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A note on the minimum reduced reciprocal Randić index of n-vertex unicyclic graphs

Akbar Ali[1,2,*], Akhlaq A. Bhatti[1]

[1]*Dept. of Sciences & Humanities, National University of Computer & Emerging Sciences, B-Block, Faisal Town, Lahore-Pakistan*

[2]*Dept. of Mathematics, University of Management & Technology, Sialkot-Pakistan*

[*]*Corresponding author: akbarali.maths@gmail.com*

Abstract

Recent studies show that the reduced reciprocal Randić (RRR) index possesses the second-best correlating ability among the several well known topological indices. Hence, it is meaningful to study the mathematical properties of the RRR index, especially bounds and characterization of the extremal elements for renowned graph families. In the present note, the unicyclic graph having minimum RRR index is characterized among the class of all n-vertex unicyclic graphs.

Keywords: Reduced reciprocal Randic′ index; topological index; unicyclic graph.

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1. Introduction

All the graphs considered in the present study are simple, finite, undirected and connected. The *vertex set* and *edge set* of a graph G will be denoted by $V(G)$ and $E(G)$ respectively. The *degree of a vertex* $u \in V(G)$ and the *edge* connecting the vertices u and v will be denoted by d_u and uv respectively. If $uv, vw \in E(G)$ but $uw \in E(G)$, then we call v and w as the *first neighbor* of u and *second neighbor* of u, respectively. The set of all first neighbors of a vertex $v \in V(G)$ will be denoted by $N(v)$. The vertices $u, v \in V(G)$ are said to be disconnected, if there does not exist any path between u and v in G. Undefined notations and terminologies from (chemical) graph theory can be found in (Harary, 1969; Trinajstić, 1992).

Topological indices are numerical quantities of a graph, which are invariant under graph isomorphisms. Randić (1975) proposed the following topological index:

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

for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons and he named it as *branching index*. Nowadays, this topological index is also known as *connectivity index* and *Randić index*. According to Gutman (2013), “Randić index is the most investigated, most often applied, and most popular among all topological indices. Hundreds of papers and a few books are devoted to this topological index”.

Many physico-chemical properties of chemical structures are dependent on the factors different from branching. In order to take these factors into account, Estrada *et al.* (1998) introduced a modified version of the Randić index and called it as *atom-bond connectivity (ABC)* index. This index is defined as:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

Details about the chemical applicability and mathematical properties of this index can be found in the survey (Gutman, 2013), papers (Ahmadi *et al.*, 2014; Dimitrov, 2014; Goubko *et al.*, 2015; Palcios, 2014; Raza *et al.*, 2016) and related references cited therein.

Inspired by work on the ABC index, Furtula *et al.* (2010) gave the following modified version of the ABC index (and hence a modified version of Randić index) under the name *augmented Zagreb index* (AZI):

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3.$$

The prediction power of AZI is better than ABC index in the study of heat of formation for heptanes and octanes (Furtula *et al.*, 2010). Details about this index can be found in the survey (Gutman, 2013), recent papers (Ali *et* *al.*, 2016a; Ali *et al.*, 2016b; Huang & Liu, 2015; Zhan *et al.*, 2015) and related references cited therein.

In Manso *et al.* (2012), a new topological index (namely *Fi* index) was proposed to predict the normal boiling point temperatures of hydrocarbons. In the mathematical definition of *Fi* index two terms are present. Gutman *et al.* (2014), recently, 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 named it as *reduced reciprocal Randić* (RRR) *index*. In the current study, we are concerned with this recently introduced modified version of the Randić index. In order to get some preliminary information on whether this index possesses any potential applicability in chemistry (especially in quantitative structure-property relationship and quantitative structure-activity relationship studies), Gutman *et al.* (2014) tested the correlating ability of several well known degree based topological indices (along with RRR index) for the case of standard heats (enthalpy) of formation and normal boiling points of octane isomers, and they concluded that AZI and RRR index has the best and second-best, respectively, correlating ability among the examined topological indices. It is worth mentioning here that among the examined topological indices, ABC index was also included which was the second-best topological index among some well known degree based topological indices according to the earlier study (Gutman & Tošović, 2013).

