

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

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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

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

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 [3, 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  $P := u_1 u_2 \dots u_r$  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	$n - 9$	$\frac{n-9}{2} + \frac{3}{\sqrt{2}} + \frac{3}{\sqrt{6}}$
$U_7$	$n \geq 9$	1	1	3	0	1	$n - 6$	$\frac{n-6}{2} + \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{2}{3}$
$U_8$	$n \geq 10$	3	0	5	0	2	$n - 10$	$\frac{n-10}{2} + \frac{3}{\sqrt{2}} + \frac{5}{\sqrt{6}} - \frac{1}{3}$

### 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	$n - 11$	$\frac{n-11}{2} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{3}{\sqrt{6}}$
$U_{11}$	$n \geq 11$	2	1	2	0	3	$n - 8$	$\frac{n-6}{2} + \frac{\sqrt{2}}{2} + \frac{\sqrt{3}}{2} + \frac{1}{\sqrt{6}}$
$U_{12}$	$n \geq 11$	0	2	2	0	1	$n - 5$	$\frac{n-5}{2} + \frac{\sqrt{2}}{2} + \frac{\sqrt{3}}{2} + \frac{1}{\sqrt{6}}$
$U_{13}$	$n \geq 12$	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.

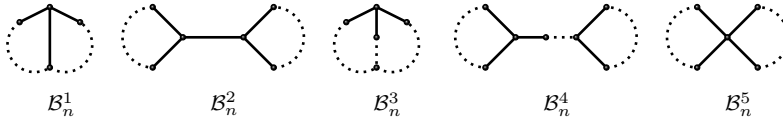
Table 5. Unicyclic graphs with ninth to fourteenth maximum Randić index

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	$n - 11$	$\frac{n-11}{2} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{3}{\sqrt{6}}$
$U_{12}$	$n \geq 11$	2	1	2	0	3	$n - 8$	$\frac{n-6}{2} + \frac{\sqrt{2}}{2} + \frac{\sqrt{3}}{2} + \frac{1}{\sqrt{6}}$
$U_{13}$	$n \geq 11$	0	2	2	0	1	$n - 5$	$\frac{n-5}{2} + \frac{\sqrt{2}}{2} + \frac{\sqrt{3}}{2} + \frac{1}{\sqrt{6}}$
$U_{14}$	$n \geq 12$	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).

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



**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.

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

**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 twelfth 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  $G \in \mathcal{B}_n \setminus \{B_i : i = 1 \text{ to } 6\}$ . 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  $f(G) \leq 2 \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 + 2 \left( 1 - \frac{1}{\sqrt{2}} \right)^2$ .

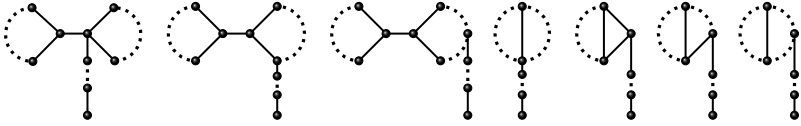
Throughout the proof, we consider  $G, G'$  and  $G'' \in \mathcal{B}_n$  on  $n$  vertices. Let  $G'$  be the graph obtained from  $G$  by attaching a pendent path to any vertex of  $G$  and  $G''$  be the graph obtained from  $G$  by attaching two pendent paths in  $G$ .

