

Augmented Sombor and Augmented Revan Sombor Indices of Certain Families of Benzenoid Systems

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Abstract: Chemical Graph Theory is a branch of Mathematical Chemistry whose focus of interest is to finding topological indices of molecular graph which correlate well with chemical properties of the chemical molecules. In this paper, we introduce the augmented Revan Sombor and reciprocal augmented Revan Sombor indices of a graph. Also we determine the augmented Revan Sombor and reciprocal augmented Revan Sombor indices of triangular benzenoids, benzenoid rhombus, benzenoid hourglass and jagged rectangle benzenoid systems.

KEYWORDS: augmented Revan Sombor index, reciprocal augmented Revan Sombor index, benzenoid.

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I. Introduction

A molecular graph is a graph such that the vertices correspond to atoms and the edges to the bonds. Chemical Graph Theory is branch of Mathematical Chemistry which has an important effect on the development of the Chemical Sciences, see [1, 2].

In this paper, we consider only a finite, simple connected graph G with a vertex set $V(G)$ and an edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v . Let $\Delta(G)$ ($\delta(G)$) denote the maximum (minimum) degree among the vertices of G . The Revan vertex degree of a vertex v in G is defined as $r_G(v) = \Delta(G) + \delta(G) - d_G(v)$. The Revan edge connecting the Revan vertices u and v will be denoted by uv . For other undefined notations and terminologies, we refer [3].

The augmented Sombor index [4] of a graph G is defined as

$$ASO(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u)^2 + d_G(v)^2}{d_G(u) + d_G(v) - 2}}$$

Recently, some augmented indices were studied, for example, in [5, 6, 7, 8, 9, 10].

We now introduce the augmented Revan Sombor index, defined as

$$ARSO(G) = \sum_{uv \in E(G)} \sqrt{\frac{r_G(u)^2 + r_G(v)^2}{r_G(u) + r_G(v) - 2}}$$

We define the reciprocal augmented Revan Sombor index as

$$RARSO(G) = \sum_{uv \in E(G)} \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u)^2 + r_G(v)^2}}$$

We consider some families of benzenoid systems. In this paper, the augmented Sombor index, augmented Revan Sombor index and reciprocal augmented Revan Sombor index of triangular benzenoids, benzenoid rhombus, benzenoid hourglass and jagged rectangle benzenoid systems are determined.

II. Results for Triangular Benzenoids

In this section, we consider the graph of triangular benzenoid T_p where p is the number of hexagons in the base graph. Clearly T_p has $\frac{1}{2}p(p+1)$ hexagons. The graph of triangular benzenoid T_4 is presented in Figure 1.

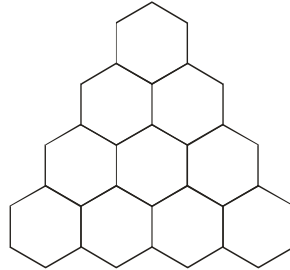


Figure 1. The graph of triangular benzenoid T_4 .

Let G be the graph of a triangular benzenoid T_p . The graph G has $p^2 + 4p + 1$ vertices and $\frac{3}{2}p(p+3)$ edges. From Figure 1, it is easy to see that the vertices of T_p are either of degree 2 or 3. Therefore $\Delta(G)=3$ and $\delta(G)=2$. Thus $r_G(u) = \Delta(G) + \delta(G) - d_G(u) = 5 - d_G(u)$. By algebraic method, we obtain that the edge set $E(G)$ can be divided into three partitions:

$$\begin{aligned} E_{22} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}, & |E_{22}| &= 6. \\ E_{23} &= \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}, & |E_{23}| &= 6p - 6. \\ E_{33} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, & |E_{33}| &= \frac{3}{2}p(p-1). \end{aligned}$$

Thus there are three types of Revan edges based on the degree of end Revan vertices of each Revan edge as given in Table 1.

