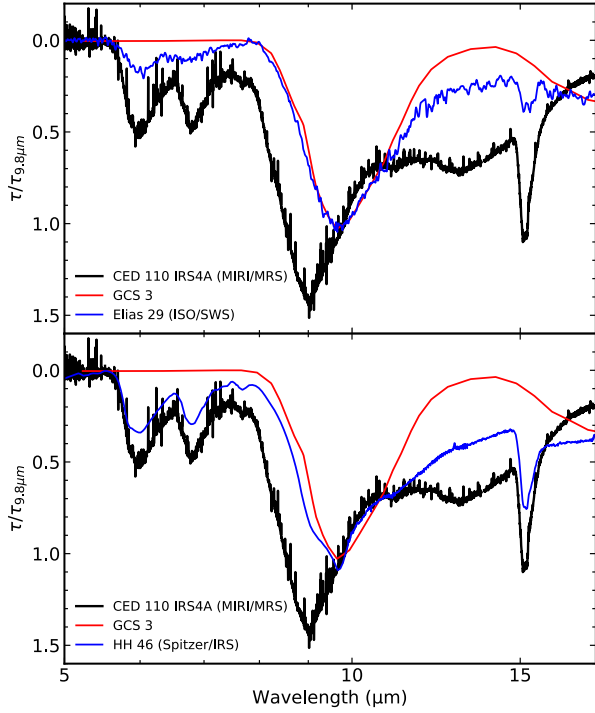


Fig 6 Silicate profiles of GCS3 (Kemper et al. 2004), Elias 29 (Boogert et al. 2000b) and HH 46 (Noriega-Crespo et al. 2004) compared to the MIRI/MRS spectrum of IRS4A. All spectra are normalised by the peak optical depth at 9.8 μm .

($n(a) \propto a^{-3.5}$) of hollow spheres (DHS) with sizes ranging from 0.1 to 1.0 μm . The effects of the grain-ice porosity and scattering are not considered in this model, which would be better reproduced with a full radiative transfer modelling. The literature focused on disk mineralogy generally reports that silicates with olivine stoichiometry dominate the 9.8 μm emission band (e.g. Olofsson et al. 2009; Sargent et al. 2009; Juhász et al. 2010; Fogerty et al. 2016; Grimbale et al. 2024), whereas silicates with pyroxene stoichiometry dominates the 9.4 μm absorption band towards protostars (Chiar & Tielens 2006; Rocha & Pilling 2015; Do-Duy et al. 2020). Although one type of silicate dominates the band profile, it is important to mention that often a combination of both kinds is needed in the fits (see Henning & Semenov (2013) for a review). The two dust components used in this paper are pyroxene ($Mg_{0.7}Fe_{0.3}SiO_3$) and olivine ($MgFeSiO_4$), and their optical constants were taken from Dorschner et al. (1995). In addition, optical constants taken from Zubko et al. (1996) were used to include amorphous carbon into the dust composition, following the standard mass ratio of 0.87/0.13 for the silicate and carbon, respectively (e.g. Woitke et al. 2016). Similarly, for the H_2O ice population, we used the same size limits as for the dust. We adopted a continuous distribution of ellipsoids (CDE) for the grain-shape correction and the optical constants were taken from Rocha et al. (2024a).

In our simplified model, we considered two populations of dust. Given the inclination of IRS4A (70°; Manoj et al. 2011), we assume that pyroxene dust dominates the absorption and comes mostly from the envelope. In contrast, olivine originates in the disk and dominates the emission profile. The model using Equation (2) is presented in Figure 7a. The values of the mass column densities of pyroxene and olivine are $5.5 \times 10^{-4} \text{ g cm}^{-2}$ and $4.3 \times 10^{-4} \text{ g cm}^{-2}$, respectively, which are on the same order of magnitude as the protostar HOPS-68 (Poteet et al. 2011).

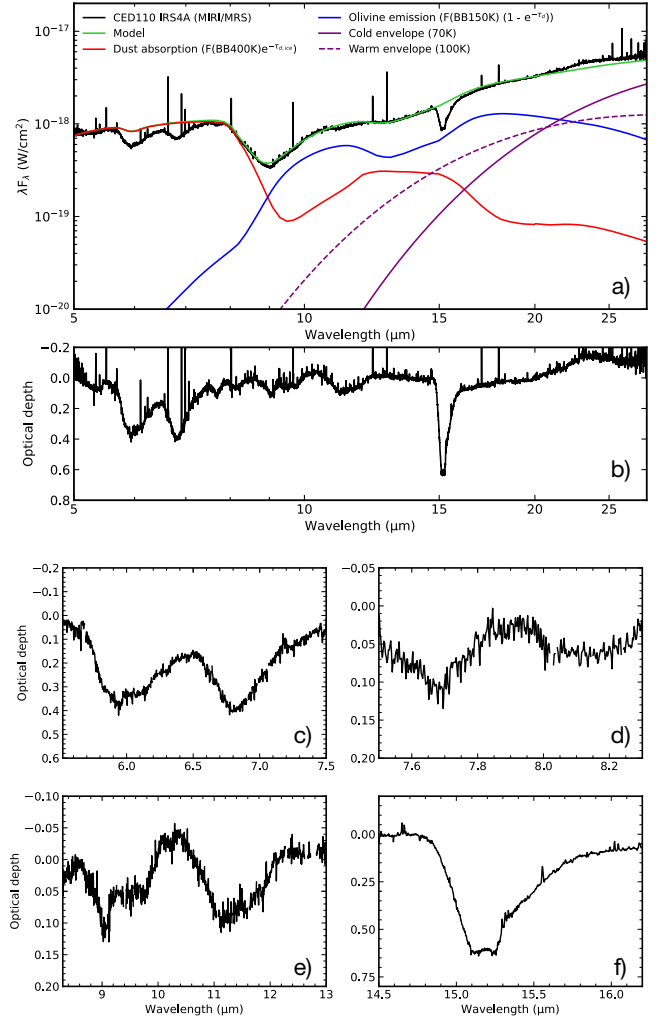


Fig. 7. Panel a shows the SED fit using Method 2 shown by the green line. The absorption component (red line) considers pyroxene and H_2O ice absorption. The emission component (blue line) considers olivine thermal emission, as well as colder dust emission (purple lines) at longer wavelengths. Panel b shows the optical depth spectrum after subtracting the green profile. Panels c–f show different absorption features that are investigated in this work.

A black-body profile with a temperature of 400 K was used to model the pyroxene and H_2O ice absorption in the MIRI range, while the olivine emission is modelled with a black-body with a temperature of 150 K. The black-body at 400 K is mostly caused by the extinct black-body from the central source (see Boogert et al. 2002, for individual radiative transfer components). The radiation field associated with the extinct black-body interacts with the dust and icy material located in regions with temperatures above and below 150 K, respectively, where 150 K is the sublimation temperature of H_2O ice (Collings et al. 2004). In the case of the dust thermal emission, radiative transfer models show that disks embedded in protostellar envelopes have temperatures around 100–200 K between 100 and 400 au (e.g. Nazari et al. 2023). In our simplified model, it is assumed that such olivine emission comes from those regions. Two other black-body emission representing optically thick dust at temperatures of 70 and 100 K are needed to fit the spectrum longwards of 20 μm . This level of theory is enough to subtract the silicate profile and the dust continuum towards Ced 110 IRS4A. Naturally, more sophisticated models aiming at reproducing both

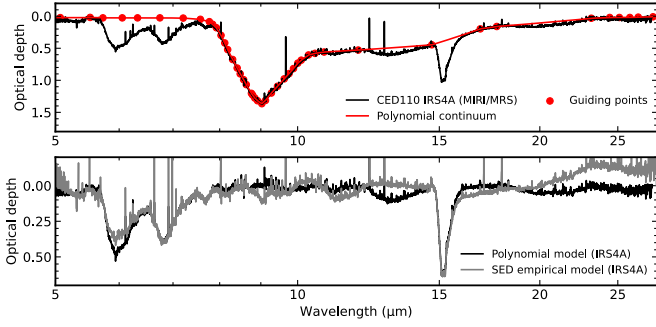


Fig 8 Silicate profile removed using polynomial functions anchored at specific guiding points. The top panel shows the fitted profile and the bottom panel compares the optical depth spectrum obtained from the polynomial and SED empirical models.

spectrum and image, as well as the silicate emission and absorption interplay, are required to fully unveil the dust nature of in that source.

After subtracting the continuum profile, clear absorption features due to ices are revealed, which are presented in Figure 7b, with the zoom-ins shown in Figures 7c–f. We note that a larger fraction of H₂O ice at 6 μm was already subtracted with the continuum based on the 3 μm, where more details are presented in Section 5.1.1. In that case, other contributions must be assumed in order to explain this absorption feature.

4.2.2. Polynomial subtraction

Because of the uncertainty in the nature of the silicate profile towards IRS4A, we also performed a silicate subtraction using a guided continuum (top panel of Figure 8). The criteria for selecting the position of these points was that they should not subtract clear absorption features other than the silicate itself. For instance, in the region between 5 and 7.2 μm the points are positioned at $\tau = 0$. From 7.5 μm onwards, the points follow the shape of the broadband at 9 μm. Longwards of 11 μm, the points trace the baseline for some strong absorption features, specifically, at 11.2, 13.0, 15.2, and 20 μm. The downside of this method is that the total subtraction of the H₂O ice libration band at 12 μm, whereas the contribution of the H₂O bending mode around 6 μm is not removed. Another limitation is that the 9 μm band is fully removed since the physical motivation of this approach is that this entire band profile is caused by radiative transfer effects instead of chemistry. We highlight that this is not a problem for the analysis of this paper since we only perform ice analysis for specific wavelength ranges.

In the bottom panel of Figure 8, we compare the optical depth spectra of IRS4A after subtracting the silicate using the polynomial and the SED empirical method. Both spectra show rather similar features between 6.4 and 7.9 μm, and for most of the CO₂ bending mode at 15.2 μm. On the other hand, some differences are seen at 6, 8.7–9.3 and 14 μm, which are discussed in this paper.

4.3. Ice fitting approach

We performed a global fit of the primary and companion source spectra covering specific spectral ranges using the ENIIGMA fitting tool (Rocha et al. 2021). This method has the advantage of accounting for multiple molecular absorption features. ENIIGMA combines laboratory spectra using a linear combination and adopts genetic modelling algorithms to search for the best fit.

Genetic algorithms are robust optimisation techniques based on the processes of biological natural selection that are aimed at finding the global minimum solution for complex problems (Holland 1975; Koza 1992). The code searches for the global minimum solution that fits the observations using the reduced chi-square function, calculated with the following equation:

$$\chi^2 = \frac{1}{d.o.f.} \sum_{i=0}^{n-1} \left(\frac{\tau_{\nu,i}^{\text{obs}} - \sum_{j=0}^{m-1} w_j \tau_{\nu,j}^{\text{lab}}}{\gamma_{\nu,i}^{\text{obs}}} \right)^2, \quad (3)$$

where *d.o.f.* is the number of degrees of freedom, γ is the error in the observational optical depth spectrum propagated from the flux error ($\sim 10\%$), n is the number of data points, ν is the wavenumber, $\tau_{\nu,i}^{\text{obs}}$ is the optical depth of the observational spectrum defined in Equation (1), $\tau_{\nu,j}^{\text{lab}}$ is the optical depth of the laboratory data, and w_j is the scaling factor. The absorbance laboratory data (*Abs*) is converted to an optical depth by equation $\tau_{\nu}^{\text{lab}} = 2.3 \text{Abs}$.

The ice column density from the best fit is calculated with the following equation:

$$N_{\text{ice}} = \frac{1}{A} \int_{\nu_1}^{\nu_2} w \cdot \tau_{\nu}^{\text{lab}} d\nu, \quad (4)$$

where A is the vibrational mode band strength of the molecule, as listed in Table 2.

ENIIGMA searches for the best fit in a vast solution space. Because of the degeneracy involved in the fit, ENIIGMA also performs a confidence interval analysis of the linear combination coefficients using a reduced χ^2 map. Based on the confidence intervals, ENIIGMA calculates the lower and upper ice column densities inside a 3σ confidence interval. In total, the ENIIGMA code evaluates around 4000 solutions based on this dataset. This represents a huge number of solutions, but it is important to mention that some mixtures may not be included in the current dataset, such as specific variations in the mixture fraction.



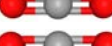
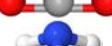





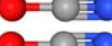






5. Results

In this section, we show the ice fits and results for Ced 110 IRS4A and IRS4B. Finally, we derive the ice column densities of the species securely or tentatively identified.

5.1. Ice analysis: Ced 110 IRS4A

We performed a more detailed analysis of the MIRI spectrum of Ced 110 IRS4A, which has a high S/N. Due to the lack of data between 3.6 and 5.0 μm we cannot measure either CO₂ (4.27 μm) or CO ice (4.67 μm). Therefore, the NIRC2 spectrum (2.6–3.6 μm) is solely used to estimate the H₂O ice column density, which can be used later to calculate the ice abundances. In this section, we analyzed the optical depth spectra between 7 and 10 μm calculated from the SED and polynomial silicate subtraction methods, as presented in Section 5.1.2. Similarities and differences from the two data are compared. In Section 5.1.3, we also analyzed the 6–8 μm optical depth data from both subtraction methods. In the case of SED subtraction, we performed analysis using the C1–C5 empirical components (Boogert et al. 2008) because this method requires subtraction of H₂O ice first. For the polynomial subtraction method, where H₂O ice is not removed, this range is used to cross check the intensity of the features derived from the fit between 7–10 μm. The chemical nature causing the 6–8 μm range is highly unknown, and a dedicated

Table 2. List of vibrational transitions and band strengths of molecules presented in this work.

