Digest Journal of Nanomaterials and Biostructures Vol. 3, No.4, December 2008, p. 251-255

TOPOLOGICAL INDICES OF NANOTUBES, NANOTORI AND NANOSTARS

H. YOUSEFI-AZARI, A. R. ASHRAFI[a], M. H. KHALIFEH
School of Mathematics, Statistics and Computer Science, University of Tehran, Tehran, I. R. Iran
[a]*Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran*

The Wiener index of a graph G is defined as $W(G) = 1/2\sum\{x,y\}\subseteq V(G)d(x,y)$, where V(G) is the set of all vertices of G and for $x,y \in V(G)$, d(x,y) denotes the length of a minimal path between x and y. In this paper, we first report our recent results on computing Wiener, PI and Balaban indices of some nanotubes and nanotori. Next, the PI and Szeged indices of a new type of nanostar dendrimers are computed for the first time.

(Received November 2, 2008; accepted November 12, 2008)

Keywords: Nanotube, Nanotori, Nanostar, Wiener index, PI index, Balaban index

1. Introduction

The first use of a graph invariant for the correlation of the measured properties of molecules with their structural features was made in 1947 by the chemist Harold Wiener, [1]. In that year, he introduced the notion of path number of a graph as the sum of the distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. Next Hosoya [2], named such graph invariants, topological index. With hundreds of topological indices one would expect that most molecules could be well characterized and their physicochemical properties correlated with the available descriptors.

Khadikar [3], defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. This newly proposed topological index, PI, does not coincide with the Wiener index (W) for acyclic (trees) molecules. The derived PI index is very simple to calculate and has a discriminating power similar to that of the W index.

Let G be a molecular graph and $x \in V(G)$. We denote by d(x), the summation of topological distances between x and all vertices of G. The Balaban index of a molecular graph G is defined by Balaban [4,5]. Then Balaban and co-authors [6,7], investigated this index even for infinite graphs.

In a series of papers, Diudea and coauthors [8-14] computed the Wiener index of some nanotubes. In this paper, we report our recent results in computing topological indices of nanotubes and nanotori. Our notation is standard and mainly taken from [15,16]. We encourage reader to consult [17-28] for discussion and background material about topological indices of nanotubes and nanotori.

2. History

In this section we describe some notations which will be kept throughout. We now recall some algebraic definitions that will be used in the paper. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-shapes of which are represented by V(G) and E(G), respectively. If e is an edge of G, connecting the vertices u and v then we write e=uv. The number of vertices of G is denoted by n. The distance between a pair of vertices u and w of G is denoted by d(u,w). Wiener index of a graph G is defined as W(G) =

$1/2\sum_{\{x,y\}\subseteq V(G)}d(x,y)$.

The Balaban index of a molecular graph G is defined as $J(G) = m/(\mu+1)\Sigma_{e=uv}[d(u)d(v)]^{-0.5}$, where m is the number of edges of G, $\mu(G) = |E(G)|-|V(G)|+1$ is the cyclomatic number of G and for every vertex x, d(x) is the summation of topological distances between x and all vertices of G.

We now define for e=uv two quantities $n_{eu}(e|G)$ and $n_{ev}(e|G)$. $n_{eu}(e|G)$ is the number of edges lying closer to the vertex u than the vertex v, and $n_{ev}(e|G)$ is the number of edges lying closer to the vertex v than the vertex u. Then the Padmakar–Ivan (PI) index of a graph G is defined as $PI(G) = \sum[n_{eu}(e|G)+ n_{ev}(e|G)]$. We notice that the edges equidistant from both ends of the edge uv are not counted in calculating the PI index of a graph. It is easy to see that $|E(G)| = N(e) + n_{eu}(e|G) + n_{ev}(e|G)$.

Graphene is a generic name for the carbon allotropes produced by laser vaporization of graphite. They include, besides the famous spherical fullerenes, nanotubes, and their closed, circular forms with toroidal shape. exist. Carbon nanotubes, the one-dimensional carbon allotropes, are intensively studied, with respect to their promise to exhibit unique physical properties: mechanical, optical, electronic, etc. However, only a relatively small number of studies on the carbon nanotoroidal cage structures

The following result determines the exact value of the Wiener index of a polyhex nanotori.

