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Thermodynamic Analysis of the Fullerene Nano Molecules Used in PDT(Photodynamic Therapy) JUN SUK KIM, YOUJUNG LEE, NIKITA PATEL, Choice Research Group — When advanced photoactive nanomaterials, such as functionalized fullerenes and carbon nanotubes(CNTs) contact Near Infrared Radiation (NIR), the resulting material behaves like a CNT nanobomb (CNT-NB), a key element in this cancer treatment. Treatment of cancer cells with CNTs with an antibody or substituted fullerenes and subsequent emission of NIR (700-1100 nm) result in the heating up of CNT-NBs. This heat is powerful, causing extermination of the bodys cancerous cells. Computational analysis of the unique structure of fullerenes and carbon nanotubes (CNTs) accounts for their high potential to be used as nanocarriers (NCs) in cancer therapy. As nanocarriers, the molecules distinct surface properties allow for enhanced function of absorption and/or bio-conjugation of various moieties. In this paper, we used Avogadro to compare the safety and stability of the CNT and fullerenes, which are doped with various types of clusters, by checking their optimized molecular energy both stereochemically and thermodynamically. The software enabled us to calculate and determine optimized energy, determine the structural formulae, and model the electronic structures of the optimized molecules.

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