Structure	Chemical formula	Name	λ [μm]	ν [cm^{-1}]	Identification	\mathcal{A} [cm molec^{-1}]	References ^(a)
	H ₂ O	Water	3.01	3322	OH str.	2.2×10^{-16}	[1]
	¹² CO	Carbon monoxide	4.67	2141	CO str.	1.4×10^{-17}	[1]
	¹² CO ₂	Carbon dioxide	4.27	2141	CO str.	1.1×10^{-16}	[1]
	¹³ CO ₂	Carbon dioxide	4.38	2283	CO str.	1.1×10^{-16}	[1]
	NH ₃	Ammonia	9.0	1111	NH str.	2.1×10^{-17}	[1]
	CH ₄	Methane	3.32	3007	CH str.	1.27×10^{-17}	[1]
	CH ₄	Methane	7.67	1303	CH ₄ def.	8.4×10^{-18}	[1]
	SO ₂	Sulfur dioxide	7.60	1320	SO ₂ str.	3.4×10^{-17}	[2]
	N ₂ O	Nitrous oxide	4.47	2337	NO str.	1.22×10^{-17}	[3]
	OCN ⁻	Cyanate ion	4.59	2166	CN str.	1.3×10^{-16}	[4]
	OCN ⁻	Cyanate ion	7.62	1312	Comb. ($2\nu_2$)	7.45×10^{-18}	[5]
	H ₂ CO	Formaldehyde	8.04	1244	CH ₂ rock	1.0×10^{-18}	[6]
	HCOOH	Formic acid	8.22	1216	C–O stretch	2.9×10^{-17}	[1]
	CH ₃ OH	Methanol	3.2–3.8	2631–3125	CH str.	1.3×10^{-16}	[1]
	CH ₃ OH	Methanol	9.74	1026	CO str.	1.8×10^{-17}	[1]
	CH ₃ OCHO	Methyl formate	8.25	1211	C–O str.	2.52×10^{-17}	[7]

Notes. [1] Bouilloud et al. (2015), [2] Boogert et al. (1997), [3] Fulvio et al. (2009), [4] van Broekhuizen et al. (2005), [5] Rocha et al. (2024b), [6] Schutte et al. (1993), [7] Terwisscha van Scheltinga et al. (2021). ^(a)References to Bouilloud et al. (2015) refer to the corrected band strength value considering a different ice density mentioned by the authors.

analysis of this part of the spectrum is deferred to future work. Other absorption features observed in the MIRI range, such as 11.2 μm and 15.2 μm are also analyzed. Since this paper does not target gas-phase species, we only briefly mention the 7.18 μm feature in Appendix F.

5.1.1. H₂O ice: 2.5–28 μm

The NIRCам and MIRI spectra of Ced 110 IRS4A (Fig. 4) show clear H₂O ice absorption features at 3 (O–H stretch), 6 (bending) and 12 μm (libration). From among these features, we used the 3 μm band to estimate the H₂O ice column density. The 6 μm band has strong overlap with other species, and the 12 μm is affected by the atypical silicate profile coming from the complex circumstellar environment of Ced 110 IRS4A (e.g. Pontoppidan & Dullemond 2005). However, the 3 μm band is the sum of PSF spectra at selected regions from NIRCам and, for this reason, we derived the H₂O ice column density by scaling the laboratory data to the observations. The analysis of the individual PSF spectra will be performed in a future work.

The IR spectra of bulk and grain-shape corrected ice spectrum of pure H₂O ice are scaled to the JWST data as shown in Figure 9. Both data at 10 K account for most of the 3 μm band, but some differences can be mentioned. For example, the grain-shape corrected spectrum using the CDE approach with $a_{\text{max}} = 1 \mu\text{m}$, does not explain the blue wing excess of the 3 μm feature, whereas it accounts for some of the red wing excess compared to the bulk ice spectrum. More differences between pure ice bulk and geometric-corrected spectrum are notable at 6 and 12 μm , where the large grain spectrum has flatter absorption features, and the 12 μm band is blue-shifted. A third laboratory spectrum, H₂O:NH₃ (10:1.6) is used in this analysis motivated by the best fits towards the two background stars in McClure et al. (2023). This spectrum shows an excellent match with the 3 μm band, and the small inflection around 2.9 μm , related to NH₃ ice. Using this ice mixture shows other NH₃ related ice features are seen at 6.2 and 9.0 μm . An absorption excess at 3.4 μm due to the formation of ammonia hydrates (Dartois & d’Hendecourt 2001) is seen in this laboratory data, which is not present in the pure H₂O ice bulk spectra. Interestingly, the intensity of this excess is comparable to the profile from large-grain spectra and highlights that

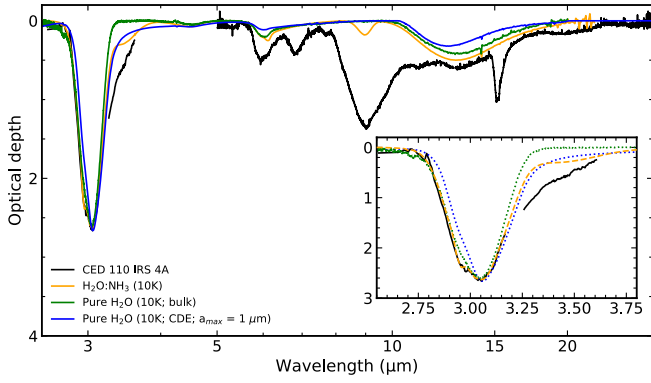


Fig 9 H₂O ice IR data compared with the optical depth spectrum of Ced 110 IRS4A prior silicate subtraction. The green and orange lines represent the pure H₂O bulk ice and H₂O:NH₃ spectra. Blue shows the CDE-corrected ice spectra of pure H₂O ice. The inset panel shows a zoom-in of the 3 μm band.

both physical and chemical phenomena play a role in creating this absorption profile.

Finally, we note that the OH dangling feature for these two protostars are not addressed in this paper, as this would require first deriving an accurate flux error from the NIRCarn observations. The OH dangling band was observed towards several lines of sight in the Chameleon I molecular cloud, as demonstrated by Noble et al. (2024).

5.1.2. 7–10 μm

The analysis of the MIRI spectrum between 7 and 10 μm of Ced 110 IRS4A was performed independently of the rest of the observational data and follows the methodology described in Rocha et al. (2024b). This approach allows us to improve the constraints on the species contributing to this range, without addressing the specific nature of the 6 and 6.8 μm bands. Despite the independent analysis of this spectral range, we used the best fit to assist the analysis of the 6 and 6.8 μm bands in Section 5.1.3.

Here, we use the ENIIGMA fitting tool to search for the best fit out of a large dataset of laboratory data listed in Table C.1. The local continuum subtraction around this spectral range and for the empirical silicate subtraction is shown in Appendix G. In the case of the polynomial method, this subtraction follows the profile reported in Figure 8.

Figure 10 presents the ENIIGMA fit for the 7–10 μm range of Ced 110 IRS4A for both silicate subtraction methods. In these two cases, there are clear absorption features at 7.67, 8.2 μm and around 9.8 μm. No absorption features at 7.2 and 7.4 μm were seen towards Ced 110 IRS4A. Additionally, in the case of the polynomial silicate subtraction, no absorption is present at 9 μm, where we would expect to see NH₃ ice. The best fits indicate that the feature at 7.67 μm is composed of CH₄:H₂O, SO₂:CH₃OH, OCN[−] (HNCO:NH₃), and N₂O. Previous analyses of this band (Gibb et al. 2004; Öberg et al. 2008; Zasowski et al. 2009) using *ISO* and *Spitzer* data have concluded that two species, namely, CH₄ and SO₂, contribute to this absorption feature. With the most recent JWST observations, a detailed analysis performed of NGC 1333 IRAS 2A and IRAS 23385+6053 by Rocha et al. (2024b) confirmed a good spectral match with CH₄, SO₂, and also OCN[−].

The next strong feature in this spectral range is seen at 8.2 μm. The fits demonstrate that HCOOH mixed with H₂O:CO₂

and with H₂O:CH₃OH contribute to this band, where the former is stronger in the data after empirical silicate subtraction. This result is aligned with Bisschop et al. (2007) and Rocha et al. (2024b), which found a good spectral match with HCOOH:H₂O:CH₃OH. In addition, this result indicates that a mixture where CO₂ ice is presented is also possible, which brings important insights into the origin of HCOOH (Qasim et al. 2019).

The subsequent spectral range between 8.6 and 10 μm is dominated by NH₃ and CH₃OH absorption features and the ENIIGMA fits are different in the two spectra given their distinct profiles. In the case of empirical silicate subtraction, a large excess is present in this entire spectral range, which is fitted with NH₃:H₂O, NH₃:CO₂, CH₃OH:CO, and CH₃OH:H₂O, along with a narrow Gaussian profile at 9.04 μm representing an unidentified feature. On the other hand, no absorption remains at 9 μm after using the polynomial method with the specified guided points. Other guiding point avoiding the 9 μm band would leave some space to fit NH₃ ice, but exactly where to place the continuum is rather challenging. The band around 9.8 μm was fitted with CH₃OH:CO and two CH₃OH:H₂O components, namely: CH₃OH:H₂O and HCOOH:CH₃OH:H₂O. Most of these features were previously found in the literature, as are the cases of NH₃:H₂O, CH₃OH:CO, and CH₃OH:H₂O (Lacy et al. 1998; Bottinelli et al. 2010; Cuppen et al. 2011; McClure et al. 2023). The reliability of the other two features, NH₃:CO₂ and the Gaussian profile, are discussed in Section 6.2.5.

Finally, we performed two complementary analyses that are shown in Appendix H (<https://doi.org/10.5281/zenodo.14281751>). First, we performed a consistency check of the components used in this fit with the entire spectral range available for the primary source, which is shown in Figure H.5. This assessment demonstrates that the intensities of the features found in this local analysis are consistent with features of those components in other wavelengths. It also indicates that additional components are needed to fit those spectral ranges. The second analysis consists of deriving Akaike information criterion (AIC) values to estimate the minimum number of components to the fit (Figure H.7). This analysis indicates that eight of the ten components are crucial to the fit. The least needed components are SO₂ and HCOOH:H₂O:CH₃OH. However, among these two, SO₂ keeps the model within the interval of a robust fit, whereas HCOOH:H₂O:CH₃OH does not.

In summary, the analysis of the spectral range between 7 and 10 μm, allows us to report IR features from CH₄, SO₂, OCN[−], NH₃, HCOOH, and CH₃OH, along with the tentative assignment of N₂O, as well as an unidentified feature at 9 μm.

5.1.3. 6 and 6.8 μm bands

The 6–7 μm interval was analysed in a similar way as in Boogert et al. (2008), which proposed the use of five empirical components to model this spectral range. As required by this method, the H₂O pure ice spectrum is subtracted, which for simplicity, is done using the bulk ice spectrum at 10 K without grain-shape correction (Fig. 9). The residual spectrum fitted using the five components is shown in Figure 11 and is likely related to different chemical species. Components C1 and C2 account for the 6 μm absorption band, where C1 can be related with a carbonyl group (C=O) and C2 with NH₃ and formate ion (e.g. HCOO[−]) deformation modes. C3 and C4 fit together the 6.8 μm, and they can be tracers of NH₄⁺ at different temperatures and chemical environments (e.g. Novozamsky et al. 2001; Gálvez et al. 2010). Finally, C5 is a broad feature covering the full range. This

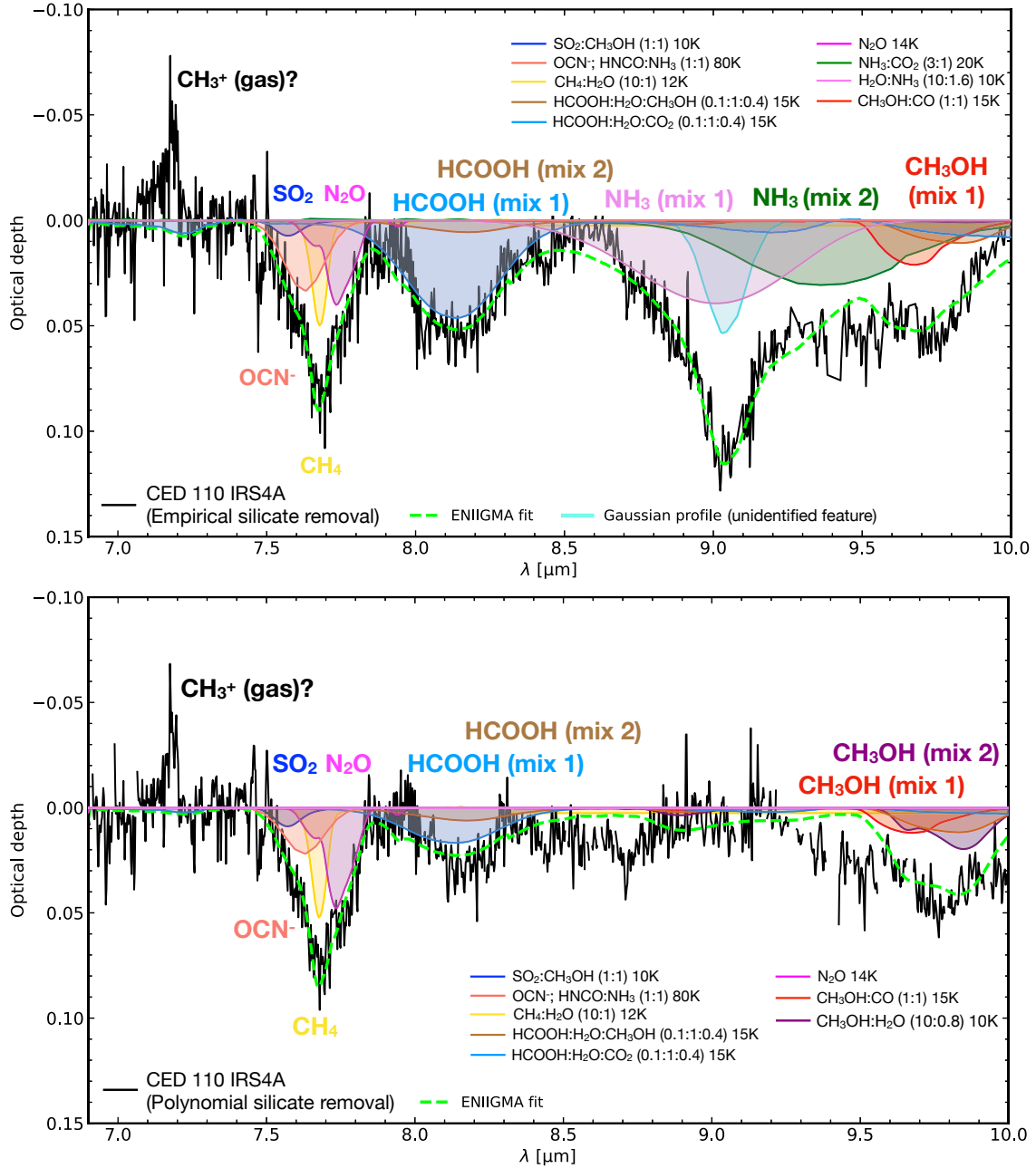


Fig 10 ENIIGMA fit (dashed green) in the range between 6.9 and 10 μm of Ced 110 IRS4A spectrum (black) after the empirical (top) and polynomial (bottom) silicate subtraction. The IR spectra of many ice species contribute to this fit and are indicated by labels and coloured areas. The terms “mix 1” and “mix 2” are used when two mixtures containing the same species are needed. The information of these mixtures is presented in the figure labels. We highlight that these best fits are based on the large laboratory ice database listed in Appendix C used to explore a variety of solutions. Other solutions can be further explored by expanding the database of species tested with new data. We refer Appendix F for a brief discussion of the CH_3^+ emission feature.

component can be linked with crystalline H_2O ice and to organic refractory material (e.g. [Gibb & Whittet 2002](#)).