Theorem 1: (Yousefi-Ashrafi). Armchair and zig-zag polyhex nanotori have the same Wiener index as follows:

$$W(TUHC_6[2p,q]) = W(TUVC_6[2p,q]) = \begin{cases} \frac{pq^2}{24}(6p^2+q^2-4) & q \le p \\ \frac{p^2q}{24}(3q^2+3pq+p^2-4) & q \ge p \end{cases}.$$

The first serious work for computing the PI index of chemical graphs was done by Khadikar and co-authors [20,21]. They introduced a method for the calculating the PI index of hexagonal chains. In [22], Deng introduced another method for calculating the PI indices of catacondensed hexagonal systems according to the lengths of their segments, and to determine the catacondensed hexagonal systems with minimum and maximum PI index.

We now report on our recent results related to PI index of nanotubes and nanotori.

Theorem 2: (Ashrafi-Loghman [17]). The PI index of the zig-zag polyhex nanotube in the terms of their circumference (2p) and their length (q), Figure 1,.is as follows:

$$PI(TUHC_6[2p,q]) = \begin{cases} p^2(9q^2-7q+2)-4pq^2 & \text{if} \quad q \le p \\ p^2(9q^2-15q+4p-2)+4pq & \text{if} \quad q \ge p \end{cases}$$

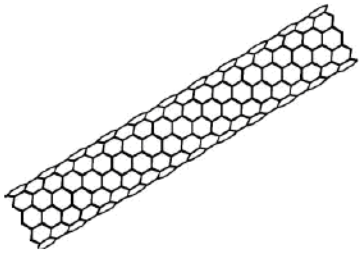

Fig. 1. A Zig-zag $TUHC_6[20,q]$.

Using a similar arguments in [18,19] Ashrafi and Loghman computed the PI index of some other nanotubes. They proved that:

Theorem 3: The PI index of armchair polyhex nanotube in the terms of their circumference (2p) and their length (q), Figure 4, is as follows:

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

where $X = 9p^2q^2 - 12p^2q - 5pq^2 + 8pq + 4p^2 - 4p$ and $Y = 9p^2q^2 - 20p^2q - pq^2 + 4pq + 4p^3 + 8p^2 - 4p$.

Theorem 4: The PI index of $TUC_4C_8(S)[4p,q]$ nanotube in the terms of their circumference (2p) and their length (q), Figure 3, is as follows:

$$PI(TUC_4C_8(S))[4p,q]) = \begin{cases} X & q \le p \\ Y & q \ge p \end{cases},$$

where $X = 36p^2q^2 - 28p^2q + 8p^2 - 8pq^2$ and $Y = 36p^2q^2 - 36p^2q - 4pq^2 + 4pq + 4p^3 + 4p^2$.

Fig. 2. An Armchair $TUVC_6[20,n]$ nanotube.

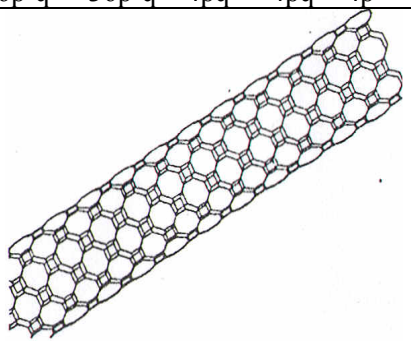

Fig. 3: $TUC_4C_8(S)$ Nanotubes.

We now investigate the Balaban index of the chemical graphs of an armchair polyhex nanotorus and $TUC_4C_8(S)$ nanotorus. For simplicity, we denote these graphs by T_1 and T_2, respectively. We first consider an armchair nanotorus T_1, Figure 1. The molecular graph of T_1 has exactly pq vertices and 3pq/2 edges, Figure 4. So the cyclomatic number of T_1 is $\mu = 3pq/2 - pq + 1 = pq/2 + 1$.

Theorem 5: The Balaban index of T_1 is as follows:

$$W(T_1) = \begin{cases} \frac{pq^2}{24}(6p^2 + q^2 - 4) & q < p \\ \frac{p^2q}{24}(3q^2 + 3pq + p^2 - 4) & q > p \end{cases}.$$

Consider the chemical graph of a $TUC_4C_8(R)$ nanotorus $T_2 = T[m,n]$, Figure 2, in which n is the number of rhombs on the level 1 and the length of torus is m.

In the end of this paper, we state a formula for the Balaban index of $TUC_4C_8(S)$ nanotori, with exactly m/2 and n/2 octagons in every row and column, respectively. Clearly, T_3 has exactly 2mn vertices and 3mn edges and so $\mu(T_3)=mn + 1$.