In Gutman *et al.* (2014), the structure of n-vertex tree having maximum RRR index and extremal n-vertex graphs with respect to RRR index were reported. The main purpose of the present note is to characterize the n-vertex unicyclic graph having minimum RRR index over the collection of all n-vertex unicyclic graphs. An n-vertex (connected) graph is called unicyclic, if it has n edges. Some extremal results for the unicyclic graphs with respect to Randić index, ABC index and AZI can be found in the papers (Gan *et al.*, 2011; Gao & Lu, 2005; Pan *et al.*, 2006; Zhan *et al.*, 2015).

2. Main result

Denote by S_n^+ the unique n-vertex unicyclic graph obtained from the n-vertex star graph S_n by adding an edge between any two pendent vertices. Many topological indices (for example ABC index, Randić index, AZI), which have S_n as an extremal graph over the set of all n-vertex trees, have also S_n^+ as an extremal graph over the set of all n-vertex unicyclic graphs. However, different approaches required to prove these results. From the definition of RRR index, it can be easily seen that $RRR(T_n) \geq RRR(S_n)$ where T_n is any n-vertex tree. Is it true that the graph S_n^+ has minimum RRR index over the set of all n-vertex unicyclic graphs? The answer is not positive. For the n-vertex unicyclic graph H_n^+ depicted in Figure 1(b), one have

$$RRR(H_n^+) = 1 + \sqrt{2}(2 + \sqrt{n-4}\,).$$

But on the other hand, $RRR(S_n^+) = 1 + 2\sqrt{n-2}$ and

$$RRR(S_n^+)\begin{cases} < RRR(H_n^+) & \text{if } 5 \leq n \leq 19, \\ = RRR(H_n^+) & \text{if } n = 20, \\ > RRR(H_n^+) & \text{if } n \geq 21. \end{cases}$$

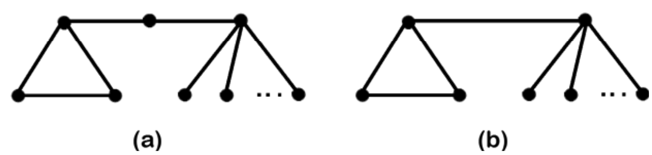

Fig. 1. (a) The n-vertex unicyclic graph H_n where n is at least 6. (b) The n-vertex unicyclic graph H_n^+ where n is at least 5.

The following theorem gives characterization of the n-vertex unicyclic graph having minimum RRR index over the collection of all n-vertex unicyclic graphs for $n \geq 4$.

Theorem 1. *For any n-vertex unicyclic graph U_n (where $n \geq 4$), the following inequalities hold:*

$$RRR(U_n)\begin{cases} \geq 1 + 2\sqrt{n-2} & \text{if } 4 \leq n \leq 16, \\ \geq 1 + 3\sqrt{2} + \sqrt{n-5} & \text{if } n \geq 17. \end{cases}$$

The equality sign in the first inequality holds if and only if $U_n \cong S_n^+$ and the equality sign in the second inequality holds if and only if $U_n \cong H_n$, where H_n is shown in Figure 1(a).

Proof. If U_n is the cycle graph. Then, routine computation yields $RRR(U_n) = n > 1 + 2\sqrt{n-2}$ for all $n \geq 4$ and $RRR(U_n) = n > 1 + 3\sqrt{2} + \sqrt{n-5}$ for all $n \geq 7$. Assume that U_n is not isomorphic to the cycle graph. Let $P(U_n) = \{u'_0, u'_1, u'_2, \ldots, u'_{p-1}\}$ be the set of all pendent vertices in U_n. For $0 \leq i \leq p-1$, suppose that $W_{u'_i}$ is the set of all those second neighbors of u'_i which are pendent. Choose a member of $P(U_n)$, 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.

3. subject to (1) and (2), the sum of degrees of first neighbors of v_0 is as small as possible.

Let $N(v_0) = \{u_0, u_1, u_2, \dots, u_{r-1}, u_r, \dots, u_{x-1}\}$ where $d_{u_i} = 1$ for $0 \le i \le r-1$ and $d_{u_i} \ge 2$ for $r \le i \le x-1$ (see Figure 2).

