

Abstract

The main goal of this work is to study abundances of several molecules, including some of potential prebiotic and we investigated the role of PAHs. We explored production channels for astrobiologically relevant nitrogenated heterocycles: pyrrole and pyridine. Furthermore, we have checked the role of the increasing or decreasing in cosmic rays rate based on theory that cosmic rays could raise the cations abundances and, therewith, intensify the complex molecules abundances. This presents simulations show us how the exploration of a small quantities of possibles path of production of heterocycles resulted already in significant abundances at least one N-heterocycle specie, the pyridine.

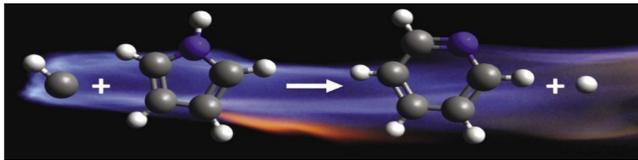
Introduction

Nitrogen:

- present in the composition of the information carrier molecule. It has odd valence number and introduces asymmetries.
- nitrogen bases; DNA & RNA

PAHs & PANHs:

- They are widely found in the interstellar medium and are resistant to radiation field in the star formation regions
- PANHs may constitute a precursor to biological information carriers
- In a further RNA world pre/probiotic scenario, assembling of PAH/PANH rich-material could perform the transition from nonliving to living matter.

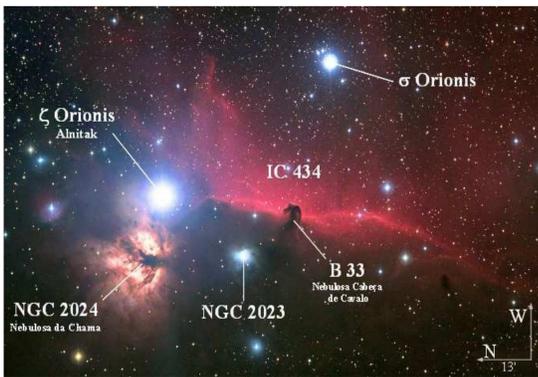


Sorkia (2010b)

Simulations

The PDR Meudon Code

- The HorseHead Nebula:
- Molecular Cloud Archetype



Horsehead Nebula: molecular cloud archetype

Horsehead Nebula Model:

- Radiation field FUV: 60 Draine
- Temperature: 15 K
- Pressure: 4×10^6 Kcm⁻³
- Density (n(H₂)): 1×10^4 cm⁻³
- Distance: 400 pc
- σ Ori (o9,5V) ~3,5 pc

Data Base

- UMIST
- KIDA
- OSU2009
- Papers

Hundreds of added reactions

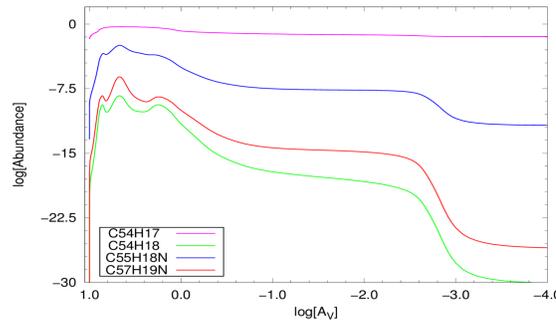
REAGENTS	PRODUCTS	γ	α	β		
C54H18	H	C54H17	H2	5.00E-008	0.5	0
C54H18	C2H	C54H17	C2H2	5.00E-008	0.5	0
C54H17	HCN	C55H18N	photon	5.00E-007	0.5	0
C55H18N	C2H2	C57H19N	H	5.00E-007	0.5	0
C57H19N	C2H4	C54H18	C5H5N	5.00E-007	0.5	0

Example: Chemical reactions, parameters and types of reaction for producing of pyrrole and pyridine involving PAHs.

