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

TAHERPOUR, Avat Arman

Univ Queensland, Sch Mol & Microbial Sci, Unusual Mol & React Intermediates Grp, Chem Bldg, Brisbane, Qld 4072 Australia

&

Islam Azad Univ, Fac Sci, Dept Chem, Arak, Iran
avatarman.taherpour@gmail.com

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
References
1. ***. PHYS WORLD 13; 2000
2. ANDERSON MR. Making connections between metallofullerenes and fullerenes: electrochemical investigations. CARBON 38:1663; 2000
3. ARELLANO JS. Interaction of molecular and atomic hydrogen with (5,5) and (6,6) single-wall carbon nanotubes. JOURNAL OF CHEMICAL PHYSICS 117:2281; 2002
4. AVOURIS P. Molecular electronics with carbon nanotubes. ACCOUNTS OF CHEMICAL RESEARCH 35:1026; 2002
5. BANDOW S. Smallest limit of tube diameters for encasing of particular fullerenes determined by radial breathing mode Raman scattering. CHEMICAL PHYSICS LETTERS 347:23; 2001
6. BARNETT R. Superconducting and charge-density wave instabilities in ultrasmall-radius carbon nanotubes. SOLID STATE COMMUNICATIONS 135:335; 2005
7. BECKE AD. DENSITY-FUNCTIONAL THERMOCHEMISTRY. 3. THE ROLE OF EXACT EXCHANGE. JOURNAL OF CHEMICAL PHYSICS 98:5648; 1993
8. BOLBOACA SD. How good can the characteristic polynomial be for correlations? INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES 8:335; 2007
10. COLLINS PG. SCI AM 283:38; 2000
11. DENNIS TJS. Isolation and characterisation of the two major isomers of [84]fullerene (C- 84). CHEMICAL COMMUNICATIONS :619; 1998
12. DRESSELHAUS MS. CARBON-FIBERS BASED ON C-60 AND THEIR SYMMETRY. PHYSICAL REVIEW B 45:6234; 1992
13. DRESSELHAUS MS. SCI FULLERENES CARBO. 1996
14. DRESSELHAUS SM. CARBON NANOTUBES SYN. 2001
15. DU YP. J CHEM INF COMP SCI 42:1128; 2002
16. FOWLER PW. ATLAS FULLERENES 30; 1995
17. FUCHS D. Extraction and chromatographic elution behavior of endohedral metallofullerenes: Inferences regarding effective dipole moments. JOURNAL OF PHYSICAL CHEMISTRY 100:725; 1996
19. HANSEN PJ. CHEMICAL APPLICATIONS OF GRAPH-THEORY. 1. FUNDAMENTALS AND TOPOLOGICAL INDEXES. JOURNAL OF CHEMICAL EDUCATION 65:574; 1988
20. HAUFLE RE. EFFICIENT PRODUCTION OF C60 (BUCKMINSTERFULLERENE), C60H36, AND THE SOLVATED BUCKIDE ION. JOURNAL OF PHYSICAL CHEMISTRY 94:8634; 1990
21. HOFFMAN KR. Spectroscopic studies of fullerenes doped with rare earth and transition metal ions. JOURNAL OF LUMINESCENCE 66:244; 1995
22. HOSOYA H. TOPOLOGICAL INDEX - NEWLY PROPOSED QUANTITY CHARACTERIZING TOPOLOGICAL NATURE OF STRUCTURAL ISOMERS OF SATURATED HYDROCARBONS. BULLETIN OF THE CHEMICAL SOCIETY OF JAPAN 44:2332; 1971
23. IIDUKA Y. CHEM COMMUN 2057:2059; 2006
25. JANDA P. Nanostructuring of highly ordered C-60 films by charge transfer. ADVANCED MATERIALS 10:1434; 1998
29. Kimura K. Evidence for substantial interaction between Gd ion and SWNT in (Gd@C-82)(n)@SWNT peapods revealed by STM studies. Chemical Physics Letters 379:340; 2003
40. Pichler T. Proof for trivalent Sc ions in Sc-2 @ C-84 from high-energy spectroscopy. Physical Review B 62:13196; 2000
44. Rehm D. Kinetics of fluorescence quenching by electron and h-atom transfer. Israel Journal of Chemistry 8:259; 1970
