ISSN 2321-807X

Computing Fifth Geometric-Arithmetic Index for Circumcoronene series of benzenoid H_k

Mohammad Reza Farahani
Department of Applied Mathematics, Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran
Mr_Farahani@Mathdep.iust.ac.ir

ABSTRACT

Let *G=(V; E)* be a simple connected graph. The sets of vertices and edges of G are denoted by *V=V(G)* and *E=E (G),* respectively. The geometric-arithmetic index is a topological index was introduced by Vukicevic and Furtula in 2009 and defined as $GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$ in which degree of vertex *u* denoted by $d_G(u)$ (or d_u for short). In 2011, *A. Graovac et al* defined a new version of *GA* index as $GA_5(G)=\sum_{uv\in E(G)}\frac{2\sqrt{S_v S_u}}{S_v+S_u}$ where $S_v=\sum_{uv\in E(G)} d_u$. The goal of this paper is to compute the fifth geometric-arithmetic index for "Circumcoronene series of benzenoid H_k $(k\geq1)$".

Indexing terms/Keywords

Molecular graph; Circumcoronene Series of Benzenoid, Geometric-Arithmetic Index;

SUBJECT CLASSIFICATION

E.g., Mathematics Subject Classification; 05C05; 05C12; 92E10.

INTRODUCTION

Let *G=(V;E)* be a simple connected graph of finite order *n*=|*V*| and the number of edges e=|E|, such that it has vertex set *V=V(G)* and edge set *E=E(G).* A general reference for the notation in graph theory is [1-3]. A molecular graph is a simple finite graph such that its vertices correspond to the atoms and the edges to the bonds.

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 a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. This theory has an important effect on the development of the chemical sciences.

In chemical graph theory, we have many different topological index of arbitrary molecular graph *G.* A topological index of a graph is a number related to a graph which is invariant under graph automorphisms. Obviously, every topological index defines a counting polynomial and vice versa. The simplest topological indices are the number of vertices and edges of the graph *G*.

Also, an important terminology of graph theory is degree of a vertex $v\in V(G)$, that it is the number of adjacent vertices with *v* and we denoted by d_v (In other words, the degree of a vertex *v* is equal to the number of its first neighbors.). If $u,v\in V(G)$ then the distance $d_G(u,v)$ (or *d(u,v)* for short) between *u* and *v* is defined as the length of (number of edges in) any shortest path in *G* connecting *u* and *v*. An edge *e=uv* of the graph *G* is joined between two vertices u and *v (d(u,v)=1).*

The Wiener index *W(G)* [4-9] is the first reported distance based topological index which have very chemical applications, mathematical properties and is defined as half sum of the distances between all the pairs of vertices in a molecular graph, which:

$$W(G)=\frac{1}{2}\sum_{v\in V(G)}\sum_{u\in V(G)} d(u,v)$$

One of important connectivity topological indices is geometric-arithmetic index of *G.* A class of geometric-arithmetic topological indices [10] may be defined as

$$GA_{general}(G)=\sum_{uv\in E(G)}\frac{2\sqrt{Q_vQ_u}}{Q_v+Q_u}$$

where Q_v is some quantity that in a unique manner can be associated with the vertex *v* of the graph *G*.
The first member of this class for $Q_v=d_v$ was considered by *Vukicevic* and *Furtula* [11], in 2009, and GA_1 index was defined as

$$GA_1(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_vd_u}}{d_v+d_u}$$

in which degree of vertex *u* denoted by $d_G(u)$ (or d_u for short).
The second member of this class was considered by *Fath-Tabar* et al. [12] by setting Q_u to be the number n_u of vertices of *G* lying closer to the vertex *u* than to the vertex *v* for the edge *uv* of the graph *G*:

$$GA_2(G)=\sum_{uv\in E(G)}\frac{2\sqrt{n_vn_u}}{n_v+n_u}$$

The third member of this class was considered by Bo *Zhou* et al.[13] by setting Q_u to be the number m_u of edges of *G* lying closer to the vertex *u* than to the vertex *v* for the edge *uv* of the graph *G*:

$$GA_3(G)=\sum_{uv\in E(G)}\frac{2\sqrt{m_vm_u}}{m_v+m_u}$$

The fourth member of this class was considered by *Ghorbani* et al.[14] in 2010 as follows:

$$GA_4(G)=\sum_{uv\in E(G)}\frac{2\sqrt{\varepsilon_v\varepsilon_u}}{\varepsilon_v+\varepsilon_u}$$

