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COMPUTATIONAL SIMULATION OF THE PHOSPHORYLATION OF THE RIBOSE IN THE PRESENCE OF WHITLOCKITE AS PRIMITIVE MINERAL IN THE PRIMITIVE EARTH

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Phosphorus plays a leading role in biochemical processes. However, lacking a volatile phase, it has not been easy to understand the phosphorylation of prebiotic molecules, such as ribose, a group present in RNA and DNA, etc. In the present work we develop the simulation of the probable mineralogical conditions of the primitive Earth and thus be able to generate a plausible scenario in which the presence of a primitive mineral allows the formation of the phosphate-ribose group. Through the *HyperChem* program we simulate the mineralogical conditions of the Primitive Earth, using a template of whitlockite as a primitive mineral. It is expected that the impact of bolides or the lightning strike will generate the dehydrogenation of whitlockite allowing the formation of reactive phosphate species that will allow the phosphorylation of ribose

Most phosphorus minerals are not chemically reactive under current conditions of temperature, pressure, and pH, so the question arises as to whether early living systems had access to a chemically reactive source of phosphorus. This is relevant because phosphorus plays a prominent role in biochemical processes, suggesting that it participated in prebiotic chemistry. However, of the main biogenic elements (C, H, O, N, S, and P), it lacks a volatile phase, so the source of this element must have been a mineral (Pasek et al. 2015). The questions arise, what kind of reactions could have prevailed in these stages? and what kind of reactivity of phosphate could occur spontaneously in the absence of enzymes? Therefore, it is necessary to construct reasonable scenarios to understand the role of the group phosphate in the origin and evolution of life on Earth (Liu et al. 2019). Currently, researchers are trying to solve these questions are faced with the lack of solid evidence of the various proposed theories about the origin of life. Therefore, the development of computational simulations allows exploring various ideas that due to their complexity are difficult to test in a laboratory; the study of the origin of the stars and the galaxy, as well as the origin of the universe are a clear example of this. It is at this point that molecular modeling techniques play an important role (Mayen et al. 2020).

Our goal is to build a possible ribose phosphorylation pathway from a template of whitlockite as a primitive mineral. Through the *HyperChem* program we will simulate the mineralogical conditions of the Primitive Earth and thus be able to develop a plausible scenario in which the presence of this primitive mineral will lead to the formation of the phosphate-ribose group of the type of the groups present in RNA and DNA. The procedure consists of 4 stages:

1. With the help of the *HyperChem* program, perform the computational simulations.
   A) Get the crystal structure of whitlockite
   B) Propose a ribose synthesis route
   C) Propose the whitlockite disassembly route emphasizing the phosphate group
   D) Suggest possible ribose phosphorylation routes
2. Compare each of the simulations and choose the most viable scenario to reproduce it experimentally.
3. Using various analytical techniques to analyze the results of the experimental phase.
4. Compare the experimental data with theoretical data.

We believe that the impact of bolides or the lightning strike will generate the dehydrogenation of whitlockite allowing the formation of reactive phosphate species that will allow the phosphorylation of ribose.

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