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*Research Article*

# On the ordering of the Randić index of unicyclic and bicyclic graphs

**Venkatesan Maitreyi[1], Suresh Elumalai[1,*] and Selvaraj Balachandran[2]**

[1]Department of Mathematics, College of Engineering and Technology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpet 603 203, India
mv3171@srmist.edu.in
*sureshkako@gmail.com

[2]Department of Mathematics, School of Arts, Sciences and Humanities, SASTRA Deemed University, Thanjavur, India
bala_maths@rediffmail.com

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**Abstract:** Let $d_x$ be the degree of the vertex $x$ in a graph $G$. The Randić index of $G$ is defined by $R(G) = \sum_{xy \in E(G)} (d_x d_y)^{-\frac{1}{2}}$. Recently, *Hasni et al.* [Unicyclic graphs with maximum Randić indices, Communication in Combinatorics and Optimization, 1 (2023), 161–172] obtained the ninth to thirteenth maximum Randić indices among the unicyclic graphs with $n$ vertices. In this paper, we correct the ordering of Randić index of unicyclic graphs. In addition, we present the ordering of maximum Randić index among bicyclic graphs of order $n$.

**Keywords:** Unicyclic graphs, Bicyclic graphs, Randić index

**AMS Subject classification:** 05C50, 05C92

## 1. Introduction

In mathematical chemistry, molecular descriptors are significant, in particular when analyzing the relationships between quantitative structure-activity and quantitative structure-property. The so-called topological indices [7] are given special consideration among them. The Randić index often called the connectivity index, is a widely studied degree-based topological index [11, 18, 19]. Milan Randić [18] initially developed it in 1976, and it is given as

* *Corresponding Author*

$$R(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{d_x d_y}}$$

The Randić index is the most often used index in chemistry and pharmacology, among the hundreds of currently used graph-based chemical structure descriptors [20, 21]. Information about these applications can be found in the books [7, 12, 14].
The graph invariant $R(G)$ features a number of interesting and challenging mathematical characteristics, which took nearly two decades to discover by mathematicians [3, 4]. As a result, there was a significantly large amount of mathematical research in this field, and numerous research articles were published. For more information, refer [1, 2, 6, 9, 16, 17].

For a simple connected graph $G = (V(G), E(G))$ with $n$ vertices and $n + c$ edges where $c = -1, 0, 1$ is called a tree, unicyclic and bicyclic respectively. In [5, 8], the trees with the maximal Randić indices, and in [4, 8, 23], the trees with minimal Randić indices are identified. In [8, 13], the maximum Randić indices of unicyclic graphs have been found. The lower bound for the unicyclic and bicyclic graphs have been obtained in [10, 22] respectively. In this article, we first present the correct ordering of Randić index of unicyclic graphs. We then provide the seventh to sixteenth maximum Randić index for bicyclic graphs.

## 2. Preliminaries

The vertex with degree one is called as a pendent vertex and the incident edge corresponding to it, is called as a pendent edge. Let $\Delta$ denote the maximum degree in a graph. A $r$-vertex path $P := u_1u_2...u_r$ in $G$ with $d_{u_1} \geq 3, d_{u_i} = 2$ for $i = 2, \dots, r-1$ and $d_{u_r} = 1$ is said to be a pendent path at $u_1$. An edge of $G$ with vertex degree $r$ and $s$ will be called an $(r, s)$-edge and $\mathcal{E}_{r,s}$ denotes the number of $(r, s)$-edges in $G$. Let $\mathcal{U}_n, \mathcal{B}_n$ denotes the collection of all connected unicyclic and bicyclic graphs of order $n$, respectively.
In [5], Caprossi et al. presented an alternate definition for $R(G)$ as follows,

$$R(G) = \frac{n}{2} - \frac{1}{2} f(G) \tag{1}$$

where

$$f(G) = \sum_{xy \in E(G)} \left( \frac{1}{\sqrt{d_x}} - \frac{1}{\sqrt{d_y}} \right)^2 .$$

$R(G)$ is decreasing on $f(G)$ for a fixed $n$. This fact will be used to identify the extremal graphs with the largest Randić indices.
Among all the unicyclic graphs, Caprossi et al. [5] identified the maximum and second maximum Randić indices (see table 1). Du and Zhou [8] obtained third, fourth and the fifth maximum Randić indices (see table 2). Li et al. [15] further extended the works and provided sixth, seventh and the eighth maximum Randić indices (see table

3). Very recently, Hasni et al. [13], classified the ninth to thirteenth maximum Randić index. (See table 4)

Table 1. Unicyclic graphs with first and second maximum Randić index (see Theorem 1,4 in [5])

| Notation | vertices | $\mathcal{E}_{1,2}$ | $\mathcal{E}_{1,3}$ | $\mathcal{E}_{2,3}$ | $\mathcal{E}_{2,4}$ | $\mathcal{E}_{3,3}$ | $\mathcal{E}_{2,2}$ | $R(G)$ |
|---|---|---|---|---|---|---|---|---|
| $U_1$ | $n \geq 3$ | 0 | 0 | 0 | 0 | 0 | $n$ | $\frac{n}{2}$ |
| $U_2$ | $n \geq 5$ | 1 | 0 | 3 | 0 | 0 | $n-4$ | $\frac{n-4}{2}+\frac{3}{\sqrt{6}}+\frac{1}{\sqrt{2}}$ |

