Iranian J. Math. Chem. 13 (1) March (2022) 19 – 32

IRANIAN JOURNAL OF
Mathematical Chemistry
Journal homepage: ijmc.kashanu.ac.ir

Original Scientific Paper

On the Difference of Atom–Bond Connectivity Index and Randić Index with Some Topological Indices

ROSLAN HASNI[1,•], MOHAMAD NAZRI HUSIN[1], FATEMEH MOVAHEDI[2], RUDRUSAMY GOBITHAASAN[1] AND MOHAMMAD HADI AKHBARI[3]

[1]Special Interest Group on Modelling and Data Analytics (SIGMDA), Faculty of Ocean Engineering Technology and Informatics, University Malaysia Terengganu, 21030 UMT Kuala Nerus, Terengganu, Malaysia
[2] Department of Mathematics, Faculty of Science, Golestan University, Gorgan, Iran
[3] Department of Mathematics, Estahban Branch, Islamic Azad University, Estahban, Iran

ARTICLE INFO

Article History:

Received: 22 February 2022
Accepted: 15 March 2022
Published online: 30 March 2022
Academic Editor: Ali Reza Ashrafi

Keywords:

Geometric-arithmetic index
Zagreb index
Randić index
Atom-bond connectivity (ABC) index

ABSTRACT

Assume G denotes a connected and simple graph with edge set $E(G)$ as well as vertex set $V(G)$. In chemical graph theory, the atom-bond connectivity ABC index as well as the Randić index of graph G are two well-defined topological indices. In addition, Ali and Du [On the difference between ABC and Randić indices of binary and chemical trees, *Int. J. Quantum Chem.* (2017) e25446] recently unveiled the distinction between Randić and ABC indices. In this report, we study the link between the difference of Randić and ABC indices with certain well-studied topological indices.

© 2022 University of Kashan Press. All rights reserved

1. INTRODUCTION

Let G resembles a simple graph possessing edge set $E(G)$ as well as vertex set $V(G)$. Subsequently, let d_u express the *degree* of vertex $u \in V(G)$. Let $\Delta(G)$ and $\delta(G)$

•Corresponding author (Email: hroslan@umt.edu.my).
DOI: 10.22052/IJMC.2022.246069.1611

express the *maximum* and *minimum* degree of G, accordingly. Then the *distance* $d_G(u,v)$ between the vertices u and v is described as the shortest path length connecting them for $u,v \in V(G)$. The greatest distance between the vertex v and any other vertices in G is termed as the *eccentricity* of v in G and is represented by $e(v)$ with respect to a vertex $v \in V(G)$. Please refer to [37] for any Graph Theory terminologies and notations not included here.

The topological indices [9] are among the many convenient tools developed by graph theory for chemists. Molecular graphs are frequently employed to model molecular and molecules compounds. One of the earliest and extensively utilized descriptors in QSAR/QSPR research [33] is molecular graphs' topological indices.

The Randić was suggested by Randić [27] in the year 1975 for evaluating the branching extent of the saturated hydrocarbons' carbon-atom skeleton, described as given below:

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The general Randić index, expressed by R_α [2] was described as

$$R_\alpha = R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha,$$

in which α denotes any real number.

The (first) geometric-arithmetic graph index was described in [34] as

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

The harmonic graph index was described in [20] as

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u + d_v}.$$

Explanation regarding the Randić index and the majority of its corresponding mathematical features may be discovered in [15, 22], the surveys [23, 28] and some recent papers [19, 21].

Estrada *et al.* [12] suggested a topological index known as atom-bond connectivity (ABC for short) index employing Randić modification index. The ABC index of G is characterised as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

When the paper [11] was published 10 years later, this index grew popular. The ABC index's mathematical features have been widely investigated since then. Readers are referred to the survey [16], the latest papers [6, 10, 14, 32, 38] and related references cited therein for further information.

In keeping with the popularity of topological indices, several scholars are interested in investigating the comparison or relationship of topological indices; for instance, refer [7, 8, 30, 40]. Consequently, Ali and Du [1] lately developed several extremal findings for binary and chemical trees in terms of the difference between the Randić index and ABC index. Wan Zuki et al. [36] investigated more extremal values of the difference between the

Randić index and ABC index for chemical trees and obtained an upper bound for such trees with given number of pendant vertices. Provided that the maximum vertex degree in T is at most 3 (4, accordingly), it is considered to be a binary tree (chemical tree, accordingly).

