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The detection of nucleobases precursors in Class 0 protostars

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Abstract. Nucleobases play an important role in the maintenance and evolution of life on Earth. All nucleobases – adenine, guanine, thymine, cytosine and uracil – were detected on meteorite. Beside this, experiments with interstellar ices analogs demonstrated the abiotic synthesis of cytosine, uracil, thymine, adenine, hypoxanthine, and xanthine from a simple mixture containing water (H_2O), carbon monoxide (CO), ammonia (NH_3), and methanol (CH_3OH), abundant and important chemical species for the molecular dynamic of the interstellar medium. The aim of the present work is the detection of the nucleobases precursor (H_2O + CO + NH_3 + CH_3OH) in star forming regions, indicating possible astrophysical targets where the abiotic synthesis of nucleobases is plausible.

Resumo. Bases nitrogenadas desempenham um importante papel na manutenção e evoulção da vida na Terra. Todas as bases nitrogenadas dos ácidos nucléicos - adenina, guanina, timina, citosina e uracila - foram detectadas em meteoritos. Além disso, experimentos com análogos de gelo interestlar demonstraram a síntese abiótica de citosina, uracila, timina, adenina, hipoxantina e xantina a partir de uma mistura de moléculas simples contendo água (H_2O), monóxido de carbono (CO), amônia (NH_3) e metanol (CH_3OH), espécies químicas abundantes e importantes para a dinâmica molecular do meio interestelar. O objetivo do presente trabalho é a detecção das espécies químicas precursoras das bases nitrogenadas (H_2O + CO + NH_3 + CH_3OH) em regiões de formação estelar, indicando assim, possíveis alvos astrofísicos onde a síntese abiótica de bases nitrogenadas é plausível.

Keywords. Astrobiology – Astrochemistry – ISM: molecules – Infrared: general

1. Introduction

The significant number of complex organic molecules, including nucleobases, found in meteorites suggests that the extraterrestrial synthesis of such molecules is plausible (Burton et al. 2012, Callahan et al. 2011, Stoks & Schwartz 1979). Nucleobases play an important role in the maintenance and evolution of life on Earth. All nucleobases – adenine ($C_5H_5N_5$), guanine ($C_5H_5N_5O$), thymine ($C_5H_6N_2O_2$), cytosine ($C_4H_5N_3O$), and uracil ($C_4H_4N_2O_2$) – were detected on Murray, Lake and Murchison meteorite fragments (Oba et al. 2022). Beside this, recent experimental studies have also demonstrated that the abiotic synthesis of purines and pyrimidines nucleobases under conditions like those found in the interstellar medium is feasible. Oba et al. (2019) and Ruf et al. (2019) reported the synthesis of nucleobases from irradiated mixtures of simple molecules, such as water (H_2O), ammonia (NH_3), methanol (CH_3OH), and carbon monoxide (CO), species commonly found in the molecular clouds (McClure et al. 2023). Experiments from Oba et al. (2019) specifically demonstrated the abiotic synthesis of adenine, thymine, cytosine, and uracil, from the UV (Lyman-alpha) irradiation of an interstellar ice analog containing H_2O + CO + NH_3 + CH_3OH. These findings reinforce the idea that all these terrestrially-important nucleobases could also to be formed in extraterrestrial environments. Despite that, nucleobases have never been directly detected in the interstellar medium, even though the ingredients needed for their synthesis according to Oba et al. (2019) (i.e., precursor molecules and energy sources) are available in the extraterrestrial medium (Thaddeus 2006). There have been attempts to detect nucleobases in molecular clouds, but none have been successful (Brünken et al. 2006, Charnley et al. 2005, Simon & Simon 1973), as detecting complex molecules, such as nucleobases, is a significant challenge. Therefore, this work aims to detect the precursor molecules of nucleobases synthesis, according to Oba et al. (2019), in prestellar regions. To achieve this, were constructed an interstellar ice analogue in the laboratory, containing H_2O + CO + NH_3 + CH_3OH, and were obtained the infrared spectrum of this ice. Subsequently, were identified the observed bands in the laboratory spectrum in the infrared observational spectra of 8 Class 0 protostars collected by the Spitzer Space Telescope. Finally, a comparative analysis, correlating the observational spectra with the laboratory spectrum.

