# Maximum Atom-Bond Sum-Connectivity Index in Unicyclic Graphs of Fixed Girth

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#### Abstract

The 
$$ABS$$
 (atom-bond sum-connectivity) index of a graph  $G$  is given by the formula:

$$ABS(G) = \sum_{xy \in E(G)} \sqrt{\frac{d_x + d_y - 2}{d_x + d_y}},$$

where  $d_x$  denotes the degree of vertex x in the graph G. The primary objective of this research paper is to identify the maximum, and second-maximum ABS index among all unicyclic graphs with a fixed girth. Additionally, we provide a characterization of the specific graphs that attain these extreme ABS values.

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## 1 Introduction

Let G be a connected, undirected, simple graph with precisely n vertices. The neighborhood set and degree of a vertex x in G are N(x) and d(x), respectively. A pendent vertex is a vertex of degree 1. An edge incident with a pendent vertex is called a pendent edge. Let G - x represent the resulting graph from G after removing a vertex x and all of its incident edges. Similarly, G - xy represents the resulting graph from G after removing the edge  $xy \in E(G)$ . On the other hand, G + xy represents the resulting graph from G by adding an edge xy between two non-adjacent vertices x and y of G. Additionally, the renaming of entity B as A is indicated by the notation A := B.

Chemical graph theory [27], an essential field within Mathematical Chemistry, is dedicated to representing and examining chemical structures through mathematical models. Within this field, topological indices play a vital role in establishing links between molecular structures and the properties crucial for advancing computer-aided drug design [11, 17]. Among these indices, the atom-bond sum-connectivity (ABS) index stands out, expressing connectivity patterns in molecular graphs as real-number values. The ABS index has garnered considerable attention in literature owing to its capability to provide valuable insights into the structure-property relationship of chemical compounds. Through the quantification of molecular connectivity features, the ABS index serves as a mathematical tool for comprehending and predicting the chemical and physical properties of molecules.

Various topological indices based on degrees have been introduced, as extensively discussed in [13, 16]. Among these, the atom-bond sumconnectivity (ABS) index represents a novel approach, formulated by incorporating fundamental concepts from the atom-bond connectivity (ABC) index and sum-connectivity (SC) index. This modified index first introduced by Furtula et al. [13] in 2013, represents a novel perspective on quantifying molecular structure. Ali et al. [5] have also defined the ABSindex for a simple connected graph G, expressed as follows:

$$ABS(G) = \sum_{xy \in E(G)} \sqrt{\frac{d_x + d_y - 2}{d_x + d_y}}.$$

They explored the properties of trees with the extremal ABS index values compared to all other chemical trees of a specified order  $n \ge 11$ . Expanding on this research, Ali et al. [6], extended the application of ABSto unicyclic graphs, determining both the maximum and minimum ABSindex values for unicyclic graphs of the same order and size. In a related study, Gowtham and Gutman [15] established several inequalities that describe the relationship between the SC and ABS indices. Additionally, Alraqad et al. [9, 10] characterized extremal trees and certain classes of graphs with a fixed order, number of pendent vertices, chromatic number, and independence number. Furthermore, [18, 25], provided a comprehensive solution for the largest ABS index observed in trees with a fixed number of leaves and matching number and diameter.

In our earlier investigation [24], we identified the first four minimum ABS indices for unicyclic graphs with a specified girth, highlighting the graphs that exhibit these extremal values. For a more comprehensive exploration of the ABS index and its implications in the realm of chemistry, interested readers can refer to the additional references [1–3, 7, 8, 22, 24].

In [14], Ge et al. derived a relationship between the ABS(L(G)) and ABS(G). They also identified the minimum ABS index among all line graphs of unicyclic graphs with a fixed number of vertices. Hussain et al. [19] established the sharp bounds for ABS index in terms of graph invariants. The study also derived a lower bound for the ABS index specifically for trees with the maximum degree. Additionally, in a recent publications [20,30], authors determined both upper and lower bounds for the ABS index of graphs by using the fixed parameters, which included the chromatic number, clique number, connectivity, matching number and domination number. Very recently, in [23], we determined the minimum values of ABS index among all unicyclic graphs of a given order with maximum degree, also we characterized the extremal graphs attaining these

minimum values.

Motivated by [24], in this study, we obtain the maximum, and secondmaximum ABS index of unicyclic graphs that consist of at least 5 vertices and girth  $\mathcal{R}$ , where  $(3 \leq \mathcal{R} \leq n)$ . Additionally, we provide a characterization of the extremal graphs that correspond to these values.

Consider  $\mathbb{U}_n$  to be collection of all unicyclic graphs with  $n \geq 5$  vertices. In a similar manner, the collection of all unicyclic graphs that have at least 5 vertices and girth  $\mathcal{R}$ , where  $3 \leq \mathcal{R} \leq n$  is known as  $\mathbb{U}_{n,\mathcal{R}}$ . It is observed that,  $\mathbb{U}_n = \bigcup_{\mathcal{R}=3}^n \mathbb{U}_{n,\mathcal{R}}$ . The cycle comprising n vertices is denoted by  $C_n$  and unique unicyclic graph comprising n vertices and girth n-1 is denoted by  $U_{n,n-1}^1$ . It is evident that  $\mathbb{U}_{n,n} = \{C_n\}$  and  $\mathbb{U}_{n,n-1} = \{U_{n,n-1}^1\}$ . In the subsequent arguments, we will specifically focus on the cases where  $(3 \leq \mathcal{R} \leq n-2)$ .

# 2 The maximum and second-maximum ABSindex among $\mathbb{U}_{n,\mathcal{R}}$

In the following part, we will discuss the maximum and second-maximum ABS index for graphs that belong to the set  $\mathbb{U}_{n,\mathcal{R}}$ , as well as the extremal graphs that corresponds to those graphs. Additionally, we determine the extremal graph that has the second-maximum ABS index for graphs  $\mathbb{U}_n$ . First, we will examine two lemmas.

**Lemma 1.** (i) Define  $f(p) = \sqrt{\frac{2}{b+p}} - \sqrt{\frac{2}{b+p-1}}$ . Consider a integer  $b \ge 3$  holds true for  $p \ge 1$ , the function f is decreasing.

- (ii) Define  $g(p) = 2\sqrt{\frac{p}{p+2}} + (p-4)\sqrt{\frac{p-1}{p+1}} (p-3)\sqrt{\frac{p-2}{p}}$ . For  $p \ge 3$ , the function g is increasing.
- (iii) Define  $h(p) = \sqrt{\frac{p}{p+2}} + (p-3)\sqrt{\frac{p-1}{p+1}} (p-3)\sqrt{\frac{p-2}{p}}$ . For  $p \ge 3$ , the function h is increasing.

