

Unveiling the whole from its parts or to see the forest for the trees

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Abstract. If biologically complex molecules as DNA were present in the extraterrestrial targets, their spectral signatures would be rather difficult to be unambiguously identified. As a matter of fact, the molecular array of a single nucleobasis will generate a tangled spectral signature. On the other hand, a part of it, e.g. bands due to the group of HNCO of guanine may have been detected but associated to smaller molecules, e.g. isocyanic acid (HNCO). However, if comprised in a nucleobasis, its detection would be misinterpreted. Five key transitions were preliminarily selected for either purines and pyrimidines that should be observed together in the same target. If this happens, it may be that we are detecting the whole from its parts.

Keywords. ISM: molecules, ISM: lines and bands, astrochemistry

1. Introduction

We live in a molecular universe. In a spiral galaxy as the Milky Way (MW), interstellar molecular clouds are the bigger and heavier baryonic components of the spiral system. The largest molecular clouds are visible to the naked eye, appearing as dark patches against the brighter background of the MW. They can be seen all over the magnificent projection of the galaxy disk on the sky, mainly from the southern hemisphere.

Biology tell us that more than 95 % of all life forms on Earth is composed by H, O, C N, P and S, sources of the known CHONPS anagram. Moreover, the genetic material of all life forms is encoded in huge molecules, formed by the long sequences of deoxyribonucleic or ribonucleic acids (DNA and RNA).

2. Molecular factories

It is well known that interstellar molecular clouds and circumstellar envelopes harbour ice grains that can act as factories of molecular synthesis. Indeed, atoms and molecules can meet and react at the surface of the ices present in the clouds, the cosmic rays and energetic photons acting as the necessary energy source for ionization and chemical reactions (e.g. [Marshall & Sadeghpour 2016](#)).

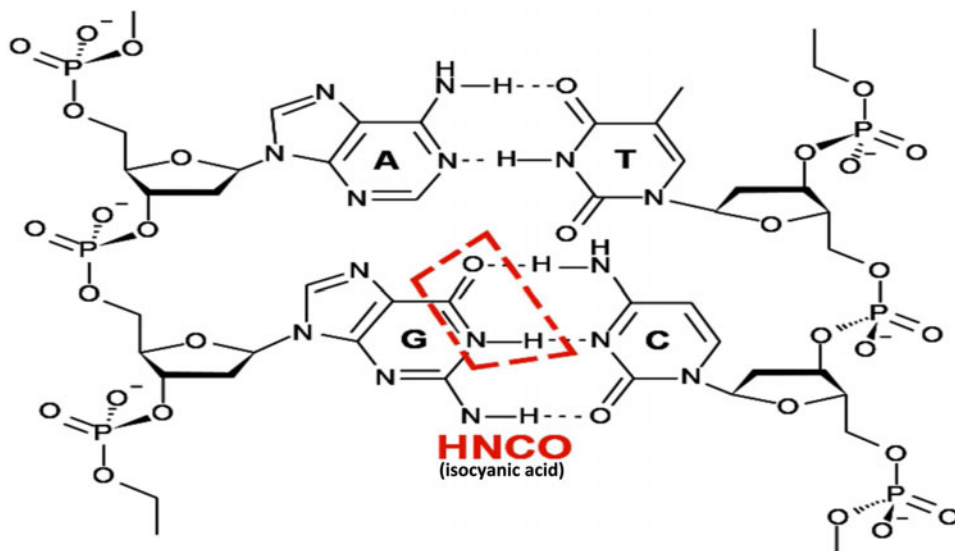


Figure 1. A small segment of a DNA molecule is depicted. The spectrum of the whole molecule is quite complex and entangled. The independent vibrational signal of a local isocyanic acid is perhaps detected, but not interpreted as coming from a part of the DNA molecule.

Surprisingly, complex, pre-biotic molecules used in biochemistry on Earth are found in the interstellar medium, in circumstellar envelopes, planetary atmospheres and cometary surfaces, asteroids and meteorites, and interplanetary dust particles (Ehrenfreund & Cami 2010).

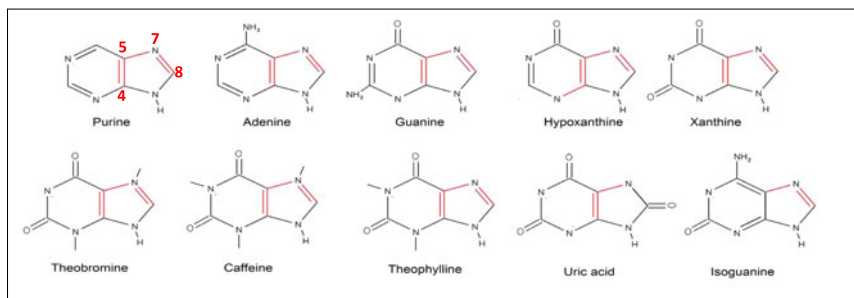
3. An organic friendly universe

We live in an organic-friendly universe: there are pre-biotic molecules everywhere in the MW, e.g., in interstellar clouds and circumstellar envelopes of forming stars, where tens of organic molecules up to 13 atoms have been detected in radiobands (<https://www.astro.uni-koeln.de/cdms>) (excluding PAHs; these compounds will not be considered in this paper). Relatively complex organic molecules (Dimethyl ether and methyl formate) have also been observed in nearby galaxies as the Magellanic Clouds (Sewilo *et al.* 2018).