where ε_u is the number of the eccentricity of vertex *u*.
A new member of the class of geometric-arithmetic topological indices was considered by *A. Graovac et al* [15] recently, by setting Q_v to be the summation S_v of degrees of all neighbors of vertex *v* in *G* $S_v=\sum_{uv\in E(G)} d_u$:

$$GA_5(G)=\sum_{uv\in E(G)}\frac{2\sqrt{S_vS_u}}{S_v+S_u}$$

Recently, *A. Iranmanesh et al* introduced [16] the *edge version of geometric-arithmetic index* on the ground of the end-vertex degree d_e and d_f of edges *e* and *f* in a line graph of *G* as follows

$$GA_e(G) = \sum_{ef \in E(L(G))} \frac{2\sqrt{d_e d_f}}{d_e + d_f}$$

where the line graph *L(G)* of a graph *G* is defined to be the graph whose vertices are the edges of *G*, with two vertices being adjacent if the corresponding edges share a vertex in *G*.

In Refs [17-25] some connectivity and geometric-arithmetic topological indices of some nanotubes and nanotorus are computed. Here our notations are standard and mainly taken from standard books of chemical graph theory [1-3].

Main Results and Discussions

The goal of this paper is to compute a closed formula of this new Connectivity index "fifth geometric-arithmetic index GA_5" of circumcoronene homologous series of benzenoid H_k $(k\geq1)$.

The circumcoronene homologous series of benzenoid is family of molecular graph, which consist several copy of benzene C_6 on circumference. The first terms of this series are H_1=benzene, H_2=coronene, H_3=circumcoronene, H_4=circumcircumcoronene, see Figure 1 and Figure 2, where they are shown. Readers can see a general represetation of H_k in Figure 2. In addition, this benzenoid molecular graph is presented in many papers, for further study and more historical details, readers can see the paper series [21-41].

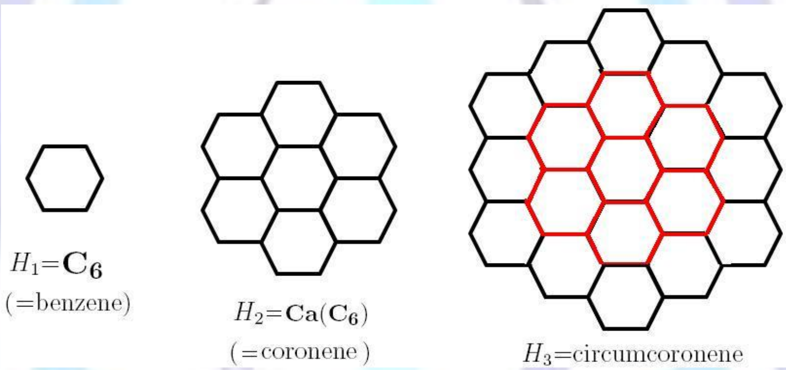

Fig. 1. The first three graphs H_1, H_2 and H_3 from the circumcoronene series of benzenoid [21].

By the above terminologies, we have following theorems. These theorems are main result in this paper.

Theorem 1. [21] Consider the graph $G=H_k$ $(k\geq2)$ is circumcoronene series of benzenoid. Then the Geometric-Arithmetic index $GA(H_k)$ is

$$GA(H_k) = 9k^2 + \left(\frac{24\sqrt{6}}{5} - 15\right)k + \left(12 - \frac{24\sqrt{6}}{5}\right)$$

Theorem 2. [22] Let *G* be the circumcoronene series of benzenoid H_k $(k\geq1)$. Then Second geometric-arithmetic index GA_2 of *G* is equal to

$$GA_2(H_k) = \frac{12}{n_k}\left(\sum_{i=1}^{k-1}(k+i)\sqrt{2k^2i^2 + 12k^3i - 4ki^3 - i^4}\right) + 6k$$

Theorem 3. [23] The third geometric-arithmetic index of circumcoronene series of benzenoid H_k $(k\geq1)$ is equal to

$$GA_3(H_k) = 6k + 6\sum_{i=1}^{k-1}\frac{k+i}{(9k^2-4k)-i}\sqrt{\frac{-9}{4}i^4 - (9k-3)i^3 + \left(\frac{18k^2+30k-3}{4}\right)i^2 + \left(\frac{54k^3-39k^2-k}{2}\right)i - 9k^3 + 3k^2}.$$