Table 2. Unicyclic graphs with third to fifth maximum Randić index (see Proposition 2.2 in [8])

| Notation | vertices | $\mathcal{E}_{1,2}$ | $\mathcal{E}_{1,3}$ | $\mathcal{E}_{2,3}$ | $\mathcal{E}_{2,4}$ | $\mathcal{E}_{3,3}$ | $\mathcal{E}_{2,2}$ | $R(G)$ |
|---|---|---|---|---|---|---|---|---|
| $U_3$ | $n \geq 5$ | 0 | 1 | 2 | 0 | 0 | $n-3$ | $\frac{n-3}{2}+\frac{2}{\sqrt{6}}+\frac{1}{\sqrt{3}}$ |
| $U_4$ | $n \geq 7$ | 2 | 0 | 4 | 0 | 1 | $n-7$ | $\frac{n-7}{2}+\frac{4}{\sqrt{6}}+\sqrt{2}+\frac{1}{3}$ |
| $U_5$ | $n \geq 8$ | 2 | 0 | 6 | 0 | 0 | $n-8$ | $\frac{n-8}{2}+\sqrt{6}+\sqrt{2}$ |

Table 3. Unicyclic graphs with sixth to eighth maximum Randić index (see Theorem 2.2 in [15])

| Notation | vertices | $\mathcal{E}_{1,2}$ | $\mathcal{E}_{1,3}$ | $\mathcal{E}_{2,3}$ | $\mathcal{E}_{2,4}$ | $\mathcal{E}_{3,3}$ | $\mathcal{E}_{2,2}$ | $R(G)$ |
|---|---|---|---|---|---|---|---|---|
| $U_6$ | $n \geq 9$ | 3 | 0 | 3 | 0 | 3 | $n-9$ | $\frac{n-7}{2}+\frac{3}{\sqrt{2}}+\frac{3}{\sqrt{6}}$ |
| $U_7$ | $n \geq 9$ | 1 | 1 | 3 | 0 | 1 | $n-6$ | $\frac{n-4}{2}+\frac{1}{\sqrt{2}}+\frac{3}{\sqrt{6}}+\frac{1}{\sqrt{3}}-\frac{2}{3}$ |
| $U_8$ | $n \geq 10$ | 3 | 0 | 5 | 0 | 2 | $n-10$ | $\frac{n-8}{2}+\frac{3}{\sqrt{2}}+\frac{5}{\sqrt{6}}-\frac{1}{3}$ |

## 3. Main Results

In Theorem 1 of [13] i.e., In Table 4, the following value has been proved as the ninth maximum Randić index.

$$R(G) = \frac{n-7}{2} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{5}{\sqrt{6}} \approx \frac{n}{2} - 0.174301497.$$

First, we note that the ninth maximum Randić index stated above is not true. Let $G$ be a $n$-vertex unicyclic graph ($n \geq 10$), with exactly two pendent paths of length atleast two attached to the same vertex of the cycle $C_k (k < n)$, then

$$R(G) = \frac{n-6}{2} + \frac{2}{\sqrt{2}} + \frac{4}{\sqrt{8}} \approx \frac{n}{2} - 0.171572875$$

Table 4. Unicyclic graphs with ninth to thirteenth maximum Randić index (see Theorem 1 in [13])

| Notation | Vertices | $\mathcal{E}_{1,2}$ | $\mathcal{E}_{1,3}$ | $\mathcal{E}_{2,3}$ | $\mathcal{E}_{2,4}$ | $\mathcal{E}_{3,3}$ | $\mathcal{E}_{2,2}$ | $R(G)$ |
|---|---|---|---|---|---|---|---|---|
| $U_9$ | $n \geq 10$ | 1 | 1 | 5 | 0 | 0 | $n-7$ | $\frac{n-7}{2}+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}+\frac{5}{\sqrt{6}}$ |
| $U_{10}$ | $n \geq 11$ | 3 | 0 | 7 | 0 | 1 | $n-11$ | $\frac{n-11}{2}+\frac{3}{\sqrt{2}}+\frac{7}{\sqrt{6}}+\frac{1}{3}$ |
| $U_{11}$ | $n \geq 11$ | 2 | 1 | 2 | 0 | 3 | $n-8$ | $\frac{n-6}{2}+\frac{2}{\sqrt{2}}+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}$ |
| $U_{12}$ | $n \geq 11$ | 0 | 2 | 2 | 0 | 1 | $n-5$ | $\frac{n-5}{2}+\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{6}}+\frac{1}{3}$ |
| $U_{13}$ | $n \geq 12$ | 3 | 0 | 9 | 0 | 0 | $n-12$ | $\frac{n-12}{2}+\frac{3}{\sqrt{2}}+\frac{9}{\sqrt{6}}$ |

It is simple to verify that, (as indicated in Table 3 and Table 4) $\frac{n}{2}-0.171572875$ lies between the eighth and the ninth maximum of Randić index:
$\frac{n-8}{2}+\frac{3}{\sqrt{2}}+\frac{5}{\sqrt{6}}-\frac{1}{3} > \frac{n-6}{2}+\frac{2}{\sqrt{2}}+\frac{4}{\sqrt{8}} > \frac{n-7}{2}+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}+\frac{5}{\sqrt{6}}.$

We now give the correct version of the ordering in Table 5.

