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Topological Relationship Between Wiener Index in contrast to the Energy and Electric Moments in TUVC6[2p, q] with Same Circumference and Various Lengths

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ABSTRACT

Topological indices are one of the oldest and most widely used descriptors in Quantitative Structure Properties Relationships (QSPR). Amongst the topological indices used as descriptors in QSPR, the Wiener index is by far the most popular index, as it has been shown that the Wiener index has a strong correlation with the chemical properties of the compound.
In this study, the relationship between some of the Wiener index in contrast to the electric moments and energy ($kJmol^{-1}$) of some armchair polyhex carbon nanotubes $TUVC_6[2p, q]$ with same circumference [2p] and various length [q] are presented. The results are performed by use of the Gaussian 98 program at the Restricted Hartree-fock (RHF) levels with the 3-21G basis set.

Keywords: Armchair carbon Nanotubes; Wiener index; Electric moment, Ab initio method; Molecular topology.

INTRODUCTION

Carbon nanotubes were first discovered in 1991 by S. Iijima [1-3]. Single Walled Carbon Nanotubes (SWNT) can be imagined as rolled-up rectangular strips of hexagonal graphite monolayers. Two of these correspond to high symmetry SWNT's; in zigzag tubes, some of the C-C bonds lie parallel to the tube axis, while in armchair tubes, some bonds are perpendicular to the axis (see scheme-1). Study about properties of nanotubes with medicinal and electronic applications have been made the highly useful and effective results for applications in different areas of science.

Graph theory [4, 5] is a branch of mathematics concerned about how networks can be encoded and their properties measured. In chemical graph theory and in mathematical chemistry, a topological index is any of several numerical parameters (which are usually graph invariants) of a graph which characterize its topology. It is a kind of a molecular descriptor

The Wiener index is the first topological index recognized in chemical graph theory, and it is often referred to as "the" topological index. Usually topological indices do not recognize double bonds and atom types (C, N, O etc.), ignore hydrogen atoms and defined for connected undirected molecular graphs only [6] .

In this study, the relationship between the Wiener topological index in contrast to the electric moments and energy ($kJmol^{-1}$) of some armchair polyhex carbon nanotubes $TUVC_6[2p, q]$ with same circumference [2p: 6] and various length [q: 3-14] are presented. The results are performed by use of the Gaussian 98 program at

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the Restricted Hartree-fock (RHF) levels and with the 3-21G basis set. The relationships between this topological index of $TUVC_6[2p, q]$ nanotubes with the mentioned molecular properties are presented and discussed.

Topological Indices

A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it does not depend on the labelling or the pictorial representation of a graph. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules. Here, we consider Wiener topological index (W).

Wiener Index

Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffins. The Wiener index [7-12] is one of the oldest molecular graph based structure descriptors and its chemical applications are well documented, see for details. In a series of papers, Diudea and coauthors [13-21] studied the mathematical property of some nanotubes. They also computed the Wiener index of some of these nanotubes.

The Wiener index of a graph G is defined as the sum of all distances between distinct vertices of G. The formula for computing the Wiener index of armchair polyhex nanotube in the terms of their circumference [2p] and their length [q], is as follow [22]:

In the case: $q \geq p$

$$WTUVC_6(p,q) = \frac{p}{12}[p^2(12q^2-2p^2+8) + 8pq(p^2+q^2-2)+3(-1+1-1)^p)]$$

In the case: $q \leq p$

$$WTUVC_6(p,q) = \frac{p}{12}[24\,p^2\,q^2 - 2q^4 - 8q^2 + 3\,(-1)^p(1-(-1)^p)]$$

Mathematical Method and Design Model

The following structure-property models are the most successful for the logarithm of Wiener index considered.

$$\text{Log } E = 0.4051(\text{ Log}W) + 5.1650 \qquad (4)$$

$R^2 = 0.9989$

$$\text{Log } Q = 1.2267(\text{ Log } W) + 2.7845 \qquad (5)$$

$R^2 = 0.9990$

$$\text{Log } H = 2.1355(\text{ Log } W) + 3.4295 \qquad (6)$$

$R^2 = 0.9949$

Computational Methods

Energy and electric polar moments and molecular topological index discussed in this report were shown in table 1. The determinant concern with the above matrixes solved by using MAPLE- 9.5 package implemented to a personal computer.

