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Theoretical and Quantitative Structural Relationship Study of the Electrochemical Properties of [M-2@C-x]@[SWCNT(5,5)-Armchair-CnH20] (M = Er and Sc, x=82 and 84, and n=20-300) Complexes

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Abstract. One of the nanoscale structures of carbon is the carbon nanotubes. These structures of carbon display an attractive variation of structural characteristics, and many useful forms have been synthesized and identified. Carbon nanotubes are either single-wall (SWCNT) or multiwall (MWCNT); the former attract attention due to their unique electronic, optical, and spectroscopic properties. One of the main recognized structures of single-walled nanotubes is the (5,5) single-walled tube. Endohedral metallofullerenes (M-n@C-x) were introduced as a new class of spherical fullerenes group with unique properties. Formation of endohedral metallofullerenes is thought to involve the transfer of electrons from the encapsulated metal atom(s) to the surrounding fullerene cage. Two of these molecules are Er-2@C-82 (1) and Sc-2@C-84 (2). A topological index is a mathematical invariant of a chemical graph, which shows a significant correlation with some chemical or physical properties. Topological indices have been successfully used to construct effective and useful mathematical methods for finding good relationships between structural data and the properties of these materials. To establish a good structural relationship between the structure of molecules Sc-2@C-84, Er-2@C-82, and [SWCNT(5,5)-Armchair-CnH20] (n = 20-190) 320, the molecular degree of unsaturation (Du) was used as one of the useful numerical and structural properties of unsaturated compounds. In this study, the relationship between this index and the free energy of electron transfer (Delta G(et)) as assessed using the Rehm-Weller equation on the basis of the first oxidation potential (E-ox(1)) of Sc-2@C84 and Er-2@C-82 for the predicted supramolecular complexes between 3-20 and the endohedral metallofullerenes Sc-2@C-84 and Er-2@C-82 as [M-2@C-x]@[SWCNT(5,5)-Armchair-CnH20] (M = Er and Sc, x = 82 and 84, and n = 20-190) 21-38 and 39-56 are presented. The results were extended for [M-2@C-x]@[SWCNT(5,5)-Armchair-CnH20] (M = Er and Sc, x = 82 and 84, and n = 200-300) 68-78 and 79-89.

Keywords. Wall carbon nanotubes; Density-functional thermochemistry; Endohedral metallofullerene; Electronic-structure; Topological indexes; Exact exchange; Fullerenes; C-60; Molecules; Isomers

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