Fullerenes, Nanotubes and Carbon Nanostructures
Volume 17, Issue 2 March 2009, pages 171 - 186.

Structural Relationship Study of Electrochemical Properties of the Nano Structures of Cis-unsaturated Thiocrown Ethers and Their Supramolecular Complexes [X-UT-Y][La@C72(C6H3Cl2)] Non-IPR Carbon Cage

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Abstract

The structure of fullerenes allows exohedral and endohedral chemistries to be distinguished. Since the discovery of the metalofullerenes as one of the class of organo-metal compounds, the unusual structures and properties of these molecules and by the many potential applications have been obtained. It has been known as the isolated pentagon rule (IPR) that all pentagons are isolated in the most stable fullerene. Endohedral metalofullerenes M@Cx 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. One of these molecules is the La@C72. It is determined that La@C72 has a non-IPR carbon cage. The addition of a dichlorophenyl radical on La@C72 leads to La@C72 (C6H3Cl2) (10-12) with a closed shell structure. Unsaturated thiocrown ethers with cis-geometry [X-UT-Y](where, UT is the abbreviation of Unsaturated Thiocrown ethers, X and Y are the numbers of carbon and sulfur atoms, respectively) 1-9 are a group of crown ethers that, in light of their conformational restriction compared to a corresponding saturated system, and the size their cavities, (1-9) demonstrate interesting properties for physicochemical studies. The supramolecular complexes of 1-9 with 10-12 have shown here to possess a host-guest interaction for electron transfer processes, and these behaviors have not previously been reported. To establish a good structural relationship between the structures of 1-9 with La@C72 (C6H3Cl2) that they were introduced here was utilized an index that is introduced by cs . This index is the ratio between the sum of carbon (nc) and sulfur atoms (ns) and the product of nc and ns for 1-9. In this study, the relationship between this index and oxidation potential (oxE1) of 1-9, as well as the free energy of electron transfer (Get , by the Rehm-Weller equation) between 1-9 and La@C72(C6H3Cl2) (10-12) as [X-UT-Y][La@C72(C6H3Cl2)-Z] (where Z is the adduct (A, B and C) isomers of dichlorophenyl group) (13-15) supramolecular complexes are presented and investigated.

Keywords: *Endohedral metalofullerenes; IPR; Non-IPR carbon cage; Rehm-Weller equation; Oxidation potential; Unsaturated thiocrown ethers; Molecular modeling; Molecular topology*

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