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MORE ON COMPARISON BETWEEN FIRST GEOMETRIC-ARITHMETIC INDEX AND ATOM-BOND CONNECTIVITY INDEX

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Abstract. The first geometric-arithmetic (GA) index and atom-bond connectivity (ABC) index are molecular structure descriptors which play a significant role in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies. Das and Trinajstić [*Chem. Phys. Lett.* **497** (2010) 149-151] showed that *GA* index is greater than *ABC* index for all those graphs (except $K_{1,4}$ and T^* , see Figure 1) in which the difference between maximum and minimum degree is less than or equal to 3. In this note, it is proved that *GA* index is greater than *ABC* index for line graphs of molecular graphs, for general graphs in which the difference between maximum and minimum degree is less than or equal to $(2\delta - 1)^2$ (where δ is the minimum degree and $\delta \ge 2$) and for some families of trees. Therefore, a partial solution to an open problem proposed by Das and Trinajstić is given.

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1. INTRODUCTION

Let G = (V, E) denote a graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ and edge set E(G) such that |E(G)| = m. Suppose that d_i is the degree of a vertex $v_i \in V(G)$ [18]. All the graphs considered in this study are simple, finite and undirected.

Topological indices are numerical parameters of a graph which are invariant under graph isomorphisms. They play a significant role in mathematical chemistry especially in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) investigations [8, 17]. A whole class of topological indices is the "geometric-arithmetic indices" whose general definition is as follows [12, 21]:

$$GA_{general} = GA_{general}(G) = \sum_{ij \in E(G)} \frac{\sqrt{Q_i Q_j}}{\frac{1}{2}(Q_i + Q_j)},$$

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where Q_i is some quantity that can be associated with the vertex v_i of the graph G in a unique manner. The first geometric-arithmetic (GA) index was proposed by Vukičević and Furtula [21] by setting Q_i as the degree d_i of the vertex v_i of the graph G:

$$GA(G) = \sum_{ij \in E(G)} \frac{\sqrt{d_i d_j}}{\frac{1}{2}(d_i + d_j)}.$$

It has been demonstrated, on the example of octane isomers, that GA index is wellcorrelated with a variety of physico-chemical properties [21]. The details about mathematical properties of the GA indices and their applications in QSPR and QSAR can be found in the survey [5] reported by Das, Gutman and Furtula.

Estrada et al. [11] proposed a topological index, known as the atom-bond connectivity (ABC) index of graph G, which is abbreviated as ABC(G) and defined as

$$ABC(G) = \sum_{ij \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}.$$

The *ABC* index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [10, 11]. Due to its physicochemical applicability, the *ABC* index has attracted significant attention from researchers in recent years and many mathematical properties of this index were reported. For instance, see the papers [3, 4, 7, 13, 14, 19, 22, 23], more precisely the recent ones [2, 9, 15, 20] and references cited therein.

A graph having maximum vertex degree at most 4 is known as a molecular graph. The line graph L(G) of a graph G has the vertex set V(L(G)) = E(G) where the two vertices of L(G) are adjacent if and only if the corresponding edges of G are adjacent; detailed properties of a line graph can be found in [18]. Some possible chemical applications of line graphs of molecular graphs were discussed in [16]. Das and Trinajstić [6] compared the GA and ABC indices for molecular graphs and for general graphs in which the difference between maximum and minimum degree is less than or equal to three. Recently, the current authors [1] derived a relation between GA index and ABC index. In the present work, these two indices are compared for line graphs of molecular graphs, for general graphs in which the difference between maximum and minimum degree is less than or equal to $(2\delta - 1)^2$ (where δ is the minimum degree and $\delta \ge 2$) and for some families of trees.

2. PRELIMINARIES

The maximum and minimum vertex degree in a graph G are denoted by Δ and δ respectively. Also, a vertex of the graph G is said to be pendant if its neighborhood contains exactly one vertex. While, an edge of a graph is said to be pendant if one of its vertices is pendant.