**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

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



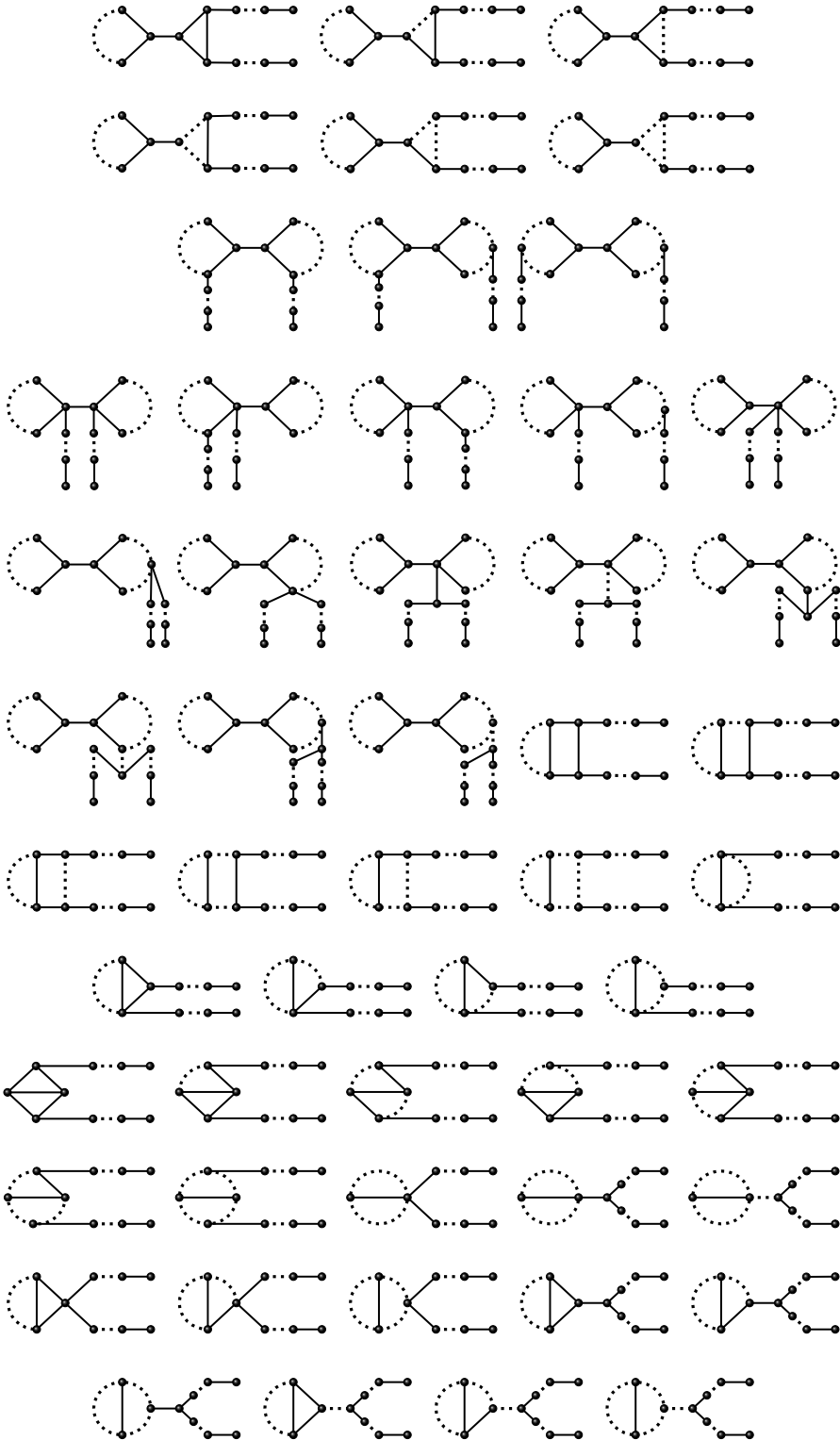
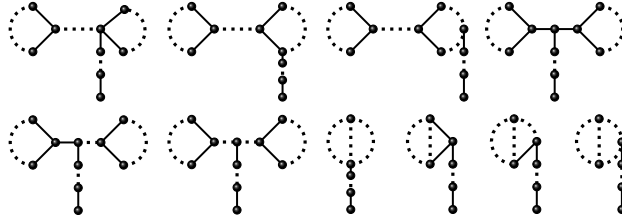


Figure 3. Graphs with exactly two pendent paths obtained from  $G \in \mathcal{B}^f$ .



