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On the Bicyclic Graphs with Minimum Reduced Reciprocal Randić Index

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ABSTRACT

The reduced reciprocal Randić (RRR) index is a molecular structure descriptor (or more precisely, a topological index), which is useful for predicting the standard enthalpy of formation and normal boiling point of isomeric octanes. In this paper, a mathematical aspect of RRR index is explored, or more specifically, the graph(s) having minimum RRR index is/are identified from the collection of all n–vertex connected bicyclic graphs for $n \geq 5$. As a consequence, the best possible lower bound on the RRR index, for n–vertex connected bicyclic graphs is obtained when $n \geq 5$.

1 INTRODUCTION

It is widely known fact that a graph can be used to represent a molecule in which atoms correspond to the vertices while the molecular bonds between atoms represent edges [1, 5]. In chemical graph theory, those graph invariants are usually referred as topological indices which are expected to correlate with some physical observable measures by experiments in such a way that theoretical predictions can be used to gain chemical insights even for not yet existing molecules [2]. Applications of topological indices in chemistry begin in 1947, when the chemist

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Wiener [6] devised a topological index, nowadays known as Wiener index, for predicting the boiling points of paraffins.

All graphs considered in this paper are simple and finite. Undefined notations and terminologies from (chemical) graph theory can be found in [1-4].

The Randić index [7] is one of the most studied and most applied topological indices, which was proposed in 1975 for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The Randić (R) index for a graph G is defined as

$$R(G) = \sum_{uv\in E(G)} (d_u d_v)^{-\frac{1}{2}},$$

where uv is the edge connecting the vertices u, v of the graph G, $E(G)$ is the edge set of G and d_u is degree of the vertex u. Determining the graphs with minimum or maximum R value from certain collections of graphs with some fixed parameters, was the topic of several publications. For instance, Bollobás and Erdős [8] identified the unique tree with minimum R value among all n–vertex trees, when $n \geq 3$. The unique graph with minimum R value was determined in [9] (respectively, in [10]) from the class of all n–vertex connected unicyclic (respectively, bicyclic) graphs, when $n \geq 5$. Details about the chemical applicability and mathematical properties of R can be found in the surveys [11, 12], recent papers [13-20] and/or related references listed therein.

Based on the successful consideration of Randić index, Manso *et al.* [21] introduced a new topological index (and named it *Fi* index) to predict the normal boiling point temperatures of hydrocarbons. In the mathematical definition of *Fi* index two terms are present. In 2014, Gutman *et al.* [22] considered one of these terms, which is given below:

$$RRR(G) = \sum_{uv\in E(G)} \sqrt{(d_u - 1)(d_v - 1)},$$

and they called it *reduced reciprocal Randić* (RRR) *index*. In [22], the RRR index was compared with several well-known topological indices for predicting the standard heats (enthalpy) of formation and normal boiling points of octane isomers, and it was concluded that RRR index deserves attention of researchers performing quantitative structure-property relationship and quantitative structure-activity relationship studies.

The study of extremal graphs with respect to the RRR index was initiated by the authors of [22]. They proved that the star graph and the complete graph have the minimum and maximum value, respectively, among all n-vertex graphs, and also posed a conjecture related to the maximum RRR value of trees. This conjecture was proved by Ren *et al.* [23]. Recently, the problem of finding graph with minimum RRR value among all n-vertex connected unicyclic graphs (n-vertex connected graphs with n edges) was solved in [24]. Main purpose of the present paper is to extend the main result of the reference [24] for connected bicyclic graphs (n-vertex connected graphs with $n+1$ edges), or more precisely, to solve the following extremal problem.

Problem 1. *Which graph(s) has/have minimum RRR index among all n-vertex connected bicyclic graphs*?

As there is only one bicyclic graph on 4 vertices, so the Problem 1 is well defined for $n \geq 5$ and thereby in the remaining part of this paper, it would be assumed that the graph under consideration has at least 5 vertices.

Nowadays, many researchers are interested in finding best possible bounds on topological indices; for example, see [25-29]. As a consequence of our main result, we obtain best possible lower bound on the RRR index, for n–vertex connected bicyclic graphs when $n \geq 5$.