(iv) Define 
$$m(p) = -\sqrt{\frac{p-1}{p+1}} - 2\sqrt{\frac{1}{p(p+2)^3}} - (p-3)\sqrt{\frac{1}{(p-1)(p+1)^3}} +$$

 $\left(\frac{p+1}{p}\right)\sqrt{\frac{p-2}{p}}$ . For  $p \ge 3$ , the function *m* is increasing. (v) Define  $o(p) = -2\sqrt{\frac{1}{(p-1)(p+1)^3}} - (p-4)\sqrt{\frac{1}{(p-2)p^3}} + \sqrt{\frac{p-2}{p^3}}$ . For  $p \geq 3$ , the function o is decreasing.

*Proof.* (i) consider the derivative function

$$f'(p) = \sqrt{\frac{1}{(b+p)^3(b+p-2)}} - \sqrt{\frac{1}{(b+p-1)^3(b+p-3)}}$$

is negative-valued under the specified constraints.

(ii) consider the derivative function

$$g'(p) = 2\sqrt{\frac{1}{p(p+2)^3}} + (p^2 + p - 5)\sqrt{\frac{1}{(p+1)^3(p-1)}} - (p^2 - p - 3)\sqrt{\frac{1}{p^3(p-2)}}$$

is positive-valued under the specified constraints.

(iii) consider the derivative function, for  $p \ge 3$ .

$$h'(p) = \sqrt{\frac{1}{p(p+2)^3}} + (p^2 + p - 4)\sqrt{\frac{1}{(p+1)^3(p-1)}} - (p^2 - p - 3)\sqrt{\frac{1}{p^3(p-2)}}$$

is positive-valued under the specified constraints.

(iv) Consider the derivative function,

$$m'(p) = -2\sqrt{\frac{1}{(p-1)(p+1)^3}} + 2(2p+1)\sqrt{\frac{1}{p^3(p+2)^5}} + (2p-1)(p-3)\sqrt{\frac{1}{(p-1)^3(p+1)^5}} + 3\sqrt{\frac{1}{p^5(p-2)}}$$

is positive-valued under the specified constraints.

(v) Consider the derivative function,

$$o'(p) = 2(2p-1)\sqrt{\frac{1}{(p-1)^3(p+1)^5}} - \left(\frac{4p^2 + 6p}{p^2(p-2)}\right)\sqrt{\frac{1}{p^3(p-2)}}$$

is negative-valued under the specified constraints.



Figure 1. Transformation 1: Graphs  $G_1$  and  $G'_1$  in Lemma 2

The proof of Lemma 2.1 in [6] does not require the condition of degrees. Consequently, Lemma 2.1 can be refined to yield the following result.

**Lemma 2.** [6] Let  $G_1$  be a connected graph that is not trivial. Let xand y be vertices such that there exists an edge  $xy \in E(G_1)$ . Furthermore,  $d_{G_1}(x), d_{G_1}(y) \ge 2$  and  $N_{G_1}(x) \cap N_{G_1}(y) = \emptyset$ . The graph  $G'_1$  is constructed by merging the edge xy into a new vertex w and then attaching a new pendent edge ww' to w. (Refer to Figure 1 for a visual representation of these graphs). Then  $ABS(G_1) < ABS(G'_1)$ .

The graph  $\mathfrak{L}_{n,\mathfrak{R}}$  is defined as a unicyclic graph comprising n vertices, where  $n - \mathfrak{R}$  pendent edges are connected to a single vertex x of the cycle  $C_{\mathfrak{R}}$ , for all  $3 \leq \mathfrak{R} \leq n - 2$ . (Refer to Figure 2 for a visual representation of these graphs).



Figure 2. The graphs  $\mathfrak{L}_{n,\mathfrak{R}}, \mathfrak{L}_{n,\mathfrak{R}}^*$  and  $\mathfrak{L}_{n,\mathfrak{R}}^*$   $(3 \leq \mathfrak{R} \leq n-2)$ 

**Theorem 1.** Let  $G \in \mathbb{U}_{n,\mathcal{R}}$ . Then

$$ABS(G) \le (n-\mathcal{R})\sqrt{\frac{n-\mathcal{R}+1}{n-\mathcal{R}+3}} + 2\sqrt{\frac{n-\mathcal{R}+2}{n-\mathcal{R}+4}} + (\mathcal{R}-2)\sqrt{\frac{1}{2}}$$

with equality if and only if  $G \cong \mathfrak{L}_{n,\mathfrak{R}}$ .

*Proof.* The theorem will be established through a mathematical induction process based on n. If  $n = \mathcal{R} + 2$  (*i.e.*,  $\mathcal{R} = n - 2$ ), then

$$ABS(\mathfrak{L}_{n,n-2}) = 2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{2}{3}} + (\mathfrak{R}-2)\sqrt{\frac{1}{2}}$$
$$= (n-\mathfrak{R})\sqrt{\frac{n-\mathfrak{R}+1}{n-\mathfrak{R}+3}} + 2\sqrt{\frac{n-\mathfrak{R}+2}{n-\mathfrak{R}+4}} + (\mathfrak{R}-2)\sqrt{\frac{1}{2}},$$

therefore the theorem is valid for  $n = \mathcal{R} + 2$ . Hence, we proceed by assuming that  $n > \mathcal{R} + 2$  and the theorem is applicable for smaller n values. Additionally, for the sake of convenience, we make the assumption that Gpossesses the maximum ABS index compared to all other graphs within  $\mathbb{U}_{n,\mathcal{R}}$ .

Consider a pendent vertex  $w \in V(G)$  and an edge  $yw \in E(G)$ . The vertex y has a degree  $\psi \geq 2$ , given that  $G \in \mathbb{U}_{n,\mathcal{R}}$ , which implies  $\psi \leq n-\mathcal{R}+2$ . We define  $N(y) = \{w, y_1, ..., y_{\psi-1}\}$  where each  $y_i$  has a degree  $\psi_i$  (i.e.,  $d(y_i) = \psi_i$ ) for each  $1 \leq i \leq \psi - 1$ . Notably, within the set  $\{y_1, ..., y_{\psi-1}\}$ , there is at least one vertex that has a degree greater than or equal to 2.

If only one vertex in  $\{y_1, ..., y_{\psi-1}\}$ , say x, has a degree greater than or equal to 2. According to Lemma 2, there is a graph  $G' \in \mathbb{U}_{n,\mathcal{R}}$  such that ABS(G) < ABS(G'). However, this contradicts our initial assumption that G has the maximum ABS index among all graphs in  $\mathbb{U}_{n,\mathcal{R}}$ .