FIGURE 1. The molecular graphs $K_{1,4}$ and T^*

The union $H \cup K$ of two graphs H and K is the graph with the vertex set $V(H) \cup V(K)$ and the edge set $E(H) \cup E(K)$. A tree in which exactly one of its vertices has degree greater than two is known as Starlike tree. Let $S(r_1, r_2, ..., r_k)$ denote the Starlike tree which has a vertex v of degree k > 2 such that the graph obtained from $S(r_1, r_2, ..., r_k)$ by removing the vertex v is $P_{r_1} \cup P_{r_2} \cup \cdots \cup P_{r_k}$ where P_{r_i} is the path graph on r_i $(1 \le i \le k)$ vertices. We say that the Starlike tree $S(r_1, r_2, ..., r_k)$ has k branches, the lengths of which are $r_1, r_2, ..., r_k$ $(r_1 \ge r_2 \ge \cdots \ge r_k \ge 1)$, and has $\sum_{i=1}^{k} r_i + 1$ vertices.

By a trivial graph, we mean a graph having one vertex. Denote by $K_{1,n}$ and K_n the Star on n + 1 vertices and complete graph on n vertices respectively. A triangle of a graph G is called odd if there is a vertex of G adjacent to an odd number of its vertices.

Lemma 1 ([18]). A graph G is a line graph if and only if G does not have $K_{1,3}$ as an induced subgraph, and if two odd triangles have a common edge then the subgraph induced by their vertices is K_4 .

3. Comparison between GA index and ABC index

If the graph *G* has $s \ge 2$ components G_1, G_2, \ldots, G_s , then from the definition of the *GA* and *ABC* indices it follows that $ABC(G) = \sum_{i=1}^{s} ABC(G_i)$ and $GA(G) = \sum_{i=1}^{s} GA(G_i)$. Moreover, if the graph *G* is trivial then $ABC(G) = GA(G) = 0 = ABC(P_2)$. Hence it is enough to restrict our considerations to non-trivial and connected graphs only. Denoted by T^* the tree on eight vertices, obtained by joining the central vertices of two copies $K_{1,3}$ by an edge (see Figure 1). To prove the first main theorem of this section, we need the following known result:

Theorem 1 ([6]). Let G be a non-trivial and connected graph with maximum degree Δ and minimum degree δ . If $\Delta - \delta \leq 3$ and $G \ncong K_{1,4}, T^*$, then GA(G) > ABC(G).

Let $m_{a,b}(G)$ be the number of edges of a graph G connecting the vertices of degree a and b. In the following theorem, we compare the GA index and the ABC index for line graph of a molecular graph:

Theorem 2. Let M be a molecular (connected) graph with $n \ge 3$ vertices and $G \cong L(M)$. Then GA(G) > ABC(G).

Proof. If $n \le 4$ or $M \cong P_n$, then it can be easily seen that *G* is a molecular graph which satisfies the hypothesis of Theorem 1 and hence the result follows. Let us assume that $n \ge 5$ and $M \not\cong P_n$. Note that $1 \le d_i \le 6$ for all vertices v_i of *G*. Hence the edges of *G* are of possible degree pairs: (6, 6), (6, 5), (6, 4), (6, 3), (6, 2), (6, 1), (5, 5), (5, 4), (5, 3), (5, 2), (5, 1), (4, 4), (4, 3), (4, 2), (4, 1), (3, 3), (3, 2), (3, 1), (2, 2), (2, 1).The values of $\theta_{ij} = \frac{2\sqrt{d_i d_j}}{d_i + d_j}$ and $\phi_{ij} = \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}$ for all above mentioned degree pairs are given in the Table 1 and Table 2 (Table 2 is taken from [6]). From these tables one can note easily that

$$\theta_{ij} - \phi_{ij} \begin{cases} \geq \frac{2\sqrt{6}}{7} - \sqrt{\frac{5}{6}} \approx -0.2130 & \text{if } (d_i, d_j) = (4, 1), (5, 1), (6, 1) \\ \approx 0.0495 & \text{if } (d_i, d_j) = (3, 1) \\ \approx 0.1589 & \text{if } (d_i, d_j) = (6, 2) \\ \approx 0.1964 & \text{if } (d_i, d_j) = (5, 2) \\ \approx 0.2357 & \text{if } (d_i, d_j) = (2, 1), (4, 2) \\ \geq \frac{2\sqrt{6}}{5} - \frac{1}{\sqrt{2}} \approx 0.2727 & \text{otherwise} \end{cases}$$
(3.1)

