

Abstract Submitted
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Thermodynamic Analysis of Compounds in the Antiaging Components and the Reactive Oxygen Species(ROS) JONG HA LEE , JAEYEON PARK, NIKITA PATEL, Choice Research Group — This research paper uses computational analysis to figure out the thermodynamic stability of various compounds used in anti-aging antioxidant. Primary method to determine such stability include finding the optimal shape based on stereochemistry. Reactive Oxidation Species (ROS) causes a shift in cell structure as it allows highly reactive chemicals to bond to the nucleus of cells. The results of such changes lead to cell aging. In this paper, we investigate the safety and stability of the components used in vitamin E such as α -, β -, γ -, and δ -tocopherol and α -, β -, γ -, and δ -tocotrienol, which reduce the level of ROS of our body cells. This is achieved via studying the stereochemistry of the compounds by using computational thermodynamic analysis and force optimizations. Molecules that we examined include a few isomers of fullerenes. Density Functional Theory (DFT), a computational chemistry technique, is used in order to model the electron properties of the compound. The research validates that chemical compounds that have lower optimization energy are more safe and effective to be used in anti-aging products.

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