We performed an additional analysis of the 6–7 μm range by accounting for areas of the bands fitted in the range between 7 and 10 μm . For instance, we consider $\text{H}_2\text{O}:\text{NH}_3$ ice at 10 K constrained from Figure 9. The contributions of other species is constrained from the local fits performed in Section 5.1.2. For example, the intensity of NH_4^+ at 6.8 μm , is derived from the same spectral data fitting the OCN^- feature at 7.6 μm in Figure 10, which is $\text{HNCO}:\text{NH}_3$ at 80 K ([Novozamsky et al. 2001](#)). The same is repeated for HCOOH (mixed with H_2O and

CO_2) and NH_3 (mixed with CO_2). The H_2CO contribution comes from the upper limit based on the 8 μm band. Figure 12a displays the individual contributions of the five laboratory spectra as well as their cumulative sum. Notably, the analysis reveals that both 6 and 6.8 μm bands are not entirely adequately explained by the species used in this analysis. In particular, the NH_4^+ feature constrained from the local fits presented in Section 5.1.2, does not account for all absorption at 6.8 μm .

The percentage contribution of each species is illustrated in Figure 12b. The component $\text{H}_2\text{O}:\text{NH}_3$, that can fit entirely the 3 μm , contributes to 30% of the 6–8 μm band. The second

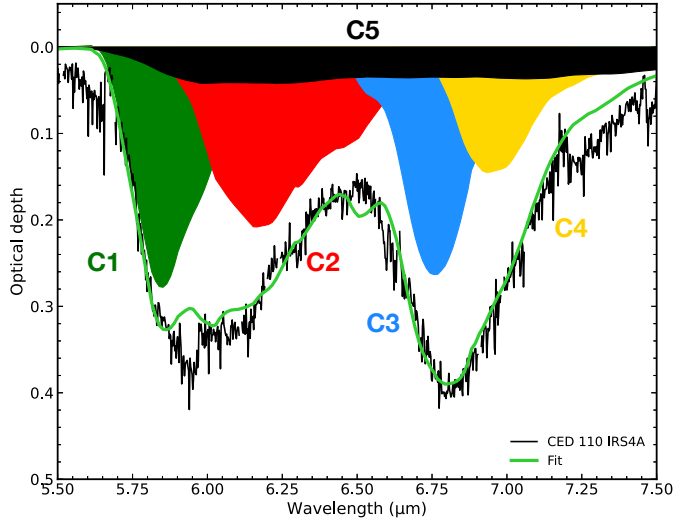


Fig 11. Spectral decomposition of the H₂O-subtracted spectrum of Ced 110 IRS4A using five empirical components from Boogert et al. (2008). See accompanying text for the meaning of components C1 to C5.

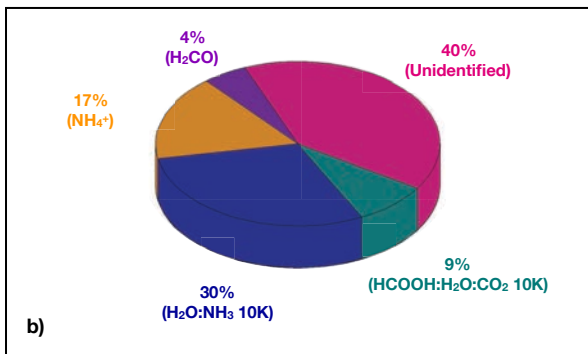
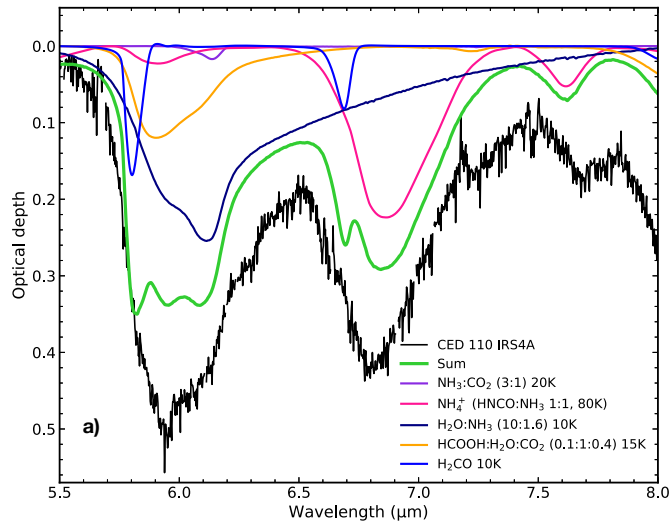


Fig 12. Simplified analysis of the 6 and 6.8 μm bands of Ced 110 IRS4A using laboratory data. H₂O ice is not subtracted in this case. Panel a shows the sum (green) of four laboratory spectra of known species. Panel b shows the fractional area of each component relative to the total area in the MIRI spectra between 5.5 and 7.5 μm . Unidentified refers to the difference between the MIRI data and the sum of the four components in the specified range. The contribution of NH₃:CO₂ is not added to the chart because it represents less than 1% of the total area.

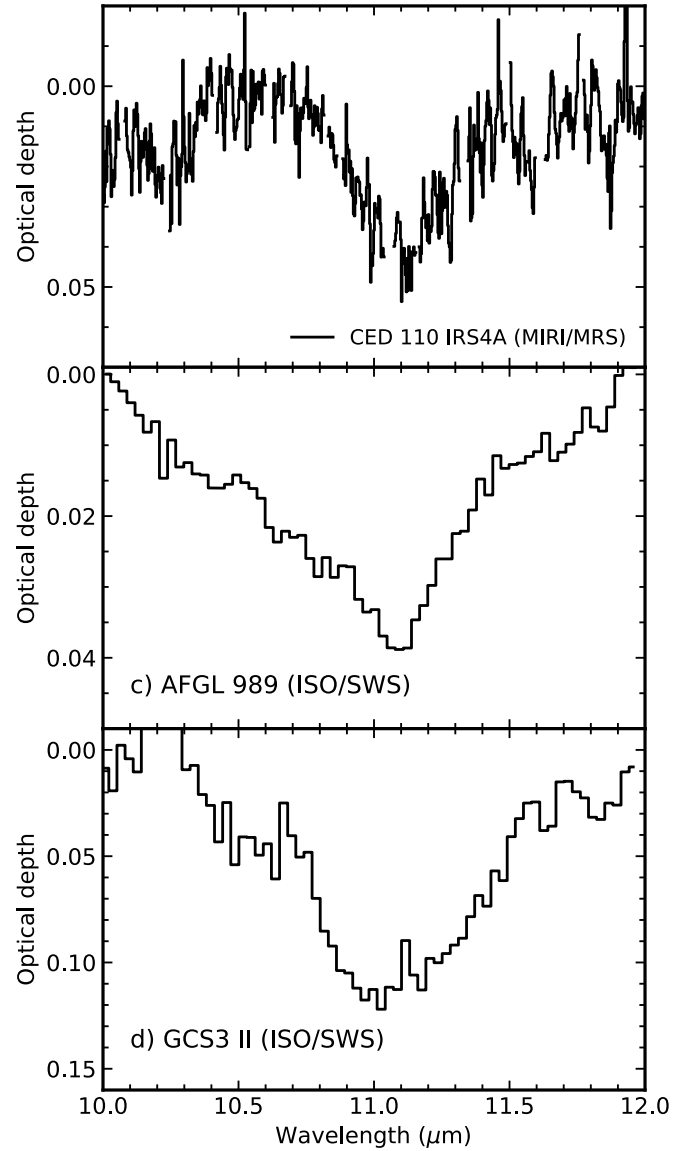


Fig 13. Comparison between the 11 μm feature towards Ced 110 IRS4A (panel a) with ISO/SWS towards a high-mass protostar AFGL 989 and the galactic center source GCS II (panels b and c).

and third most prominent features are the NH₄⁺ (17%), and HCOOH:H₂O:CO₂ accounts for 9%. Finally, H₂CO ice contributes with 4% as estimated from the upper limits based on the 8 μm band. Subtracting these four species, an area of 40% remains to be fitted. This simple analysis illustrates that an important portion of the 6–7 μm remains unknown. Candidates can be some of the carriers of the C1 to C5 components shown in Figure 11.

5.1.4. 11.2 μm

The analysis of the 11.2 μm band is performed by using the optical depth spectrum after polynomial silicate subtraction as presented in Figure 13a. This procedure was needed because the silicate subtraction performed with the SED modelling underpredicts the absorption profile at this range, which is noticed by the negative optical depth values (see Fig. 7). For comparison, data from the *Infrared Space Observatory* using the Short

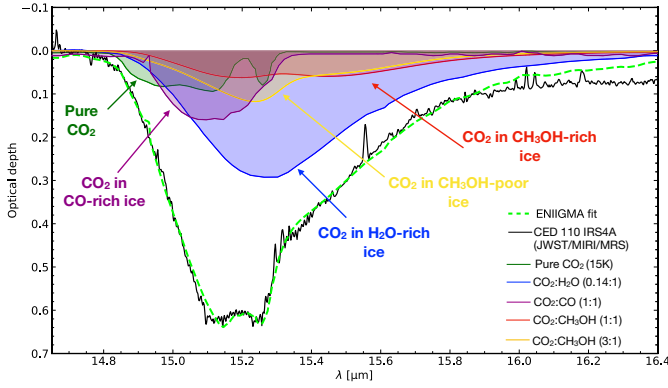


Fig 14 ENIIGMA fit of the CO₂ ice bending mode towards Ced 110 IRS4A. The fit performed with five components indicate contributions of CO₂ pure and mixed with H₂O, CO, and CH₃OH.

Wavelength Spectrometer (SWS) data of AFGL 989 and GCS3 II from Do-Duy et al. (2020) are presented, both with an absorption feature at 11.2 μm.

We calculated the fraction of crystalline silicate using the following equation from Poteet et al. (2013):

$$\frac{N_{\text{cr}}}{N_{\text{cr}} + N_{\text{am}}} = \frac{\tau_{\text{cr}}(\lambda_p)\kappa_{\text{am}}}{\tau_{\text{cr}}(\lambda_p)\kappa_{\text{am}} + \tau_{\text{am}}(\lambda_p)\kappa_{\text{cr}}}, \quad (5)$$

where N_{cr} and N_{am} are the dust column densities of the crystalline and amorphous dust, respectively. Similarly, τ_{cr} and τ_{am} are the optical depths in the two ice morphologies, κ_{cr} and κ_{am} , the mass-opacity values and λ_p the wavelength at the peak of the feature.

The optical depth values for the crystalline and amorphous dust are 0.06 (Fig. 13) and 2.8 (estimated from the empirical silicate subtraction), respectively. The mass-opacity values at 11.2 μm are $\kappa_{\text{am}} = 3.5 \times 10^3 \text{ cm}^2 \text{ g}^{-1}$ and $\kappa_{\text{cr}} = 6.0 \times 10^3 \text{ cm}^2 \text{ g}^{-1}$. The crystalline to amorphous dust ratio is 1.2%, which is consistent with values in the majority of YSOs (e.g. Demyk et al. 1999; Wright et al. 2016; Do-Duy et al. 2020).

5.1.5. 15.2 μm

We analysed the 15.2 μm feature using the continuum subtraction method from the SED model. In this particular example, we have adopted the same ice components used previously by Pontoppidan et al. (2008) to fit the spectrum, namely, CDE corrected spectrum of pure CO₂ ice, CO₂:H₂O (0.14:1), CO₂:CO (1:1), CO₂:CO (0.21:1). In addition, to these data, we added CO₂:CH₃OH mixtures with five different proportions, 1:1, 1:3, 1:10, 10:1, 3:1. This spectral decomposition reveals that the double peak in this feature is mostly caused by the presence of pure CO₂ ice, which indicates ice segregation or distillation due to thermal processing (Dartois et al. 1999; Ehrenfreund et al. 1999). Pure CO₂ also has a prominent blue wing that contributes to the short-wavelength shoulder of the 15 μm band. The red wing of this band is dominated by CO₂ in a H₂O rich environment and CO₂:CH₃OH (1:1). Other two components due to CO₂ in a CO-rich ice and CO₂:CH₃OH (3:1) contribute to an increase in the optical depth at 15.2 μm. Overall, this fit illustrates that the majority of the 15.2 μm band is dominated by CO₂ in H₂O ice-rich environment, which is aligned with Pontoppidan et al. (2008). In addition, the mixture with CH₃OH ice agrees with recent results Brunken et al. (2024a) for ¹³CO₂ ice at 4.38 μm.

A statistical analysis was performed to decide on the minimum number of components providing the best fit, and what is the effect of adding more components to the fit. For this analysis, both χ^2 and AIC are calculated. This result is presented in Appendix H. It indicates that a number of five components are needed to have both low χ^2 and AIC, which are the components displayed in Figure 14.

5.2. Ice fits: Ced 110 IRS4B

A global fit covering the range between 2.5 and 5.0 μm of the NIRSpect data of Ced 110 IRS4B was performed using the ENIIGMA fitting tool. The MIRI/MRS data is not included in this fit because of the low S/N and flux overlap with the primary source at longer wavelengths. Figure 15 shows the best fit with 7 components, namely, H₂O:NH₃, H₂O:CO₂, CO:CO₂ (10 and 70 K), CO₂:CH₃OH, CO:CH₃OH, and pure CO. The top panel of Figure 15 shows the overall fit highlighting the major absorption features at 3, 4.27 and at 4.67 μm. The bottom panels show zoom-ins of the three strong absorption features, where there is an inset displaying the 4.38 μm band in the middle panel.

