Monte Carlo simulation of amino acid synthesis driven by UV irradiation in protoplanetary disks and primitive Earth atmosphere

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Introduction: Electric discharge or UV/gamma-ray irradiation experiments and analyses of carbonaceous chondrites suggest that amino acid synthesis can have happened on icy dust surface in molecular clouds or a protoplanetary disk, but the mechanism is still undiscovered. Although a large part of amino acids detected in these studies are suggested to exist in the form of precursors, their structures are not clear at the present, either. Not only the experiments but also the theoretical simulations will be effective to examine the synthesis mechanism of the amino acid and the structures of the precursors and their generation processes. However, in order to perform simulations that produce complex organic matters such as those detected in experiments and meteorites, the chemical kinetic method by rate equations with assumed reaction network and the ab-initio quantum chemistry calculation with high computational cost may not be the best tools. In this study, we adopted the Monte Carlo chemical reaction simulation without the assumed network developed by Takehara et al. [1], which is computationally accelerated by simplifications but enables us to grasp the global synthesis paths of formation of complex organic compound. While the previous work [1] focused on sugar synthesis, we here explored the amino acid synthesis driven by UV irradiation that could have taken place in molecular clouds and protoplanetary disks by the Monte Carlo simulation.

Method: Modifying the classical graph-theoretic matrix model for chemical reactions [2] to be applied for UV photosynthesis of complex organic molecules, Takehara et al. [1] developed a numerical scheme to forwardly explore chemical reaction sequences from simple molecules with Monte Carlo approach. By representing chemical bonds of reactant molecules as a matrix, all the possible chemical reactions are derived automatically. We choose one from them under the probability weighted with the Arrhenius' equation. The products are assumed to be new starting materials, and the next reaction is chosen by the same operation again. We can proceed with a chemical reaction pathway by repeating this process. This novel simulation enables us to forwardly explore complex reaction pathways without preparing any reaction networks. Consequently, we can access the global picture of not only amino acid synthesis, but also the formation of any compounds. Takehara et al. [1] utilized this method and clarified new reaction pathway to form sugars which is different from the conventional formose reaction. They also succeeded to reproduce relative production rates between sugars and sugar alcohols and between sugars and deoxysugars that were obtained by experiments [3, 4]. Now, we applied their method to the simulation of amino acid and its precursor syntheses.

Results and discusstion: The result showed rapid increase of amino acids after UV irradiation phase stopped. They include various kinds of amino acids that are also detected in experiments such as glycine, alanine, serine and so on. These are formed in the decomposition process of relatively large unstable molecular species that are formed by UV irradiation. Therefore, we may need to take account of not only the bottom-up mechanism by UV irradiation, but also decomposing procceses after that. We also focused on the formation of amino acid precursors and found that the amide group that could be a part of the precursors survived relatively stably. In contrast to the process of increasing amino acids, the bonds formed during UV irradiation remained dominant in the production of amide group. Hence, it is suggested that amino acid precursors may form mostly independently of the synthesis of amino acids. At the same time, our result indicates the complex organic matter formed by UV irradiation would randomly contain the structure that could provide amino acids by hydrolysis.

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