Indian Journal of Fundamental and Applied Life Sciences ISSN: 2231– 6345 (Online)
An Open Access, Online International Journal Available at www.cibtech.org/sp.ed/jls/2014/04/jls.htm
2014 Vol. 4 (S4), pp. 1-3/Bahrami
Research Article

COMPUTING SOME STRUCTURAL PROPERTIES OF NANOTUBES BY BIO-MATHEMATICS MODELLING

***Amir Bahrami**
Department of Mathematics, Mahshahr Branch, Islamic Azad University, Mahshahr, Iran
**Author for Correspondence*

ABSTRACT
Topological descriptors, other graph measures, and in a broader sense, graph-theoretical methods, have been proven as powerful tools to perform biological network analysis. In this paper, counting descriptor called "Padmakar Ivan ", of T-Junction carbon nanotubes is determined.

Keywords: *Topological Descriptors, Padmakar Ivan Index, T-Junction Carbon Nanotubes*

INTRODUCTION
Gutman (1994) was intended to examine a few Wiener – number related quantities, which can be considered as generalization of Wiener-number concept. One of these quantities is W* (Gutman, 1994). Gutman was attacking the problem of W* of benzenoid chains (un-branched catacondensed Benzenoids). This offer from Gutman provided researchers to learn much more of graph-theoretical topological indices and other related graph-theoretical concepts (Khadikar *et al.*, 1994).

After that, Khadikar to remove this lacuna, proposed another index in 2000, which he named Padmakar-Ivan index and abbreviated as PI (Gutman *et al.*, 1995). It is worth mentioning that Padmakar is the first name of Khadikar, while Ivan is the first name of Gutman, Khadikar [29] conceived this index while attempting simultaneous estimation of Wiener and Szeged indices of benzenoids using elementary cut method. The Padmakar-Ivan index is defined it as below:

The PI index of a molecular graph is defined by the following expression:

$PI = PI(G) = \Sigma e \in E(G)[n_{eu}(e \mid G) + n_{ev}(e \mid G)]$

Here, we define edge of G connecting the vertices u and v, as $e = uv \in E(G)$. The quantities neu and n_{ev} are the number of edges closer to u and v respectively. In calculating PI index edges equidistance from both end of the edge *uv* are not counted. The PI index of acyclic and cyclic graphs differs. However, the main interest of proposing a topological index for cyclic graph alone remained unresolved.

The PI index is very simple to calculate and has disseminating power similar to that of the Wiener and Szeged indices. Khadikar and coauthors investigated numerous chemical and biological applications in that PI index and they found PI index superior to both Wiener and Szeged indices (Khadikar *et al.*, 1995, 2000). In this paper, we consider for the first time a class of T-Junction nanotubes and compute the PI index of molecular graph of T-Junction carbon nanotubes.

Our notation is standard and mainly taken from Trinajestic (1983).

RESULTS AND DISCUSSION
A 3-way junction nanotubes (or 3-way intersection) are a type of road intersection with three arms. A Y junction (or Y intersection) generally has 3 arms of equal size. A T junction (or T intersection) also has 3 arms, but one of the arms is generally a minor road connecting to larger road**.**In this section the PI index of Structural models of symmetric T-junctions carbon nanotube (figure 1) is determined. For this computation, Suppose that G [m,n}] is the molecular graph symmetric Y-Junctions carbon nanotubes (figure 1). In the following theorem we compute the Padmakar-Ivan index of G, Figure 1.
Theorem PI index of the molecular graph of G=G[m,n], is equal to:

$$PI(G) = 124mn \times \begin{cases} 56m(n^2 + 12n^3 - 16) & if \ \ m < n \\ 144n(m^3 + 44m^2 - 14) & if \ \ m \geq n \end{cases}$$

where m, n are the number of vertices in every parts of sections of G.

Proof. For Computing PI index of molecular graph of T-junction nanotube, we khnow that, if Gu,e = {x | dG(u,x) < dG(v,x)}, Gv,e = { x | dG(u,x) > dG(v,x)} and Ge = {x | dG-{e}(u,x) - dG-{e}(v,x) = ±1} then neu(e|G) = |E(Gu,e)|, nev(e|G) = |E(Gv,e)| and N(e) = |E(Ge)|. Here for any subset U of the vertex set V = V(G), |E(U)| denotes the number of edges of G between the vertices of U. It is easy to see that |E(G)| = N(e) + neu(e|G) + nev(e|G).

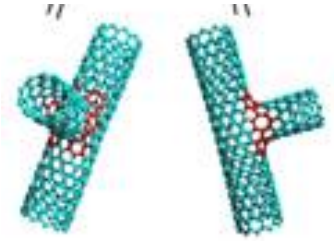

Figure 1: T-Junction Carbon Nanotubes

By very hard computation and formula of direct product of molecular graphs for PI index above formula is determined.

ACKNOWLEDGEMENT

This research is supported by the research council of the Mahshahr Branch, Islamic Azad University, Mahshahr, Iran.

REFERENCES

Balaban AT (1976). *Chemical Applications of Graph Theory* (Academic Press) London (UK).

Bonchev D (1983). *Information Theoretic Indices for Characterization of Chemical Structures* (Research Studies Press) Latchworth.

Bonchev D and Roouvray DH (1993). *Chemical Graph Theory: Introduction and Fundamentals* (Gordon and Breach Science Publishers) New York (NY).

Gutman I (1994). Formula for the Wiener Number of Trees and Its Extension to Graphs Containing Cycles, Graph Theory Notes New York **27** 9-15.

Gutman I, Gaurilovic N, Nankovic D, Khadikar PV, Deshpande NV and Kale PP (1994). Dependence of Spectral Moments of Benzenoid Hydrocarbons on Molecular Structure. The Case of Linear Polyacenes, *Journal of the Serbian Chemical Society* **59** 519-524.

Gutman I, Khadikar PV, Rajput PV and Karmarkar S (1995). The Szeged Index of Polyacenes, *Journal of the Serbian Chemical Society* **60** 759-764.

Khadikar PV, Deshpande NV, Kale PP and Gutman I (1994). Spectral Moments of Polyacenes, *Journal of Chemical Information and Computer Sciences* **34** 1181-1183.

Khadikar PV, Deshpande NV, Kale PP, Dobrynin A, Gutman I and Domotor G (1995). The Szeged Index and an Analogy with the Wiener Index, *Journal of Chemical Information and Computer Sciences* **35** 547-550.

Khadikar PV, Karmarkar S and Agrawal VK (2000). PI Index of Polyacenes and its Use in Developing QSPR, *National Academy Science Letters* **23** 124-128.
Kier LB and Hall LH (1976). *Molecular Connectivity in Chemistry and Drug Research* (Research Studies Press) Latchworth.
Kier LB and Hall LH (1986). *Molecular Connectivity in Structure-Analysis* (Research Studies Press) Latchworth.
Trinajstic N (1983). *Chemical Graph Theory* (CRC Press) Boca Raton, FL **I and II**.