The 3 μm feature is dominated by H₂O ice (O–H stretch), which is mixed with CO₂ and NH₃. Ammonia has a natural vibrational mode at 2.9 μm (N–H stretch) and, when mixed with H₂O ice, a broad profile peaking at 3.5 μm called ammonia hydrate is activated (Dartois & d’Hendecourt 2001; Moore et al. 2007). A small contribution to the broad 3 μm feature also comes from CH₃OH mixed with CO. Another important aspect to highlight is the absorption excess in the red wing of the 3 μm band that has not been fitted with the ice components adopted in this work. The nature of this band is mostly associated with grain growth effects and larger chemical species.

The second major absorption feature in the Ced 110 IRS4 spectrum is the 4.27 μm band, which is associated with ¹²CO₂ ice. The fits indicate that this band is composed of CO₂:H₂O, and CO:CO₂ at two temperatures, 10 and 70 K. For the warm component, we found a range between 60 and 80 K that fit well the observations, as presented in Figure D.2. CO₂ ice is known to be a reliable temperature tracer of protostellar ices from analysis of the 4.38 μm (Boogert et al. 2000a; Brunken et al. 2024a) and 15 μm bands (Gerakines et al. 1999; Keane et al. 2001; Pontoppidan et al. 2008; Kim et al. 2012).

The ¹³CO₂ band at 4.38 μm is another important feature to highlight. All four CO₂ components used to fit the 4.27 μm band are also present here and agree with recent ¹³CO₂ ice results from Brunken et al. (2024a). Nevertheless, the absorption profile is not fully reproduced in the global fit. Mostly the peak at 4.38 μm and the long-wavelength side are not well fitted. In principle, increasing the contributions from CO₂:CH₃OH, H₂O:CO₂, and CO:CO₂ (low T) would improve the fit. However, this approach is not reasonable because the concurrent fit between 2.5 and 5 μm already takes into account contributions in other wavelengths. This is still an open question that requires further analysis with a larger number of sources and ideally considering both ¹²CO₂ and ¹³CO₂ bands.

The feature at 4.67 μm associated with the CO ice is the third major ice band in the NIRSpect data of Ced 110 IRS4. The fits indicate that three CO components are needed to interpret the shape of the CO band, namely, pure CO, CO:CO₂ and CO:CH₃OH, which is aligned with previous studies (Pontoppidan et al. 2003; Cuppen et al. 2011; McClure et al. 2023). Only the cold CO:CO₂ component contributes to the CO ice absorption since 60–80 K is beyond the CO ice desorption.

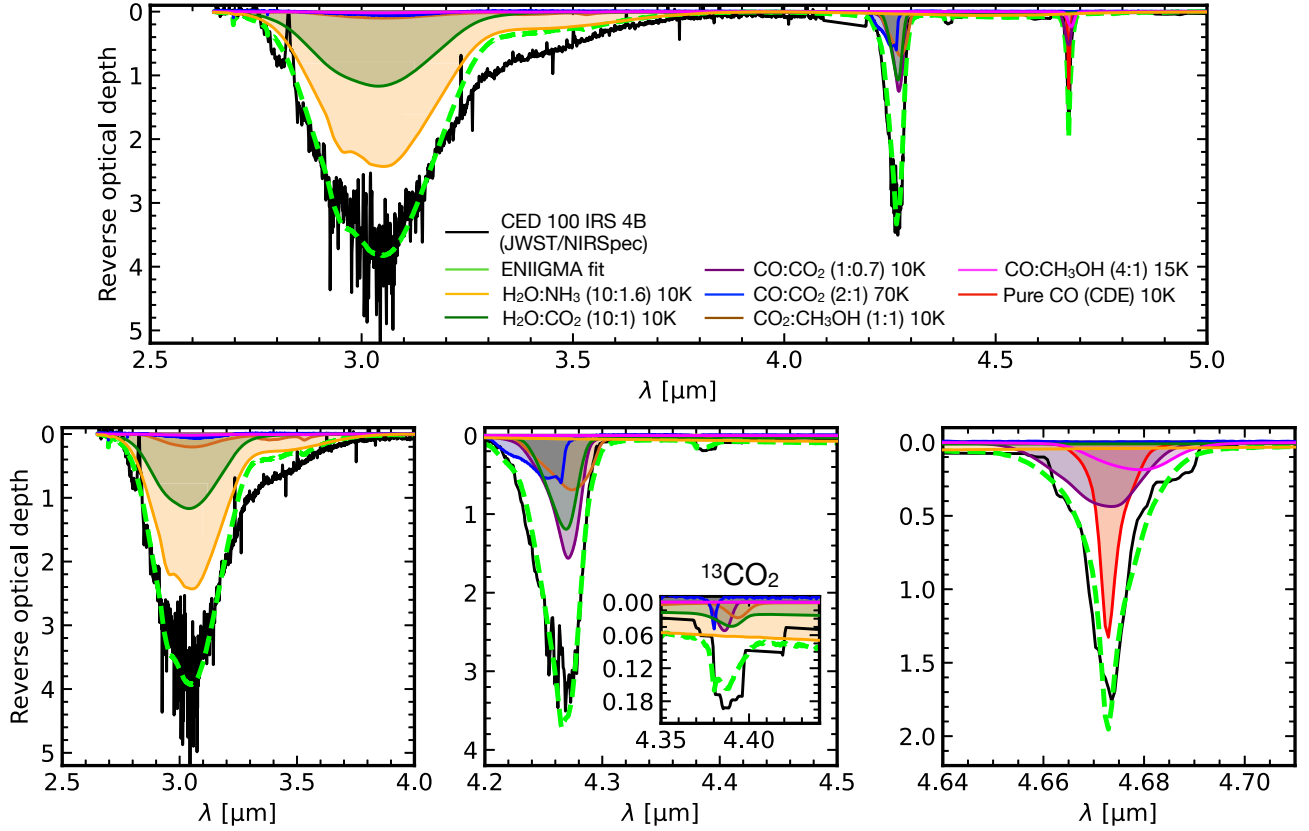


Fig 15 ENIIGMA fit (green) between 2.5 and 5 μm of the Ced 110 IRS4B spectrum (black). Top panel shows the global fit, and bottom panels displays details of specific regions, namely, H_2O , CO_2 , and CO.

The pure CO ice in this work is fitted using grain-shape correction assuming the CDE approach and grain size ranging from 0.1 to 1 μm . The lack of accurate optical constants for ice mixtures precludes the use of grain-shape correction for all species in the fit. Additionally, weaker bands are less affected by grain-shape correction (e.g. Tielens et al. 1991).

A consistency check of this fit was performed in the mid-IR spectral range as presented in Figure H.6 of Appendix H. The lower quality of the MIRI/MRS data precludes further analyses of this range. However, the components fitting the NIR range are consistent with the Mid-IR, and no overshooting of the absorption features is found. In fact, the H_2O ice libration band and the CO_2 bending mode at 12 and 15.2 μm , respectively, are relatively well fitted.

Other minor features, such as OCN^- (4.6 μm), ^{13}CO (4.78 μm) and OCS (4.9 μm) were not addressed in this paper. If present, these features are strongly blended with CO gas emission lines, which is required to be accurately removed prior to the ice analysis.

5.3. Ice column densities

The ice column densities of the chemical species identified towards Ced 110 IRS4A and IRS4B were calculated using Equation (4) and are presented in Table 3. The ice abundances with respect to H_2O ice are also calculated and compared with the literature values in LYSOs and comet 67P/Churyumov–Gerasimenko (67P/C-G).

The ice column densities of H_2O in Ced 110 IRS4A and $^{13}\text{CO}_2$ in Ced 110 IRS4B were calculated using simplified methods. In the former, the H_2O ice was calculated from the

$\text{H}_2\text{O}:\text{NH}_3$ ice mixture scaled to the NIRCам spectrum as shown in Figure 9. This approach was used because the libration band is affected by the silicate emission and are therefore excluded from the global fits. In the latter, the band area at 4.38 μm is used to derive the $^{13}\text{CO}_2$ ice column density because the ENIIGMA fits do not account for all the absorption in the NIRSspec data. Upper limits for NH_4^+ and H_2CO towards Ced 110 IRS4A were derived. In the former case, we used the sum of components C3 and C4 (Fig. 11), whereas in the latter, we adopted the band of the 5.8 μm band shown in Figure 12. Excluding these cases, all ice column densities were calculated directly from the ENIIGMA fitting tool and the error bars were derived from the confidence intervals presented in Appendix H. In the case of SO_2 , Ced 110 IRS4A has the same abundance of sulfur dioxide ice as NGC1333 IRAS 2A (Rocha et al. 2024b), despite the lower ice column density. The abundance of CO ice in Ced 110 IRS4B being close to the lower limit of what is found in LYSOs could point to a heating event where part of CO ice sublimates.

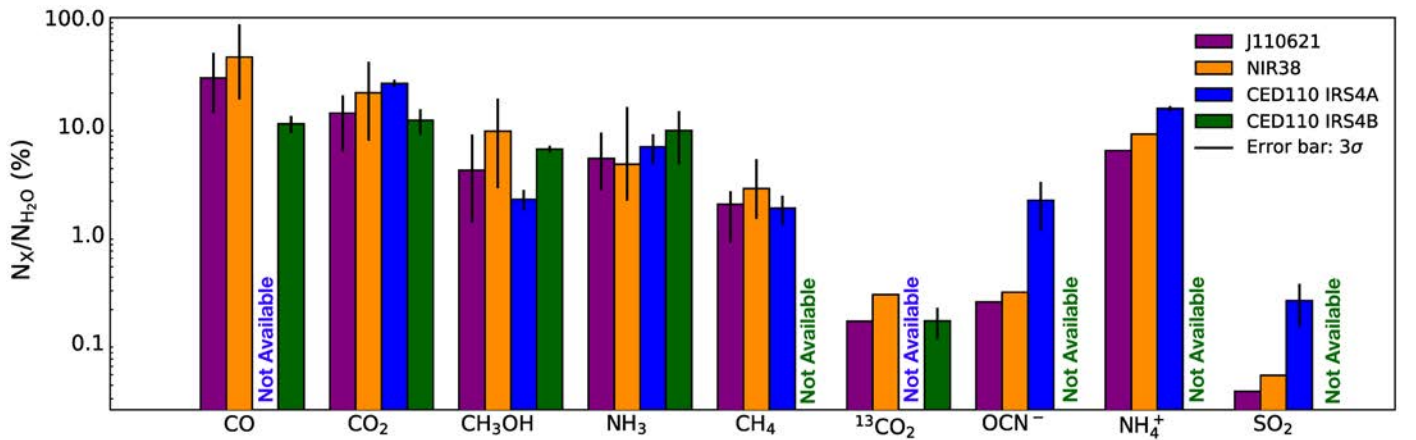
An important result from these values is the $^{12}\text{CO}_2/^{13}\text{CO}_2$ ratio, which is 71^{+88}_{-68} . This interval is similar to the values found for the two background stars presented in McClure et al. (2023), which range between 69 and 87. This ratio cannot be derived for IRS4A since the observations do not cover the 4.38 μm band. A recent work using JWST data by Brunken et al. (2024b) derived $^{12}\text{CO}_2/^{13}\text{CO}_2$ ratios of 85 ± 23 , 76 ± 12 , and 97 ± 17 when derived from the $^{12}\text{CO}_2$ ice bands at 2.7, 4.27 and 15.2 μm , which are consistent with the isotope ratio towards Ced 110 IRS4B.

Comparisons of the ice column densities and abundances between two protostars are not conclusive since different wavelengths were analysed for both sources. Nevertheless, it seems that the companion source hosts more ice material than

Table 3. Ice column densities and abundances with respect to H₂O ice towards Ced 110 IRS4A and IRS4B compared with literature values.

Species	N_{ice} (10^{17} cm ⁻²)		$X_{\text{H}_2\text{O}}$ (%)		Literature (% H ₂ O)			
	IRS4A ^(a)	IRS4B	IRS4A	IRS4B	LYSOs ^(b)	NIR38 ^(e)	J110621 ^(f)	Comet 67P/C-G ^(f)
H ₂ O	45.2±2.3	63.5 ^{69.3} _{48.1}	100	100	100	100	100	100
¹² CO ₂	11.1 ^{15.0} _{9.7}	7.1 ^{7.9} _{6.8}	24.5	11.2	28 ³⁷ ₂₃	20.1 ^{38.7} _{7.3}	13.0 ^{19.0} _{6.1}	4.7±1.4
¹³ CO ₂	...	0.1±0.01	...	0.2	...	0.3	0.3	...
¹² CO	...	6.6 ^{7.2} _{5.9}	...	10.4	21 ³⁵ ₁₂	43.1 ^{65.4} _{20.0}	27.5 ^{47.2} _{13.0}	3.1±0.9
CH ₄	0.78 ^{1.0} _{0.52} (0.80 ^{1.12} _{0.55})	...	1.7 (1.8)	...	4.5 ⁶ ₃	2.6 ^{4.8} _{1.4}	1.9 ^{2.4} _{0.9}	0.340±0.07
SO ₂	0.11 ^{0.17} _{0.06} (0.09 ^{0.15} _{0.07})	...	0.2 (0.2)	...	0.2 ^c	0.05	0.04	0.127±0.100
NH ₃	2.88 ^{3.86} _{1.90} (0.0)	5.7 ^{6.3} _{2.1}	6.4 (0.0)	8.9	6 ⁸ ₄	4.4 ^{10.6} _{2.1}	5.0 ^{8.6} _{2.5}	0.67±0.20
HCOOH	0.92 ^{1.28} _{0.56} (0.41 ^{0.61} _{0.22})	...	2.0 (0.9)	...	<0.5–4 ^(d) , 1.0 ^(c)	0.013±0.008
CH ₃ OH	0.94 ^{1.3} _{0.70} (0.89 ^{1.05} _{0.67})	3.85 ^{5.2} _{2.7}	2.1 (2.0)	6.1	6 ¹² ₅	8.9 ^{17.7} _{2.6}	3.9 ^{8.2} _{2.5}	0.21±0.06
OCN ⁻	0.92 ^{1.4} _{0.46} (0.63 ^{0.82} _{0.35})	...	2.0 (1.4)	...	0.6 ^{0.8} _{0.4} , 1.2 ^(c)	0.3	0.3	...
N ₂ O	0.81 ^{1.10} _{0.53} (0.85 ^{1.21} _{0.55})	...	1.8 (1.9)
Upper limits								
NH ₄ ⁺	<6.5	...	<14.3	...	11 ¹⁵ ₇	<6	<8	...
H ₂ CO	<3.4	...	<7.5	...	~6	0.32±0.1

Notes. This table shows literature values for LYSOs, the two field stars probing lines of sight towards Chameleón I (NIR38 and J110621), and the comet 67P/G-C. ^(a)Values inside parentheses are calculated based on the data after polynomial silicate subtraction. ^(b)When not indicated otherwise, the values correspond to the median and lower and upper quartile values from summarised by Boogert et al. (2015), ^(c)Rocha et al. (2024b); IRAS 2A, ^(d)Öberg et al. (2011), ^(e)McClure et al. (2023), ^(f)Rubin et al. (2019).