$r_G(u), r_G(v) \setminus e = uv \in E(G)$	(3, 3)	(3, 2)	(2, 2)
Number of edges	6	$6p - 6$	$\frac{3}{2}p(p-1)$

Table 1. Revan edge partition of T_p

Theorem 1. Let T_p be the triangular benzenoid. Then

$$ASO(G) = \frac{3}{2}\sqrt{\frac{9}{2}}p^2 + \frac{3}{2}\sqrt{\frac{13}{3}}p - \frac{3}{2}\sqrt{\frac{9}{2}}p + 6\sqrt{4} - 6\sqrt{\frac{13}{3}}.$$

Proof: Let G be the graph of a triangular benzenoid T_p .

The augmented Sombor index of T_p is

$$\begin{aligned} ASO(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d_G(u)^2 + d_G(v)^2}{d_G(u) + d_G(v) - 2}} \\ &= 6\sqrt{\frac{2^2 + 2^2}{2+2-2}} + (6p-6)\sqrt{\frac{2^2 + 3^2}{2+3-2}} + \frac{3}{2}p(p-1)\sqrt{\frac{3^2 + 3^2}{3+3-2}} \\ &= \frac{3}{2}\sqrt{\frac{9}{2}}p^2 + \frac{3}{2}\sqrt{\frac{13}{3}}p - \frac{3}{2}\sqrt{\frac{9}{2}}p + 6\sqrt{4} - 6\sqrt{\frac{13}{3}}. \end{aligned}$$

Theorem 2. Let T_p be the triangular benzenoid. Then

$$ARSO(G) = 3p^2 + 6\sqrt{\frac{13}{3}}p - 3p + 6\sqrt{\frac{9}{2}} - 6\sqrt{\frac{13}{3}}$$

Proof: Let G be the graph of a triangular benzenoid T_p .

The augmented Revan Sombor index of T_p is

$$\begin{aligned} ARSO(G) &= \sqrt{\frac{r_G(u)^2 + r_G(v)^2}{r_G(u) + r_G(v) - 2}} \\ &= 6\sqrt{\frac{3^2 + 3^2}{3 + 3 - 2}} + (6p - 6)\sqrt{\frac{2^2 + 3^2}{2 + 3 - 2}} + \frac{3}{2}p(p - 1)\sqrt{\frac{2^2 + 2^2}{2 + 2 - 2}} \\ &= 3p^2 + 6\sqrt{\frac{13}{3}}p - 3p + 6\sqrt{\frac{9}{2}} - 6\sqrt{\frac{13}{3}} \end{aligned}$$

Theorem 3. Let T_p be the triangular benzenoid. Then

$$RARSO(G) = \frac{3}{4}p^2 + 6\sqrt{\frac{3}{13}}p - \frac{3}{4}p + 6\sqrt{\frac{2}{9}} - 6\sqrt{\frac{3}{13}}$$

Proof: Let G be the graph of a triangular benzenoid T_p .

The reciprocal augmented Revan Sombor index of T_p is

$$\begin{aligned} RARSO(G) &= \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u)^2 + r_G(v)^2}} \\ &= 6\sqrt{\frac{3 + 3 - 2}{3^2 + 3^2}} + (6p - 6)\sqrt{\frac{2 + 3 - 2}{2^2 + 3^2}} + \frac{3}{2}p(p - 1)\sqrt{\frac{2 + 2 - 2}{2^2 + 2^2}} \\ &= \frac{3}{4}p^2 + 6\sqrt{\frac{3}{13}}p - \frac{3}{4}p + 6\sqrt{\frac{2}{9}} - 6\sqrt{\frac{3}{13}} \end{aligned}$$

III. Results for Benzenoid Rhombus

In this section, we consider the graph of a benzenoid rhombus R_p . The benzenoid rhombus R_p is obtained from two copies of a triangular benzenoid T_p by identifying hexagons in one of their base rows. The graph of benzenoid rhombus R_4 is presented in Figure 2.

