Montes Taurus J. Pure Appl. Math. 6 (3), 131–145, 2024

Montes Taurus Journal of Pure and Applied Mathematics
https://www.mtjpamjournal.com

MTJPAM
ISSN: 2687-4814

Mathematical inequalities for novel generalized atom-bond connectivity related descriptors

Bheemanna Sarveshkumar [a], Basavaraju Chaluvaraju [b], Veerabhadraiah Lokesha [c]

[a] Department of Mathematics, Bangalore University, Jnana Bharathi Campus, Bangalore-560 056, India
[b] Department of Mathematics, Bangalore University, Jnana Bharathi Campus, Bangalore-560 056, India
[c] Registrar (Evaluation), Bangalore City University, Central College Campus, Bangalore-560 0001, India

Abstract

The significance of the (i, j, k)-variants of atom-bond connectivity (ABC) indices lies in the fact that their special privilege, for suitably-picked potential gains of the variants i, j and k, concur with a long shot a large portion of as of late considered atom-bond accessibility-related indices. In this paper, we obtain some mathematical inequalities based on the sign of the variants (i, j, k) in terms of degree, order and size, characterizations, and within comparisons, along with some bounds in terms of existing descriptors.

Keywords: Molecular descriptors, ABC indices, AZI indices, (i, j, k)-variant ABC indices

2020 MSC: 05A20, 05C07, 05C09, 26D15, 97H30

1. Introduction

The graphs in this article are simple, non-empty, and finite with $|V(G)| = p$ and $|E(G)| = q$ denoting the cardinality of the vertex set and edge set of a graph $G = (V, E)$, respectively. As a vertex has degree (or valency) $d_G(u)$, that vertex is in the neighborhood set u. Also, $d_G(e) = d_G(u) + d_G(v) - 2$ is the degree of an edge $e = uv$ in G.

A molecular (chemical) graph is a graph wherein the vertices compare to the particles and the edges to the obligations of a molecule. The unique value that can be computed from the molecular graph and used to portray some property of the invisible particle is supposed to be a molecular structure descriptor (topological index). These are applicable to investigate their connections with chemical documentation, structure-property relationships, isomer discrimination, structure-activity interactions, pharmaceutical drug design, and many other topics that are possible to use. The basic definitions and terminology for graph theory and chemical graph theory follow Harary [27] and Trinajstic [45], respectively. For more explanations of the above matters in terms of Mathematical properties and their chemical applicability, we refer to [6, 8, 22, 25, 31, 33, 34, 44, 46].

As described in [14], Estrada et al. introduced the ABC index of a graph G and it is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(e)}{d_G(u)d_G(v)}}.$$

†*Article ID:* MTJPAM-D-23-00012

Email addresses: sarveshbub@gmail.com (Bheemanna Sarveshkumar), bchaluvaraju@gmail.com (Basavaraju Chaluvaraju), v.lokesha@gmail.com (Veerabhadraiah Lokesha)

Received:3 June 2023, Accepted:18 December 2023, Published:2 March 2024

⋆*Corresponding Author:* Veerabhadraiah Lokesha

This descriptor is a valuable predictive index in the study of the heat of formation of alkanes [13] and [17]. For more information about ABC-related indices, we refer to [1, 4, 7], [9]-[12], [19]-[21], [23, 24, 28], [36]-[38], [41, 47, 49, 50].

2. (i, j, k)-ABC indices

Let $x = d_G(u)$, $y = d_G(v)$ and $z = d_G(e)$ with $uv \in E(G)$. Then, we define the different types of (i, j, k)-ABC related valency descriptors (indices) of a connected graph $G = (V, E)$ as

(i) $ABC^1_{(i,j,k)}(G) = \sum_{uv\in E(G)} \left([x^i + y^i][z^j]\right)^k$

(ii) $ABC^2_{(i,j,k)}(G) = \sum_{uv\in E(G)} \left([x^i + y^i] + z^j\right)^k$

(iii) $ABC^3_{(i,j,k)}(G) = \sum_{uv\in E(G)} \left(x^i\, y^i\, z^j\right)^k$

(iv) $ABC^4_{(i,j,k)}(G) = \sum_{uv\in E(G)} \left([x^i\, y^i] + z^j\right)^k$

(v) $ABC^5_{(i,j,k)}(G) = \sum_{uv\in E(G)} \left(\frac{z^j}{x^i + y^i}\right)^k$

(vi) $ABC^6_{(i,j,k)}(G) = \sum_{uv\in E(G)} \left(\frac{z^j}{x^i\, y^i}\right)^k,$

where $i, j, k \in \mathbb{R}$ (Set of real numbers).

In general, for any $i, j, k \in \mathbb{R}$ and k, an (i, j, k)-ABC related valency descriptors of a connected graph G is defined as

$$ABC^t_{(i,j,k)}(G) = \sum_{uv\in E(G)} \left([x^i * y^i] o\, z^j\right)^k,$$

where $x = d_G(u)$, $y = d_G(v)$ and $z = d_G(e)$ with $uv \in E(G)$, where $*$ and o the two binary compositions.

2.1. The particular values of i, j and k in (i, j, k)-ABC indices:

For specific values of the $i, j, k \in \mathbb{R}$, the majority of previously investigated degree-based topological indices are special cases of the (i, j, k)-ABC indices as in the Table 1.

3. Special classes of graphs

Theorem 3.1. *Let G be a regular graph with $p \geq 2$ and $deg(v) = r : \forall v \in V(G)$. Then*

(i) $ABC^1_{(i,j,k)}(G) = q2^{(i+j)k}\left[r^i(r-1)^j\right]^k$

(ii) $ABC^2_{(i,j,k)}(G) = q\left[2r^i + (2(r-1))^j\right]^k$

(iii) $ABC^3_{(i,j,k)}(G) = q2^{jk}r^{2ik}(r-1)^{jk}$

(iv) $ABC^4_{(i,j,k)}(G) = q\left[r^{2i} + 2^j(r-1)^j\right]^k$

(v) $ABC^5_{(i,j,k)}(G) = q2^{(j-i)^k}\left[\frac{(r-1)^j}{r^i}\right]^k$

(vi) $ABC^6_{(i,j,k)}(G) = q2^{jk}\left[\frac{(r-1)^j}{r^{2i}}\right]^k$,

where $i, j, k \in \mathbb{R}$.

Proof. Let G be a regular graph with $p \geq 2$ and $i, j, k \in \mathbb{R}$. If $d_G(v) = r : \forall v \in V(G)$ and $2q = pr$, then the desired results (i)-(vi) follows. □

