CARBON NANOPARTICLES: QUANTUM-MECHANICAL AND QSAR MODELING OF FULLERENE C_{60} SOLUBILITY IN ORGANIC SOLVENTS

Tetyana Petrova\textsuperscript{1}, Bakhtiyor F. Rasulev\textsuperscript{1}, Andrey A. Toropov\textsuperscript{1}, Danuta Leszczynska\textsuperscript{2}, Jerzy Leszczynski\textsuperscript{1}

\textsuperscript{1}Interdisciplinary Center for Nanotoxicity, Department of Chemistry and Biochemistry, Jackson State University, Jackson, MS 39217, USA
\textsuperscript{2}Department of Civil and Environmental Engineering, Jackson State University, 1400 J.R. Lynch St, Jackson, MS 39217, USA

Abstract: The interaction between nanostructured materials and living systems is of fundamental and practical interest and will determine the biocompatibility, potential utilities and applications of novel nanomaterials in biological settings. C\textsubscript{60} and its derivatives, because of their large size, stability and hydrophobic character, may prove to have values as diagnostic or therapeutic agents in medicine. The solution property, such as solubility, of C\textsubscript{60} has been of great interest to numerous fullerene investigators owing to its fundamental importance and practical interest in fullerene research. Fullerenes are sparingly soluble in many solvents. The dependence of fullerene’s solubility on molecular structure of the solvent must be understood in order to efficiently separate different members of the fullerene family from each other and from their precursors or derivatives. Current work was devoted to the investigation of the solubility of fullerene C\textsubscript{60} in 122 organic solvents using \textit{ab initio} quantum-chemical calculations in combination with quantitative structure-property relationship (QSPR) tools. The employed GA-MLRA approach augmented by application of quantum-chemical calculations yields reliable results, allowing one to build simple, interpretable and transparent models that can be used for future predictions of C\textsubscript{60} solubility in various organic solvents and to provide basics for understanding of this mechanism. The additional quantum-mechanical calculations of C\textsubscript{60} solubility by different methods (DFT, HF, semi-empirical methods) using thermodynamically based polarized continuum model (CPCM) showed an interesting parabolic correlation of total energy of solvated fullerene and experimental solubility. This approach can be used as good preliminary predictor for fullerenes’ solubility in various solvents.

Keywords: Fullerene, quantum-chemical calculation, quantitative structure-property relationships