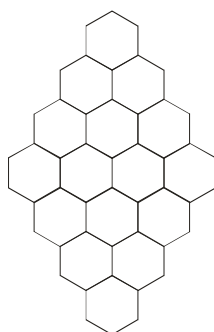


Figure 2. The graph of benzenoid rhombus R_4

Let G be the graph of a benzenoid rhombus R_p . The graph G has $2p^2 + 4p$ vertices and $3p^2 + 4p - 1$ edges. From Figure 2, it is easy to see that the vertices of R_p are either of degree 2 or 3. Therefore $\Delta(G)=3$ and $\delta(G)=2$. Thus $r_G(u) = \Delta(G) + \delta(G) - d_G(u) = 5 - d_G(u)$. By calculation, we obtain that the edge set $E(G)$ can be divided into three partitions:

$$\begin{aligned} E_{22} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}, & |E_{22}| &= 6. \\ E_{23} &= \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}, & |E_{23}| &= 8(p - 1). \end{aligned}$$

$$E_{33} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, \quad |E_{33}| = 3p^2 - 4p + 1.$$

Thus there are three types of Revan edges based on the degree of end Revan vertices of each Revan edge as given in Table 2.

$r_G(u), r_G(v) \setminus uv \in E(G)$	(3, 3)	(3, 2)	(2, 2)
Number of edges	6	$8(p - 1)$	$3p^2 - 4p + 1$

Table 2. Revan edge partition of R_p

Theorem 4. Let R_p be the benzenoid rhombus. Then

$$ASO(G) = 9\sqrt{\frac{1}{2}}p^2 + 8\sqrt{\frac{13}{3}}p - 12\sqrt{\frac{1}{2}}p + 12 - 8\sqrt{\frac{13}{3}} + 3\sqrt{\frac{1}{2}}.$$

Proof: Let G be the graph of a benzenoid rhombus R_p .

The augmented Sombor index of R_p is

$$\begin{aligned} ASO(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d_G(u)^2 + d_G(v)^2}{d_G(u) + d_G(v) - 2}} \\ &= 6\sqrt{\frac{2^2 + 2^2}{2+2-2}} + (8p - 8)\sqrt{\frac{2^2 + 3^2}{2+3-2}} + (3p^2 - 4p + 1)\sqrt{\frac{3^2 + 3^2}{3+3-2}} \\ &= 9\sqrt{\frac{1}{2}}p^2 + 8\sqrt{\frac{13}{3}}p - 12\sqrt{\frac{1}{2}}p + 12 - 8\sqrt{\frac{13}{3}} + 3\sqrt{\frac{1}{2}}. \end{aligned}$$

Theorem 5 . Let R_p be the benzenoid rhombus. Then

$$ARSO(G) = 6p^2 + 8\sqrt{\frac{13}{3}}p - 8p + 18\sqrt{\frac{1}{2}} - 8\sqrt{\frac{13}{3}} + 2.$$

Proof: Let G be the graph of a benzenoid rhombus R_p .

The augmented Revan Sombor index of R_p is

$$\begin{aligned} ARSO(G) &= \sum_{uv \in E(G)} \sqrt{\frac{r_G(u)^2 + r_G(v)^2}{r_G(u) + r_G(v) - 2}} \\ &= 6\sqrt{\frac{3^2 + 3^2}{3+3-2}} + (8p - 8)\sqrt{\frac{2^2 + 3^2}{2+3-2}} + (3p^2 - 4p + 1)\sqrt{\frac{2^2 + 2^2}{2+2-2}} \\ &= 6p^2 + 8\sqrt{\frac{13}{3}}p - 8p + 18\sqrt{\frac{1}{2}} - 8\sqrt{\frac{13}{3}} + 2. \end{aligned}$$

Theorem 6. Let R_p be the benzenoid rhombus. Then

$$RARSO(G) = \frac{3}{2}p^2 + 8\sqrt{\frac{3}{13}}p - 2p + 6\sqrt{\frac{2}{9}} - 8\sqrt{\frac{3}{13}} + \frac{1}{2}.$$

Proof: Let G be the graph of a benzenoid rhombus R_p .

