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Formation and destruction of organic molecules in the upper atmosphere of Titan

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Abstract. In this work we introduce an atmospheric code to simulate molecular abundances in Titan's upper atmosphere, including mass loss. The retrieved abundances verify the possible formation of complex organic compounds, such as HC_3N, CH_3CN, and C_2H_5CN, in a Titan-like environment, allowing the production of even bigger molecules. Ion fragments are also observed in our abundances, since the model takes into account a Saturn's magnetospheric particle inflow. We present the main differences between considering Titan's atmosphere with and without this inflow, and the roles these magnetospheric particles play in the fragmentation of atmospheric molecules.

Resumo. Neste trabalho introduzimos um modelo atmosférico para simular abundâncias moleculares na alta atmosfera de Titã, incluindo sua perda de massa. As abundâncias encontradas mostram a possível formação de compostos orgânicos complexos em um ambiente similar a Titã, como HC_3N, CH_3CN e C_2H_5CN, permitindo a produção de moléculas ainda maiores. Fragmentos iônicos também são observados, já que o modelo leva em conta a influência de partículas da magnetosfera de Saturno adentrando a atmosfera. Apresentamos as principais diferenças entre considerar a atmosfera de Titã com e sem a influência dessas partículas, e o papel que elas têm na fragmentação de compostos amosféricos.

Keywords. Planets and satellites: atmospheres – Astrochemistry – Astrobiology

1. Introduction

Perhaps one of the most interesting objects in the Solar System, Titan is known to be the only body besides the Earth to form and destroy complex organic molecules in its atmosphere. With a composition of about 95% N_2 (molecular nitrogen) and 3% CH_4 (methane), Titan's atmosphere is irradiated by the UV sunlight, dissociating or ionizing its main molecules into smaller fragments, allowing the production of bigger ones. This process occurs in the upper parts of the atmosphere.

As these compounds become bigger, they condense to lower altitudes, forming clouds and hazes, and continue to accrete material. Eventually, an aerosol layer is formed in the stratosphere, at about 100–300 km. Titan's upper atmosphere is also influenced by Saturn's magnetosphere, and mass loss processes are observed. Particles such as ions and electrons from Saturn's magnetosphere interact with compounds in Titan's outer atmosphere, and outflows ions ($HCNH^+$, $C_2H_5^+$) can be seen, along with an inflow of O^+ from Enceladus.

Our work simulates the abundance of molecules in Titan's upper atmosphere considering these escape processes, which occur at about 1400 km and above. We used a chemical model by Pinotti & Boechat-Roberty (2016), regarding a few corrections to utilize the model for a planetary atmosphere.

2. Methodology

2.1. Selection of species

We first selected to include in our model chemical compounds that were previously observed in Titan's atmosphere, as well as its fragments. Only C, H, O and N-bearing molecules were considered.

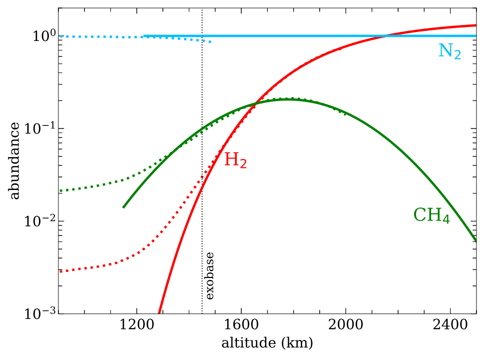

Figure 1. Abundances of N_2, CH_4, and H_2 used in our simulations. Dotted lines correspond to De La Haye et al., (2008) model, and solid lines are our adjusts above the exobase.

2.2. List of reactions

The UMIST Database (McElroy et al., 2013) was the source for the reactions' constants, and a correction had to be made to consider an atmospheric medium instead of an interstellar one. We also applied a correction factor to consider not only UV radiation from the Sun, but also plasma particles from Saturn's magnetosphere, which are known to be the second main source of energy to inflow Titan's atmosphere.

2.3. Continuity equations

Each molecule i has its own continuity equation (equation 1), which includes the flux variation according to the altitude ($d\Phi_i/dz$), the production rate (P_i) of all the reactions involving the specie i, and the loss rate (L_i). Initial parameters include the

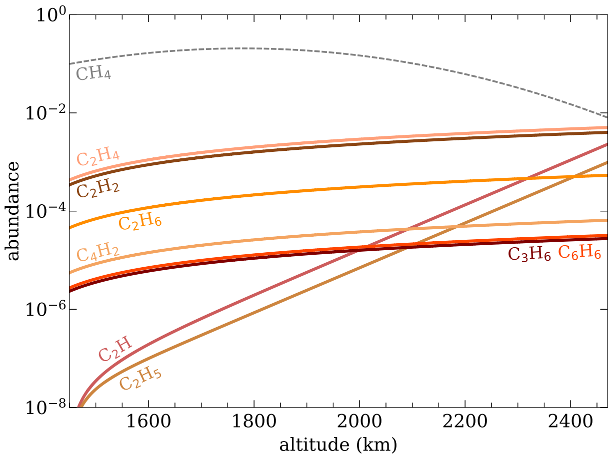

Figure 2. Abundances of hydrocarbon molecules simulated by our model. Dashed line is CH_4 (the same as in Fig. 1) for comparison.

