EXPLORATION OF THE RELEVANCE OF FORMALDEHYDE AND THE HYDROXYMETHYL RADICAL IN ASTROCHEMISTRY AND ASTROBIOLOGY

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Abstract

Analyzing astrophysical ices of H_2O and CO_2 using PROCODA allows for the investigation of numerous chemical reactions, among which formaldehyde (H_2CO) and the hydroxyformyl radical (HOCO) stand out, both of which are highly important to astrochemistry and astrobiology. In astrochemistry, H_2CO and HOCO are essential for the formation of complex organic compounds such as methanol and amino acids, playing a role in reactions within molecular clouds and protoplanetary disks. Their presence provides crucial insights into the physical and chemical conditions of these environments and influences the dynamics of planetary systems. In astrobiology, these molecules are significant as they can be precursors to essential life-building compounds such as sugars and amino acids. The detection of H_2CO and HOCO in comets, asteroids, and the moons of gas giants suggests that the building blocks of life may exist in various extraterrestrial environments. Studying these compounds can enhance our understanding of astrobiology, particularly concerning the formation of complex organic compounds and amino acids.

Keywords: Astrochemistry, astrobiology, formaldehyde, hydroxyformyl radical.

Knowledge Area: Exact and Earth Sciences – Astronomy

Introduction

aIn this work, we will present several chemical reactions that are important for the field of astrobiology, derived from the analysis of an $H_2O:CO_2$ ice irradiated by cosmic rays. Among the relevant molecules are formaldehyde (H_2CO) and the hydroxylformyl radical (HOCO), organic molecules that play a significant role in the formation of complex organic molecules (COMs) such as methanol and some amino acids.

Using PROCODA code, we were able to analyze these molecules individually, allowing for a thorough analysis at three different stages of production and consumption until they reach chemical equilibrium (CE).

Formaldehyde is a simple molecule, but it is of great importance in prebiotic chemistry. It is an intermediate in the abiotic carbon cycle and is present in various cosmic environments. Its prebiotic relevance is highlighted by its ability to participate in various addition and redox reactions, resulting in biologically significant products such as sugars and amino acids. In particular, formaldehyde can be a precursor to ribose and other sugars, which are essential for the formation of RNA (Cleaves et al., 2008). Experimental and theoretical studies indicate that formaldehyde can also be formed by meteorite and asteroid impacts, contributing to the synthesis of important biomolecules, such as amino acids and sugars.

The hydroxylformyl radical (HOCO) is a reactive species that can play a significant role in prebiotic chemical reactions. For example, the formation of sugars and other organic compounds in impact reactions and plasma conditions suggests that radicals like HOCO may be involved in intermediate stages of these reactions (M. Ferus et al., 2019). Additionally, the presence of reactive species in interstellar and planetary environments can facilitate the formation of complex molecules from simple precursors such as formaldehyde (Sorakayala Thripati et al., 2013).

Complex organic molecules (COMs) are essential for understanding chemical complexity in star-forming regions, as they are precursors to materials that can promote habitability in primitive planetary systems. This summary synthesizes the findings of several studies on the evolution and distribution of these molecules in different star-forming environments (W. Rocha et al., 2024).

Methodology

Based on a detailed investigation of the chemical evolution of ice composed of H_2O:CO_2 molecules under the influence of cosmic ray irradiation, we used the latest version of the PROCODA code, as referenced in the works of Pilling et al. (2022b) and Pilling et al. (2023a). The main focus of this study was the analysis of molecules identified as relevant within this context, particularly those with a higher susceptibility to forming complex organic molecules (COMs) (Moraes in progress).

These molecules, identified as key in the chemical evolution under astrophysical conditions, were highlighted and analyzed in greater depth. To achieve this, PROCODA, in its second module, allowed the individualized processing of data for each molecule. This processing enabled a detailed analysis of the consumption and production of each molecule over time, providing a clear view of how these molecules evolve at different stages of irradiation.

Specifically, the analysis was conducted at three distinct time intervals: 1.5 s, 25.01 s, and 2495.5 s, corresponding to the chemical equilibrium (CE) phase of the system, as described by Moraes (in progress). These times were selected to capture different stages of chemical evolution, from the initial moments of irradiation to the point of chemical equilibrium (CE), allowing for a comprehensive understanding of the chemical dynamics.

This focus on the temporal behavior of molecules under the influence of cosmic rays is essential for understanding the underlying mechanisms of complex organic molecule formation in astrophysical environments. By detailing the consumption and production of the molecules in question, the study not only identifies the most promising pathways for COM formation but also contributes to advancing knowledge of the chemical processes occurring in the interstellar space, providing crucial data for future research in astrochemistry and astrobiology.