The reciprocal augmented Revan Sombor index of R_p is

$$RARSO(G) = \sum_{uv \in E(G)} \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u)^2 + r_G(v)^2}}$$

$$\begin{aligned}
 &= 6\sqrt{\frac{3+3-2}{3^2+3^2}} + (8p-8)\sqrt{\frac{2+3-2}{2^2+3^2}} + (3p^2-4p+1)\sqrt{\frac{2+2-2}{2^2+2^2}} \\
 &= \frac{3}{2}p^2 + 8\sqrt{\frac{3}{13}}p - 2p + 6\sqrt{\frac{2}{9}} - 8\sqrt{\frac{3}{13}} + \frac{1}{2}.
 \end{aligned}$$

IV. Results for Benzenoid Hourglass

In this section, we consider the graph of benzenoid hourglass X_p which is obtained from two copies of a triangular benzenoid T_p by overlapping hexagons. The graph of benzenoid hourglass is shown in Figure 3.

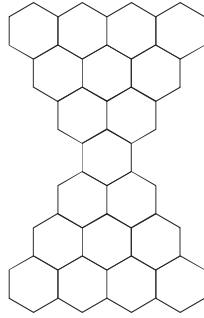


Figure 3. The graph of benzenoid hourglass

Let G be the graph of a benzenoid hourglass X_p . The graph G has $2(p^2 + 4p - 2)$ vertices and $3p^2 + 9p - 4$ edges. From Figure 3, it is easy to see that the vertices of benzenoid hourglass X_p are either of degree 2 or 3. Therefore $\Delta(G) = 3$ and $\delta(G) = 2$. Thus $r_G(u) = \Delta(G) + \delta(G) - d_G(u) = 5 - d_G(u)$. By algebraic method, we obtain that the edge set $E(X_p)$ can be divided into three partitions:

$$\begin{aligned}
 E_{22} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}, & |E_{22}| &= 8. \\
 E_{23} &= \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}, & |E_{23}| &= 4(3p - 4). \\
 E_{33} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, & |E_{33}| &= 3p^2 - 3p + 4.
 \end{aligned}$$

Thus there are three types of Revan edges based on the degree of end Revan vertices of each Revan edge as given in Table 3.

$r_G(u), r_G(v) \setminus uv \in E(G)$	(3, 3)	(3, 2)	(2, 2)
Number of edges	8	$4(3p - 4)$	$3p^2 - 3p + 4$

Table 3. Revan edge partition of X_p

Theorem 7. Let X_p be the benzenoid hourglass. Then

$$ASO(G) = \frac{9}{2}p^2 + 12\sqrt{\frac{13}{3}}p - 9\sqrt{\frac{1}{2}}p + 16 - 16\sqrt{\frac{13}{3}} + 12\sqrt{\frac{1}{2}}.$$

Proof: Let G be the graph of a benzenoid hourglass X_p . The augmented Sombor index of X_p is

$$\begin{aligned}
 ASO(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d_G(u)^2 + d_G(v)^2}{d_G(u) + d_G(v) - 2}} \\
 &= 8\sqrt{\frac{2^2 + 2^2}{2+2-2}} + (12p-16)\sqrt{\frac{2^2 + 3^2}{2+3-2}} + (3p^2-3p+4)\sqrt{\frac{3^2 + 3^2}{3+3-2}} \\
 &= \frac{9}{2}p^2 + 12\sqrt{\frac{13}{3}}p - 9\sqrt{\frac{1}{2}}p + 16 - 16\sqrt{\frac{13}{3}} + 12\sqrt{\frac{1}{2}}
 \end{aligned}$$

Theorem 8 . Let X_p be the benzenoid hourglass. Then

$$ARSO(G) = 6p^2 + 12\sqrt{\frac{13}{3}}p - 6p + 24\sqrt{\frac{1}{2}} - 16\sqrt{\frac{13}{3}} + 8.$$

Proof: Let G be the graph of a benzenoid hourglass X_p .

