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Research Article

GENERAL MULTIPLICATIVE REVAN INDICES OF POLYCYCLIC AROMATIC HYDROCARBONS AND BENZENOID SYSTEMS

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ABSTRACT

Recently multiplicative Revan indices were studied. In this paper, we introduce the general first and second multiplicative Revan indices. Furthermore we determine the multiplicative Revan indices, multiplicative hyper-Revan indices, general first and second multiplicative Revan indices for polycyclic aromatic hydrocarbons and jagged rectangle benzenoid systems.

INTRODUCTION

Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d_G(v)$ denote the degree of a vertex v in a graph G. Let $\Delta(G)(\delta(G))$ denote the maximum (minimum) degree among the vertices of G. The Revan vertex degree $r_G(v)$ 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.

A topological index is a numerical parameter mathematically derived from the graph structure. Several topological indices have been considered in Theoretical Chemistry.

The first and second Revan indices were introduced by Kulli in [2]. They are defined as

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

$$R_2(G) = \sum_{uv \in E(G)} r_G(u) r_G(v).$$

Recently, Revan indices were studied, for example, in [3, 4, 5, 6, 7].

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

$$RII_1(G) = \prod_{uv \in E(G)} \left[r_G(u) + r_G(v) \right],$$

$$RII_2(G) = \prod_{uv \in E(G)} r_G(u) r_G(v). \qquad (1)$$

These indices were introduced by Kulli in [5].

The first and second multiplicative hyper-Revan indices [5] of a graph G are respectively defined as

$$HRII_1(G) = \prod_{uv \in E(G)} \left[r_G(u) + r_G(v) \right]^2,$$

$$HRII_2(G) = \prod_{uv \in E(G)} \left[r_G(u) r_G(v) \right]^2. \qquad (2)$$

We now introduce the general first and second multiplicative Revan indices of a graph G as

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$$RII_1^a(G)=\sum_{uv\in E(G)}\left[r_G(u)+r_G(v)\right]^a,$$

$$RII_2^a(G)=\sum_{uv\in E(G)}\left[r_G(u)r_G(v)\right]^a. \quad (3)$$

Recently many multiplicative indices were studied, for example, in [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19].

In this paper, we compute the multiplicative Revan indices and the general multiplicative Revan indices for polycyclic aromatic hydrocarbons PAH_n and jagged rectangle benzenoid systems $B_{m,n}$. For more information about polycyclic aromatic hydrocarbons and jagged-rectangle benzenoid systems see [20].

Results for Polycyclic Aromatic Hydrocarbons

In this section, we focus on the molecular graph, structure of the family of polycyclic aromatic hydrocarbons, denoted PAH_n. The first three members of the family of polycyclic aromatic hydrocarbons are depicted in Figure 1.

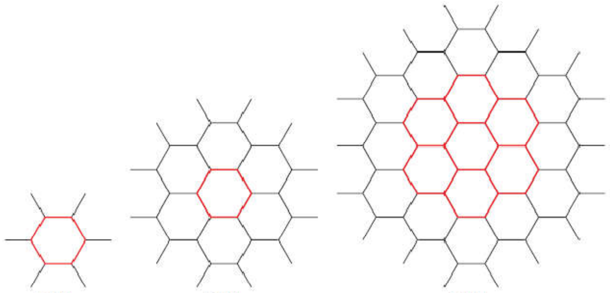

Figure 1

In the following theorem, we compute the general multiplicative Revan index of PAH_n.

Theorem 1. Let PAH_n be the family of polycyclic hydrocarbons. Then

$$RII_1^a(PAH_n)=4^{6an}\times 2^{(9n^2-3n)a}. \quad (4)$$

Proof: Let $G = PAH_n$ be the molecular graph in the family of polycyclic aromatic hydrocarbons. We see that the vertices of G are either of degree 1 or 3. Thus $\Delta(G)$=3 and $\delta(G)$=1 and hence $r_G(u) = \Delta(G)+\delta(G) - d_G(u) = 4 - d_G(u)$. By calculation, we obtain that G has $6n^2+6n$ vertices and $9n^2+3n$ edges, see [20]. In G, there are two types of edges based on the degree of end vertices of each edge as follows:

$E_{13} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\}, |E_{13}| = 6n$.
$E_{33} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, |E_{33}| = 9n^2 - 3n$.

