Digest Journal of Nanomaterials and Biostructures Vol. 4, No.3, September 2009, p. 507-510

PADMAKAR-IVAN, OMEGA AND SADHANA POLYNOMIAL OF $HAC_5C_6C_7$ NANOTUBES

JAVAD YAZDANI, AMIR BAHRAMI[a*]

Nanoscience and Nanotechnology Research Center, Razi University, Kermanshah, Iran .

[a]*Young Researchers Club, Islamic Azad University, Garmsar Branch, Garmsar, Iran.*

Padmakar-Ivan ,Omega and Sadhana polynomials of a molecular graph are important in computing PI,Omega and Sadhana indices. These indices are most important in some physico chemical structures of molecules. In this paper, Padmakar-Ivan ,Omega and Sadhana polynomials of $HAC_5C_6C_7$ nanotubes are determined.

(Received June 28, 2009; accepted July 4, 2009)

Keywords: Padmakar-Ivan polynomial, Omega polynomial, Sadhana polynomial, $HAC_5C_6C_7$ nanotubes .

1. Introduction

We consider three representations of molecules as graphs:molecular graphs, topological pharmacophore graphs and reduced graphs.In molecular graph,vertices are atom types, edges are bond type.

In the fields of chemical graph theory and in mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound[1] Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure.[2-4]

The simplest topological indices do not recognize double bonds and atom types (C, N, O etc.) and ignore hydrogen atoms ("hydrogen suppressed") and defined for connected undirected molecular graphs only.[5] More sophisticated topological indices also take into account the hybridization state of each of the atoms contained in the molecule.

The Hosoya index is the first topological index recognized in chemical graph theory, and it is often referred to as the topological index.[6-7]

Other examples include the Wiener index, Padmakar-Ivan, Omega and Sadhana indices[8-9].These indices have some polynomials such that defined in [10].These polynomials**,** are useful to determine descriptors .We continue a new method to compute this polynomials for $HAC_5C_6C_7$ nanotubes.

*Corresponding author: bahrami@khayam.ut.ac.ir

2. Main Results and Discussion

In this section some applied polynomials of $HAC_5C_6C_7$ nanotubes are determined.For this computation , suppose that G= $HAC_5C_6C_7[4p,2q]$ nanotubes.

2.1. PI polynomial of $HAC_5C_6C_7[4p,2q]$ nanotubes

The PI polynomial of a graph G as $PI(G;X) = \Sigma_{\{u,v\}\subseteq V(G)} x^{N(u,v)}$, where for an edge $e = uv$, $N(u,v) = n_{eu}(e|G) + n_{ev}(e|G)$ and zero otherwise and we defined for the edge $e = uv$ of G 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. This polynomial is most important to compute the PI index and another topological indices. In this section, the PI Polynomial of the molecular graph of G = $HAC_5C_6C_7[4p,2q]$ nanotube are computed, when p is divisible by 4. Suppose $E_1 = E(G)$, is the set of all edges of G, respectively. Define $N_G(e) = |E_1| -(n_{eu}(e|G)+n_{ev}(e|G))$ .Then

$$PI(G,X) = \sum_{e\in E(G)} X^{|E(G)|-N(e)} + \binom{|V(G)|+1}{2} - |E(G)|.$$

But $|E_1| = 9pq+p/4$. Thus for computing the PI polynomial of G, it is enough to calculate $N_G(e)$, for every $e \in E_1$.
In the following theorem we compute the PI Polynomial of G, Figure 1.

Theorem 2.1.1. $PI(G,x) = q\, x^{9pq-p/4} + p\, x^{9pq+ p/4 - 6q} + 4q\, x^{9pq -15/4 p+2} -9pq-p/4 + \binom{|V(G)|+1}{2}$;
Where $|V(G)| = 3/2\, p^2 q+7/2q +p$.

Proof. To compute the PI polynomial of G, it is enough to calculate N(e). To do this, we consider three cases that e is vertical, horizontal or oblique. If e is horizontal then a similar argument as in Lemma 1 of Ref. 22 shows that N(e) = p/2. If e is a vertical edge on hexagons or heptagons then N(e) = 6q, 2(2q+1), respectively. Finally, if e is an oblique edge on hexagons or heptagons then N(e) = 4p–2. So we have:
$PI(G,x) = q\, x^{9pq-p/4} + p\, x^{9pq+ p/4 - 6q} + 4q\, x^{9pq -15/4 p+2} + \binom{|V(G)|+1}{2} - |E_1|$; Where
$|V(G)| = 3/2\, p^2 q+7/2q +p$ and $|E_1| = 9pq+p/4$; which completes the proof. ■

2.2. Omega and Sadhana Polynomials of $HAC_5C_6C_7[4p,2q]$ Nanotube

Let G be an arbitrary graph. Two edges $e = uv$ and $f = xy$ of G are called *codistant* (briefly: *e co f)* if they obey the topologically parallel edges relation. Let m (G, c) be the number of *qoc* strips of length c (*i.e.*, the number of cut-off edges) in the graph G; for the sake of simplicity, m (G,c) will hereafter be written as m (see [10]). Two counting polynomials have been defind on the ground of *qoc* strips:

$$\Omega(G,x) = \sum_c m \cdot x^c \qquad (1)$$

and

$$\mathrm{Sd}\,(G, x) = \sum_{c} m\, x^{|E(G)|-c} \qquad (2)$$

In the following theorem we compute the Omega and Sadhana polynomial of G ,Figure1.