For $n \geq 3$, provided that G denotes an n-vertex connected graph, the difference of ABC and Randić indices is expressed by $ABC - R$ index and is characterized as follows:

$$(ABC - R)(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u + d_v - 2} - 1}{\sqrt{d_u d_v}}.$$

Notice that $(ABC - R)(G) \geq 0$ with equality attains when G is isomorphic to P_3, the 3-vertex path graph. We consider $n \geq 4$ for the remaining part of this paper.

The first Zagreb index may also be represented as a sum over G edges [17],

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

Further results on Zagreb indices please refer to [13, 35, 39], recent surveys [3, 4] and the references cited therein.

The reciprocal products' sum degrees of adjacent vertices' pairs [31] is equal to the modified second Zagreb index $\mathcal{M}_2^*(G)$, that is,

$$\mathcal{M}_2^*(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

In [18], the latest version of Zagreb indices is characterized as given below:

$$M_1^*(G) = \sum_{uv \in E(G)} [e(u) + e(v)],$$
$$M_1^{**}(G) = \sum_{u \in V(G)} (e(u))^2,$$
$$M_2^*(G) = \sum_{uv \in E(G)} e(u)e(v).$$

The disparity between the two topological indices was not taken into account, considering the apparent cause that it might have positive, zero, or negative values for structurally similar graphs. We expect to fill up some of the gaps in this work. We establish some new relations between the difference of ABC and Randić indices with some well-known topological indices.

2. Relation Between the Difference of ABC Index and Randić Index with Respect to Other Topological Indices

This section contains some relations between the difference of ABC index and Randić index (or $ABC - R$ index) with some other topological indices. We will make use of the following mathematical inequalities of real number sequences.

Theorem 1. (Jensen's inequality [25, 24]) *Let $p = (p_i)$, $i = 1,2, \dots, n$, resembles a sequence of non-negative real numbers, as well as $a = (a_i)$, $i = 1,2, \dots, n$, resembles a sequences of positive real numbers. Therefore, for any real number r with $r \geq 1$ or $r \leq 0$,*

$$\sum_{i=1}^{n} p_i a_i^r \sum_{i=1}^{n} p_i \left(\frac{\sum_{i=1}^{n} p_i a_i}{\sum_{i=1}^{n} p_i} \right)^r . \quad (1)$$

Theorem 2. ([29, 24]) *Let $a = (a_i)$ and $b = (b_i)$, $i = 1,2, \dots, n$, resembles two sequences of positive real numbers. With any $r \geq 0$,*

$$\sum_{i=1}^{n} \frac{a_i^{r+1}}{b^r} \frac{\left(\sum_{i=1}^{n} a_i\right)^{r+1}}{\left(\sum_{i=1}^{n} b_i\right)^{r}}. \tag{2}$$

We develop an upper bound for the difference of Randić and ABC indices in regards to the first Zagreb index.

Theorem 3. *Let G denote a graph with m edges, minimum degree δ and the first Zagreb index $M_1(G)$. Therefore*

$$(ABC - R)(G) \leq \sqrt{(M_1(G) - m)\frac{m}{\delta^2}}.$$

Proof. Let G resembles a graph possessing m edges, minimum degree δ as well as the first Zagreb index $M_1(G)$. Notice that $\delta d_v \Delta$ for each $v \in V(G)$ and by the Cauchy-Schwarz inequality, we acquire

$$\begin{aligned}
(ABC - R)(G) &= \sum_{uv\in E(G)} \frac{\sqrt{d_u+d_v-2}-1}{\sqrt{d_u d_v}} \\
&\leq \sqrt{\sum_{uv\in E(G)} \left(\sqrt{d_u + d_v - 2} - 1\right)^2 \sum_{uv\in E(G)} \frac{1}{d_u d_v}} \\
&= \sqrt{\sum_{uv\in E(G)} \left(d_u + d_v - 2 + 1 - 2\sqrt{d_u + d_v - 2}\right) \sum_{uv\in E(G)} \frac{1}{d_u d_v}} \\
&< \sqrt{\sum_{uv\in E(G)} (d_u + d_v - 1) \sum_{uv\in E(G)} \frac{1}{d_u d_v}} \\
&\leq \sqrt{(M_1(G) - m)\frac{m}{\delta^2}}.
\end{aligned}$$

The proof is now completed. ■

In regards to the modified second Zagreb index, we now establish lower and upper bounds for the difference between the Randić and ABC indices.

Theorem 4. *Let G resembles a graph having m edges, minimum degree δ, maximum degree Δ as well as modified second Zagreb index $\mathcal{M}_2^*(G)$. Therefore*

$$(\sqrt{2\delta - 2} - 1)\sqrt{\mathcal{M}_2^*(G) + \frac{m(m-1)}{\Delta^2}} \leq (ABC - R)(G) \leq (\sqrt{2\Delta - 2} - 1)\sqrt{\mathcal{M}_2^*(G) + \frac{m(m-1)}{\delta^2}},$$

having equality if and only if G denotes a regular graph.