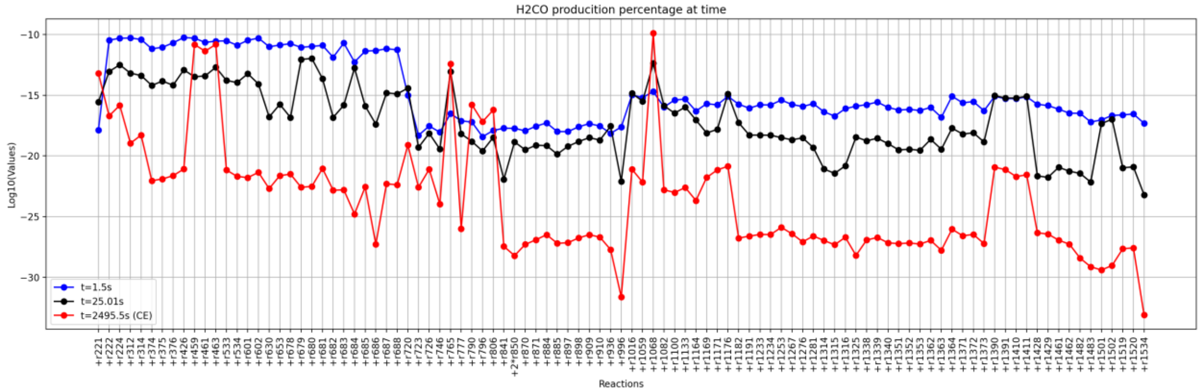
Results

In the initial stage of chemical evolution, molecules begin to form from simple molecular precursors present in astrophysical environments. During this phase, the production rate of new molecules can be quite high, as shown in Figures 1a and 1b, especially when there is an available energy source, such as cosmic rays. These energy sources are capable of inducing chemical reactions by providing the necessary energy to break and form chemical bonds, thereby promoting the synthesis of new molecular species.

Simultaneously, these newly formed molecules start to interact and react with other chemical species present in the environment, leading to their consumption. The consumption rate during this initial phase is highly dependent on the availability of reactants and environmental conditions, such as temperature, medium density, and radiation intensity. In environments where reactants are abundant and conditions are favorable, these reactions can occur quickly and efficiently, consuming the molecules as rapidly as they are produced.

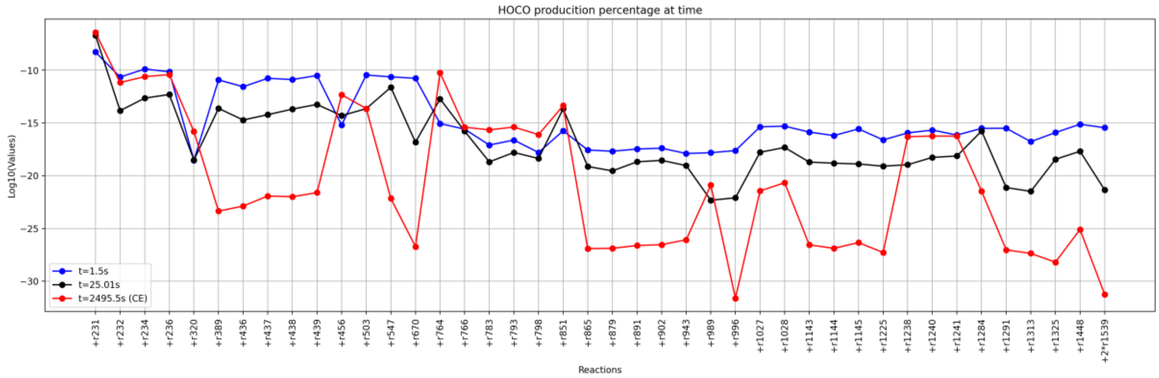
Over time, the system evolves toward a state of chemical equilibrium, resulting in molecular concentrations that remain constant over time. Chemical equilibrium is a dynamic state where reactions continue to occur but in a balanced manner, without changes in the relative concentrations of the species involved.

