Iranian Journal of Mathematical Chemistry, Vol. 3, Supplement 1, December 2012, pp. s51 – s58 **IJMC**

On Counting Polynomials of Some Nanostructures

MODJTABA GHORBANI• AND MAHIN SONGHORI

Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785-136, I. R. Iran

(*Received May 29, 2011*)

ABSTRACT

The Omega polynomial $\Omega(x)$ was recently proposed by Diudea, based on the length of strips in given graph *G*. The Sadhana polynomial has been defined to evaluate the Sadhana index of a molecular graph. The PI polynomial is another molecular descriptor. In this paper we compute these three polynomials for some infinite classes of nanostructures.

Keywords: Omega polynomial, PI polynomial, nanostar dendrimers.

1. INTRODUCTION

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-sets of which are represented by *V*(*G*) and *E*(*G*), respectively. Suppose *G* is a connected molecular graph and $x, y \in V(G)$. The distance $d(x, y)$ between *x* and *y* is defined as the length of a minimum path between x and y. Two edges $e = ab$ and $f = xy$ of *G* are called codistant, "*e* co *f*", if and only if $d(a, x) = d(b, y) = k$ and $d(a, y) = d(b, x) = k+1$ or vice versa, for a non-negative integer *k*. For some edges of a connected graph *G* there are the following relations satisfied [1 – 4]:

$$e\ co\ e \tag{1}$$

$$e\ co\ f \Leftrightarrow f\ co\ e \tag{2}$$

$$e\ co\ f,\ f\ co\ h \Rightarrow e\ co\ h \tag{3}$$

though the relation (3) is not always valid.

Let $C(e) := \{f \in E(G);\ f\ co\ e\}$ denote the set of edges in *G*, codistant to the edge $e \in E(G)$. If relation *co* is an equivalence relation (*i.e.*, all the elements of *C*(*e*) satisfy the relations (1) to (3)), then *G* is called a *co-graph*. Consequently, *C*(*e*) is called an *orthogonal*

•Author to whom correspondence should be addressed.(e-mail:mghorbani@srttu.edu)

cut "oc" of G and $E(G)$ is the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k$ and $Ci \cap Cj = \emptyset$ for $i \neq j, i, j = 1,2,..,k$.

The Omega polynomial $\Omega(x)$ for counting *qoc* strips in G was defined by Diudea as $\Omega(x) = \sum_c m(G,c) \times x^c$ with $m(G, c)$ being the number of strips of length c. The summation runs up to the maximum length of *qoc* strips in G. If G is bipartite then a *qoc* starts and ends out of G and so $\Omega(G,1) = r/2$, in which r is the number of edges in out of G.

The Sadhana index $Sd(G)$ for counting *qoc* strips in G was defined by Khadikar et al. [5, 6] as $Sd(G) = \Sigma_c m(G,c)(|E(G)| - c)$, where $m(G, c)$ is the number of strips of length c. The Sadhana polynomial $Sd(x)$ was defined by Ashrafi and his co–authors [7] as $Sd(x) = \Sigma_c m(G,c) x^{|E| - c}$. By definition of omega polynomial, one can obtain the Sadhana polynomial by replacing x^c with $x^{|E|-c}$ in omega polynomial. Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at $x = 1$.

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 $|G|$. Let U be the subset of vertices of $V(G)$ which are closer to u than v and V be the subset of vertices of $V(G)$ which are closer to v than u:

$$U = \{u_i \mid u_i \in V(G),\ d(u,u_i) < d(u_i,v)\},$$

$$V = \{v_i \mid v_i \in V(G),\ d(v,v_i) < d(v_i,v)\}.$$

Let now $U = \prec U, E_1 \succ$, $V = \prec V, E_2 \succ$, then $n_1(e) = |E_1|$ are the number of edges nearer to u than v and $n_2(e) = |E_2|$ are the number of edges nearer to v than u. In all case of cyclic graphs there are edges equidistant to the both ends of the edges. Such edges are not taken into account. Then, the *PI* index [8,9] is defined as:

$$PI(G) = \sum_{e \in E} [n_1(e) + n_2(e)]. \tag{4}$$

Similar to the case of Sadhaa index, the *PI* polynomial was defined as:

$$PI(x) = \sum_{e \in E} x^{[n_1(e)+n_2(e)]}. \tag{5}$$

So, the PI index is the first derivative of $PI(x)$ at $x = 1$. Given an edge $e = uv \in E(G)$ of G, we define the distance of e to a vertex $w \in V(G)$ as the minimum of the distances of its edges to w, *i.e.*,

$$d(w, e) := \min\{d(w, u), d(w, v)\}.$$

Note that in this definitions the edges *equidistant* from the two ends of the edge $e = uv$ i.e., edges f with $d(u, f) = d(v, f)$ are not counted. We call such edges *parallel* to e. This implies that we can write $PI(x) = \sum_{e \in E(G)} x^{|E|-|N(e)|}$, where $N(e)$ is set of all parallel edges with e.

Here our notations are standard and mainly taken from standard book of graph theory such as [10]. We encourage reader to consult the work of Khadikar for discussion and background material about the PI index [11 – 15].

2. NANOSTAR DENDRIMERS

The goal of this section is computation of PI, Omega and Sadhana polynomials of nanostar dendrimer G_n, depicted in Figure 1. To do this, consider the following fundamental proposition:

Proposition 1. Let G be a bipartite graph and $e \in E(G)$. Then $C(e) = N(e)$.

By using Proposition 1 we can reformulate three mentioned counting polynomials as follows:

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

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

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

where $m(G, c)$ is the number of strips of length c.

Now we are ready to compute three counting polynomials of nanostar dendrimer G_n. At first consider G_1, in Figure 2. Obviously, there are two different strips, *e. g*. F_1 and F_2. On the other hand there are 36 strips of type F_1 and 9 strips of type F_2. Further, $|F_1| = 2$ and $|F_2| = 1$. Hence by using Theorem 1, we have

$$\Omega(x) = 9x^2 + 3x,\ Sd(x) = 9x^{19} + 3x^{20},\ \ PI(x) = 18x^{19} + 3x^{20}.$$

Let us consider the graph of G_2 depicted in Figure 1. Similar to the last case, there are two different strips, namely F_1 and F_2, in which $|F_1| = 2$ and $|F_2| = 1$. On the other hand there are 36 strips of type F_1 and 9 strips of type F_2. Further, $|F_1| = 2$ and $|F_2| = 1$. This implies

$$\Omega(x) = 36x^2 + 9x,\ Sd(x) = 9x^{85} + 3x^{86},\ \ PI(x) = 72x^{85} + 9x^{86}.$$

In generally, in G_n there are two strips F_1 and F_2, with $|F_1| = 2$ and $|F_2| = 1$. By counting strips equivalent with F_1 and F_2 respectively, it is easy to see that there are $9 + 27\times2^{n-2}$ strips of type F_1 and $3 + 12 \times 2^{n-2}$ cut edges. Thus we proved the following Theorem:

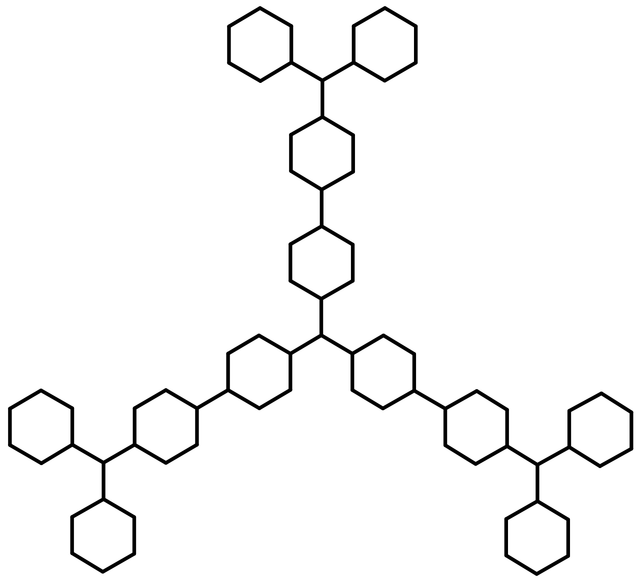

Figure 1. 2*D* Graph of Nanostar Dendrimer G_n for $n = 2$.

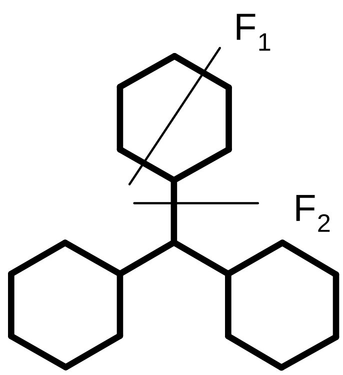

Figure 2. 2*D* Graph of Nanostar Dendrimer G_n for $n = 1$.

Theorem 2. Consider the nanostar dendrimer G_n, for $n \geq 2$. Then

$$\Omega(x) = (9 + 27 \times 2^{n-2})x^2 + (3 + 12 \times 2^{n-2})x,$$

$$Sd(x) = (9 + 27 \times 2^{n-2})x^{|E|-2} + (3 + 12 \times 2^{n-2})x^{|E|-1},$$

$$PI(x) = 2(9 + 27 \times 2^{n-2})x^{|E|-2} + (3 + 12 \times 2^{n-2})x^{|E|-1},$$

where $|E| = |E(G_n)| = 33 \times 2^n - 45$.

3. FULLERENE GRAPHS

Carbon exists in several allotropic forms in nature. Fullerenes are zero-dimensional nanostructures, discovered experimentally in 1985 [16]. Fullerenes are carbon–cage molecules in which a number of carbon atoms are bonded in a nearly spherical configuration. The most famous fullerenes are [5, 6] fullerenes, *e. g* fullerenes with pentagonal and hexagonal faces. In this section we study [3, 6] fullerenes. Let *t, h, n* and *m* be the number of triangles, hexagons, carbon atoms and bonds between them, in a given fullerene *C*. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (3p + 6h)/3$, the number of edges is $m = (3t + 6h)/2 = (3/2)n$ and the number of faces is $f = t + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(3t + 6h)/3 - (3t + 6h)/2 + t + h = 2$, and therefore $t = 4$. This implies that such molecules, made entirely of *n* carbon atoms, have 4 triangles and $(n/2) - 2$ hexagonal faces.

In this section we compute Omega polynomial and Sadhana polynomial of an infinite class of fullerene graphs, namely C_{8n} fullerenes, see Figures 3, 4. In other words, this family of fullerenes has exactly $8n$ vertices and $12n$ edges.

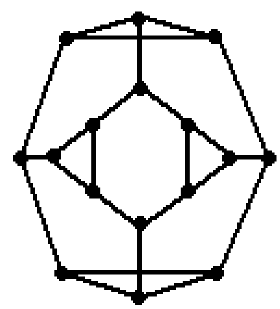

Figure 3. 2*D* Graph of Fullerene C_{8n} for $n = 2$.

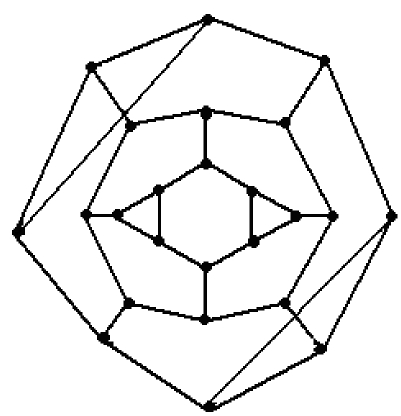

Figure 4. 2*D* Graph of Fullerene C_{8n} for $n = 3$.