Fig. 16. Ice abundances relative to H₂O ice for the protostars Ced 110 IRS4A and Ced 110 IRS4B compared to the two lines of sight towards field stars behind the Chameleón I molecular cloud, NIR38 and J110621.

the primary source. The only exception is ¹²CO₂. Despite the saturation of the 4.27 μm band in the NIRSpec data of Ced 110 IRS4B, the error bars still indicate lower amount of CO₂ ice. In comparison with LYSO abundances, all values are within the ranges previously found in the literature. It is also worth mentioning that the ice column density values estimated from the data after empirical and polynomial continuum subtraction are different in the cases of NH₃, HCOOH, and OCN⁻, which are lower by a 100, 55, and 30%, respectively.

Finally, Figure 16 displays a bar plot with the ice abundances relative to H₂O ice compared to the molecular cloud values towards the background stars NIR38 and J110621. In the case of the minor species in IRS4A, we used abundances derived after SED empirical subtraction of the continuum and silicate. No significant difference in the ice abundance is observed for

the molecules addressed in this work. Only OCN⁻, NH₄⁺, and SO₂ seem to be enhanced in Ced 110 IRS4A compared to the molecular cloud. In fact, in the cases of these two ions, Boogert et al. (2015) suggested an enhancement in the median values from background stars to low-mass protostars.

6. Discussion

6.1. Thermal processing

Both Ced 110 sources show evidence of thermal processing characterised by the CO₂ ice band. In the case of IRS 4A, the bending mode of CO₂ ice at 15.2 μm shows that the double peak can be due to pure CO₂ ice that has stemmed from ice segregation in the case of H₂O:CO₂. Another possible explanation may be the ice

distillation of $\text{CO}_2:\text{CO}$, as well as CO_2 interacting with a complex molecule (e.g. Dartois et al. 1999). Distinguishing between the two scenarios is beyond the scope of this work. The fraction of pure CO_2 in the fits is 8.2%, which is consistent with the values found by Brunken et al. (2024a) for other protostars. The two $\text{CO}_2:\text{CH}_3\text{OH}$ data can also be used as thermal ice tracers. For example, the mixture with 3:1 proportion can indicate a colder region where a larger fraction of CO_2 is mixed with CH_3OH . On the other hand, the 1:1 mixture would be associated with a higher temperature where most CO_2 ice has sublimated.

In the case of IRS 4B, the evidence of thermal processing also comes from the CO_2 stretch mode at $4.27\text{ }\mu\text{m}$. In past works, a short-wavelength shoulder ($4.23\text{ }\mu\text{m}$) was also used as a tracer of ice thermal processing as can be noted in de Graauw et al. (1996) and Gerakines et al. (1999). This feature is present in IRS 4B, which is associated with $\text{H}_2\text{O}:\text{CO}_2$ (0.7:1) after CO distillation (see Section 3 and Appendix D). Performing a simultaneous fit of the two strong $^{12}\text{CO}_2$ bands $4.27\text{ }\mu\text{m}$ and $15.2\text{ }\mu\text{m}$ would be important to rule out degeneracies in the analysis and obtain an accurate conclusion on the CO_2 ice composition. Unfortunately, this is not possible for IRS4A and IRS4B since there is no data coverage for both sources in these ranges. This type of analysis was performed by Keane et al. (2001) who found that annealed CO_2 ice mixtures (e.g. $\text{H}_2\text{O}:\text{CO}_2:\text{CH}_3\text{OH}$) are needed to reproduce both the $4.27\text{ }\mu\text{m}$ and $15.2\text{ }\mu\text{m}$ in the spectrum of the source S 140:IRS1. The CO_2 bending mode in S 140:IRS1 is more pronounced than in Ced 110 IRS4A, which likely indicate a warmer environment (see Dartois et al. 1999). Our results are similar to the findings of Keane et al. (2001) regarding the need for a polar ice mixture to hold CO_2 ice when warming up, as well as the notion that the short-wavelength shoulder of the CO_2 stretching mode in the observations can be attributed to ice thermal processing.

In a recent paper, Brunken et al. (2024a) used JWST data to show that warmer sources present a prominent short-wavelength profile in the $^{13}\text{CO}_2$ ice band at $4.38\text{ }\mu\text{m}$, where the intensity is proportional to the level of thermal processing. A similar trend was previously found toward high-mass protostars (Boogert et al. 2000b). The $4.38\text{ }\mu\text{m}$ absorption profile is not covered in IRS 4A, while in IRS 4B, the presence of a blue profile is not fully clear. However, we note that this feature is convoluted with a forest of CO gas-phase lines, which can affect the shape of the $^{13}\text{CO}_2$ band in the secondary source of the Ced 110 system.

6.2. Chemical environment

This section is focused on discussing the chemical environment of the Ced 110 IRS4 system and how it compares with the Chameleon I molecular cloud.

6.2.1. Absence of the $7.2\text{ }\mu\text{m}$ and $7.4\text{ }\mu\text{m}$ bands in IRS4A

Unlike NIR38 and J110621, which display clear absorption features around $7.2\text{ }\mu\text{m}$ and $7.4\text{ }\mu\text{m}$ (see Fig. 3 in McClure et al. 2023) indicative of COMs, Ced 110 IRS4A exhibits no absorption in this range. The absence of these two features can have either a physical or a chemical origin, or both.

In Figure 17, we show a potential correlation between the H_2O ice column density towards different YSOs and the intensity of the $7.2\text{ }\mu\text{m}$ band. H_2O ice is simply used here as a tracer of material along the line of sight. Extinction parameters are not used to avoid complications arising from the total-to-selective extinction and the size distribution of grains that change the extinction law (e.g. Cardelli et al. 1989; Pontoppidan et al.

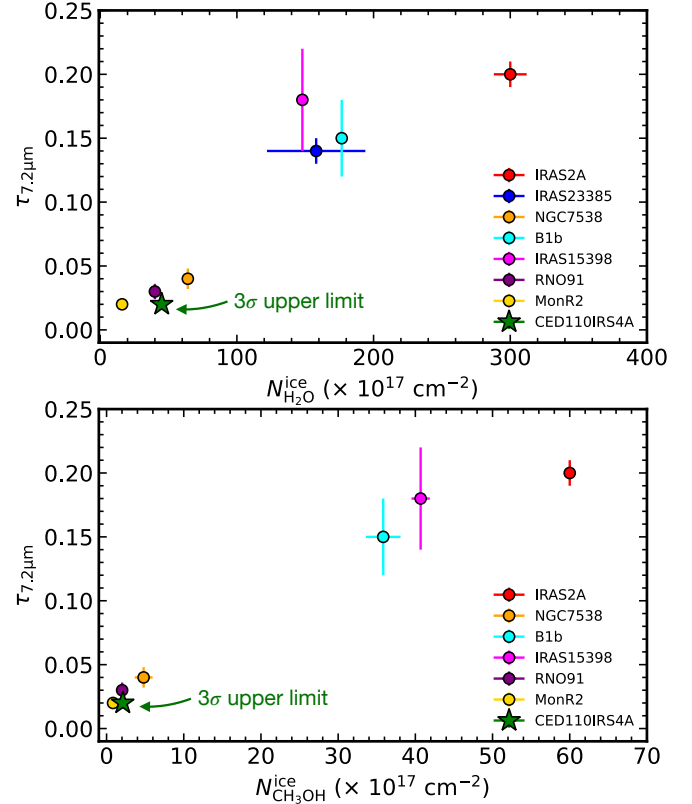


Fig. 17. Correlation between the H_2O and CH_3OH ice column densities and the intensity of the $7.2\text{ }\mu\text{m}$ band for different protostars. Ced 110 IRS4A is indicated by the green star and corresponds to a 3σ upper limit.

2024). It should be noted that higher peak intensities at $7.2\text{ }\mu\text{m}$ may be related to a high ice material along the line of sight, whereas shallow features are likely due to less material between the source and the observer. This correlation still holds for Ced 110 IRS4A if we consider a 3σ upper limit for the optical depth. This value is consistent with other sources observed with ISO and Spitzer (e.g. RNO91 and Mon R2 IRS3; Boogert et al. 2008) with similar H_2O ice column densities.

If the absence of the $7.2\text{ }\mu\text{m}$ band in Ced 110 IRS4A is entirely due to the low column density material along the line of sight, this implies that the source inclination plays an important role in tracing these bands. Consequently, the non-detection of these bands does not imply the absence of icy COMs and HCOO^- . On the other hand, a chemical argument can be invoked. For example, the ice mixtures $\text{NH}_3:\text{HCOOH}$ and $\text{H}_2\text{O}:\text{NH}_3:\text{HCOOH}$ are known to form HCOO^- , peaking at 7.2 and $7.4\text{ }\mu\text{m}$, whereas other mixtures do not lead to this same chemical product (e.g. $\text{HNCO}:\text{NH}_3$; Novozamsky et al. 2001). This would imply that no reaction between NH_3 and HCOOH occurred in this source. A third possibility is that strong gas-phase emission lines hide the ice's absorption profiles. For instance, van Gelder et al. (2024) showed that SO_2 gas-phase emission can also affect the shape of the $7.4\text{ }\mu\text{m}$ feature due to the P-branch emission profile. However, no SO_2 gas is seen towards Ced 110 IRS4A (see van Gelder et al. 2024).

Finally, it is important to highlight the non-detection of gas-phase COMs in this source, including CH_3OH gas (van Gelder 2022). According to Nazari et al. (2022), the absence of CH_3OH gas emission does not imply the lack of these molecules in the source. In fact, the presence of a disk with relatively large grains

reduces the CH_3OH emission by more than an order of magnitude (see also [Nazari et al. 2024b](#)). From this perspective, the absence of 7.2 and 7.4 μm bands is more likely to result from the physical evolution and geometry of the source than the chemical evolution of the ices.

6.2.2. CH_4 , SO_2 , OCN^- , and NH_4^+

In a H_2O ice mixture, CH_4 is found to fit the 7.67 μm towards Ced 110 IRS4A well. This is aligned with other recent analyses of spectrally resolved JWST data ([Rocha et al. 2024b](#); [Chen et al. 2024](#)) as well as the formation mechanism of these two species via hydrogenation ([Tielens et al. 1991](#); [Öberg et al. 2011](#)). SO_2 ice has been proposed to contribute to the short-wavelength side of the 7.67 μm band ([Öberg et al. 2008](#)) and it was confirmed statistically in IRAS2A ([Rocha et al. 2024b](#)), as well as for Ced 110 IRS4A (see Figure H.2 of Appendix H). Despite the fact that SO_2 mixed with CH_3OH produces the best fit, it is important to note that no other SO_2 ice data is currently available. [Boogert et al. \(2022\)](#) found a good correlation between OCS and CH_3OH ices, which is likely related to a common formation pathway from the CO ice. Concluding whether SO_2 can be mixed with CH_3OH and if this mixture is the best carrier of the short-wavelength wing of the 7.67 μm requires more study with a comprehensive list of SO_2 -containing ice mixtures.

Finally, OCN^- was also proposed by [Rocha et al. \(2024b\)](#) as one of the carriers of the short-wavelength wing of the 7.67 μm . In the case of [Rocha et al. \(2024b\)](#), the presence of OCN^- in IRAS2A was confirmed by the band at 4.6 μm (CN stretch), also due to this negative ion. Unfortunately, there is no data in this range for Ced 110 IRS4A. However, this band has been ubiquitously identified in YSOs and is likely to be present in this source. OCN^- can be formed via acid-base reactions or ice irradiation (e.g. [Schutte & Khanna 2003](#)). As discussed by [van Broekhuizen et al. \(2005\)](#), an OCN^- abundance of $\sim 1\%$ is observed for a large number of YSOs. This is consistent OCN^- abundances formed in irradiated ices ($\sim 1.5\%$) with a NH_3 ice abundance of around 5% with respect to H_2O ice. These values are aligned with what is found in this work. A better estimation of OCN^- ice in IRS4A will highly benefit of observations at 4.6 μm . In the case of NH_4^+ , it is known to be the carrier of the band at 6.85 μm since CH_3OH cannot account for the entire absorption ([Bottinelli et al. 2010](#)). Similarly to OCN^- , this ion can be formed via acid-base reactions or ice irradiation (e.g. [Schutte & Khanna 2003](#); [Pilling et al. 2010](#)).

A direct comparison between the MIRI data of Ced 110 IRS4A and NIR38 and J110621 is hampered because of the spectral resolution in both cases. However, it is possible to conclude that CH_4 share similar chemical conditions in both cases, whereas SO_2 and OCN^- would benefit from a higher spectral resolution towards NIR38 and J110621 data to obtain secure conclusions.

