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Topological relationship between electric quadrupole, hexadecapole moments, energy and Padmakar–Ivan index in armchair polyhex nanotubes TUVC$_6$[2p,q]

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ABSTRACT

The electric quadrupole, hexadecapole moments, energy (kJmol $^{-1}$) for some armchair polyhex carbon nanotubes TUVC$_6$[2p,q] are performed by Beck-Lee-Yang-Parr [B3LYP] on 3-21G basis set using the standard procedure indices GAUSSIAN 98, then the Padmakar-Ivan (PI) index of TUVC$_6$[2p,q] nanotubes in the terms of their circumference (2p) and lengh (q) is calculated and the relationships between the Padmakar-Ivan index of TUVC$_6$[2p,q] nanotubes with the above mentioned molecular properties is studied.

Keywords: Padmakar-Ivan index; Armchair polyhex nanotubes; Graph theory; QSPR; Electric hexadecapole moment; Electric quadrupole moment

INTRODUCTION

Carbon nanotubes (CNTs) were first discovered in 1991 by Iijima [1]. CNTs are peri-condensed benzenoids composed of sp^2 carbon atoms, which in turn are ordered in a graphite-like hexagonal pattern. CNTs may be derived from graphite by rolling up the rectangular sheets along certain vectors, Figure a. Rectangular sheets may be rolled up along a vertical axis, yielding zig-zag CNTs, or along the horizontal axis, yielding armchair CNTs, Figure b.

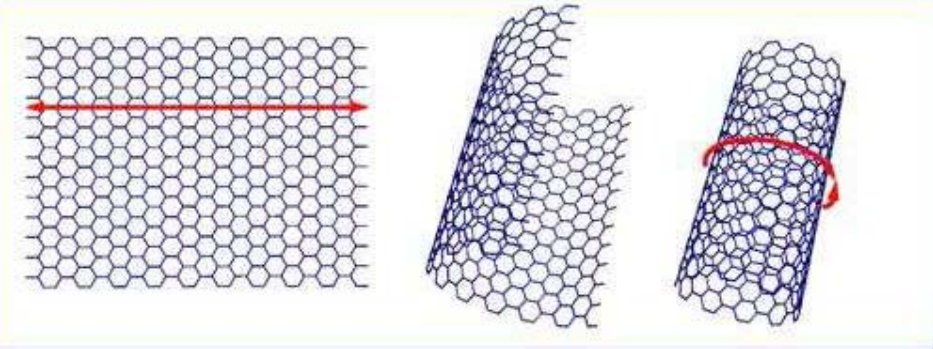

Figure a. Graphite to armchair CNT from [2].

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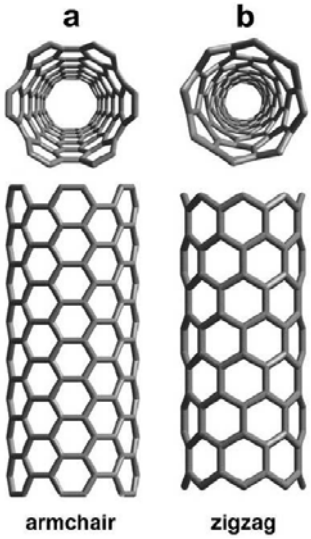

Figure b. Armchair and zig-zag CNT from [2].

Single wall carbon nanotubes (SWNT's) can display metallic or semiconducting character depending on their chiralities and diameters [3-5] similar to the aforementioned idea exploited extensively in crystals [6], quantum structures can also be produced in SWNT's [7-14].

Molecular descriptors play a decisive role for evaluating large virtual libraries and to predict biological or physicochemical properties of compounds. Topological indices are an important class of molecular descriptors, based on the graph of a molecule.

Chemical graph theory has been extensively applied to predict the physical properties of small molecules through quantitative structure-property relationships (QSPR). This has been accomplished by demonstrating strong correlation between physical properties and one or more topological indices. Extending the application of topological indices to single wall nanotubes can lead to potential problems for such models. The oldest topological indices is the Wiener index [15,16,18].

Recently, a new topological index, namely, Padmakar–Ivan index, abbreviated as PI has been mentioned. In ref [19], the PI index of a zig-zag polyhex nanotube has been computed. Deng [20,21] computed the PI index of the catacondensed hexagonal systems and some other nanotubes. The present authors in ref [22] computed the PI index of the armchair polyhex nanotube.

Throughout this paper T= TUVC6[2p,q] denotes an arbitrary armchair nanotube, in the term of their circumference (2p) and their length (q), Figure c.