2. MAIN RESULTS

In order to prove the main result, we need some definitions. If $uv, vw \in E(G)$ but $uw \not\in E(G)$, then the vertex v and the vertex w will be called *first neighbor* of u and *second neighbor* of u, respectively. Denote by $N_G(u)$ (or simply by $N(u)$) the set of all first neighbors of u in G. The minimum and maximum degree of G will be denoted by $\delta(G)$ and $\Delta(G)$, respectively. A vertex with degree one is known as a pendent vertex. Now, we are in a position to prove the main result, which gives the complete solution of Problem 1.

Theorem 1. *Among all n–vertex connected bicyclic graphs,*

- *$\tilde{B}_n$ is the only graph with minimum RRR value for $5 \leq n \leq 9$;*
- *$\hat{B}_n$ is the only graph with minimum RRR value for $10 \leq n \leq 13$;*
- *$\hat{B}_n$ and B'_n are the only graphs with minimum RRR value for $n = 14$;*
- *B'_n is the only graph with minimum RRR value for $n \geq 15$, where the graphs $\tilde{B}_n$, $\hat{B}_n$* and B'_n are depicted in Figure 1.

Proof. We note that there are only five non-isomorphic connected bicyclic graphs on 5 vertices. These graphs, together with their RRR index, are depicted in Figure 2. Hence, the result is true for $n = 5$.

Now, we assume that B_n is an n-vertex connected bicyclic graph for $n \geq 6$. If $\Delta(B_n) = n - 1$, then B_n must be isomorphic to one of the graphs $B_n^{(1)}$, $B_n^{(2)}$, shown in Figure 3.

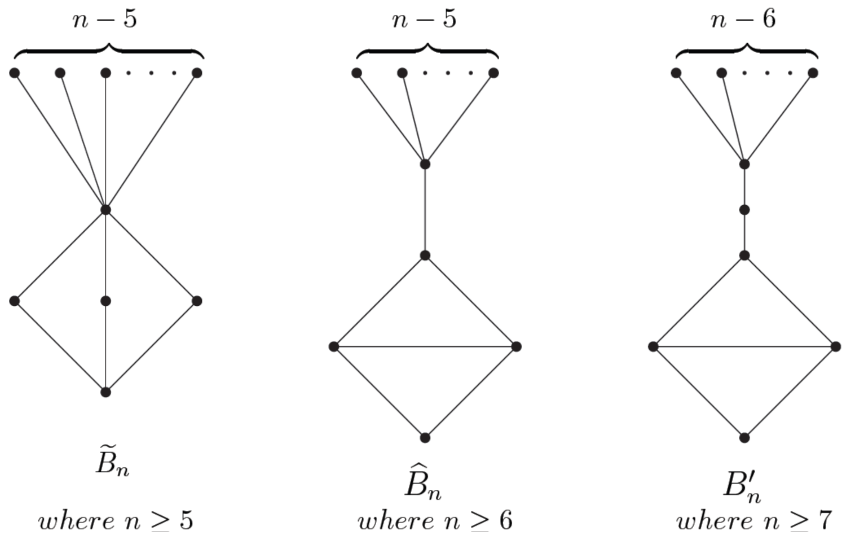

Figure 1. The graphs $\tilde{B}_n$, $\hat{B}_n$ and B'_n.

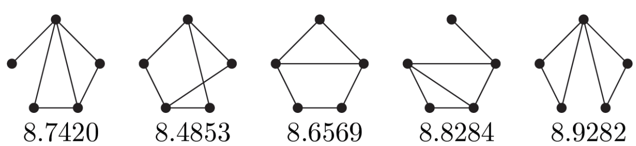

Figure 2. All the non-isomorphic connected bicyclic graphs on 5 vertices together with their RRR index.

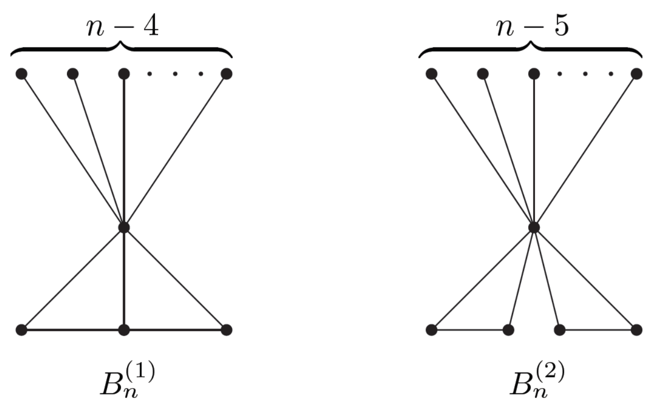

Figure 3. The graphs $B_n^{(1)}$ and $B_n^{(2)}$.

