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On Augmented Revan Index and its Polynomial 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 propose the augmented Revan index and augmented Revan polynomial of a graph. Also we determine the augmented Revan index and its polynomial of triangular benzenoids, benzenoid rhombus, benzenoid hourglass and jagged rectangle benzenoid systems.

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1. 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 Zagreb index [3] of a graph G is defined as

$$AZI(G) = \sum_{uv\in E(G)} \left(\frac{d_G(u)\, d_G(v)}{d_G(u) + d_G(v) - 2}\right)^3.$$

This topological index has proved to a valuable predictive index in the study of the heat formation in octanes and heptanes, whose prediction power is better than atom bond connectivity index, see [4]. This index was also studied, for example, in [5–9]. We now introduce the augmented Revan index, defined as

$$ARI(G) = \sum_{uv\in E(G)} \left(\frac{r_G(u)\, r_G(v)}{r_G(u) + r_G(v) - 2}\right)^3. \tag{1}$$

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Considering the augmented Revan index, we define the augmented Revan polynomial as

$$ARI\,(G,x) = \sum_{uv\in E(G)} x^{\left(\frac{r_G(u)r_G(v)}{r_G(u)+r_G(v)-2}\right)^3}. \tag{2}$$

Recently, many topological indices were studied, for example, in [10–16]. For more information and recent results about Revan indices, see [17–26]. We consider some families of benzenoid systems. In this paper, the augmented Revan index and its polynomial of triangular benzenoids, benzenoid rhombus, benzenoid hourglass and jagged rectangle benzenoid systems are determined. For more information about benzenoids see [27, 28].

2. 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.

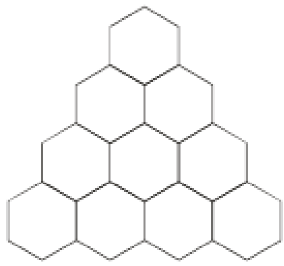

Figure 1. **The graph of triangular benzenoid T_4.**

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:

$$E_{22} = \{uv \in E(G)|d_G(u) = d_G(v) = 2\}, \qquad |E_{22}| = 6.$$

$$E_{23} = \{uv \in E(G)|d_G(u) = 2, d_G(v) = 3\}, \quad |E_{23}| = 6p-6.$$

$$E_{33} = \{uv \in E(G)|d_G(u) = d_G(v) = 3\}, \qquad |E_{33}| = \frac{3}{2}p\,(p-1)\,.$$

Thus there are three types of Revan edges based on the degree of end Revan vertices of each Revan edge as given in Table 1. In the following theorem, we compute the augmented Revan index and augmented Revan polynomial of T_p.

$r_G(u), r_G(v)\backslash e = uv \in E(G)$	(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 2.1. *Let T_p be the triangular benzenoid. Then*

(1). $ARI\,(T_p) = 12p^2 + 36p + \frac{651}{32}$.

(2). $ARI\,(T_p, x) = 6x^{\frac{729}{64}} + \left(\frac{3}{2}p^2 + \frac{9}{2}p - 6\right)x^8$.

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

(1). By using Equation (1) and Table 1, the augmented Revan index of T_p is

$$\begin{aligned} ARI(T_p) &= \sum_{uv\in E(G)} \left(\frac{r_G(u)\,r_G(v)}{r_G(u)+r_G(v)-2}\right)^3 \\ &= \left(\frac{3\times 3}{3+3-2}\right)^3 6 + \left(\frac{3\times 2}{3+2-2}\right)^3 (6p-6) + \left(\frac{2\times 2}{2+2-2}\right)^3 \frac{3}{2}p(p-1) \\ &= 12p^2 + 36p + \frac{651}{32}. \end{aligned}$$

(2). By using Equation (2) and Table 1, the augmented Revan polynomial of T_p is

$$\begin{aligned} ARI(T_p, x) &= \sum_{uv\in E(G)} x^{\left(\frac{r_G(u)r_G(v)}{r_G(u)+r_G(v)-2}\right)^3} \\ &= 6x^{\left(\frac{3\times 3}{3+3-2}\right)^3} + (6p-6)\,x^{\left(\frac{3\times 2}{3+2-2}\right)^3} + \frac{3}{2}p(p-1)\,x^{\left(\frac{2\times 2}{2+2-2}\right)^3} \\ &= 6x^{\frac{729}{64}} + (6p-6)\,x^8 + \frac{3}{2}p(p-1)\,x^8 \\ &= 6x^{\frac{729}{64}} + \left(\frac{3}{2}p^2 + \frac{9}{2}p - 6\right) x^8. \end{aligned}$$

□

3. 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.

