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Research Article

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A New Version of the Edge Geometric-Arithmetic Index

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Abstract

In this paper, we consider the second of the edge version of geometric-arithmetic (GA_{e2}) index of graphs belonging to the class of geometric-arithmetic indices. It is nearly related to the new versions of vertex Szeged index and vertex PI index of line graphs. The main properties of GA_{e2} are considered, such as upper and lower bounds. We compare the second version of the edge geometric-arithmetic indices for some graphs, $TUC_4C_6C_8[p, q]$ nanotorus and molecular octane isomers.

Keywords : Geometric-arithmetic index; Line graph; PI index; Szeged index; Degree of a vertex; Octane isomers; Molecular graph; Nanotorus.

1 Introduction

ONe of the branch of theoretical chemistry is mathematical 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 that applies graph theory to mathematical modeling of chemical phenomena. A molecular graph is a simple connected graph such that its vertices correspond to the atoms and the edges to the bonds. In many states, the hydrogen atoms are omitted. By IUPAC terminology, a topological index is a numerical value related to chemical structure of correlation of chemical structure with different physical properties, chemical or biological activity. Throughout this research G is a simple connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. A topological index is a numeric quantity from the structure of a graph that is invariant under automorphisms of the graph under consideration. A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry has been began in 1947 when chemist Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties variety of alkanes known as paraffin.

The concept of geometric-arithmetic indices has been introduced in the chemical graph theory. A single number that can be used to characterize some property of the graph of molecular is called a topological index for that graph. There are numerous topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [12]. Vukicevic and Furtula [13, 14, 15, 16], proposed a topological index named the geometric-arithmetic index

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as:

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

where d_u denotes the degree of the vertex u in G, in [2, 3, 4, 5, 6].

It is natural which we introduce the edge version of geometric-arithmetic index based on the end-vertex degrees of edges in ling graph of G as follows:

$$GA_e(G) = \sum_{e=fs\in E(L(G))} \frac{2\sqrt{d_f \cdot d_s}}{d_f + d_s} \tag{1.1}$$

where d_f denotes the degree of the edge f in G [7, 8, 9, 10, 11]. In this work we focus our attention to another member of this class which we denote by GA_{e2} be referred to as the second version of the edge geometric-arithmetic index [1].

Let $e = fs$ be an edge of line graph $L(G)$ of G, connecting the vertices f and s. Define the sets:

$$N(e, f, L(G)) = \{x \in V(L(G)) \mid d(x, f) < d(x, s)\},$$
$$N(e, s, L(G)) = \{x \in V(L(G)) \mid d(x, f) > d(x, s)\}.$$

Consisting, respectively, of vertices of $L(G)$ lying closer to f than to s, and lying closer to s than to f. The number of such vertices is then

$$n_f(e) = |N(e, f, L(G))|,$$
$$n_s(e) = |N(e, s, L(G))|.$$

We know that $f \in N(e, f, L(G))$, $s \in N(e, s, L(G))$ so that $n_f(e) \geq 1$, $n_s(e) \geq 1$.

In this paper we define the new version of the Szeged index and PI index as:

$$Sz_v(L(G)) = \sum_{e=fs\in E(L(G))} n_f(e) \cdot n_s(e), \tag{1.2}$$

$$PI_v(L(G)) = \sum_{e=fs\in E(L(G))} [n_f(e) + n_s(e)] \tag{1.3}$$

Also we define the second version of the edge geometric-arithmetic index as:

$$GA_{e2}(G) = \sum_{e=fs\in E(L(G))} \frac{\sqrt{n_f(e).n_s(e)}}{\frac{1}{2}[n_f(e) + n_s(e)]} \tag{1.4}$$

Remark 1.1 *In a line graph $L(G)$ of G, we have $d_e = d_u + d_v - 2$, here $e = uv \in E(G)$. Then the number of edges in a line graph is:*

$$|E(L(G)| = \frac{1}{2} \sum_{e_i=u_iv_i\in E(G)} (u_i + v_i - 2) \times |E_i|$$

where

$$|E_i| = |\{(e_i) \mid e_i \in E(G), 1 \leq i \leq |E(G)|, (e_i) = (du_i, dv_i)\}|.$$

Remark 1.2 *For each $e = fs \in E(L(G))$ that $n_s(e) = n_f(e)$. Then:*

$$GA_{e2}(G) = |E(L(G))|.$$

In this paper, we compare the second version of the edge geometric-arithmetic indices for some graphs, $TUC_4C_6C_8[p, q]$ nanotorus and molecular octane isomers.