Routine calculations yield

$$RRR\left(B_n^{(1)}\right) = \left(2 + \sqrt{2}\right)\sqrt{n-2} + 2\sqrt{2}$$

and

$$RRR\left(B_n^{(2)}\right) = 4\sqrt{n-2} + 2.$$

Simple comparison gives

$$RRR\left(B_n^{(j)}\right) > \begin{cases} 3\left(\sqrt{n-3}+\sqrt{2}\right) = RRR\left(\tilde{B}_n\right) & for\ \ 6 \le n \le 9, \\ \sqrt{2}\left(\sqrt{n-5}+2\right)+6 = RRR\left(\hat{B}_n\right) & for\ \ 10 \le n \le 13, \\ 5\sqrt{2}+6 = RRR\left(\hat{B}_{14}\right) = RRR(B'_{14}) & for\ \ n = 14, \\ \sqrt{n-6}+3\left(2+\sqrt{2}\right) = RRR(B'_n) & for\ \ n \ge 15, \end{cases}$$

where $j = 1,2$. Now, we suppose that $\Delta(B_n) \le n-2$ where $n \ge 6$. If B_n does not contain any pendent vertex, then B_n must be isomorphic to one of the graphs $B_n^{(3)}$, $B_n^{(4)}$, depicted in Figure 4. It holds that

$$RRR\left(B_n^{(3)}\right) = \begin{cases} n+2(2\sqrt{2}-1) & if\ k = 0, \\ n+6\sqrt{2}-5 & otherwise. \end{cases}$$

and

$$RRR\left(B_n^{(4)}\right) = \begin{cases} n+4\sqrt{3}-3 & if\ q = 1, \\ n+2(2\sqrt{2}-1) & if\ q = 2, \\ n+6\sqrt{2}-5 & otherwise. \end{cases}$$

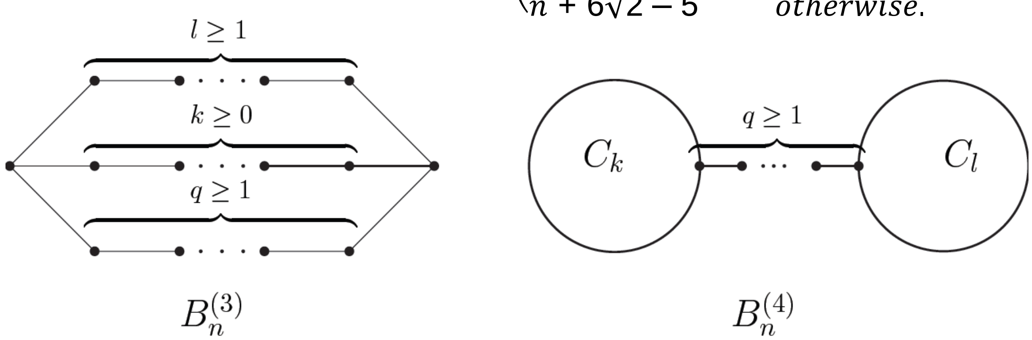

Figure 4. The graphs $B_n^{(3)}$ and $B_n^{(4)}$.

After simple comparison, we have

$$RRR\left(B_n^{(s)}\right) > \begin{cases} 3\left(\sqrt{n-3}+\sqrt{2}\right) = RRR\left(\tilde{B}_n\right) & for\ \ 6 \le n \le 9, \\ \sqrt{2}\left(\sqrt{n-5}+2\right)+6 = RRR\left(\hat{B}_n\right) & for\ \ 10 \le n \le 13, \\ 5\sqrt{2}+6 = RRR\left(\hat{B}_{14}\right) = RRR(B'_{14}) & for\ \ n = 14, \\ \sqrt{n-6}+3\left(2+\sqrt{2}\right) = RRR(B'_n) & for\ \ n \ge 15, \end{cases}$$

where $s = 3,4$. In what follows, we assume that $\delta(B_n) = 1$ and $\Delta(B_n) \le n-2$ where $n \ge 6$. Let $P(B_n) = \{u'_0, u'_1, u'_2, \ldots, u'_{p-1}\}$ be the set of all pendent vertices of B_n. For $0 \le i \le p-1$, suppose that $W_{u'_i}$ is the set of all those second neighbors of u'_i which are pendent. We choose a member of $P(B_n)$, say $u'_0 = u_0$ (without loss of generality), such that