**Table 5.** **Unicyclic graphs with ninth to fourteenth maximum Randić index**

| Notation | Vertices | $\mathcal{E}_{1,2}$ | $\mathcal{E}_{1,3}$ | $\mathcal{E}_{2,3}$ | $\mathcal{E}_{2,4}$ | $\mathcal{E}_{3,3}$ | $\mathcal{E}_{2,2}$ | $R(G)$ |
|---|---|---|---|---|---|---|---|---|
| $U_9$ | $n \geq 10$ | 2 | 0 | 0 | 4 | 0 | $n-6$ | $\frac{n-6}{2}+\frac{2}{\sqrt{2}}+\frac{4}{\sqrt{8}}$ |
| $U_{10}$ | $n \geq 10$ | 1 | 1 | 5 | 0 | 0 | $n-7$ | $\frac{n-7}{2}+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}+\frac{5}{\sqrt{6}}$ |
| $U_{11}$ | $n \geq 11$ | 3 | 0 | 7 | 0 | 1 | $n-11$ | $\frac{n-11}{2}+\frac{3}{\sqrt{2}}+\frac{7}{\sqrt{6}}+\frac{1}{3}$ |
| $U_{12}$ | $n \geq 11$ | 2 | 1 | 2 | 0 | 3 | $n-8$ | $\frac{n-6}{2}+\frac{2}{\sqrt{2}}+\frac{1}{\sqrt{3}}+\frac{2}{\sqrt{6}}$ |
| $U_{13}$ | $n \geq 11$ | 0 | 2 | 2 | 0 | 1 | $n-5$ | $\frac{n-5}{2}+\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{6}}+\frac{1}{3}$ |
| $U_{14}$ | $n \geq 12$ | 3 | 0 | 9 | 0 | 0 | $n-12$ | $\frac{n-12}{2}+\frac{3}{\sqrt{2}}+\frac{9}{\sqrt{6}}$ |

## 4. Bicyclic Graphs Maximizing Randić indices :

Let $\mathcal{B}_n$ be the collection of graphs with $n$ vertices and $n+1$ edges. A graph $G \in \mathcal{B}_n$ is called as a bicyclic graph. Bicyclic graphs without pendent vertices are classified as follows (see Figure 1).

$$\mathcal{B}^{I} = \mathcal{B}_n^1 \cup \mathcal{B}_n^2 = \left\{\mathcal{E}_{2,3}=4, \mathcal{E}_{3,3}=1, \mathcal{E}_{2,2}=n-4\right\}$$
$$\mathcal{B}^{II} = \mathcal{B}_n^3 \cup \mathcal{B}_n^4 = \left\{\mathcal{E}_{2,3}=6, \mathcal{E}_{2,2}=n-5\right\}$$
$$\mathcal{B}^{III} = \mathcal{B}_n^5 = \left\{\mathcal{E}_{2,4}=4, \mathcal{E}_{2,2}=n-3\right\}$$

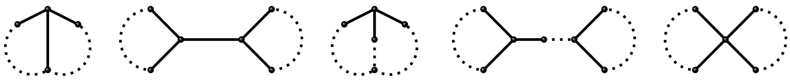


**Figure 1.** **Classification of Bicyclic graphs**

Among the collection $\mathcal{B}_n$, the two class of graphs $(\mathcal{B}_n^1 \cup \mathcal{B}_n^2)$ with maximum Randić index was determined by Caprossi et al.[5], the second to fifth maximum Randić indices was determined by Du and Zhou [8] and the sixth maximum Randić index was determined by Li et al. [15] (See Table 6).

Table 6. Bicyclic graphs with first six maximum Randić index (See Theorem 5 in [5], Proposition 2.3 in [8] and Theorem 2.3 in [15] )