2. Methodology

2.1. Laboratory interstellar ice analog spectrum

The experiment was performed at the Van de Graaff Laboratory of the Pontifical Catholic University of Rio de Janeiro (PUC-Rio). The experimental apparatus consisted of a high-vacuum chamber, a Fourier Transform Infrared Spectrometer (FTIR – Jasco FT-IR-4200) and a simple holder with a ZnSe substrate which can be cooled down to 15 K using a closed-cycle helium cryostat (Sumitomo HC-4E). The base pressure of the chamber during the experiments was of the order of 10^{-8} mbar. A H_2O:CO:NH_3:CH_3OH gas mixture was deposited onto the cooled ZnSe substrate. This mixture has the same composition and proportion as used in the experiment where Oba et al. (2019) demonstrated the abiotic synthesis of nucleobases. The gas mix-

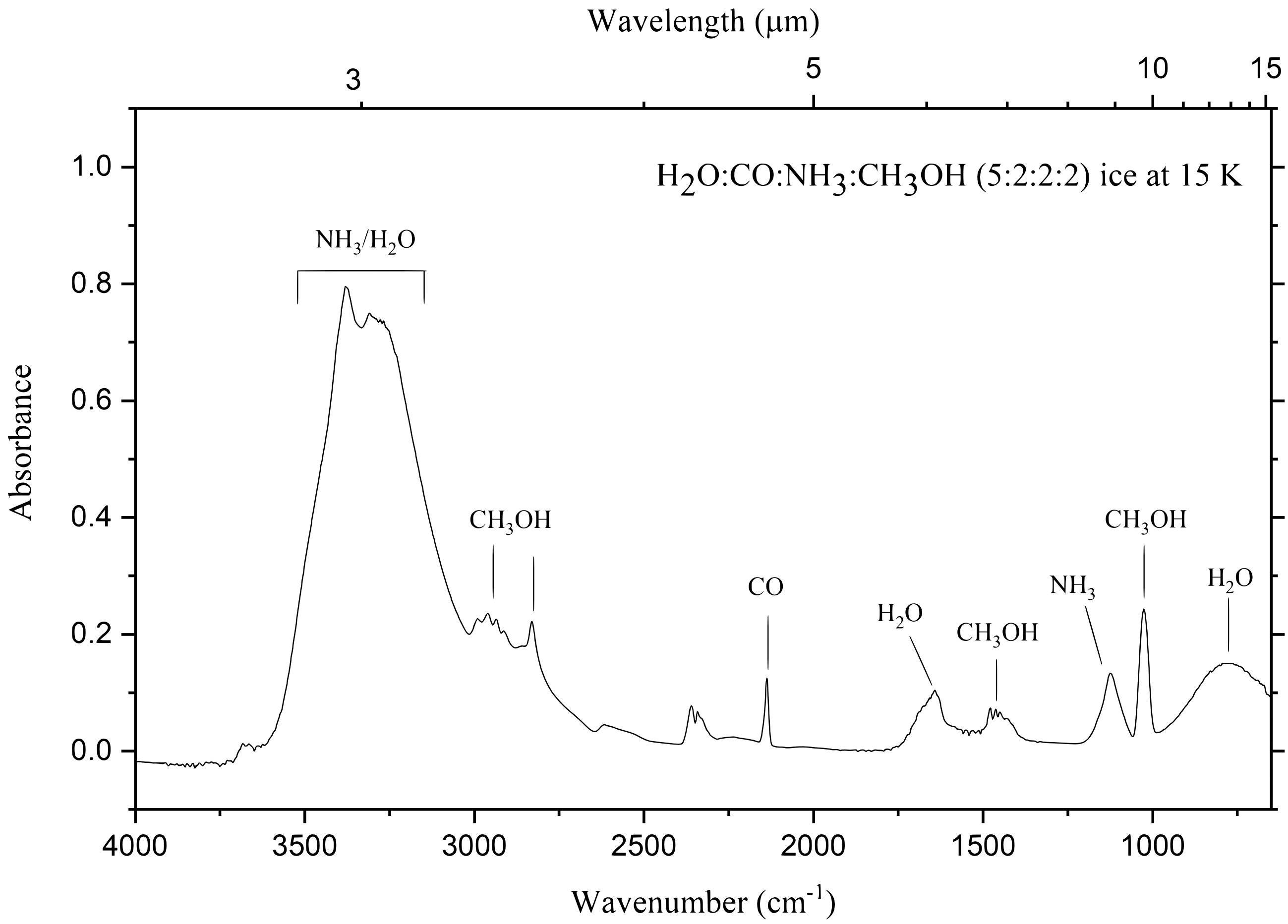

Figure 1. The mid-infrared spectrum of an interstellar ice analogue containing H_2O:CO:NH_3:CH_3OH at 15 K.