The particular values of i, j, k in (i, j, k)-ABC indices
$ABC^1_{(1,0,1)}(G) = M_1(G)$, the first Zagreb index, [26].
$ABC^3_{(1,0,1)}(G) = M_2(G)$, the second Zagreb index, [26].
$ABC^1_{(-1,0,1)}(G) = ReM_1(G)$, the redefined first Zagreb index, [40].
$ABC^1_{(-1,0,-1)}(G) = ReM_1(G)$, the redefined second Zagreb index, [40].
$ABC^1_{(2,0,1)}(G) = F(G)$, the Forgotten index, [16].
$ABC^1_{(1,0,\frac{-1}{2})}(G) = \chi(G)$, the sum connectivity index, [52].
$ABC^1_{(1,0,2)}(G) = HM_1(G)$, the first hyper Zagreb index, [43].
$ABC^3_{(-1,1,\frac{1}{2})}(G) = ABC(G)$, the ABC-index, [14].
$ABC^3_{(1,0,2)}(G) = HM_2(G)$, the second hyper Zagreb index, [48]
$2ABC^1_{(1,0,-1)}(G) = H(G)$, the Harmonic index, [15].
$ABC^3_{(1,0,\frac{-1}{2})}(G) = R(G)$, the Randic index, [39].
$ABC^3_{(1,0,\frac{1}{2})}(G) = RR(G)$, the reciprocal Randic index, [39].
$ABC^3_{(1,-1,3)}(G) = AZI(G)$, the Augmented Zagreb index, [18].
$ABC^3_{(1,0,-1)}(G) = MM_2(G)$, the Modified Zagreb index, [18].
$ABC^3_{(1,0,b)}(G) = R^b(G)$, the general Randic index, [5].
$ABC^1_{(a-1,0,1)}(G) = M^a_1(G)$, the general first Zagreb index, [35].
$ABC^1_{(0,1,1)}(G) = I_{Pl}(G)$, the Platt number, [3].
$ABC^3_{(1,-1,\frac{1}{2})}(G) = RABC(G)$, the Reciprocal ABC, [2].
$\frac{1}{2}ABC^1_{(1,0,1)}(G) = SK(G)$, the SK index, [42].
$ABC^1_{(a,0,b)}(G) = KA^1_{(a,b)}(G)$ the first (a, b)-KA indices, [32].
$\frac{1}{2}ABC^3_{(1,0,1)}(G) = SK_1(G)$, the first SK index, [42].
$\frac{1}{4}ABC^1_{(1,0,2)}(G) = SK_2(G)$, the second SK index, [42].
$ABC^1_{(a,0,b)}(G) = KA^1_{(a,b)}(G)$ the second (a, b)-KA indices, [32].
$ABC^1_{(-2,0,\frac{1}{2})}(G) = BSO(G)$, the Banhatti Sombor index, [30].
$ABC^1_{(1,0,b)}(G) = \chi^b(G)$, the general sum Connectivity index, [51].
$ABC^1_{(1,0,1)}(G) + ABC^3_{(1,0,1)}(G) = GO_1(G)$, the first Gaurava index, [29].

Table 1. The particular values of i, j, k in (i, j, k)-ABC indices to other valency based topological indices (molecular descriptors)

By Theorem 3.1, we have the particular values of the cycle C_p; $p \geq 3$ with $r = 2$ and the complete graph K_p; $p \geq 2$ with $r = p - 1$.

Theorem 3.2. *Let $K_{m,n}$ be a complete bipartite graph. Then*

(i) $ABC^1_{(i,j,k)}(K_{m,n}) = mn\left[(m^i + n^i)(m + n - 2)^j\right]^k$

(ii) $ABC^2_{(i,j,k)}(K_{m,n}) = mn\left[(m^i + n^i) + (m + n - 2)^j\right]^k$

(iii) $ABC^3_{(i,j,k)}(K_{m,n}) = (mn)^{ik+1}(m + n - 2)^{jk}$

(iv) $ABC^4_{(i,j,k)}(K_{m,n}) = mn\left[(mn)^i + (m + n - 2)^j\right]^k$

(v) $ABC^5_{(i,j,k)}(K_{m,n}) = mn\left[\dfrac{(m+n-2)^j}{(m^i+n^i)^k}\right]$

(vi) $ABC^6_{(i,j,k)}(K_{m,n}) = (mn)^{1-ik}(m+n-2)^{jk}$,

where $i, j, k \in \mathbb{R}$.

Proof. Let $K_{m,n}$ be a complete bipartite graph with m, n vertex partitions and $i, j, k \in \mathbb{R}$. Since $p = m+n$ and $q = mn$ for all edge $uv \in E(G)$ and by the definitions of (i, j, k)-ABC indices with $x = m = d_G(u)$, $y = n = d_G(v)$ and $z = d_G(e) = m+n-2$. Hence, the results (i)-(vi) follows. □

By Theorem 3.2, we have the particular values of the star $K_{1,p-1}$; $p \geq 2$ with $m = 1$ and $n = p-1$.
Further, for any three positive real numbers i, j, and k, we have

$$0 \leq ABC^t_{(i,j,k)}(K_{m,n}) \leq mn\left[(m^i * n^i)o(m+n-2)^j\right]^k,$$

where $*$ and o are binary composition with respected to addition (+) or multiplication (×) and $1 \leq t \leq 6$.

4. Inequalities in terms of size and degree

Theorem 4.1. *Let G be any connected graph with* $p \geq 3$ *vertices. Then the value of* $ABC^1_{(i,j,k)}(G)$ *lies between* $q2^{k(1+j)}\left[\delta(G)^i(\delta(G)-1)^j\right]^k$ *and* $q2^{k(1+j)}\left[\Delta(G)^i(\Delta(G)-1)^j\right]^k$ *or* $q2^{k(1+j)}\left[\delta(G)^i(\Delta(G)-1)^j\right]^k$ *and* $q2^{k(1+j)}\left[\Delta(G)^i(\delta(G)-1)^j\right]^k$. *Further, the equality holds if and only if the graph G is regular.*

We present the following claims before proving the preceding theorem.

Claim 4.2. If $i, j, k \geq 0$ or $i, j, k \leq 0$, then

$$q2^{k(1+j)}\left[\delta(G)^i(\delta(G)-1)^j\right]^k \leq ABC^1_{(i,j,k)}(G) \leq q2^{k(1+j)}\left[\Delta(G)^i(\Delta(G)-1)^j\right]^k.$$

Proof. We know that $\delta(G) \leq x, y \leq \Delta(G)$ and $2\delta(G)-2 \leq z \leq 2\Delta(G)-2$.

Case 1. When $i, j, k \geq 0$, for any $i, j \geq 0$, the above inequalities becomes

$$\delta(G)^i \leq \left\{x^i, y^i\right\} \leq \Delta(G)^i, (2\delta(G)-2)^j \leq z^j \leq (2\Delta(G)-2)^j$$

$$2\delta(G)^i \leq x^i + y^i \leq 2\Delta(G)^i, 2^j(\delta(G)-1)^j \leq z^j \leq 2^j(\Delta(G)-1)^j.$$

Every term in the above inequality is non-negative. By taking the product of those inequalities, we have

$$2\delta(G)^i 2^j(\delta(G)-1)^j \leq (x^i+y^i)z^j \leq 2\Delta(G)^i 2^j(\Delta(G)-1)^j.$$

For any non-negative value of k, the above inequality becomes

$$\left[2^{1+j}\delta(G)^i(\delta(G)-1)^j\right]^k \leq \left[\left(x^i+y^i\right)z^j\right]^k \leq \left[2^{1+j}\Delta(G)^i(\Delta(G)-1)^j\right]^k$$

$$2^{k(1+j)}\left[\delta(G)^i(\delta(G)-1)^j\right]^k \leq \left[\left(x^i+y^i\right)z^j\right]^k \leq 2^{k(1+j)}\left[\Delta(G)^i(\Delta(G)-1)^j\right]^k.$$

Case 2. When $i, j, k \leq 0$, we have for any $i, j \leq 0$,

$$\Delta(G)^i \leq x^i, y^i \leq \delta(G)^i, (2\Delta(G)-2)^j \leq z^j \leq (2\delta(G)-2)^j$$

$$2\Delta(G)^i \leq x^i + y^i \leq 2\delta(G)^i, 2^j(\Delta(G)-1)^j \leq z^j \leq 2^j(\delta(G)-1)^j.$$

Since each term in the above inequalities is non-negative. Hence the product of those inequalities are

$$2\Delta(G)^i 2^j(\Delta(G)-1)^j \le \left(x^i + y^i\right) z^j \le 2\delta(G)^i 2^j\left(\delta(G)-1\right)^j$$

$$2^{1+j}\Delta(G)^i(\Delta(G)-1)^j \le \left(x^i + y^i\right) z^j \le 2^{1+j}\delta(G)^i(\delta(G)-1)^j.$$

The above inequity can be rewritten for any non-positive value of k.

$$2^{k(1+j)}[\delta(G)^i(\delta(G)-1)^j]^k \le \left[\left(x^i + y^i\right) z^j\right]^k \le 2^{k(1+j)}\left[\Delta(G)^i(\Delta(G)-1)^j\right]^k.$$

By Case 1 and Case 2, the inequality satisfies for each $uv \in E(G)$. By taking the sum of those inequalities, we have

$$q2^{k(1+j)}[\delta(G)^i(\delta(G)-1)^j]^k \le ABC^1_{(i,j,k)}(G) \le q2^{k(1+j)}[\Delta(G)^i(\Delta(G)-1)^j]^k.$$

This completes the proof. □

Similarly, we have the following claims for changing the values of real numbers i, j, k and omitting the proofs.