| Notation | Vertices | $\mathcal{E}_{1,2}$ | $\mathcal{E}_{1,3}$ | $\mathcal{E}_{2,3}$ | $\mathcal{E}_{2,4}$ | $\mathcal{E}_{3,3}$ | $\mathcal{E}_{2,2}$ | $R(G)$ |
|---|---|---|---|---|---|---|---|---|
| $B_1 \in \mathcal{B}^I$ | $n \geq 6$ | 0 | 0 | 4 | 0 | 1 | $n-4$ | $\frac{n-4}{2}+\frac{4}{\sqrt{6}}+\frac{1}{3}$ |
| $B_2 \in \mathcal{B}^{II}$ | $n \geq 7$ | 0 | 0 | 6 | 0 | 0 | $n-5$ | $\frac{n-5}{2}+\sqrt{6}$ |
| $B_3$ | $n \geq 7$ | 1 | 0 | 3 | 0 | 3 | $n-6$ | $\frac{n-4}{2}+\frac{3}{\sqrt{6}}+\frac{1}{\sqrt{2}}$ |
| $B_4$ | $n \geq 9$ | 1 | 0 | 5 | 0 | 2 | $n-7$ | $\frac{n-7}{2}+\frac{5}{\sqrt{6}}+\frac{1}{\sqrt{2}}+\frac{2}{3}$ |
| $B_5 \in \mathcal{B}^{III}$ | $n \geq 9$ | 0 | 0 | 0 | 4 | 0 | $n-3$ | $\frac{n-3}{2}+\sqrt{2}$ |
| $B_6$ | $n \geq 10$ | 1 | 0 | 7 | 0 | 1 | $n-8$ | $\frac{n-6}{2}+\frac{1}{\sqrt{2}}+\frac{7}{\sqrt{6}}-\frac{2}{3}$ |

A pendent path of length one and two in $G$ contributes to $f(G)$ at least $\left(1-\frac{1}{\sqrt{3}}\right)^2$ and $\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2$, respectively and $\left(1-\frac{1}{\sqrt{3}}\right)^2 > \left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2$. Let us consider the following functions $\phi(x) = \left(1-\frac{1}{\sqrt{x}}\right)^2$ and $\psi(x) = \left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{x}}\right)^2$. Both $\phi(x)$ and $\psi(x)$ are increasing for $x \geq 3$, therefore $p$ pendent paths in $G$ contributes to $f(G)$ at least $p\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right]$, and using the identity (1) immediately leads to the following upper bound for $R(G)$ with given $p$ pendent vertices.

**Lemma 1.** *Let $G$ be a simple graph with $p$ pendent vertices, then*

$$R(G) \leq \frac{n}{2} - \frac{p}{2}\left[\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2\right] \tag{2}$$

We now define the following graphs which are used in the main results.

$$B_7 = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{33} = 5, \mathcal{E}_{23} = 2, \mathcal{E}_{12} = 2, \mathcal{E}_{22} = n-8\Big\}$$
$$B_8 = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{33} = 3, \mathcal{E}_{23} = 2, \mathcal{E}_{13} = 1, \mathcal{E}_{22} = n-5\Big\}$$
$$B_9 = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{23} = 9, \mathcal{E}_{12} = 1, \mathcal{E}_{22} = n-9\Big\}$$
$$B_{10} = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{33} = 4, \mathcal{E}_{23} = 4, \mathcal{E}_{12} = 2, \mathcal{E}_{22} = n-9\Big\}$$
$$B_{11} = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{33} = 2, \mathcal{E}_{23} = 4, \mathcal{E}_{13} = 1, \mathcal{E}_{22} = n-6\Big\}$$
$$B_{12} = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{34} = 1, \mathcal{E}_{24} = 3, \mathcal{E}_{23} = 2, \mathcal{E}_{12} = 1, \mathcal{E}_{22} = n-6\Big\}$$
$$B_{13} = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{33} = 3, \mathcal{E}_{23} = 6, \mathcal{E}_{12} = 2, \mathcal{E}_{22} = n-10\Big\}$$
$$B_{14} = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{33} = 1, \mathcal{E}_{23} = 6, \mathcal{E}_{13} = 1, \mathcal{E}_{22} = n-7\Big\}$$
$$B_{15} = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{33} = 5, \mathcal{E}_{23} = 1, \mathcal{E}_{13} = 1, \mathcal{E}_{12} = 1, \mathcal{E}_{22} = n-7\Big\}$$
$$B_{16} = \Big\{G|G \in \mathcal{B}_n \text{ and } \mathcal{E}_{34} = 2, \mathcal{E}_{33} = 1, \mathcal{E}_{24} = 2, \mathcal{E}_{23} = 2, \mathcal{E}_{12} = 2, \mathcal{E}_{22} = n-8\Big\}$$

**Theorem 1.** *Among the $n$-vertex bicyclic graphs $\mathcal{B}_n$,*
*(i) For $n \geq 10$, the graphs in $B_7$ have the seventh maximum Randić index, which equals*

$$\frac{n-8}{2} + \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{2}} + \frac{5}{3}.$$

*(ii) For $n \geq 10$, the graphs in $B_8$ have the eighth maximum Randić index, which equals*

$$\frac{n-3}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}}.$$

*(iii) For $n \geq 10$, the graphs in $B_9$ have the ninth maximum Randić index, which equals*

$$\frac{n-9}{2} + \frac{9}{\sqrt{6}} + \frac{1}{\sqrt{2}}.$$

*(iv) For $n \geq 10$, the graphs in $B_{10}$ have the tenth maximum Randić index, which equals*

$$\frac{n-9}{2} + \frac{4}{\sqrt{6}} + \frac{2}{\sqrt{2}} + \frac{4}{3}.$$

*(v) For $n \geq 10$, the graphs in $B_{11}$ have the eleventh maximum Randić index, which equals*

$$\frac{n-6}{2} + \frac{4}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{2}{3}.$$