2 The Main Results

In this section we will show the second edge GA index for some graphs C_n, P_n and S_n which are the cycle, Path and star graphs respectively.
In the next propositions, we suppose the graph G is a connected.

Lemma 2.1 *Let G be any graph with n vertices and m edges. Therefore, we have:*

$$|E(L(G))| = \frac{1}{2} \sum_{x\in V(G)} d_x^2 - m \tag{2.5}$$

where d_x is the degree of vertex x, that $x \in V(G)$.

Proof. We have $|E(L(G))| = \sum_{x\in V(G)} \binom{d_x}{2}$ and $\sum_{x\in V(G)} d_x = 2m$. Therefore,

$$\begin{aligned} |E(L(G))| &= \sum_{x\in V(G)} \binom{d_x}{2} \\ &= \frac{1}{2} \sum_{x\in V(G)} d_x^2 - \frac{1}{2} \sum_{x\in V(G)} d_x \\ &= \frac{1}{2} \sum_{x\in V(G)} d_x^2 - m. \end{aligned}$$

Theorem 2.1 *The second edge GA index of some familiar graphs C_n, P_n and S_n is:*

1. $GA_{e2}(C_n) = |E(L(C_n))| = n$
2. $GA_{e2}(S_n) = |E(L(S_n))| = \binom{n-1}{2}$
3. $GA_{e2}(P_n) = \sum_{i=1}^{n-2} \frac{2\sqrt{n-i-1}}{n-1}$.

Proof.
1. If $e = fs \in E(L(C_n))$ then

$$n_s(e) = n_f(e) = \begin{cases} \frac{n}{2} & n \text{ is even} \\ \frac{n-1}{2} & n \text{ is odd} \end{cases}.$$

Also, $L(C_n) = C_n$ then

$$\begin{aligned} GA_{e2}(C_n) &= \sum_{e=fs\in E(L(C_n))} \frac{\sqrt{n_f(e)\cdot n_f(e)}}{\frac{1}{2}[n_f(e)+n_f(e)]} \\ &= \sum_{e=fs\in E(L(C_n))} 1 \\ &= |E(L(C_n))| = |E(C_n)| = n. \end{aligned}$$

2. Now, if $e = fs \in E(L(S_n))$ then $n_s(e) = n_f(e) = 1$ and $L(S_n) = K_{n-1}$ then

$$\begin{aligned} GA_{e2}(S_n) &= \sum_{e=fs\in E(L(S_n))} \frac{\sqrt{n_f(e)\cdot n_s(e)}}{\frac{1}{2}[n_f(e)+n_s(e)]} \\ &= \sum_{e=fs\in E(L(S_n))} 1 \\ &= |E(L(S_n))| = |E(K_{n-1})| \\ &= \binom{n-1}{2}. \end{aligned}$$

3. Now, if $e = fs \in E(L(P_n))$ then $n_s(e) + n_f(e) = 1$ and $L(P_n) = P_{n-1}$ then

$$\begin{aligned} GA_{e2}(P_n) &= \sum_{e=fs\in E(L(P_n))} \frac{\sqrt{n_f(e).n_s(e)}}{\frac{1}{2}[n_f(e)+n_s(e)]} \\ &= \sum_{i=1}^{n-2} \frac{2\sqrt{n-i-1}}{n-1}. \end{aligned}$$

Theorem 2.2 *Let G a graph with n vertices, m edges and $|E(L(G))| = m'$, then*

$$GA_{e2}(G) \leq m' = \frac{1}{2}\sum_{x\in V(G)} d_x^2 - m \tag{2.6}$$

with equality if and only if $G \cong S_n$ or $G \cong C_n$ for $n \geq 3$.