1. the number of elements in W_{u_0} is as large as possible;
2. subject to (1), the first neighbor (say v_0) of u_0 has degree as small as possible (let $d_{v_0} = x$ and $N(v_0) = \{u_0, u_1, u_2, \ldots, u_{r-1}, u_r, \ldots, u_{x-1}\}$ where $d_{u_i} = 1$ for $0 \le i \le r-1$ and $d_{u_i} \ge 2$ for $r \le i \le x-1$);
3. subject to (1) and (2), $\sum_{i=r}^{x-1} d_{u_i}$ is as small as possible;
4. subject to (1), (2) and (3), $\max\{d_{u_r}, d_{u_{r+1}}, \ldots, d_{u_{x-1}}\}$ is as small as possible.

It is evident that $x \ge 2$. If B^*_{n-1} is the graph obtained from B_n by removing the vertex u_0, then

$$RRR(B_n) = RRR(B^*_{n-1}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\sum_{i=r}^{x-1} \sqrt{d_{u_i} - 1}. \tag{1}$$

Now, we have the following six cases: Case 1. $r \le x-3$; Case 2. $r = x-2$ and both of $d_{u_{x-2}}$ and $d_{u_{x-1}}$ are greater than 2; Case 3. $r = x-2$, one of $d_{u_{x-2}}$, $d_{u_{x-1}}$ is 2 and other is greater than 2; Case 4. $r = x-2$ and $d_{u_{x-2}} = d_{u_{x-1}} = 2$; Case 5. $r = x-1$ and $d_{u_{x-1}} > 2$; Case 6. $r = x-1$ and $d_{u_{x-1}} = 2$.

For $t = 1, 2, \ldots, 6$ and $n \ge 6$, let $\mathbb{B}_n^{(t)}$ be the collection of all those n-vertex connected bicyclic graphs which

- have at least one pendent vertex,
- have maximum vertex degree at most $n-2$ and
- fall in Case t.

Claim 1. If $B_n \in \mathbb{B}_n^{(1)}$, then $RRR(B_n) \ge 3\left(\sqrt{n-3} + \sqrt{2}\right)$ with equality if and only if $B_n \cong \tilde{B}_n$.

Proof of Claim 1. The claim will be proved by induction on n. For $n = 6$, the claim follows from Figure 5.

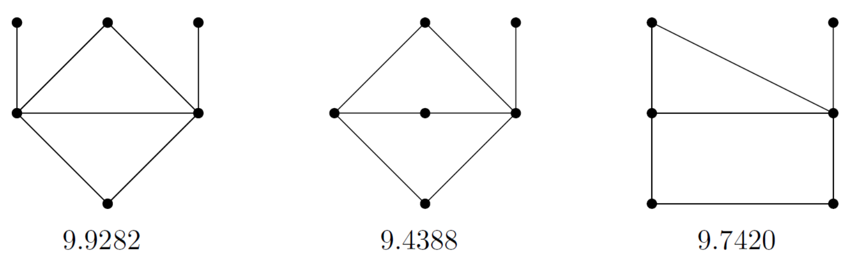

Figure 5. All the non-isomorphic members of $\mathbb{B}_6^{(1)}$ together with their RRR index.

Let us assume that $n \ge 7$. Bearing in mind the condition $r \le x-3$, inductive hypothesis and the fact $x \le n-2$, from Equation (1) we have

$$RRR(B_n) \geq RRR(\tilde{B}_{n-1}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)(x-r)$$
$$\geq 3(\sqrt{2} + \sqrt{n-4}) + 3\left(\sqrt{x-1} - \sqrt{x-2}\right)$$
$$\geq 3(\sqrt{2} + \sqrt{n-4}) + 3\left(\sqrt{n-3} - \sqrt{n-4}\right) = RRR(\tilde{B}_n).$$

The equality $RRR(B_n) = RRR(\tilde{B}_n)$ holds if and only if $x = n-2, x-r = 3$ and $B^*_{n-1} \cong \tilde{B}_{n-1}$, that is $B_n \cong \tilde{B}_n$. This completes the proof of Claim 1.