Theorem 4. [24] Let *G* be the circumcoronene series of benzenoid H_k $(\forall k\geq1)$. Then the eccentric geometric-arithmetic index GA_4 of H_k is equal to

ISSN 2321-807X

$$GA_4(H_k)=\sum_{i=2}^{k}12(i-1)\left(\frac{2\sqrt{4i^2+(8k-6)i+4k^2-6k+2}}{4i+4k-3}+\frac{\sqrt{4i^2+(8k-10)i+4k^2-10k+6}}{4i+4k-5}\right)+6k$$

Theorem 5. [25] For the graphs from the circumcoronene series of benzenoid H_k $\forall$ $k\geq 1$

$$GA_e(H_k)=6k^2(3k-4)+\frac{48\sqrt{k-1}}{7}+\frac{24\sqrt{6}}{5}$$

Theorem 6. Consider the graph $G=H_k$ $(k\geq 1)$ is circumcoronene series of benzenoid. Then

$$GA_5(H_k) = 9k^2+(\frac{24\sqrt{6}}{5}-15)k+(12-\frac{24\sqrt{6}}{5})$$

Proof. Let G be the circumcoronene series of benzenoid H_k for all integer number $k\geq 1$ (Figure 2). The number of vertices/atoms in this benzenoid molecular graph is equal to $|V(H_k)|=6k^2$ and the number of vertices as degrees 2 and 3 are equal to $|V_2|=6k$ and $|V_3|=6k(k-1)$, (we denote $V_i:=\{v\in V(G)\,|\,d_i=i\}$) thus obviously the number of edges/bonds of G is $|E(H_k)|=\frac{3\times 6k(k-1)+2\times 6k}{2}=9k^2-3k$. Also, it is easy to see that the edge set of H_k can be divide in to three partitions, e.g. E_4, E_5 and E_6 as follow:

- For every $e_6=uv$ belong to E_6, $d_v=d_u=3$.
- For every $e_5=xy$ belong to E_5, then $d_x=2$ and $d_y=3$.
- For every $e_4=ab$ belong to E_4, then $d_a=d_b=2$.

From Figure 2, we mark the members of E_4, E_5 and E_6 by red, green and black color and obviously the size of these three edge types are equal to 6, $12(k-1)$ and $9k^2-15k+6$, respectively.
According to Figure 2, one can see that the summation of degrees of vertices of this benzenoid graph have four types, such that for vertices $a,b\in V_2$ & $ab\in E_4$ $S(a)= d_b+3=5$ $(S(b)= d_a+3)$. And also, for vertices $x\in V_2$ & $y_1,y_2\in V_3$ and edges xy_1, $xy_2\in E_5$ $S(x)=d_{y1}+d_{y2}=6$ and $S(y_i)= 2+2+3=7$. It is easy to see that for all other vertices u, v from V_3 and all other edges $e=uv$ belong to E_6 $S(u)= d_v+3+3=9$ $(S(v)=d_u+3+3)$.

Now, by arrangement above formula, we have:

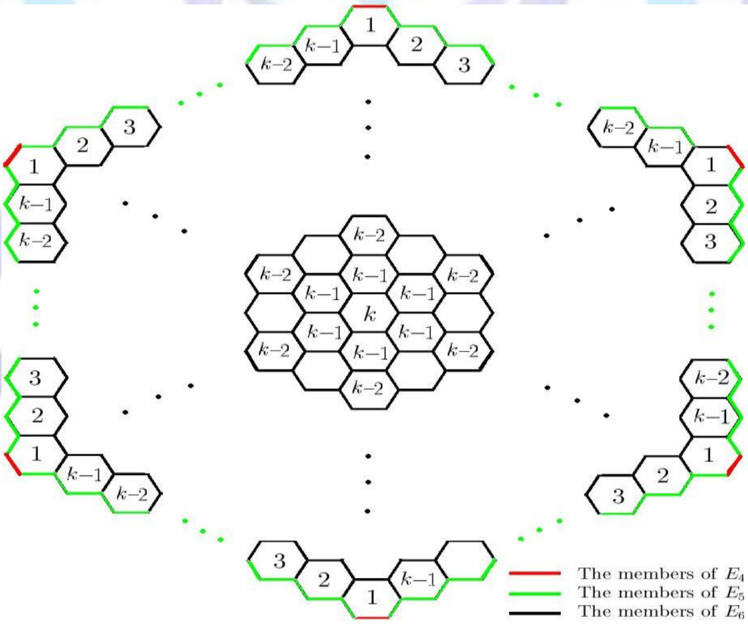

Fig. 2. The circumcoronene series of benzenoid H_k, $k\geq 1$, with edges marking [21].

