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CONNECTIVITY REVAN INDICES OF CHEMICAL STRUCTURES IN DRUGS

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ABSTRACT

In Medical Science, the methods of topological descriptor computation can help to obtain the available pharmacological, biological, chemical and medical information of drugs. So that the connectivity indices are applied to measure the chemical characteristics of drugs. In this paper, we introduce the atom bond connectivity Revan index and geometric-arithmetic Revan indices of a molecular graph. Furthermore, we determine the sum connectivity Revan index, atom bond connectivity Revan index and geometric-arithmetic Revan index of chemically interesting drugs like jagged-rectangle benzenoid systems and polycyclic aromatic hydrocarbons.

Keywords: chemical graph, connectivity Revan indices, benzenoid system, polycyclic aromatic hydrocarbon.
Mathematics Subject Classification : 05C05, 05C07, 05C90..

I. INTRODUCTION

Let G be a finite, simple connected graph with vertex set $V(G)$ and 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 terminology, the readers are referred to [1].

A topological index is a numerical parameter mathematically derived from the graph structure. Numerous degree based indices were introduced such as Zagreb index, Banhatti index, reverse index, Revan index, Gourava index and so on. There are many research papers on some special nanomaterial molecular structures which may be referred to Alikhani et al. [2], Akhtar et al. [3], Ashrafi et al. [4], Gao et al. [5, 6, 7], Husin et al. [8], Kulli [9, 10, 11, 12, 13, 17, 18].

In [19], the sum connectivity Revan index of a graph G is defined as

$$SR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_G(u) + r_G(v)}}. \qquad (1)$$

One of the best known topological index is the product connectivity Revan index, introduced by Kulli in [15]. The product connectivity Revan index of a graph G is defined as

$$PR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_G(u) r_G(v)}}. \qquad (2)$$

Recently, Revan indices were studied, for example, in [14, 16].

Motivated by the definition of the product connectivity Revan index, we introduce the atom bond connectivity Revan index and geometric-arithmetic Revan index of a molecular graph as follows:

The atom bond connectivity Revan index of a graph G is defined as

$$ABCR(G) = \sum_{uv \in E(G)} \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u) r_G(v)}}. \qquad (3)$$

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The geometric-arithmetic Revan index of a graph G is defined as

$$GAR(G) = \sum_{uv \in E(G)} \frac{2\sqrt{r_G(u) r_G(v)}}{r_G(u) + r_G(v)}. \qquad (4)$$

In this paper, the sum connectivity Revan index, product connectivity Revan index, atom bond connectivity Revan index and geometric-arithmetic Revan index of jagged-rectangle systems and polycyclic aromatic hydrocarbons are determined. For more information about benzenoid systems and polycyclic aromatic hydrocarbons see [20].

II. RESULTS FOR BENZENOID SYSTEMS $B_{M,N}$

In this section, we consider the chemical graph structure of a jagged-rectangle benzenoid system, symbolized by $B_{m,n}$, for $m, n \in N$. Three chemical graphs of a jagged-rectangle benzenoid system are depicted in Figure 1.

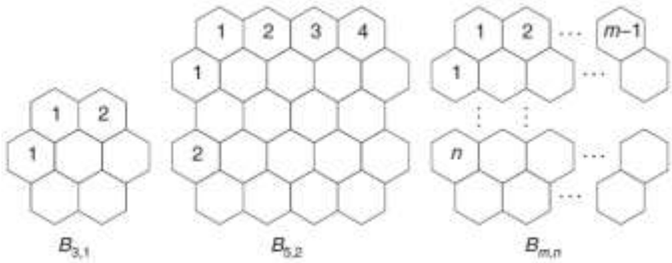

Figure-1. Chemical graphs of a jagged-rectangle benzenoid system

Let G be the chemical graph in the family 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 $|V(G)|=4mn+4m+2n-2$ and $|E(G)|=6mn+5m+n-4$. In $(B_{m,n})$, 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 there are three types of revan edges based on the revan degree of end revan vertices of each revan edge as given in Table 1.

Table 1. Revan edge partition of $B_{m,n}$

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

In the following theorem, we compute the sum connectivity Revan index of $B_{m,n}$.