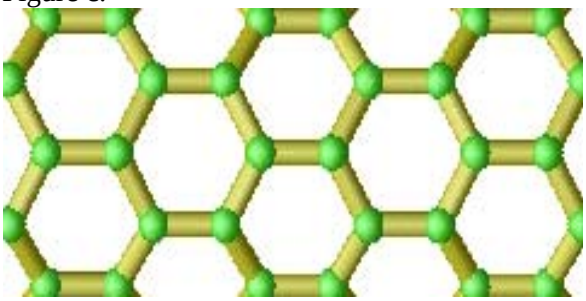

Figure c. A Armchair Polyhex Lattice with p=3 and q=5.

MATHEMATICAL METHODS

To compute the PI index of the graph T= $TUVC_6[2p,q]$, we [22], assume that E= E(T) is the set of all edges and

$$N(e) = |E| - \left(n_{eu}(e|G) + n_{ev}(e|G)\right).$$

Then

$$PI(T) = |E|^2 - \sum_{e\in E} N(e).But|E(T)| = p(3q-2)$$

and so

$$PI(T) = p^2(3q-2)^2 - \sum_{e\in E} N(e).)$$

Therefore, to compute the PI index of T, it is enough to calculate N(e), for every $e \in E$. To calculate N(e), we consider two cases that e is horizontal or non- horizontal:

1) If e is an horizontal edge then

$$N(e)= \begin{cases} q-1 & e \in T_{2k} \\ q+1 & e \in T_{2k-1} \\ q & \text{otherwise} \end{cases}$$

where Ti denotes the set of all horizontal edges of the i^{th} row of the armchair polyhex lattice.

2) If e is a non- horizontal edge in the k^{th} row, $1 \le k \le p$, of the armchair polyhex lattice of T=$TUVC_6[2p,q]$, then

$$N(e)= \begin{cases} 2p + 2(k-1) & q \ge p + k \\ 2q - 2 & q \le p + k \end{cases}$$

3) If $q \le 2p$ then:

$$N(E_{1,1}) = N(E_{q,1}), N(E_{2,1}) = N(E_{(q-1),1}), ..., N(E_{S,1}) = N(E_{(s+1+b),1}), where\ s = [q/2]$$

is the greatest integer less than or equal to $q/2$, and $b=[(q+1)/2]-[q/2]$.

4) If q > 2p then:

$N\left(E_{1,1}\right)=N\left(E_{q,1}\right), N\left(E_{2,1}\right)=N\left(E_{(q-1),1}\right)$ and $,.....,N\left(E_{p,1}\right)=N\left(E_{((q-p+1),1}\right),$

$n\left(E_{(p+1)1}\right)=N\left(E_{(p+2)1}\right)=....=N\left(E_{(q-p)1}\right)=N\left(E_{p1}\right)$

.

On this basis, the final equation for calculating the PI index of armchair polyhex nanotube is:

$$PI\left(TUVC_6[2p,q]\right)=\begin{cases}\begin{cases}X-p & q\le p+1\\ Y-p & q\ge p+1\end{cases} & 2\mid p \quad \& \; 2\mid q-1\\ \begin{cases}X & q\le p+1\\ Y & q\ge p+1\end{cases} & \text{otherwise}\end{cases}$$

where:

$$X=9p^2q^2-12p^2q-5pq^2+8pq+4p^2-4p$$

$$Y=9p^2q^2-20p^2q-pq^2+4pq+4p^3+8p^2-4p$$

The value of the determinants of electric moments discussed in this report solved by using MAPLE-9.5 package implemented to a Personal computer.

Graphs

The graphs are produced drawing the Microsoft Office Excel-2003 program.

Discussion and designing QSPR models

Topological indices have proven to be very useful in QSPR models, especially when a physical property such as electrical moments is modeled for a specific family of molecular graphs. Therefore, QSPR modeling the reduces topological correlation between the two sets of numbers via an algebraic expression. (one set of numbers represents the properties, and the other set represents the structures of molecules under study).

There are several ways of topological design of QSPR models. Here we outline one possible strategy which contains five steps:

Step 1. Get a reliable source of experimental data for a given set of molecules. This initial set of molecules is called the training set [23,24]. The data in this set must be reliable and accurate. The quality of the selected data is important because it will affect all the following steps.

Step 2. The topological index is selected and computed. This is also an important step because selecting the appropriate topological index (or indices) can facilitate finding the most accurate model.

Step 3. The two sets of numbers are then statistically analyzed using a suitable algebraic expression.

The QSPR model is thus a regression model, and one must be careful about its statistical stability. Chance factors could yield spuriously accurate correlations. The quality of the QSPR models can be conveniently measured by the correlation coefficient r and standard deviations. A good QSPR model must have r > 0.99, while s depends on the property. For example, for boiling point, s < 5 ^{0}C. Therefore, step 3 is a central step in the design of the structure-property models.

Step 4. Predictions are modeled for the values of the molecular property for species that are not part of the training set via the obtained initial QSPR model. The unkown molecules are structurally related to the initial set of compounds.