Theorem 6: The Balaban index of a $TUC_4C_8(S)$ nanotorus, Figure 3, is as follows:

$$J(T_2) = \begin{cases} \frac{54mn^2}{(mn+2)(6n^2 + 3nm + m^2 - 4)} & n \le m \\ \frac{54mn^2}{(mn+2)(6m^2 + 3mn + n^2 - 4)} & m < n \end{cases}.$$

3. Main results

The subject of Nanostar is one of the main topics of Nanobiotechnology. In recent years, the Nanostar, a phenylacetylene dendrimer, has attracted attention due to its potential applications. The Nanostar absorbs ultraviolet photons at its terminal groups and the energy transfers from the periphery to the core where it is collected with 99% efficiency and then it is emitted in the visible range. This energy transfer process is in the order of picoseconds. Due to its localized excitations, the Nanostar was studied as the sum of separate units, which are 24 two-ring systems, 4 three-ring systems, 2 four-ring systems and a core. The aim of this section is computing the PI index of two types of Nanostars I and II, Figures 3 and 4.

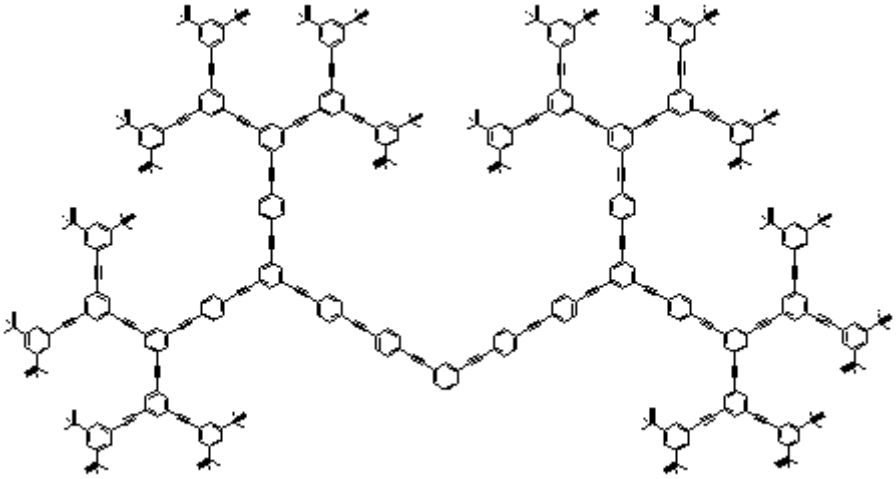

Fig. 3. A Nanostar of Type I, with n = 3 and k = 1.

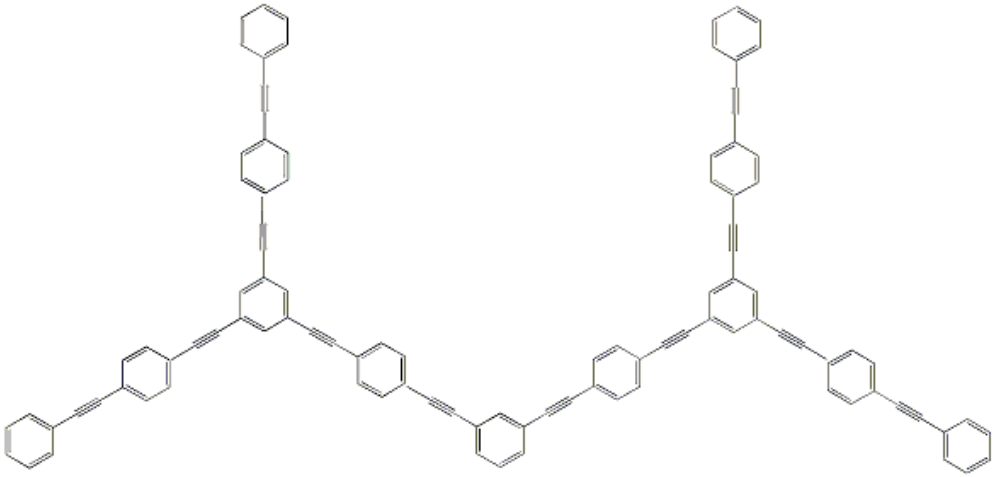

Fig. 4. A Nanostar of Type II, with n = 3 and k = 1.