Hence, it follows that there must be at least 2 vertices in the set  $\{y_1, ..., y_{\psi-1}\}$  that have a degree of at least 2 (and thus  $\psi \geq 3$ ). Consequently, we define G'' as the graph obtained by deleting vertex w from G, i.e., G'' := G - w, it follows that  $G'' \in \mathbb{U}_{n-1,\mathcal{R}}$ .

Utilizing Lemma 1 (i) and (ii) along with the assumption from the induction hypothesis, we can derive the following.

$$\begin{split} ABS(G) &= ABS(G'') + \sum_{i=1}^{\psi-1} \left[ \sqrt{\frac{\psi+\psi_i-2}{\psi+\psi_i}} - \sqrt{\frac{(\psi-1)+\psi_i-2}{(\psi-1)+\psi_i}} \right] + \sqrt{\frac{\psi-1}{\psi+1}} \\ &\leq ABS(G'') + \sqrt{\frac{\psi-1}{\psi+1}} + 2\sqrt{\frac{\psi}{\psi+2}} - 2\sqrt{\frac{\psi-1}{\psi+}} + (\psi-3) \left[ \sqrt{\frac{\psi-1}{\psi+1}} - \sqrt{\frac{\psi-2}{\psi}} \right] \\ &= ABS(G'') + 2\sqrt{\frac{\psi}{\psi+2}} + (\psi-4)\sqrt{\frac{\psi-1}{\psi+1}} - (\psi-3)\sqrt{\frac{\psi-2}{\psi}} \\ &\leq (n-1-\Re)\sqrt{\frac{(n-1)-\Re+1}{(n-1)-\Re+3}} + 2\sqrt{\frac{(n-1)-\Re+2}{(n-1)-\Re+4}} + (\Re-2)\sqrt{\frac{1}{2}} \\ &+ 2\sqrt{\frac{\psi}{\psi+2}} + (\psi-4)\sqrt{\frac{\psi-1}{\psi+1}} - (\psi-3)\sqrt{\frac{\psi-2}{\psi}} \\ &\leq (n-\Re-1)\sqrt{\frac{n-\Re}{n-\Re+2}} + 2\sqrt{\frac{n-\Re+1}{n-\Re+3}} + (\Re-2)\sqrt{\frac{1}{2}} \\ &+ 2\sqrt{\frac{n-\Re+2}{n-\Re+4}} + (n-\Re-2)\sqrt{\frac{n-\Re+1}{n-\Re+3}} - (n-\Re-1)\sqrt{\frac{n-\Re}{n-\Re+2}} \\ &= (n-\Re)\sqrt{\frac{n-\Re+1}{n-\Re+3}} + 2\sqrt{\frac{n-\Re+2}{n-\Re+4}} + (\Re-2)\sqrt{\frac{1}{2}} \end{split}$$

equality occurs if and only if G'' is isomorphic to  $\mathfrak{L}_{n-1,\mathfrak{R}}$ , where  $d(y) = \psi = n - \mathfrak{R} + 2$ , with exactly 2 vertices in  $\{y_1, ..., y_{\psi-1}\}$  have a degree of 2, while the remaining  $(\psi - 3)$  vertices in  $\{y_1, ..., y_{\psi-1}\}$  have a degree of 1. In other words,  $G \cong \mathfrak{L}_{n,\mathfrak{R}}$ . Therefore,  $\mathfrak{L}_{n,\mathfrak{R}}$  is the unique graph within the set  $\mathbb{U}_n$  that exhibits the maximum *ABS* index among all graphs.

To determine the second-maximum ABS index among the graphs in  $\mathbb{U}_{n,\mathfrak{R}}$ , we will need to utilize some additional lemmas.

**Transformation 2:** Let H be a connected graph that is nontrivial. Let  $xy \in E(H)$  such that  $d_H(x) = d_H(y) = 2$ . Additionally, the other neighbors of x and y have a degree of at least 2 in H. Now create a new graph  $G_2$  from H by connecting  $\mu - 2$  pendent edges to x and  $\psi - 2$  pendent edges to y (where  $\mu \ge \psi \ge 3$ ), respectively. Additionally, create another graph  $G'_2$  from H by connecting the  $\mu + \psi - 4$  pendent edges to x. (Refer to Figure 3 for a visual representation of these graphs.)



Figure 3. Illustration of Transformation 2

**Lemma 3.** Let  $G_2$  and  $G'_2$  be the graphs in Figure 3. Then  $ABS(G_2) < ABS(G'_2)$ .

*Proof.* Consider that  $N_H(x) = \{y, w\}$  where  $d_H(w) = s \ge 2$ , and  $N_H(y) = \{x, w'\}$  where  $d_H(w') = t \ge 2$ . Given that  $(\mu \ge \psi \ge 3)$ , then

$$\begin{aligned} ABS(G_2) - ABS(G'_2) \\ &= \left( (\mu - 2)\sqrt{\frac{\mu - 1}{\mu + 1}} + \sqrt{\frac{\mu + s - 2}{\mu + s}} + (\psi - 2)\sqrt{\frac{\psi - 1}{\psi + 1}} + \sqrt{\frac{\psi + t - 2}{\psi + t}} \right) \\ &- \left( (\mu - 2)\sqrt{\frac{\mu + \psi - 3}{\mu + \psi - 1}} + \sqrt{\frac{\mu + \psi + s - 4}{\mu + \psi + s - 2}} + (\psi - 2)\sqrt{\frac{\mu + \psi - 3}{\mu + \psi - 1}} + \sqrt{\frac{t}{2 + t}} \right) \\ &= (\mu - 2)\left(\sqrt{\frac{\mu - 1}{\mu + 1}} - \sqrt{\frac{\mu + \psi - 3}{\mu + \psi - 1}}\right) + \left(\sqrt{\frac{\mu + s - 2}{\mu + s}} - \sqrt{\frac{\mu + \psi + s - 4}{\mu + \psi + s - 2}}\right) \\ &+ (\psi - 2)\left(\sqrt{\frac{\psi - 1}{\psi + 1}} - \sqrt{\frac{\mu + \psi - 3}{\mu + \psi - 1}}\right) + \left(\sqrt{\frac{\psi + t - 2}{\psi + t}} - \sqrt{\frac{t}{2 + t}}\right) \\ &\leq (\psi - 2)\left(\sqrt{\frac{\psi - 1}{\psi + 1}} - \sqrt{\frac{\mu + \psi - 3}{\mu + \psi - 1}}\right) + \left(\sqrt{\frac{\psi}{\psi + 2}} - \sqrt{\frac{1}{2}}\right) \end{aligned}$$

if  $\mu = \psi = 3$ , then

$$ABS(G_2) - ABS(G'_2) = \left(\sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}}\right) + \left(\sqrt{\frac{3}{5}} - \sqrt{\frac{1}{2}}\right) = 0$$