**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

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

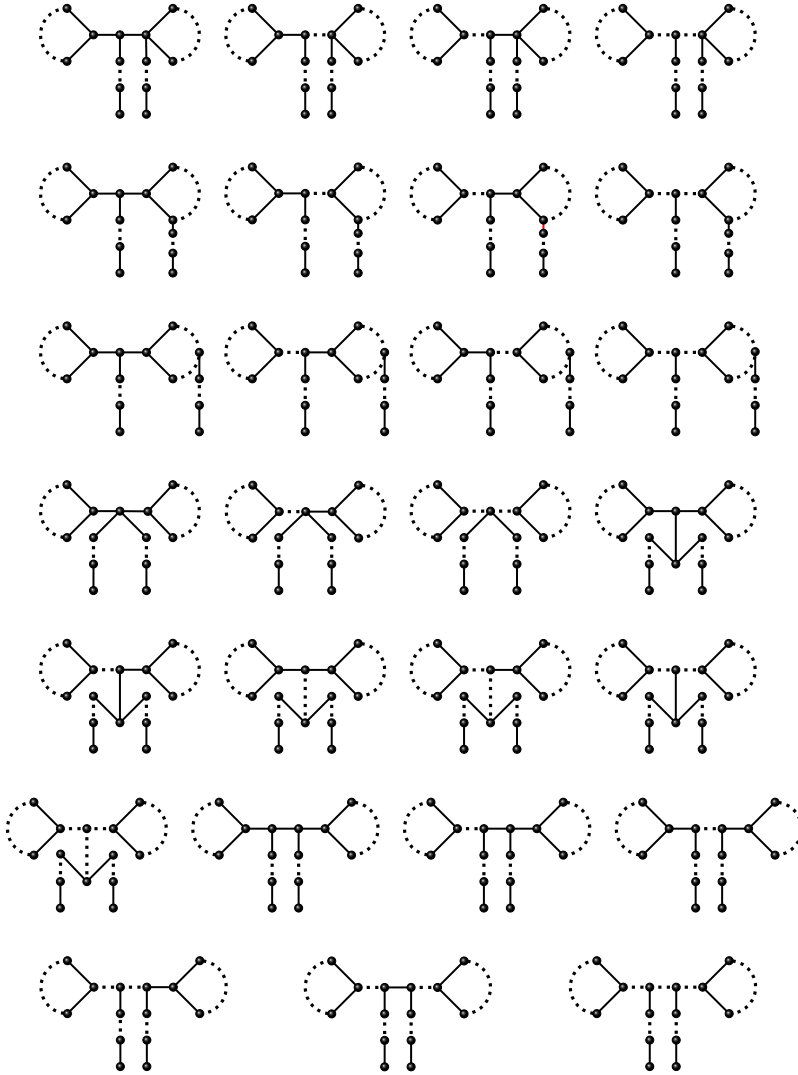
*Subcase 2.2 :* If  $G''$  obtained from  $G \in \mathcal{B}^{II}$ . The various possible graph structures can be constructed from Figure 3 by replacing the edge  $xy \in E(G'')$  ( with  $d_x = 3, d_y = 3$  ) by a path of length atleast two and the remaining cases are depicted in figure 5.

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  $G \in \mathcal{B}^{II}$ .

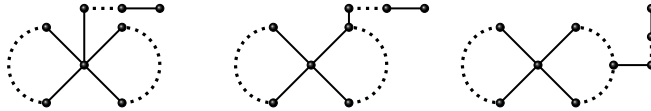
If  $P_1 = P_2 = 1$ , then

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

*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



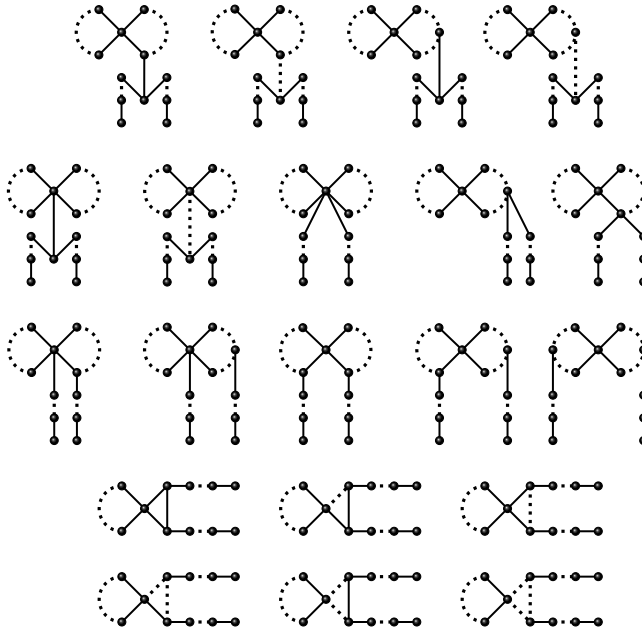
**Figure 6.** Graphs with exactly one pendent path obtained from  $G \in \mathcal{B}^{III}$ .

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

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

□

**Conflict of Interest:** The authors declare that there is no competing interest related to this paper.

**Data Availability:** Data sharing is not applicable to this article as no data sets were generated or analyzed during the current study.

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