$$GA_5(H_k) = \sum_{e=uv\in E(H_k)}\frac{2\sqrt{S(v)S(u)}}{S(v)+S(u)}$$

$$= 6\left(\frac{2\sqrt{5\times 5}}{5+5}\right)+6\left(\frac{2\sqrt{5\times 7}}{5+7}\right)+2\times 6(k-2)\left(\frac{2\sqrt{6\times 7}}{6+7}\right)+6(k-1)\left(\frac{2\sqrt{7\times 9}}{7+9}\right)+|E(H_{k-1})|\frac{2\sqrt{9\times 9}}{9+9}$$

ISSN 2321-807X

$$= 6+\sqrt{35}+\frac{24(k-2)\sqrt{42}}{13}+\frac{9(k-1)\sqrt{7}}{4}+9k^2-21k+12$$

Finally, Fifth Geometric-Arithmetic index of circumcoronene series of benzenoid H_k is equal to

$$GA_5(H_k) = 9k^2+\left(\frac{24\sqrt{42}}{13}+\frac{9\sqrt{7}}{4}-21\right)+\left(18+\sqrt{35}-\frac{48\sqrt{42}}{13}-\frac{9\sqrt{7}}{4}\right). \square$$

Here, we complete the proof of Theorem 6.■

REFERENCES

[1] D.B. West. An Introduction to Graph Theory. Prentice-Hall. (1996).

[2] N. Trinajstić. Chemical Graph Theory. CRC Press, Bo ca Raton, FL. (1992).

[3] R. Todeschini and V. Consonni. Handbook of Molecular Descriptors. Wiley, Weinheim. (2000).

[4] H. Wiener, Structural Determination of Paraffin Boiling Points. *J. Am. Chem. Soc. 69*, 17. (1947).

[5] A.A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. 66, 211–249, (2001).

[6] D.E. Needham, I.C. Wei and P.G. Seybold. Molecular modeling of the physical properties of alkanes. *J. Am. Chem. Soc.* 110, 4186. (1988).

[7] G. Rucker and C. Rucker. On topological indices, boiling points, and cycloalkanes. *J. Chem. Inf. Comput. Sci.* 39, 788. (1999).

[8] W. C. Shiu and P. C. B. Lam. The Wiener number of a hexagonal net. *Discrete Appl. Math.* 73, 101-111. (1997).

[9] B. Zhou and I. Gutman. Relations between Wiener, Hyper-Wiener and Zagreb Indices. *Chemical Physics Letters.* 394, 93-95. (2004).

[10] B. Furtula, A. Graovac and D. Vukičević, Atom–bond connectivity index of trees, Disc. Appl. Math., 157 (2009), 2828 - 2835.

[11] 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.

[12] GH. Fath-Tabar, B. Furtula and I. Gutman, A new geometric--arithmetic index, J. Math. Chem., 47 (2010), 477 – 486.

[13] B. Zhou, I. Gutman, B. Furtula and Z. Du, On two types of geometric-arithmetic index, Chem. Phys. Lett., 482 (2009), 153 – 155.

[14] 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.

[15] A. Graovac, M. Ghorbani and M. A. HosseinZadeh. Computing fifth geometric-arithmetic index for nanostar dendrimers, Journal of Mathematical NanoScience, 1(1), 2011, 33-42.

[16] A. Mahmiani, O. Khormali and A. Iranmanesh. On the Edge Version of Geometric-Arithmetic Index, *Digest J. Nanomate, Bios*., **7**(2)., 411–414. (2012).

[17] M.R. Farahani. Computing some connectivity indices of Nanotubes. *Advances in Materials and Corrosion* 1(2012) 57-60.

[18] M.R. Farahani. Fifth Geometric-Arithmetic Index of $TURC_4C_8(S)$ Nanotubes. Journal of Chemica Acta. 2(1) (2013).

[19] M. Ghorbani and M. Ghazi. Computing Some Topological Indices of Triangular Benzenoid. *Digest. J. Nanomater. Bios.* 5, (4), 1107-1111. (2010).

