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Origin of Life Theory: Study of Prebiotically Plausible Photochemical Reactions

by

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Abstract

UV-irradiation is considered as one of the most important selection factors that might have driven the early molecular evolution. It is an important source of energy that could have selectively promoted prebiotic chemical reactions. Furthermore, exposure of the chemistry on early Earth to sunlight resulted in remarkable enrichment of photostable biomolecular building blocks and photodestruction of other compounds. The main goal of this thesis was to study selected prebiotically plausible photochemical reactions by means of theoretical calculations. This work describes state-of-the-art quantum chemical calculations and simulations of the photodynamics of small and medium-sized molecules, relevant to prebiotic chemistry. The results of the calculations allowed to clarify the molecular mechanisms underlying the photochemistry and photostability of several crucial intermediate molecules, which might have participated in the early abiogenesis. The described studies also revealed how water may directly participate in the photorelaxation mechanisms of these chromophores. Most importantly, the joint experimental and theoretical studies showed that theoretical simulations may be used as an important tool in proposing new prebiotically plausible reaction sequences.