It is claimed that

$$\sum_{b=2}^{6} m_{1,b}(G) \le \lfloor \frac{|V(G)|}{2} \rfloor \le \lfloor \frac{|E(G)|}{2} \rfloor.$$
(3.2)

The right inequality obviously holds because *G* contains atleast one cycle. To prove the left inequality it is enough to show that no two pendent edges of *G* are adjacent. Contrarily, suppose that $e_1 = uv$ and $e_2 = uw$ are pendent edges of *G*. Since $n \ge 5$, order of *G* is at least 4. This implies that there exists a vertex *t* (different from v, w) adjacent with *u* in *G*. Then the graph obtained by removing all vertices except u, v, w, t of *G* is $K_{1,3}$, a contradiction to the Lemma 1. Now, we consider two cases: *Case 1*. If $m_{1,b}(G) = 0$ for all $b \ge 4$, then it follows from (3.1) that $\theta_{ij} - \phi_{ij} > 0$

for all edges $ij \in G$ and hence GA(G) > ABC(G).

Case 2. If $m_{1,b}(G) = 0$ not for all $b \ge 4$.

If $m_{2,5}(G) = m_{2,6}(G) = 0$, then from (3.1) and (3.2), it follows that

$$GA(G) - ABC(G) = \sum_{ij \in E(G)} (\theta_{ij} - \phi_{ij}) > 0$$
(3.3)

If at least one of $m_{2,5}(G), m_{2,6}(G)$ is nonzero. Consider the edge $e = xy \in G$ where degree of x and y is two and c (c = 5, 6) respectively. Let l denote number of vertices of degree two which are adjacent with y. Then $1 \le l \le 2$ for otherwise $K_{1,3}$ would be an induced subgraph of G. Note that the vertex y lies on either of the cliques K_{c-1}, K_c of G and hence the edges with possible degree pairs of these

TABLE 1. Values of θ_{ij} and ϕ_{ij} for all edges with degrees (d_i, d_j) where $5 \le d_i \le 6$ and $d_i \ge d_j$

| (d_i, d_j) | (6,6) | (6,5) | (6,4) | (6,3) | (6,2) | (6,1) | (5,5) | (5,4) | (5,3) | (5,2) | (5,1) |
|---------------|---------------------------------|-------------------------|-----------------------|---------------------------------|----------------------|-----------------------|-----------------------|---------------------------------|-----------------------|------------------------|----------------------|
| θ_{ij} | 1 | $\frac{2\sqrt{30}}{11}$ | $\frac{2\sqrt{6}}{5}$ | $\frac{2\sqrt{2}}{3}$ | $\frac{\sqrt{3}}{2}$ | $\frac{2\sqrt{6}}{7}$ | 1 | $\frac{4\sqrt{5}}{9}$ | $\frac{\sqrt{15}}{4}$ | $\frac{2\sqrt{10}}{7}$ | $\frac{\sqrt{5}}{3}$ |
| ϕ_{ij} | $\frac{1}{3}\sqrt{\frac{5}{2}}$ | $\sqrt{\frac{3}{10}}$ | $\frac{1}{\sqrt{3}}$ | $\frac{1}{3}\sqrt{\frac{7}{2}}$ | $\frac{1}{\sqrt{2}}$ | $\sqrt{\frac{5}{6}}$ | $\frac{2\sqrt{2}}{5}$ | $\frac{1}{2}\sqrt{\frac{7}{5}}$ | $\sqrt{\frac{2}{5}}$ | $\frac{1}{\sqrt{2}}$ | $\frac{2}{\sqrt{5}}$ |