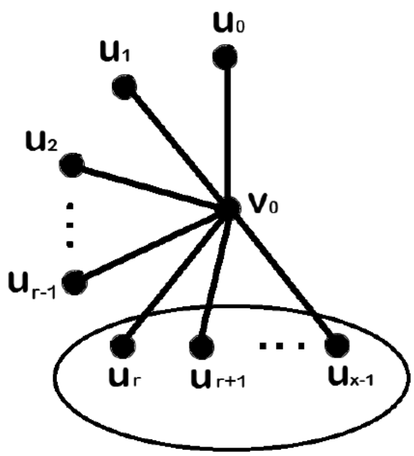

Fig. 2. The presentation of an n-vertex unicyclic graph U_n used in the proof of Theorem 1.

If U'_{n-1} is the graph obtained from U_n by removing the vertex u_0, then

$$RRR(U_n) = RRR(U'_{n-1}) + \sum_{i=1}^{x-1} \sqrt{(x-1)(d_{u_i}-1)} - \sum_{i=1}^{x-1} \sqrt{(x-2)(d_{u_i}-1)} \quad (1)$$

We will discuss three cases:

Case 1. Either the vertex v_0 is adjacent with at least two non-pendent vertices or v_0 is adjacent with exactly one non-pendent vertex, say u_{x-1} such that $d_{u_{x-1}} \ge 5$ (that is either $r \le x-2$ or $r = x-1, d_{u_{x-1}} \ge 5$).

Let $\mathcal{U}_n^{(1)}$ be the collection of all those n-vertex unicyclic graphs (different from the cycle graph) which fall in this case. By using induction on n, we will prove that the only one graph, namely S_n^+, has the minimum RRR value among all the members of $\mathcal{U}_n^{(1)}$. Then the desired result will follow from the fact that

$$RRR(S_n^+) = 1 + 2\sqrt{n-2} > 1 + 3\sqrt{2} + \sqrt{n-5} = RRR(H_n) \quad \text{for all } n \ge 17.$$

For $n = 4$, there are only two non-isomorphic unicyclic graphs namely C_n and S_n^+ and hence the result holds for $n = 4$. For $n = 5$, all the non-isomorphic members of $\mathcal{U}_n^{(1)}$ are depicted in the Figure 3 along with their RRR values.

Fig. 3. All the non-isomorphic members of $\mathcal{U}_5^{(1)}$ together with their RRR values.

Now, suppose that $U_n \in \mathcal{U}_n^{(1)}$ and $n \ge 6$. By virtue of inductive hypothesis and from Equation (1), one have

$$RRR(U_n) \ge 1 + 2\sqrt{n-3} + \left(\sqrt{x-1} - \sqrt{x-2}\right) \sum_{i=1}^{x-1} \sqrt{d_{u_i} - 1} \quad (2)$$

with equality if and only if $U'_{n-1} \cong S_{n-1}^+$. We discuss two subcases:

Subcase 1.1. If $r \ge 2$. From Inequality (2) it follows that

$$RRR(U_n) \ge 1 + 2\sqrt{n-3} + \left(\sqrt{x-1} - \sqrt{x-2}\right) \sum_{i=\mathrm{r}}^{x-1} \sqrt{d_{u_i} - 1} \quad (3)$$

According to the definition of $U_n \in \mathcal{U}_n^{(1)}$, either $r \le x-2$ or $r = x-1, d_{u_{x-1}} \ge 5$. If $r \le x-2$, then Inequality (3) implies that

$$RRR(U_n) \ge 1 + 2\sqrt{n-3} + \left(\sqrt{x-1} - \sqrt{x-2}\right)(x-r)$$

$$\geq 1 + 2\sqrt{n-3} + 2\left(\sqrt{x-1} - \sqrt{x-2}\right)$$
$$\geq 1 + 2\sqrt{n-3} + 2\left(\sqrt{n-2} - \sqrt{n-3}\right)$$
$$= 1 + 2\sqrt{n-2}.$$

The equality $RRR(U_n) = 1 + 2\sqrt{n-2}$ holds if and only if $x = n-1, x-r = 2$, $d_{u_i} = 2$ for all $i \geq r$ and $U'_{n-1} \cong S^+_{n-1}$.