Step 5. The predictions are tested with unknown molecules by experimental determination of the predicted properties. This step is rather involved because it requires acquiring or preparing the test molecules.

The following structure-property models are the most successful for logarithmic values of Padmakar-Ivan (PI) considered:

(1): Log E= -0.0019(LogPI)^3 + 0.0421(LogPI)2+ 0.2089(LogPI) +5.4926 R2= 1

(2): Log Q= 0.0009 (LogPI)^3 + 0.0595 (LogPI)^2+ 0.8606(LogPI) + 3.4546 R2=1

(3): Log H= $0.0220(LogPI)^3$ – $0.1646(LogPI)^2$+ 2.5249 (LogPI)+3.6344 R2= 1

RESULTS AND DISCUSSION

The value of Padmakar–Ivan index, energy ($kJmol^{-1}$), electric quadrupole, hexadecapole moments of armchair polyhex nanotubes $TUVC_6[2p,q]$ with p:4, q: (3 to 14) were shown in table 1 .

The energy and electric quadrupole, hexadecapole moments of these nanotubes were performed by Beck-Lee-Yang-Parr (B_3LYP) on 3-21G basis set using the standard procedure indices GAUSSIAN 98.

The value of the topological index discussed in this report increases with the number of q in $TUVC_6[2p,q]$ or the number of carbon in nanotubes and increases their length.

According to the data of table 2. the logarithmic values of Padmakar-Ivan increase by increasing the values of logarithmic electric quadrupole, hexadecapole moments of armchair polyhex carbon nanotubes $TUVC_6[2p,q]$ with p: 4, q: (3,5,7,9,12,14) .

In figs. [1-3] it is attempted to show two dimensional diagrams of the relationship between the logarithmic values of Padmakar-Ivan index and logarithmic values of energy ($kJmol^{-1}$), quadrupole, hexadecapole moments of $TUVC_6[2p,q]$ with p:4, q:(3,5,7,9,12,14).

In those curves, there is good correlation between the values.

After the calculation the Padmakar-Ivan index 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 (eques, 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.

Electric quadrupole and hexadecapole moments of armchair polyhex carbon nanotubes $TUVC_6[2p,q]$ with p: 4, q: (4 to13) were performed by Beck-Lee-Yang-Parr (B_3LYP) on 3-21G basis set using the standard procedure indices GAUSSIAN 98.

The results of these calculations are shown indices tables (3-5). We use eques (1-3) to predict the electric quadrupole and hexadecapole moments of $TUVC_6[2p,q]$ with p: 4 q: (4,6,8,11,13) .

We compare the predicted and GAUSSIAN values of $TUVC_6[2p,q]$ with p: 4, q: (4 to 13), [see tables (3-5)].

CONCLUSIONS

In the first part of this study, the quantum mechanics methodology was used to determine the energy, electric quadrupole, hexadecapole moments of armchair polyhex carbon nanotubes $TUVC_6[2p,q]$ with p: 4, q: (4 to 13)

The relationships between the Padmakar-Ivan index with the above mentioned molecular properties has been studied.

Futhermore, the results of such studies were used to get into the quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) subjects.

The graph-theoretical approach to QSPR is based on a well-defined mathematical representation of the molecular structure. In this report we presented a strategy for designing the QSPR based on topological indices. The instructive example was directed to the design of the structure-property model for predicting the electric quadrupole and hexadecapole moment of armchair polyhex carbon nanotubes $TUVC_6[2p,q]$ with p: 4 , q: (3 to14). In the most accurate QSPR models for nanotubes energy, electric quadrupole, hexadecapole moments are based on Log PI.

The study of QSPR show that energy and electric quadrupole and hexadecapole moments of $TUVC_6[2p,q]$ with p: 4, q: (4 to 13) could be well predicted.

Table 1. The values of circumference (2p), length (q), energy ($kJmol^{-1}$), electric quadrupole, hexadecapole moments and Padmakar-Ivan (PI) index of armchair polyhex carbon nanotubes $TUVC_6[2p,q]$ with p: 4, q: (3,5,7,9,12,14)

$TUVC_6$ [2p,q]		**E**	**Quadrupole**	**Hexadecapole**	**PI**
P	q	$kJmol^{-1}$	moment	moment	Index
4	3	2383806.4670	2450963.2800	$-9/2247 \times 10^{9}$	680
4	5	3975381.5180	11591566.9500	$-1/30559 \times 10^{11}$	2344
4	7	5566812.0130	32159802.6600	$-1/1013 \times 10^{11}$	5096
4	9	7158147.6400	68728406.4500	$-2/5142 \times 10^{12}$	8968
4	12	9545218.8000	167764417.8000	$-1/0679 \times 10^{13}$	16880
4	14	11136631.9200	26619141.2000	$-2/3084 \times 10^{13}$	23552

