$\Pi(G,x)$ polynomial and $\Pi(G)$ index of Armchair Polyhex Nanotubes $TUAC_6[m,n]$

Mohammad Reza Farahani

Department of Applied Mathematics, Iran University of Science and Technology (IUST),
 Narmak, Tehran 16844, Iran

E-mail address: Mr_Farahani@Mathdep.iust.ac.ir, MrFarahani88@Gmail.com

ABSTRACT

Let G be a simple connected graph with the vertex set $V = V(G)$ and the edge set $E = E(G)$, without loops and multiple edges. For counting *qoc* strips in G , Omega polynomial was introduced by Diudea and was defined as $\Omega(G,x) = \sum_c m(G,c)x^c$, where $m(G,c)$ be the number of *qoc* strips of length c in the graph G . Following Omega polynomial, the Sadhana polynomial was defined by Ashrafi et al as $Sd(G,x) = \sum_c m(G,c)x^{|E(G)|-c}$. In this paper we compute the Pi polynomial $\Pi(G,x) = \sum_c m(G,c)x^{|E(G)|-c}$ and Pi index $\Pi(G) = \sum_c c \times m(G,c)(|E(G)|-c)$ of an infinite class of “Armchair Polyhex Nanotubes $TUAC_6[m,n]$ ”.

Keywords: Molecular Graph; Armchair Polyhex Nanotubes and Nanotori; Omega polynomial; Pi polynomial; Pi index.

1. INTRODUCTION

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which being denoted by $V(G)$ and $E(G)$, respectively. Suppose G is a connected molecular graph and $u,v \in V(G)$. The distance $d(u,v)$ between u and v is defined as the length of a minimum path between u and v . Two edges $e = uv$ and $f = xy$ of G are *co* if and only if $d(u,x) = d(v,y) = k$ and $d(u,y) = d(v,x) = k+1$ or vice versa, for a non-negative integer k .

The relation “*co*” is reflexive and symmetric but it is not necessary to be transitive, obviously. Set $C(e) = \{f \in E(G) \mid e \text{ co } f\}$, denote the subset of edges in G , *co*-distant to the edge e . If the relation “*co*” is transitive on $C(e)$ then $C(e)$ is called an *orthogonal cut* (denoted by *oc*) of G [1-10]. The graph G is called *co-graph* if and only if the edge set $E(G)$ a union of disjoint orthogonal cuts. Observe *co* is a theta Θ relation, (Djoković [11], and Winkler [12]):

$$d(x,u) + d(y,v) \neq d(x,v) + d(y,u)$$

Theta Θ is a *co*-relation if and only if G is a partial cube, as Klavžar [13] correctly stated in a recent paper. Relation Θ is reflexive and symmetric but need not be transitive.

If any two consecutive edges of an edge-cut sequence are topologically parallel within the same face of the covering, such a sequence is called a *quasi-orthogonal cut qoc* strip.

Let $m(G,c)$ be the number of *qoc* strips of length c in the graph G . For counting “opposite edge strips” qocs of $E(G)$, *M.V. Diudea* introduced the *Omega polynomial* of G [1-10] and was defined as

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

It is easy to see that the first derivative of Omega polynomial $\Omega(G, x)$ (in $x = 1$) equals the number of edges in the graph. Following Omega polynomial, the Sadhana polynomial was defined by *Ashrafi* and co-authors [14] in 2008, as

$$Sd(G,x) = \sum_c m(G,c)x^{|E(G)|-c}$$

The Sadhana index $Sd(G)$ for counting *qoc* strips in G was defined by *Khadikar et. al* [15-17] as first derivative of sadhana polynomial evaluated at $x=1$

$$Sd(G) = Sd'(G, x) = \sum_{i=1}^k (|E(G)| - c_i)$$

Another polynomial also related to the Sadhana polynomial is the *Pi* polynomial $\Pi(G, x)$ and defined as:

$$\Pi(G,x) = \sum_c m(G,c).c.x^{|E(G)|-c}$$

The first derivative (computed at $x=1$) of this counting polynomial provide its topological index:

$$\Pi(G) = \Pi'(G,x) = \sum_c c \times m(G,c)(|E(G)| - c)$$

$\Omega(G,x)$ polynomial count codistant edges in G while $Sd(G,x)$ and $\Pi(G,x)$, non-codistant edges.

In chemical, physics and nano sciences, we have the appealing structure, especially symmetric structure with chemical constitution purporting [18,19]. One of the nanotube is *Polyhex Nanotubes*, that the structure of polyhex nanotubes is consisting of the cycles with length six C_6 in columns. Since polyhex nanotubes have more practical in the chemical, physics and nano science (see Figure 1). In Figures 1 and 2, one can see that the 3-dimensional and 2-dimentional graph of Armchair polyhex nanotubes $TUAC_6[m,n]$, where m,n are the numbers of rows/columns of hexagon (C_6) in 2-dimentional perception $TUAC_6[m,n]$. In a series of papers [18-30], some properties and applications and more historical details of nanotubes are presented and studied.

