Digest Journal of Nanomaterials and Biostructures Vol. 4, No.3, September 2009, p. 403 – 406

COMPUTING OMEGA AND SADHANA POLYNOMIALS OF C_{12N+4} FULLERENE

ALI REZA ASHRAFI, MODJTABA GHORBANI*, MARYAM JALALI
Institute of Nanoscience and Nanotechnology,
University of Kashan, Kashan 87317−51167, I. R. Iran

The omega polynomial Ω(G,x) for counting qoc strips in G was defined by Diudea as $\Omega(G,x)=\sum_c m(G,c)\times x^c$ with m(G,c) being the number of strips of length c. The Sadhana polynomial Sd(G,x) was defined by Ashrafi and co-authors as $Sd(G,x)=\sum_c m(G,c)\times x^{|E|-c}$. In this paper we compute the omega polynomial and then Sadhana polynomial of an infinite family of fullerenes .

(Received June 6, 2009; accepted July 20, 2009)

Keywords: Omega and Sadhana Polynomial, Fullerene graph, Topological Index.

1. Introduction

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. Fullerenes C_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].

Mathematical calculations are absolutely necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures [3-5]. This theory had an important effect on the development of the chemical sciences. This paper reflects an attempt for studying nanostructures by using graph theory. 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 ∈ 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 co-distant, "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. It is easy to see that the relation "co" is reflexive and symmetric but it is not necessary to be transitive.

Set C(e):= {f ∈ E(G) | f 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. The Omega polynomial Ω(G,x) for counting qoc strips in G was defined by Diudea as $\Omega(G,x)=\sum_c m(G,c)\times x^c$ 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 [6-10].

Corresponding author: Modjtaba.ghorbani@gmailyahoo.com)

The CI index was introduced by P. E. John and co-authors[11] for plane bipartite graphs as $CI(G) = \Omega'(G,x)^2 - (\Omega'(G,x) + \Omega''(G,x)\big|_{x=1}$. Klavzar[12] noticed that CI(G)=0 provided that G contains a single quasi-orthogonal cut. He also introduced an infinite series of such examples by complete bipartite graphs $K_{2,2k+1}$, $k \geq 1$, that is, $CI(K_{2,2k+1})=0$ for any $k \geq 1$.

The Sadhana index Sd(G) for counting qoc strips in G was defined by Khadikar et al[13,14] as $Sd(G,x) = \sum_c m(G,c)(|E(G)| - c)$, where m(G,c) is the number of strips of length c. The Sadhana polynomial Sd(G,x) was defined by Ashrafi and co-authors[15] as $Sd(G,x) = \sum_c m(G,c) \times x^{|E|-c}$. 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.

The aim of this study is to compute the Omega polynomial and then Sadhana polynomial of some nano structures. To do this, we first draw these compounds by HeperChem [16] and then compute their adjacency and distance matrices by TopoCluj [17]. Next, we apply some GAP [18] programs to compute the number of parallel edges for a given edge of these nanomaterials. Final step of this process is analyzing data obtained by our GAP programs. These programs are accessible from the authors upon request. Herein, our notation is standard and taken from the standard book of graph theory [19-26].

2. Results

The aim of this section is to compute the Omega and Sadhana polynomials of an infinite family of fullerenes with 12n+4 carbon atoms and 18n+6 bonds (figure 1).

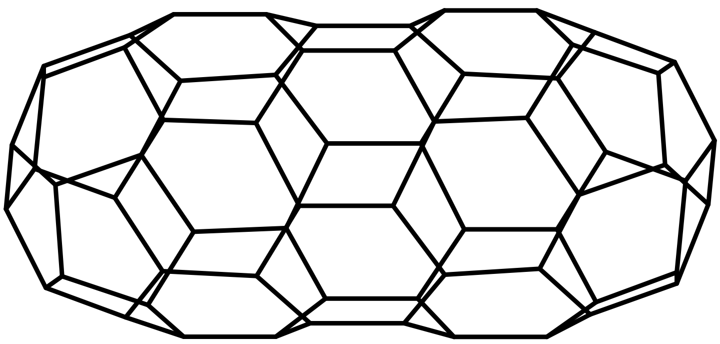

Fig. 1. graph of fullerene C_{12n+4}.

Theorem1. The omega polynomial of fullerene graph C_{12n+4} is as follows:

$$\Omega(C_{12n+4},x) = 18x + 4x^2 + (n-2)x^6 + 8x^{n-1} + 4x^n.$$

proof. By fig. 2, there are five distinct cases of qoc strips. We denote the corresponding edges by $e_1, e_2, \ldots, e_5$. By table 1 one can see that $|C(e_1)|=2$, $|C(e_2)| = n-1$, $|C(e_3)| = n$, $|C(e_4)| = 1$ and $|C(e_5)| = 6$. On the other hand, there are 4, 8, 4, 18 and n-2 similar edges for each of edges e_1, e_2, e_3, e_4 and e_5, respectively. So, we have $\Omega(C_{12n+4},x) = 18x + 4x^2 + (n-2)x^6 + 8x^{n-1} + 4x^n$.

