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量子化学計算による星間ダストでのグリシン生成の研究
Quantum chemical calculations of glycine formation in the interstellar medium

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Amino acids in the primitive earth may have been originated in the interstellar medium (ISM). Many amino acids and their precursors were found in the meteorites and were detected in laboratory experiments of UV irradiation on interstellar ice analogs. Moreover, various organic molecules were detected in molecular clouds; recently the detection of amino acid has been expected, especially by ALMA

In this study, we would like to make clear the mechanism of the simplest amino acid, glycine formation in the ISM using accurate quantum chemical calculation (density functional theory; DFT). Glycine formation pathway via hydantoin, which is glycine precursor detected in Murchison meteorite, were investigated. At first, the reactions in the gas-phase were examined. As a result, it was unlikely that glycine was formed during the lifetime of molecular clouds. However, there is a possibility that the reactions proceed with catalysis or the outside energies such as UV and heat.

Organic molecules in the ISM are considered to be generated on icy interstellar dust grains. In a previous study, the reaction barriers in aminoacetonitrille precursor formation pathway become lower with water molecules than those in the gas-phase, since water molecules on the ice core can play crucially a proton-transfer role, facilitating the basic transformations in the glycine formation pathways, [1]. We investigate the hydantoin and glycine formation pathway with one water molecule as a simplest model of ice.

[1] D. M. Koch, et.al. J. Phys. Chem. C112, 2972 (2008)

Keywords: interstellar medium, amino acid