Proof. We have:

$$\sqrt{n_f(e)\cdot n_s(e)} \leq \frac{n_f(e)+n_s(e)}{2}$$

for all edges $e = fs \in E(L(G))$, so

$$\begin{aligned} GA_{e2}(G) &= \sum_{e=fs\in E(L(G))} \frac{\sqrt{n_f(e)\cdot n_s(e)}}{\frac{1}{2}[n_f(e)+n_s(e)]} \\ &\leq \sum_{e=fs\in E(L(G))} 1 \\ &= |E(L(G))| = m'. \end{aligned}$$

By Theorem 2.1, we get an equality.
Conversely, if:

$$\begin{aligned} GA_{e2}(G) &= \sum_{e=fs\in E(L(G))} \frac{\sqrt{n_f(e)\cdot n_s(e)}}{\frac{1}{2}[n_f(e)+n_s(e)]} \\ &= m' = \sum_{e=fs\in E(L(G))} 1 \end{aligned}$$

Then $n_s(e) = n_f(e)$ holds for all edges $e = fs \in E(L(G))$, i. e., if and only if $G \cong S_n$ or $G \cong C_n$ for $n \geq 3$.

Theorem 2.3 *For any graph G with $|E(L(G))| = m' > 1$, then*

$$GA_{e2}(G) \leq \sqrt{Sz_v(L(G)) + m'(m'-1)} \tag{2.7}$$

with equality if and only if, $G \cong S_n(n \geq 3)$ or $G \cong C_3$.

Proof.

$$\begin{aligned} [GA_{e2}(G)]^2 &= \sum_{fs} \frac{4n_f(e).n_s(e)}{[n_f(e)+n_s(e)]^2} \\ &\quad + 2\sum_{fs\neq f's'} \frac{2\sqrt{n_f(e)\cdot n_s(e)}}{n_f(e)+n_s(e)} \\ &\quad \cdot \frac{2\sqrt{n_{f'}(e')\cdot n_{s'}(e')}}{n_{f'}(e')+n_{s'}(e')} \\ &\leq \sum_{fs}[n_f(e)\cdot n_s(e)] \\ &\quad + 2\sum_{fs\neq f's'} (1)\cdot(1) \\ &= \sum_{fs}[n_f(e)\cdot n_s(e)] + 2\frac{m'(m'-1)}{2} \\ &= Sz_v(L(G)) + m'(m'-1). \end{aligned}$$

If $G \cong S_n$ $(n \geq 3)$ or $G \cong C_3$ then $GA_{e2}(G) = Sz_v(L(G)) = m'$, so equality is occurs.

Theorem 2.4 *Let G a graph with m edges and $|E(L(G))|= m'$. Then*

$$GA_{e2}(G) \geq \frac{2m'\sqrt{m-1}}{m} \tag{2.8}$$

with equality if and only if $G \cong S_3$.

Proof. Without loos of generality we may choose the vertices of the edge $e = fs \in E(L(G))$ so that $n_f(e) \geq n_s(e)$. Then, we get $\frac{n_f(e)}{n_s(e)} = x$ and

$$\frac{\sqrt{n_f(e) \cdot n_s(e)}}{\frac{1}{2}[n_f(e) + n_s(e)]} = \frac{2\sqrt{x}}{x+1}.$$

The variable x assumes values in $1 \leq x \leq m - 1$. In that interval the function, $f(x) = \dfrac{2\sqrt{x}}{x+1}$ monotonically decreases. Because,

$$\begin{aligned} f'(x) &= \frac{\frac{1}{\sqrt{x}}(x+1) - 2\sqrt{x}}{(x+1)^2} \\ &= \frac{1-x}{(x+1)^2\sqrt{x}} \leq \circ. \end{aligned}$$

Therefore, $\frac{2\sqrt{x}}{x+1} \geq \frac{2\sqrt{m-1}}{(m-1)+1} = \frac{2\sqrt{m-1}}{m}$ then

$$\begin{aligned} GA_{e2}(G) &= \sum_{e=fs\in E(L(G))} \frac{\sqrt{n_f(e) \cdot n_s(e)}}{\frac{1}{2}[n_f(e) + n_s(e)]} \\ &= \sum_{|E(L(G))|} \frac{2\sqrt{x}}{x+1} \\ &\geq \sum_{|E(L(G))|=m'} \frac{2\sqrt{m-1}}{m} \\ &= \frac{2m'\sqrt{m-1}}{m} \end{aligned}$$

with equality if and only if $G \cong S_3$.

