# Theoretical Study of Structural Relationships and Electrochemical Properties of Supramolecular [Tetracyclines].Cn Complexes

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**Abstract:** Tetracyclines are a broad spectrum of antibiotics that are commonly used in human pathologies as well as in veterinary medicine as animal nutrition and feed additives for cattle growth. The electrochemical oxidation of the tetracycline antibiotics was studied at various carbon electrodes including glassy carbon (GC), as deposited BDD (boron-doped diamond thin film) and anodized BDD electrodes using cyclic voltammetry. Since the discovery of fullerenes (Cn), one of the main classes of carbon compounds, the unusual structures and physiochemical properties of these molecules have been discovered, and many potential applications and physicochemical properties have been introduced. Up to now, various empty carbon fullerenes with different numbers on,o such as C60, C70, C76, C82 and C86, have been obtained. Topological indices are digital values that are assigned based on chemical composition. These values are purported to correlate chemical structures with various chemical and physical properties. They have been successfully used to construct effective and useful mathematical methods to establish clear relationships between structural data and the physical properties of these materials. In this study, the number of carbon atoms in the fullerenes was used as an index to establish a relationship between the structures of Tetracycline (TC), Chlortetracycline (CTC), Doxytetracycline (DTC) and Oxyteracycline (OTC), 1-4 and fullerenes Cn (n=60, 70, 76, 82 and 86), which create [Tetracyclines].Cn, A-1 to A-5 ([TC].Cn), B-1 to B-5 ([CTC].Cn), C-1 to C-5 ([DTC].Cn) and D-1 to D-5 ([OTC].Cn). The relationship between the number of carbon atoms and the free energies of electron transfer (Get(1) to Get(4) ) are assessed using the Rehm-Weller equation for A-1 to A-5, B1 to B-5, C-1 to C-5 and D-1 to D-5 supramolecular [Tetracyclines].Cn complexes 5-24. Calculations are presented for the four reduction potentials ( Red.E1 to Red.E4 ) of fullerenes Cn . The results were used to calculate the four free-energies of electron transfer (Get(1) to Get(4) ) of supramolecular complexes A-1 to A-19 to B-1 to B-19, C-1 to C-19 and D-1 to D-19 (5-81) for fullerenes C60 to C300.

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