Digest Journal of Nanomaterials and Biostructures Vol. 4, No.1, March 2009, p. 141 - 144

VERTEX PI INDEX OF V- PHENYLENIC NANOTUBES AND NANOTORI

A. BAHRAMI[*], J. YAZDANI[a]
Young Researchers Club, Islamic Azad University , Garmsar Branch , Garmsar , Iran
[a]*Nanoscience and Nanotechnology Research Center, Razi University, Kermanshah, Iran.*

In series of papers, P.V. Khadikar introduced a new topological index and named it as Padmakar–Ivan (PI) Index. This index is found very useful in nano technology, particularly in making and characterizing carbon nanotubes and nanotori. In this paper the vertex PI index of V-phenylenic nanotubes and nanotori, is computed.

(Received January 24, 2009; accepted February 13, 2009)

Keywords: Molecular graphs, vertex PI index, V-phenylenic nanotube and nanotorous.

1. Introduction

Let G be a molecular graph, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. A topological index of G is a real number related to the molecular graph of G. It must be a structural invariant, i.e., it does not depend on the labelling or the pictorial representation of the graph. The Wiener index W is the first topological index proposed to be used in chemistry [1-4]. It was introduced in 1947 by Harold Wiener for characterization of alkanes. This index is defined as the sum of all distances between distinct vertices. The vertex PI index is a new topological index proposed by the present authors [5-8.] It is defined by $PI_v(G) = \sum_{e=uv\in E(G)}[n_u(e) + n_v(e)]$, where $n_u(e)$ is the number of vertices of G lying closer to u and $n_v(e)$ is the number of vertices of G lying closer to v.

In Refs [9-13] the PI and Szeged indices of some hexagonal graphs containing nanotubes and nanotorus are computed. In this paper, we continue this work to compute the vertex PI index of molecular graphs related to V-phenylenic nanotubes and nanotori. Our notation is standard and mainly taken from Refs [14, 15].

2.Main Results

The novel phenylenic and naphthylenic lattices proposed can be contructed from a square net embedded on the toroidal surface. In this section, the vertex PI index of a V-phenylenic nanotube and nanotorus are computed. Following Diudea [16] we denote a V-Phenylenic nanotube by G=VPHX[m,n]. We also denote a V-Phenylenic nanotorus by H=VPHY[m,n].

2.1. Vertex PI index of V-Phenylenic nanotube

In the following theorem we compute , the vertex PI index of the molecular graph G in Figure 1.

Theorem1. $PI_v(G)= \begin{cases} \alpha_1 & if\ m \neq n \\ \alpha_2 & if\ m = n \end{cases}$; where

α_1 =12|n-m| β^3-3|n-m|+12mn|n-m|-18|n-m| β^2+12|n-m| β +12 β^2(n-m)^2-12 β (n-m)^2+3(n-m)^2-12 β^3-12mn+6 β^2+18m^{3}n-12m^4+21m^3-9m^2-18m^{2}n+24m^{2}n^2-24mn^2, $\beta = \min(m,n)$

And α_2 =18m^{3}n-12m^4+21m^3-9m^2-18m^{2}n+24m^{2}n^2-24mn^2+12n^3+21n^2-30n+6mn-3.

Proof. We first notice v = |V(T)| =6mn. To compute the vertex PI index of G, we assume that A, B and C to be the set of all vertical, oblique and horizontal edges, respectively. Then we have:

$PI_v(G)=\sum_{e\in E}(n_u(e)+n_v(e)) = \sum_{e\in A}(n_u(e)+n_v(e))+\sum_{e\in B}(n_u(e)+n_v(e))+\sum_{e\in C}(n_u(e)+n_v(e)) =$

$$2\sum_{i=1}^{n-1}\{(6mi)+(6nm-6mi)(2m)\}+\sum_{i=1}^{n-1}\{(3mi)+(6nm-3mi)(2n)\}+\sum_{e\in C}(n_u(e)+n_v(e))$$

= 18m^{3}n-12m^4+21m^3-9m^2-18m^{2}n+24m^{2}n^2-24mn^2+ $\sum_{e\in C}(n_u(e)+n_v(e))$