Table 2. Logarithm values of energy, electric quadrupole, hexadecapole moments, Padmakar-Ivan index of armchair polyhex carbon nanotube $TUVC_6[2p,q]$ with p:4, q:(3,5,7,9,12,14)

$TUVC_6$[2p,q]		**Log E**	**Log Q**	**Log H**	**Log PI**
p	q				
4	3	6.3773	6.3893	9.9649	2.8325
4	5	6.5994	6.0641	11.1158	3.3699
4	7	6.7456	6.5073	11.8513	3.7072
4	9	6.8548	7.8371	12.4004	3.9527
4	12	6.9798	8.2247	13.0286	4.2273
4	14	7.0467	8.4252	13.3633	4.3720

Table 3. Comparison between predicted (Models 1-3) and Gaussian values of elecrtric quadrupole moments of armchair polyhex carbon nanotube $TUVC_6[2p,q]$ with p:4, q: (4,6,8,11,13)

$TUVC_6$ [2p,q]		**Log Q(Gauss)**	**Log Q(Calc)**	**[Log Q(Gauss) -Log Q (Calc)]**
p	q		Log PI	Log PI
4	4	6.7678	6.7759	-0.0081
4	6	7.3026	7.3056	- 0.0030
4	8	7.6864	7.6857	+0.0007
4	11	8.1069	8.1080	-0.0011
4	13	8.3245	8.3306	-0.0061

Table 4. Comparison between predicted (Models 1-3) and Gaussian values of electric hexadecapole moments of armchair polyhex carbon nanotube TUVC6[2p,q] with p: 4, q: (4,6,8,11,13)

$TUVC_6$ [2p,q]		**Log H(Gauss)**	**Log H(Calc)**	**[Log H(Gauss) -Log H(Calc)]**
p	q		Log PI	Log PI
4	4	10.6207	10.6285	0.0078
4	6	11.5141	11.5173	0.0032
4	8	12.1425	13.1455	0.0030
4	11	12.8384	12.8386	0.0002
4	13	13.2016	13.2032	0.0016

Table 5. Comparison between predicted (Models 1-3) and Gaussian values of energy of armchair polyhex carbon nanotube TUVC6[2p,q] with p: 4, q: (4,6,8,11,13)

$TUVC_6$ [2p,q]		**Log E(Gauss)**	**Log E(Calc)**	**[Log E(Gauss) -Log E(Calc)]**
p	q		Log PI	Log PI
4	4	6.5024	6.5063	-0.0039
4	6	6.6786	6.6817	-0.0031
4	8	6.8036	6.8073	-0/0037
4	11	6.9420	6.9464	-0.0044
4	13	7.0146	6.0194	-0.0048

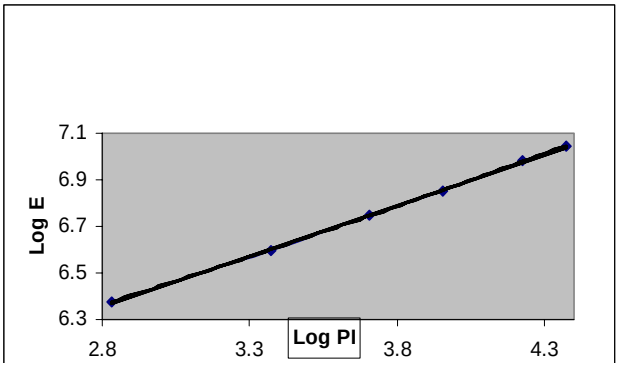

Fig.1. The curve of the Log PI versus Log E

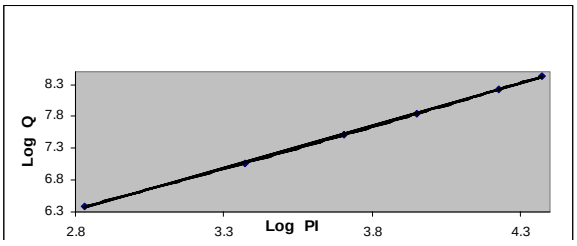

Fig.2. The curve of the Log PI versus Log Q .

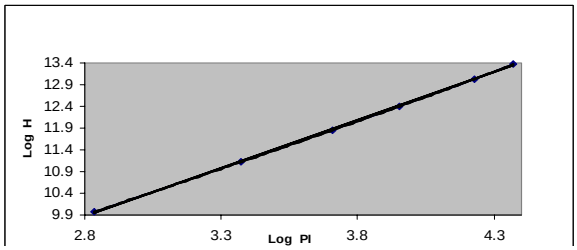

Fig.3. The curve of the Log PI versus Log H .

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