Our structures optimization and the total energy calculations are performed by use of the Gaussian 98 program at the Restricted Hartree-fock (RHF) levels with the 3-21G basis set.

Graphs

The Microsoft office Excel-2003 program was utilized for drawing the graphs of results.

RESULTS AND DISSCUSSION

The values of energy ($kJmol^{-1}$), electric quadrupole, hexadecapole moments of armchair polyhex carbon nanotubes $TUVC_6[2p, q]$, (C_{18}, C_{30}, C_{42}, C_{54}, C_{66}, C_{78}, C_{84}), with [p: 3, q: 3, 5, 7, 9, 11, 13, 14] increasing in tube length and number of carbon were shown in table 1.

Energy and electric moments of these nanotubes were performed at the Restricted Hartree-fock (RHF) levels on 3-21G basis set using the standard procedure in Gaussian 98 package.

The values of the Wiener topological index discussed in this report increase with the number of carbon or increase in nanotube length [q], (see table.1). In accordance with the data of table.2, the logarithm values of Wiener index increase by increasing value of the logarithmic energy and electric quadrupole, hexadecapole moments of armchair carbon nanotubes $TUVC_6[2p,q]$ in (C_{18}, C_{30}, C_{42}, C_{54}, C_{66}, C_{78}, C_{84}).

The equations 1 to 3 were utilized to predict the values of the energy and electric quadrupole, hexadecapole moments of $TUVC_6[2p, q]$ with same circumference [2p: 6], various lengths [q: 4, 6, 8, 10, 12] or (C_{24}, C_{36}, C_{48}, C_{60}, C_{72}).

In tables 3, the predicted and Gaussian values of the related data due to the armchair carbon nanotubes $TUVC_6[2p, q]$ in (C_{24}, C_{36}, C_{48}, C_{60}, C_{72}) were compared.

In figures 1, 2 and 3 ,,was attempted to show two dimensional diagrams of the relationship between logarithmic values of W index and

logarithmic values energy and logarithmic electric hexadecapole moments of $TUVC_6$ [2p, q] in (C_{18}, C_{30}, C_{42}, C_{54}, C_{66}, C_{78}, C_{84}).

In those curves, there are good correlation between the value after calculating, the indices previously defined, partial least squares regression was performed and the best model was taken as the one presenting the optimal value of prediction coefficient, taking into account the number of descriptors used [Eq.1-3] That is, if the election of a major number of parameters did not justify the quality of the model, it was rejected. Furthermore the results of such studies were used to get into the quantitative structure-property relationship (QSPR) subjects.

CONCLUSION

The most accurate QSPR models for $TUVC_6$[2p, q] electric quadrupole, hexadecapole moment are based on Log W. The results show that energy and electric quadrupole and hexadecapole moments of some $TUVC_6$ [2p, q] such as (C_{24}, C_{36}, C_{48}, C_{60}, C_{72}) could be well predicted by utilizing the model. In this study, The relationship between W index with the molecular properties (the electric moments and energy) has been studied and model for designing the quantitative structure-property relationships based on topological indices was presented.

Table1. The values of energy (E/kJmol^{-1}), electric quadrupole (Q), hexadecapole (H) Moments and Wiener index (W) of armchair polyhex carbon nanotubes $TUVC_6$[2p, q]. (C_{18}, C_{30}, C_{42}, C_{54}, C_{66}, C_{78}, C_{84})