In the present work we compute the *Pi* polynomial $\Pi(G,x)$ and *Pi* index $\Pi(G)$ for an infinite class of Nano-structure “*Armchair Polyhex Nanotubes TUAC₆*”. Throughout this paper our notation is standard and mainly taken from standard book of graph theory such as [31-36].

Figure 1. A 3-dimentional lattice of *Armchair Polyhex Nanotubes* $TUAC_6$.

Figure 2. A 2-dimentional lattice of *Armchair Polyhex Nanotubes* $TUAC_6[m,n]$ and its hotizontal edge e_i and oblique edges f_i and h_i .

2. RESULTS AND DISCUSSION

In this section we present explicit formulas for the *Pi* polynomial $\Pi(G,x)$ and *Pi* index $\Pi(G)$ of an *Armchair Polyhex Nanotubes* $TUAC_6$.

Theorem 1. Consider the Armchair polyhex nanotubes $TUAC_6[m,n] \forall m,n \in N$; the *Pi* polynomials and its index are calculated by formulas:

$$\Pi(TUAC_6[m,n], x) = 2m[(n+1)x^{6mn+4m-n-1} + (2n+1)x^{6mn+4m-2n-1}]$$

and
$$\Pi(TUAC_6[m,n]) = 23[18mn^2 + 24mn - 5n^2 + 8m - 6n - 2]$$

Proof. Let $G = TUAC_6[m,n]$ be the the Armchair polyhex nanotubes and m and n be the number of hexagons in rows and columns of G .

From Figures 1 and 2, it is easy to see that the number of vertices/carbon atoms and edges/chemical bonds of $TUAC_6[m,n]$, are equal to $|V(TUAC_6[m,n])| = 4m(n+1)$ and $|E(TUAC_6[m,n])| = 6mn+4m$.

By according to Figure 2, we denote all horizontal edge in i^{th} column by e_i and all oblique edges in i^{th} column by f_i (right) and h_i (left), then one can see that for all *quasi-orthogonal cuts* $C(e_i)$, $C(f_j)$ and $C(h_l)$:

There are $2m$ number of $C(e_i)$ with size $|C(e_i)| = n+1$ and m number of $C(f_j)$ and $C(h_l)$ with same size $|C(f_j)| = |C(h_l)| = 2n+1$. So we have the following relations for Armchair polyhex nanotubes $G = TUAC_6[m,n]$:

$$\begin{aligned} \Pi(TUAC_6[m,n],x) &= \sum_c c \times m(TUAC_6[m,n],c) x^{|E(TUAC_6[m,n])|-c} \\ &= \sum_c 2m \times |C(e_i)|.x^{6mn+4m-|C(e_i)|} + \sum_c m \times |C(f_i)|.x^{6mn+4m-|C(f_i)|} + \sum_c m \times |C(h_i)|.x^{6mn+4m-|C(h_i)|} \\ &= 2m \times (n+1)x^{6mn+4m-n-1} + m \times (2n+1)x^{6mn+4m-2n-1} + m \times (2n+1)x^{6mn+4m-2n-1} \\ &= 2m[(n+1)x^{6mn+4m-n-1} + (2n+1)x^{6mn+4m-2n-1}] \end{aligned}$$

The first derivative (computed at $x=1$) of $\Pi(TUAC_6[m,n],x)$ polynomial provide the Pi index of an *Armchair Polyhex Nanotubes* $TUAC_6$ as follows:

$$\begin{aligned} \Pi(TUAC_6[m,n]) &= \Pi'(TUAC_6[m,n],1) \\ &= \sum_c c \times m(TUAC_6[m,n],c) (|E(TUAC_6[m,n])|-c) \\ &= 2m[(n+1)(6mn+4m-n-1) + (2n+1)(6mn+4m-2n-1)] \\ &= 23[18mn^2 + 24mn - 5n^2 + 8m - 6n - 2] \end{aligned}$$

and this completes the proof.

3. CONCLUSION

In this paper, I was counting a new counting topological polynomial and its index for a family of carbon nanotubes "Armchair polyhex nanotubes $TUAC_6[m,n]$ ". $\Pi(G,x)$ polynomial and its index are useful for counting the *quasi-orthogonal cut qoc* strip in structure of connected nanotubes and connected nanostructures.