Proof. Let G resembles a graph having m edges, minimum degree δ, maximum degree Δ including the modified second Zagreb index $\mathcal{M}_2^*(G)$. We recognise that $2\delta d_i + d_j 2\Delta$ for all edges $v_i v_j \in E(G)$ and $\delta d_i \Delta$ for all vertices $v_i \in V(G)$. By the $ABC - R$ index's definition, we obtain

$$(ABC-R(G))^2=\sum_{u_iv_j\in E(G)}\frac{\left(\sqrt{d_i+d_j-2}-1\right)^2}{d_id_j}$$
$$+2\sum_{u_iv_j\neq v_rv_s\in E(G)}\left(\frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\right)\left(\frac{\sqrt{d_r+d_s-2}-1}{\sqrt{d_rd_s}}\right)$$
$$\leq\sum_{u_iv_j\in E(G)}\frac{\left(\sqrt{2\Delta-2}-1\right)^2}{d_id_j}+\sum_{u_iv_j\neq v_rv_s\in E(G)}\left(\frac{\sqrt{2\Delta-2}-1}{\delta}\right)\left(\frac{\sqrt{2\Delta-2}-1}{\delta}\right)$$
$$=\left(\sqrt{2\Delta-2}-1\right)^2\left(\mathcal{M}_2^*(G)+\frac{m(m-1)}{\delta^2}\right).$$

Similarly,

$$(ABC-R(G))^2=\sum_{u_iv_j\in E(G)}\frac{\left(\sqrt{d_i+d_j-2}-1\right)^2}{d_id_j}$$
$$+2\sum_{u_iv_j\neq v_rv_s\in E(G)}\left(\frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\right)\left(\frac{\sqrt{d_r+d_s-2}-1}{\sqrt{d_rd_s}}\right)$$
$$\geq\sum_{u_iv_j\in E(G)}\frac{\left(\sqrt{2\delta-2}-1\right)^2}{d_id_j}+\sum_{u_iv_j\neq v_rv_s\in E(G)}\left(\frac{\sqrt{2\delta-2}-1}{\Delta}\right)\left(\frac{\sqrt{2\delta-2}-1}{\Delta}\right)$$
$$=\left(\sqrt{2\delta-2}-1\right)^2\left(\mathcal{M}_2^*(G)+\frac{m(m-1)}{\Delta^2}\right).$$

The equalities are true if and only if $d_u+d_v=2\Delta=2\delta$, for each $uv\in E(G)$ indicating that G refers to a regular graph. ∎

Theorem 5. *Let G resembles a graph having $n\geq 3$ vertices, m edges, minimum degree δ as well as maximum degree Δ. Therefore*

$$\frac{\sqrt{2\delta-2}-1}{\Delta}<(ABC-R)(G)<m\sqrt{2\Delta-2}.$$

Proof. For the lower bound, we obtain

$$(ABC-R)(G)=\sum_{u_iv_j\in E(G)}\frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}>\frac{\sum_{u_iv_j\in E(G)}\sqrt{d_i+d_j-2}-1}{\sum_{u_iv_j\in E(G)}\sqrt{d_id_j}}.$$

Provided that $2\delta\leq d_i+d_j\leq 2\Delta$ for all edges $v_iv_j\in E(G)$, we acquire

$$\frac{\sum_{u_iv_j\in E(G)}\sqrt{d_i+d_j-2}-1}{\sum_{u_iv_j\in E(G)}\sqrt{d_id_j}}>\frac{\sqrt{2\delta-2}-1}{\Delta}.$$

Since

$$\sum_{u_iv_j\in E(G)}\frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}<\sum_{u_iv_j\in E(G)}\sqrt{d_i+d_j-2},$$

and by employing the Cauchy-Schwarz inequality, we get

$$\sum_{u_iv_j\in E(G)}\sqrt{d_i+d_j-2}<\sqrt{\sum_{u_iv_j\in E(G)}1\sum_{u_iv_j\in E(G)}(d_i+d_j-2)}.$$

Provided that $2\delta\leq d_i+d_j\leq 2\Delta$ for all edges $v_iv_j\in E(G)$, we obtain

$$\sqrt{\sum_{u_iv_j\in E(G)}1\sum_{u_iv_j\in E(G)}(d_i+d_j-2)}<\sqrt{\sum_{u_iv_j\in E(G)}1\sum_{u_iv_j\in E(G)}2\Delta-2}$$
$$=m\sqrt{2\Delta-2}.$$