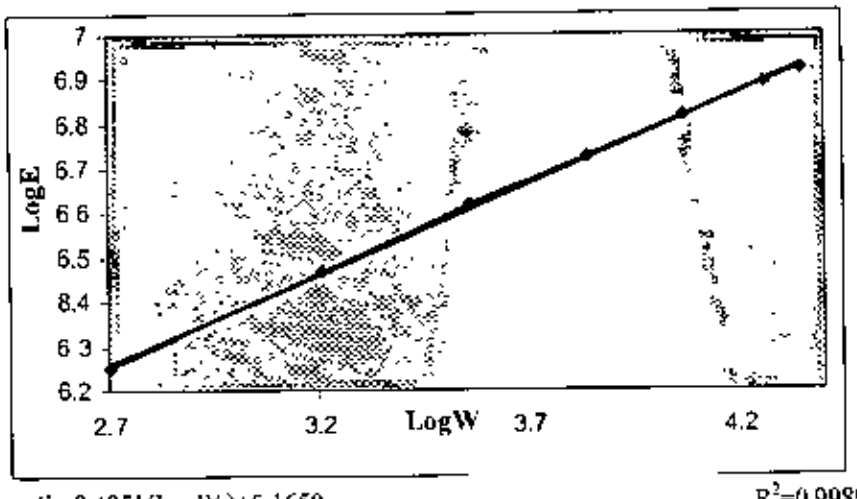
$TUVC_6$[2p,q]	E(kJmol^{-1})	Q Moment	H Moment	W Index
C_{18}	1775952.3790	1171598.3540	1552150596	507
C_{30}	2961763.3360	5528717.6190	20964456420	1611
C_{42}	4147462.8530	15185345.7400	1.13273E+11	3651
C_{54}	5333030.1760	32204157.3000	4.13293E+11	6915
C_{66}	6518765.9810	60413894.9900	1.10807E+12	11691
C_{78}	7704392.0160	99167167.8000	2.55255E+12	18267
C_{84}	8297239.4350	125268644	7.58195E+12	22320

Table2. Logarithmic values of energy, electric quadrupole and hexadecapole moments, Wiener index of armchair polyhex carbon nanotube $TUVC_6$[2p, q]. [p: 3, q: 4, 6, 8, 10, 12]

$TUVC_6$[2p,q]	Log E	Log Q	Log H	Log W
C_{18}	6.2494	6.0687	9.1909	2.705
C_{30}	6.4715	6.7426	10.3215	3.2071
C_{42}	6.6178	7.1814	11.0541	3.5624
C_{54}	6.7269	7.5079	11.6162	3.8398
C_{66}	6.8141	7.7811	12.0445	4.0678
C_{78}	6.8867	7.9964	12.4069	4.2616
C_{84}	6.9189	8.0978	12.8798	4.3487

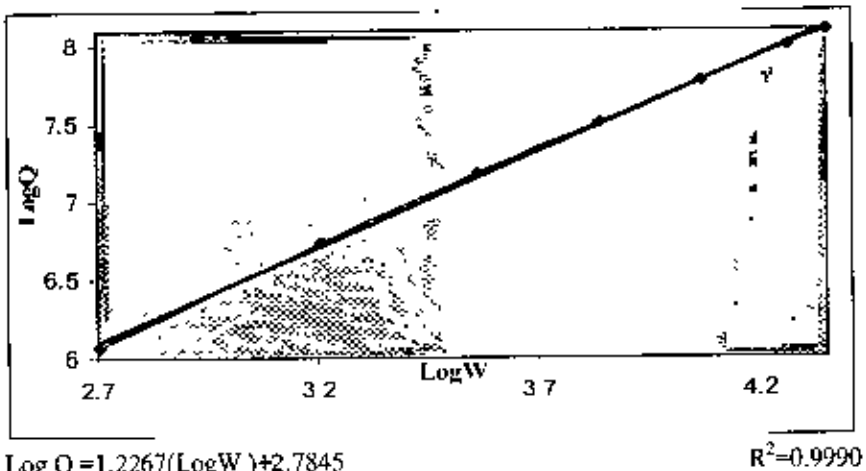
Table3. Comparison between predicted (Models 1, 2, 3) and Gaussian values of electric hexadecapole moments of armchair polyhex carbon nanotube $TUVC_6$[2p, q], [p: 3, q: 4, 6, 8, 10, 12]

