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

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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 $$GA(G) = \sum_{uv \in E(G)} \frac{2d_u d_v}{d_u + d_v},$$ in which degree of vertex $u$ denoted by $d_u (u)$ (or $d_u$ for short). In 2011, A. Graovac et al defined a new version of $GA$ index as $$GA_s(G) = \sum_{uv \in E(G)} \frac{2S_u S_v}{S_u + S_v}$$ where $S_u = \sum_{v \in E(G)} d_v$. The goal of this paper is to compute the fifth geometric-arithmetic index for "Circumcoronene series of benzenoid $H_k (k \geq 1)$".

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 $d_{u,v}$ (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:

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

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

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

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

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

in which degree of vertex $u$ denoted by $d_u(u)$ (or $d_u$ for short).

The second member of this class was considered by Fath-Tabar et al. [12] by setting $Q_v$ to be the number $n_v$ 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 $Q_v$ to be the number $m_v$ 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:

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

where $\epsilon_v$ 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

\[
GA_e(G) = \sum_{e,f \in E(L(G))} \frac{2\sqrt{d_e d_f}}{d_e + d_f}
\]

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 \(H_k (k \geq 1)\).

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 \(H_1=\text{benzene}, H_2=\text{coronene}, H_3=\text{circumcoronene}, H_4=\text{circumcircumcoronene}\), see Figure 1 and Figure 2, where they are shown. Readers can see a general representation 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].

**Theorem 1.** [21] Consider the graph \(G=H_k (k \geq 2)\) is circumcoronene series of benzenoid. Then the Geometric-Arithmetic index \(GA_5(H_k)\) is

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

**Theorem 2.** [22] Let \(G\) be the circumcoronene series of benzenoid \(H_k (k \geq 1)\). Then Second geometric-arithmetic index \(GA_2\) of \(G\) is equal to

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

**Theorem 3.** [23] The third geometric-arithmetic index of circumcoronene series of benzenoid \(H_k (k \geq 1)\) is equal to

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

**Theorem 4.** [24] Let \(G\) be the circumcoronene series of benzenoid \(H_k (\forall k \geq 1)\). Then the eccentric geometric-arithmetic index \(GA_4\) of \(H_k\) is equal to

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

By the above terminologies, we have following theorems. These theorems are main result in this paper.
GA_d(H_k) = \sum_{i=1}^{k-1} \left( \frac{2\sqrt{4i^2 + 8k - 6i + 4k^2 - 6k + 2}}{4i + 4k - 3} + \frac{2\sqrt{4i^2 + 8k - 10i + 4k^2 - 10k + 6}}{4i + 4k - 5} \right) + 6k

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

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

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

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

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 \( V_i := \{ v \in V \ | \ d_i = i \} \) thus obviously the number of edges/bonds of \( G \) is \( |E(H_k)| = 3 \times 6k - 1 + 2 \times 6k = 9k^2 - 3k \). 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 \( e_{\theta} = uv \) belong to \( E_6 \), \( d_v = d_u = 3 \).
- For every \( e_{\theta} = xy \) belong to \( E_5 \), then \( d_x = 2 \) and \( d_y = 3 \).
- For every \( e_{\theta} = ab \) 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 \( a, b, c, d \in V_2 \) & \( a, b, \& c \in E_4 \) and \( d \in E_5 \). And also, for vertices \( x, y, z, \& w \in V_3 \) and edges \( x, y \in E_5 \), \( S(x) = d_x + d_y = 6 \) and \( S(y) = 2 + 2 + 3 = 7 \). It is easy to see that for all other vertices \( u, v \) from \( V_3 \) and all other edges \( e = uv \) belong to \( E_6 \), \( S(u) = d_u + d_v = 9 \) and \( S(v) = d_u + d_v = 3 + 3 + 3 \).

Now, by arrangement above formula, we have:

\[ GA_5(H_k) = \sum_{e_{\theta} \in E(H_k)} \frac{2S v S u}{S v + S u} \]

\[ = 6 \frac{2\sqrt{5} x 5}{5 + 5} + 6 \frac{2\sqrt{5} x 7}{5 + 7} + 2 x 6 k - 2 \frac{2\sqrt{7} x 9}{6 + 7} + 6 k - 1 \frac{2\sqrt{7} x 9}{7 + 9} + |E(H_k)| \frac{2\sqrt{9} x 9}{9 + 9} \]

Fig. 2. The circumcoronene series of benzenoid \( H_k, k \geq 1 \), with edges marking [21].
Finally, Fifth Geometric-Arithmetic index of circumcoronene series of benzenoid $H_k$ is equal to

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

Here, we complete the proof of Theorem 6. ■

REFERENCES


