

## 宇宙ダスト上のアミノ酸生成過程についての理論的研究 Theoretical investigation of amino acid formations on interstellar dusts

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Molecular evolution in the interstellar space remains unsolved. Formations of molecules in space have been extensively studied by experiments and space observations. Formations of complex organic molecules are expected in the interstellar space. In fact, some amino acids were found in meteorites and amino acids were detected after UV irradiation of interstellar ice analogs.

In the amino acid formation in space, many precursors and molecular evolution pathways are expected. Among these possible pathways, it is very important to know the energy profiles and molecular structures in the major formation pathways. In this study, possible amino acid formation pathways are investigated by using accurate quantum chemistry methods at the density functional theory levels.

Two formation pathways of glycine and alanine were examined: (1) hydrolysis of aminoacetonitrile and (2) hydrolysis of hydantoin derivatives. In the aqueous solution model, Polarizable Continuum Model was used.

Calculated formation energy of glycine is the most stable in the formation pathway in vacuum and no excessively stable intermediates existed. In aqueous solution, hydantoin pathway was slightly unstabilized. In conclusion, glycine production is considered to be occurred easily if the components exist. Similar trend is expected for the alanine production.