Theorem 1. The sum connectivity Revan index of a jagged-rectangle benzenoid system $B_{m,n}$ is given by

$$SR(B_{m,n}) = 3mn + \left(\frac{4}{\sqrt{5}} + \frac{1}{2}\right)m + \left(\frac{2}{\sqrt{6}} + \frac{4}{\sqrt{5}} - \frac{5}{2}\right)n + \left(\frac{1}{\sqrt{6}} - \frac{1}{\sqrt{5}} - \frac{1}{2}\right)4.$$

Proof: From equation (1) and using Table 1, we derive

$$SR(B_{m,n}) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_G(u) + r_G(v)}}$$

$$= (2n+4)\left(\frac{1}{\sqrt{3+3}}\right) + (4m+4n-4)\left(\frac{1}{\sqrt{3+2}}\right) + (6mn+m-5n-4)\left(\frac{1}{\sqrt{2+2}}\right)$$

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$$= 3mn + \left(\frac{4}{\sqrt{5}} + \frac{1}{2}\right)m + \left(\frac{2}{\sqrt{6}} + \frac{4}{\sqrt{5}} - \frac{5}{2}\right)n + \left(\frac{1}{\sqrt{6}} - \frac{1}{\sqrt{5}} - \frac{1}{2}\right)4.$$

In the following theorem, we compute the product connectivity Revan index of $B_{m,n}$.

Theorem 2. The product connectivity Revan index of a jagged-rectangle benzenoid system $B_{m,n}$ is given by

$$PR(B_{m,n}) = 3mn + \left(\frac{4}{\sqrt{6}} + \frac{1}{2}\right)m + \left(\frac{4}{\sqrt{6}} - \frac{11}{6}\right)n - \left(\frac{4}{\sqrt{6}} + \frac{2}{3}\right)$$

Proof: From equation (2) and using Table 1, we derive

$$PR(B_{m,n}) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_G(u) r_G(v)}}$$

$$= (2n+4)\left(\frac{1}{\sqrt{3\times 3}}\right) + (4m+4n-4)\left(\frac{1}{\sqrt{3\times 2}}\right) + (6mn+m-5n-4)\left(\frac{1}{\sqrt{2\times 2}}\right)$$

$$= 3mn + \left(\frac{4}{\sqrt{6}} + \frac{1}{2}\right)m + \left(\frac{4}{\sqrt{6}} - \frac{11}{6}\right)n - \left(\frac{4}{\sqrt{6}} + \frac{2}{3}\right)$$

In the following theorem, we determine the atom bond connectivity Revan index of $B_{m,n}$.

Theorem 3. The atom bond connectivity Revan index of a jagged-rectangle benzenoid system $B_{m,n}$ is given by

$$ABCR(B_{m,n}) = \frac{6}{\sqrt{2}}mn + \frac{5}{\sqrt{2}}m + \left(\frac{4}{3} - \frac{1}{\sqrt{2}}\right)n + \left(\frac{8}{3} - \frac{8}{\sqrt{2}}\right)$$

Proof: From equation (3) and using Table 1, we deduce

$$ABCR(B_{m,n}) = \sum_{uv \in E(G)} \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u) r_G(v)}}$$

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

$$= \frac{6}{\sqrt{2}}mn + \frac{5}{\sqrt{2}}m + \left(\frac{4}{3} - \frac{1}{\sqrt{2}}\right)n + \left(\frac{8}{3} - \frac{8}{\sqrt{2}}\right)$$

In the following theorem, we compute the geometric-arithmetic Revan index of $B_{m,n}$.

Theorem 4. The geometric-arithmetic Revan index of a jagged-rectangle benzenoid system $B_{m,n}$ is given by

$$GAR(B_{m,n}) = 6mn + \left(\frac{8\sqrt{6}}{5} + 1\right)m + \left(\frac{8\sqrt{6}}{5} - 3\right)n - \frac{8\sqrt{6}}{5}.$$

Proof: From equation (4) and using Table 1, we deduce

$$GAR(B_{m,n}) = \sum_{uv \in E(G)} \frac{2\sqrt{r_G(u) r_G(v)}}{r_G(u) + r_G(v)}$$

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

$$= 6mn + \left(\frac{8\sqrt{6}}{5}+1\right)m + \left(\frac{8\sqrt{6}}{5}-3\right)n - \frac{8\sqrt{6}}{5}.$$

III. RESULTS FOR POLYCYCLIC AROMATIC HYDROCARBONS PAH_N.

In this section, we focus on the chemical graph of the family of polycyclic aromatic hydrocarbons, symbolized by PAH_n. The first three members of the family PAH_n are presented in Figure 2.