Claim 4.3. If $i, j \le 0, k \ge 0$ or $i, j \ge 0, k \le 0$, then

$$q2^{k(1+j)}\left[\Delta(G)^i(\Delta(G)-1)^j\right]^k \le ABC^1_{(i,j,k)}(G) \le q2^{k(1+j)}\left[\delta(G)^i(\delta(G)-1)^j\right]^k.$$

Claim 4.4. If $i, k \ge 0, j \le 0$ or $i, k \le 0, j \ge 0$,

$$q2^{k(1+j)}\left[\delta(G)^i(\Delta(G)-1)^j\right]^k \le ABC^1_{(i,j,k)}(G) \le q2^{k(1+j)}\left[\Delta(G)^i(\delta(G)-1)^j\right]^k.$$

Claim 4.5. If $i \ge 0, j, k \le 0$ or $i \le 0, \ \ j, k \ge 0$, then

$$q2^{k(1+j)}\left[\Delta(G)^i(\delta(G)-1)^j\right]^k \le ABC^1_{(i,j,k)}(G) \le q2^{k(1+j)}\left[\delta(G)^i(\Delta(G)-1)^j\right]^k.$$

Proof of the Theorem 4.1 follows from claims 4.2 to 4.5. Further, the equality holds good for regular graph G with $d_G(v) = d_G(u)$.

Theorem 4.6. *Let G be a connected graph with $p \ge 3$. Then the value of $ABC^2_{(i,j,k)}(G)$ lies between $q\left[2\delta(G)^i + 2^j(\delta(G)-1)^j\right]^k$ and $q\left[2\Delta(G)^i + 2^j(\Delta(G)-1)^j\right]^k$ or $q\left[2\Delta(G)^i + 2^j(\delta(G)-1)^j\right]^k$ and $q\left[2\delta(G)^i + 2^j(\Delta(G)-1)^j\right]^k$. Further, the equality holds if and only if the graph G is regular.*

We present the following claims before proving the preceding theorem.

Claim 4.7. If $i, j, k \ge 0$ or $i, j, k \le 0$, then

$$q\left[2\delta(G)^i + 2^j(\delta(G)-1)^j\right]^k \le ABC^2_{(i,j,k)}(G) \le q\left[2\Delta(G)^i + 2^j\left(\Delta(G)-1\right)^j\right]^k.$$

Proof. We know that $\delta(G) \le x, y \le \Delta(G)$ and $2\delta(G) - 2 \le z \le 2\Delta(G) - 2$.

Case 1. When $i, j, k \ge 0$, for any $i, j \ge 0$,

$$2\delta(G)^i + 2^j(\delta(G)-1)^j \le x^i + y^i + z^j \le 2\Delta(G)^i + 2^j(\Delta(G)-1)^j.$$

For any non-negative value k, the above inequality becomes

$$\left[2\delta(G)^i + 2^j(\delta(G)-1)^j\right]^k \le \left[x^i + y^i + z^j\right]^k \le \left[2\Delta(G)^i + 2^j(\Delta(G)-1)^j\right]^k.$$

Case 2. When $i, j, k \le 0$, we have for any $i, j \le 0$,

$$2\Delta(G)^i + 2^j(\Delta(G)-1)^j \le x^i + y^i + z^j \le 2\delta(G)^i + 2^j(\delta(G)-1)^j.$$

For any non-positive value of k, the above inequality becomes

$$\left[2\delta(G)^i + 2^j(\delta(G) - 1)^j\right]^k \leq \left[x^i + y^i + z^j\right]^k \leq \left[2\Delta(G)^i + 2^j(\Delta(G) - 1)^j\right]^k.$$

The final equation of Case 1 and Case 2 are the same, which satisfies each edge $uv \in E(G)$. By taking the sum of those inequalities, we have

$$q\left[2\delta(G)^i + 2^j(\delta(G) - 1)^j\right]^k \leq ABC^2_{(i,j,k)}(G) \leq q\left[2\Delta(G)^i + 2^j(\Delta(G) - 1)^j\right]^k.$$

This completes the proof. □

Similarly, we have the following claims for changing the values of real numbers i, j, k and omitting the proofs.

Claim 4.8. If $i, j \leq 0, k \geq 0$ or $i, j \geq 0, k \leq 0$, then

$$q\left[2\Delta(G)^i + 2^j(\Delta(G) - 1)^j\right]^k \leq ABC^2_{(i,j,k)}(G) \leq q\left[2\delta(G)^i + 2^j(\delta(G) - 1)^j\right]^k.$$

Claim 4.9. If $i, k \geq 0, j \leq 0$ or $i, k \leq 0, j \geq 0$, then

$$q\left[2\delta(G)^i + 2^j(\Delta(G) - 1)^j\right]^k \leq ABC^2_{(i,j,k)}(G) \leq q\left[2\Delta(G)^i + 2^j(\delta(G) - 1)^j\right]^k.$$

Claim 4.10. If $i \geq 0, j, k \leq 0$ or $i \leq 0, j, k \geq 0$, then

$$q\left[2\Delta(G)^i + 2^j(\delta(G) - 1)^j\right]^k \leq ABC^2_{(i,j,k)}(G) \leq q\left[2\delta(G)^i + 2^j(\Delta(G) - 1)^j\right]^k.$$

Proof of the Theorem 4.6 follows from claims 4.7 to 4.10. Further, the equality holds good for regular graph G with $d_G(v) = d_G(u)$.

Theorem 4.11. *Let G be a connected graph with $p \geq 3$ vertices. Then the value of $ABC^3_{(i,j,k)}(G)$ lies between $q2^{jk}\delta(G)^{2ik}(\delta(G)-1)^{jk}$ and $q2^{jk}\Delta(G)^{2ik}(\Delta(G)-1)^{jk}$ or $q2^{jk}\Delta(G)^{2ik}(\delta(G)-1)^{jk}$ and $q2^{jk}\delta(G)^{2ik}(\Delta(G)-1)^{jk}$. Further, the equality holds if and only if the graph G is regular.*

We present the following claims before proving the preceding theorem.