The Role of PAHs

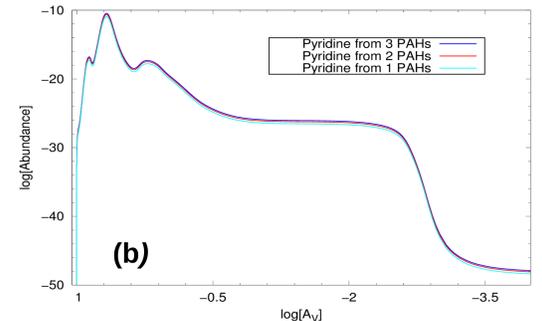
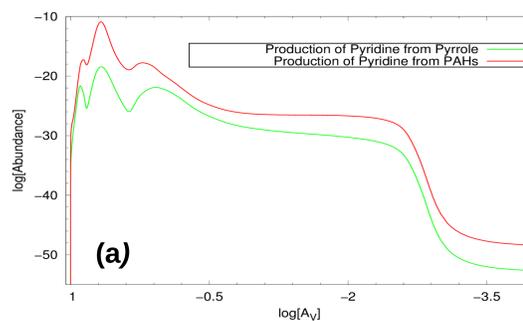
PAHs e PANHs:

Circuncoronene as a typical PAH



Horsehead Nebula PDR model abundance results for PAH circuncoronene and its dehydrogenated form besides PANHs formed from C54H18 as a function of optical depth in V band A V.

Pyrrole and Pyridine: possible nucleobases parents

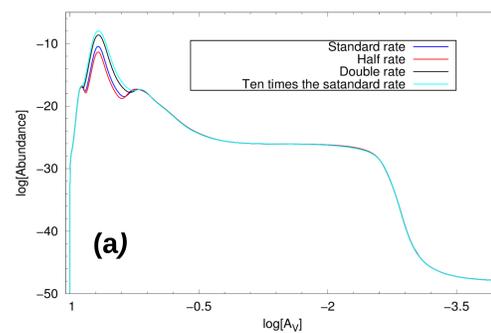


Pyridine production from diferent channels: a) from pyrrole and circuncoronene; b) from coronene, ovalene and circuncoronene

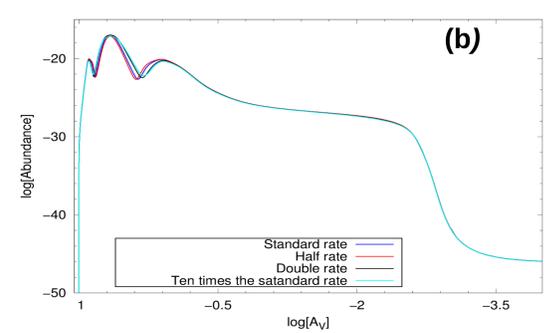
PAHs act as catalysts in the complex molecules formation.

The Role of Cosmic Rays

Pyridine

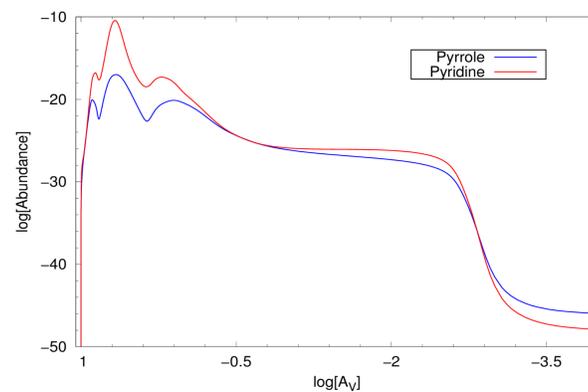


Pyrrole



Abundance results for standard, twice, tenfold and a half the amount the standard cosmic rays ionization rate for a) pyridine b) pyrrole

Increasing the cosmic rays ionization rate promotes increased molecular complexity



Abundance results for production of pyrrole and pyridine as a function of optical depth in V band A V.

Pyrrole seems to be most abundant in the cloud edge, but it becomes less abundant than pyridine in inner regions. This behavior is similar for both species also to the photochemical model for Titan's atmosphere.

The results indicate that the PAHs can be important in production intermediate species of N-heterocycles, as illustrated by the high abundance obtained for pyridine in modeling Nebula horse head.

In the same way, cosmic rays must be important and their rates should studied better.

References:

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