Iranian Journal of Mathematical Chemistry, Vol. 3, Supplement 1, December 2012, pp. s45 – s50

IJMC

Geometric – Arithmetic Index of Hamiltonian Fullerenes

H. R. MOSTAFAEI[1], A. ZAEEMBASHI[2,*] AND M. OSTAD RAHIMI[3]

[1]*Department of Statistics, Tehran North Branch, Islamic Azad University, Tehran, Iran & Department of Economics Energy, Institute for International Energy Studies (IIES), Tehran, Iran*
[2]*Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785-136, I. R. Iran*
[3]*Department of mathematics, Tehran North Branch, Islamic Azad University, Tehran, Iran*

(*Received May 31, 2011*)

ABSTRACT

A graph that contains a Hamiltonian cycle is called a Hamiltonian graph. In this paper we compute the first and the second geometric – arithmetic indices of Hamiltonian graphs. Then we apply our results to obtain some bounds for fullerene.

Keywords: Fullerene graphs, Hamiltonian graphs, geometric –arithmetic index.

1. INTRODUCTION

Throughout this paper graph means simple connected graph. Let G be a connected graph with vertex and edge sets $V(G)$ and E(G), respectively. Suppose Λ denotes the class of all graphs. A map is called a topological index, if $G \cong H$ implies that $Top(G) = Top(H)$. Obviously, the maps Top_1 and Top_2 defined as the number of edges and vertices, respectively, are topological indices. The Wiener index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph, [1]. If $x, y \in V(G)$ then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y. The eccentricity of a vertex u in G was also defined as $\varepsilon(u) = \mathrm{Max}\{d(x, u) \mid x \in V(G)\}$.

*Author correspondence should be addressed. (E-mail: azaeembashi@srttu.edu)

Nowadays thousands and thousands topological indices are defined for different goals, such as stability of alkanes, the strain energy of cycloalkanes, prediction of boiling point and etc. One of the important topological index is the geometric – arithmetic index (GA) considered by Vukičević and Furtula [2, 3] as

$$GA(G) = \sum_{uv\in E} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u)+\deg(v)},$$

in which degree of vertex u denoted by $deg(u)$.

Fathtabar et. al [4] introduced a new version of geometric – arithmetic index and named it GA_2 index. It was defined as follows:

$$GA_2(G) = \sum_{uv\in E} \frac{2\sqrt{n(u)n(v)}}{n(u)+n(v)},$$

where, $n(u)$ is the number of vertices of G closer to u than to v. Zhou and his coauthors [5] introduced the third version of geometric – arithmetic index, namely GA_3 index, which is defined as follows:

$$GA_3(G) = \sum_{uv\in E} \frac{2\sqrt{m(u)m(v)}}{m(u)+m(v)},$$

where, $m(u)$ is the number of edges of G closer to vertex u than to vertex v. Ghorbani et. al [6] introduced GA_4 index based on eccentricity of vertices. In other words, it defines as follows:

$$GA_4(G) = \sum_{uv\in E} \frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}.$$

Carbon exists in several allotropic forms in nature. Fullerenes are zero–dimensional nanostructures, discovered experimentally in 1985 [7]. Fullerenes are carbon–cage molecules in which a number of carbon atoms are bonded in a nearly spherical configuration. Let p, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (5p + 6h)/3$, the number of edges is $m = (5p + 6h)/2 = 3/2n$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(5p + 6h)/3 - (5p + 6h)/2 + p + h = 2$, and therefore $p = 12$, $n = 2h + 20$ and $m = 3h + 30$. This implies that such molecules, made entirely of n carbon atoms, have 12 pentagonal and $(n/2 - 10)$ hexagonal faces, while $n \neq 22$ is a natural number equal or greater than 20 [8]. The aim of this paper is to compute two versions of geometric arithmetic indices of fullerenes. Through this paper, our notations are standard and taken from the standard book of graph theory [9–11]. We encourage reader to references [12–15].

2. MAIN RESULTS AND DISCUSSION

Before going to calculate these topological indices for fullerenes, we must compute some bounds for Hamiltonian graphs. In the field of graph theory a Hamiltonian path is a path which visits each vertex exactly once. A Hamiltonian cycle is a cycle which visits each vertex exactly once and also returns to the starting vertex. A graph that contains a Hamiltonian cycle is called a Hamiltonian graph.