[20] L. Xiao, S. Chen, Z. Guo and Q. Chen. The Geometric-Arithmetic Index of Benzenoid Systems and Phenylenes *Int. J. Contemp. Math. Sciences*. 5, (45), 2225-2230, (2010).

[21] M.R. Farahani. Computing Randic, Geometric-Arithmetic and Atom-Bond Connectivity indices of Circumcoronene Series of Benzenoid. *Int. J. Chem. Model*. 5(4), In press (2013).

[22] M.R. Farahani. GA_2 index of Circumcoronene Series of Benzenoid H_k. Submitted for publish, 2013.

[23] M.R. Farahani. Using the Cut Method to Computing GA_3 of Circumcoronene Series of Benzenoid H_k. *Int J Chem Model*. 5(2) in press (2013).

[24] M.R. Farahani. Computing a New Connectivity Index for a Famous Molecular Graph of Benzenoid Family. *Journal of Chemica Acta,* 2, (2013) 26-31.

[25] M.R. Farahani. The Edge Version of Geometric-Arithmetic Index of Benzenoid Graph. *Submitted for publish*, (2012).

[26] J. Brunvoll, B. N. Cyvin and S.J. Cyvin. Enumeration and Classification of Benzenoid Hydrocarbons. Symmetry and Regular Hexagonal Benzenoids. *J. Chem. Inf. Comput. Sci.* 27, 171-177. (1987).

[27] V. Chepoi and S. Klavžar. Distances in benzenoid systems: Further developments. *Discrete Mathematics.* 192, 27-39. (1998).

[28] J.R. Dias. From benzenoid hydrocarbons to fullerene carbons. *MATCH Commun. Math. Comput. Chem.* 4, 57-85. (1996).

[29] M.V. Diudea. *Studia Univ. Babes-Bolyai*. 4, 3-21. (2003).

[30] A. Dress and G. Brinkmann. Phantasmagorical fulleroids, *MATCH Commun. Math. Comput. Chem.* 33, 87-100. (1996).

[31] M.R. Farahani and M.P. Vlad. On the Schultz, Modified Schultz and Hosoya polynomials and Derived Indices of Capra-designed planar Benzenoids. *Studia Univ. Babes-Bolyai*. 57(4) In press, (2012).

[32] M.R. Farahani. On the Schultz polynomial, Modified Schultz polynomial, Hosoya polynomial and Wiener index of circumcoronene series of benzenoid, *J. Applied Mathe. & Informatics.* 31(3) in press, (2013).

[33] M.R. Farahani. Zagreb index, Zagreb Polynomial of Circumcoronene Series of Benzenoid. Advances in Materials and Corrosion. 2 (2013) 16-19

[34] M. Goldberg. A class of multi-symmetric polyhedra. *Tohoku Math. J.* 43, 104-108. (1937).

[35] A. Ilic, S. Klavžar and D. Stevanovic. Calculating the Degree Distance of Partial Hamming Graphs. *MATCH Commun. Math. Comput. Chem.* 63, 411-424, (2010).

[36] S. Klavžar and I. Gutman. Bounds for The Schultz Molecular Topological Index of benzenoid Systems in Terms of Wiener Index. *J. Chem. Inf. Comput. Sci.* 37, (4), 741-744. (1997).

[37] S. Klavžar. A Bird's Eye View of The Cut Method and a Survey of Its Applications in Chemical Graph Theory. *MATCH Commun. Math. Comput. Chem.* 60, 255-274. (2008).

[38] S. Klavžar, I. Gutman and B. Mohar. Labeling of Benzenoid Systems which Reflects the Vertex-Distance Relations. *J. Chem. Inf. Comput. Sci.* 35, 590-593. (1995).

[39] S. Klavžar and I. Gutman. A Comparison of the Schultz Molecular Topological Index with the Wiener Index. *J. Chem. Inf. Comput. Sci.* 36, 1001-1003. (1996).

[40] K. Salem, S. Klavžar and I. Gutman. On the role of hypercubes in the resonance graphs of benzenoid graphs. *Discrete Mathematics.* 13(8) 306, (2003).

[41] A. Soncini, E. Steiner, P.W. Fowler, R.W.A. Havenith, and L.W. Jenneskens. Perimeter Effects on Ring Currents in Polycyclic Aromatic Hydrocarbons, Circumcoronene and Two Hexabenzocoronenes. *Chem. Eur.* J. 9, 2974-2981. (2003).