If $r = x - 1$ and $d_{u_{x-1}} \geq 5$, then $x < n-2$ and the graph U'_{n-1} must be different from S^+_{n-1}, and hence from Equation (1) one have

$$RRR(U_n) > 1 + 2\sqrt{n-3}$$
$$+2\left(\sqrt{x-1} - \sqrt{x-2}\right)$$
$$> 1 + 2\sqrt{n-3}$$
$$+2\left(\sqrt{n-3} - \sqrt{n-4}\right)$$
$$> 1 + 2\sqrt{n-2}.$$

Subcase 1.2. If $r = 1$. Then, either $x \geq 3$ or $x = 2, d_{u_1} \geq 5$. From the definition of u_0, it follows that the set $W_{u'_i}$ is empty for all $u'_i \in P(U_n)$. It means that no two pendent edges are adjacent.

If $x \geq 4$, then among the vertices $u_1, u_2, \ldots, u_{x-1}$ at least two are disconnected in $U_n - v_0$ (because otherwise U_n contains more than one cycle, a contradiction. The graphs $U_n - v_0$ and U_n considered in this subcase are shown in Figure 4).

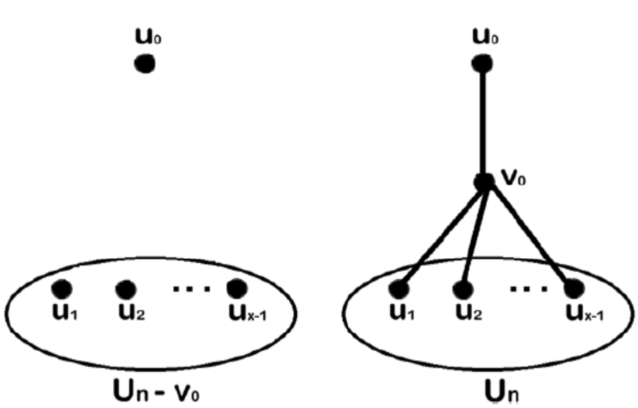

Fig. 4. The graphs U_n and $U_n - v_0$ used in Subcase 1.2 of the proof of Theorem 1.

Without loss of generality, let u_1 and u_2 be disconnected in $U_n - v_0$ and suppose that C_j (for $j = 1,2$) is the component of $U_n - v_0$ containing u_j. Since $d_{u_i} \geq 2$ in U_n for all $i \geq 1$, so both the components C_1 and C_2 must be non-trivial. Note that at least one of the components C_1 and C_2, (say C_1) contains a pendent vertex which must not be a member of $N(v_0)$. Also, recall that no two pendent edges of U_n are adjacent. This implies that there exist $w_1 \in V(C_1) \cap P(U_n)$ and $w_1w_2 \in E(C_1) \cap E(U_n)$ such that degree of w_2 in U_n is at most 3, which contradicts the definition of u_0. Hence $x = 2$ or 3. It can be easily noted that the graph U'_{n-1} is different from S^+_{n-1} in this subcase. Now, we consider further two subcases:

Subcase 1.2.1. If $x = 3$. Then, from Equation (1) it follows that

$$RRR(U_n) > 1 + 2\sqrt{n-3}$$
$$+\left(\sqrt{2} - 1\right)\left(\sqrt{d_{u_1} - 1} + \sqrt{d_{u_2} - 1}\right)$$
$$\geq 1 + 2\sqrt{n-3} + 2\left(\sqrt{2} - 1\right)$$
$$> 1 + 2\sqrt{n-2}, \quad \text{because} \quad n \geq 6.$$

Subcase 1.2.2. If $x = 2$ and $d_{u_1} \geq 5$. Then, from Equation (1) we have

$$RRR(U_n) > 1 + 2\sqrt{n-3} + \sqrt{d_{u_1} - 1}$$
$$\geq 3 + 2\sqrt{n-3} > 1 + 2\sqrt{n-2}.$$

Therefore, for any $U_n \in \mathcal{U}_n^{(1)}$ we have $RRR(U_n) \geq RRR(S^+_n)$ with equality if and only if $U_n \cong S^+_n$.

Case 2. The vertex v_0 is adjacent with exactly one non-pendent vertex, say u_{x-1} such that $d_{u_{x-1}} = 3$ or 4 (that is $r = x - 1$ and $d_{u_{x-1}} = 3$ or 4).