*(vi) For $n \geq 10$, the graphs in $B_{12}$ have the twelveth maximum Randić index, which equals*

$$\frac{n-6}{2}+\frac{2}{\sqrt{6}}+\frac{3}{2\sqrt{2}}+\frac{1}{2\sqrt{3}}+\frac{1}{\sqrt{2}}.$$

*(vii) For $n \geq 10$, the graphs in $B_{13}$ have the thirteenth maximum Randić index, which equals*

$$\frac{n-8}{2}+\frac{6}{\sqrt{6}}+\frac{2}{\sqrt{2}}.$$

*(viii) For $n \geq 10$, the graphs in $B_{14}$ have the fourteenth maximum Randić index, which equals*

$$\frac{n-7}{2}+\frac{6}{\sqrt{6}}+\frac{1}{\sqrt{3}}+\frac{1}{3}.$$

*(ix) For $n \geq 10$, the graphs in $B_{15}$ have the fifteenth maximum Randić index, which equals*

$$\frac{n-7}{2}+\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{2}}+\frac{5}{3}.$$

*(x) For $n \geq 10$, the graphs in $B_{16}$ have the sixteenth maximum Randić index, which equals*

$$\frac{n-8}{2}+\frac{2}{\sqrt{6}}+\frac{1}{\sqrt{3}}+\frac{3}{\sqrt{2}}+\frac{1}{3}.$$

*Proof.* Let $G \in \mathcal{B}_n \backslash \{B_i : i = 1 \text{ to } 6\}$. To prove the above results, it is enough to prove that any $G \in \mathcal{B}_n$ will be less than $\frac{n-8}{2}+\frac{2}{\sqrt{6}}+\frac{1}{\sqrt{3}}+\frac{3}{\sqrt{2}}+\frac{1}{3}$ (which is claimed to be the sixteenth maximum $R(G)$ value) must have $i$th maximum $R(G)$ value, for $i \geq 17$. From (1), it is clear that $R$ has a value at least

$$\frac{n}{2}-\frac{1}{2}\left[2\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{4}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+2\left(1-\frac{1}{\sqrt{2}}\right)^2\right]$$

if and only if $f(G) \leq 2\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{4}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+2\left(1-\frac{1}{\sqrt{2}}\right)^2.$

Throughout the proof, we consider $G, G'$ and $G'' \in \mathcal{B}_n$ on $n$ vertices. Let $G'$ be the graph obtained from $G$ by attaching a pendent path to any vertex of $G$ and $G''$ be the graph obtained from $G$ by attaching two pendent paths in $G$.

**Case 1.** Graphs $G', G''$ constructed from the class $\mathcal{B}^I$.

If $G \in \mathcal{B}^I$, then $R(G) = \frac{n}{2} - 2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2$ with $f(G) = 4\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2 = f(B_1)$.

*Subcase 1.1 :* If $G'$ constructed from $G \in \mathcal{B}^I$, then $G'$ has the following possibilities depicted in Figure 2. Assuming the length of the pendent path is at least two, then

$$\begin{aligned} f(G') &\geq \left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{4}}\right)^2+3\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(1-\frac{1}{\sqrt{2}}\right)^2 = f(B_{12}) \\ &> 7\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(1-\frac{1}{\sqrt{2}}\right)^2 = f(B_6) \\ &> 5\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(1-\frac{1}{\sqrt{2}}\right)^2 = f(B_4) \\ &> 3\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(1-\frac{1}{\sqrt{2}}\right)^2 = f(B_3). \end{aligned}$$

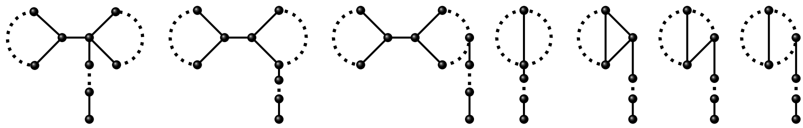

**Figure 2.** **Graphs with exactly one pendent path obtained from $G \in \mathcal{B}^I$.**

Next, we consider the pendent path of length exactly one in figure 2, then we get

$$\begin{aligned} f(G') &\geq 6\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(1-\frac{1}{\sqrt{3}}\right)^2=f(B_{14})\\ &\geq 4\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(1-\frac{1}{\sqrt{3}}\right)^2=f(B_{11})\\ &\geq 2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(1-\frac{1}{\sqrt{3}}\right)^2=f(B_8). \end{aligned}$$