Hence, we obtain that G has two types of revan edges based on the revan degree of end revan vertices of each revan edge as follows:

$RE_{31} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 1\}, |RE_{31}| = 6n$.
$RE_{11} = \{uv \in E(G) \mid r_G(u) = r_G(v) = 1\}, |RE_{11}| = 9n^2 - 3n$.

To compute $RII_1^a(PAH_n)$ we see that

$$RII_1^a(PAH_n)=\prod_{uv\in E(G)}\left[r_G(u)+r_G(v)\right]^a=\prod_{RE_{31}}\left[r_G(u)+r_G(v)\right]^a\times\prod_{RE_{11}}\left[r_G(u)+r_G(v)\right]^a$$

$$=\left[(3+1)^a\right]^{6n}\times\left[(1+1)^a\right]^{9n^2-3n}$$

$$=4^{6an}\times 2^{(9n^2-3n)a}.$$

We obtain the following results by Theorem 1.

Corollary: Let PAH_n be the family of polycyclic aromatic hydrocarbons. Then

$$RII_1(G)=4^{6n}\times 2^{9n^2-3n}.$$

Proof: Put a = 1 in equation (4), we get the desired result.

Corollary: Let PAH_n be the family of polycyclic aromatic hydrocarbons. Then

$$HRII_1(PAH_n)=4^{12n}\times 2^{18n^2-6n}.$$

Proof: Put a = 2 in equation (4), we get the desired result.

In the following theorem, we compute the general second multiplicative Revan index of PAH_n.

Theorem 2: Let PAH_n be the family of polycyclic aromatic hydrocarbons, Then

$$RII_2^a(PAH_n)=3^{6an}. \quad (5)$$

Proof: Let $G = PAH_n$ be the molecular graph in the family of polycyclic aromatic hydrocarbons. Then from equation (3) and by cardinalities of the revan edge partition of PAH_n, we have

$$RII_2^a(PAH_n)=\prod_{uv\in E(G)}\left[r_G(u)r_G(v)\right]^a=\prod_{RE_{31}}\left[r_G(u)r_G(v)\right]^a\times\prod_{RE_{11}}\left[r_G(u)r_G(v)\right]^a$$

$$=\left[(3\times1)^a\right]^{6n}\times\left[(1\times1)^a\right]^{9n^2-3n}$$

$$=3^{6an}.$$

We obtain the following results by Theorem 2.

Corollary: Let PAH_n be the family of polycyclic aromatic hydrocarbons. Then
$RII_2(PAH_n) = 3^{6n}$.

Proof: Put a = 1 in equation (5), we get the desired result.

Corollary: Let PAH_n be the family of polycyclic aromatic hydrocarbons. Then $HRII_2(PAH_n) = 3^{12n}$.
Proof: Put a = 2 *in* equation (5), w get the desired result.

Results for Benzenoid systems

In this section, we 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 molecular graphs of a jagged rectangle benzenoid system are given in Figure 2.

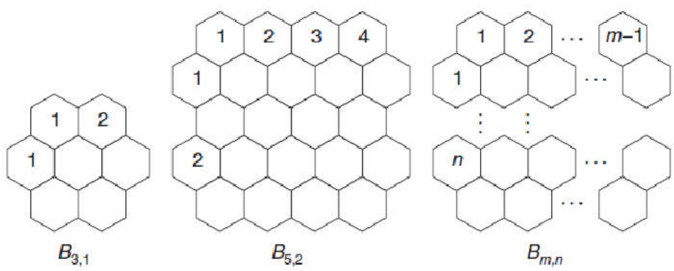

Figure 2

In the following theorem, we compute the general first multiplicative Revan index of $B_{m,n}$.

Theorem 3: Let $B_{m,\ n}$ be the family of a jagged rectangle benzenoid system. Then

$$RII_1^a\left(B_{m,n}\right)=6^{a(2n+4)}\times 5^{a(4m+4n-4)}\times 4^{a(6mn+m-5n-4)} \qquad (6)$$

Proof: Let $G = B_{m,n}$ be the molecular graph of a jagged rectangle benzenoid system. 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, see [20].