Lemma 1. Let G be Hamiltonian graphs. Then,

$$2 \leq \deg(u) \leq \Delta \text{ and } 2 \leq \varepsilon(u) \leq \lfloor n/2 \rfloor.$$

Proof. Since G has a Hamiltonian cycle, so every vertex is adjacent with at least two vertices. On the other hand, the maximum distance between two vertices in a cycle is $\lfloor n/2 \rfloor$ and this completes the proof.

Example 2. Consider the fullerene graph C_{20}, Figure 1. This fullerene graph is vertex transitive and so, for every $x \in V(G)$, $\varepsilon(x) = 5$. Since C_{20} is the smallest fullerene, thus for every fullerene graph such as F and $x \in V(F)$ we have $\varepsilon(x) \geq 5$.

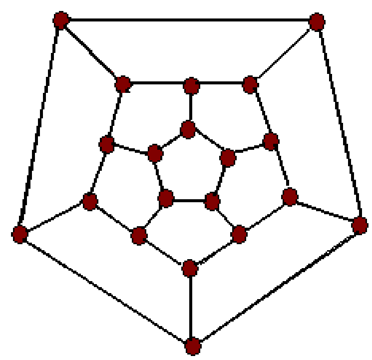

Figure 1. Graph of fullerene C_{20}.

Theorem 3. Let F_n be a fullerene graph with n vertices. Then

$$15 \leq GA_4(F_n) \leq 3n^2/20.$$

Proof. Since the number of vertices of a fullerene graph is even, $\lfloor n/2 \rfloor = n/2$. Thus for every vertex u in $V(F_n)$, $\varepsilon(u) \leq n/2$. This implies:

$$GA_4(G) = \sum_{uv \in E} \frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)} \leq \frac{2|E|}{10} \times \frac{n}{2} = \frac{3n^2}{20}$$

and

$$GA_4(G)=\sum_{uv\in E}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}\geq\frac{2\times 5\times|E|}{n}=\frac{2\times 5\times 3n}{2\times n}=15\,.$$

Corollary 4. For a Hamiltonian graph G, we have

$$\frac{2|E|}{\Delta}\leq GA(G)\leq\frac{\Delta|E|}{2}.$$

Corollary 5. For every fullerene graph F we have $GA(F) = |E| = 3n/2$.

It is well known fact if G and H be Hamiltonian graphs, then Cartesian product $G\times H$ is also a Hamiltonian graph. Also we know every cycle is Hamiltonian. So, the proof of the following proposition is straightforward:

Proposition 6. The graph of nanotorus $S = C_n \times C_m$ is Hamiltonian.

Since C_n is vertex transitive so, for every pair of vertices such as x and y, we have $\varepsilon(x)=\varepsilon(y)$. On the other hand, $\varepsilon_{G\times H}((x,y))=\varepsilon_G(x)+\varepsilon_H(y)$. This implies that

$$GA_4(C_n\times C_m)=\sum_{((a,b),(x,y)\in E(C_n\times C_m)}\frac{2\sqrt{\varepsilon_{C_n\times C_m}((a,b))\varepsilon_{C_n\times C_m}((x,y))}}{\varepsilon_{C_n\times C_m}((a,b))+\varepsilon_{C_n\times C_m}((x,y))}$$

$$=\sum_{((a,b),(x,y)\in E(C_n\times C_m)}\frac{2\sqrt{[\varepsilon_{C_n}(a)+\varepsilon_{C_m}(b)][\varepsilon_{C_n}(x)+\varepsilon_{C_m}(y)]}}{[\varepsilon_{C_n}(a)+\varepsilon_{C_m}(b)]+[\varepsilon_{C_n}(x)+\varepsilon_{C_m}(y)]}$$

$$=|E(C_n\times C_m)|\,.$$

Since, $|E(G\times H)|=|V(H)||E(G)|+|V(G)||E(H)|$, thus we proved the following theorem:

Theorem 7.

$$GA_4(C_n\times C_m)=2nm\,.$$

Lemma 6 [16]. The molecular graph of a polyhex nanotorus $T[p, q]$ (Figures 2,3) is vertex transitive.