ture was previously prepared in a separate chamber, kept at 10^{-6} mbar. During the mixture deposition, the main chamber pressure was kept at $(5 \pm 3) \times 10^{-7}$ mbar, resulting in a deposition rate of $6.12x10^{15}$ $cm^{-1}.s^{-1}$. After the ice deposition, the infrared spectrum was collected.

2.2. Observational spectra

Were analyzed the infrared spectrum of 8 Class 0 protostars (Table 1), because its circumstellar disk is considered a genuine chemical laboratory for synthesizing biomolecules and a strong candidate for detecting new molecular species, such as nucleobases (Bergantini et al. 2017). We collected spectroscopy data using the Infrared Spectrometer (IRS) aboard the Spitzer Space Telescope at low resolution (R 60-130) and short wavelengths (SL2 5.13 - 7.60 μm and - SL1 7.46 – 14.29 μm) (Houck et al. 2004). These spectra were obtained from the c2d Legacy program "From Molecular Cores to Planet-Forming Disks", and the data were collected in September 2005.

The software SMART (Higdon et al. 2004) was utilized for data processing. Initially, the data were orthogonalized, and bad pixels were removed using IRSCLEAN. Next, the background was subtracted using the pair of nods subtraction method, and the spectra were extracted using the "automatic optimal extraction" function. This method provides a better signal-to-noise ratio for weak sources by using the profile distribution function of instrumental points to weigh the data. Next, the spectra were divided by the spectrum of the standard star HR 2194, which was extracted and processed similarly. An IDL (Interactive Data Language) routine was developed for the continuum subtraction,

Table 1. Class 0 protostars investigated

Target	R.A (J2000)	Decl (J2000)	Cloud
RNO 91	16 34 29.32	-15 47 01.4	L43
L1489 IRS	04 04 43.07	+26 18 56.4	Taurus
R CrA IRS 5	19 01 48.03	- 36 57 21.6	CrA
L1014 IRS	21 24 07.51	+49 59 09.0	L1014
IRAS 08242-5050	08 25 43.78	-51 00 35.6	HH 46
IRAS 03235+3004	03 26 37.45	+30 15 27.9	Perseus
2MASS J17112317	17 11 23.13	-27 24 32.6	B59
B1b	03 33 20.34	+31 07 21.4	Perseus

and a high-order polynomial was fitted in the following wavelength ranges: 5.40-5.60, 6.40-6.60, and 7.30-8.00 μm for SL2 and 8.25-8.75, 9.23-9.37, and 9.98-10.40 μm for SL1. The continuum level was subtracted, and the flux was converted to optical depth (Whittet et al. 2007). For the correlation between observational and laboratory data an IDL routine was wrote.

3. Results

3.1. Laboratory spectrum of H_2O:CO:NH_3:CH_3OH ice

The mid-infrared spectrum of an interstellar ice analogue containing the precursor molecules of nucleobases (H_2O:CO:NH_3:CH_3OH) is shown in Figure 1. The characterization of each band can be observed in the Figure 1, and their respective wavelengths, wavenumbers, and assignments can be found in Table 2, according with Bouilloud et al. (2015 - Ref. a) and Zhu et al. (2020 - Ref. b).