Claim 4.12. If i, j, k are of the same sign or $ik, jk \geq 0$, then

$$q2^{jk}\delta(G)^{2ik}(\delta(G) - 1)^{jk} \leq ABC^3_{(i,j,k)}(G) \leq q2^{jk}\Delta(G)^{2ik}(\Delta(G) - 1)^{jk}.$$

Proof. We know that, $\delta(G) \leq x, y \leq \Delta(G)$ and $2\delta(G) - 2 \leq z \leq 2\Delta(G) - 2$.
For any i, j, k with the same sign or $ik, jk \geq 0$, we have

$$\delta(G)^{2ik} \leq x^{ik}y^{ik} \leq 2\Delta(G)^{2ik}, 2^{jk}(\delta(G) - 1)^{jk} \leq z^{jk} \leq 2^{jk}(\Delta(G) - 1)^{jk}.$$

Since each term in the above inequalities is non-negative. Hence the product of corresponding terms is

$$\delta(G)^{2ik}2^{jk}(\delta(G) - 1)^{jk} \leq x^{ik}y^{ik}z^{jk} \leq \Delta(G)^{2ik}2^{jk}(\Delta(G) - 1)^{jk}.$$

The above inequalities hold for each edge $uv \in E(G)$. By taking the sum of those inequalities, we have

$$q2^{jk}\delta(G)^{2ik}(\delta(G) - 1)^{jk} \leq ABC^3_{(i,j,k)}(G) \leq q2^{jk}\Delta(G)^{2ik}(\Delta(G) - 1)^{jk}.$$

This completes the proof. □

Similarly, we have the following claims for changing the values of real numbers i, j, k and omitting the proofs.

Claim 4.13. If $ik, jk \leq 0$, then

$$q2^{jk}\Delta(G)^{2ik}(\Delta(G) - 1)^{jk} \leq ABC^3_{(i,j,k)}(G) \leq q2^{jk}\delta(G)^{2ik}(\delta(G) - 1)^{jk}.$$

Claim 4.14. If $ik \leq 0$ and $jk \geq 0$, then

$$q2^{jk}\Delta(G)^{2ik}(\delta(G)-1)^{jk} \leq ABC^3_{(i,j,k)}(G) \leq q2^{jk}\delta(G)^{2ik}(\Delta(G)-1)^{jk}.$$

Claim 4.15. If $ik \geq 0$ and $jk \leq 0$, then

$$q2^{jk}\delta(G)^{2ik}(\Delta(G)-1)^{jk} \leq ABC^3_{(i,j,k)}(G) \leq q2^{jk}\Delta(G)^{2ik}(\delta(G)-1)^{jk}.$$

Proof of the Theorem 4.11 follows from claims 4.12 to 4.15. Further, the equality holds for regular graph G with $d_G(v) = d_G(u)$.

Theorem 4.16. *Let G be a connected graph with $p \geq 3$. Then the value of $ABC^4_{(i,j,k)}(G)$ lies between $q\left[\delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k$ and $q\left[\Delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k$ or $q\left[\delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k$ and $q\left[\Delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k$. Further, the equality holds if and only if the graph G is regular.*

We present the following claims before proving the preceding theorem.

Claim 4.17. If $i, j, k \geq 0$ or $i, j, k \leq 0$, then

$$q\left[\delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k \leq ABC^4_{(i,j,k)}(G) \leq q\left[\Delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k.$$

Proof. We know that $\delta(G) \leq x, y \leq \Delta(G)$ and $2\delta(G) - 2 \leq z \leq 2\Delta(G) - 2$.

Case 1. When $i, j, k \geq 0$, for any $i, j \geq 0$,

$$\delta(G)^{2i} + 2^j(\delta(G)-1)^j \leq (x^i y^i) + z^j \leq \Delta(G)^{2i} + 2^j(\Delta(G)-1)^j.$$

For any non-negative value of k, the above inequality becomes

$$\left[\delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k \leq \left[(x^i y^i) + z^j\right]^k \leq \left[\Delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k.$$

Case 2. When $i, j, k \leq 0$, for any $i, j \leq 0$,

$$\Delta(G)^{2i} + 2^j(\Delta(G)-1)^j \leq (x^i y^i) + z^j \leq \delta(G)^{2i} + 2^j(\delta(G)-1)^j.$$

The above inequity can be rewritten for any non-positive value of k.

$$\left[\delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k \leq \left[(x^i y^i) + z^j\right]^k \leq \left[\Delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k.$$

The final equation of Case 1 and Case 2 are the same, which satisfies each edge $uv \in E(G)$. By taking the sum of those inequalities, we have

$$q\left[\delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k \leq ABC^4_{(i,j,k)}(G) \leq q\left[\Delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k.$$

This completes the proof. □

Similarly, we have the following claims for changing the values of real numbers i, j, k and omitting the proofs.

Claim 4.18. If $i, j \leq 0, k \geq 0$ or $i, j \geq 0, k \leq 0$, then

$$q\left[\Delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k \leq ABC^4_{(i,j,k)}(G) \leq q\left[\delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k.$$

Claim 4.19. If $i, k \geq 0, j \leq 0$ or $i, k \leq 0, j \geq 0$, then

$$q\left[\delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k \leq ABC^4_{(i,j,k)}(G) \leq q\left[\Delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k.$$

Claim 4.20. If $i \geq 0, j, k \leq 0$ or $i \leq 0, j, k \geq 0$, then

$$q\left[\Delta(G)^{2i} + 2^j(\delta(G)-1)^j\right]^k \leq ABC^4_{(i,j,k)}(G) \leq q\left[\delta(G)^{2i} + 2^j(\Delta(G)-1)^j\right]^k.$$

Proof of the Theorem 4.16 follows from claims 4.17 to 4.20. Further, the equality holds for regular graph G with $d_G(u) = d_G(v)$.

By changing the values of real numbers i, j, k in Theorems 4.1 and 4.11, we have the following result without proof.

Theorem 4.21. *Let G be a connected graph with $p \geq 3$. Then*

(i) $ABC^5_{(i,j,k)}(G) = ABC^1_{(i,-j,-k)}(G)$.

(ii) $ABC^6_{(i,j,k)}(G) = ABC^3_{(i,-j,-k)}(G)$.

5. Inequalities among the novel generalized ABC indices

This section shows some inequalities among the novel generalized ABC indices. For any positive reals $a_1, a_2, \ldots, a_n$, then we use the following well-known generalized version of the arithmetic mean-geometric mean inequality.

Theorem 5.1. *Let $a_1, a_2, \ldots, a_n$ be a any positive real numbers. Then*

$$\frac{a_1 + a_2 + \cdots + a_n}{n} \geq \sqrt[n]{a_1 a_2 \ldots a_n}.$$

Further, if $a_1 = a_2 = \cdots = a_n$ the equality holds.

Theorem 5.2. *Let G be a connected graph with $i, j, k > 0$ and $p \geq 3$. Then*

(i) $ABC^2_{(i,j,k)}(G) \geq 3^k ABC^3_{\left(i,j,\frac{k}{3}\right)}(G)$.

(ii) $ABC^1_{(i,j,k)}(G) \geq 2^k ABC^3_{\left(\frac{i}{2},j,k\right)}(G)$.

(iii) $ABC^6_{\left(\frac{i}{2},j,k\right)}(G) \geq 2^k ABC^5_{(i,j,k)}(G)$.

Proof. Consider G to be a connected graph with $i, j, k > 0$ and $p \geq 3$ vertices. If $x, y, z > 0$ and $i, j \in \mathbb{R}$, then the exponential values x^i, y^i, z^j are positive. By Theorem 5.1, we have

$$x^i + y^i + z^j \geq 3\left(x^{\frac{i}{3}} y^{\frac{i}{3}} z^{\frac{j}{3}}\right).$$

For any positive value of k, we have

$$\left[x^i + y^i + z^j\right]^k \geq 3^k \left[(x^i y^j) z^j\right]^{\frac{k}{3}}.$$

The above inequalities hold good for each edge $uv \in E(G)$. Therefore the sum of those inequalities becomes

$$\sum_{uv \in E(G)} \left[(x^i + y^i) + z^j\right]^k \geq 3^k \sum_{uv \in E(G)} \left[(x^i y^i) z^j\right]^{\frac{k}{3}}.$$

Thus the result (i) follows.
Similarly, by using Theorem 5.1, the desired results of (ii) and (iii) follow. □

We have the following result without proof by choosing $k < 0$ in Theorem 5.2.