The proof is then completed. ∎

Theorem 6. *Let G resembles a graph having m edges, p pendant vertices, minimum degree δ as well as maximum degree Δ. Therefore*

$$\frac{\sqrt{2\delta-2}-1}{\Delta}(m-p)+\frac{\sqrt{\delta-1}-1}{\sqrt{\Delta}}p \le (ABC-R)(G) \le \frac{\sqrt{2\Delta-2}-1}{\delta}(m-p)+\frac{\sqrt{\Delta-1}-1}{\sqrt{\delta}}p$$

with equality if and only if G resembles a regular graph.

Proof. Provided that $2\delta \le d_i + d_j \le 2\Delta$ for all edges $v_iv_j \in E(G)$ and $\delta \le d_i \le \Delta$ for all vertices $v_i \in V(G)$. In addition to from the $ABC-R$ index's definition, we obtain

$$\begin{aligned}(ABC-R)(G) &= \sum_{\substack{u_iv_j\in E(G)\\ d_i,d_j\neq 1}} \frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}} + \sum_{\substack{u_iv_j\in E(G)\\ d_i=1}} \frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\\
&\le \sum_{\substack{u_iv_j\in E(G)\\ d_i,d_j\neq 1}} \frac{\sqrt{2\Delta-2}-1}{\delta} + \sum_{\substack{u_iv_j\in E(G)\\ d_i=1}} \frac{\sqrt{1+d_j-2}-1}{\sqrt{d_j}}\\
&\le \sum_{\substack{u_iv_j\in E(G)\\ d_i,d_j\neq 1}} \frac{\sqrt{2\Delta-2}-1}{\delta} + \sum_{\substack{u_iv_j\in E(G)\\ d_i=1}} \frac{\sqrt{1+\Delta-2}-1}{\sqrt{\delta}}\\
&= \frac{\sqrt{2\Delta-2}-1}{\delta}(m-p)+\frac{\sqrt{\Delta-1}-1}{\sqrt{\delta}}p.\end{aligned}$$

Similarly,

$$\begin{aligned}(ABC-R) &= \sum_{\substack{u_iv_j\in E(G)\\ d_i,d_j\neq 1}} \frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}} + \sum_{\substack{u_iv_j\in E(G)\\ d_i=1}} \frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\\
&\ge \sum_{\substack{u_iv_j\in E(G)\\ d_i,d_j\neq 1}} \frac{\sqrt{2\delta-2}-1}{\Delta} + \sum_{\substack{u_iv_j\in E(G)\\ d_i=1}} \frac{\sqrt{1+d_j-2}-1}{\sqrt{d_j}}\\
&\ge \sum_{\substack{u_iv_j\in E(G)\\ d_i,d_j\neq 1}} \frac{\sqrt{2\delta-2}-1}{\Delta} + \sum_{\substack{u_iv_j\in E(G)\\ d_i=1}} \frac{\sqrt{1+\delta-2}-1}{\sqrt{\Delta}}\\
&= \frac{\sqrt{2\delta-2}-1}{\Delta}(m-p)+\frac{\sqrt{\delta-1}-1}{\sqrt{\Delta}}p.\end{aligned}$$

The equalities are true if and only if $d_u + d_v = 2\Delta = 2\delta$, for every $uv \in E(G)$ indicating that G resembles a regular graph. ■

We now determine an upper bound for the difference of Randić and ABC indices with respect to Randić index.

Theorem 7. *Let G resembles a tree having n vertices. Therefore*

$$(ABC-R)(G) \le R(G)\left(\sqrt{n-2}-1\right),$$

with equality if and only if G denotes a star graph.

Proof . Provided that $d_i + d_j \le n$, for every $u_iv_j \in E(G)$. Moreover, from the $ABC-R$ index's definition, we obtain

$$(ABC-R)(G) = \sum_{u_iv_j\in E(G)} \frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}} \leq \sum_{u_iv_j\in E(G)} \frac{\sqrt{n-2}-1}{\sqrt{d_id_j}}$$
$$= \sqrt{n-2}-1\sum_{u_iv_j\in E(G)} \frac{1}{\sqrt{d_id_j}}$$
$$= \left(\sqrt{n-2}-1\right)R(G).$$

The equality is true if and only if $d_u + d_v = n$, for every $uv \in E(G)$, implying that G expresses a star graph. ■

Theorem 8. *Let G resembles a graph having m edges, minimum degree δ as well as maximum degree Δ. Therefore*

$$(ABC-R)(G) \leq m\left(\frac{\sqrt{2\Delta-2}-1}{\delta}\right).$$

with equality holds if and only if G denotes a regular graph.