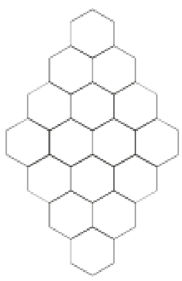

Figure 2. **The graph of benzenoid rhombus** R_4

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:

$$E_{22} = \{uv \in E(G) | d_G(u) = d_G(v) = 2\}, \quad |E_{22}| = 6.$$

$$E_{23} = \{uv \in E(G) | d_G(u) = 2, d_G(v) = 3\}, \quad |E_{23}| = 8(p-1).$$

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

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.

$r_G(u), r_G(v) \backslash uv \in E(G)$	(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**

In the following theorem, we compute the augmented Revan index and augmented Revan polynomial of R_p.

Theorem 3.1. *Let G be the graph of a benzenoid rhombus R_p. Then*

(1). $ARI\left(R_p\right) = 24p^2 - 32p + \frac{395}{32}$.

(2). $ARI\left(R_p, x\right) = 6x^{\frac{729}{64}} + \left(3p^2 + 4p - 7\right) x^8$.

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

(1). By using equation (1) and Table 2, the augmented Revan index of R_p is

$$\begin{aligned} ARI\left(R_p\right) &= \sum_{uv \in E(G)} \left(\frac{r_G(u)\, r_G(v)}{r_G(u) + r_G(v) - 2}\right)^3 \\ &= \left(\frac{3\times 3}{3+3-2}\right)^3 6 + \left(\frac{3\times 2}{3+2-2}\right)^3 8\left(p-1\right) + \left(\frac{2\times 2}{2+2-2}\right)^3 \left(3p^2 - 4p + 1\right) \\ &= 24p^2 - 32p + \frac{395}{32}. \end{aligned}$$

(2). By using equation (1) and Table 2, the augmented Revan polynomial of R_p is

$$\begin{aligned} ARI\left(R_p, x\right) &= \sum_{uv \in E(G)} x^{\left(\frac{r_G(u) r_G(v)}{r_G(u)+r_G(v)-2}\right)^3} \\ &= 6x^{\left(\frac{3\times 3}{3+3-2}\right)^3} + 8\left(p-1\right) x^{\left(\frac{3\times 2}{3+2-2}\right)^3} + \left(3p^2 - 4p + 1\right) x^{\left(\frac{2\times 2}{2+2-2}\right)^3} \\ &= 6x^{\frac{729}{64}} + \left(3p^2 + 4p - 7\right) x^8. \end{aligned}$$

□

4. 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.

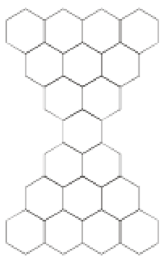

Figure 3. **The graph of benzenoid hourglass**

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:

$$E_{22} = \{uv \in E(G)|d_G(u) = d_G(v) = 2\}, \qquad |E_{22}| = 8.$$

$$E_{23} = \{uv \in E(G)|d_G(u) = 2, d_G(v) = 3\}, \quad |E_{23}| = 4(3p-4).$$

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

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.

$r_G(u), r_G(v)\backslash uv \in E(G)$	(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**

In the following theorem, we determine the augmented Revan index and augmented Revan polynomial of X_p.

Theorem 4.1. *Let G be the graph of a benzenoid hourglass X_p. Then*

(1). $ARI\,(X_p) = 24p^2 + 72p - \frac{39}{8}$.

(2). $ARI\,(X_p, x) = 8x^{\frac{729}{64}} + \left(3p^2 + 9p - 12\right)x^8$.