References

- [1] M.V. Diudea, *Carpath. J. Math.* 22 (2006) 43--47.
- [2] M.V. Diudea, S. Cigher, A.E. Vizitiu, O. Ursu, P.E. John. *Croat. Chem. Acta* 79(3), (2006) 445-448.
- [3] P.E. John, A.E. Vizitiu, S. Cigher, M.V. Diudea, *MATCH Commun. Math. Comput. Chem.* 57 (2007) 479-484.
- [4] M.V. Diudea, S. Cigher, P.E. John. *MATCH Commun. Math. Comput. Chem.* 60 (2008) 237-250.
- [5] M.V. Diudea, S. Cigher, P.E. John, *MATCH Commun. Math. Comput. Chem.* 60 (2008) 237-250.
- [6] M.V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology*, NOVA, New York, 2002.
- [7] A.E. Vizitiu, S. Cigher, M.V. Diudea, M.S. Florescu, *MATCH Commun. Math. Comput. Chem.* 57(2) (2007) 479-484.
- [8] M.V. Diudea, A. Ilić, *Carpath. J. Math.* 20(1) (2009) 177-185.
- [9] M.V. Diudea, *MATCH Commun. Math. Comput. Chem.* 2010, 64, 569.
- [10] A.R. Ashrafi, M. Jalali, M. Ghorbani, M.V. Diudea. *MATCH, Commun. Math. Comput. Chem.* 60 (2008), 905-916.
- [11] D.Ž. Djoković, *J. Combin. Theory Ser. B* 14 (1973) 263.
- [12] P.M. Winkler, *Discrete Appl. Math.* 8 (1984) 209.
- [13] S. Klavžar, *MATCH Commun. Math. Comput. Chem.* 59 (2008) 217.
- [14] A.R. Ashrafi, M. Ghorbani, M. Jalali, *Int. J. Chem.* 47A(4) (2008) 535-537.
- [15] P.V. Khadikar, S. Joshi, A. V. Bajaj, D. Mandloi, *Med. Chem. Lett.* 14 (2004) 1187-1191.
- [16] P.V. Khadikar, V. K. Agrawal, S. Karmarkar. *Bioorg. Med. Chem.* 2(10) (2002) 3499-3507.
- [17] P.V. Khadikar, D. Mandoli, Sadhana, *Bioinformatics Trends* 1 (2006) 51-63.
- [18] S. Iijima, *Nature* 354 (1001) 56.
- [19] D.S. Bethune, C.H. Kiang, M.S. Devries, G. Gorman, R. Savoy, J. Vazquez, A. Beyers, *IBID* 363 (1993) 605.
- [20] I. Gutman, S. Klavžar, *ACH Models Chem.* 133 (1996) 389-399.
- [21] M.V. Diudea, *MATCH, Commun. Math. Comput. Chem.* 45 (2002) 109-122.
- [22] A.R. Ashrafi, G. R. Vakili-Nezhaad, *Journal of Physics: Conference Series* 29 (2006) 181-184.
- [23] S. Yousefi, H. Yousefi-Azari, A.R. Ashrafi, M. H. Khalifeh, *JSUT* 33(3) (2008) 7-11.
- [24] A. Iranmanesh, Y. Alizadeh, *Digest. J. Nanomater. Bios* 4 (2009) 607-611.
- [25] H. Shabani, A.R. Ashrafi, *Digest. J. Nanomater. Bios* 4 (2009) 423-428.

-
- [26] S. Alikhani, M.A. Iranmanesh, *Digest. J. Nanomater. Bios* 5 (2010) 1-7.
- [27] M.R. Farahani, *Proceedings of the Romanian Academy Series B Chemistry* 15(1) (2013) 3-6.
- [28] M.R. Farahani, *Journal of Advances in Physics* 3(1) (2013) 191-196.
- [29] M.R. Farahani, *Acta Chim. Slov.* 59 (2012) 779-783.
- [30] M.R. Farahani, *Le Matematiche* 69(2) (2014).
- [31] N. Trinajstić, *Chemical Graph Theory*, (second ed.) CRC Press, Boca Raton, FL, (1992).
- [32] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Weinheim, Wiley-VCH, (2000).
- [33] N. Trinajstić, I. Gutman, *Croat. Chem. Acta* 75 (2002) 329-356.
- [34] Mohammad Reza Farahani, *International Letters of Chemistry, Physics and Astronomy* 12 (2014) 56-62.
- [35] Mohammad Reza Farahani, *International Letters of Chemistry, Physics and Astronomy* 12 (2014) 63-68.
- [36] Mohammad Reza Farahani, *International Letters of Chemistry, Physics and Astronomy* 13(1) (2014) 71-76.

(Received 17 June 2014; accepted 27 June 2014)