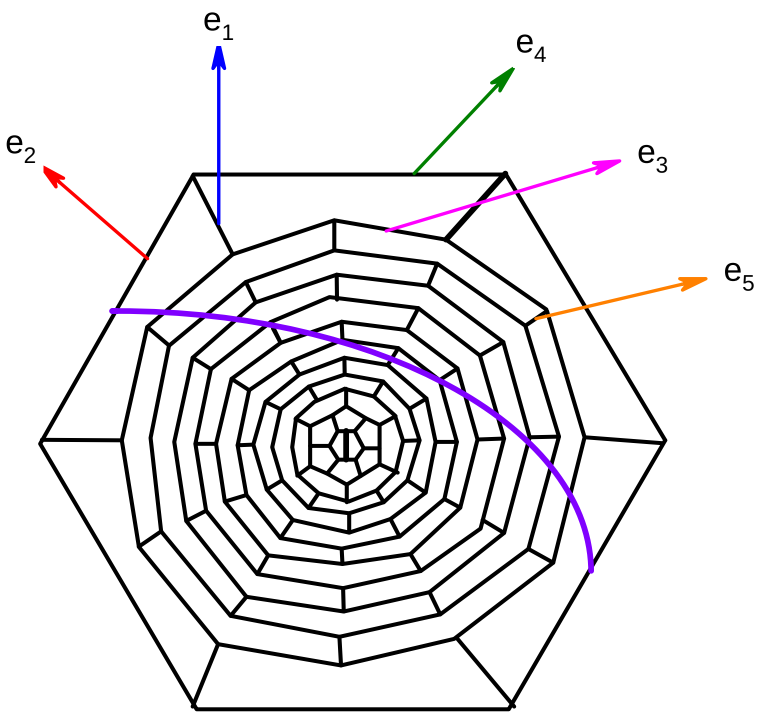

Fig. 2. The qoc strips of edges e_1, e_2, …, e_5 in graph of fullerene C_{12n+4}.

Table 1. The number of co-distant edges of e_i, $1 \le i \le 5$.

No.	Number of co-distant edges	Type of Edges
4	2	e_1
8	n-1	e_2
4	n	e_3
18	1	e_4
n-2	6	e_5

Corollary2. The Sadhana polynomial of fullerene graph C_{12n+4} is as follows:

$$Sd(C_{12n+4}, x) = 4x^{17n+6} + 8x^{17n+7} + (n-2)x^{18n} + 4x^{18n+4} + 18x^{18n+5}.$$

Corollary3. The Sadhana index of fullerene graph C_{12n+4} is $18n^2 + 564n + 186$.

References

[1] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R.E. Smalley Nature **318**, 162 (1985).
[2] H. W. Kroto, J. E. Fichier, D. E Cox, The Fulerene, Pergamon Press, New York, 1993.
[3] N. Trinajstić, "Chemical Graph Theory", CRC Press, Boca Raton, FL 1992.

[4] I. Gutman, O.E. Polansky. “Mathematical Concepts in Organic Chemistry”, Springer-Verlag, New York, 1986.
[5] M. A. Johnson, G.M. Maggiora, “Concepts and Applications of Molecular Similarity”, Wiley Interscience, New York 1990.
[6] P. E. John, A. E. Vizitiu, S. Cigher and M. V. Diudea, MATCH Commun. Math. Comput.Chem. **57**, 479 (2007).
[7] M. V. Diudea, S. Cigher, A. E. Vizitiu, O. Ursu and P. E. John, Croat. Chem. Acta, **79**, 445 (2006).
[8] E. Vizitiu, M. V. Diudea, Studia Univ. Babes-Bolyai, 2006 (accepted).
[9] A. E. Vizitiu, S. Cigher, M. V. Diudea, M. S. Florescu, MATCH Commun. Math. Comput. Chem. **57**, 457 (2007).
[10] M. V. Diudea, Carpath. J. Math., **22**, 43 (2006).
[11] P. E. John, A. E. Vizitiu, S. Cigher and M. V. Diudea, MATCH Commun. Math.Comput. Chem., **57**, 479 (2007).
[12] S. Klavzar, MATCH Commun. Math. Comput. Chem., **59**, 217 (2008).
[13] P. V. Khadikar, S. Joshi, A. V. Bajaj and D. Mandloi, Bioorg. Med.Chem. Lett., 14, 1187 (2004).
[14] P. V. Khadikar, V. K. Agrawal and S. Karmarkar, Bioorg. Med. Chem., 10, 3499 (2002).
[15] A. R. Ashrafi, M. Ghorbani and M. Jalali, Ind. J. Chem., **47A**, 535 (2008).
[16] HyperChem package Release 7.5 for Windows, (Hypercube Inc., Florida, USA) 2002.
[17] M. V. Diudea, O. Ursu and L. Nagy Cs, TOPOCLUJ(Babes-Bolyai University, Cluj), 2002.
[18] GAP, Groups, Algorithms and Programming, (Lehrstuhl De fur Mathematik, RWTH, Aachen), 1992.
[19] H. Yousefi, A. Bahrami, J. Yazdani and A. R. Ashrafi, J. Comput. Theor. Nanosci., **3**, 604 (2007).
[20] A.R. Ashrafi, M. Ghorbani and M. Jalali, Digest Journal of Nanomaterials and Biostructures , **3**(4), 245 (2008).
[21] A. R. Ashrafi, H. Saati and M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **3**(4), 227 (2008).
[22] M. Ghorbani, and M. Jalali, Digest Journal of Nanomaterials and Biostructures, **3**(4), 269 (2008).
[23] A. R. Ashrafi and M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4** (2), 313 (2009).
[24] M. Ghorbani and A. R. Ashrafi, J. Comput. Theor. Nanosci. **3**, 803 (2006).
[25] A. R. Ashrafi, M. Jalali, M. Ghorbani and M. V. Diudea, MATCH Commun. Math. Comput. Chem. **60**(3), 905 (2008).
[26] M. V. Diudea, Fullerenes, Nanotubes, and Carbon Nanostructures, **10**, 273 (2002).