So we can consider that  $\mu \geq 4$  and  $\psi \geq 3$ . Hence

$$ABS(G_2) - ABS(G'_2) \leq (\psi - 2) \left(\sqrt{\frac{\psi - 1}{\psi + 1}} - \sqrt{\frac{\mu + \psi - 3}{\mu + \psi - 1}}\right) + \left(\sqrt{\frac{\psi}{\psi + 2}} - \sqrt{\frac{1}{2}}\right) < 0$$

Therefore,  $ABS(G_2) - ABS(G'_2) < 0$ 



Figure 4. Illustration of Transformation 3

**Transformation 3:** Let H be a connected graph that is nontrivial. Let  $xy \in E(H)$  such that  $d_H(x) = d_H(y) = 2$ , and their remaining neighbors in H also have a degree of 2. Now create a new graph  $G_3$  from H by connecting  $\mu - 2$  pendent edges to x and  $\psi - 2$  pendent edges to y, where  $(\mu \ge \psi \ge 3)$ , respectively. Additionally, create another graph  $G'_3$  from H by connecting  $\mu - 1$  and  $\psi - 3$  pendent edges to x and y, respectively. (Refer to Figure 4 for a visual representation of these graphs.)

**Lemma 4.** Let  $G_3$  and  $G'_3$  be the graphs in Figure 4. Then  $ABS(G_3) < ABS(G'_3)$ .

*Proof.* Using Lemma 1 (iii), for  $p \ge 3$  the function h(p) is increasing function. Given that  $\mu \ge \psi \ge 3$ , then

$$\begin{aligned} ABS(G_3) - ABS(G'_3) \\ &= \left( (\mu - 2)\sqrt{\frac{\mu - 1}{\mu + 1}} + \sqrt{\frac{\mu}{\mu + 2}} + (\psi - 2)\sqrt{\frac{\psi - 1}{\psi + 1}} + \sqrt{\frac{\psi}{\psi + 2}} \right) \\ &- \left( (\mu - 1)\sqrt{\frac{\mu}{\mu + 2}} + \sqrt{\frac{\mu + 1}{\mu + 3}} + (\psi - 3)\sqrt{\frac{\psi - 2}{\psi}} + \sqrt{\frac{\psi - 1}{\psi + 1}} \right) \\ &= \left( \sqrt{\frac{\psi}{\psi + 2}} + (\psi - 3)\sqrt{\frac{\psi - 1}{\psi + 1}} - (\psi - 3)\sqrt{\frac{\psi - 2}{\psi}} \right) \\ &- \left( \sqrt{\frac{\mu + 1}{\mu + 3}} + (\mu - 2)\sqrt{\frac{\mu}{\mu + 2}} - (\mu - 2)\sqrt{\frac{\mu - 1}{\mu + 1}} \right) \\ &= h(\psi) - h(\mu + 1) < 0 \end{aligned}$$

Therefore  $ABS(G_3) - ABS(G'_3) < 0.$ 



Figure 5. Illustration of Transformation 4

**Transformation 4:** Let H be a connected graph that is nontrivial. Let two distinct vertices x and y have a degree of 2 and such that  $xy \notin E(H)$ . Additionally, the remaining neighbors of x and y in H also have a degree of 2. Now create a new graph  $G_4$  from H by connecting  $\mu - 2$  pendent edges to x and  $\psi - 2$  pendent edges to y where ( $\mu \ge \psi \ge 3$ ), respectively. Additionally, create another graph  $G'_4$  from H by connecting  $\mu - 1$  and  $\psi - 3$ pendent edges to x and y. (Refer to Figure 5 for a visual representation of these graphs.)

**Lemma 5.** Let  $G_4$  and  $G'_4$  be the graphs in Figure 5. Then  $ABS(G_4) < ABS(G'_4)$ .

*Proof.* Using Lemma 1 (ii), for  $p \ge 3$  the function g(p) is increasing. Since  $\mu \ge \psi \ge 3$ , then

$$\begin{aligned} ABS(G_4) - ABS(G'_4) \\ &= \left( (\mu - 2)\sqrt{\frac{\mu - 1}{\mu + 1}} + 2\sqrt{\frac{\mu}{\mu + 2}} + (\psi - 2)\sqrt{\frac{\psi - 1}{\psi + 1}} + 2\sqrt{\frac{\psi}{\psi + 2}} \right) \\ &- \left( (\mu - 1)\sqrt{\frac{\mu}{\mu + 2}} + 2\sqrt{\frac{\mu + 1}{\mu + 3}} + (\psi - 3)\sqrt{\frac{\psi - 2}{\psi}} + 2\sqrt{\frac{\psi - 1}{\psi + 1}} \right) \\ &= \left( 2\sqrt{\frac{\psi}{\psi + 2}} + (\psi - 4)\sqrt{\frac{\psi - 1}{\psi + 1}} - (\psi - 3)\sqrt{\frac{\psi - 2}{\psi}} \right) \\ &- \left( 2\sqrt{\frac{\mu + 1}{\mu + 3}} + (\mu - 3)\sqrt{\frac{\mu}{\mu + 2}} - (\mu - 2)\sqrt{\frac{\mu - 1}{\mu + 1}} \right) \\ &= g(\psi) - g(\mu + 1) < 0 \end{aligned}$$

Therefore  $ABS(G_4) - ABS(G_4') < 0.$ 



Figure 6. The graph sets  $\mathfrak{L}^1_{n,\mathfrak{R}}$  and  $\mathfrak{L}^2_{n,\mathfrak{R}}$   $(3 \leq \mathfrak{R} \leq n-2)$ 

We consider two sets of unicyclic graphs comprising n vertices for  $3 \leq \mathcal{R} \leq n-2$ . The first set denoted by  $\mathfrak{L}^{1}_{n,\mathcal{R}}$  consists of graphs created by attaching  $\mu$  and  $\psi$  pendent edges ( $\mu \geq \psi \geq 1$  and  $\mu + \psi = n - \mathcal{R}$ ) to two distinct vertices x and y of the cycle  $C_{\mathcal{R}}$ , respectively. The second set of unicyclic graphs comprising n vertices denoted by  $\mathfrak{L}^{2}_{n,\mathcal{R}}$  created by connecting  $\psi$  pendent edges  $(1 \leq \psi \leq n - \mathcal{R} - 1)$  to a pendent vertex y of  $\mathfrak{L}_{n-\psi,\mathcal{R}}$  (as shown in Figure 6 for visual representation).