To compute the last summation, we suppose that U = $\sum_{e\in C}(n_u(e)+n_v(e))$ and consider two separate cases, as follows:

Case 1: m ≠ n

In this case we have:

$$U = 2\sum_{i=1}^{|m-n|-1}\{(2\beta)(S_\beta+(6\beta-3)i))+(6mn-S_\beta-(6\beta-3)i\},$$

where S_i = 3+9+15+… + (6i-3) and $\beta = \min(m,n)$. Hence in this case, the vertex PI index of G is equal to: 12|-m+n| β^3-3|-m+n|+12mn|-m+n|-18|-m+n| β^2+12|-m+n| β +12 β^2(-m+n)^2-12 β (-m+n)^2+3(-m+n)^2-12 β^3-12mn+6 β^2+18m^{3}n-12m^4+21m^3-9m^2-18m^{2}n+24m^{2}n^2-24mn^2, $\beta = \min(m,n)$

Case2: m = n

In this case we have U = 4n(S_n+6n-3)+(6nm- S_n-(6n+3)) and so the vertex PI index of G is equal to: 18m^{3}n-12m^4+21m^3-9m^2-18m^{2}n+24m^{2}n^2-24mn^2+12n^3+21n^2-30n+6mn-3, and proof is completed.▲

2.2. Vertex PI index of V-Phenylenic nanotorus

In the end of this section, we compute the vertex PI index of H ; figure 2.

Theorem 2. $PI_v(H)= \begin{cases} \lambda_1 & if\ m \neq n \\ \lambda_2 & if\ m = n \end{cases}$; where

λ_1 = 12m^{2}n^2+18mn^3-9mn^2-33mn-12m^{2}n+24|(m-n)|β^3-6|(m-n)|+24mn|(m-n)|-36|(m-n)|β^2+24|(m-n)|β+24β^2(m-n)^2-24β(m-n)^2+6(m-n)^2-24β^3+12β^2 ; $\beta = \min(m,n)$

And λ_2 = 12m^{2}n^2+18mn^3-9mn^2-3mn-12m^{2}n+12n^3+21n^2-18n+3

Proof. To prove the theorem, we apply a similar method as in Theorem 1. It is easily seen that v = |V(H)| =6mn. we assume that A, B and C to be the set of all vertical, oblique and horizontal edges, respectively. then we have:

$$PI_v(G)=\sum_{e\in E}(n_u(e)+n_v(e)) = \sum_{e\in A}(n_u(e)+n_v(e))+\sum_{e\in B}(n_u(e)+n_v(e)) + \sum_{e\in C}(n_u(e)+n_v(e))$$

$$=2\sum_{i=1}^{n-1}\{(6mi)+(6nm-6mi)(2m)\}+2\sum_{i=1}^{n-1}\{(3mi)+(6nm-3mi)(2n)\}+\sum_{e\in C}(n_u(e)+n_v(e))$$

$$= 12m^2n^2+18mn^3-9mn^2-9mn-12m^2n+\sum_{e\in C}(n_u(e)+n_v(e))$$

To compute the last summation, we suppose that U = $\sum_{e\in C}(n_u(e)+n_v(e))$ and consider two separate cases, as follows:

Case 1: m$\neq$ n

In this case we have:

$$U=4\sum_{i=1}^{|m-n|-1}\{(2\beta)(S_\beta+(6\beta-3)i))+(6mn-S_\beta-(6\beta-3))i\},$$

Where S_i = 3+9+15+… + (6i-3) and $\beta = \min(m,n)$. Hence in this case, the vertex PI index of H is equal to 12m^{2}n^2+18mn^3-9mn^2-33mn-12m^{2}n+24|(m-n)|β^3-6|(m-n)|+24mn|(m-n)|-36|(m-n)|β^2+24|(m-n)|β+24β^2(m-n)^2-24β(m-n)^2+6(m-n)^2-24β^3+12β^2 ; $\beta = \min(m,n)$

Case2: m=n

In this case we have U = 4n(S_n+6n-3)+(6nm- S_n-6n+3) and so the vertex PI index of H is equal to 12m^{2}n^2+18mn^3-9mn^2-3mn-12m^{2}n+12n^3+21n^2-18n+3,which completes the proof. ▲