Theorem 5.3. *Let G be a connected graph with $i, j, k < 0$ and $p \geq 3$. Then*

(i) $ABC^2_{(i,j,k)}(G) \leq 3^k ABC^3_{\left(i,j,\frac{k}{3}\right)}(G)$.

(ii) $ABC^1_{(i,j,k)}(G) \leq 2^k ABC^3_{\left(\frac{i}{2},j,k\right)}(G)$.

(iii) $ABC^6_{\left(\frac{i}{2},j,k\right)}(G) \leq 2^k ABC^5_{(i,j,k)}(G)$.

6. Inequalities in terms of other degree-based indices

First, we get the relationship between $ABC^t_{(i,j,k)}(G)$ for $1 \leq t \leq 6$ with $ij > 0$ and the general Randic index $R^\alpha(G) = \sum_{uv\in E(G)} (d_G(u)d_G(v))^\alpha$, where α is any real number, see [5].

Theorem 6.1. *Let G be a connected graph with $p \geq 3$. Then*

(i) *For any $i, j, k \in \mathbb{R}$ with same sign,*

$$\frac{2^{k(1+j)}}{\Delta^{ik}}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jk} R^{\alpha_1}(G) \leq ABC^1_{(i,j,k)}(G) \leq \frac{2^{k(1+j)}}{\delta^{ik}}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jk} R^{\alpha_1}(G),$$

where $\alpha_1 = k(i+j) \in \mathbb{R}$.

(ii) *For any $i, j \in \mathbb{R}$ with the same sign and k is any natural number $\mathbb{N}$,*

$$\sum_{r=1}^{k}\binom{k}{r}\frac{2^{k-r+jr}}{\Delta^{ik-ir}}\left(\frac{1}{\Delta}-\frac{1}{\delta^2}\right)^{jr} R^{\alpha_2}(G) \leq ABC^2_{(i,j,k)}(G) \leq \sum_{r=1}^{k}\binom{k}{r}\frac{2^{k-r+jr}}{\delta^{ik-ir}}\left(\frac{1}{\delta}-\frac{1}{\Delta^2}\right)^{jr} R^{\alpha_2}(G),$$

where $\alpha_2 = ik - ir + jr \in \mathbb{R}$.

(iii) *For any $i, j, k \in \mathbb{R}$ with same sign,*

$$\left|\frac{2}{\delta}-\frac{2}{\Delta^2}\right|^{jk} R^{\alpha_1}(G) \leq ABC^3_{(i,j,k)}(G) \leq \left|\frac{2}{\Delta}-\frac{2}{\delta^2}\right|^{jk} R^{\alpha_1}(G),$$

where $\alpha_1 = k(i+j) \in \mathbb{R}$.

(iv) *For any $i, j \in \mathbb{R}$ with the same sign and $k \in \mathbb{N}$,*

$$\sum_{r=1}^{k}\binom{k}{r}2^{jr}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jr} R^{\alpha_2}(G) \leq ABC^4_{(i,j,k)}(G) \leq \sum_{r=1}^{k}\binom{k}{r}2^{jr}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jr} R^{\alpha_2}(G),$$

where $\alpha_2 = ik - ir + jr \in \mathbb{R}$.

(v) *For any $i, j, k \in \mathbb{R}$ with same sign,*

$$2^{k(j-1)}\delta^{ik}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jk} R^{\alpha_3}(G) \leq ABC^5_{(i,j,k)}(G) \leq 2^{k(j-1)}\Delta^{ik}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jk} R^{\alpha_3}(G),$$

where $\alpha_3 = k(j-i) \in \mathbb{R}$.

(vi) *For any $i, j, k \in \mathbb{R}$ with same sign,*

$$\left|\frac{2}{\Delta}-\frac{2}{\delta^2}\right|^{jk} R^{\alpha_3}(G) \leq ABC^6_{(i,j,k)}(G) \leq \left|\frac{2}{\delta}-\frac{2}{\Delta^2}\right|^{jk} R^{\alpha_3}(G),$$

where $\alpha_3 = k(j-i) \in \mathbb{R}$.

Proof. Let G be a connected graph with $p \geq 3$. If $x = d_G(u)$, $y = d_G(v)$ and $z = d_G(e) = x+y-2$ with $uv \in E(G)$, then

(i) For any $i, j, k \in \mathbb{R}$ with same sign, we have

$$\begin{aligned}\left((x^i+y^i)z^j\right)^k &= \left((x^i+y^i)(x+y-2)^j\right)^k \text{ for } ij > 0\\ &= \left(x^{i+j}y^{i+j}\left(\frac{1}{x^i}+\frac{1}{y^i}\right)\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^j\right)^k\\ &= x^{k(i+j)}y^{k(i+j)}\left(\frac{1}{x^i}+\frac{1}{y^i}\right)^k\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{jk}.\end{aligned}$$

$$\frac{2^{k(1+j)}}{\Delta^{ik}}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jk} \le \left(\frac{1}{x^i}+\frac{1}{y^i}\right)^k\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{jk} \le \frac{2^{k(1+j)}}{\delta^{ik}}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jk}$$

$$\implies \frac{2^{k(1+j)}}{\Delta^{ik}}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jk} x^{k(i+j)}y^{k(i+j)} \le \left((x^i+y^i)z^j\right)^k \le \frac{2^{k(1+j)}}{\delta^{ik}}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jk} x^{k(i+j)}y^{k(i+j)}.$$

The above inequality satisfies each edge $uv \in E(G)$.
For $\alpha_1 = k(i+j) \in \mathbb{R}$, the sum of those inequalities becomes

$$\frac{2^{k(1+j)}}{\Delta^{ik}}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jk} R^{\alpha_1}(G) \le ABC^1_{(i,j,k)}(G) \le \frac{2^{k(1+j)}}{\delta^{ik}}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jk} R^{\alpha_1}(G).$$

(ii) For any $i, j \in \mathbb{R}$ with the same sign and $k \in \mathbb{N}$, we have

$$\begin{aligned}\left((x^i+y^i)+z^j\right)^k &= \sum_{r=1}^{k}\binom{k}{r}(x^i+y^i)^{k-r}z^{jr}\\ &= \sum_{r=1}^{k}\binom{k}{r}\left(\frac{1}{x^i}+\frac{1}{y^i}\right)^{k-r}\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{jr} x^{ik-ir+jr}y^{ik-ir+jr}.\end{aligned}$$

$$\frac{2^{k-r+jr}}{\Delta^{ik-ir}}\left(\frac{1}{\Delta}-\frac{1}{\delta^2}\right)^{jr} \le \left(\frac{1}{x^i}+\frac{1}{y^i}\right)^k\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{jk} \le \frac{2^{k-r+jr}}{\delta^{ik-ir}}\left(\frac{1}{\delta}-\frac{1}{\Delta^2}\right)^{jr}.$$

The above inequality satisfies each $uv \in E(G)$.
For $\alpha_2 = ik - ir + jr \in \mathbb{R}$, the sum of those inequalities becomes

$$\begin{aligned}\implies \sum_{r=1}^{k}\binom{k}{r}\frac{2^{k-r+jr}}{\Delta^{ik-ir}}\left(\frac{1}{\Delta}-\frac{1}{\delta^2}\right)^{jr} R^{\alpha_2}(G) &\le ABC^2_{(i,j,k)}(G)\\ &\le \sum_{r=1}^{k}\binom{k}{r}\frac{2^{k-r+jr}}{\delta^{ik-ir}}\left(\frac{1}{\delta}-\frac{1}{\Delta^2}\right)^{jr} R^{\alpha_2}(G).\end{aligned}$$