At first suppose $n = 2$, Figure 3. By computing number of strips and their sizes Omega and Sadhana polynomials are as follows:

$$\Omega(G,x) = 2x^2 + 4x^6 + 2x^4 \text{ and } Sd(G,x) = 2x^{34} + 4x^{30} + 2x^{32}.$$

When $n = 3$, Figure 4, one can see that $\Omega(G,x) = 2x^2 + 4x^6 + 2x^4$ and

$Sd(G,x) = 2x^{34} + 4x^{30} + 2x^{32}$. By computing this method we have the following Theorem for Omega and Sadhana polynomials of [3, 6] fullerene graphs:

Theorem 3. Consider the fullerene graph C_{8n} (Figure 5). Then:

$$\Omega(F_{8n},x) = \begin{cases} 2x^2 + (n-1)x^4 + 4x^{2n} & 2\mid n \\ 2x^2 + (n-1)x^4 + 2x^n + 3x^{2n} & 2\nmid n \end{cases},$$

$$Sd(F_{8n},x) = \begin{cases} 2x^{12n-2} + (n-1)x^{12n-4} + 4x^{10n} & 2\mid n \\ 2x^{12n-2} + (n-1)x^{12n-4} + 2x^{11n} + 3x^{10n} & 2\nmid n \end{cases}.$$

Proof. To compute qoc strips we should to consider two cases:

Case 1: n is even. According to Figure 5(a), there are 3 strips such as $C(e_1)$, $C(e_2)$ and $C(e_3)$ with $|C(e_1)| = 2$ ‘$|C(e_2)| = 4$ and $|C(e_3)| = 2n$. On the other hand, there are 2, $n-1$, 4 stripes of types $C(e_1)$, $C(e_2)$ and $C(e_3)$, respectively. This completes the first claim.

Case 2: n is odd. n is even. According to Figure 5(b), there are 4 strips such as $C(e_1)$, $C(e_2)$, $C(e_3)$ and $C(e_4)$ with $|C(e_1)| = 2$ ‘$|C(e_2)| = 4$, $|C(e_3)| = n$ and $|C(e_4)| = 2n$. On the other hand, there are 2, $n-1$, 2, 3 stripes of types $C(e_1)$, $C(e_2)$, $C(e_3)$ and $C(e_4)$, respectively. This completes the proof.

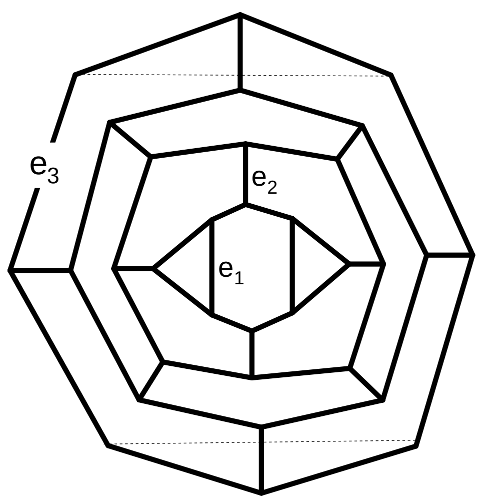

Figure 5(a). 2D Graph of Fullerene C_{8n}, n is Even.