**Lemma 6.** Let  $G \in \mathfrak{L}^{1}_{n,\mathcal{R}}$ (i) If  $\mathfrak{R} = 3$ , then

$$ABS(G) \le (n-4)\sqrt{\frac{n-3}{n-1}} + \sqrt{\frac{n-1}{n+1}} + \sqrt{\frac{n-2}{n}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{3}{5}}$$

maintains equality holds if and only if  $\psi = 1$ . (ii) If  $4 \leq \Re \leq n - 2$ , then

$$ABS(G) \le (n - \mathcal{R} - 1)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + 2\sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + (\mathcal{R} - 3)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{3}{5}}$$

maintains equality holds if and only if  $xy \notin E(G)$  and  $\psi = 1$ .

*Proof.* Assuming  $\mathcal{R} = 3$ , it follows that  $xy \in E(G)$ . we can apply Lemma 4 to draw the following conclusion:

$$ABS(G) \le (n-4)\sqrt{\frac{n-3}{n-1}} + \sqrt{\frac{n-1}{n+1}} + \sqrt{\frac{n-2}{n}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{3}{5}}$$

maintains equality if and only if  $\mu = n - 4$  and  $\psi = 1$ . Hence proved (i).

Assume for the moment that  $4 \leq \Re \leq n-2$ . If  $xy \in E(G)$ , then by Lemma 4, we derive the following conclusion:

$$ABS(G) \le (n - \mathcal{R} - 1)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + \sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + \sqrt{\frac{n - \mathcal{R} + 2}{n - \mathcal{R} + 4}} + (\mathcal{R} - 2)\sqrt{\frac{1}{2}} + \sqrt{\frac{3}{5}}$$

maintains equality if and only if  $\mu = n - \Re - 1$  and  $\psi = 1$  both hold true.

If  $xy \notin E(G)$ , then we can apply Lemma 5 to derive the following conclusion:

$$ABS(G) \le (n - \mathcal{R} - 1)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + 2\sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + (\mathcal{R} - 3)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{3}{5}}$$

maintains equality if and only if  $\mu = n - \mathcal{R} - 1$  and  $\psi = 1$  both hold true.

Since

$$\begin{split} & \left( (n - \mathcal{R} - 1)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + \sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + \sqrt{\frac{n - \mathcal{R} + 2}{n - \mathcal{R} + 4}} + (\mathcal{R} - 2)\sqrt{\frac{1}{2}} + \sqrt{\frac{3}{5}} \right) \\ & - \left( (n - \mathcal{R} - 1)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + 2\sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + (\mathcal{R} - 3)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{3}{5}} \right) \\ & = \sqrt{\frac{n - \mathcal{R} + 2}{n - \mathcal{R} + 4}} - \sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} \\ & \leq \sqrt{\frac{4}{6}} - \sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} < 0 \end{split}$$

therefore (ii) holds.

**Lemma 7.** Consider  $G \in \mathfrak{L}^2_{n,\mathfrak{R}}$ . Then

$$ABS(G) \le (n - \Re - 2)\sqrt{\frac{n - \Re}{n - \Re + 2}} + 3\sqrt{\frac{n - \Re + 1}{n - \Re + 3}} + (\Re - 2)\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}}.$$

maintains equality holds if and only if  $\psi = 1$ .

*Proof.* Since there is only one graph in  $\mathfrak{L}^{2}_{n,\mathfrak{R}}$ , the statement of the lemma is trivially true for the case  $n - \mathfrak{R} = 2$ . Therefore, we proceed by assuming that  $n - \mathfrak{R} \geq 3$ . Let

$$\begin{split} f(\psi) &= ABS(G) = \sqrt{\frac{n-\Re+1}{n-\Re+3}} + 2\sqrt{\frac{n-\Re+2-\psi}{n-\Re+4-\psi}} + (\Re-2)\sqrt{\frac{1}{2}} \\ &+ (n-\Re-1-\psi)\sqrt{\frac{n-\Re+1-\psi}{n-\Re+3-\psi}} + \psi\sqrt{\frac{\psi}{\psi+2}} \end{split}$$

where  $1 \le \psi \le n - \mathcal{R} - 1$ . Hence

$$f'(\psi) = -\sqrt{\frac{n - \mathcal{R} + 1 - \psi}{n - \mathcal{R} + 3 - \psi}} - 2\sqrt{\frac{1}{(n - \mathcal{R} + 2 - \psi)(n - \mathcal{R} + 4 - \psi)^3}} - (n - \mathcal{R} - 1 - \psi)\sqrt{\frac{1}{(n - \mathcal{R} + 1 - \psi)(n - \mathcal{R} + 3 - \psi)^3}} + \sqrt{\frac{\psi}{\psi + 2}} + \sqrt{\frac{\psi}{(\psi + 2)^3}}$$

If  $1 \le \psi \le \left\lfloor \frac{n - \Re}{2} \right\rfloor$  (i.e.,  $\psi + 2 \le n - \Re + 2 - \psi$ ), then by Lemma 1 (iv)

(with  $p = n - \mathcal{R} + 2 - \psi \ge 3$ ), leading to:

$$\begin{aligned} f'(\psi) &= -\sqrt{\frac{n-\Re+1-\psi}{n-\Re+3-\psi}} - 2\sqrt{\frac{1}{(n-\Re+2-\psi)(n-\Re+4-\psi)^3}} \\ &- (n-\Re-1-\psi)\sqrt{\frac{1}{(n-\Re+1-\psi)(n-\Re+3-\psi)^3}} + \left(\frac{\psi+3}{\psi+2}\right)\sqrt{\frac{\psi}{\psi+2}} \\ &+ \left(\frac{n-\Re+3-\psi}{n-\Re+2-\psi}\right)\sqrt{\frac{n-\Re-\psi}{n-\Re+2-\psi}} - \left(\frac{n-\Re+3-\psi}{n-\Re+2-\psi}\right)\sqrt{\frac{n-\Re-\psi}{n-\Re+2-\psi}} \end{aligned}$$

$$\leq -\sqrt{\frac{n - \Re + 1 - \psi}{n - \Re + 3 - \psi}} - 2\sqrt{\frac{1}{(n - \Re + 2 - \psi)(n - \Re + 4 - \psi)^3}} \\ - (n - \Re - 1 - \psi)\sqrt{\frac{1}{(n - \Re + 1 - \psi)(n - \Re + 3 - \psi)^3}} \\ + \left(\frac{n - \Re + 3 - \psi}{n - \Re + 2 - \psi}\right)\sqrt{\frac{n - \Re - \psi}{n - \Re + 2 - \psi}} \\ = -\sqrt{\frac{p - 1}{p + 1}} - 2\sqrt{\frac{1}{p(p + 2)^3}} - (p - 3)\sqrt{\frac{1}{(p - 1)(p + 1)^3}} + \left(\frac{p + 1}{p}\right)\sqrt{\frac{p - 2}{p}} < 0.$$