Let $\mathcal{U}_n^{(2)}$ be the family of all those n-vertex unicyclic graphs (different from the cycle graph) which fall in this case. Note that n must be at least 5 in this case. By using induction on n, we will prove that the only one graph, namely H^+_n, has the minimum RRR value among all the members of $\mathcal{U}_n^{(2)}$. Then the desired result will follow from the following fact:

$$RRR(H^+_n) = 1 + 2\sqrt{2} + \sqrt{2(n-4)}$$
$$> \begin{cases} 1 + 2\sqrt{n-2} \text{ for } 5 \leq n \leq 16, \\ 1 + 3\sqrt{2} + \sqrt{n-5} \text{ for } n \geq 17. \end{cases}$$

It can be easily seen that $\mathcal{U}_5^{(2)}$ has only one element, namely H_5^+. Also, all the non-isomorphic members of $\mathcal{U}_6^{(2)}$ are depicted in the Figure 5 along with their RRR values.

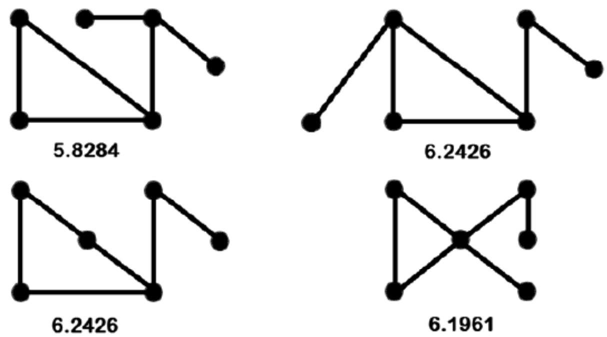

Fig. 5. All the non-isomorphic members of $\mathcal{U}_6^{(2)}$ together with their *RRR* values.

Hence the result holds for $n = 5$ and $n = 6$. Suppose that $U_n \in \mathcal{U}_n^{(2)}$ and $n \geq 7$. By using the inductive hypothesis in Equation (1), we have

$$RRR(U_n) \geq 1 + 2\sqrt{2} + \sqrt{2(n-5)} + \left(\sqrt{x-1} - \sqrt{x-2}\right)\sqrt{d_{u_{x-1}} - 1} \quad (4)$$

with equality if and only if $U'_{n-1} \cong H_{n-1}^+$. It can be easily observed that $x \leq n-3$. According to the definition of $U_n \in \mathcal{U}_n^{(2)}$, $d_{u_{x-1}} = 3$ or 4. Hence from Inequality (4), it follows that

$$\begin{aligned} RRR(U_n) &\geq 1 + 2\sqrt{2} + \sqrt{2(n-5)} \\ &\quad + \sqrt{2}\left(\sqrt{x-1} - \sqrt{x-2}\right) \\ &\geq 1 + 2\sqrt{2} + \sqrt{2(n-5)} \\ &\quad + \sqrt{2}\left(\sqrt{n-4} - \sqrt{n-5}\right) \\ &= 1 + 2\sqrt{2} + \sqrt{2(n-4)}. \end{aligned}$$

The equality $RRR(U_n) = 1 + 2\sqrt{2} + \sqrt{2(n-4)}$ holds if and only if $x = n-3$, $d_{u_{x-1}} = 3$ and $U'_{n-1} \cong H_{n-1}^+$.

Therefore, for any $U_n \in \mathcal{U}_n^{(2)}$ we have $RRR(U_n) \geq RRR(H_n^+)$ with equality if and only if $U_n \cong H_n^+$.

Case 3. The vertex v_0 is adjacent with exactly one non-pendent vertex, say u_{x-1} such that $d_{u_{x-1}} = 2$ (in other words, $r = x-1$ and $d_{u_{x-1}} = 2$).

Let $\mathcal{U}_n^{(3)}$ be the class of all those n-vertex unicyclic graphs (different from the cycle graph) which fall in this case. Note that n must be at least 6 in this case. By using induction on n, we will prove that the only one graph, namely H_n, has the minimum RRR value among all the members of $\mathcal{U}_n^{(3)}$. Then the desired result will follow from the following inequality

$$\begin{aligned} RRR(H_n) &= 1 + 3\sqrt{2} + \sqrt{n-5} \\ &> 1 + 2\sqrt{n-2} \quad \text{for} \quad 6 \leq n \leq 16. \end{aligned}$$

It can be easily seen that $\mathcal{U}_6^{(3)}$ has only one member, namely H_6. Also, all the non-isomorphic members of $\mathcal{U}_7^{(3)}$ are depicted in the Figure 6 along with their RRR values.

