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Explanation of the Electron Transfer Mechanism from β-Carotene to N-Pentyl Peroxyl Radical by Density Functional Theory Method

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Abstract : Weak oxidizing radicals, such as alkyl peroxyl derivatives, react with carotenoids through hydrogen atom transfer to form neutral carotenoid radicals. Using the DFT method, it has been observed that s-cis-β-carotene is more stable than all-transforms. In the context of this study, an attempt is made to explain the reaction mechanism of the isomers of β-carotene, which exhibits antioxidant properties, with n-pentyl peroxide, one of the alkyl peroxyl molecules, using the Density Functional Theory (DFT) method. The cis and transforms of β-carotene are used in the study to determine which form is more reactive. For this purpose, Natural Bond Orbital (NBO) charges of all optimized structures are calculated, and electron transfer is determined by examining electron transitions between Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO). Additionally, the radical character and reaction mechanism of β-carotene in a radical environment are attempted to be explained based on the calculations. The theoretical inclination of whether β-carotene in cis or transforms is more active in reaction is also discussed. All these calculations are performed in the gas phase using the Integral Equation Formalism Polarizable Continuum Model IEFPCM method with dichloromethane as the solvent.

Keywords : β-carotene, n-pentyl peroxyl radical, DFT, TD-DFT
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