$$\begin{split} & \text{If} \left\lfloor \frac{n-\mathcal{R}+1}{2} \right\rfloor \leq \psi \leq n-\mathcal{R}-1 \text{ (i.e., } \psi+2 \geq n-\mathcal{R}+3-\psi \text{ ), then} \\ & \text{by Lemma 1 (v) (with } p=n-\mathcal{R}+3-\psi \text{), leading to:} \end{split}$$

$$\begin{split} f'(\psi) &= -\sqrt{\frac{\psi}{\psi+2}} - 2\sqrt{\frac{1}{(n-\mathcal{R}+2-\psi)(n-\mathcal{R}+4-\psi)^3}} \\ &- (n-\mathcal{R}-1-\psi)\sqrt{\frac{1}{(n-\mathcal{R}+1-\psi)(n-\mathcal{R}+3-\psi)^3}} + \sqrt{\frac{\psi}{\psi+2}} + \sqrt{\frac{\psi}{(\psi+2)^3}} \\ &\geq -2\sqrt{\frac{1}{(p-1)(p+1)^3}} - (p-4)\sqrt{\frac{1}{(p-2)p^3}} + \sqrt{\frac{p-2}{p^3}} > 0. \end{split}$$

This suggests that for  $1 \leq \psi \leq \left\lfloor \frac{n-\Re}{2} \right\rfloor$ ,  $f(\psi)$  is increasing and for  $\left\lfloor \frac{n-\Re+1}{2} \right\rfloor \leq \psi \leq n-\Re-1$ ,  $f(\psi)$  is decreasing. Therefore the maximum

value of  $f(\psi)$  is  $max \{f(1), f(n - \mathcal{R} - 1)\}$ . Since  $n - \mathcal{R} \ge 3$ , we have

$$\begin{split} f(n-\Re-1) &- f(1) \\ &= \left( (n-\Re-1)\sqrt{\frac{n-\Re-1}{n-\Re+1}} + \sqrt{\frac{n-\Re+1}{n-\Re+3}} + (\Re-2)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{3}{5}} \right) \\ &- \left( (n-\Re-2)\sqrt{\frac{n-\Re}{n-\Re+2}} + \sqrt{\frac{n-\Re+1}{n-\Re+3}} + 2\sqrt{\frac{n-\Re+1}{n-\Re+3}} + (\Re-2)\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}} \right) \\ &= (n-\Re-1)\sqrt{\frac{n-\Re-1}{n-\Re-1+2}} - 2\sqrt{\frac{n-\Re+1}{n-\Re+3}} - (n-\Re-2)\sqrt{\frac{n-\Re}{n-\Re+2}} + 2\sqrt{\frac{3}{5}} - \sqrt{\frac{1}{3}} \\ &\leq (3-1)\sqrt{\frac{3-1}{3+1}} - 2\sqrt{\frac{3+1}{3+3}} - (3-2)\sqrt{\frac{3}{3+2}} + 2\sqrt{\frac{3}{5}} - \sqrt{\frac{1}{3}} < 0. \end{split}$$

As a result, the conclusion of Lemma 7 is valid.

The collection of unicyclic graph comprising n vertices denoted by  $\mathfrak{L}_{n,3}^*$ created by connecting n-4 and one pendent edge to 2 adjacent vertices x and y of a triangle. For  $4 \leq \mathfrak{R} \leq n-2$ , the collection of unicyclic graph comprising n vertices denoted by  $\mathfrak{L}_{n,\mathfrak{R}}^*$  created by connecting  $n-\mathfrak{R}-1$ and one pendent edge to 2 non-adjacent vertices x and y of the cycle  $C_{\mathfrak{R}}$ (as shown in figure 2 for visual representation). It is important to note that  $\mathfrak{L}_{n,\mathfrak{R}}^* \subseteq \mathfrak{L}_{n,\mathfrak{R}}^1$  and there are  $\left\lfloor \frac{\mathfrak{R}}{2} \right\rfloor - 1$  unicyclic graphs in  $\mathfrak{L}_{n,\mathfrak{R}}^*$  for each  $4 \leq \mathfrak{R} \leq n-2$ . We can now determine the second-maximum *ABS* index among all graphs in  $\mathbb{U}_{n,\mathfrak{R}}$ .

**Theorem 2.** Let  $G \in \mathbb{U}_{n,\mathcal{R}}$  and  $G \ncong \mathfrak{L}_{n,\mathcal{R}}$ . (i) If  $\mathcal{R} = 3$ , then

$$ABS(G) \le (n-4)\sqrt{\frac{n-3}{n-1}} + \sqrt{\frac{n-1}{n+1}} + \sqrt{\frac{n-2}{n}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{3}{5}}$$

maintains equality if and only if  $G \cong \mathfrak{L}_{n,3}^*$ . (ii)If  $4 \leq \mathfrak{R} \leq n-2$ , then

$$ABS(G) \le (n - \mathcal{R} - 1)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + 2\sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + (\mathcal{R} - 3)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{3}{5}}$$

maintains equality if and only if  $G \cong \mathfrak{L}^*_{n,\mathcal{R}}$ .

*Proof.* Suppose G is a graph with a unique cycle C, where  $C := y_1 y_2 \dots y_{\mathcal{R}} y_1$ .

Then there exists at least one vertex among  $\{y_1, y_2, ..., y_R\}$  have a degree of at least 3. For the sake of the proof, let

$$P := (n-4)\sqrt{\frac{n-3}{n-1}} + \sqrt{\frac{n-1}{n+1}} + \sqrt{\frac{n-2}{n}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{3}{5}},$$

for  $\mathcal{R} = 3$ , or

$$P := (n - \mathcal{R} - 1)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + 2\sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + (\mathcal{R} - 3)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{3}{5}}$$

for  $4 \leq \Re \leq n-2$ . Similarly,

$$Q := (n - \mathcal{R} - 2)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + 3\sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + (\mathcal{R} - 2)\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}}.$$

If G has at least 3 vertices among  $\{y_1, y_2, ..., y_{\mathcal{R}}\}$  have a degree of at least 3. Then by using Lemmas 2, 3, (or 5), and 6, a graph  $G_1 \in \mathfrak{L}^1_{n,\mathcal{R}}$  can be found such that  $ABS(G) < ABS(G_1) \leq P$ .