Figure 1a – H_2CO Producition



Source: Author

Figure 1b – HOCO Producition



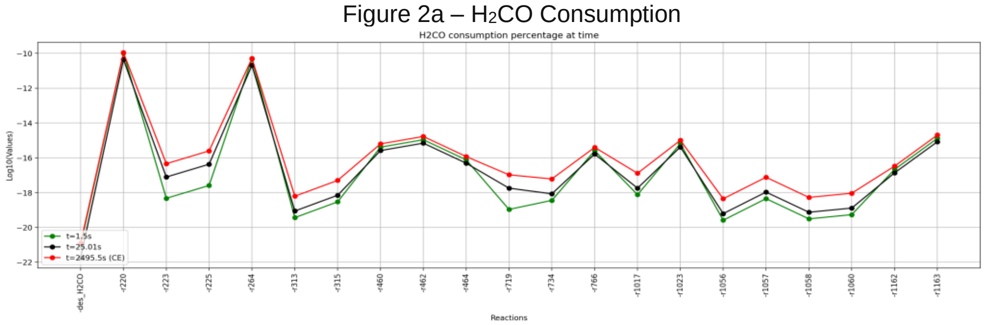
Source: Author

The study of the consumption and production of molecules in space is fundamental for understanding the chemistry that occurs in astrophysical environments. It provides valuable insights into the chemical evolution of structures such as molecular clouds, protoplanetary disks, and other cosmic scenarios. Understanding these dynamics is crucial for deciphering the processes that lead to the formation of complex organic molecules, which may be precursors to life.

In Figures 2a and 2b, we can observe the most dominant reactions, as was presented in Figures 1a and 1b. Among them, the reactions that stand out for the production and consumption of H_2CO are: H_2CCO + R → C + H_2CO; CH_3OCHOH + R → H_2CO + CH_3O; C + H_2O_2 → O + H_2CO; and H_2CO + R → H + HCO, across all time intervals.

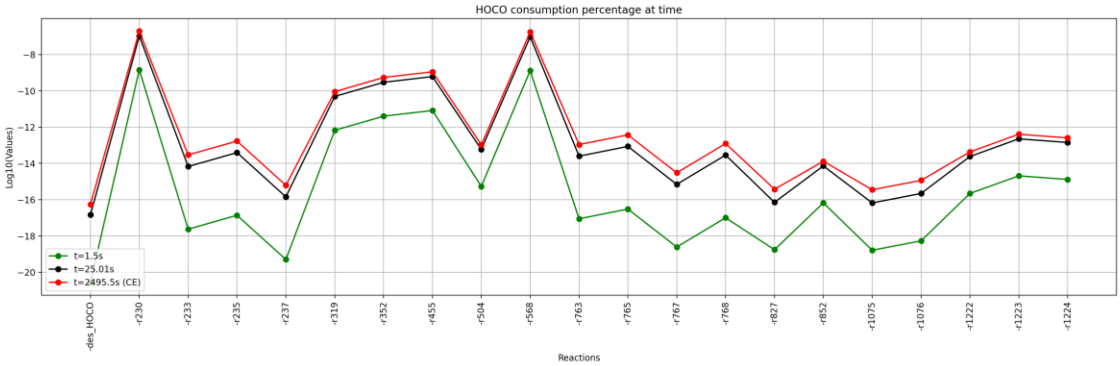
For HOCO, the reactions are: H + CO_2 → HOCO, for all three time intervals, and HOCO + R → H + CO_2, also for all three time intervals, respectively.

Figure 2a – H_2CO Consumption



Source: Author

Figure 2b – HOCO Consumption



Source: Author

Discussion

The presence of simple organic molecules in interstellar ices, comets, and other frozen surfaces in space is a topic of increasing interest in astrochemistry and astrobiology. Among these molecules, formaldehyde (H_2CO) and the hydroxylcarbonyl radical (HOCO) stand out due to their implications in the formation of more complex organic molecules, which are essential for the emergence of life.

Formaldehyde and the hydroxylcarbonyl radical (HOCO), for example, can produce formic acid (HCOOH), which in turn is a crucial element for the formation of more complex molecules. Formic acid can participate in several important chemical reactions for the synthesis of biomolecules. It can act as a donor of formyl groups, which are needed for the formation of various essential organic substances.

In prebiotic environments, formic acid can contribute to chemical reactions under low-energy conditions, helping to catalyze the formation of more complex organic compounds, such as amino acids and nucleotides.

Conclusion

In this study, we can analyze and observe the importance of formaldehyde and the hydroxylcarbonyl radical in astrophysical ices. With the simple presence of these molecules in the interstellar medium, we can advance research into even more complex matters. These molecules play crucial roles as key components in a complex network of chemical reactions that culminate in the formation of complex organic molecules, which are essential for life as we know it. The detection of these compounds in a variety of spatial environments, from molecular clouds to protoplanetary disks, reinforces the notion that the chemistry essential for life is not exclusive to Earth but is instead widely distributed throughout the universe. This significantly increases the likelihood that environments conducive to the formation of amino acids and other prebiotic molecules may exist in different locations in the cosmos. Consequently, the continued study of these compounds in space ices is not only relevant but essential for deepening our understanding of the origin and potential distribution of life in the universe.

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