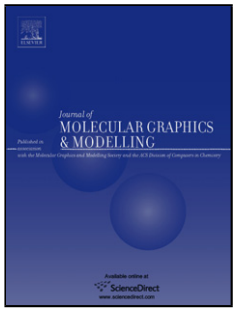

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PII: S1093-3263(16)30339-4
DOI: http://dx.doi.org/doi:10.1016/j.jmgm.2017.03.017
Reference: JMG 6878

To appear in: *Journal of Molecular Graphics and Modelling*

Received date: 28-10-2016
Revised date: 23-3-2017
Accepted date: 24-3-2017

Please cite this article as: Don Betowski, Predicted phototoxicities of carbon nano-material by quantum mechanical calculations, Journal of Molecular Graphics and Modellinghttp://dx.doi.org/10.1016/j.jmgm.2017.03.017

Predicted phototoxicities of carbon nano-material by quantum mechanical calculations

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Abstract

The purpose of this research was to develop a predictive model for the phototoxicity potential of carbon nanomaterials (fullerenols and single-walled carbon nanotubes). This model is based on the quantum mechanical (*ab initio*) calculations on these carbon-based materials and comparison of the triplet excited states of these materials to published work relating phototoxicity of polynuclear aromatic hydrocarbons (PAH) to their predictive triplet excited state energy. A successful outcome will add another tool to the arsenal of predictive methods for the U.S. EPA program offices as they assess the toxicity of compounds in use or coming into commerce.

The basis of this research was obtaining the best quantum mechanical structure of the carbon nanomaterial and was fundamental in determining the triplet excited state energy. The triplet excited state, in turn, is associated with the phototoxicity of the material.

This project relies heavily on the interaction of the predictive results (physical chemistry) and the experimental results obtained by biologists and toxicologists. The results of the experiments (toxicity testing) will help refine the predictive model, while the predictions will alert