*Subcase 1.2 :* If $G''$ constructed from $G \in \mathcal{B}^I$ by considering two pendent paths $P_1$ and $P_2$. The various possibilities of $G''$ are depicted in Figure 3. The pendent paths $P_1$ and $P_2$ are subdivided into three possible combinations, we get the following results. If both $P_1$ and $P_2$ are of length at least two, then

$$\begin{aligned} f(G'') &\geq 2\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{4}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{4}}\right)^2+2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+2\left(1-\frac{1}{\sqrt{2}}\right)^2=f(B_{16})\\ &\geq 6\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+2\left(1-\frac{1}{\sqrt{2}}\right)^2=f(B_{13})\\ &\geq 4\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+2\left(1-\frac{1}{\sqrt{2}}\right)^2=f(B_{10})\\ &\geq 2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+2\left(1-\frac{1}{\sqrt{2}}\right)^2=f(B_7). \end{aligned}$$

Next, we consider the pendent path $P_1$ with length one and $P_2$ with length at least two in Figure 2, then we get

$$f(G'') \geq \left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+\left(1-\frac{1}{\sqrt{2}}\right)^2+\left(1-\frac{1}{\sqrt{3}}\right)^2=f(B_{15}).$$

If both $P_1$ and $P_2$ are of length one, then

$$f(G'') \geq 2\left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)^2+2\left(1-\frac{1}{\sqrt{3}}\right)^2.$$