The augmented Revan Sombor index of X_p is

$$\begin{aligned} ARSO(G) &= \sqrt{\frac{r_G(u)^2 + r_G(v)^2}{r_G(u) + r_G(v) - 2}} \\ &= 8\sqrt{\frac{3^2 + 3^2}{3 + 3 - 2}} + (12p - 16)\sqrt{\frac{2^2 + 3^2}{2 + 3 - 2}} + (3p^2 - 3p + 4)\sqrt{\frac{2^2 + 2^2}{2 + 2 - 2}} \\ &= 6p^2 + 12\sqrt{\frac{13}{3}}p - 6p + 24\sqrt{\frac{1}{2}} - 16\sqrt{\frac{13}{3}} + 8. \end{aligned}$$

Theorem 9 . Let X_p be the benzenoid hourglass. Then

$$RARSO(G) = \frac{3}{2}p^2 + 12\sqrt{\frac{3}{13}}p - \frac{3}{2}p + 8\sqrt{\frac{2}{9}} - 16\sqrt{\frac{3}{13}} + 2.$$

Proof: Let G be the graph of a benzenoid hourglass X_p . The reciprocal augmented Revan Sombor index of X_p is

$$\begin{aligned} RARSO(G) &= \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u)^2 + r_G(v)^2}} \\ &= 8\sqrt{\frac{3 + 3 - 2}{3^2 + 3^2}} + (12p - 16)\sqrt{\frac{2 + 3 - 2}{2^2 + 3^2}} + (3p^2 - 3p + 4)\sqrt{\frac{2 + 2 - 2}{2^2 + 2^2}} \\ &= \frac{3}{2}p^2 + 12\sqrt{\frac{3}{13}}p - \frac{3}{2}p + 8\sqrt{\frac{2}{9}} - 16\sqrt{\frac{3}{13}} + 2. \end{aligned}$$

V. Results for Jagged Rectangle Benzenoid Systems

We now focus on the molecular graph structure of a jagged rectangle benzenoid system. This system is denoted by $B_{m,n}$ for all $m, n \in \mathbb{N}$. Three chemical graphs of a jagged rectangle benzenoid system are shown in Figure 4.

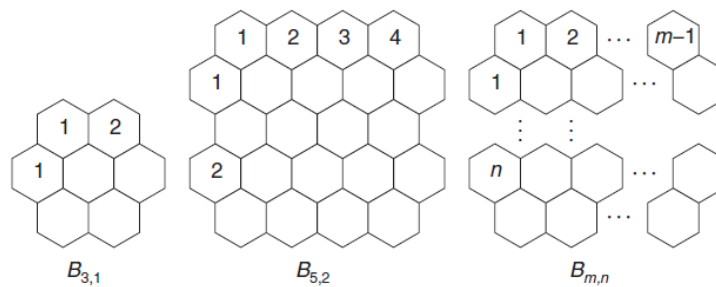


Figure-4

Let G be the graph of a jagged rectangle benzenoid system $B_{m,n}$. From Figure 4, it is easy to see that the vertices of G are either of degree 2 or 3. Thus $\Delta(G) = 3$ and $\delta(G) = 2$. Therefore $r_G(u) = \Delta(G) + \delta(G) - d_G(u) = 5 - d_G(u)$. By calculation, we obtain that G has $4mn + 4m + 2n - 2$ vertices and $6mn + 5m + n - 4$ edges. In G , there are three types of edges based on the degree of end vertices of each edge as follows:

$$\begin{aligned} E_{22} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}, & |E_{22}| &= 2n + 4. \\ E_{23} &= \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}, & |E_{23}| &= 4m + 4n - 4. \\ E_{33} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, & |E_{33}| &= 6mn + m - 5n - 4. \end{aligned}$$

Thus G has three types of Revan edges based on the revan degree of end revan vertices of each revan edge as given in Table 4.

$r_G(u), r_G(v) \setminus uv \in E(G)$	(3, 3)	(3, 2)	(2,2)
Number of edges	$2n + 4$	$4m + 4n - 4$	$6mn + m - 5n - 4$

Table 4. Revan edge partition of $B_{m, n}$

Theorem 10. Let $B_{m, n}$ be the jagged rectangle benzenoid system. Then

$$ASO(G) = 18\sqrt{\frac{1}{2}mn} + 4\sqrt{\frac{13}{3}m} + 3\sqrt{\frac{1}{2}m} + 4n + 4\sqrt{\frac{13}{3}n} - 15\sqrt{\frac{1}{2}n} + 8 + 4\sqrt{\frac{13}{3}} - 12\sqrt{\frac{1}{2}}.$$