3 Comparison to GA_e and GA_{e2} Indices for Octan Isomer

In this section, comparison between GA_2 and GA_{e2} indices for octane isomers have been done. In Table 1 as seen, the GA_e, GA_{e2} and GA_2 indices of the octane isomers. The correlation between GA_e and GA_{e2} is illustrated in Fig. 1.

By consideration of Fig. 1, some relations between two versions of geometric-arithmetic Indices can be investigated. There is existence a correlation between GA_e and GA_{e2}. The data points **15**, **13**, **5**, **9**, **8**, **7**, **2**, and **1** form an almost perfect straight line with decreasing slope. If we show the number of tertiary and quaternary carbon atoms by n_3 and n_4, we may immediately check that for these isomers (n_3, n_4) is equal to $(0, 2)$, $(1, 1)$, $(0, 1)$, $(2, 0)$, $(1, 0)$, and $(0, 0)$, respectively. It is important that both GA_e and GA_{e2} are decreasing functions of the extent of branching of the molecular skeleton. The molecules **15**, **13**, **5**, **9**, and **2** are all branched at the very end of their carbon-atom chains and the molecular graph **1** is a path graph with 8 vertices (P_8).

The before mentioned described relations between GA_e and GA_{e2}, that hold not only for each octanes, but for all chemical trees, shows that these indices depend in the similar way on one structural feature, but have a various dependence on some other details of molecular structure. This hopes that GA_e and GA_{e2} will two be simultaneously usable in QSPR and QSAR researches. By

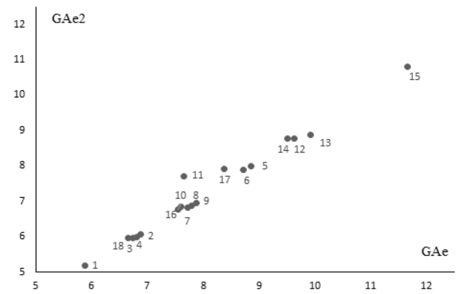

Figure 1: The edge geometric-arithmetic index (GA_e) of the octane isomers vs. their second edge version of geometric-arithmetic index (GA_{e2}). The numbering is same as in Table 1.

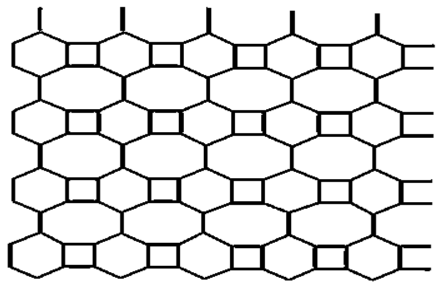

Figure 2: The graph of $TUC_4C_6C_8[p, q]$ nanotorus.

Table 1: The GA_e, GA_{e2} and GA_2 indices of the octane isomers for details see text and Fig. 1.