47. Shen HJ. The compressive mechanical properties of C-n (n=20, 60, 80, 180) and endohedral M@C-60 (M = Na, Al, Fe) fullerene molecules. Molecular Physics 105:2405; 2007
48. SHERIGARA BS. Electrocatalytic properties and sensor applications of fullerenes and carbon nanotubes. ELECTROANALYSIS 15:753; 2003
49. SLANINA Z. Ca@C-82 isomers: Computed temperature dependency of relative concentrations. JOURNAL OF CHEMICAL PHYSICS 120:3397; 2004
50. SLANINA Z. MATCH COMMUN MATH CO 44:335; 2001
51. SMALLEY RE. DOPING THE FULLERENES. ACS SYMPOSIUM SERIES 481:141; 1992
52. SMITH BW. NATURE 396:3239; 1998
53. SRIVASTAVA D. Computational nanotechnology with carbon nanotubes and fullerenes. COMPUTING IN SCIENCE & ENGINEERING 3:42; 2001
54. SRIVASTAVA D. P IEEE SUP:97; 1997
55. SRIVASTAVA D. Nanoplasticity of single-wall carbon nanotubes under uniaxial compression. PHYSICAL REVIEW LETTERS 83:2973; 1999
57. SUENAGA K. Direct imaging of Sc-2@C-84 molecules encapsulated inside single-wall carbon nanotubes by high resolution electron microscopy with atomic sensitivity. PHYSICAL REVIEW LETTERS 90:ARTN055506; 2003
59. TAHERPOUR A. Quantitative relationship study of mechanical structure properties of empty fullerenes. FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES 16:196; 2008
60. TAHERPOUR A. The structural relationship between Randic indices, adjacency matrixes, distance matrixes and maximum wave length of linear simple conjugated polyene compounds. JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 726:183; 2005
61. TAHERPOUR AA. 2 INT C CHEM ED SUST; 2004
62. TAHERPOUR AA. AUST J ED CHEM 65:37; 2005
63. TAHERPOUR AA. Structural relationship between degree of unsaturation with polarizability of (5,5) armchair single-wall carbon nanotubes. FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES 15:279; 2007
64. TAHERPOUR AA. NANO TUBES CARBON NAN 17:26; 2009
65. TOPOL IA. Experimental determination and calculations of redox potential descriptors of compounds directed against retroviral zinc fingers: Implications for rational drug design. PROTEIN SCIENCE 10:1434; 2001
66. TOUZIK A. Nanostructuring of potassium fulleride layers. EUROPHYSICS LETTERS 60:411; 2002
67. WANG CR. A scandium carbide endohedral metallofullerene: (Sc2C2)@C-84. ANGEWANDTE CHEMIE-INTERNATIONAL EDITION 40:397; 2001
68. WEAVER JH. XPS PROBES OF CARBON-CAGED METALS. CHEMICAL PHYSICS LETTERS 190:460; 1992
69. WIENER H. J AM CHEM SOC 17:20; 1947
70. XIE QS. ELECTROCHEMICAL DETECTION OF C-60(6-) AND C-70(6-) - ENHANCED STABILITY OF FULLERIDES IN SOLUTION. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 114:3978; 1992
71. YAKOBSON BI. MECH PROPERTIES CARB :293; 2001
72. YAKOBSON BI. Nanomechanics of carbon tubes: Instabilities beyond linear response. PHYSICAL REVIEW LETTERS 76:2511; 1996
73. YANNONI CS. SCANDIUM CLUSTERS IN FULLERENE CAGES. SCIENCE 256:1191; 1992
74. ZHANG M. Thermogravimetric analysis for the array of C-60 molecules formed in single-wall carbon nanotube. CHEMICAL PHYSICS LETTERS 369:680; 2003
75. ZHOU ZY. Electronic structure of tubular aromatic molecules derived from the metallic (5,5) armchair single wall carbon nanotube. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 126:3597; 2004