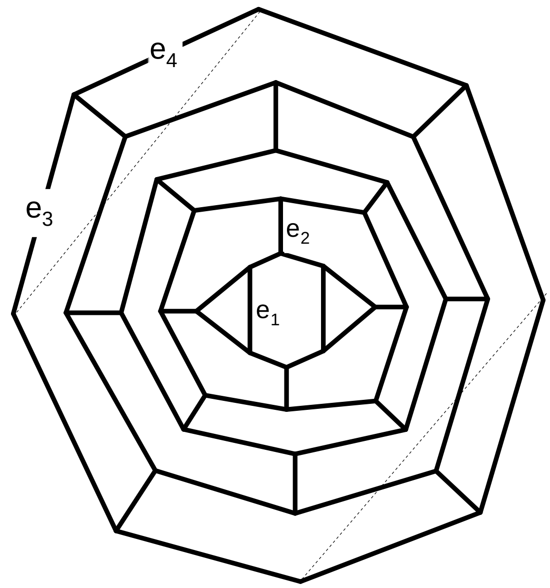

Figure 5(b). 2*D* Graph of Fullerene C_{8n}, n is Odd.

REFERENCES

1. M. V. Diudea, S. Cigher, A. E. Vizitiu, O. Ursu and P. E. John, Omega polynomial in tubular nanostructures, *Croat. Chem. Acta.* **79** (2006) 445 – 448.
2. A. E. Vizitiu, S. Cigher, M. V. Diudea and M. S. Florescu, Omega polynomial in ((4,8)3) tubular nanostructures, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 457 – 462.
3. M. V. Diudea, Note on omega polynomial, *Carpath. J. Math.* **22** (2006) 43 – 47.
4. M. V. Diudea, Phenylenic and naphthylenic tori, *Fullerenes, Nanotubes and Carbon Nanostructures* **10** (2002) 273 – 292.
5. P. V. Khadikar, S. Joshi, A .V. Bajaj and D. Mandloi, A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts, *Bioorg. Med. Chem. Lett.* **14** (2004) 1187 – 1191.
6. P. V. Khadikar, V. K. Agrawal and S. Karmarkar, Prediction of lipophilicity of polyacenes using quantitative structure – activity *relationships*, *Bioorg. Med. Chem.* **10** (2002) 3499 – 3507.
7. A. R. Ashrafi, M. Ghorbani and M. Jalali, Computing Sadhana polynomial of V - phenylenic nanotubes and nanotori, *Ind. J. Chem.* **47A** (2008) 535 – 537.
8. P. V. Khadikar, On a novel structural descriptor PI, *Nat. Acad. Sci. Lett.* **23** (2000) 113 – 118.
9. P. V. Khadikar, S. Karmarkar, V. K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, *J. Chem. Inf. Comput. Sci.* **41** (2001) 934 – 949.
10. N. Trinajstić, *Chemical Graph Theory*, CRC Press, *Boca Raton*, FL, 1992.

11. P. V. Khadikar, S. Karmarkar, V. K. Agrawal PI index of polyacenes and its use in developing QSPR, *Nat. Acad. Sci. Lett.* **23** (2000) 124 – 128.
12. P. V. Khadikar, M. V. Diudea, J. Singh, P. E. John, A. Shrivastava, S. Singh, S. Karmarkar, M. Lakhwani, P. Thakur, Use of PI index in computer–aided designing of bioactive compounds, *Curr. Bioact. Comp.* **2** (2006) 19 – 56.
13. P. E. John, P. V. Khadikar, J. A. Singh, Method for computing the PI index of benzenoid hydrocarbons using orthogonal cuts, *J. Math. Chem.* **42** (2007) 37 – 45.
14. P. V. Khadikar, D. Mandloi, A. K. Bajaj, *Novel applications of PI index*: Prediction of the ultrasonic sound velocity in N–alkanes, *Oxid. Commun.* **27** (2004) 29 – 33.
15. A. R. Ashrafi, M. Jalali, M. Ghorbani and M. V. Diudea, Computing PI and omega polynomials of an infinite family of fullerenes, *MATCH Commun. Math. Comput. Chem.* **60 (3)** (2008) 905 – 916.
16. H. W. Kroto, J. R. Heath, S. C. O’Brien, R. F. Curl and R.. Smalley, C_{60}: buckminsterfullerene, *Nature* **318** (1985) 162 – 163.