Iranian Journal of Mathematical Chemistry, Vol. 1, No. 1, April 2010, pp. 105 – 110

IJMC

Computing Vertex PI, Omega and Sadhana Polynomials of $F_{12(2n+1)}$ Fullerenes

MODJTABA GHORBANI

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

(*Received January 10, 2010*)

ABSTRACT

The topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. The vertex PI polynomial is defined as $PI_v(G) = \sum_{e=uv} n_u(e) + n_v(e)$. Then Omega polynomial $\Omega(G,x)$ for counting qoc strips in G is defined as $\Omega(G,x) = \sum_c m(G,c)x^c$ with m(G,c) being the number of strips of length c. In this paper, a new infinite class of fullerenes is constructed. The vertex PI, omega and Sadhana polynomials of this class of fullerenes are computed for the first time.

Keywords: Fullerene, vertex PI polynomial, Omega polynomial, Sadhana polynomial.

1. INTRODUCTION

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. Fullerenes F_n can be drawn for n = 20 and for all even n ≥ 24. They have *n* carbon atoms, 3n/2 bonds, 12 pentagonal and n/2-10 hexagonal faces. The most important member of the family of fullerenes is C_{60} [1,2].

Let ∑ be the class of finite graphs. A topological index is a function Top from ∑ into real numbers with this property that Top(G) = Top(H), if G and H are isomorphic.

Let G = (V,E) be a connected bipartite graph with the vertex set V = V(G) and the edge set E = E(G), without loops and multiple edges. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than u. The vertex PI index is a topological index which is introduced in [3]. It is defined as the sum of $[n_u(e) + n_v(e)]$, over all edges of a graph G. 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. For some edges of a connected graph G there are the following relations satisfied [4,5]:

$$e\ co\ e$$
$$e\ co\ f \Leftrightarrow f\ co\ e$$
$$e\ co\ f\ ,\ f\ co\ h \Rightarrow e\ co\ h$$

though the last relation is not always valid.

Set $C(e):= \{f \in E(G) \mid f \text{ co } e\}$. If the relation "co" is transitive on C(e) then C(e) is called an orthogonal cut "oc" of the graph G. The graph G is called co-graph if and only if the edge set E(G) is the union of disjoint orthogonal cuts.

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. Three counting polynomials have been defined [6-8] on the ground of qoc strips:

$\Omega(G,x) = \sum_c m \cdot x^c$, $\Theta(G,x) = \sum_c m \cdot c \cdot x^c$ and $\Pi(G,x) = \sum_c m \cdot c \cdot x^{e-c}$. $\Omega(G,x)$ and $\Theta(G,x)$ polynomials count equidistant edges in G while $\Pi(G,x)$, non-equidistant edges. In a counting polynomial, the first derivative (in x=1) defines the type of property which is counted; for the three polynomials they are:

$$\Omega'(G,1) = \sum_c m.c = |E(G)|,\ \Theta'(G,1) = \sum_c m.c^2 \text{ and } \Pi'(G,1) = \sum_c m.c.(e-c).$$

If G is bipartite, then a qoc starts and ends out of G and so Ω(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. [9,10] as $Sd(G)=\sum_c m(G,c)(|E(G)|-c)$, where m(G,c) is the number of strips of length c. We now define the Sadhana polynomial of a graph G as $Sd(G,x) = \sum_c m(G,c) \cdot x^{|E|-c}$. 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(G, x) evaluated at x = 1. Herein, our notation is standard and taken from the standard book of graph theory [11-17].

Example 1. Let C_n denotes the cycle of length n.

$$\Omega(C_n,x) = \begin{cases} \frac{n}{2}x^2 & 2\mid n \\ nx & 2\nmid n \end{cases} \text{ and } Sd(C_n,x) = \begin{cases} \frac{n}{2}x^{n-2} & 2\mid n \\ nx^{n-1} & 2\nmid n \end{cases}.$$

Example 2. Suppose K_n denotes the complete graph on n vertices. Then we have:

$$\Omega(K_n,x)=\begin{cases}\frac{n}{2}(x^{\frac{n}{2}}+x^{\frac{n}{2}-1}) & 2\mid n\\ nx^{\frac{n-1}{2}} & 2\nmid n\end{cases} \text{ and } Sd(K_n,x)=\begin{cases}\frac{n}{2}(x^{\frac{n}{2}(n-2)}+x^{\frac{n^2}{2}-n+1}) & 2\mid n\\ nx^{(n-1)(n-2)/2} & 2\nmid n\end{cases}.$$

Example 3. Let T_n be a tree on n vertices. We know that $|E(T_n)|=n-1$. So,

$$\Omega(T_n,x)=\Theta(T_n,x)=(n-1)x,\ Sd(T_n,x)=\Pi(T_n,x)=(n-1)x^{n-2}.$$

2. Main Results and Discussion

The aim of this section is to compute the counting polynomials of equidistant (Omega, Sadhana and Theta polynomials) of an infinite family $F_{12(2n+1)}$ of fullerenes with 12(2n+1) carbon atoms and 36n+18 bonds (the graph $F_{12(2n+1)}$, Figure 1 is n = 4).