Remaining claims will also be proved by induction on n.

Claim 2. If $B_n \in \mathbb{B}_n^{(2)}$, then

$$RRR(B_n) \geq \begin{cases} RRR\left(B_n^{\dagger}\right) & if\ \ n = 6, \\ RRR\left(B_n^{(5)}\right) & if\ \ n \geq 7, \end{cases}$$

where the graphs $B_n^{\dagger}$ and $B_n^{(5)}$ are shown in Figure 6. The equalities $RRR(B_6) = RRR\left(B_6^{\dagger}\right)$ and $RRR(B_n) = RRR\left(B_n^{(5)}\right)$ (for≥ 7) hold if and only if $B_6 \cong B_6^{\dagger}$ and $B_n \cong B_n^{(5)}$ respectively.

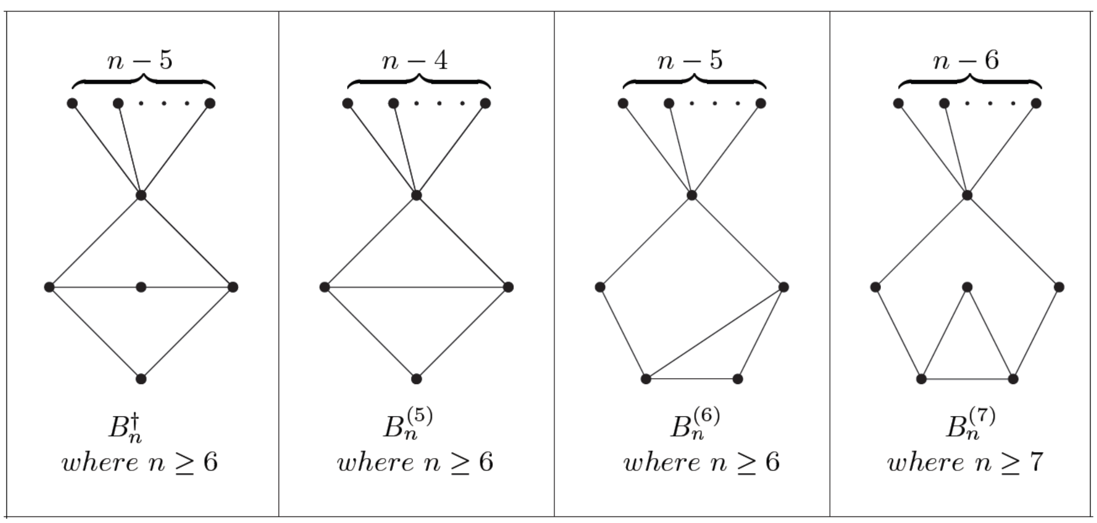

Figure 6. The graphs $B_n^{\dagger}$, $B_n^{(5)}$,$B_n^{(6)}$ and $B_n^{(7)}$.

Proof of Claim 2. For $n = 6$ and $n = 7$, the claim follows from Figures 7 and 8, respectively. Assume that $n \geq 8$. Using the inductive hypothesis in Equation (1), we get

$$\begin{aligned} RRR(B_n) &\geq RRR\left(B_{n-1}^{(5)}\right) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\left(\sqrt{d_{u_{x-2}} - 1} + \sqrt{d_{u_{x-1}} - 1}\right) \\ &\geq 2\left[1 + \sqrt{2} + \sqrt{2(n-4)}\right] + 2\sqrt{2}\left(\sqrt{x-1} - \sqrt{x-2}\right) \\ &\geq 2\left[1 + \sqrt{2} + \sqrt{2(n-4)}\right] + 2\sqrt{2}\left(\sqrt{n-3} - \sqrt{n-4}\right) = RRR\left(B_n^{(5)}\right). \end{aligned}$$