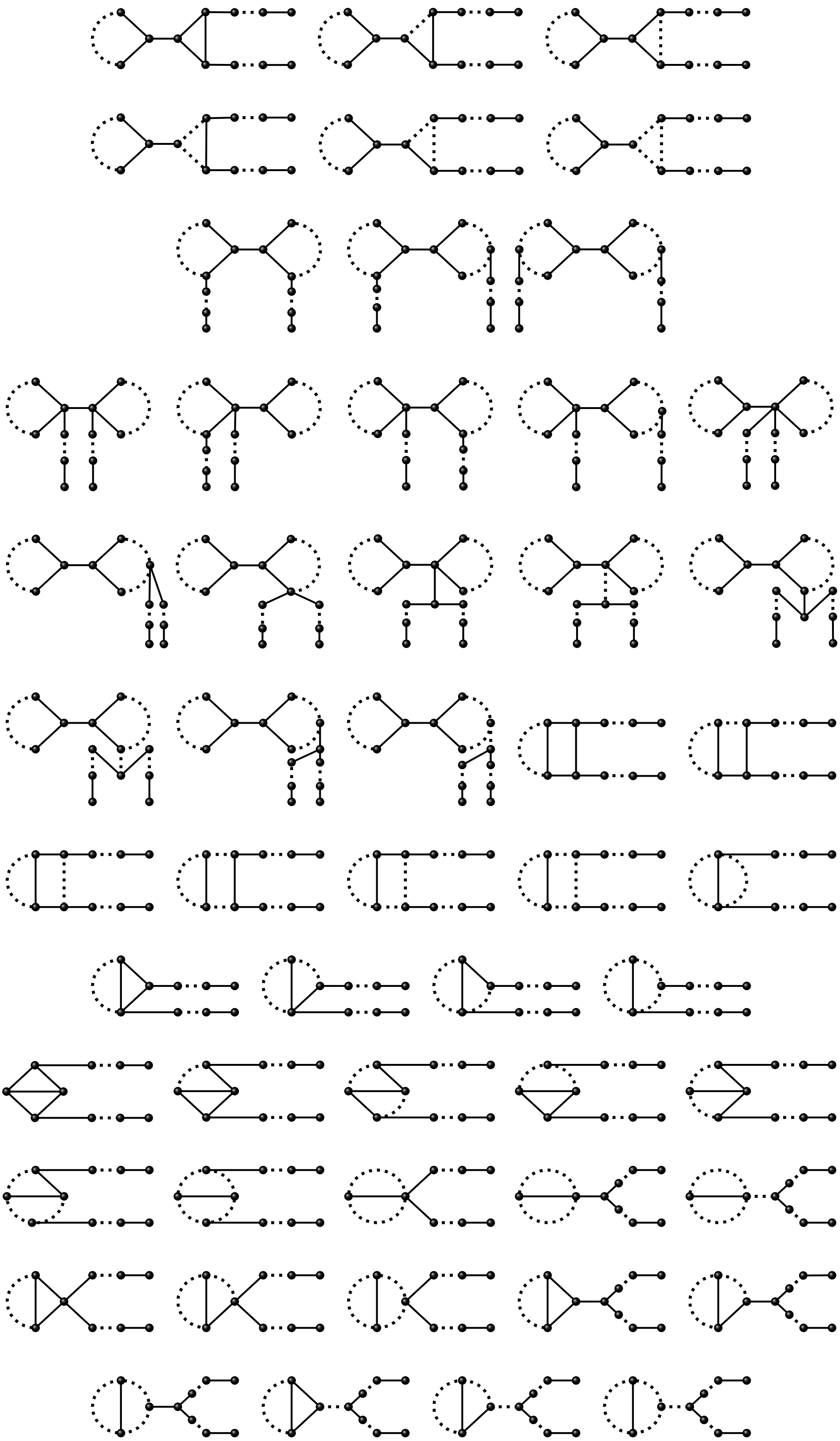

**Figure 3.** **Graphs with exactly two pendent paths obtained from $G \in \mathcal{B}^I$.**

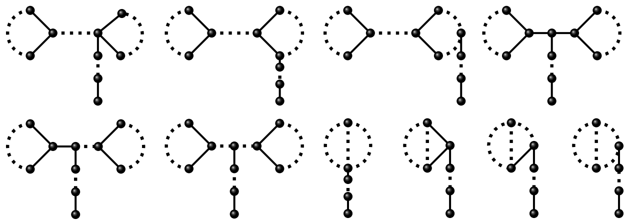

**Figure 4.** **Graphs with exactly one pendent path obtained from $G \in \mathcal{B}^{II}$.**

*Case 2 :* Graphs $G', G''$ constructed from the class $\mathcal{B}^{II}$.
If $G \in \mathcal{B}^{II}$, then $R(G) = \frac{n}{2} - 3\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2$ with $f(G) = 6\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 = f(B_2)$.
*Subcase 2.1* : If $G'$ constructed from $G \in \mathcal{B}^{II}$, then $G'$ has the following possibilities depicted in Figure 4. Suppose the length of the pendent path is at least two, then

$$\begin{aligned} f(G') &\geq 9\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{2}}\right)^2 = f(B_9) \\ &> 7\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{2}}\right)^2 = f(B_6). \end{aligned}$$

If the length of pendent path is exactly one in figure 4, then we get

$$\begin{aligned} f(G') &\geq 6\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{3}}\right)^2 = f(B_{14}) \\ &\geq 4\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{3}}\right)^2 = f(B_{11}). \end{aligned}$$

*Subcase 2.2* : If $G''$ obtained from $G \in \mathcal{B}^{II}$. The various possible graph structures can be constructed from Figure 3 by replacing the edge $xy \in E(G'')$ ( with $d_x = 3, d_y = 3$ ) by a path of length atleast two and the remaining cases are depicted in figure 5.
If $P_1 \geq 2$ and $P_2 \geq 2$, then

$$\begin{aligned} f(G'') &\geq 6\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + 2\left(1 - \frac{1}{\sqrt{2}}\right)^2 = f(B_{13}) \\ &\geq 4\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + 2\left(1 - \frac{1}{\sqrt{2}}\right)^2 = f(B_{10}). \end{aligned}$$

If $P_1 = 1$ and $P_2 \geq 2$, then

$$f(G'') \geq 3\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{2}}\right)^2.$$

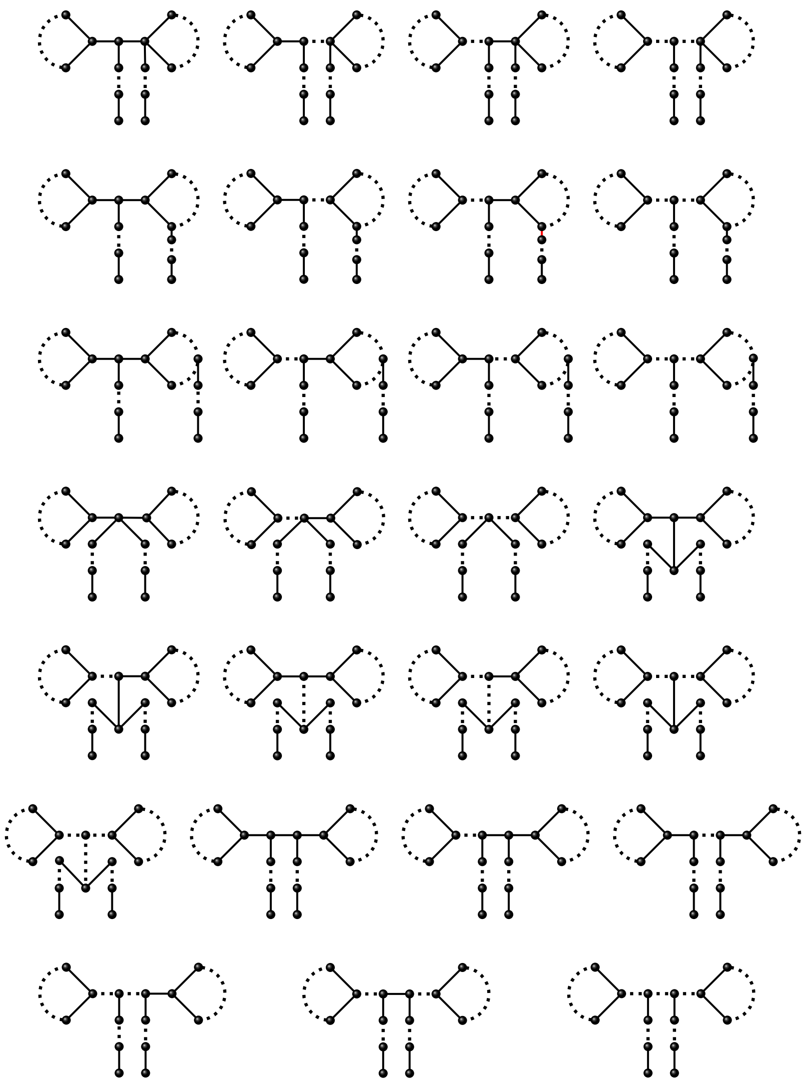

**Figure 5.** **Graphs with exactly two pendent paths obtained from $G \in \mathcal{B}^{II}$.**

If $P_1 = P_2 = 1$, then

$$f(G'') \geq 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + 2\left(1 - \frac{1}{\sqrt{3}}\right)^2.$$

