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Theoretical Investigation of a Mechanism of Chirality Induction for Amino Acids in the Early Solar System

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Present terrestrial life is consisted of L-form amino acids, which are ones of enantiomers. Although L-form and D-form amino acids are generated equivalently by chemical synthesis in a laboratory, only L-form is produced in protein biosynthesis. The origin of chirality for amino acids is not revealed yet and remains as one of the big mysteries in the studies of molecular evolution and the origin of life. To explain it, it is thought that racemic amino acids in interstellar space were destructed asymmetrically by the irradiation of circularly polarized light (CPL) in the early solar system and enantiomeric excess was induced.

Recently, some observational and experimental results supporting this hypothesis have been reported. Amino acids and their precursors have been found in meteorites and their abundances are also biased to L-form. Besides, high circular polarization was observed in the Orion massive star-forming region (OMC-1). In a laboratory, the asymmetric decomposition of amino acid enantiomers by CPL irradiation has been reported. Moreover, it was experimentally proved that low enantiomeric excess could become higher and one enantiomer eventually became dominant. These results support that the origin of life was derived from outside the earth and the chirality of amino acids in life and the inclination found in meteorites should be same derivation. However, some problems to explain this hypothesis are remained, i.e. the mechanism of generation process of amino acids in space and the interaction between amino acid and CPL are not revealed.

To resolve them, the analysis of photo-properties of amino acids is now vital. Especially, the study for the UV light absorbability of amino acids and the destruction or decomposition process is imperative since enantiomeric excess should be mainly derived from the isomerization of racemic amino acids by CPL irradiation. In that sense, the analyses of the excited states for amino acids and their structural changes are important. In particular, it is necessary to study the mechanism of the bond dissociation of a chiral carbon and the carbon connecting to it since it plays a key role for the isomerization reaction.

In this study, we theoretically determined the excited states and potential energy surfaces (PES) for alanine, valine, and isovaline, which are ones of basic amino acids for life and found in meteorites. We first investigated the most stable structures in space at the density functional theory (DFT) level. Then we analyzed the isomerization processes. Especially, their energies, absorption intensities, and circular dichroism (CD) spectra were calculated to predict CPL-induced decompositions of amino acids. C-C bond dissociation pathways were examined in this study.

In the results, we found that the peaks of CD for the amino acids existed in the region of 8-12 eV (100-150 nm wavelength). Four plausible reaction pathways are extracted. For Alanine, the peaks of the absorbance and CD exist at the excitation energy of 9.81 eV. It may lead to the structural decomposition of D-form alanine. For valine, the peaks are found at the excitation energies of 10.00 eV and 10.91 eV. For isovaline, the excitation energy of 9.32 eV is applied to the conditions. These four curves are energetically likely to induce the bond dissociation of C-C and have the peaks of absorption intensity and CD at the ground state.

These results suggest the irradiation of vacuum-ultraviolet (VUV) CPL with the wavelength 110-135 nm for amino acids in space could induce enantiomeric excess. Furthermore, the pathways obtained in this study could be one of the clues to establish the hypothesis that enantiomeric excess based on isomerization was induced by the irradiation of VUV-CPL.

Keywords: enantiomer, amino acid, polarized light, proto-solar nebula