6.2.3. HCOOH

The best fits of Ced 110 IRS4A indicate that HCOOH may exist in two different chemical environments with different polarity levels, namely, $\text{HCOOH}:\text{CO}_2:\text{H}_2\text{O}$ and $\text{HCOOH}:\text{CH}_3\text{OH}:\text{H}_2\text{O}$, where the former is more prominent. Laboratory experiments from [Qasim et al. \(2019\)](#) showed that $\text{HCOOH}:\text{CO}_2$ can be formed in both H_2O -rich or CO-rich environments via $\text{H} + \text{HOCO}$. In the CO-rich case, H_2CO may also be formed, which is a precursor of CH_3OH . In the H_2O -rich case, HCOOH and CO_2 are the main products (adsorption of atomic carbon as source of

C), with the latter being the most abundant. In that case, it is possible that the Ced 110 IRS4A environment where HCOOH is found is dominated by H_2O instead of CO ice. It is worth noting that the amount of HCOOH used to fit the 8.2 μm feature does not overpredict the C=O stretch at 5.8 μm (see Figure H.5 of Appendix H).

No detailed spectral fits were made for NIR38 and J110621 in the range of 8 μm because the MIRI/LRS data suffered from wavelength calibration issues. For this reason, no HCOOH assignment was made for this dataset. Future analysis of the data with correct and improved wavelength calibration will help to address the presence of HCOOH in the molecular cloud.

6.2.4. CH_3OH and NH_3

CH_3OH ice is detected in both sources. Based on the MIRI data of Ced 110 IRS4A, CH_3OH probes environments with CO, CO_2 and likely H_2O ices, where the latter is continuum dependent. All these three conditions are supported via laboratory experiments (e.g. [Fuchs et al. 2009](#); [Qasim et al. 2018](#)). In the case of IRS4B, CH_3OH is found mixed with CO_2 and CO, which is consistent with IRS4A. The non-detection of CH_3OH mixed with H_2O is due to the lack of quality data at 9.8 μm . In the case of NH_3 , the best fits suggest a mixture between NH_3 and H_2O , which is aligned with the formation pathways of these two species. The other component, $\text{NH}_3:\text{CO}_2$ is discussed in Section 6.2.5.

The chemical environments where CH_3OH and NH_3 were found are consistent with what is found for NIR38 and J110621. This strongly suggests that the chemical environment of CH_3OH ice is established prior to the protostellar stage in the molecular cloud.

6.2.5. Other small features

Here, we briefly discuss other species that are needed to achieve the best fit. However, confirming the presence of these particular components in ices will require further systematic studies in a large sample of sources.

$\text{NH}_3:\text{CO}_2$ ice: this ice mixture fits the absorption excess at 9.4 μm . Such excess was also observed towards NIR38 and J110621 after subtracting the silicate and is not fitted with $\text{NH}_3:\text{H}_2\text{O}$, $\text{CH}_3\text{OH}:\text{CO}$, or $\text{CH}_3\text{OH}:\text{H}_2\text{O}$. The ice mixture $\text{NH}_3:\text{CO}_2$ is plausible to be formed in ices as demonstrated in the laboratory (e.g. [Bossa et al. 2008](#); [James et al. 2021](#)). However, the presence of this component is highly dependent of the silicate subtraction method. In fact, [Bottinelli et al. \(2010\)](#) noted that the choice of the continuum can affect the shape of the NH_3 ice band. To provide a sense of variability of the NH_3 band at 9 μm , Figure 18 compares the observed spectrum with other NH_3 -containing ices. From the fitting perspective, pure NH_3 and $\text{NH}_3:\text{CO}$ also have the ammonia umbrella mode around 9.4 μm , but their profiles are sharper than in the case of $\text{NH}_3:\text{CO}_2$. A final conclusion on the presence of $\text{NH}_3:\text{CO}_2$ in the ice requires an accurate silicate subtraction, which is not trivial and depends on the dust composition of the source.

N_2O ice: assignments for nitrogen oxides (N_xO_y) around 7.7 μm , including N_2O , NO_2 , and NO were proposed in [Grim et al. \(1989\)](#), and many laboratory experiments have confirmed their formation in interstellar ice analogues (e.g. [Congiu et al. 2012](#); [Fedoseev et al. 2012, 2016](#)). Nevertheless, the secure detection of these features in ices remains elusive despite recent tentative detection by [Nazari et al. \(2024a\)](#) based on JWST/NIRSpec data of protostars. N_2O is often not included in major chemical models. For example, [Agúndez & Wakelam \(2013\)](#) addressed the

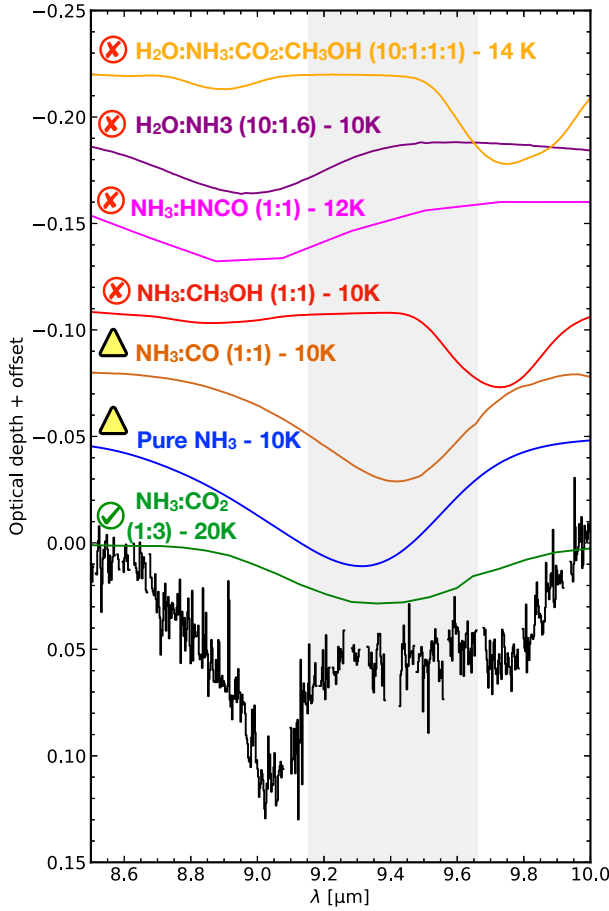


Fig 18 NH_3 umbrella mode in different ice mixtures compared with the MIRI spectrum of Ced 110 IRS4A. The best fit of the grey shaded area is indicated with the green check mark and other possible solutions with the yellow triangle. Excluded solutions are given by the red cross.

gas-phase formation of NO and NO_2 , but not N_2O . However, N_2O ice is suggested as a candidate to explain the gas-phase abundance of NO likely originated from ice sublimation in the dust trap of the planet-forming disk Oph-IRS 48 (Leemker et al. 2023).

In Figure 19a, we compare different laboratory spectra with the MIRI/MRS data of Ced 110 IRS4A between 7.4 and 8.2 μm . The N_2O IR features are affected by energetic processing and the chemical environment. For example, Bergantini et al. (2022) showed that the spectral profile of the 7.7 μm band changes upon bombardment with heavy ions ($^{136}\text{Xe}^{23+}$) of 90 MeV. While the peak position does not change with the irradiation, a prominent red wing arises associated with other nitrogen oxides, which is compatible with the spectral profile seen in Ced 110 IRS4A. A small feature at 7.67 μm from N_2O_4 is also formed. Further chemical studies are needed to clarify whether N_2O ice can exist in pure form or not. For example, segregation studies could elucidate whether N_2O behaves as other molecules that segregate and form small clusters at higher temperatures as is the case of $\text{H}_2\text{O}:\text{CO}_2$ (Ehrenfreund et al. 1997). Another example of how the N_2O band changes with the chemical environment is seen in the IR spectra of pure N_2O ice (Hudson et al. 2017), and the mixtures with H_2O (Bergantini et al. 2022) and CO_2 (Pereira et al. 2018). Both pure N_2O and $\text{N}_2\text{O}:\text{H}_2\text{O}$ ices have a peak at 7.8 μm , but the band of the pure ice is broader. In the case of $\text{N}_2\text{O}:\text{CO}_2$, the band has a peak at 7.72 μm . Other two laboratory spectra are

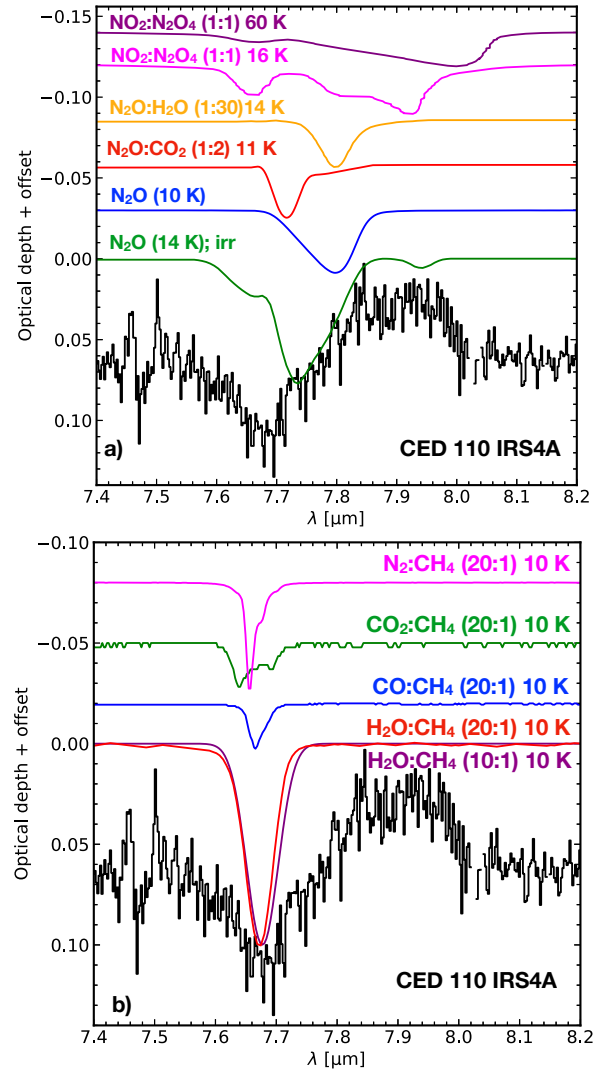


Fig. 19. N_2O IR ice spectra from different experiments compared with the optical depth spectrum of Ced 110 IRS4A between 7.4 and 8.2 μm . The panel a displays IR features of nitrogen oxides ice data, whereas the panel b shows the CH_4 ice band mixed with other molecules.

compared to the observational data, $\text{NO}_2:\text{N}_2\text{O}_4$ at 16 and 60 K from Fulvio et al. (2009) and Fulvio et al. (2019), but no good match with the observation is found. In Figure 19b, we show that only CH_4 ice in different mixtures cannot explain the blue and red wings of the 7.67 μm .

Unidentified feature at 9 μm – A narrow band is seen at 9.04 μm in the spectrum of Ced 110 IRS4A. It is unclear if this feature is a consequence of the atypical silicate profile or it is indeed associated with an additional species. In fact, no laboratory data in our list of IR spectra matched this band. Other solid-phase species can be an alternative, such as SiO_2 and nano-sized silicate dust that peaks at the exact same position and has a narrow profile (Guiu et al. 2021). However, the corresponding long wavelength band counterparts are not seen in the MIRI/MRS data. Another candidate for this feature is ammonium sulfate $(\text{NH}_4)_2\text{SO}_4$ (Garland et al. 2005), which shows a narrow strong band at 8.96 μm . The caveat related to this species comes from the condensation models from Janssen et al. (2023), which suggest that although a fraction of sulfur condense to solids, a higher amount remains in the gas phase.

6.3. Ced 110 IRS4 sources and other protostars observed with JWST

The overall ice inventory with secure detections observed towards Ced IRS4A and IRS4B is similar to other protostars observed with JWST presented in Brunken et al. (2024a,b), Tyagi et al. (2024), and Slavicinska et al. (2025). The first major difference compared to other protostellar environments is the absence of both the 7.2 and 7.4 μm bands. These two features are identified towards the hot core and hot corinos, IRAS 2A and IRAS 23385 (Rocha et al. 2024b), observed with JWST and many other sources with other telescopes. However, a better comparison should be done with other protostars with a similar age of Ced 110 IRS4 sources. Second, Ced 110 IRS4A shows an atypical silicate profile that has not yet been seen in the sources observed with JWST. Finally, Ced 110 IRS4A show a likely CH_3^+ emission around 7.18 μm . So far, CH_3^+ was only detected towards mature protoplanetary disks, such as d203-506 (Berné et al. 2023) and TW Hya (Henning et al. 2024). Other differences are motivated by the lack of data or difficulties in the spectral analysis. For example, HDO ice that is detected towards the protostars HOPS 370 and IRAS 20126+4104 (Slavicinska et al. 2024) cannot be investigated in the case of IRS4B due to the NIRSpec spectral gap at 4 μm , whereas for IRS4A no observational data is available. Regarding the presence of complex cyanides (Nazari et al. 2024a), the spectral region around 4.4 μm is strongly blended with CO gas emission lines. A more detailed line removal is required before the ice analysis of that band.

7. Conclusions

In this paper, we present the first analysis of the JWST data targeting the binary system Ced 110 IRS4A and IRS4B. ENIIGMA fits were performed on the NIRSpec data of IRS4B and MIRI of IRS4A because of the high quality of the data. Other spectral ranges were mostly used for consistency assessments. Below we summarize the main conclusions found in this work:

- Overall, the Ced 110 IRS4A and IRS4B show the same ice mixtures regarding major species and CH_3OH , as observed in the Chameleon I molecular cloud towards the background stars NIR38 and J110621. This includes similar ice abundances and suggests that the chemical composition of protostars is set at earlier stages.
- The first major difference between the protostars and the Chameleon I molecular cloud is the absence of the 7.2 and 7.4 μm features in the protostar. This is not conclusive evidence for the lack of COMs or HCOO^- . Instead, it can be related to the low ice column density due to the source inclination. This is supported by the relation between the intensity of the 7.2 μm band and the H_2O ice column density.
- The second major difference between the protostars and the Chameleon I molecular cloud is the evidence of thermal processing in the protostar. In the primary source, evidence is traced by the 15.2 μm band profile of CO_2 ice, which indicates distillation or segregation. In the companion source, the CO_2 ice stretch mode at 4.27 μm shows that a warm (~ 60 – 80 K) ice component ($\text{H}_2\text{O}:\text{CO}_2$ after CO distillation) is needed to provide a good fit to the data. In both cases, CO_2 ices are tracing the superimposition of cold (~ 10 K) and warm (~ 60 – 80 K) regions, which is consistent with a temperature gradient along the line of sight to the protostars.
- The $^{12}\text{CO}_2/^{13}\text{CO}_2$ ratio for the companion source ranges between 68 and 88. This is similar to the result found for

the two background stars in the same host cloud presented in McClure et al. (2023).