Theorem 4. The omega polynomial of fullerene graph $F_{12(2n+1)}$ for $n \geq 2$ is as follows:

$$\Omega(F_{12(2n+1)},x)=12x^{3}+12x^{2n-2}+6x^{n-1}+3x^{2n+4}.$$

Proof. By figure 1, there are four distinct cases of qoc strips. We denote the corresponding edges by f_1, f_2, f_3 and f_4. By the table 1 proof is completed.

Edge	#Co distance	Number of edges
f_1	3	12
f_2	2n-2	12
f_3	2n+4	3
f_4	n-1	6

Table 1. The Number of Equidistant Edges**.**

Corollary 5. The Sadhana polynomial of fullerene graph $F_{12(2n+1)}$ is as follows:

$$Sd(F_{12(2n+1)},x)=12x^{36n+15}+12x^{34n+20}+6x^{35n+19}+3x^{34n+14}.$$

Now, we are ready to compute the vertex PI polynomial of fullerene graph $F_{12(2n+1)}$. It is well-known fact that an acyclic graph T does not have cycles and so $n_u(e|G) + n_v(e|G) = |V(T)|$. Thus $PI_v(T) = |V(T)|.|E(T)|$. Since a fullerene graph F has 12 pentagonal faces, $PI_v(F) < |V(F)|.|E(F)|$. Let G be a connected graph. The PI_v polynomials of G are defined as $PI_v(G;x)=\sum_{e=uv\in E(G)}x^{n_u(e|G)+n_v(e|G)}$.Obviously $PI'_v(G,1)=PI_v(G)$ and $PI_v(G,1)$ =

$|E(G)|$. Define $N(e) = |V| - (n_u(e) + n_v(e))$. Then $PI_v(G) = \sum_{e=uv}[|V| - N(e)] = |V||E| - \sum_{e=uv} N(e)$ and we have:

$$PI_v(G,x) = \sum_{e=uv\in E(G)} x^{n_u(e)+n_v(e)} = \sum_{e=uv\in E(G)} x^{|V(G)|-N(e)}$$
$$= x^{|V(G)|}\sum_{e=uv\in E(G)} x^{-N(e)}.$$

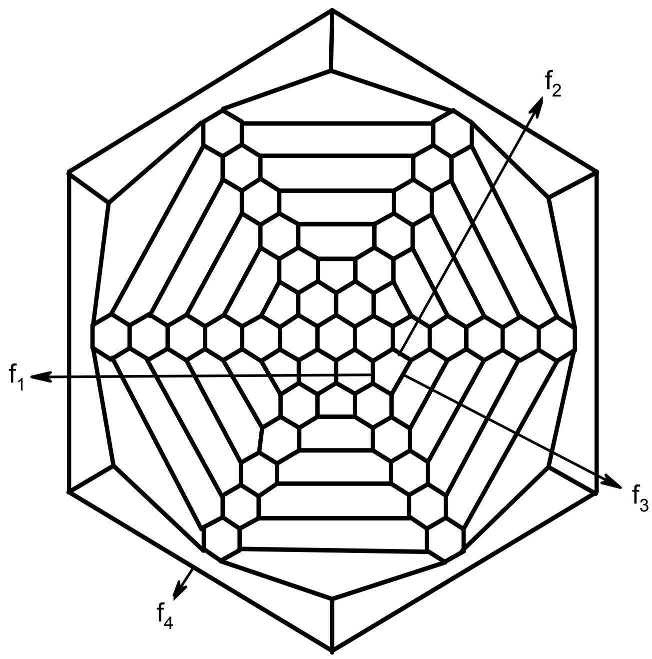

Figure1. The graph of fullerene $F_{12(2n+1)}$ for n = 4.

Example 6. Suppose F_{30} denotes the fullerene graph on 30 vertices, see Figure 2. Then $PI_v(F_{30}, x) = 10x^{20} + 10x^{22} + 20x^{26} + 5x^{30}$ and so $PI_v(F_{30}) = 1090$.

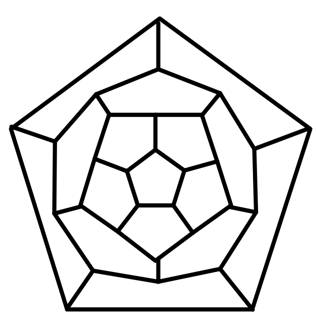

Figure 2. The Fullerene Graph F_{30}.

