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F-REVAN INDEX AND F-REVAN POLYNOMIAL OF SOME FAMILIES OF BENZENOID SYSTEMS

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Abstract: Recently, the Revan vertex degree concept is defined in graph theory. In this paper, we propose the F-Revan index of molecular graph. Considering the F-Revan index, we define the F-Revan polynomial of a molecular graph. Furthermore, we compute the F-Revan index and F-Revan polynomial of triangular benzenoid, benzenoid rhombus, benzenoid hourglass and jagged rectangle benzenoid system.'

Keywords: F-Revan index, F-Revan polynomial, benzenoid.

Mathematics Subject Classification**:** 05C07, 05C12, 05C35.

1. INTRODUCTION

In this paper, we consider finite simple connected graphs. Let G be a graph with a vertex set $V(G)$ and edge set $E(G)$. Let $d_G(v)$ denote the degree of a vertex v in a graph G, which 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. We refer to [1] for undefined term and notation.

Chemical graph theory is a branch of Mathematical chemistry which has an important effect on the development of the Chemical Sciences. A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. A topological index is a numeric quantity from the structure graph of a molecule. Numerous such topological indices have been considered in Theoretical Chemistry and have found some applications, especially in *QSAR*/*QSPR* research, see [2].

The first and second Revan indices of a graph G are defined as

$$R_1(G)=\sum_{uv\in E(G)}\left[r_G(u)+r_G(v)\right],\qquad R_2(G)=\sum_{uv\in E(G)} r_G(u)r_G(v).$$

These Revan indices were introduced by Kulli in [3]. For more information and recent results about Revan indices, see [4, 5, 6, 7, 8, 9, 10, 11, 12].

The forgotten topological index or F-index of a graph G is defined as

$$F(G)=\sum_{u\in V(G)} d_G(u)^3=\sum_{uv\in E(G)}\left[d_G(u)^2+d_G(v)^2\right].$$

This index was studied by Furtula and Gutman in [13]. Furthermore, it was also studied, for example, in [14, 15, 16, 17, 18, 19, 20,21].

Motivated by the definition of the F-index and its applications, we propose the F-Revan index and F_1-Revan index of a molecular graph as follows:

The F-Revan index of a molecular graph G is defined as

$$FR(G)=\sum_{uv\in E(G)}\left[r_G(u)^2+r_G(v)^2\right]. \qquad (1)$$

The F_1-Revan index of a molecular graph G is defined as

$$F_1R(G)=\sum_{u\in F(G)} r_G(u)^3.$$

Considering the F-Revan index, we propose the F-Revan polynomial of a molecular graph G as

$$FR(G,x)=\sum_{uv\in E(G)} x^{\left[r_G(u)^2+r_G(v)^2\right]}. \qquad (2)$$

The study of benzenoids has received much attention in the mathematical and chemical literature, see [22, 23]. In this paper, we compute the F-Revan index and F-Revan polynomial of triangular benzenoid, benzenoid rhombus, benzenoid hourglass and jagged rectangle benzenoid system.

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.

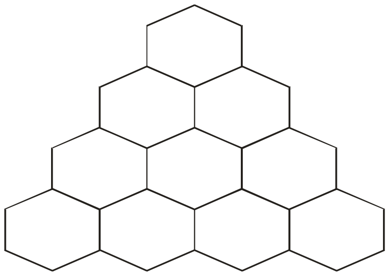

Figure 1. The graph of triangular benzenoid T_4.

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:

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

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

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

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.

Table 1. Revan edge partition 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	$6p - 6$	$\frac{3}{2}p(p-1)$

In the following theorem, we compute the *F*-Revan index and *F*-Revan polynomial of this type of benzenoid.

Theorem 1. Let T_p be a triangular benzenoid. Then

(1) $FR(T_p) = 12p^2 + 66p + 32$.

(ii) $FR(T_p, x) = 6x^{18} + 6(p - 1)x^{13} + \frac{3}{2}p(p-1)x^8$.

Proof: (i) Let T_p be a triangular benzenoid. By using equation (1) and Table 1, the F-Revan index of T_p is given by

$$FR(T_p)=\sum_{uv\in E(T_p)}\left[r_{T_p}(u)^2+r_{T_p}(v)^2\right]$$

$$=(3^2+3^2)6+(3^2+2^2)(6p-6)+(2^2+2^2)\frac{3}{2}p(p-1)$$

$$=12p^2+66p+32.$$

(ii) By using equation (2) and Table 1, the F-Revan polynomial of T_p is given by

$$FR(T_p, x) = \sum_{uv \in E(T_p)} x^{\left[r_{T_p}(u)^2 + r_{T_p}(v)^2\right]}$$

$$= 6x^{(3^2+3^2)} + 6(p-1)x^{(3^2+2^2)} + \frac{3}{2}p(p-1)x^{(2^2+2^2)}.$$

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

3. RESULTS FOR BENZENOID RHOMBUS

In this section, we consider the graph of 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.

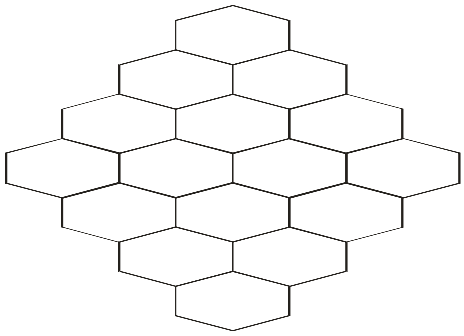

Figure 2. The graph of benzenoid rhombus R_4

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:

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

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

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

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.

