Theoretical study on the alanine formation in interstellar space and the origin of the homochirality

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Abstract

One of the biggest misteries in astrobiology is the origin of the homochirality of amino acids. Why living organisms on the earth selected the L-form amino acid has not been solved yet. In recent years, L-form excesses have been detected in meteorites, besides the circular polarized light (CPL) can be observed in star forming regions. Therefore, a formation of enantiomeric excess from extra-terrestrial environment can be debated scientifically. There exist some laboratory experimental results that CPL can induce the homochirality of amino acid by ~ 1 %.

In the present study, we investigated two major alanine formation pathways: radical and Strecker pathways by using the density functional theory (DFT). We evaluated the key intermediate states with searching their stable conformations and determined the transition states to estimate the reaction rates in the alanine formation. Then, circular dichroism (CD) spectra of all the intermediate states were calculated at the symmetry-adapted cluster-configuration interaction (SAC-CI) theoretical level to characterize the chiral photoabsorption properties. We found that some alanine precursors, nitrile precursors of $HOCHCH_3CN$ and NH_2CHCH_3CN, have high chiral absorption property at Lyman-α wavelength (121nm) region, and they can be attributed to the origin of the alanine homochirality. Detailed theoretical results are presented.

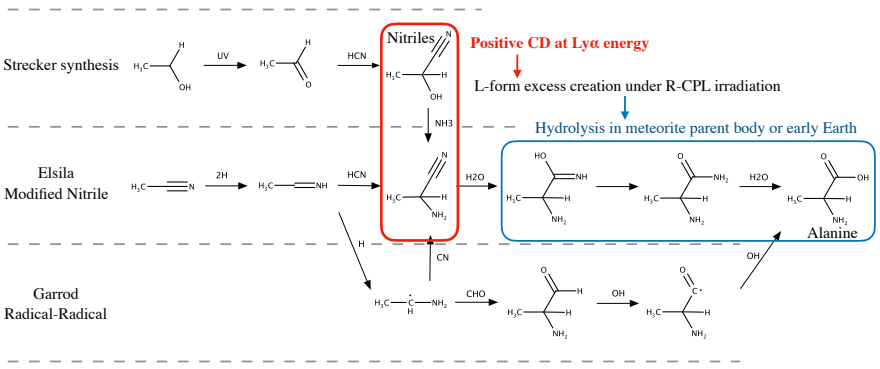

Figure 1: Conceptional diagram of three alanine formation pathways and enantiomeric excess creation mechanism. The D-form nitrile precursors surrounding red line undergoes asymmetric photolysis by R-CPL to form L-enantiomeric excess. Subsequently, these molecules are hydrolyzed inside the meteoritic parent body or on the early earth to become alanine, and finally L-form enantiomeric excess of alanine is created.