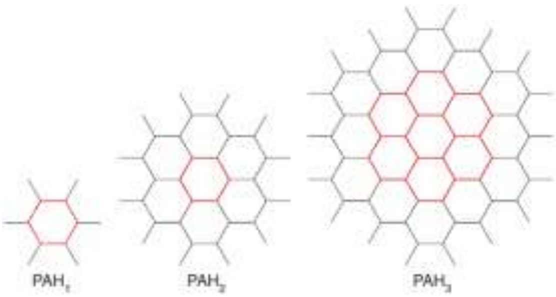

Figure 2. First three elements of PAH_n

Let G be the chemical graph in the family of polycylic aromatic hydrocarbons PAH_n. It is easy to see that the vertices G are either of degree 1 or 3. Therefore $\Delta(G)=3$ and $\delta(G)=1$. 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. In G, there are two types of edges based on the degree of end vertices of each edge as follows:

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

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

Table 2. Revan edge partition of PAH_n

$r_G(u), r_G(v)\backslash uv \in E(G)$	(3, 1)	(1, 1)
Number of edges	$6n$	$9n^2 - 3n$

In the following theorem, we determine the sum connectivity Revan index of PAH_n.

Theorem 5. The sum connectivity Revan index of a polycyclic aromatic hydrocarbon PAH_n is

$$SR(PAH_n) = \frac{9}{\sqrt{2}}n^2 + \left(3 - \frac{3}{\sqrt{2}}\right)n.$$

Proof: Using equation (1) and Table 2, we deduce

$$SR(PAH_n) = \sum_{uv\in E(G)} \frac{1}{\sqrt{r_G(u)+r_G(v)}}$$

$$= 6n\left(\frac{1}{\sqrt{3+1}}\right) + (9n^2-3n)\left(\frac{1}{\sqrt{1+1}}\right) = \frac{9}{\sqrt{2}}n^2 + \left(3 - \frac{3}{\sqrt{2}}\right)n.$$

In the next theorem, we determine the product connectivity Revan index of PAH_n.

Theorem 6. The product connectivity Revan index of a polycyclic aromatic hydrocarbon PAH_n is

$$PR(PAH_n) = 9n^2 + \left(2\sqrt{3} - 3\right)n.$$

Proof: Using equation (2) and Table 2, we deduce

$$PR(PAH_n) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_G(u) r_G(v)}}$$

$$= 6n\left(\frac{1}{\sqrt{3 \times 1}}\right) + \left(9n^2 - 3n\right)\left(\frac{1}{\sqrt{1 \times 1}}\right) = 9n^2 + \left(2\sqrt{3} - 3\right)n.$$

In the following theorem, we determine the atom bond connectivity Revan index of PAH_n.

Theorem 7. The atom bond connectivity Revan index of a polycyclic aromatic hydrocarbon PAH_n is

$$ABCR(PAH_n) = 2\sqrt{6}n.$$

Proof: Using equation (3) and Table 2, we deduce

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

$$= 6n\left(\sqrt{\frac{3+1-2}{3\times 1}}\right) + \left(9n^2 - 3n\right)\left(\sqrt{\frac{1+1-2}{1\times 1}}\right)$$

$$= 2\sqrt{6}n$$

In the next theorem, we compute the geometric-arithmetic Revan index of PAH_n.

Theorem 8. The geometric-arithmetic Revan index of a polycyclic aromatic hydrocarbon PAH_n is

$$GAR(PAH_n) = 9n^2 + \left(\sqrt{3} - 1\right)3n.$$

Proof: Let G be the graph in the family of polycyclic aromatic hydrocarbons PAH_n. By using equation (4) and Table 2, we deduce

$$GAR(PAH_n) = \sum_{uv \in E(G)} \frac{2\sqrt{r_G(u) r_G(v)}}{r_G(u) + r_G(v)} = 6n\left(\frac{2\sqrt{3 \times 1}}{3+1}\right) + \left(9n^2 - 3n\right)\left(\frac{2\sqrt{1 \times 1}}{1+1}\right)$$

$$= 9n^2 + \left(\sqrt{3} - 1\right)3n.$$

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