#	*Octanes*	GA_e	GA_{e2}	GA_2
1	*n-Octane*	5.88562	5.18621	5.99142
2	*2-Methyl heptane*	6.88220	6.07356	5.78683
3	*3-Methyl heptane*	6.74823	5.97858	5.68461
4	*4-Methyl heptane*	6.80481	5.98878	5.65286
5	*2,2-Dimethyl hexane*	8.85485	7.99310	5.48002
6	*3,3-Dimethyl hexane*	8.72088	7.90068	5.34605
7	*2,3-Dimethyl hexane*	7.72058	6.82612	5.44827
8	*2,4-Dimethyl hexane*	7.78520	6.86593	5.48002
9	*2,5-Dimethyl hexane*	7.87878	6.96091	5.58224
10	*3,4-Dimethyl hexane*	7.55675	6.77094	5.37780
11	*2,3,4-Trimethyl pentane*	7.65686	7.71348	5.24368
12	*2,2,3-Trimethyl pentane*	9.62232	8.78548	5.17321
13	*2,2,4-Trimethyl pentane*	9.91857	8.88046	5.27543
14	*2,3,3-Trimethyl pentane*	9.51680	8.78803	5.14146
15	*2,2,3,3-Tetramethyl butane*	11.65686	10.8	4.96863
16	*3-Ethyl-2-methyl pentane*	7.59716	6.85001	5.34605
17	*3-Ethyl-3-methyl pentane*	8.36923	7.92799	5.24383
18	*3-Ethyl hexane*	6.65466	5.96267	5.55064

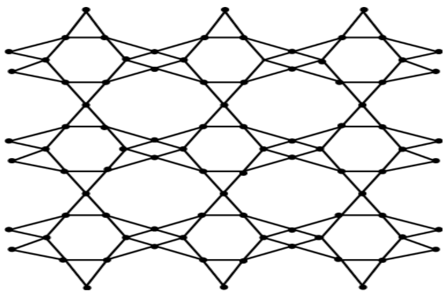

Figure 3: The graph of $L(TUC_4C_6C_8[3,3])$ nanotorus.

Equality (1.4) and Table 1, we get the following result.

Corollary 3.1 *Comparison to the second of the edge version of Geometric-arithmetic indices of the octane isomers are:*

1. $GA_{e2}(n-Octane \cong P_8) < GA_2(n-Octane)$
2. GA_{e2}*(other moleculars)*$>$ GA_2*(other moleculars)*

4 Computation GA_e and GA_{e2} Indices for $TUC_4C_6C_8[p,q]$ Nanotorus

In Fig. 2, the graph of $TUC_4C_6C_8[5,4]$ nanotorus is indicated. Also this graph is a cubic graph and 3-regular graph. Also, in Table 2 the type of edges, their numbers and amount of ξ_i of $TUC_4C_6C_8[p,q]$ nanotorus is shown where $\xi_i = \left(2\sqrt{d_{u_i} \cdot d_{v_i}}\right)/(d_{u_i} + d_{v_i})$ at correlation GA index. According to the Table 2, Remark 1.2 and

Table 2: The type of edges, their numbers and amount of ξ_i of $TUC_4C_6C_8[p,q]$ nanotorus

Number of edges	ξ_i	Type of edges
$9pq$	1	$(3,3)$

$|E(TUC_4C_6C_8\,[p,q])| = 9pq$, we have:

$$|E(L(K))| = \frac{1}{2}\left[(3+3-2)(9pq)\right] = 18pq.$$

In the Fig. 3, the line graph of $TUC_4C_6C_8[3,3]$ nanotorus is shown. Then, we have the following theorem.

Theorem 4.1 *The edge GA and GA_2 indices of $K = TUC_4C_6C_8[p,q]$ nanotorus is*

$$GA_e(K) = GA_{e2}(K) = 18pq.$$

Proof. Since $L(TUC_4C_6C_8[p,q])$ is 4-regular graph then by according to Remark 1.1 and Fig. 3, we have: $GA_e(K) = |E(L(K))| = 18pq$.

Now, for all edges $e = fs \in E(L(K))$, we have: $n_s(e) = n_f(e) = \frac{|V(L(K))|}{2}$, and by according to Remark 1.2, then:

$$GA_{e2}(G) = \sum_{e=fs\in E(L(G))} \frac{\sqrt{n_f(e).n_s(e)}}{\frac{1}{2}[n_f(e)+n_s(e)]} = |E(L(K))| = 18pq.$$

Then $GA_e(K) = GA_{e2}(K) = 18pq$.

5 Conclusion

By using the graph theory techniques, we get the bound for the second version of the edge geometric-arithmetic index and expressed exact values were exacted. We compare the second version of the edge geometric-arithmetic indices for some graphs, $TUC_4C_6C_8[p,q]$ nanotorus and molecular octane isomers.

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