*Case 3:* Graphs $G', G''$ constructed from the class $\mathcal{B}^{III}$.
If $G \in \mathcal{B}^{III}$, then $R(G) = \frac{n}{2} - 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2$ with $f(G) = 4\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2 = f(B_5)$.
*Subcase 3.1* : If $G'$ constructed from $G \in \mathcal{B}^{III}$, then $G'$ has the following possibilities

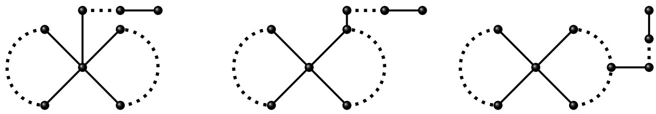

**Figure 6.** **Graphs with exactly one pendent path obtained from $G \in \mathcal{B}^{III}$.**

depicted in Figure 6. Consider the length of the pendent path is at least two, then

$$f(G') \geq 3\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2 + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right)^2 + 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{2}}\right)^2 = f(B_{12}).$$

If the length of the pendent path is one, then

$$f(G') \geq 3\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2 + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{3}}\right)^2.$$

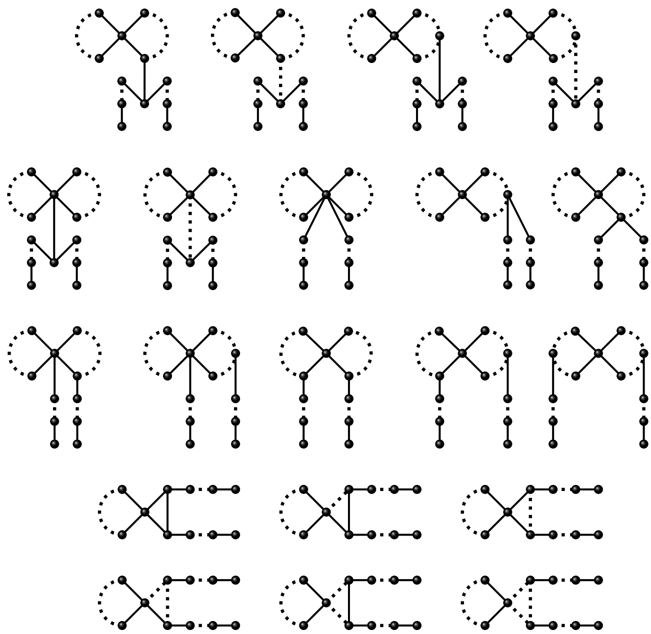

**Figure 7.** **Graphs with exactly two pendent paths obtained from $G \in \mathcal{B}^{III}$.**

*Subcase 3.2* : If $G''$ constructed from $G \in \mathcal{B}^{III}$ considering the two pendent paths $P_1$ and $P_2$. The various possibilities of graphs are depicted in Figure 7. If $P_1 \geq 2$ and $P_2 \geq 2$, then we get

$$f(G'') \geq 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2 + 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + 2\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right)^2 + 2\left(1 - \frac{1}{\sqrt{2}}\right)^2 = f(B_{16}).$$

If $P_1 = 1$ and $P_2 \geq 2$, then

$$f(G'') \geq 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2 + 2\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(1 - \frac{1}{\sqrt{3}}\right)^2.$$

If $P_1 = P_2 = 1$, then

$$f(G'') \geq 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2 + 2\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right)^2 + 2\left(1 - \frac{1}{\sqrt{3}}\right)^2.$$

By comparing the values of $f(G'), f(G'')$ in cases 1, 2 and 3, we conclude any bicyclic graph with atmost 2 pendent vertices other than $B_i$ $\{i = 1, 2...16\}$ will have

$$f(G) > 2\left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right)^2 + 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}}\right)^2 + 2\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + 2\left(1 - \frac{1}{\sqrt{2}}\right)^2.$$

*Case 4:* If $G^* \in \mathcal{B}_n$ with at least three pendent paths, then from Lemma 1, we get

$$f(G^*) \geq k\left[\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{2}}\right)^2\right] > 3\left[\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 + \left(1 - \frac{1}{\sqrt{2}}\right)^2\right].$$

It is easy to see that $f(G^*) > f(B_{16})$, this concludes that any $G \in \mathcal{B}_n$ will have the following order

$$f(G) > f(B_{16}) > f(B_{15}) > f(B_{14}) > f(B_{13}) > f(B_{12}) > f(B_{11}) > f(B_{10}) > f(B_9) > f(B_8) > f(B_7).$$

□

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