Proof. By the $ABC-R$ index's definition and from Cauchy-Scharwz inequality, we obtain

$$(ABC-R(G))^2 = \left(\sum_{u_iv_j\in E(G)} \frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\right)^2$$
$$\leq m\sum_{u_iv_j\in E(G)} \left(\frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\right)^2$$
$$\leq m\sum_{u_iv_j\in E(G)} \left(\frac{\sqrt{2\Delta-2}-1}{\delta}\right)^2$$
$$= m^2\left(\frac{\sqrt{2\Delta-2}-1}{\delta}\right)^2.$$

The equalities are true if and only if $d_u + d_v = 2\Delta = 2\delta$, for every $uv \in E(G)$, implying that G resembles a regular graph. ■

Lemma 1. (Pólya-Szegö inequality [26]). *Given that* $0 < m_1 \leq x_i \leq M_1$ *as well as* $0 < m_2 \leq y_i \leq M_2$, *for* $1 \leq i \leq n$. *Then*

$$\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i^2 \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} x_iy_i\right)^2. \quad (3)$$

Theorem 9. *Let G resembles a graph having m edges, minimum degree δ as well as maximum degree $\Delta > 1$. Therefore*

$$(ABC-R)(G) \geq \frac{m\frac{\sqrt{2\delta-2}-1}{\Delta}}{\frac{1}{2}\left(\sqrt{\frac{\Delta(\sqrt{2\Delta-2}-1)}{\delta(\sqrt{2\delta-2}-1)}}+\sqrt{\frac{\delta(\sqrt{2\delta-2}-1)}{\Delta(\sqrt{2\Delta-2}-1)}}\right)},$$

with equality if and only if G denotes a regular graph.

Proof. For $x_i = \frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_i d_j}}$, $y_i = 1$, $M_1 = \frac{\sqrt{2\Delta-2}-1}{\delta}$, $m_1 = \frac{\sqrt{2\delta-2}-1}{\Delta}$ and $M_2 = m_2 = 1$, by Inequality (3), we have

$$\sum_{u_iv_j\in E(G)} \left(\frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\right)^2 \sum_{u_iv_j\in E(G)} 1 \leq \frac{1}{4}\left(\sqrt{\frac{\Delta(\sqrt{2\Delta-2}-1)}{\delta(\sqrt{2\delta-2}-1)}} + \sqrt{\frac{\delta(\sqrt{2\delta-2}-1)}{\Delta(\sqrt{2\Delta-2}-1)}}\right)^2 \left(\sum_{u_iv_j\in E(G)} \frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\right)^2. \quad (4)$$

Furthermore, provided that $2\delta d_i + d_j 2\Delta$ for all edges $v_iv_j \in E(G)$, we now obtain

$$\sum_{u_iv_j\in E(G)} \left(\frac{\sqrt{d_i+d_j-2}-1}{\sqrt{d_id_j}}\right)^2 \sum_{u_iv_j\in E(G)} 1 \sum_{u_iv_j\in E(G)} \left(\frac{\sqrt{2\delta-2}-1}{\Delta}\right)^2 \sum_{u_iv_j\in E(G)} 1 = m^2\left(\frac{\sqrt{2\delta-2}-1}{\Delta}\right)^2. \quad (5)$$

Now the proof follows immediately from Inequalities 4 and 5. The equalities are true if and only if $d_u + d_v = 2\Delta = 2\delta$, for every $uv \in E(G)$, implying that G resembles a regular graph. ∎

Thus, we now give an upper bound for the difference of Randić and ABC indices in respect to general Randić index R_α when $\alpha = -1$.

Theorem 10. *Let G resembles a connected graph having m edges. Therefore*

$$(ABC - R)(G) \leq \sqrt{m\left(\sqrt{2\Delta-2}-1\right)\left(\frac{m\sqrt{2\Delta-2}}{\delta^2} - R_{-1}(G)\right)}.$$