Powner, Gerland & Sutherland (2009), Jeilani *et al.* (2016) and Hudson *et al.* (2012) have shown that primitive abiogenic reactions in the primordial soup of simple molecules as hydrogen cyanide (HCN), glycoaldehyde and formamide may generate life building blocks as pyrimidines and purines. Thus, relatively straightforward prebiotic chemical reactions may form the robust code of the biosphere on Earth, which is based on nucleic acids. Why then, it is so difficult to address their detection in astrophysical targets? At least a part of the answer could be based on the fact that a) their characteristic IR bands are complex and often overlap with the features due to other species, making it difficult to safely identify them and b) the best wavelength range to collect spectra of complex molecules, the mid-IR, is only accessible by means of expensive, cooled spectroscopes.

4. Detecting the whole from its parts?

Our work hypothesis is that maybe only partial (i.e, local) transitions coming from big molecules have been identified, but are not interpreted as such. Could it be that we are seeing the trees and missing the forest as a whole? In Figure 1 a small part of a DNA is shown. The sugar-phosphate backbones can be seen at the extreme left and right



Spectral signatures for the purine family

in-plane ring vibration (“breathing” movement): 9 lines between 14.4 and 6.7 μm

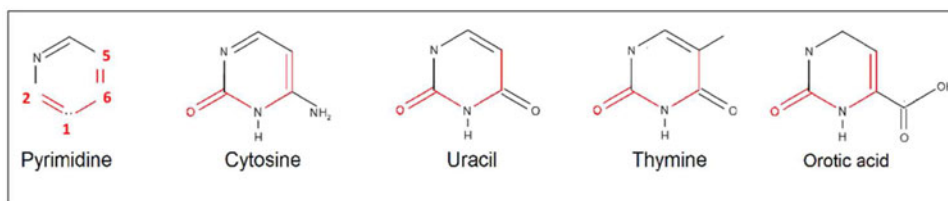
out-of-plane ring vibration (“butterfly” movement): lines at 43.47 and 34.96 μm

$\text{N}^7 - \text{C}^5$ in-ring bond: line at 8.10 μm

$\text{N}^7 - \text{C}^8$ in-ring double bond: 5 lines between 6.75 and 8.40 μm

$\text{C}^4 - \text{C}^5$ in-ring double bond: 3 common lines at 6.37, 6.25 and 5.93 μm

Figure 2. Five proposed preliminary spectral characteristics of the purine family (sketched on the top) (approximate wavelengths). If they are detected together in the same astronomical target we may be seeing the forest (the nucleobases) for the trees (the local transitions within them).



Spectral signatures for the pyrimidine family

Out-of-plane ring vibration (“chair” movement): 3 lines between 43.10 – 51.54 μm

$\text{C}^5 - \text{C}^6$ in-ring double bond: lines at 5.94 and 6.19 μm

$\text{N}^1 - \text{C}^6$ in-ring single bond: line at 6.79 μm

$\text{C}^2 - \text{N}^1$ in-ring bond: lines at 6.79 and 13.18 μm

$\text{C}^2 - \text{O}$ double bond: lines between 5.62 and 5.88 μm

Figure 3. The same for the pyrimidine family (on the top).

and the alternate nitrogen containing bases (pyrimidines and purines) are seen towards the center. A HNC/O fragment is highlighted in the base pairing between a guanine (G) and a cytosine (C). The independent vibrational feature of an isocyanic acid is perhaps detected, but not interpreted as coming from a part of the bigger structure, as a guanine molecule. Nucleic acids may be present in the interstellar medium, but their spectra are quite complex and entangled. Within the spectral forest of IR or radio spectra, parts of such a complex molecule could be detected as simple, local transitions. Although nucleic acids may be there, we only see parts of the whole.

We propose to define spectral signatures of the two nucleobases families (purines and pyrimidines) by selecting a number of local transitions within the molecules. In order to enhance the signal, the chosen transitions should be present in all types of nucleobases (there are 5 types of pyrimidines and 10 types of purines). Five transitions were preliminarily proposed for each family and shown in Figures 2 and 3. If they are detected together at the same astronomical target, we are perhaps seeing the forest (the nucleobases) through detection of the trees (local transitions within these nucleobases).

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Discussion

KEDZIORA-CHUDCZER: Can you comment on the chirality of these discussed compounds?

JANOT-PACHECO: Indeed, chirality may play a certain role in the transitions of complex organic molecules. We intend to include this aspect of the problem in the future.