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

(1). By using equation (1) and Table 3, the augmented Revan index of X_p is

$$\begin{aligned} ARI\,(X_p) &= \sum_{uv\in E(G)} \left(\frac{r_G\,(u)\, r_G\,(v)}{r_G\,(u) + r_G\,(v) - 2}\right)^3 \\ &= \left(\frac{3\times 3}{3+3-2}\right)^3 8 + \left(\frac{3\times 2}{3+2-2}\right)^3 4\,(3p-4) + \left(\frac{2\times 2}{2+2-2}\right)^3 \left(3p^2 - 3p + 4\right) \\ &= 24p^2 + 72p + \frac{39}{8}. \end{aligned}$$

(2). By using equation (2) and Table 3, the augmented Revan polynomial of X_p is

$$\begin{aligned} ARI\,(X_p, x) &= \sum_{uv\in E(G)} x^{\left(\frac{r_G(u)r_G(v)}{r_G(u)+r_G(v)-2}\right)^3} \\ &= 8x^{\left(\frac{3\times3}{3+3-2}\right)^3} + 4\,(3p-4)\,x^{\left(\frac{3\times2}{3+2-2}\right)^3} + \left(3p^2-3p+4\right)x^{\left(\frac{2\times2}{2+2-2}\right)^3} \\ &= 8x^{\frac{729}{64}} + \left(3p^2 + 9p - 12\right)x^8. \end{aligned}$$

□

5. 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 $m, n \in N$. Three chemical graphs of a jagged rectangle benzenoid system are shown in Figure 4.

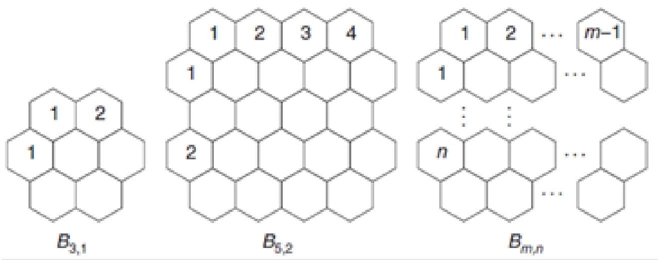

Figure 4.

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:

$$E_{22} = \{uv \in E(G) | d_G(u) = d_G(v) = 2\}, \qquad |E_{22}| = 2n + 4.$$

$$E_{23} = \{uv \in E(G) | d_G(u) = 2, d_G(v) = 3\}, \quad |E_{23}| = 4m + 4n - 4.$$

$$E_{33} = \{uv \in E(G) | d_G(u) = d_G(v) = 3\}, \qquad |E_{33}| = 6mn + m - 5n - 4.$$

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.

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

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

In the following theorem, we determine the augmented Revan index and augmented Revan polynomial of $B_{m,n}$.

Theorem 5.1. *Let $B_{m,n}$ be the jagged rectangle benzenoid system. Then*

(1). $ARI\,(B_{m,n}) = 48mn + 40m + \frac{473}{32}n - \frac{295}{32}$.

(2). $ARI\,(B_{m,n}, x) = (2n + 4)\,x^{\frac{729}{64}} + (6mn + 5m - n - 8)\,x^8$.

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

(1). By using equation (1) and Table 4, the augmented Revan index of $B_{m,n}$ is

$$\begin{aligned} ARI\,(B_{m,n}) &= \sum_{uv \in E(G)} \left(\frac{r_G\,(u)\,r_G\,(v)}{r_G\,(u) + r_G\,(v) - 2} \right)^3 \\ &= \left(\frac{3 \times 3}{3 + 3 - 2} \right)^3 (2n + 4) + \left(\frac{3 \times 2}{3 + 2 - 2} \right)^3 (4m + 4n - 4) + \left(\frac{2 \times 2}{2 + 2 - 2} \right)^3 (6mn + m - 5n - 4) \\ &= 48mn + 40m + \frac{473}{32}n - \frac{295}{32}. \end{aligned}$$

(2). By using equation (2) and Table 4, the augmented Revan polynomial of $B_{m,n}$ is

$$ARI\,(B_{m,n}, x) = \sum_{uv \in E(G)} x^{\left(\frac{r_G(u) r_G(v)}{r_G(u) + r_G(v) - 2} \right)^3}$$

$$= (2n+4)\,x^{\left(\frac{3\times 3}{3+3-2}\right)^3} + (4m+4n-4)\,x^{\left(\frac{3\times 2}{3+2-2}\right)^3} + (6mn+m-5n-4)\,x^{\left(\frac{2\times 2}{2+2-2}\right)^3}$$

$$= (2n+4)\,x^{\frac{729}{64}} + (6mn+5m-n-8)\,x^8.$$

□

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