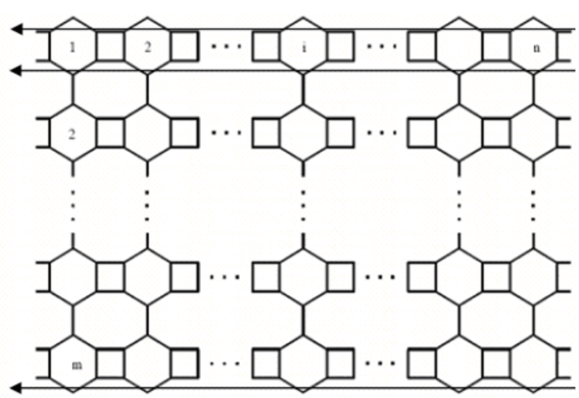

Fig. 1. The Molecular Graph of V-Phenylenic Nanotube.

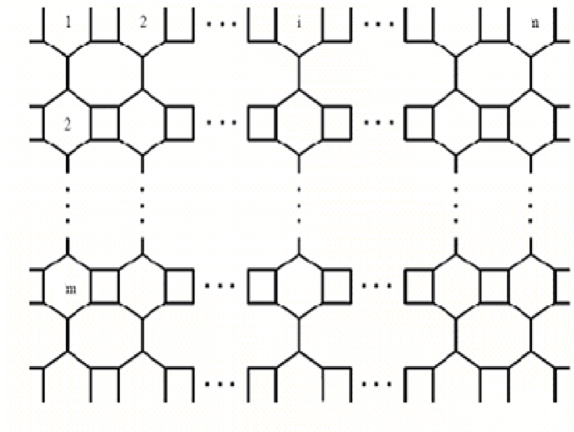

Fig. 2. The Molecular Graph of V-Phenylenic Nanotorus.

3. Conclusions

In chemical graph theory, mathematical chemistry and mathematical physics, a topological index is any of several numerical parameters (which are usually graph invariants) of a molecular graph which characterize its topology. It is a kind of a molecular descriptor. In this paper, counting topological index called "Vertex PI index ", of V-phenylenic nanotubes and nanotori were determined.

References

[1] H. Wiener, J. Am. Chem. Soc, **69** ,17 (1947).
[2]R.Todeschini , V. Consonni, Handbook of Molecular Descriptors, Wiley, Weinheim, 2000.
[3] D.E. Needham, I.C. Wei, P.G. Seybold, J. Am. Chem. Soc. **110** ,4186 (1988).
[4] G. Rucker, C. Rucker, J. Chem. Inf. Comput. Sc, **39**,788 (1999).
[5] M.H.Khalifeh,H. Yousefi-Azari, A.R.Ashrafi,Discrete Appl. Math**, 156**,1780 (2008).
[6] M.H.Khalifeh,H. Yousefi-Azari, A.R.Ashrafi., Linear Alg.Appl ,**429**,2702 (2008).
[7] I. Gutman, A. R.Ashrafi, Croatica Chemica Acta **81** ,63 (2008).
[8] A.R Ashrafi, M.Ghorbani, M. .**,** J. Theor. Comput.Chem,**7**,221 (2008).
[9] A.R.Ashrafi and A.Loghman, J. Comput. Theor. Nanosci**, 3**, 378 (2006).
[10] S.Y ousefi , A.R.Ashrafi, MATCHCommun. Math. Comput.Chem, **55**, 169 (2006).
[11] M. V. Diudea, M. S. Florescu, P. V. Khadikar: MATCHCommun. Math. Comput.Chem, **58** ,233 (2007).
[12] H. Yousefi Azari, J. Yazdani, A. Bahrami, A. R. Ashrafi,J.Serb.Chem.Soc , **72**, 1063 (2007).
[13] A.Bahrami,J.Yazdani, Digest Journal of Nanomaterials and Biostructures ,**3**, 265 (2008).
[14] P.J. Cameron, Combinatorics: Topics, Techniques, Algorithms, Cambridge University Press, Cambridge, 1994.
[15] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton**,** FL. 1992
[16] M.V. Diudea, Fuller. Nanotub. Carbon Nanostruct , **10**, 273 (2002).