$TUVC_6$[2p,q]	$LogE_{(Cal)}$-$LogE_{(Gauss)}$	$LogQ_{(Cal)}$-$LogQ_{(Gauss)}$	$LogH_{(Cal)}$-$LogH_{(Gauss)}$
C24	-0.0014	-0.0004	-0.0224
C36	-0.0096	-0.0220	-0.0327
C48	-0.0085	-0.0286	-0.1022
C60	-0.0040	-0.0105	0.0493
C72	0.0017	-0.0020	-0.2016



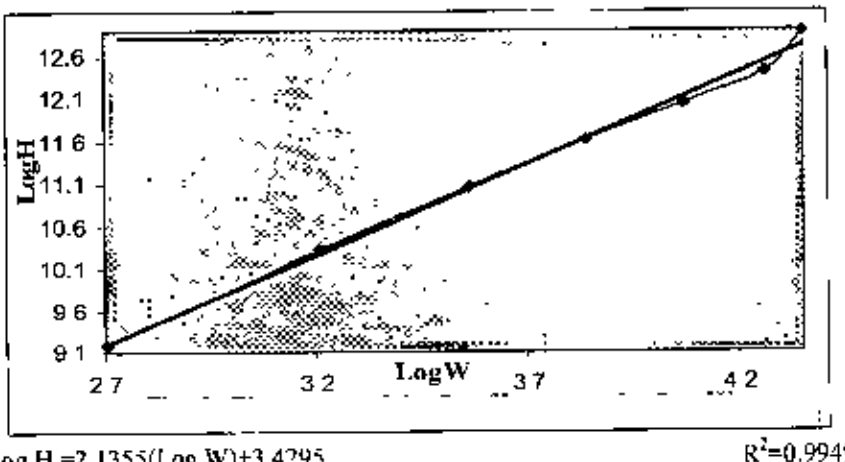
LogE =0 4051(LogW)+5.1650 R^2=0.9989
LogE=0.0066(LogW)^3-0 0983(LogW)^2+0 8504(LogW)+4 5379 R^2=1.0000

Fig.1. The curve of the LogE versus the LogW



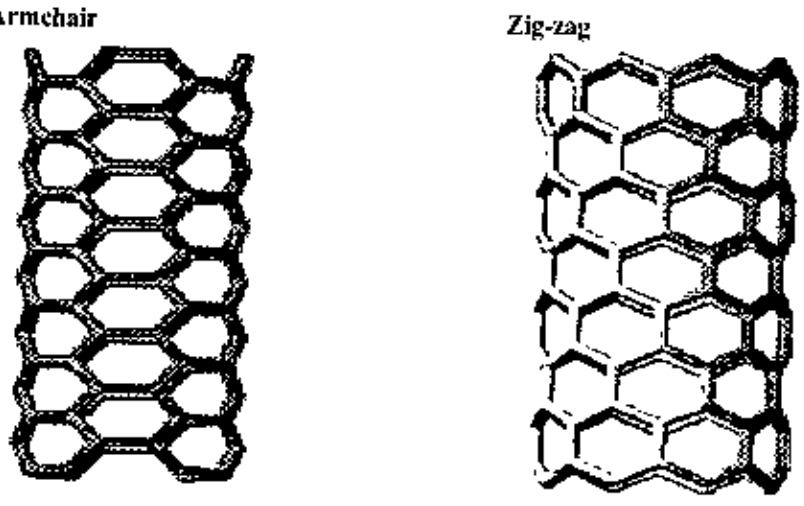
Log Q =1.2267(LogW)+2.7845 R^2=0.9990
LogQ=0 0313(LogW)^3-0.4127(LogW)^2-2.9582(LogW)+0.4683 R^2=1.0000

Fig.2. The curve of the LogQ versus the LogW



Log H =2.1355(Log W)+3.4295 R^2=0.9949
LogH=0.4765(LogW)^3-5.0196(LogW)^2+19 493 (LogW)-16.247 R^2=0.9968

Fig.3. The curve of the LogH versus the LogW



Scheme1. Two types of single-wall nanotubes.

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