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Thermodynamic Analysis of Compounds in Sunscreen and the Cancer-Causing Reactive Oxygen Species (ROS) RICHARD KYUNG, JOHYUN LEE, Choice Research Group — This research paper uses computational analysis to determine the physical and thermodynamic stability of various compounds used in sunscreen. The two primary methods to determine such stability include finding the optimal shape of the materials and computing the measures of oxidizing ability. Reactive Oxidation Species (ROS) causes a harmful shift in cell structure as it allows highly reactive chemicals to bond to the nucleus of cells. The results of such changes that occur within cells are mutated cells, which can be the leading cause of cancer. In this paper, we investigate the safety of the components used in sunscreens and the possibility of replacing existing chemical compounds to reduce the level of ROS. This is achieved via studying the shape and reactivity of the structures by using computational thermodynamic analysis and force optimizations. Molecules that we examined include oxybenzone, octocrylene, metal oxides, and fullerenes. Density Functional Theory (DFT), a computational chemistry technique, is used in order to model the electron properties of the compound. The results of the computational analysis validate that oxide chemical compounds and fullerene derivatives, which have lower optimzation energy, are more safe and effective to be used in suncreen.

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