- Tentative ice detections of N_2O and $\text{NH}_3:\text{CO}_2$ towards Ced 110 IRS4A were presented. Both cases would contribute to enhancing the N budget observed in protostars. Finally, a narrow unidentified feature at 9 μm is shown, which does not match with the IR ice spectrum considered in this work.

The binary system Ced 110 IRS4A and IRS4B has proven to be a challenging protostellar system. Further studies require a sophisticated radiative transfer model to help in the interpretation of this object. In particular, a precise fit of the atypical silicate profile will be highly beneficial to understanding the dust and ice evolution in these sources. Additionally, further studies of a large sample of sources would be required to investigate common ice mixtures towards different types of objects, aimed at unveiling the intricate chemical nature of the ices.

Data availability

Appendices G and H can be found on Zenodo (<https://doi.org/10.5281/zenodo.14281751>).

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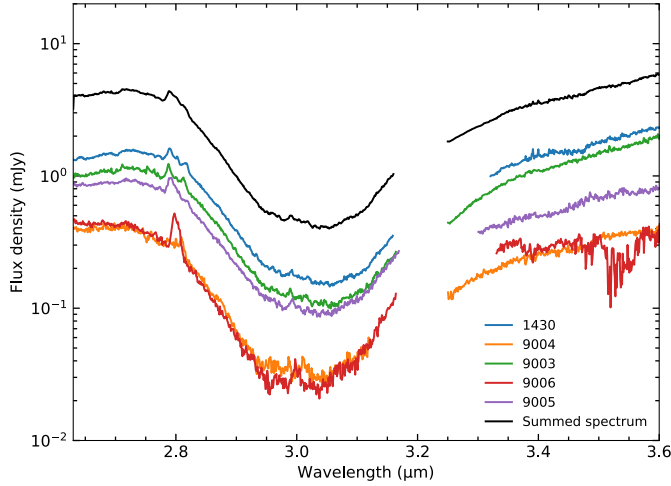


Fig. A.1. Extracted spectrum using the PSF method of different regions around Ced 110 IRS4A as indicated in Figure 2. Individual spectra are shown in colour and the sum of these individual data is presented in black. While the emission line at 2.8 μm is due to $\text{H}_2\text{O}(3)$ line, the strong absorption features at 3.55 μm in the region 9006 (red) is due to extraction artifact.

Appendix A: NIRCcam spectrum

The protostars Ced 110 IRS4A and IRS4B were observed using the NIRCcam Wide Field Slitless Spectroscopy. Spectral extraction was performed at different positions of the two sources as indicated in Figure 2. The individual and summed spectra are shown in Figure A.1. The spectral gaps are due to the physical separation between detectors in the field of view. The summed NIRCcam spectrum is added together with the MIRI spectrum, and the combined data is used in the ice analysis demonstrated in this paper.

Appendix B: Comparison between MIRI/MRS and Spitzer/IRS

The primary source, Ced 110 IRS4A was observed with *Spitzer* in 2005, as part of the program “Spectroscopy of protostellar, protoplanetary and debris disks” (P.I. J. R. Houck). This spectrum was originally published by Manoj et al. (2011), where the data reduction steps are detailed. The spectral data was downloaded from the Spitzer Heritage Archive catalogue⁴ based on the astronomical observation request (AOR) 12692224. A comparison between the *Spitzer*/InfraRed Spectrometer (IRS) and the MIRI spectrum is shown in Figure B.1. When roughly spectrally resolved, both data show similar absorption features. The *Spitzer* spectrum has an enhanced flux longwards of 10 μm due to the larger slit width compared to MIRI (e.g. *Spitzer* 14–36 μm : 10.2"; MIRI/MRS: 4"). The spectral range between 6.5 and 10 μm is fully resolved in the MIRI range, which allowed the analysis performed in Section 5.1.2. In addition, a clear feature at 6.8 μm is visible in the MIRI/MRS spectrum, as well as multiple emission lines which are not labelled in this paper.

Appendix C: List of laboratory data

A comprehensive list of molecules was used in this paper to search for the best fit of the region between 6.8 and 10 μm for

⁴ <https://irsa.ipac.caltech.edu/data/SPITZER/docs/spitzerdataarchives/>

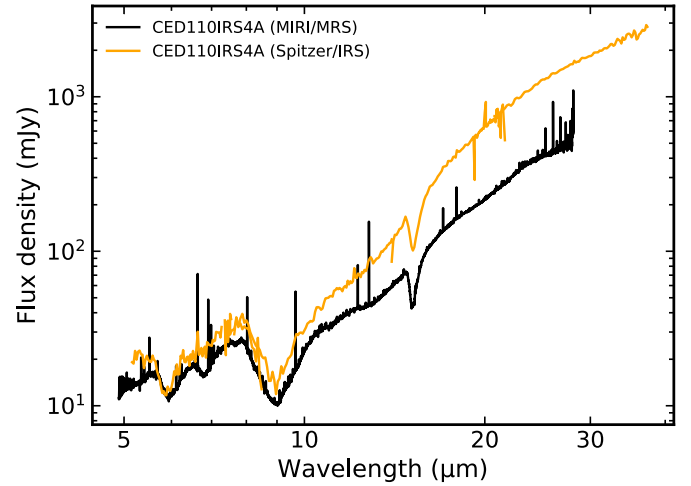


Fig. B.1. Comparison between the MIRI/MRS and *Spitzer*/IRS spectrum of Ced 110 IRS4A. The nominal spectral resolving power of both data at 7 μm are ~ 3000 and 600, respectively.

Ced 110 IRS4A and between 2.5–5.0 μm for Ced 110IRS4B. This list includes COMs in different mixtures as well as simple molecules. The full list is shown in Table C.1.

Table C.1. Laboratory data tested in the global fit performed with ENIIGMA.

Label	Temperature (K)	Resolution (cm ⁻¹)	Database ^a	Reference
Simple molecules (less than 6 atoms) and hydrocarbons				
H ₂ O	15–160	2.0	LIDA	[1]
CH ₄	10–30	1.0	OCdb	[2]
CO	10	1.0	LIDA	[3]
HCOOH	15–165	1.0	LIDA	[4]
NH ₃ :CO ₂ (3:1)	20	1.0	...	[5]
H ₂ O:CO ₂ (10:1)	10	1.0	LIDA	[6]
H ₂ O:CO ₂ (1:10)	10	1.0	LIDA	[6]
H ₂ O:CO ₂ (1:6)	10	1.0	LIDA	[6]
H ₂ O:CO ₂ (1:1)	10	1.0	LIDA	[6]
H ₂ O:CO ₂ :CH ₄ (10:1:1)	10	2.0	UNIVAP	[7]
H ₂ O:CO (1:0.14)	10	1.0	LIDA	[3]
SO ₂ :CH ₃ OH (1:1)	15	1.0	LIDA	[8]
H ₂ O:CH ₄ (10:1)	15	1.0	UNIVAP	[7]
H ₂ O:NH ₃ (10:1.6)	10	2.0	LIDA	[9]
CO:CO ₂ (2:1)	40–80	0.5	LIDA	[10]
CO:CO ₂ (1:0.7)	10	0.5	LIDA	[10]
CO ₂ :CH ₃ OH (1:1)	10	1.0	LIDA	[6]
CO ₂ :CH ₃ OH (3:1)	10	1.0	LIDA	[6]
CO ₂ :CH ₃ OH (1:3)	10	1.0	LIDA	[6]
C ₂ H ₂	15	1.0	NASA	[11]
C ₂ H ₄	15	1.0	NASA	[12]
C ₂ H ₆	15	1.0	NASA	[12]
HCOOH:H ₂ O:CO ₂ (0.1:1.0:0.4)	15	1.0	LIDA	[4]
N ₂ O (irr.)	14	1.0	...	[13]
N ₂ O	10	1.0	...	[13]
N ₂ O:H ₂ O (1:30)	14	1.0	...	[13]
NO ₂ :N ₂ O ₄ (1:1)	16	1.0	...	[14]
NO ₂ :N ₂ O ₄ (1:1)	60	1.0	...	[14]
Ions ^c				
OCN ⁻ : HNCO:NH ₃ (1:1)	15	1.0	LIDA	[15]
HCOO ⁻ : H ₂ O:NH ₃ :HCOOH (100:2.6:2)	14–210	1.0	LIDA	[16]
HCOO ⁻ : NH ₃ :HCOOH (1.3:1)	14–210	1.0	LIDA	[16]
COMs (more than 6 atoms)				
CH ₃ OH	10–120	1.0	OCdb	[2]
CH ₃ CHO	15–120	1.0	LIDA	[17]
CH ₃ CN	15–150	1.0	LIDA	[18]
CH ₃ OCH ₃	15–100	1.0	LIDA	[17]
CH ₃ COCH ₃	15–100	1.0	LIDA	[19]
CH ₃ CH ₂ OH	15–150	1.0	LIDA	[17]
CH ₃ OCHO	15–120	1.0	LIDA	[20]
CH ₃ COOH	10	1.0	NASA	[21]
CH ₃ NH ₂	10	1.0	LIDA	[22]
CH ₃ CH ₂ CH ₂ OH	13	1.0	NASA	[23]
HC(O)CH ₂ CH ₃	10	1.0	NASA	[24]
CH ₃ CH ₂ OH:H ₂ O (1:20)	15–160	1.0	LIDA	[17]
CH ₃ CH ₂ OH:CO (1:20)	15, 30	1.0	LIDA	[17]
CH ₃ CH ₂ OH:CH ₃ OH (1:20)	15–150	1.0	LIDA	[17]

Table C.1. Continued.

Label	Temperature ^(a) (K)	Resolution (cm ⁻¹)	Database ^(b)	Reference
CH ₃ CH ₂ OH:CO:CH ₃ OH (1:20:20)	15–150	1.0	LIDA	[17]
CH ₃ CHO:H ₂ O (1:20)	15–120	1.0	LIDA	[17]
CH ₃ CHO:CO (1:20)	15, 30	1.0	LIDA	[17]
CH ₃ CHO:CH ₃ OH (1:20)	15–140	1.0	LIDA	[17]
CH ₃ CHO:CO:CH ₃ OH (1:20:20)	15–120	1.0	LIDA	[17]
CH ₃ OCH ₃ :H ₂ O (1:20)	15–160	1.0	LIDA	[17]
CH ₃ OCH ₃ :CO (1:20)	15, 30	1.0	LIDA	[17]
CH ₃ OCH ₃ :CH ₃ OH (1:20)	15–120	1.0	LIDA	[17]
CH ₃ OCH ₃ :CO:CH ₃ OH (1:20:20)	15–100	1.0	LIDA	[17]
CH ₃ COCH ₃ :H ₂ O (1:20)	15–160	1.0	LIDA	[19]
CH ₃ COCH ₃ :CO (1:20)	15, 30	1.0	LIDA	[19]
CH ₃ COCH ₃ :CO ₂ (1:20)	15–100	1.0	LIDA	[19]
CH ₃ COCH ₃ :CH ₃ OH (1:20)	15–140	1.0	LIDA	[19]
CH ₃ COCH ₃ :H ₂ O:CO ₂ (1:2.5:2.5)	15–160	1.0	LIDA	[19]
CH ₃ COCH ₃ :CO:CH ₃ OH (1:2.5:2.5)	15–140	1.0	LIDA	[19]
CH ₃ OCHO:H ₂ O (1:20)	15–120	1.0	LIDA	[20]
CH ₃ OCHO:CO (1:20)	15–120	1.0	LIDA	[20]
CH ₃ OCHO:H ₂ CO (1:20)	15–120	1.0	LIDA	[20]
CH ₃ OCHO:CO:H ₂ CO:CH ₃ OH (1:20:20:20)	15–120	1.0	LIDA	[20]
CH ₃ COOH:H ₂ O (1:20)	10	1.0	NASA	[21]
CH ₃ NH ₂ :H ₂ O (1:20)	15–150	1.0	LIDA	[22]
CH ₃ NH ₂ :NH ₃ (1:20)	15–150	1.0	LIDA	[22]
CH ₃ NH ₂ :CH ₄ (1:20)	15–150	1.0	LIDA	[22]
CH ₃ CN:H ₂ O (1:20)	15–150	1.0	LIDA	[22]
CH ₃ CN:CO (1:20)	15–100	1.0	LIDA	[18]
NH ₂ CHO:H ₂ O (7:100)	15–160	1.0	LIDA	[25]
NH ₂ CHO:CO (4:100)	15–34	1.0	LIDA	[25]
HCOCH ₂ OH:H ₂ O (1:18)	10	1.0	NASA	[26]
CH ₃ OH:CO (1:4)	15	1.0	LIDA	[27]
CH ₃ OH:NH ₃ (1:1)	15	1.0	UNIVAP	[28]
CH ₃ OH:H ₂ O (10:0.8)	10	1.0	...	[29]
HCOOH:H ₂ O:CH ₃ OH (0.1:1.0:0.4)	15	1.0	LIDA	[14]

Notes. [1] Öberg et al. (2007); [2] Hudgins et al. (1993); [3] Ehrenfreund et al. (1997); [4] Bisschop et al. (2007); [5] James et al. (2021); [6] Ehrenfreund et al. (1999); [7] Rocha et al. (2017); [8] Boogert et al. (1997); [9] http://strw.leidenuniv.nl/~schutte/database/H2O_NH3_20_10K; [10] Schutte (1999); [11] Hudson et al. (2014a); [12] Hudson et al. (2014b); [13] Bergantini et al. (2022); [14] Fulvio et al. (2009); [15] Novozamsky et al. (2001); [16] Gálvez et al. (2010); [17] Terwisscha van Scheltinga et al. (2018); [18] Rachid et al. (2022); [19] Rachid et al. (2020); [20] Terwisscha van Scheltinga et al. (2021); [21] No reference found - taken from the NASA Ice Database (Pure: <https://science.gsfc.nasa.gov/691/cosmicice/spectra/refspect/Acids/CH3COOH/ACETIC-w.txt>, Mixture: https://science.gsfc.nasa.gov/691/cosmicice/spectra/8_compounds/Combined_spectra_2018-12-20.xlsx); [22] Rachid et al. (2021); [23] Hudson & Gerakines (2019); [24] Yarnall et al. (2020); [25] Slavicinska et al. (2023); [26] Hudson et al. (2005); [27] Cuppen et al. (2011); [28] Rocha et al. (2020); [29] Dawes et al. (2016).^a Each spectral data was recorded for the temperature indicated in this table. ^bLIDA: The Leiden Ice Database for Astrochemistry (<https://icedb.strw.leidenuniv.nl/>); OCdb: The Optical Constant Database (<https://ocdb.smce.nasa.gov/>); UNIVAP: <https://www1.univap.br/gaa/nkabs-database/data.htm>; NASA Cosmic Ice Laboratory: <https://science.gsfc.nasa.gov/691/cosmicice/spectra.html>. ^c Only in the case of the ions, the ratios of the mixtures correspond to the deposition values. The ratios of the products are not available.