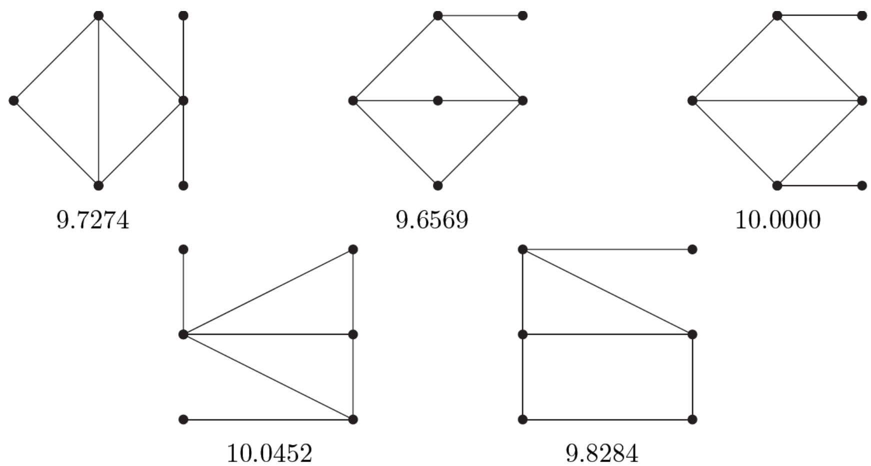

Figure 7. All the non-isomorphic members of $\mathbb{B}_6^{(2)}$ together with their RRR index.

The equality $RRR(B_n) = RRR\left(B_n^{(5)}\right)$ holds if and only if $x = n-2$, $d_{u_{x-1}} = d_{u_{x-2}} = 3$ and $B_{n-1}^* \cong B_{n-1}^{(5)}$.

Claim 3. If $B_n \in \mathbb{B}_n^{(3)}$, then $RRR(B_n) \geq RRR\left(B_n^{(6)}\right)$ with equality if and only if $B_n \cong B_n^{(6)}$, where the graph $B_n^{(6)}$ is shown in Figure 6.

Proof of Claim 3. The claim is obvious for $n = 6$, as Figure 9(a) suggests. Suppose that $n \geq 7$. It can be easily observed that $x \leq n-3$ because $B_n \in \mathbb{B}_n^{(3)}$. From Equation (1), it follows that

$$\begin{aligned} RRR(B_n) &\geq RRR(B_{n-1}^{(6)}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\left(\sqrt{d_{u_{x-2}} - 1} + \sqrt{d_{u_{x-1}} - 1}\right) \\ &\geq (1 + \sqrt{2})\left(\sqrt{n-5} + \sqrt{x-1} - \sqrt{x-2}\right) + 2 + 3\sqrt{2} \\ &\geq (1 + \sqrt{2})\sqrt{n-4} + 2 + 3\sqrt{2} = RRR\left(B_n^{(6)}\right). \end{aligned}$$

We note that the equality $RRR(B_n) = RRR\left(B_n^{(6)}\right)$ holds if and only if $x = n-3$, one of $d_{u_{x-2}}, d_{u_{x-1}}$ is 2 and other is 3, and $B_{n-1}^* \cong B_{n-1}^{(6)}$.