Proof. Setting $r = 2$, $a_{uv} = \frac{1}{\sqrt{d_ud_v}}$ and $p_{uv} = \sqrt{d_u + d_v - 2} - 1$ for every $uv \in E(G)$, applying Theorem 1 as well as definition of $ABC - R$ index, we obtain

$$\begin{aligned}
\frac{m\sqrt{2\Delta-2}}{\delta^2} - R_{-1}(G) &\geq \sum_{uv\in E(G)} \frac{\sqrt{d_u+d_v-2}}{d_ud_v} - \sum_{uv\in E(G)} \frac{1}{d_ud_v} \\
&= \sum_{uv\in E(G)} \frac{\sqrt{d_u+d_v-2}-1}{d_ud_v} \\
&= \sum_{uv\in E(G)} \frac{\sqrt{d_u+d_v-2}-1}{\left(\sqrt{d_ud_v}\right)^2} \\
&\geq \sum_{uv\in E(G)} \left(\sqrt{d_u+d_v-2}-1\right)\left(\frac{\sum_{uv\in E(G)} \frac{\sqrt{d_u+d_v-2}-1}{\sqrt{d_ud_v}}}{\sum_{uv\in E(G)} \sqrt{d_u+d_v-2}-1}\right)^2 \\
&= \frac{\left(\sum_{uv\in E(G)} \frac{\sqrt{d_u+d_v-2}-1}{\sqrt{d_ud_v}}\right)^2}{\sum_{uv\in E(G)} \left(\sqrt{d_u+d_v-2}-1\right)} \\
&= \frac{(ABC-R)^2}{\sum_{uv\in E(G)} \sqrt{d_u+d_v-2} - \sum_{uv\in E(G)} 1}
\end{aligned}$$

$$\geq \frac{(ABC-R)^2}{m(\sqrt{2\Delta-2}-1)},$$

which implies the desired bound. ■

An upper bound for the difference of Randić and ABC indices in respect to general Randić index R_α when $\alpha = -\frac{1}{4}$ is given below.

Theorem 11. *Let G resembles a connected graph having m edges as well as minimum degree δ. Thus*

$$(ABC-R)(G) \geq \frac{(R_{-\frac{1}{4}}(G))^2\sqrt{2\delta-2}}{m}.$$

Proof. Setting $r=1$, $a_{uv} = \frac{1}{\sqrt[4]{d_u d_v}}$ and $b_{uv} = \frac{1}{\sqrt{d_u+d_v-2}-1}$ for every $uv \in E(G)$, applying Theorem 2 and definition of $ABC-R$ index, we obtain

$$(ABC-R)(G) = \sum_{uv\in E(G)} \frac{\left(\frac{1}{\sqrt[4]{d_u d_v}}\right)^2}{\frac{1}{\sqrt{d_u+d_v-2}-1}}$$

$$\geq \frac{\left(\sum_{uv\in E(G)} \frac{1}{\sqrt[4]{d_u d_v}}\right)^2}{\left(\sum_{uv\in E(G)} \frac{1}{\sqrt{d_u+d_v-2}-1}\right)}$$

$$= \frac{\left(R_{-\frac{1}{4}}(G)\right)^2}{\left(\sum_{uv\in E(G)} \frac{1}{\sqrt{d_u+d_v-2}-1}\right)}$$

$$\geq \frac{\left(R_{-\frac{1}{4}}(G)\right)^2}{\left(\sum_{uv\in E(G)} \frac{1}{\sqrt{d_u+d_v-2}}\right)}$$

$$\geq \frac{(R_{-\frac{1}{4}}(G))^2}{\frac{m}{\sqrt{2\delta-2}}},$$

as well as implying the desired bound. ■

Therefore, we introduce a relation between the difference of Randić and ABC indices with geometric-arithmetic index.

Theorem 12. *Let G resembles a connected graph having $\delta \geq 2$ edges and geometric-arithmetic index $GA(G)$. Therefore*

$$(ABC-R)(G) \leq \frac{(GA(G))^{2/3}\Delta^{2/3}(\sqrt{2\Delta-2}-1)}{\delta^{5/3}}.$$

Proof. Setting $r = 2$, $a_{uv} = \frac{\sqrt{d_u+d_v-2}-1}{\sqrt{d_u d_v}}$ and $b_{uv} = \frac{2\sqrt{d_u d_v}}{d_u+d_v}$ for every $uv \in E(G)$, applying Theorem 2 as well as definition of $ABC - R$ index, we obtain

$$\frac{\left(\sqrt{2\Delta-2}-1\right)^3 \Delta^2}{\delta^{\frac{10}{3}}} \geq \sum_{uv\in E(G)} \frac{\left(\sqrt{d_u+d_v-2}-1\right)^3 (d_u+d_v)^2}{4\sqrt[3]{(d_u d_v)^5}}$$

$$= \sum_{uv\in E(G)} \frac{\left(\frac{\sqrt{d_u+d_v-2}-1}{\sqrt{d_u d_v}}\right)^3}{\left(\frac{2\sqrt{d_u d_v}}{d_u+d_v}\right)^2}$$

$$\geq \frac{\left(\sum_{uv\in E(G)} \frac{\sqrt{d_u+d_v-2}-1}{\sqrt{d_u d_v}}\right)^3}{\left(\sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\right)^2}$$

$$= \frac{((ABC-R)(G))^3}{(GA(G))^2},$$

as well as implying the desired bound. ■

Relation between the difference of Randić and ABC indices with Harmonic index is provided below.