abundances of the three main molecules: N_2, CH_4, and H_2, from De La Haye et al., (2008), featured in Fig. 1.

$$-\frac{d(\Phi_i)}{dz} + P_i - L_i = 0 \therefore -\frac{d(x_i n_{N_2} v_i)}{dz} + P_i - L_i = 0 \qquad (1)$$

3. Results

We solve the continuity equation above 1450 km (exobase) for each molecule in the model, obtaining their abundances (x_i in equation 1). Significant species were found to have high abundances, especially hydrocarbons (Fig. 2) and nitriles (Fig. 3 and 4). Ethylene (C_2H_4), acetylene (C_2H_2), and ethane (C_2H_6) are the three most abundant hydrocarbon products above the exobase, which agrees with *Cassini-Huygens* observations along the middle and lower atmosphere.

A high abundance of HCN, N, and an increasing CN abundance are derived by our results, meaning the production of cyanide triple-bonds, which will later form complex nitriles, such as acetonitrile (CH_3CN), cyanoacetylene (HC_3N), and propionitrile (C_2H_5CN), all featured on 3. Hydrogen cyanide's protonated form, $HCNH^+$, and its isometer, $HNCH^+$, are the highest abundances along the ions 4, participating in the formation of complex molecules as well.

We were also able to observe the magnetospheric influence in the abundances of small molecules and ions. Complex molecules were not affected by magnetospheric particles.

4. Conclusions

Our model estimates the abundance of prebiotic precursors, which could form molecules such as glycine and adenine. The former can be produced by reacting water, formaldehyde, and hydrogen cyanide.

$$HCN + H_2CO + H_2O \rightarrow C_2H_5NO_2$$

The latter is formed in the synthesis of 5 hydrogen cyanide molecules.

$$5\ HCN \rightarrow C_5H_5N_5$$

The production of both prebiotic compounds in Titan was previously studied in laboratory experiments by Wayne (2018) and Pilling et al., (2009), respectively.

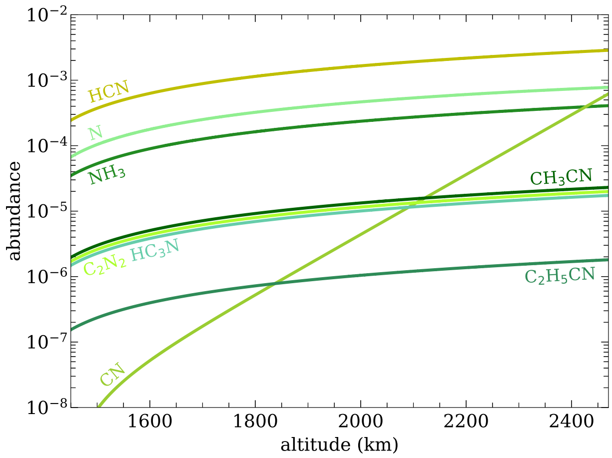

Figure 3. Abundances of nitrogen-bearing molecules simulated by our model.

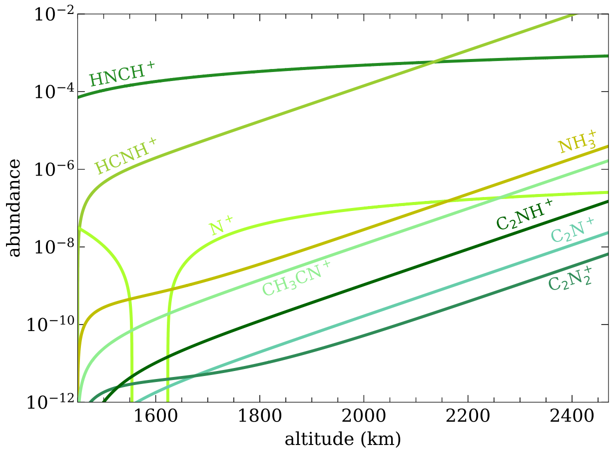

Figure 4. Abundances of nitrogen-bearing ions simulated by our model.

5. Perspectives

Future work involve upgrading the model by Pinotti & Boechat-Roberty (2016), describing a complete atmosphere instead of only the upper layers, and possibly including Titan's induced magnetic field. Considering a different database (e.g. KIDA) is also an idea that can help us consider new compounds in the model, such as PAHs and S or P-bearing molecules.

We also intend to invest in laboratory experiments to verify the stability of the most abundant complex organic molecules according to our model, especially the ones with an astrobiological interest. The work done so far will be featured in Novais et al. (in prep.).

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