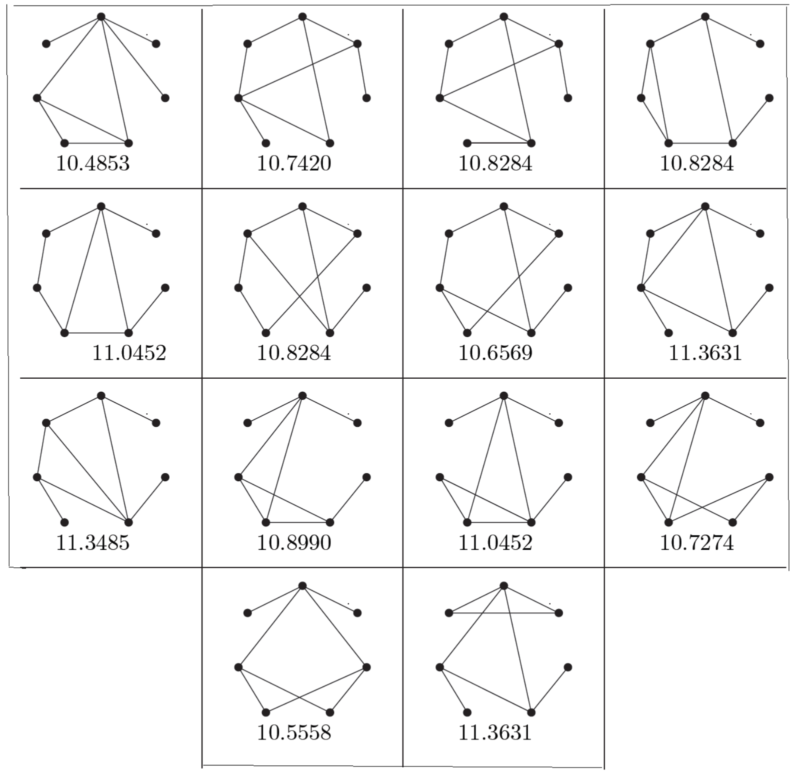

Figure 8. All the non-isomorphic members of $\mathbb{B}_7^{(2)}$ together with their RRR index.

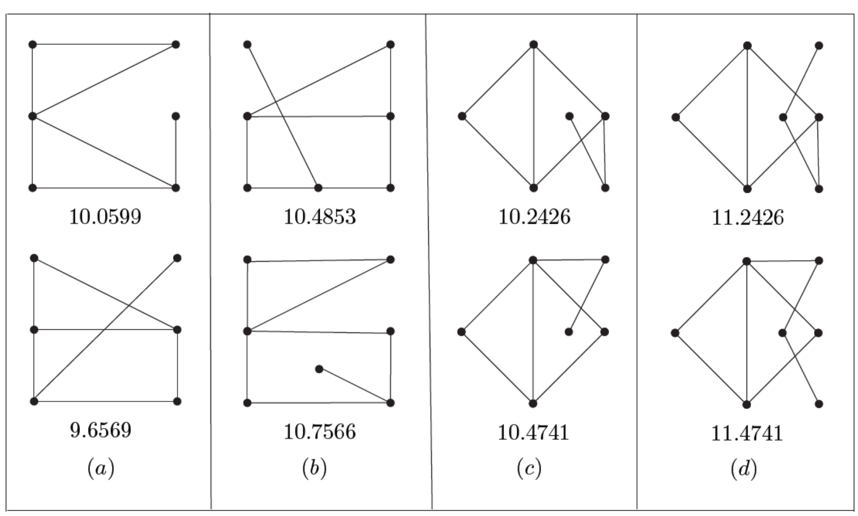

Figure 9. Parts (a), (b), (c), (d) correspond to the all non-isomorphic elements of $\mathbb{B}_6^{(3)}, \mathbb{B}_7^{(4)}, \mathbb{B}_6^{(5)}, \mathbb{B}_7^{(6)}$, respectively, together with their RRR index.

Claim 4. If $B_n \in \mathbb{B}_n^{(4)}$, then $RRR(B_n) \geq RRR\left(B_n^{(7)}\right)$ with equality if and only if $B_n \cong B_n^{(7)}$, where the graph $B_n^{(7)}$ is depicted in Figure 6.

Proof of Claim 4. We observe that the collection $\mathbb{B}_6^{(4)}$ is empty. For $n = 7$, the claim follows from Figure 9(b). Now, we assume that $n \geq 8$. It is evident that $x \leq n-4$ as $B_n \in \mathbb{B}_n^{(4)}$. From Equation (1), it follows that

$$RRR(B_n) \geq RRR\left(B_{n-1}^{(7)}\right) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\left(\sqrt{d_{u_{x-1}} - 1} + \sqrt{d_{u_{x-2}} - 1}\right)$$

$$= 2\sqrt{n-6} + 4\sqrt{2} + 2 + 2\left(\sqrt{x-1} - \sqrt{x-2}\right)$$

$$\geq 2\sqrt{n-5} + 4\sqrt{2} + 2 = RRR\left(B_n^{(7)}\right).$$

The equality $RRR(B_n) = RRR(B_n^{(7)})$ holds if and only if $x = n-4$ and $B_{n-1}^{*} \cong B_{n-1}^{(7)}$.

Claim 5. If $B_n \in \mathbb{B}_n^{(5)}$, then $RRR(B_n) \geq \sqrt{2}\left(\sqrt{n-5} + 2\ \right) + 6$ with equality if and only if $B_n \cong \hat{B}_n$.

