

MONTE CARLO SIMULATION OF PHOTOCHEMICAL SYNTHESIS OF AMINO ACIDS IN A PROTOPLANETARY DISK

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The discoveries of complex organic molecules (COMs) in the interstellar medium suggest the universality of organic synthesis in space and possibly provide clues to the origin of life. Laboratory experiments have shown that even amino acids, the building blocks of life, can be synthesized in ice exposed to UV radiation which mimics interstellar ice. Photochemical synthesis is therefore considered to be one of the formation mechanisms of COMs. However, there are still significant uncertainties in photochemistry and ice chemistry because of technical problems inherent in analysis and observation, for example. Here, we investigate amino acid synthesis in protoplanetary disks using new Monte Carlo simulation that applies the classical graph-theoretic matrix model for chemical reaction. This method was originally proposed by Takehara et al. to study sugar synthesis driven by UV irradiation. We have improved it to allow more practical consideration of radicals that play an important role in photochemistry. Molecules in our simulation form only covalent bonds or radicals, and one step of chemical reaction is restricted to the recombination of two different bonds. These constraints allow us to automatically generate chemical reaction pathways without preparing a reaction network. Consequently, we can access the global picture of not only amino acid synthesis, but also the formation of any compounds. The result showed rapid increase of amino acids after UV irradiation stopped. We found that these amino acids are produced by radical reactions rather than the Strecker-type reaction. More detailed formation mechanisms and its dependence on the initial composition of the molecules are discussed. The discoveries of complex organic molecules (COMs) in the interstellar medium suggest the universality of organic synthesis in space and possibly clues to the origin of life. Laboratory experiments have shown that even amino acids, the building blocks of life, can be synthesized in ice exposed to UV radiation which mimics interstellar ice. Photochemical synthesis is therefore considered to be one of the formation mechanisms of COMs. However, there are still significant uncertainties in photochemistry and ice chemistry because of technical problems inherent in analysis and observation, for example. Here, we investigate amino acid synthesis in protoplanetary disks using new Monte Carlo simulation that applies the classical graph-theoretic matrix model for chemical reaction. This method was originally proposed by Takehara et al. to study sugar synthesis driven by UV irradiation. We have improved it to allow more practical consideration of radicals that play an important role in photochemistry. Molecules in our simulation form only covalent bonds or radicals, and one step of chemical reaction is restricted to the recombination of two different bonds. These constraints allow us to automatically generate chemical reaction pathways without preparing a reaction network. Consequently, we can access the global picture of not only amino acid synthesis, but also the formation of any compounds. The result showed rapid increase of amino acids after UV irradiation stopped. We found that these amino acids are produced by radical reactions rather than the Strecker-type reaction. More detailed formation mechanisms and its dependence on the initial composition of the molecules are discussed.

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