(iii) For any $i, j, k \in \mathbb{R}$ with same sign, we have

$$\begin{aligned}\left(x^iy^iz^j\right)^k &= x^{ki}y^{ki}(y+x-2)^{kj}\\ &= x^{k(i+j)}\,y^{k(i+j)}\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{kj}.\end{aligned}$$

$$x^{k(i+j)}\,y^{k(i+j)}\left|\frac{2}{\Delta}-\frac{2}{\delta^2}\right|^{jk} \le \left(x^iy^iz^j\right)^k \le x^{k(i+j)}\,y^{k(i+j)}\left|\frac{2}{\delta}-\frac{2}{\Delta^2}\right|^{jk}.$$

The above inequality satisfies each $uv \in E(G)$.
For $\alpha_1 = k(i+j) \in \mathbb{R}$, the sum of those inequalities becomes

$$\left|\frac{2}{\Delta}-\frac{2}{\delta^2}\right|^{jk} R^{\alpha_1}(G) \le ABC^3_{(i,j,k)}(G) \le \left|\frac{2}{\delta}-\frac{2}{\Delta^2}\right|^{jk} R^{\alpha_1}(G).$$

(iv) For any $i, j \in \mathbb{R}$ with the same sign and $k \in \mathbb{N}$, we have

$$\begin{aligned}\left((x^iy^i)+z^j\right)^k &= \sum_{r=1}^{k}\binom{k}{r}(x^iy^i)^{k-r}z^{jr}\\ &= \sum_{r=1}^{k}\binom{k}{r}\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{jr}x^{ik-ir+jr}y^{ik-ir+jr}.\end{aligned}$$

$$2^{jr}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jr} \le \left(\frac{1}{x^i}+\frac{1}{y^i}\right)^k\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{jk} \le 2^{jr}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jr}.$$

The above inequality satisfies each $uv \in E(G)$. For $\alpha_2 = ik - ir + jr \in \mathbb{R}$, the sum of those inequalities becomes

$$\begin{aligned}\sum_{r=1}^{k}\binom{k}{r}2^{jr}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jr}R^{\alpha_2}(G) &\le ABC^4_{(i,j,k)}(G)\\ &\le \sum_{r=1}^{k}\binom{k}{r}2^{jr}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jr}R^{\alpha_2}(G).\end{aligned}$$

(v) For any $i, j, k \in \mathbb{R}$ with same sign, we have

$$\begin{aligned}\left(\frac{z^j}{x^i+y^i}\right)^k &= \left(\frac{(x+y-2)^j}{x^i+y^i}\right)^k\\ &= \left(\frac{x^{j-i}y^{j-i}}{\left(\frac{1}{x^i}+\frac{1}{y^i}\right)}\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^j\right)^k\\ &= \frac{x^{k(j-i)}y^{k(j-i)}}{\left(\frac{1}{x^i}+\frac{1}{y^i}\right)^k}\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{jk}.\end{aligned}$$

$$\begin{aligned}2^{k(j-1)}\Delta^{-ik}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jk} &\le \left(\frac{1}{x^i}+\frac{1}{y^i}\right)^{-k}\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{jk}\\ &\le 2^{k(j-1)}\delta^{-ik}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jk}.\end{aligned}$$

$$\begin{aligned}2^{k(j-1)}\Delta^{-ik}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jk}x^{k(j-i)}y^{k(j-i)} &\le \left(\frac{(z^j}{x^i+y^i}\right)^k\\ &\le 2^{k(j-1)}\delta^{-ik}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jk}x^{k(j-i)}y^{k(j-i)}.\end{aligned}$$

The above inequality satisfies each $uv \in E(G)$.
For $\alpha_3 = k(j-i) \in \mathbb{R}$, the sum of those inequalities becomes

$$2^{k(j-1)}\Delta^{-ik}\left|\frac{1}{\Delta}-\frac{1}{\delta^2}\right|^{jk}R^{\alpha_3}(G) \le ABC^5_{(i,j,k)}(G) \le 2^{k(j-1)}\delta^{-ik}\left|\frac{1}{\delta}-\frac{1}{\Delta^2}\right|^{jk}R^{\alpha_3}(G).$$

(vi) For any $i, j, k \in \mathbb{R}$ with same sign, we have

$$\begin{aligned}\left(\frac{z^j}{x^iy^i}\right)^k &= x^{-ik}y^{-ik}(x+y-2)^{jk}\\ &= x^{k(j-i)}\,y^{k(j-i)}\left(\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}\right)^{kj}.\end{aligned}$$

$$x^{(kj-ki)}\, y^{(kj-ki)} \left|\frac{2}{\Delta} - \frac{2}{\delta^2}\right|^{jk} \leq \left(\frac{z^j}{x^i y^i}\right)^k \leq x^{(kj-ki)}\, y^{(kj-ki)} \left|\frac{2}{\delta} - \frac{2}{\Delta^2}\right|^{jk}.$$

The above inequality satisfies each $uv \in E(G)$.
For $\alpha_3 = k(j-i) \in \mathbb{R}$, the sum of those inequalities becomes

$$\left|\frac{2}{\Delta} - \frac{2}{\delta^2}\right|^{jk} R^{\alpha_3}(G) \leq ABC^6_{(i,j,k)}(G) \leq \left|\frac{2}{\delta} - \frac{2}{\Delta^2}\right|^{jk} R^{\alpha_3}(G).$$

□

By above theorem, analogously we obtain the inequalities of $ABC^t_{(i,j,k)}(G)$ for $1 \leq t \leq 6$ with $ij < 0$ in terms of the general Randic index $R^\alpha(G)$ as follows.

Theorem 6.2. *Let G be a any connected graph with $p \geq 3$. Then*

(i) *For any $i, j, k \in \mathbb{R}$ with $ij < 0$,*

$$\frac{2^{k(1+j)}}{\delta^{ik}} \left|\frac{1}{\delta} - \frac{1}{\Delta^2}\right|^{jk} R^{\alpha_1}(G) \leq ABC^1_{(i,j,k)}(G) \leq \frac{2^{k(1+j)}}{\Delta^{ik}} \left|\frac{1}{\Delta} - \frac{1}{\delta^2}\right|^{jk} R^{\alpha_1}(G),$$

where $\alpha_1 = k(i+j) \in \mathbb{R}$.

(ii) *For any $i, j \in \mathbb{R}$ with $ij < 0$ and $k \in \mathbb{N}$,*

$$\sum_{r=1}^{k} \binom{k}{kr} \frac{2^{k-r+jr}}{\delta^{ik-ir}} \left(\frac{1}{\delta} - \frac{1}{\Delta^2}\right)^{jr} R^{\alpha_2}(G) \leq ABC^2_{(i,j,k)}(G) \leq \sum_{r=1}^{k} \binom{k}{r} \frac{2^{k-r+jr}}{\Delta^{ik-ir}} \left(\frac{1}{\Delta} - \frac{1}{\delta^2}\right)^{jr} R^{\alpha_2}(G),$$

where $\alpha_2 = ik - ir + jr \in \mathbb{R}$.