If G has exactly 2 vertices among  $\{y_1, y_2, ..., y_{\mathcal{R}}\}$  have a degree of at least 3. Then by using Lemmas 2, 4, (or 5) and 6, a graph  $G_2 \in \mathfrak{L}^1_{n,\mathcal{R}}$  can be found such that  $ABS(G) < ABS(G_2) \leq P$  maintains equality if and only if  $G \in \mathfrak{L}^*_{n,\mathcal{R}}$ .

Hence, it can be assumed that there is exactly one vertex among  $\{y_1, y_2, ..., y_{\mathcal{R}}\}$  have a degree of at least 3. As  $G \ncong \mathfrak{L}_{n,\mathcal{R}}$ , there must be at least one non-pendent vertex that is located outside C. If, according to Lemma 2 and 7, there exists at least two non-pendent vertex that is located outside C, then allows to finding a graph  $G_3 \cong \mathfrak{L}^2_{n,\mathcal{R}}$  such that  $ABS(G) < ABS(G_3) \leq Q$ . Assuming there is only one non-pendent vertex outside of C, implying that  $G \cong \mathfrak{L}^2_{n,\mathcal{R}}$ . By using Lemma 7, we can deduce that  $ABS(G) \leq Q$ , with equality holding if and only if  $\psi = 1$ .

Comparing the values of P and Q is essential for proving the theorem.

If  $\mathcal{R} = 3$ , then

$$\begin{aligned} Q - P &= \left( (n-5)\sqrt{\frac{n-3}{n-1}} + 3\sqrt{\frac{n-2}{n}} + (1)\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}} \right) \\ &- \left( (n-4)\sqrt{\frac{n-3}{n-1}} + \sqrt{\frac{n-2}{n}} + \sqrt{\frac{n-1}{n+1}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{3}{5}} \right) \\ &= -\sqrt{\frac{n-3}{n-1}} + 2\sqrt{\frac{n-2}{n}} + \sqrt{\frac{1}{3}} - \sqrt{\frac{n-1}{n+1}} - \sqrt{\frac{3}{5}} \\ &\leq -\sqrt{\frac{2}{3}} + 2\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} < 0. \end{aligned}$$

So (i) holds. If  $4 \leq \Re \leq n-2$ , then

$$\begin{aligned} Q - P &= \left( (n - \mathcal{R} - 2)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + 3\sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + (\mathcal{R} - 2)\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}} \right) \\ &- \left( (n - \mathcal{R} - 1)\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + 2\sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + (\mathcal{R} - 3)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{3}{5}} \right) \\ &= -\sqrt{\frac{n - \mathcal{R}}{n - \mathcal{R} + 2}} + \sqrt{\frac{n - \mathcal{R} + 1}{n - \mathcal{R} + 3}} + \sqrt{\frac{1}{3}} + \sqrt{\frac{1}{2}} + -2\sqrt{\frac{3}{5}} \\ &\leq -\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{3}{5}} + \sqrt{\frac{1}{3}} - 2\sqrt{\frac{3}{5}} < 0. \end{aligned}$$

This suggests (ii), and as a result, the proof confirming the theorem has been explored.

The following corollary can be drawn by using Theorem 1 and Theorem 2 respectively.

**Corollary 1.** Let  $\mathfrak{L}_{n,\mathfrak{R}}$ , and  $\mathfrak{L}^*_{n,\mathfrak{R}}$  be the graphs defined as above. (i) If n = 5, then

$$ABS(\mathfrak{L}_{5,3}) > ABS(\mathfrak{L}_{5,3}^*) > ABS(u_{5,4}) > ABS(u_{5,3}) > ABS(C_5)$$

(ii) If  $n \ge 6$ , then

$$\begin{split} ABS(\mathfrak{L}_{n,3}) > &ABS(\mathfrak{L}_{n,3}^*) > ABS(\mathfrak{L}_{n,4}) > ABS(\mathfrak{L}_{n,4}^*) > \dots > ABS(\mathfrak{L}_{n,n-2}) \\ > &ABS(\mathfrak{L}_{n,n-2}^*) > ABS(u_{n,n-1}) > ABS(C_n) \end{split}$$

*Proof.* Since

$$ABS(\mathfrak{L}_{5,3}) = 3.8893 > ABS(\mathfrak{L}_{5,3}^*) = 3.7799 > ABS(u_{5,4}) > ABS(u_{5,3})$$
$$> ABS(C_5)$$

This verifies that (i) valid.

Now we prove (ii). We utilize Theorem 1 and Theorem 2, to establish that  $ABS(\mathfrak{L}_{n,\mathfrak{R}}) > ABS(\mathfrak{L}_{n,\mathfrak{R}}^*)$  for each  $3 \leq \mathfrak{R} \leq n-2$ . Since

$$ABS(\mathfrak{L}_{n,n-2}^*) = (\Re - 2)\sqrt{\frac{1}{2}} + 4\sqrt{\frac{3}{5}}$$
$$ABS(U_{n,n-1}) = (n - \Re + 3)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{3}{5}}$$

and  $ABS(C_n)=n\sqrt{\frac{1}{2}}$  We can see that,  $ABS(\mathfrak{L}^*_{n,n-2})>ABS(u^*_{n,n-1})>ABS(C_n)$ 

To establish (ii), we need to prove that  $ABS(\mathfrak{L}_{n,\mathcal{R}}^*) > ABS(\mathfrak{L}_{n,\mathcal{R}+1})$  for each value of  $\mathcal{R}$ , where  $3 \leq \mathcal{R} \leq n-3$ . If  $\mathcal{R} = 3$ , then utilize Theorem 2(i)

$$\begin{split} ABS(\mathfrak{L}_{n,3}^*) - ABS(\mathfrak{L}_{n,4}) \\ &= \left( (n-4)\sqrt{\frac{n-3}{n-1}} + \sqrt{\frac{n-1}{n+1}} + \sqrt{\frac{n-2}{n}} + \sqrt{\frac{2}{4}} + \sqrt{\frac{3}{5}} \right) \\ &- \left( (n-4)\sqrt{\frac{n-3}{n-1}} + 2\sqrt{\frac{n-2}{n}} + 2\sqrt{\frac{1}{2}} \right) \\ &= \sqrt{\frac{n-1}{n+1}} - \sqrt{\frac{n-2}{n}} + \sqrt{\frac{3}{5}} - \sqrt{\frac{1}{2}} > 0 \end{split}$$

Therefore,  $ABS(\mathfrak{L}_{n,3}^*) > ABS(\mathfrak{L}_{n,4})$ . For each  $4 \leq \mathfrak{R} \leq n-3$  (and hence