TABLE 2. Values of θ_{ij} and ϕ_{ij} for all edges with degrees (d_i, d_j) where $2 \le d_i \le 4$ and $d_i \ge d_j$

| (d_i, d_j) | (4,4) | (4,3) | (4,2) | (4,1) | (3,3) | (3,2) | (3,1) | (2,2) | (2,1) |
|--------------------------|---|---|--|----------------------------|-------------------------|--|---|--------------------------------|--|
| $	heta_{ij} \ \phi_{ij}$ | $\frac{1}{\frac{1}{2}\sqrt{\frac{3}{2}}}$ | $\frac{\frac{4\sqrt{3}}{7}}{\frac{1}{2}\sqrt{\frac{5}{3}}}$ | $ \begin{array}{c} \frac{2\sqrt{2}}{3} \\ \frac{1}{\sqrt{2}} \end{array} $ | 0.8 $\frac{\sqrt{3}}{2}$ | $\frac{1}{\frac{2}{3}}$ | $\frac{\frac{2\sqrt{6}}{5}}{\frac{1}{\sqrt{2}}}$ | $\frac{\frac{\sqrt{3}}{2}}{\sqrt{\frac{2}{3}}}$ | $\frac{1}{\frac{1}{\sqrt{2}}}$ | $\frac{2\sqrt{2}}{3}$ $\frac{1}{\sqrt{2}}$ |

cliques in *G* are (6,6), (6,5), (6,4), (6,3), (5,5), (5,4), (5,3), (4,4), (4,3), (3,3). For all these degree pairs $\theta_{ij} - \phi_{ij} \ge 0.2727$. Moreover, corresponding to every clique K_d (d = 4,5,6) of *G*, there exist at most 2*d* edges with degree pairs (2,*c*) in *G*, where vertex of degree *c* (that is *y*) lies on K_d . Since the size of K_d is $\frac{d(d-1)}{2} \ge 2d$ for $d \ge 5$. Therefore, if *G* does not have clique K_4 , then by using (3.1) and (3.2) one can easily see that the inequality (3.3) holds. If *G* has clique K_4 . It can be easily seen that no edge with degree pairs (2,6) can be incident with any vertex of the clique K_4 . This implies, corresponding to every clique K_4 there exist at most 8 edges with degree pairs (2,5), but the size of K_4 is 6. Hence

$$\frac{8(0.1964) + 6(0.2727)}{14} \approx 0.2291 > 0.2130.$$

This completes the proof.

Now, we prove that conclusion of Theorem 2 remains true if minimum degree is $k \ge 2$ and the difference between maximum and minimum degree is less than or equal to $(2k-1)^2$. To proceed, we need the following lemma:

Lemma 2. If $f(x, y) = (x + y)^2 x^2 - (x + \frac{y}{2})^2 (2x + y - 2)$, $k \le x \le k + (2k - 1)^2$ and $0 \le y \le (2k - 1)^2$ where $k \ge 2$ then f(x, y) > 0.

Proof. Step 1. Firstly we take x = k, then

$$g(y) = f(k, y) = (k + y)^2 k^2 - (k + \frac{y}{2})^2 (2k + y - 2)$$

and g'(y) > 0 implies that $\alpha < y < \beta$, where

$$\alpha = \frac{2}{3}(1 - 3k + 2k^2) - \frac{2}{3}\sqrt{1 + 4k^2 - 6k^3 + 4k^4}$$

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and

$$\beta = \frac{2}{3}(1 - 3k + 2k^2) + \frac{2}{3}\sqrt{1 + 4k^2 - 6k^3 + 4k^4}$$

It means that g is increasing in the interval (α, β) and decreasing in the intervals $(-\infty, \alpha)$ and (β, ∞) . Since $\alpha < 0 < \beta < (2k-1)^2$, so g is increasing in $(0, \beta)$ and decreasing in $(\beta, (2k-1)^2)$. Moreover, $g(0) = k^2 \{k^2 - 2(k-1)\} > 0$ and $g((2k-1)^2) = k^4 + k^2 - \frac{k}{2} + \frac{1}{4} > 0$. It follows that g(y) > 0 for all $y \in [0, (2k-1)^2]$.