(iii) *For any $i, j, k \in \mathbb{R}$ with $ij < 0$,*

$$\left|\frac{2}{\Delta} - \frac{2}{\delta^2}\right|^{jk} R^{\alpha_1}(G) \leq ABC^3_{(i,j,k)}(G) \leq \left|\frac{2}{\delta} - \frac{2}{\Delta^2}\right|^{jk} R^{\alpha_1}(G),$$

where $\alpha_1 = k(i+j) \in \mathbb{R}$.

(iv) *For any $i, j \in \mathbb{R}$ with $ij < 0$ and $k \in \mathbb{N}$,*

$$\sum_{r=1}^{k} \binom{k}{r} 2^{jr} \left|\frac{1}{\Delta} - \frac{1}{\delta^2}\right|^{jr} R^{\alpha_2}(G) \leq ABC^4_{(i,j,k)}(G) \leq \sum_{r=1}^{k} \binom{k}{r} 2^{jr} \left|\frac{1}{\delta} - \frac{1}{\Delta^2}\right|^{jr} R^{\alpha_2}(G),$$

where $\alpha_2 = ik - ir + jr \in \mathbb{R}$.

(v) *For any $i, j, k \in \mathbb{R}$ with $ij < 0$,*

$$2^{k(j-1)} \Delta^{ik} \left|\frac{1}{\delta} - \frac{1}{\Delta^2}\right|^{jk} R^{\alpha_3}(G) \leq ABC^5_{(i,j,k)}(G) \leq 2^{k(j-1)} \delta^{ik} \left|\frac{1}{\Delta} - \frac{1}{\delta^2}\right|^{jk} R^{\alpha_3}(G),$$

where $\alpha_3 = k(j-i) \in \mathbb{R}$.

(vi) *For any $i, j, k \in \mathbb{R}$ with $ij < 0$,*

$$\left|\frac{2}{\delta} - \frac{2}{\Delta^2}\right|^{jk} R^{\alpha_3}(G) \leq ABC^6_{(i,j,k)}(G) \leq \left|\frac{2}{\Delta} - \frac{2}{\delta^2}\right|^{jk} R^{\alpha_3}(G),$$

where $\alpha_3 = k(j-i) \in \mathbb{R}$.

Now, we obtain an inequality of $ABC^1_{(i,j,k)}(G)$ in terms of the first general Zagreb index

$$M_1^{b+1}(G) = \sum_{uv\in E(G)} \left[d_G(u)^b + d_G(v)^b\right],$$

where $b \in \mathbb{R}$ and the general sum connectivity index $\chi^b(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]^b$. For more details, we refer to [35] and [51].

Theorem 6.3. *Let G be any connected graph with $p \geq 3$. Then*

$$M_1^{b+1}(G) \sum_{r=1}^{jk} \theta_r(\delta)^{jk-r} \leq ABC^1_{(i,j,k)}(G) \leq \chi^b(G) \sum_{r=1}^{jk} \theta_r(\Delta)^{jk-r},$$

where $\theta_r = (-1)^r(2)^{jk}\binom{jk}{r}$ and $i, j, k \in \mathbb{N}$.

Proof. Let G be any connected graph with $p \geq 3$. If $x, y \in \mathbb{N}$, $uv \in E(G)$, then by AM-GM inequalities, $x^{ik} + y^{ik} \leq \left(x^i + y^i\right)^k \leq (x+y)^{ik}$ and applying binomial expansion $(x+y-2)^{ik} = \sum_{r=1}^{jk}(-2)^r\binom{jk}{r}(x+y)^{jk-r}$, becomes $(x^i + y^i)^k(x+y-2)^{jk} = \left((x^i + y^i)z^j\right)^k$. Therefore

$$\left(x^{ik} + y^{ik}\right) \sum_{r=1}^{jk} H_r(x+y)^{jk-r} \leq \left((x^i + y^i)z^j\right)^k \leq (x+y)^{ik} \sum_{r=1}^{jk} H_r(x+y)^{jk-r},$$

where $H_r = (-2)^r\binom{jk}{r}$.
The above inequality satisfies each edge $uv \in G$. Taking the sum of those inequalities, we have

$$M_1^{b+1}(G) \sum_{r=1}^{jk} \theta_r(\delta)^{jk-r} \leq ABC^1_{(i,j,k)}(G) \leq \chi^b(G) \sum_{r=1}^{jk} \theta_r(\Delta)^{jk-r},$$

where $\theta_r = (-1)^r(2)^{jk}\binom{jk}{r}$. For any non zero integral numbers $a = ik = b$. Hence the desired result follows. □

7. Conclusions and open problems

Being novel (i, j, k)-variant ABC-related valency descriptors of a molecular graph G, it lies on the claim that their unique cases, for pertinently chosen values of the parameters i, j and k, with the vast majority of previously considered vertex degree-based topological indices. For comparative advantages, applications, and the mathematical viewpoint, numerous questions are proposed by this article, among which are the following.

1. Find the extremal values and graphs of the (i, j, k)-ABC indices.
2. Find the values of (i, j, k)-ABC indices of some chemical graph classes and explore some results in the QSTR / QSAR / QSPR Model.
3. Obtain the relationship among (i, j, k)-ABC indices for other topological indices based on degree/distance/spectral invariants.

Acknowledgments

This paper is Dedicated to Honor Professor Yilmaz Simsek on his 60th Birth Anniversary.
The authors would like to thank the reviewers for their valuable comments and suggestions to improve the quality of the paper.

Author Contributions: All authors have contributed equally to this manuscript. The manuscript's final version has been approved by all authors for publication.

Conflict of Interest: The authors have stated that they do not have any conflicts of interest to disclose.

Funding (Financial Disclosure): The first author, B. Sarveshkumar, acknowledges the financial support provided by the University Grants Commission, New Delhi, in the form of the Junior Research Fellowship (UGC-Ref-No:959/CSIR-UGC NET JUNE 2018).

References

[1] M. B. Ahmadi, D. Dimitrov, I. Gutman and S. A. Hosseini, *Disproving a conjecture on trees with minimal Atom-Bond connectivity index*, MATCH Commun. Math. Comput. Chem. **72**, 685–698, 2019.

[2] K. N. Anil Kumar, N. S. Basavarajappa, M. C. Shanmukha and A. Usha, *Reciprocal Atom-Bond connectivity and Fourth Atom-Bond connectivity indices for Polyphenylene structure of molecules*, Eurasian Chem. Commun. **2 (12)**, 1202–1209, 2020.

[3] M. M. Belavadi and T. A. Mangam, *Platt number of total graphs*, Int. J. Appl. Math. **31 (5)**, 593–602, 2018.

[4] M. Bianchi, A. Cornaro, J. L. Palacios and A. Torriero, *New upper bounds for the ABC index*, MATCH Commun. Math. Comput. Chem. **76**, 117–130, 2016.

[5] B. Bollobas and P. Erdos, *Graphs of extremal weights*, Ars Combin. **50**, 225–233, 1998.

[6] P. Bosch, P. Molina, E. D. Rodriguez and J. M. Sigarreta, *Inequalities on the generalized ABC index*, Mathematics **9 (10)**, 2021; Article ID: 1151.

[7] B. Chaluvaraju and A. B. Shaikh, Different Versions of Atom-Bond Connectivity Indices of some molecular structures: Applied for the treatment and prevention of COVID-19, Polycycl Aromat. Compd. **42 (6)**, 3748–3761, 2022.

[8] B. Chaluvaraju, H. S. Boregowda and I. N. Cangul, *Some inequalities for the first general Zagreb index of graphs and line graphs*, Proc. Natl. Acad. Sci. India, Sect. A, Phys. Sci. **91 (1)**, 79–88, 2021.

[9] K. C. Das, *Atom-Bond connectivity index of graphs*, Discrete Appl. Math. **158**, 1181–1188, 2010.