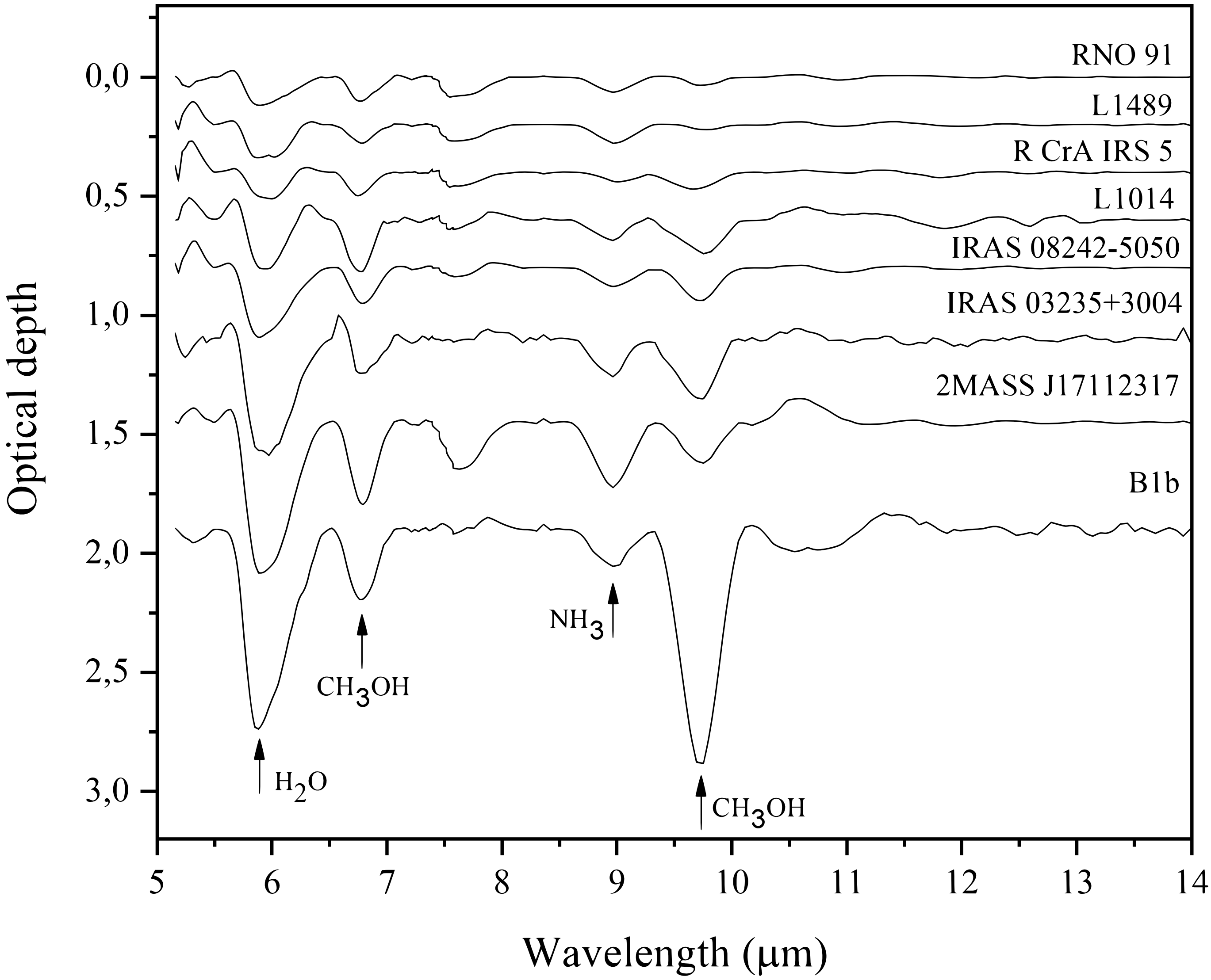

Figure 2. The infrared spectrum of eight protostars observed by Spitzer-IRS.

Table 2. Assignment of observed bands in the H_2O:CO:NH_3:CH_3OH ice spectrum.

Molecule	λ (μm)	ν (cm^{-1})	Assignment	Ref.
NH_3	2.96	3379	a-stretch	a
H_2O	3.04	3287	a-stretch	a
CH_3OH	3.38	2960	a-stretch	a, b
CH_3OH	3.53	2830	s-stretch	a, b
CO	4.68	2136	C-O stretch	a
H_2O	5.99	1670	H–O–H bend	a
CH_3OH	6.84	1462	CH_3 bend	a
NH_3	9.00	1110	umbrella mode	a
CH_3OH	9.75	1026	C–O stretch	a
H_2O	12.92	774	Libration mode	a

Were aimed the detection of the observed bands in the laboratory spectrum in the astrophysical targets of interest. As the observational data were collected in the SL1 and SL2 modules of the Spitzer IRS, covering a range from 5.13 to 14.29 μm, we focused our search on the bands observed in this range (1949 to 700 cm^{-1}, approximately). In other words, we targeted the 5.99 μm (1670 cm^{-1}) band of water, the 6.84 μm (1462 cm^{-1}) band of methanol, the 9.0 μm (1110 cm^{-1}) band of ammonia, and the 9.75 μm (1026 cm^{-1}) band of methanol, as well.