Theorem 7. The vertex PI polynomial of fullerene graph $F_{12(2n+1)}$ for $n \geq 2$ is as follows:

$$PI_v(F_{12(2n+1)}, x) = 24x^{24n-64} + 12x^{24n-44} + 12x^{24n-12} + 6(n-3)x^{24n-4} + 24x^{24n-2} + 24x^{24n} + 24x^{24n+6} + 24x^{24n+8} + 24x^{24n+10} + 6(5n-22)x^{24n+12}.$$

Proof. From Figures 3, one can see that there are ten types of edges of fullerene graph $F_{12(2n+1)}$. We denote the corresponding edges by e_1, e_2, … ,e_{10}. By table 2 the proof is completed.

Edge	Number of vertex which are codistance from two ends of edges	Num
e_1	0	6(5n-22)
e_2	2	12
e_3	4	12
e_4	6	24
e_5	12	24
e_6	14	24
e_7	16	6(n-3)
e_8	24	12
e_9	56	12
e_{10}	76	24

Table 2. Computing N(e) for Different Edges.

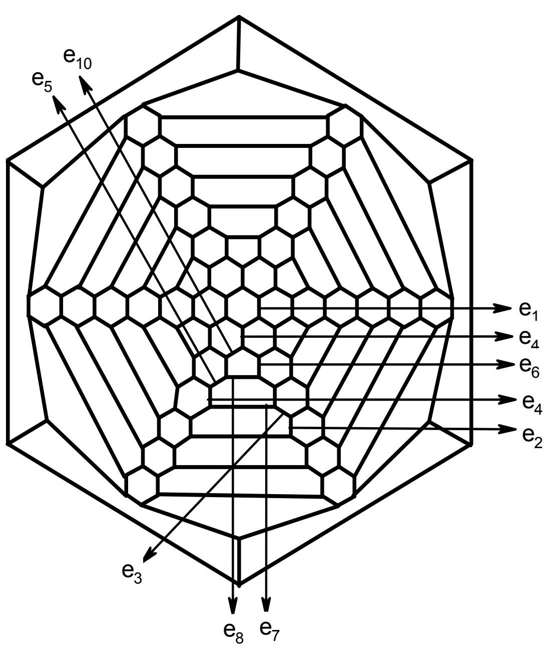

Figure 3. Types of Edges of Fullerene Graph $F_{12(2n+1)}$.

REFERENCES

[1] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl and R.E. Smalley *Nature,* **318**, 162, 1985.
[2] H. W. Kroto, J. E. Fichier and D. E Cox, The Fulerene, Pergamon Press, New York, 1993.
[3] M. H. Khalifeh, H. Yousefi-Azari and A. R. Ashrafi, *Disc. Appl. Math.*, 2007, doi: 10.1016/j.dam.2007.08.041.
[4] B. E. Sagan, Y.-N. Yeh and P. Zhang, *Int. J. Quantum Chem*., **60**, 959, 1996.
[5] P. E. John, A. E. Vizitiu, S. Cigher, and M. V. Diudea, MATCH Commun. Math. Comput. Chem., **57**, 479, 2007.
[6] M. V. Diudea, S. Cigher, A. E. Vizitiu, O. Ursu and P. E. John, *Croat. Chem. Acta*, **79**, 445, 2006.
[7] A. E. Vizitiu, S. Cigher, M. V. Diudea and M. S. Florescu, *MATCH Commun. Math. Comput. Chem.*, **57**, 457, 2007.
[8] M.V. Diudea, *Fullerenes, Nanotubes, and Carbon Nanostructures*, **10**, 273, 2002.
[9] P. V. Khadikar, S. Joshi, A. V. Bajaj and D. Mandloi, *Bioorg. Med .Chem. Lett.*, **14**, 1187, 2004.
[10] P. V. Khadikar, V. K. Agrawal and S. Karmarkar, *Bioorg. Med. Chem.*, **10**, 3499, 2002.
[11] N. Trinajstic, Chemical Graph Theory, CRC Press, *Boca Raton, FL*, 1992.
[12] A. R. Ashrafi, M. Ghorbani and M. Jalali, *Indian J. Chem*., **47**, 535, 2008.
[13] A. R. Ashrafi and M. Ghorbani, *MATCH Commun. Math. Comput. Chem.*, **60**(2), 359, 2008.
[14] M. Ghorbani and A. R. Ashrafi, *J. Comput. Theor. Nanosci.***,** **3**, 803, 2006.
[15] A. R. Ashrafi, M. Ghorbani and M. Jalali, *Digest Journal of Nanomaterials and Biostructures*, **3**(4), 245, 2008.
[16] A. R. Ashrafi, M. Jalali, M. Ghorbani, *MATCH Commun. Math.Comput. Chem*., **60**(3), 905, 2008.
[17] M. Ghorbani and M. Jalali, *MATCH Commun. Math.Comput. Chem*., **62**(3), 353, 2009.