核酸塩基の前生物的な生成過程の理論的解明
Theoretical elucidation of prebiotic formation processes into nucleobases

*小松 勇[1,2]、鈴木 大輝[1,2]
*Yu Komatsu[1,2], Taiki Suzuki[1,2]

1. アストロバイオロジーセンター 、2. 国立天文台
1. Astrobiology Center, 2. National Astronomical Observatory of Japan

As argued [1], the comets and meteorites may have provided a large amount of prebiotic molecules to the Early Earth. However, where and how such organic molecules were built is still controversial.

Recently, volatile glycine (NH2CH2COOH) has been detected in the coma of comet 67P/Churyumov-Gerasimenko by the ROSINA mass spectrometer [2], with giving us clues to glycine's interstellar origin. Moreover, in addition to various amino acids, nucleobases, such as purine, uracil, guanine, and xanthine have been identified in the meteorite (e.g., [3]). These studies suggest the formation of prebiotic molecules in the extreme condition prior to the early Earth chemistry.

If prebiotic molecules are built from small atoms or radicals in the cold ISM, the prebiotic molecules must have almost barrier-less formation paths. On the other hand, the bombardment of comets and/or asteroids would have provided very high temperature condition for chemical reactions, which may have led to the decomposition and formation of further complex prebiotic molecules. To understand the formation processes, the quantum chemical calculation is a powerful tool. The previous quantum chemical calculation has already reported the promising chemical paths to amino acids and nucleobases (e.g., [4]).

Here we investigated the possible pathway of pyrimidine, purine, uracil and thymine by the automated exploration of chemical reaction pathways. We have already discovered key dissociations for each molecule. For example, uracil and thymine, the pyrimidine type of nucleobase, have lower barriers to dissociate into an isocyanic acid, which corresponds to the previous laboratory experience, and the rest molecule. Pyrimidine and purine, which are skeleton structures of nucleobases and do not poses any oxygen atoms, have high barriers, implying to require high temperature environment like the bombardment, even though we did not exclude all possibilities of radical reactions. Detailed discussions will be provided on our poster.

References

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