Corollary 7.

$$GA(T[p,q]) = E(T[p,q]).$$

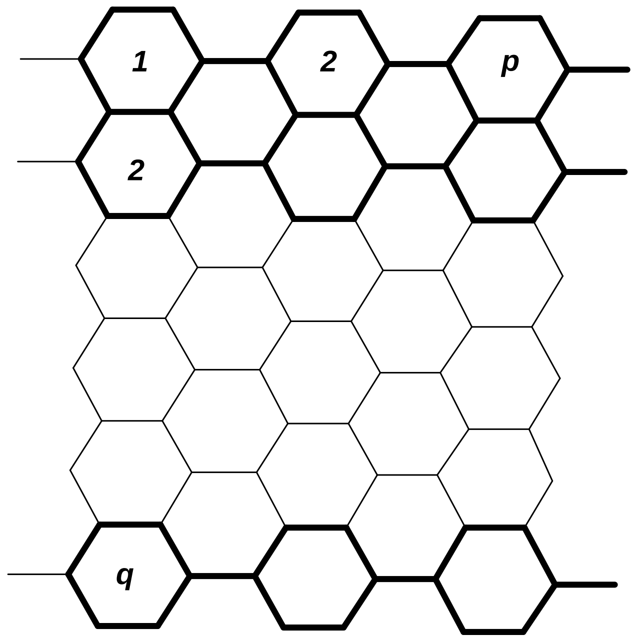

Figure 2. A 2-Dimensional Lattice for *T*[*p, q*].

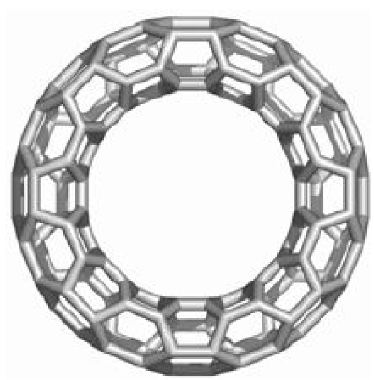

Figure 3. The Zig–Zag Polyhex Nanotorus *T*[*p, q*].

REFERENCES

1. H. Wiener, Structural determination of the paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
2. D. Vukičević and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem*. **46** (2009) 1369 − 1376.
3. B. Furtula, A. Graovac and D. Vukičević, Atom–bond connectivity index of trees, *Disc. Appl. Math.* **157** (2009) 2828 – 2835.

4. G. H. Fath–Tabar, B. Furtula, I. Gutman, A new geometric--arithmetic index, *J. Math. Chem*. **47** (2010) 477 – 486.
5. B. Zhou, I. Gutman, B. Furtula and Z. Du, On two types of geometric–arithmetic index, *Chem. Phys. Lett*. **482** (2009) 153 – 155.
6. M. Ghorbani and A. Khaki, A note on the fourth version of geometric–arithmetic index, Optoelectron. *Adv. Mater. – Rapid Comm*. **4(12)** (2010) 2212–2215.
7. 8. H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl and R. E. Smalley, C_{60}: Buckminsterfullerene, *Nature* **318** (1985) 162–163.
8. H. W. Kroto, J. E. Fichier and D. E Cox, *The Fullerene*, Pergamon Press, New York, 1993.
9. N. Trinajstić and I. Gutman, *Mathematical Chemistry*, *Croat. Chem. Acta* **75** (2002) 329 – 356.
10. M. V. Diudea, (Ed.), *QSPR/QSAR Studies by Molecular Descriptors*, NOVA, New York, 2001.
11. D. B. West, *Introduction to Graph theory*, Prentice Hall, Upper Saddle River, 1996.
12. M. Ghorbani, Computing vertex PI, omega and Sadhana polynomials of $F_{12(2n+1)}$ fullerenes, *Iranian. J. Math. Chem.* **1** (2010) 105 – 110.
13. A. Graovac and M. Ghorbani, A new version of atom–bond connectivity index, *Acta Chim. Slov.* **57** (2010) 609 – 612
14. A. R. Ashrafi and M. Ghorbani, A study of fullerene by MEC polynomial, *Electronic Materials Letters* **6(2)** (2010) 87 – 90.
15. S. Gupta, M. Singh and A. K. Madan, Application of graph theory: relationship of eccentric connectivity index and wiener's index with anti-inflammatory activity, *J. Math. Anal. Appl*. **266** (2002) 259 – 268.
16. A. R. Ashrafi, M. Ghorbani, Eccentric connectivity index of fullerenes, in: Novel Molecular Structure Descriptors – Theory and Applications I, I. Gutman and B. Furtula (eds.), *University of Kragujevac*, 2010, *pp.* 183–192.