Appendix D: CO:CO₂ and H₂O:CO₂ ice mixtures

Section 5.2 shows that CO:CO₂ at 70 K, combined with other ice mixtures, fits well the CO₂ ice band at 4.27 μm for Ced 110 IRS4B. In Figure D.1 we show a brief comparison of this IR spectrum with other laboratory data with similar conditions. Left, middle and right panels highlight the specific absorption features of H₂O, CO₂ and CO ice, respectively. At 70 K, CO is no longer in the ice as indicated in the right panel. Nevertheless, the CO₂ band of this CO:CO₂ mixture shows a prominent enhancement at the blue wing of the CO₂ ice feature, which can be due to ice distillation due to the CO sublimation. We highlight, however, that this data have H₂O ice contamination, as presented in the left panel, which corresponds to 70% of the CO₂ ice column density. By visual inspection of the spectra, we did not find evidence of contamination from other species.

To check whether the presence of H₂O in the ice can induce the blue wing excess of the CO₂ band in the CO:CO₂ data, we compare this profile with that of H₂O:CO₂ (1:1) at 70 K. Middle panel shows no enhancement of the CO₂ blue wing profile in that case. In this case, it is possible to conclude that the ice distillation can affect the CO₂ IR feature, and therefore it is a tracer of thermal evolution of the ice.

In Figure D.2 we replace the CO:CO₂ IR spectra at 70 K (best fit) by other spectra of the same ice mixture at 50, 60 and 80 K to have a sense of the variability of the fit. No calculation was performed using data recorded at 90 K because the ¹²CO₂ ice feature is no longer visible in the laboratory IR spectrum. As presented in the right panels, the fits of the ¹²CO₂ ice band changes according to the temperature of the CO:CO₂ ice spectra. The blue shoulder of ¹²CO₂ is prominent at 60 and 80 K, but not at 50 K. This causes the fit of ¹²CO₂ at 50 K to be dominated by the H₂O:CO₂ ice component, which is not enough to explain the blue shoulder profile in the data of Ced 110 IRS4B. Better fits are obtained in the cases data from CO:CO₂ at 60 and 80 K. The fitness score of both fits compared to the best fit is 15 and 8%, respectively. Given the saturation of the ¹²CO₂ ice band, these differences are not significant. Therefore, the solutions with CO₂ ice at 60, 70, and 80 K are acceptable since a better constrain requires the detection of the peak of ¹²CO₂ ice band.

Appendix E: CO rotational–vibrational line subtraction for Ced 110 IRS4B

The CO rovibrational lines are removed before tracing the continuum SED. This step is necessary to disentangle the ice features that are blended with emission lines. The continuum is traced by using a function called “top-hat” (Erb 2024; Rubinstein et al. 2024) to perform a baseline under the bottom of the emission features, but avoiding the regions where multiple emission features create a quasi-continuum profile. The baseline profile and the continuum subtracted CO lines are shown in Figure E.1. No further analysis of these CO forest lines that includes extinction correction and rotational diagrams are presented in this paper, but they will be discussed in a future work.

Appendix F: Emission profile at 7.18 μm

In recent works, methyl cation (CH₃⁺) was detected in a protoplanetary disk, called d203-506, located in the Orion star-forming region (Berné et al. 2023) and in the protoplanetary disk TW Hya (Henning et al. 2024). Accurate molecular data was calculated by Changala et al. (2023) that allowed further study of

the CH₃⁺ features in both d203-506 and TW Hya. In Figure F.1 (bottom), we presents the comparison between the observation and model from Changala et al. (2023) of the 7.18 μm band in the case of d203-506. The model assumes an excitation temperature of $T_{\text{ex}} = 700$ K. A similar emission profile was observed in the MIRI/MRS spectrum of Ced 110 IRS4A, which is different from the profile from d203-506 when compared by eye. In Figure F.1, we overlaid the same gas-phase model of CH₃⁺ from Changala et al. (2023). By visual examination, this model seems to also match the protostar observation. The continuum subtracted spectrum also display absorption lines, which will require further study to interpret them.

Berné et al. (2023) shows that this molecular ion is formed via a two-step process. Molecular H₂ is excited by a strong FUV field, and reacts with C⁺. Next, a sequence of hydrogen abstraction reactions leads to the formation of CH₃⁺. Addressing the best model to fit the data in the case of the CH₃⁺ is beyond the scope of this work. For this reason, we consider that CH₃⁺ is only tentatively detected in the protostar Ced 110 IRS4A. Further works will address this possibility, as well as discuss the likely chemical and physical origin of this ion.

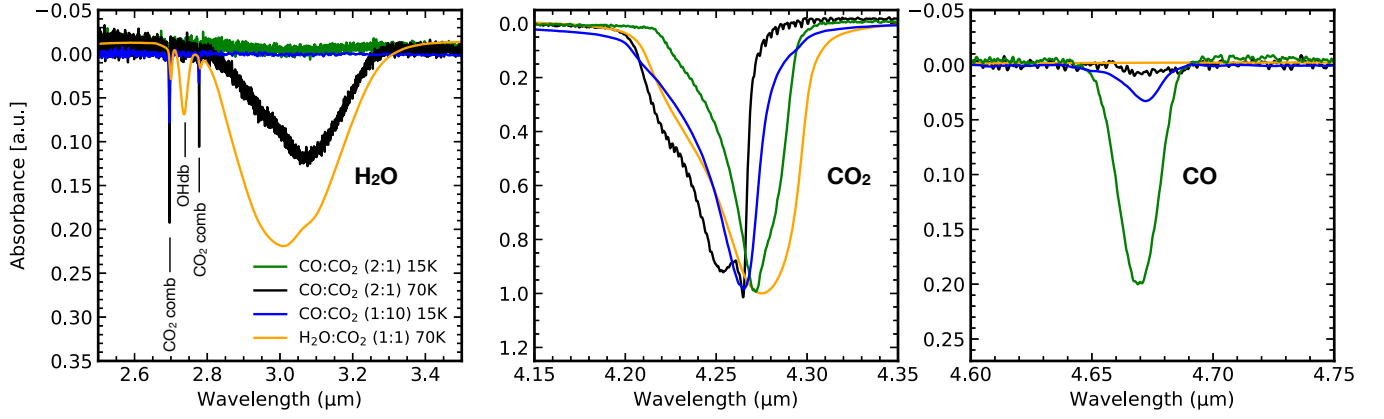


Fig D.1. Comparison between laboratory spectra of CO:CO₂ and H₂O:CO₂. The individual features of these molecules are presented.

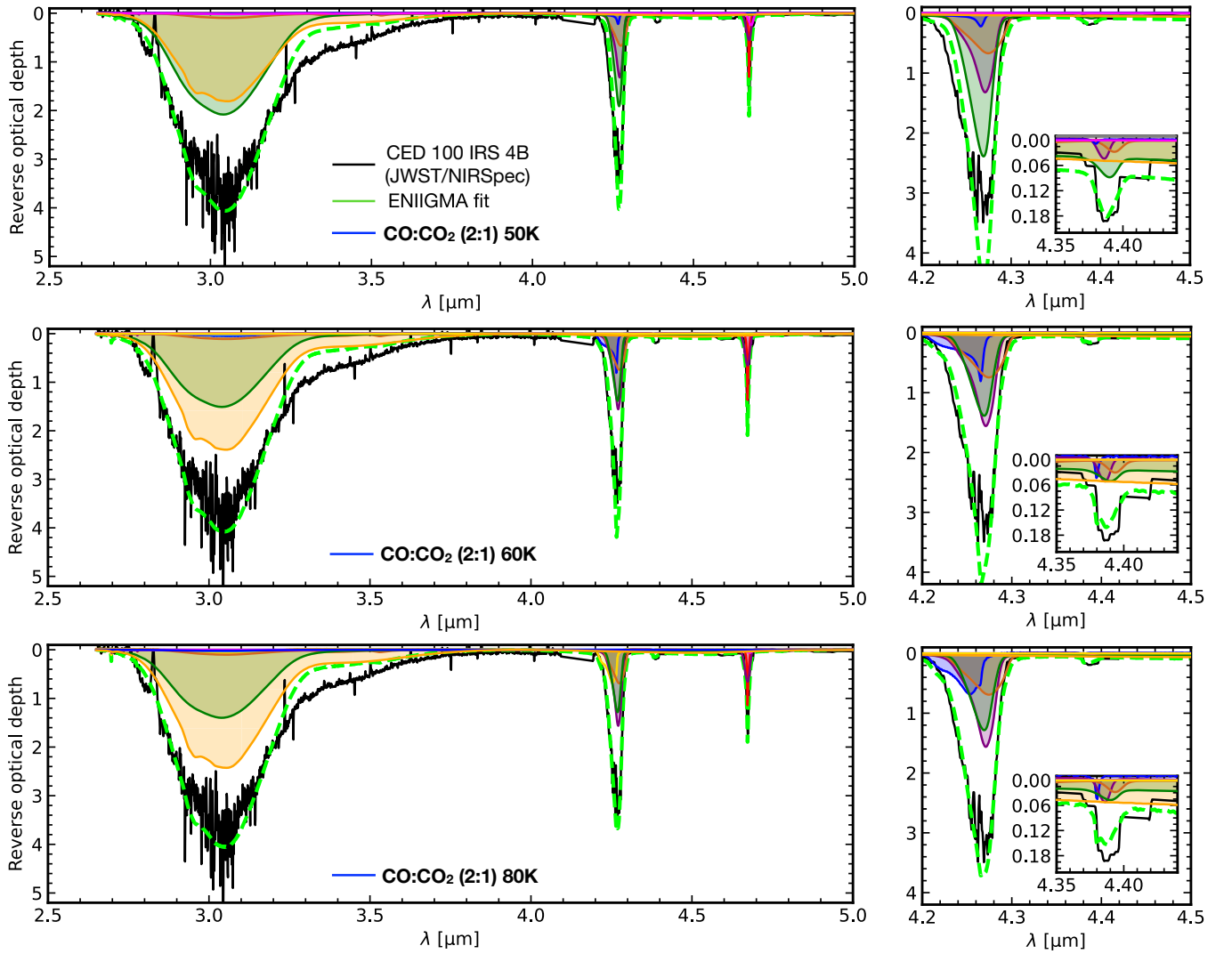


Fig D2. ENIIGMA fits of the NIRSpec range of Ced 110 IRS4B by assuming IR spectra of the CO:CO₂ ice mixture at 50 (top), 60 (middle) and 80 K (bottom). Left panels shows the full spectral range, and the right plots show a zoom-in of the ¹²CO₂ and ¹³CO₂ ice absorption features.

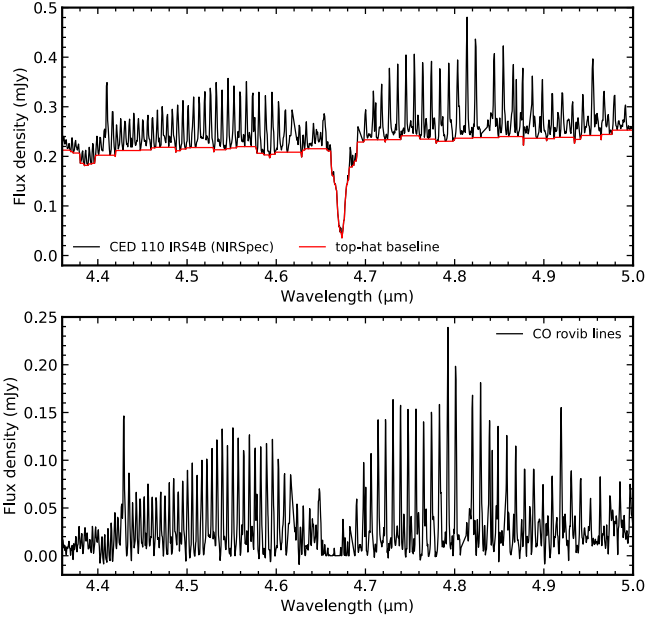


Fig E.1. Subtraction of the CO gas rotational-vibrational lines in the NIRSpec data of Ced 110IRS4B. Both P ($4.3 \leq \lambda \text{ (}\mu\text{m)} \leq 4.56$) and Q ($4.65 \leq \lambda \text{ (}\mu\text{m)} \leq 5.0$) branches are visible in this spectrum. Top panel shows the observational data with the baseline, and bottom panel shows the continuum-subtracted spectrum.

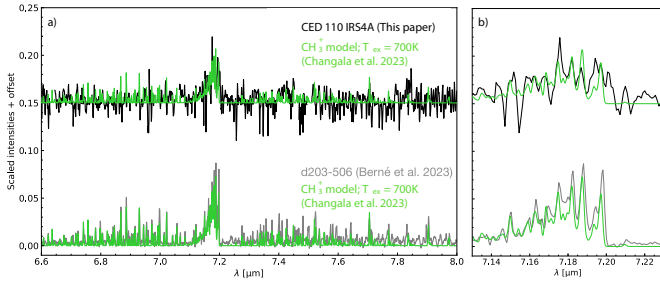


Fig F.1. Comparison between the methyl cation feature from the Orion propylid (Berné et al. 2023, bottom, $R = 3800$) and from Ced 110 IRS4A (top) overlaid with the gas-phase model from Changala et al. (2023). Panel b shows a zoom-in of panel a around $7.18 \text{ }\mu\text{m}$.