Theorem 13. *Let G resembles a graph having m edges, minimum degree δ and maximum degree Δ, as well as Harmonic index $H(G)$. Therefore*

$$(ABC - R)(G) \geq \frac{m\sqrt{2\Delta-2}}{\delta} - H(G).$$

Proof. By using geometric and arithmetic inequalities and definition of $ABC - R$ index, we possess

$$(ABC - R)(G) = \sum_{uv\in E(G)} \frac{\sqrt{d_u+d_v-2}-1}{\sqrt{d_u d_v}}$$

$$\geq \sum_{uv\in E(G)} \frac{2\sqrt{d_u+d_v-2}-2}{d_u+d_v}$$

$$= \sum_{uv\in E(G)} \frac{2\sqrt{d_u+d_v-2}}{d_u+d_v} - \sum_{u_i v_j\in E(G)} \frac{2}{d_u+d_v}$$

$$\geq \frac{m\sqrt{2\Delta-2}}{\delta} - H(G),$$

as well as implying the desired bound. ■

3. CONCLUSIONS

We derived some bounds for the difference of Randić index and atom-bond connectivity ABC index (shortly called $ABC - R$ index) in this research, as well as its connection with certain other topological indices. Given the amount of study done on the Randić and atom-bond connectivity indices, it is suprising that these two well-known indices were not compared directly. Hence, this study fills the gap and may act as an eye-opener for further research into the characterization of graphs with maximum or minimum values for the difference of Randić and ABC indices. Moreover, Chen and Guo [5] demonstrated that when one edge is removed from a graph, the ABC index of the graph reduces. It is also worth looking at what occurs to the $ABC - R$ index when an edge is removed.

To round off the paper, we suggest the following open issues:

Problem 1. Does the bound to be obtained better than the existing ones and it is possible to sharpen the bounds to be obtained?

Problem 2. Characterize the graphs with maximum or minimum values for the difference of Randić and (ABC) indices with certain parameters, for instance, matching number, chromatic number, domination number etc.

Problem 3. Study the behaviour of the $ABC - R$ index either increase or decrease when any edge is deleted.

ACKNOWLEDGEMENT. The authors would like to thank the anonymous referee for his/her constructive and valuable comments which improved the paper. A very deep appreciation to Dr. Akbar Jahanbani from Azarbaijan Shahid Madani University, Tabriz, Iran for fruitful discussions and ideas that resulted in many theorems in this paper.

REFERENCES

1. A. Ali and Z. Du, On the difference between atom-bond connectivity index and Randić index of binary and chemical trees, *Int. J. Quantum Chem.* **117** (2017) e25446.
2. B. Bollobás and P. Erdös, Graphs of extremal weights, *Ars Combin.* **50** (1998) 225–233.
3. B. Borovićanin, K. C. Das, B. Furtula and I. Gutman, Zagreb indices: Bounds and extremal graphs, in: I. Gutman, B. Furtula, K. C. Das, E. Milovanović and I. Milovanović (Eds.), *Bounds in Chemical Graph Theory-Basics*, Univ. Kragujevac, Kragujevac, 2017, pp. 76–153.
4. B. Borovićanin, K. C. Das, B. Furtula and I. Gutman, Bounds for Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 17–100.
5. J. Chen and X. Guo, Extreme atom-bond connectivity index of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 713–722.
6. Q. Cui, Q. Qian and L. Zhong, The maximum atom-bond connectivity index for graphs with edge-connectivity one, *Discrete Appl. Math.* **220** (2017) 170–173.