Theorem2.2. 1. $\Omega(G, x) = p/2\, x^{q} + 6qx^{p} + (4q+2)\, x^{p/4} + (8p-4)x^{2q}$
and $Sd(G,x) = p/2\, x^{9pq+p/4-q} + 6qx^{9pq-3p/4} + (4q+2)\, x^{9pq} + (8p-4)x^{9pq+p/4-2q}$.

Proof. To compute the omega polynomial of G, it is enough to calculate C(*e*) for every e in E(G) To do prove, suppose that $E(G) = C_1 \cup \ldots \cup C_5$ such that

$C_i = \{ e \in E(G) \mid e \text{ co } A_i \}$; $1 \le i \le 5$.

Thus by tables 1 the proof is completed.

Table 1. C (A_i) and m(A_i) for Every edge A_i in graph G.

Edge	C(A_i)	M (A_i)
A_1	q	p/2
A_2	p	6q
A_3	p/4	2(2q+1)
A_4	2q	4p-2
A_5	2q	4p-2

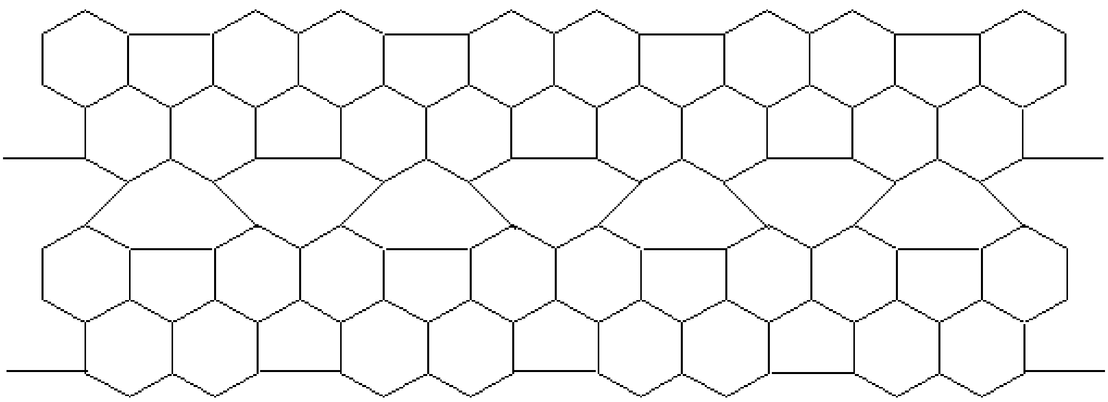

Figure 1. 2-Dimensional Lattice of the $HAC_5C_6C_7$[16,8] Nanotube

3. Conclusion

Carbon nanotubes (CNTs) are nano-objects that have raised great expectations in a number of different applications, including field emission, energy storage, molecular electronics, atomic force microscopy, and many others. Because of this importance, in this paper some properties of $HAC_5C_6C_7$ Nanotubes and Nanotori, were determined.

Acknowledgement

This work supported by Young Researchers Club,Islamic Azad University, Garmsar Branch, Garmsar, Iran .

References

[1] J. Devillers, A.T. Balaban, Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breace Science Publisher, Amsterdam, 2000.
[2] L.B. Kier, L.H. Hall, Molecular Structure Description, Academic Press, New York, 1999.
[3] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, New York, 2000.
[4] J. Devillers, Comparative QSAR, Taylor and Francis, Philadelphia, 1998.
[5] N. Trinajstic, Chemical Graph Theory, 2^{nd} revised ed., CRC Press, Boca Raton, FL, 1992.
[6] H. Wiener, J. Am. Chem. Soc, **69**, 17 (1947).
[7] I. Gutman, Y.N. Yeh, S.L. Lee, Y.L. Luo, , Indian J. Chem, **32**, 651 (1999).
[8] H. Wiener , J. Amer. Chem.Soc,**69**, 17 (1947).
[9] P.V. Khadikar, Nat Acad Sci Lett-India, **23**, 113 (2000).
[10] A.Bahrami, J. Yazdani, Digest Journal of Nanomaterials and Biostructures , **3**, 309(2008).