Suppose G = G(n,k) is the graph of a Nanostar of type I. From Figure 3, we can see that if e is an edge of a hexagon of G then N(e) = 2, otherwise N(e) = 1. We assume that A is the set of all hexagons, B is the set of all edges outside A, a = |A| and b = |B|. We calculate that $a = 1 + 2n + 2^2(n-1) + 2^3(n-2) + \ldots + 2^{k+1}(n-k) + 2^{k+1}$ and $b = a-1+2^{k+2}$. Therefore, $\sum_{e\in A} N(e) = 12a$ and $\sum_{e\in B} N(e) = b$. Hence $PI(G) = |E(G)|^2 - \sum_{e\in A} N(e) - \sum_{e\in B} N(e) = 36a^2 + b^2 + 12ab - 12a - b$. We now compute the PI index of the Nanostar H = H(n,k) of type II, Figure 4. A similar argument as above, shows that if e is an edge of a hexagon of H then N(e) = 2, otherwise N(e) = 1. Suppose A, B, a, and, b are defined as above. Then $a = 1 + k(1+2 + 2^2 + \ldots + 2^n) = 1 + k(2^{n+1} - 1)$

and b = a – 1. Therefore, $\sum_{e\in A} N(e) = 12a$ and $\sum_{e\in B} N(e) = b$. Hence PI(G) = $|E(G)|^2$ – $\sum_{e\in A} N(e) - \sum_{e\in B} N(e)$ = $36a^2 + b^2 + 12ab - 12a - b$.

We end our paper with the following open questions:

Question 1: Is there a simple closed formula for the Szeged indices of a Nanostar of types I and II?

Question 2: Is it true that for every positive integer n, there exists a Nanostar T with this condition that PI(T) = n or Sz(T) = n?

References

[1] H. Wiener, J. Am. Chem. Soc.. **69**, 17 (1947).
[2] H. Hosoya, Bull. Chem. Soc. Japan, **44,** 2332 (1971).
[3] P.V. Khadikar, On a Novel Structural Descriptor PI, Nat. Acad. Sci. Lett. **23**, 113 (2000).
[4] A. T. Balaban, Chem. Phys. Letters **89**, 399 (1982).
[5] A. Balaban, Pure Appl. Chem. **55**, 199 (1983).
[6] A.T. Balaban, P. Filip, MATCH Commun. Math. Comput. Chem., **16,** 163 (1984).
[7] A. T. Balaban, N. Ionescu-Pallas, T. S. Balaban, MATCH Commun. Math. Comput. Chem., **17**, 121 (1985).
[8] M. V. Diudea, B. Parv, P. E. John, O. Ursu, A. Graovac, MATCH Commun. Math. Comput. Chem. **49**, 23 (2003).
[9] M. V. Diudea, I. Silaghi-Dumitrescu, B. Parv, MATCH Commun. Math. Comput. Chem. **44** 117 (2001).
[10] M. V. Diudea, B. Parv, E. C. Kirby, Azulenic tori, MATCH Commun. Math. Comput. Chem., **47,** 53 (2003).
[11] M. V. Diudea, Graphenes from 4-valent tori, Bull. Chem. Soc. Jpn., **75,** 487 (2002).
[12] M. V. Diudea, Hosoya Polynomial in Tori**,** MATCH Commun. Math. Comput. Chem. **45**, 109 (2002).
[13] P. E. John, M. V. Diudea, Wiener Index of Zig-zag Polyhex Nanotubes, Croat. Chem. Acta, **77,** 127 (2004).
[14] M. V. Diudea, M. Stefu, B. Parv, P. E. John, Wiener Index of Armchair Polyhex Nanotubes, Croat. Chem. Acta, **77,** 111 (2004).
[15] P. J. Cameron, Combinatorics: Topics, Techniques, Algorithms, Cambridge University Press, Cambridge, 1994.
[16] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL. 1992.
[17] A. R. Ashrafi, A. Loghman, PI Index of Zig-Zag Polyhex Nanotubes, MATCH Commun. Math. Comput. Chem. **55**(2), 447 (2006).
[18] A. R. Ashrafi, A. Loghman, PI Index of Armchair Polyhex Nanotubes, Ars Combinatoria, **80,** 193 (2006).
[19] A. R. Ashrafi, A. Loghman, J. Comput. and Theor. Nanosci., **3,** 378 (2006).
[20] P. V. Khadikar, Nat. Acad. Sci. Lett. 23, 113 (2000).
[21] P. V. Khadikar, P. P. Kale, N, V, Deshpande, S. Karmarkar, V. K. Agrawal, J. Math. Chem.. 29, 143 (2001).
[22] H. Deng, Math. Comput. Chem. 55(2), 453 (2006).