Table 2. Revan edge partition of R_p

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

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

Theorem 2. Let R_p be the benzenoid rhombus. Then

(i) $FR(R_p) = 24p^2 + 72p + 12$.

(ii) $FR(R_p, x) = 6x^{18} + 8(p-1)x^{13} + (3p^2 - 4p + 1)x^8$.

Proof: (i) Let R_p be a benzenoid rhombus. By using equation (1) and Table 2, the F-Revan index of R_p is given by

$$FR(R_p) = \sum_{uv \in E(R_p)} \left[r_{R_p}(u)^2 + r_{R_p}(v)^2\right]$$

$$= (3^2 + 3^2)6 + (3^2 + 2^2)8(p-1) + (2^2 + 2^2)(3p^2 - 4p + 1)$$

$$= 24p^2 + 72p + 12.$$

(ii) By using equation (2) and Table 2, the F-Revan polynomial of R_p is given by

$$FR(R_p, x) = \sum_{uv \in E(R_p)} x^{\left[r_{R_p}(u)^2 + r_{R_p}(v)^2\right]}$$

$$= 6x^{(3^2+3^2)} + 8(p-1)x^{(3^2+2^2)} + (3p - 4p + 1)x^{(2^2+2^2)}$$

$$= 6x^{18} + 8(p-1)x^{13} + (3p-4p+1)x^{8}.$$

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.

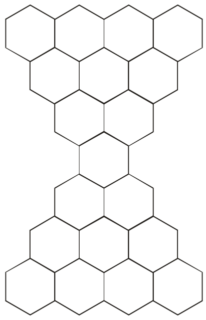

Figure 3. The graph of benzenoid hourglass

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:

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

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.

Table 3. Revan edge partition of X_p

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

In the following theorem, we determine the F-Revan index and F-Revan polynomial of this type of benzenoid.

Theorem 3. Let X_p be the benzenoid hourglass. Then

(1) $FR(X_p) = 24p^2 + 132p - 32$.

(2) $FR(X_p, x) = 8x^{18} + 4(3p - 4)x^{13} + (3p^2 - 3p + 4)x^8$.

Proof: (i) Let X_p be a benzenoid hourglass. By using equation (1) and Table 3, the F-Revan index of a benzenoid hourglass X_p is given by

$$FR(X_p) = \sum_{uv\in E(X_p)} \left[r_{X_p}(u)^2 + r_{X_p}(v)^2 \right]$$
$$= (3^2+3^2)8 + (3^2+2^2)4(3p-4) + (2^2+2^2)(3p^2-3p+4)$$
$$= 24p^2 + 132p - 32.$$

(ii) By using equation (2) and Table 3, the F-Revan polynomial of a benzenoid hourglass X_p is given by

$$FR(X_p, x) = \sum_{uv\in E(X_p)} x^{\left[r_{X_p}(u)^2 + r_{X_p}(v)^2 \right]}$$
$$= 8x^{(3^2+3^2)} + 4(3p-4)x^{(3^2+2^2)} + (3p^2-3p+4)x^{(2^2+2^2)}$$
$$= 8x^{18} + 4(3p-4)x^{13} + (3p^2-4p+4)x^{8}.$$

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 systems are shown in Figure 4.

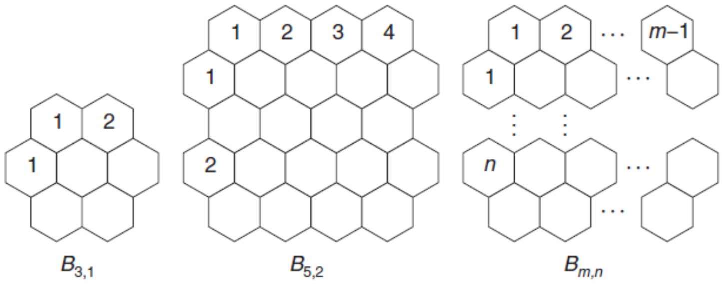

Figure-4

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:

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

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

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

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

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

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

In the following theorem, we determine the F-Revan index and F-Revan polynomial of this type of benzenoid.

Theorem 4. Let $B_{m,n}$ be a jagged rectangle benzenoid system. Then

(i) $FR(B_{m,n}) = 48mn + 60m + 48n - 12$.

(ii) $FR(B_{m,n}, x) = (2n + 4)x^{18} + (4m + 4n - 4)x^{13} + (6mn + m - 5n - 4)x^{8}$.

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

(i) By using equation (1) and Table 4, the F-Revan index of $B_{m,n}$ is given by

$$FR(X_{m,n}) = \sum_{uv\in E(G)} \left[r_G(u)^2 + r_G(v)^2 \right]$$

$$= (3^2 + 3^2)(2n + 4) + (3^2 + 2^2)(4m + 4n - 4) + (2^2 + 2^2)(6mn + m - 5p - 4)$$

$$= 48mn + 60m + 48n - 12.$$

(ii) By using equation (2) and Table 4, the F-Revan polynomial of $B_{m,n}$ is given by

$$FR(X_{m,n}, x) = \sum_{uv\in E(G)} x^{\left[r_G(u)^2 + r_G(v)^2 \right]}$$

$$= (2n + 4)x^{(3^2+3^2)} + (4m + 4n - 4)x^{(3^2+2^2)} + (6mn + m - 5n + 4)x^{(2^2+2^2)}$$

$$= (2n + 4)x^{18} + (4m + 4n - 4)x^{13} + (6mn + m - 5n - 4)x^{8}.$$

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