 $n \geq 7$ ), we have

$$\begin{split} ABS(\mathfrak{L}_{n,\mathfrak{R}}^*) &- ABS(\mathfrak{L}_{n,\mathfrak{R}+1}) \\ &= \left( (n-\mathfrak{R}-1)\sqrt{\frac{n-\mathfrak{R}}{n-\mathfrak{R}+2}} + 2\sqrt{\frac{n-\mathfrak{R}+1}{n-\mathfrak{R}+3}} + (\mathfrak{R}-3)\sqrt{\frac{2}{4}} + 2\sqrt{\frac{3}{5}} \right) \\ &- \left( (n-\mathfrak{R}+1)\sqrt{\frac{n-\mathfrak{R}+2}{n-\mathfrak{R}+4}} + 2\sqrt{\frac{n-\mathfrak{R}+3}{n-\mathfrak{R}+5}} + (\mathfrak{R}-1)\sqrt{\frac{1}{2}} \right) \\ &> 0 \end{split}$$

So the assertion of the corollary holds.

Hence, the only graph in  $\mathbb{U}_n$  with the maximum ABS index is the  $\mathfrak{L}_{n,3}$  graph. The only graph in  $\mathbb{U}_n$  with the second-maximum ABS is  $\mathfrak{L}_{n,3}^*$  graph; this is demonstrated by Theorem 1, 2 and Corollary 1.

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## References

- K. Aarthi, S. Elumalai, S. Balachandran, S. Mondal, Extremal values of the atom-bond sum-connectivity index in bicyclic graphs, *J. Appl. Math. Comput.* 69 (2023) 4269–4285.
- [2] A. M. Albalahi, E. Milovanović, A. Ali, General atom-bond sumconnectivity index of graphs, *Mathematics* 11 (2023) 1–15.
- [3] A. M. Albalahi, Z. Du, A. Ali, On the general atom-bond sumconnectivity index, AIMS Math. 8 (2023) 23771–23785.
- [4] A. Ali, K. C. Das, D. Dimitrov, B. Furtula, Atom-bond connectivity index of graphs: a review over extremal results and bounds, *Discr. Math. Lett.* 5 (2021) 68–93.
- [5] A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sumconnectivity index, J. Math. Chem. 60 (2022) 2081–2093.

- [6] A. Ali, I. Gutman, I. Redžepović, Atom-bond sum-connectivity index of unicyclic graphs and some applications, *El. J. Math.* 5 (2023) 1–7.
- [7] A. Ali, I. Gutman, I. Redžepović, J. P. Mazorodze, A. M. Albalahi, A. E. Hamza, On the difference of atom-bond sum-connectivity and atom-bond-connectivity indices, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 725–740.
- [8] A. Ali, I. Z. Milovanović, E. Milovanović, M. Matejić, Sharp inequalities for the atom-bond (sum) connectivity index, J. Math. Ineq. 17 (2023) 1411–1426.
- [9] T. A. Alraqad, I.Z. Milovanović, H. Saber, A. Ali, J. P. Mazorodze, A. A. Attiya, Minimum atom-bond sum-connectivity index of trees with a fixed order and/or number of pendent vertices, *AIMS Math.* 9 (2024) 3707–3721.
- [10] T. A. Alraqad, H. Saber, A. Ali, A. M. Albalahi, On the maximum atom-bond sum-connectivity index of graphs, *Open Math.* 22 (2024) #20230179.
- [11] S. C. Basak, A. Bhattacharjee, Computational approaches for the design of mosquito repellent chemicals, *Curr. Med. Chem.* 27 (2020) 32–41.
- [12] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London, 2008.
- [13] B. Furtula, I. Gutman, M. Dehmer, On structure-sensitivity of degree based topological indices, *Appl. Math. Comput.* **219** (2013) 8973– 8978.
- [14] Y. Ge, Z. Lin, J. Wang, Atom-bond sum-connectivity index of line graphs, *Discr. Math. Lett.* **12** (2023) 196–200.
- [15] K. J. Gowtham, I. Gutman, On the difference between atom-bond sum-connectivity and sum-connectivity indices, Bull. Cl. Sci. Math. Nat. Sci. Math. 47 (2022) 55–65.
- [16] I. Gutman, Degree based topological indices, Croat. Chem. Acta 86 (2013) 351–361.
- [17] D. M. Hawkins, S. C. Basak, X. Shi, QSAR with few compounds and many features J. Chem. Inf. Comput. Sci. 41 (2001) 663–670.
- [18] Y. Hu, F. Wang, On the maximum atom-bond sum-connectivity index of trees, MATCH Commun. Math. Comput. Chem. 91 (2024) 709–723.

- [19] Z. Hussain, H. Liu, H. Hua, Bounds for the atom-bond sumconnectivity index of graphs, MATCH Commun. Math. Comput. Chem., accepted.
- [20] F. Li, Q. Ye, H. Lu, The greatest values for atom-bond sumconnectivity index of graphs with given parameters, *Discr. Appl. Math.* 344 (2024) 188–196.
- [21] G. Liu, Y. Zhu, J. Cai, On the Randic index of unicyclic graphs with girth g, MATCH Commun. Math. Comput. Chem. 58 (2007) 127–138.
- [22] V. Maitreyi, S. Elumalai, S. Balachandran, The minimum ABS index of trees with given number of pendent vertices, arXiv: 2211.05177v1[math.CO] (2022).
- [23] P. Nithya, S. Elumalai, S. Balachandran, Minimum atom-bond sumconnectivity index of unicyclic graphs with maximum degree, *Discr. Math. Lett.* 13 (2024) 82–88.
- [24] P. Nithya, S. Elumalai, S. Balachandran, S. Mondal, Smallest ABS index of unicyclic graphs with given girth, J. Appl. Math. Comput. 69 (2023) 3675–3692.
- [25] S. Noureen, A. Ali, Maximum atom-bond sum-connectivity index of *n*-order trees with fixed number of leaves, *Discr. Math. Lett.* **12** (2023) 26–28.
- [26] M. Randić, Characterization of molecular branching, J. Am. Chem. Soc. 97 (1975) 6609–6615.
- [27] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.
- [28] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
- [29] S. Wagner, H. Wang, Introduction to Chemical Graph Theory, CRC Press, Boca Raton, 2018.
- [30] Y. Zhang, H. Wang, G. Su, K. C. Das, Extremal problems on the atom-bond sum-connectivity indices of trees with given matching number or domination number, *Discr. Appl. Math.* 345 (2024) 190– 206.
- [31] B. Zhou, N. Trinajstić, On a novel connectivity index, J. Math. Chem. 46 (2009) 1252–1270.