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 revan edge as follows:

$RE_{33} = \{uv \in E(G) \mid r_G(u) = r_G(v) = 3\}$, $|RE_{33}| = 2n + 4$.
$RE_{32} = \{uv \in E(G) \mid r_G(u) = 3,\ r_G(v) = 2\}$, $|RE_{32}| = 4m + 4n - 4$.
$RE_{22} = \{uv \in E(G) \mid r_G(u) = r_G(v) = 2\}$, $|RE_{22}| = 6mn + m - 5n - 4$.

To compute $RII_1^a\left(B_{m,n}\right)$, we see that

$$RII_1^a\left(B_{m,n}\right)=\prod_{uv\in E(G)}\left[r_G(u)+r_G(v)\right]^a$$

$$=\prod_{RE_{33}}\left[r_G(u)+r_G(v)\right]^a\times\prod_{RE_{32}}\left[r_G(u)+r_G(v)\right]^a\times\prod_{RE_{22}}\left[r_G(u)+r_G(v)\right]^a$$

$$=\left[(3+3)^a\right]^{2n+4}\times\left[(3+2)^a\right]^{4m+2n-4}\times\left[(2+2)^a\right]^{6mn+m-5n-4}$$

$$=6^{a(2n+4)}\times 5^{a(4m+4n-4)}\times 4^{a(6mn+m-5n-4)}.$$

We obtain the following results by Theorem 3.

Corollary: Let $B_{m,\ n}$ be the family of a jagged rectangle benzenoid system. Then

$$RII_1\left(B_{m,n}\right)=6^{2n+4}\times 5^{4m+4n-4}\times 4^{6mn+m-5n-4}.$$

Proof: Put a=1 in equation (6), we get the desired result.

Corollary: Let $B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

$$HRII_1\left(B_{m,n}\right)=6^{2(2n+4)}\times 5^{2(4m+4n-4)}\times 4^{2(6mn+m-5n-4)}.$$

Proof: Put a=2 in equation (6), we get the desired result.

Theorem 4*:* Let $B_{m,\ n}$ be the family of a jagged rectangle benzenoid system. Then

$$RII_2^a\left(B_{m,n}\right)=9^{a(2n+4)}\times 6^{a(4m+4n-4)}\times 4^{a(6mn+m-5n-4)}. \qquad (7)$$

Proof: Let $G= B_{m,\ n}$ be the molecular graph of a jagged rectangle benzenoid system. Then from equation (3) and by cardinalities of the revan edge partition of $B_{m,\ n}$, we have

$$RII_2^a\left(B_{m,n}\right)=\prod_{uv\in E(G)}\left[r_G(u)r_G(v)\right]^a$$

$$=\prod_{RE_{33}}\left[r_G(u)r_G(v)\right]^a\times\prod_{RE_{32}}\left[r_G(u)r_G(v)\right]^a\times\prod_{RE_{22}}\left[r_G(u)r_G(v)\right]^a$$

$$=\left[(3\times 3)^a\right]^{2n+4}\times\left[(3\times 2)^a\right]^{4m+2n-4}\times\left[(2\times 2)^a\right]^{6mn+m-5n-4}$$

$$=9^{a(2n+4)}\times 6^{a(4m+4n-4)}\times 4^{a(6mn+m-5n-4)}.$$

We obtain the following results by Theorem 4.

Corollary: Let $B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

$$RII_2\left(B_{m,n}\right)=9^{2n+4}\times 6^{4m+4n-4}\times 4^{6mn+m-5n-4}.$$

Proof: Put a=1 in equation (7), we get the desired result.

Corollary: Let $B_{m,\ n}$ be the family of a jagged rectangle benzenoid system. Then

$$HRII_2\left(B_{m,n}\right)=9^{2(2n+4)}\times 6^{2(4m+4n-4)}\times 4^{2(6mn+m-5n-4)}.$$

Proof: Put a = 2 in equation (7), we get the desired result.

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