Step 2. Now we take $y = y_0$, where y_0 is any fixed integer in the interval $[0, (2k - 1)^2]$. Let $h(x) = f(x, y_0)$ then

$$h'(x) = (2x + y_0) \left[(2x^2 + 2 - 3x) + \left(2x - \frac{3}{2}\right) y_0 \right] > 0$$

for all $x \ge k \ge 2$. Hence $h(x) = f(x, y_0)$ is increasing in $[k, \infty)$. Combining both the results proved in Step 1 and Step 2, we have the lemma.

Theorem 3. Let G be a connected graph with maximum degree Δ and minimum degree $\delta \geq 2$. If $\Delta - \delta \leq (2\delta - 1)^2$ then GA(G) > ABC(G).

Proof. Let us consider the quantity

$$\Gamma = d_i^2 d_j^2 - \frac{1}{4} (d_i + d_j)^2 (d_i + d_j - 2), \qquad (3.4)$$

where d_i and d_j are the degrees of vertices v_i and v_j respectively in G. Since $\delta \le d_i, d_j \le \Delta \le \delta + (2\delta - 1)^2$ this implies that $|d_i - d_j| \le (2\delta - 1)^2$. Without loss of generality we can suppose that $d_i \ge d_j$ then $d_i = d_j + \theta$ for some θ ; $0 \le \theta \le (2\delta - 1)^2$ and (3.4) becomes

$$\Gamma = (d_j + \theta)^2 d_j^2 - (d_j + \frac{\theta}{2})^2 (2d_j + \theta - 2), \qquad (3.5)$$

where $\delta \le d_j \le \delta + (2\delta - 1)^2$ and $0 \le \theta \le (2\delta - 1)^2$. Now, from Lemma 2 and (3.5), we have the desired result.

If the condition $\Delta - \delta \le (2\delta - 1)^2$ is replaced by $\Delta - \delta \le (2\delta - 1)^2 + 1$ in Theorem 3, then the conclusion may not be true. For instance, consider the complete bipartite graph $K_{r,s}$, if we take $r = \delta \ge 2$ and $s = (2\delta - 1)^2 + \delta + 1$ then

$$GA(K_{r,s}) = \frac{2\left[\delta((2\delta-1)^2+\delta+1)\right]^{\frac{1}{2}}}{(2\delta-1)^2+2\delta+1} < \sqrt{\delta((2\delta-1)^2+2\delta-1)((2\delta-1)^2+\delta+1)} = ABC(K_{r,s}).$$

On the other hand, consider the graph G obtained by joining any vertex of K_{12} to a vertex of K_3 by an edge. Then $\Delta = 12, \delta = 2$ which means that $\Delta - \delta = 10 > (2(2) - 1)^2$, but GA(G) > ABC(G). We have the following result:

Theorem 4. If G is a connected graph with minimum degree $\delta \ge 2$ and $|d_i - d_j| \le (2\delta - 1)^2$ for all edges $ij \in E(G)$, then GA(G) > ABC(G).

Proof. The proof is similar to the proof of Theorem 3 and hence it is omitted. \Box

A stronger version of the above result can be analogously proved:

Theorem 5. Let G be a connected graph with minimum degree $\delta \ge 2$ and $|d_i - d_j| \le (2k-1)^2$ for all edges $ij \in E(G)$, where $k = \min\{d_i, d_j\}$. Then GA(G) > ABC(G).

The current authors recently derived the following relation between GA index and ABC index:

Theorem 6 ([1]). Let G be a connected graph and minimum degree $\delta \ge 2$, then

$$\frac{\sqrt{2(n-2)}}{n-1}GA(G) \le ABC(G) \le \frac{n+1}{4\sqrt{n-1}}GA(G).$$

with left equality if and only if $G \cong K_n$ and right equality if and only if $G \cong C_3$.

Let δ_1 be the minimum non-pendant vertex degree in G. Now, we compare GA index and ABC index for trees.

Theorem 7. If *T* is a tree with $n \ge 3$ vertices such that $m_{1,b} = 0$ for all $b \ge 4$ and $\Delta - \delta_1 \le (2\delta_1 - 1)^2$, then GA(T) > ABC(T).