[10] K. C. Das, I. Gutman and B. Furtula, *On Atom-Bond connectivity index*, Chem. Phys. Lett. **511**, 452–454, 2011.

[11] K. C. Das, J. M. Rodriguez and J. M. Sigarreta, *On the generalized ABC index of graphs*, MATCH Commun. Math. Comput. Chem. **87**, 147–169, 2022.

[12] D. Dimitrov, *Efficient computation of trees with minimal atom-bond connectivity index*, Appl. Math. Comput. **224**, 663–670, 2013.

[13] E. Estrada, *Atom-bond connectivity and the energetic of branched alkanes*, Chem. Phys. Lett. **463**, 422–425, 2008.

[14] E. Estrada, L. Torres, L. Rodriguez and I. Gutman, *An atom-bond connectivity index: modelling the enthalpy of formation of alkanes*, Indian J. Chem. **37A**, 849–855, 1998.

[15] S. Fajtlowicz, *On conjectures of Graffiti-II*, Congr. Numer. **60**, 187–197, 1987.

[16] B. Furtula and I. Gutman, *A forgotten topological index*, J. Math. Chem. **53**, 1184–1190, 2015.

[17] B. Furtula, I. Gutman and K. C. Das, *On atom-bond connectivity molecular structure descriptors*, J. Serb. Chem. Soc. **81**, 271–276, 2016.

[18] B. Furtula, A. Graovac and D. Vukicevic, *Augmented Zagreb index*, J. Math. Chem. **48**, 370–380, 2010.

[19] Y. Gao and Y. Shao, *The smallest ABC index of trees with n pendent vertices*, MATCH Commun. Math. Comput. Chem. **76**, 141–158, 2016.

[20] M. Goubko, C. Magnant, P. Salehi Nowbandegani and I. Gutman, *ABC index of trees with fixed number of leaves*, MATCH Commun. Math. Comput. Chem. **74**, 697–702, 2015.

[21] A. Graovac and M. Ghorbani, *A new version of atom–bond connectivity index*, Acta Chim. Slov. **57**, 609–612, 2010.

[22] I. Gutman, *Degree-based topological indices*, Croat. Chem. Acta. **86**, 351–361, 2013.

[23] I. Gutman and B. Furtula, *Trees with smallest atom-bond connectivity index*, MATCH Commun. Math. Comput. Chem. **68**, 131–136, 2012.

[24] I. Gutman, B. Furtula and M. Ivanovic, *Notes on trees with minimal atom-bond connectivity index*, MATCH Commun. Math. Comput. Chem. **67**, 467–482, 2012.

[25] I. Gutman, V. R. Kulli, B. Chaluvaraju and H. S. Boregowda, *On Banhatti and Zagreb indices*, J. Int. Math. Virtual Inst. **7**, 53–67, 2017.

[26] I. Gutman and N. Trinajstic, *Graph theory and molecular orbitals, total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17**, 535–538, 1972.

[27] F. Harary, *Graph theory*, Addison Wesley, Reading Mass, 1969.

[28] S. A. Hosseini, M. B. Ahmadi and I. Gutman, *Kragujevac trees with minimal atom-bond connectivity index*, MATCH Commun. Math. Comput. Chem. **71**, 5–20, 2014.

[29] V. R. Kulli, *The Gourava indices and coindices of graphs*, Ann. Pure and Appl. Math. **14 (1)**, 33–38, 2017.

[30] V. R. Kulli, *On Banhatti-Sombor indices*, SSRG Int. J. Appl. Chem. **8 (1)**, 21–25, 2021.

[31] V. R. Kulli, *Graph indices*, In: Hand Book of Research on Advanced Applications of Graph Theory in Modern Society (Ed. by M. Pal, S. Samanta and A. Pal), pp. 66–91, 2020.

[32] V. R. Kulli, *The (a, b)-KA indices of polycyclic aromatic hydrocarbons and benzenoid systems*, Int. J. Math. Trends and Technol. **65**, 115–120, 2019.

[33] V. R. Kulli, B. Chaluvaraju and H. S. Boregowda, *The product connectivity Banhatti index of a graph*, Discuss. Math. Graph Theory **39 (2)**, 505–517, 2019.

[34] V. R. Kulli, D. Vyshnavi and B. Chaluvaraju, *computation of (a,b)-KA Indices of some special graphs*, Int. J. Math. Comb. **3**, 62–76, 2021.

[35] X. Li and J. Zheng, *A unified approach to the extremal trees for different indices*, MATCH Commun. Math. Comput. Chem. **54 (1)**, 195–208, 2005.

[36] W. Lin, J. Chen, C. Ma, Y. Zhang, J. Chen, D. Zhang and F. Jia, *On trees with minimal ABC index among trees with given number of leaves*, MATCH Commun. Math. Comput. Chem. **76**, 131–140, 2016.

[37] C. Magnant, P. S. Nowbandegani and I. Gutman, *Which tree has the smallest ABC index among trees with k leaves?*, Discrete Appl. Math. **194**, 143–146, 2015.
[38] J. L. Palacios, *A resistive upper bound for the ABC index*, MATCH Commun. Math. Comput. Chem. **72**, 709–713, 2014.
[39] M. Randic, *Characterization of molecular branching*, J. Am. Chem. Soc. **97 (23)**, 6609–6615, 1975.
[40] P. S. Ranjini, V. Lokesha and A. Usha, *Relation between phenylene and hexagonal squeeze using harmonic index*, Int. J. Graph Theory **1**, 116–121, 2013.
[41] B. Sarveshkumar, V. R. Kulli and B. Chaluvaraju, *Some inequalities on generalized degree based indices: An* (a,b)*-KA indices and coindices*, Proc. Jangjeon Math. Soc. **26 (1)**, 43–53, 2023.
[42] V. Shigehalli and R. Kanabur, *Computing degree-based topological indices of polyhex nanotubes*, J. Math. Nanosci. **6**, 47–55, 2016.
[43] G. H. Shirdel, H. Rezapour and A. M. Sayadi, *The hyper-Zagreb index of graph operations*, Iran. J. Math. Chem. **4 (2)**, 213–220, 2013.
[44] T. Sistani, *New upper bounds on the spectral radius of graphs*, J. Math. Ext. **14 (4)**, 53–66, 2020.
[45] N. Trinajstic, *Chemical graph theory*, Routledge, 2018.
[46] R. Todeschini and V. Consonni, *Molecular descriptors for chemoinformatics*, Wiley–VCH, Weinheim, 2009.
[47] V. Vivin and K. Kalira, *Equitable coloring of Mycielskian of some graphs*, J. Math. Ext. **11 (3)**, 1–18, 2017.
[48] G. Wei, M. R. Farahani and M. K. Siddiqui, *On the First and second Zagreb and first and second hyper-Zagreb indices of carbon nanocones* $CNC_k[n]$, J. Comput. Theor. Nanosci. **13**, 7475–7482, 2016.
[49] R. Xing, B. Zhou and Z. Du, *Further results on atom-bond connectivity index of trees*, Discrete Appl. Math. **158**, 1536–1545, 2010.
[50] J. Xu, J. B. Liu, A. Bilal, U. Ahmad, H. M. A. Siddiqui, B. Ali and M. R. Farahani, *Distance degree index of some derived graphs*, Mathematics **7 (3)**, 2019; Article ID: 283.
[51] B. Zhou and N. Trinajstic, *On general sum-connectivity index*, J. Math. Chem. **47 (1)**, 210–218, 2010.
[52] B. Zhou and N. Trinajstic, *On a novel connectivity index*, J. Math. Chem. **46**, 1252–1270, 2009.