3.2. Detection of nucleobase precursors in class 0 protostars

It was possible to detect the water (5.99 μm), methanol (6.84 and 9.75 μm), and ammonia (9.0 μm) bands in the eight protostars analyzed, as shown in Figure 2.

3.3. Correlation between laboratory and observational data

Even though the laboratory spectrum is under conditions as close as possible to those found in the cold regions of protostellar discs, there are still many variables that cannot be replicated in the laboratory. In other words, the chemical environment of the spectra is still quite distinct. Nevertheless, a significant coincidence in the central wavelength of the observed bands in the laboratory spectrum and the observational spectrum can be noted, as shown in Figure 3. In essence, it is possible to reproduce reliable models in the laboratory for the detection of chemical species in the interstellar medium.

4. Conclusions

In this study, we identified eight astrophysical targets where the future detection of nucleobases is promising, given that the precursor chemical species for their synthesis have been detected in

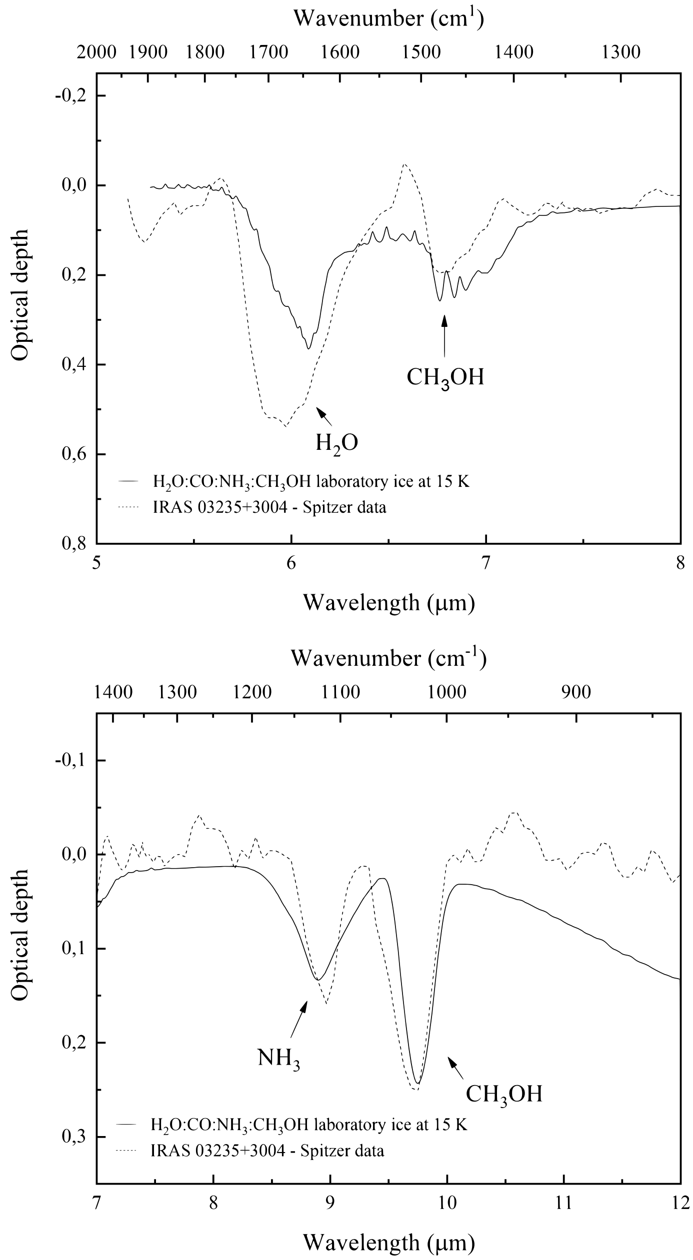

Figure 3. Correlation between water, methanol, and ammonia bands in the observational and laboratory spectrum

these targets. Through an integrated laboratory and observational study, it was possible to detect the bands of water, methanol, and ammonia in eight Class 0 protostars. Despite differences in the chemical environment where the spectra were obtained, a good correlation was observed between the laboratory data and those collected by the Spitzer Space Telescope. In other words, it is possible to reproduce reliable models in the laboratory for the detection of chemical species in the interstellar medium. Using a similar methodology, we can search for new molecules, such as nucleobases, in interstellar environments.

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