Proof of Claim 5. From Figure 9(c), we conclude that the claim holds for $n = 6$. Now, let $n \geq 7$. The definition of $\mathbb{B}_n^{(5)}$ guaranties that $x \leq n-4$. Equation (1) implies that

$$RRR(B_n) \geq RRR(\hat{B}_{n-1}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\sqrt{d_{u_{x-1}} - 1}$$

$$\geq \sqrt{2}\left(\sqrt{n-6} + \sqrt{x-1} - \sqrt{x-2} + 2\ \right) + 6$$

$$\geq \sqrt{2}\left(\sqrt{n-5} + 2\ \right) + 6 = RRR(\hat{B}_n).$$

The equation $RRR(B_n) = RRR(\hat{B}_n)$ holds if and only if $x = n-4, d_{u_{x-1}} = 3$ and $B_{n-1}^{*} \cong \hat{B}_{n-1}$.

Claim 6. If $B_n \in \mathbb{B}_n^{(6)}$, then $RRR(B_n) \geq RRR(B_n')$ with equality if and only if $B_n \cong B_n'$.

Proof of Claim 6. Obviously, the collection $\mathbb{B}_6^{(6)}$ is empty. For $n = 7$, the claim follows from Figure 9(d). Let us assume that $n \geq 8$. Clearly, it holds that $x \leq n - 5$ because $B_n \in \mathbb{B}_n^{(6)}$. From Equation (1), we have

$$RRR(B_n) \geq RRR(B'_{n-1}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\sqrt{d_{u_{x-1}} - 1}$$

$$= \sqrt{n-7} + 3(2+\sqrt{2}) + \sqrt{x-1} - \sqrt{x-2}$$

$$\geq \sqrt{n-6} + 3(2+\sqrt{2}) = RRR(B'_n).$$

The equality $RRR(B_n) = RRR(B'_n)$ holds if and only if $x = n - 5$ and $B^*_{n-1} \cong B'_{n-1}$.

For $n \geq 6$, if a graph G has minimum RRR index among all n-vertex connected bicyclic graphs then, Claims 1-6 guaranty that the graph G must belongs to the collection $\{\tilde{B}_n, B_6^{\dagger}, B_n^{(5)}, B_n^{(6)}, B_n^{(7)}, \hat{B}_n, B'_n\}$. But, the RRR index of the graphs $\tilde{B}_n, B_6^{\dagger}, B_n^{(5)}, B_n^{(6)}, B_n^{(7)}, \hat{B}_n, B'_n$ are given as

$$RRR\left(B_6^{\dagger}\right) = 4(\sqrt{2}+1), \quad RRR(\tilde{B}_n) = 3\left(\sqrt{n-3} + \sqrt{2}\right),$$

$$RRR(\hat{B}_n) = \sqrt{2}\left(\sqrt{n-5} + 2\right) + 6, \quad RRR(B'_n) = \sqrt{n-6} + 3(2+\sqrt{2}),$$

$$RRR\left(B_n^{(5)}\right) = 2\left(1 + \sqrt{2} + \sqrt{2(n-3)}\right),$$

$$RRR\left(B_n^{(6)}\right) = (1+\sqrt{2})\sqrt{n-4} + 2 + 3\sqrt{2},$$

$$RRR\left(B_n^{(7)}\right) = 2\sqrt{n-5} + 4\sqrt{2} + 2.$$

After elementary comparison, we get the desired result. ■

The following corollary is a direct consequence of Theorem 1.

Corollary 1. *For $n \geq 5$, if B_n is any n-vertex connected bicyclic graph then the following inequalities hold:*

$$RRR(B_n) \geq \begin{cases} 3\left(\sqrt{n-3} + \sqrt{2}\right) & if \;\; n \leq 9, \\ \sqrt{2}\left(\sqrt{n-5} + 2\right) + 6 & if \;\; 10 \leq n \leq 13, \\ 5\sqrt{2} + 6 & if \;\; n = 14, \\ \sqrt{n-6} + 3(2+\sqrt{2}) & if \;\; n \geq 15. \end{cases}$$

The equality sign in the first, second and fourth inequality holds if and only if $B_n \cong \tilde{B}_n$, $B_n \cong \hat{B}_n$ and $B_n \cong B'_n$ respectively, where the graphs $\tilde{B}_n$, $\hat{B}_n$ and B'_n are depicted in Figure 1. Also, the equality sign in the third inequality holds if and only if either $B_n \cong \hat{B}_n$ or $B_n \cong B'_n$.

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