Proof: Let G be the jagged rectangle benzenoid system $B_{m, n}$. The augmented Sombor index of $B_{m, n}$ is

$$\begin{aligned} ASO(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d_G(u)^2 + d_G(v)^2}{d_G(u) + d_G(v) - 2}} \\ &= (2n + 4)\sqrt{\frac{2^2 + 2^2}{2 + 2 - 2}} + (4m + 4n + 4)\sqrt{\frac{2^2 + 3^2}{2 + 3 - 2}} + (6mn + m - 5n - 4)\sqrt{\frac{3^2 + 3^2}{3 + 3 - 2}} \\ &= 18\sqrt{\frac{1}{2}mn} + 4\sqrt{\frac{13}{3}m} + 3\sqrt{\frac{1}{2}m} + 4n + 4\sqrt{\frac{13}{3}n} - 15\sqrt{\frac{1}{2}n} + 8 + 4\sqrt{\frac{13}{3}} - 12\sqrt{\frac{1}{2}}. \end{aligned}$$

Theorem 11. Let $B_{m, n}$ be the jagged rectangle benzenoid system. Then

$$ARSO(G) = 12mn + 4\sqrt{\frac{13}{3}m} + 2m + 6\sqrt{\frac{1}{2}n} + 4\sqrt{\frac{13}{3}n} - 10n + 12\sqrt{\frac{1}{2}} + 4\sqrt{\frac{13}{3}} - 8.$$

Proof: Let G be the jagged rectangle benzenoid system $B_{m, n}$. The augmented Revan Sombor index of $B_{m, n}$ is

$$\begin{aligned} ARSO(G) &= \sum_{uv \in E(G)} \sqrt{\frac{r_G(u)^2 + r_G(v)^2}{r_G(u) + r_G(v) - 2}} \\ &= (2n + 4)\sqrt{\frac{3^2 + 3^2}{3 + 3 - 2}} + (4m + 4n + 4)\sqrt{\frac{2^2 + 3^2}{2 + 3 - 2}} + (6mn + m - 5n - 4)\sqrt{\frac{2^2 + 2^2}{2 + 2 - 2}} \\ &= 12mn + 4\sqrt{\frac{13}{3}m} + 2m + 6\sqrt{\frac{1}{2}n} + 4\sqrt{\frac{13}{3}n} - 10n + 12\sqrt{\frac{1}{2}} + 4\sqrt{\frac{13}{3}} - 8. \end{aligned}$$

Theorem 12. Let $B_{m, n}$ be the jagged rectangle benzenoid system. Then

$$RARSO(G) = 3mn + 4\sqrt{\frac{3}{13}m} + \frac{1}{2}m + 2\sqrt{\frac{2}{9}n} + 4\sqrt{\frac{3}{13}n} - \frac{5}{2}n + 4\sqrt{\frac{2}{9}} + 4\sqrt{\frac{3}{13}} - 2.$$

Proof: Let G be the jagged rectangle benzenoid system $B_{m, n}$.

The reciprocal augmented Revan Sombor index of $B_{m, n}$ is

$$\begin{aligned} RARSO(G) &= \sum_{uv \in E(G)} \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u)^2 + r_G(v)^2}} \\ &= (2n + 4)\sqrt{\frac{3 + 3 - 2}{3^2 + 3^2}} + (4m + 4n + 4)\sqrt{\frac{2 + 3 - 2}{2^2 + 3^2}} + (6mn + m - 5n - 4)\sqrt{\frac{2 + 2 - 2}{2^2 + 2^2}} \\ &= 3mn + 4\sqrt{\frac{3}{13}m} + \frac{1}{2}m + 2\sqrt{\frac{2}{9}n} + 4\sqrt{\frac{3}{13}n} - \frac{5}{2}n + 4\sqrt{\frac{2}{9}} + 4\sqrt{\frac{3}{13}} - 2. \end{aligned}$$

VI. Conclusion

In this paper, the augmented Sombor index, augmented Revan Sombor index and reciprocal augmented Revan Sombor index of triangular benzenoids, benzenoid rhombus, benzenoid hourglass and jagged rectangle benzenoid systems are determined

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