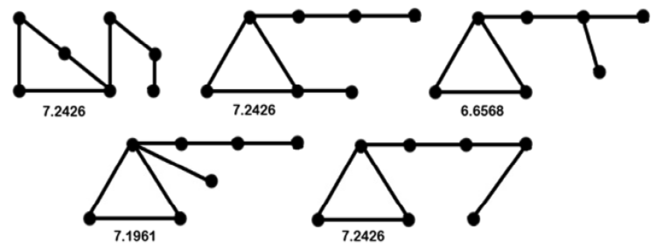

Fig. 6. All the non-isomorphic members of $\mathcal{U}_7^{(3)}$ together with their *RRR* values.

Hence the result holds for $n = 6$ and $n = 7$. Suppose that $U_n \in \mathcal{U}_n^{(3)}$ and $n \geq 8$. Bearing in mind the inductive hypothesis and the fact $d_{u_{x-1}} = 2$, from Equation (1) one have

$$RR(U_n) \geq 1 + 3\sqrt{2} + \sqrt{n-6} + \left(\sqrt{x-1} - \sqrt{x-2}\right) \quad (5)$$

with equality if and only if $U'_{n-1} \cong H_{n-1}$. It should be noted that $x \leq n-4$. From Inequality (5), it follows that

$$RRR(U_n) \geq 1 + 3\sqrt{2} + \sqrt{n-5}.$$

The equality $RRR(U_n) = 1 + 3\sqrt{2} + \sqrt{n-5}$ holds if and only if $x = n-4$ and $U'_{n-1} \cong H_{n-1}$.

Therefore, for any $U_n \in \mathcal{U}_n^{(3)}$ we conclude that $RRR(U_n) \geq RRR(H_n)$ where the equality sign holds if and only if $U_n \cong H_n$. This completes the proof.

3. Conclusion

We have studied an extremal graph theoretical problem related to a recently introduced graph invariant, *reduced reciprocal Randić* (*RRR*) *index*,which possesses potential applicability in chemistry (especially in quantitative structure-property relationship and quantitative structure-activity relationship studies). More precisely, we have proved that the unique graph S_n^+ (obtained from the n-vertex star graph S_n by adding an edge between any two pendent vertices) has the minimum RRR index in the collection of all n-vertex unicyclic graphs for $4 \leq n \leq 16$ and the unique graph H_n (depicted in Figure 1(a)) has the minimum RRR index in the before said collection for $n \geq 17$. It seems that the presented proof technique also works for charactering graphs with minimum RRR index among all n-vertex bicyclic graphs. Thereby, it would be interesting to characterize these aforementioned bicyclic graphs with respect to the RRR index in future.

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نُبذة حول الحد الأدنى من مؤشر رانديك (Randić) المتبادل المُخفَض لرسومات ن-فرتكس (n-vertex) البيانية أحادية الدورة

أكبر علي[1,2,*]، [1]أخلاق بهاتي
[1]قسم العلوم والعلوم الإنسانية، الجامعة الوطنية للحاسوب والعلوم الناشئة، بلوك ب،
مدينة فيصل، لاهور – باكستان
[2]قسم الرياضيات، جامعة الإدارة والتكنولوجيا، سايلكوت، باكستان
akbarali.maths@gmail.com

خلاصة

تُبين الدراسات الحالية أن مؤشر رانديك (Randić) المُتبادل المُخفَض (RRR) لديه ثاني أفضل قدرة ربط بين العديد من المؤشرات الطبوغرافية المعروفة. لذلك، فمن المُجدي دراسة الخصائص الرياضية لمؤشر رانديك المُتبادل المُخفض (RRR)، وخصوصاً حدود وخصائص عناصر القيم القصوى لعائلات رسوم بيانية مشهورة. في النُبذة الحالية، يُميز الرسم البياني أحادي الدورة الذي لديه الحد الأدنى من مؤشر رانديك المُتبادل المُخفض (RRR) بين أوساط جميع رسوم ن- فرتكس (n-vertex) البيانية أحادية الدورة.