7. K. C. Das, S. Das and B. Zhou, Sum-connectivity index of a graph, *Front. Math. China* **11** (1) (2016) 47–54.
8. K. C. Das and N. Trinajstić, Comparison between the first geometric-arithmetic index and atom-bond connectivity index, *Chem. Phys. Lett.* **497** (2010) 149–151.
9. J. Devillers and A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, The Netherlands, 1999.
10. D. Dimitrov, On the structural properties of trees with minimal atom-bond connectivity index II: Bounds on B_1- and B_2-branches, *Discrete Appl. Math.* **204** (2016) 90–116.
11. E. Estrada, Atom-bond connectivity and energetic of branched alkanes, *Chem. Phys. Lett.* **463** (2008) 422–425.
12. E. Estrada, L. Torres, L. Rodriguez and I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem. Sect. A* **37** (1998) 849–855.
13. B. Furtula, I. Gutman and S. Ediz, On the difference of Zagreb indices, *Discrete Appl. Math.* **178** (2014) 83–88.
14. Y. Gao and Y. Shao, The smallest ABC index of trees with n pendant vertices, *MATCH Commun. Math. Comput. Chem.* **76** (1) (2016) 141–158.
15. I. Gutman and B. Furtula, *Recent Results in the Theory of Randić Index*, in: *Mathematical Chemistry Monograph* **6**, University of Kragujevac, Kragujevac, 2008.
16. I. Gutman, B. Furtula, M. B. Ahmadi, S. A. Hosseini, P. S. Nowbandegani and M. Zarrinderakht, The ABC index conundrum, *Filomat* **27** (2013) 1075–1083.
17. I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
18. M. Ghorbani and M. A. Hosseinzadeh, A new version of Zagreb indices, *Filomat* **26** (1) (2012) 93–100.
19. N. M. Husin, R. Hasni, Z. Du and A. Ali, More results on extremum Randić indices of (molecular) trees, *Filomat* **32** (10) (2018) 3581–3590.
20. S. M. Hosamani, B. B. Kulkarni, R. G. Boli and V. M. Gadag: QSPR analysis of certain graph theoretical matrices and their corresponding energy, *Appl. Math. Nonlin. Sci.* **2** (2017) 131–150.
21. J. Li, S. Balachandran, S. K. Ayyaswamy and Y. B. Venkatakrishnan, The Randić indices of trees, unicyclic graphs and bicyclic graphs, *Ars Combin.* **127** (2016) 409–419.

22. X. Li and I. Gutman, Mathematical aspects of Randić-type molecular structure descriptors, in: *Mathematical Chemistry Monograph* **1**, University of Kragujevac, Kragujevac, Serbia, 2006.
23. X. Li and Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.
24. J. B. Liu, M. M. Matejić, E. I. Milovanović and I. Z. Milovanović, Some new inequalities for the forgotten topological index and coindex of graphs, *MATCH Commun. Math. Comput. Chem.* **84** (3) (2020) 719–738.
25. D. S. Mitrinović, J. E. Pečarić and A. M. Fink, *Classical and New Inequalities in Analysis*, Dordrecht, Netherlands: Kluwer, 1993.
26. G. Pólya and G. Szegö, *Problems and Theorems in Analysis, Series, Integral Calculus, Theory of Functions*, Springer-Verlag, Berlin, 1972.
27. M. Randić, On characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975) 6609–6615.
28. M. Randić, On the history of the Randić index and emerging hostility towards chemical graph theory, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 5–124.
29. J. Radon, Theorie und Anwendungen der absolut additiven Mengenfunktionen, *Sitzungsber. Acad. Wissen. Wien.* **122** (1913) 1295–1438.
30. Z. Raza, A. A. Bhatti and A. Ali, More comparison between the first geometric-arithmetic index and atom-bond connectivity index, *Miskolc Math. Notes* **17** (1) (2016) 561–570.
31. P. S. Ranjini, V. Lokesha and I. N. Cangul, On the Zagreb indices of the line graphs of the subdivision graphs, *Appl. Math. Comput.* **218** (2011) 699–702.
32. Z. Shao, P. Wu, Y. Gao, I. Gutman and Z. Zhang, On the maximum ABC index of graphs without pendent vertices, *Appl. Math. Comput.* **315** (2017) 298–312.
33. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.
34. 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.
35. J. F. Wang and F. Belardo, A lower bound for the first Zagreb index and its applications, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 35–56.
36. W. N. N. N. Wan Zuki, Z. Du, M. K. Jamil and R. Hasni, Extremal trees with respect to the difference between atom-bond connectivity index and Randić index, *Symmetry* **12** (2020) 1591.
37. D. B. West, *Introduction to Graph Theory*, 2nd Ed., Prentice Hall, Inc., Upper Saddle River, NJ, USA, 2001.
38. R. Xing, B. Zhou and F. M. Dong, On the atom-bond connectivity index of connected graphs, *Discrete Appl. Math.* **159** (2011) 1617–1630.

39. K. Xu, K. C. Das and S. Balachandran, Maximizing the Zagreb indices of (n, m)-graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 641–654.
40. L. Zhong and Q. Cui, On a relation between the atom-bond connectivity and the first geometric-arithmetic indices, *Discrete Appl. Math.* **185** (2015) 249–253.