Proof. Let us consider the difference

$$GA(T) - ABC(T) = \sum_{\substack{ij \in E(T), \\ d_i \neq 1 \neq d_j}} (\theta_{ij} - \phi_{ij}) + \sum_{\substack{ij \in E(T), \\ d_i = 1 \text{ or } d_j = 1}} (\theta_{ij} - \phi_{ij}) + \sum_{\substack{ij \in E(T), \\ d_i = 1 \text{ or } d_j = 1}} (\theta_{ij} - \phi_{ij})$$

As $m_{1,b} = 0$ for all $b \ge 4$, from (3.1) it follows that

$$\sum_{\substack{ij \in E(T), \\ d_i = 1 \text{ or } d_j = 1}} (\theta_{ij} - \phi_{ij}) > 0$$

Now, we have to prove that

$$\sum_{\substack{ij \in E(T), \\ d_i \neq 1 \neq d_j}} (\theta_{ij} - \phi_{ij}) > 0$$

To do so, let $d_i, d_j \ge 2$ then using the same technique, adopted in the proof of Theorem 3, we have

$$d_i^2 d_j^2 - \frac{1}{4} (d_i + d_j)^2 (d_i + d_j - 2) > 0$$

which is equivalent to

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} > \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}$$

which implies that

$$\sum_{\substack{ij \in E(T), \\ d_i \neq 1 \neq d_j}} \left(\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} \right) > 0.$$

This completes the proof.

Now, for Starlike tree, we have the following result.

Theorem 8. Let
$$S = S(r_1, r_2, ..., r_k)$$
 be a Starlike tree.
(1) If $r_i \ge 4$ for all i , then $GA(S) > ABC(S)$.
(2) If $r_i \ge 2$ for all i and $\frac{\sum_{i=1}^{k} r_i}{k} \ge 4$, then $GA(S) > ABC(S)$.
(3) If $\frac{\sum_{i=1}^{k} r_i}{k} \ge 8$, then $GA(S) > ABC(S)$.

Proof. (1) The edges of S with possible degree pairs are: (2, 1), (2, 2), (k, 2). From Table 2 we have

$$\theta_{ij} - \phi_{ij} \approx \begin{cases} 0.2357 & \text{if } (d_i, d_j) = (2, 1) \\ 0.2929 & \text{if } (d_i, d_j) = (2, 2) \end{cases}$$
(3.6)

Moreover, the function $f(k) = \theta_{2k} - \phi_{2k} = \left(\frac{2\sqrt{2k}}{k+2} - \frac{1}{\sqrt{2}}\right)$ is decreasing in $(2,\infty)$ and $f(k) \to -\frac{1}{\sqrt{2}} \approx -0.7071$ when $k \to \infty$. Hence we have $f(k) > -\frac{1}{\sqrt{2}} \approx -0.7071$ for all k. Since $r_i \ge 4$ for all i, this implies that there are k edges with degree pairs (1,2), k edges with degree pairs (2,k) and at least 2k edges with degree pairs (2,2) in S. This completes the proof of part (1).

Note that $\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} > -1$ if $(d_i, d_j) = (1, k)$ for all k. Using the same technique, adopted in the proof of part (1), one can easily prove parts (2) and (3).

Let W_n be the wheel graph of order n. Then

$$GA(W_n) = (n-1)\left(1 + \frac{2\sqrt{3(n-1)}}{n+2}\right)$$

and

$$ABC(W_n) = (n-1)\left(\frac{2}{3} + \sqrt{\frac{n}{3(n-1)}}\right).$$

It can be easily verified that $GA(W_n) > ABC(W_n)$ for $4 \le n \le 194$ and $GA(W_n) < ABC(W_n)$ for $n \ge 195$. Is there any graph *G* with the property GA(G) = ABC(G)?

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All our attempts to find such a graph were unsuccessful. We end this section with the following conjecture.

Conjecture 1. If G is a non-trivial and connected graph, then $GA(G) \neq ABC(G)$.

4. CONCLUSION

In [6], comparison between GA index and ABC index for general trees and general graphs was left as an open problem. Theorems 2 - 8 provide a partial solution of this open problem. The complete solution of the said problem remains a task for the future.

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