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Sum Augmented and Multiplicative Sum Augmented Indices of Some Nanostructures

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Abstract. We put forward the sum augmented index, multiplicative sum augmented index of a graph. We determine the sum augmented index and the multiplicative sum augmented index for polycyclic aromatic hydrocarbons and jagged rectangle benzenoid systems.

Keywords: sum augmented index, multiplicative sum augmented index, polycyclic aromatic hydrocarbon, benzenoid system.

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*09, 05*C*92

1. Introduction

Let $G = (V, E)$ be a finite, simple connected graph. Let $d(u)$ denote the degree of a vertex u [1, 2].

In the modeling of Mathematics, a molecular or a chemical graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. Topological indices are useful for finding correlations between the structure of a chemical compound and its physicochemical properties [3].

The augmented Zagreb index [4] is defined as

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

This topological index has been found to be a useful predictive indicator in the research on heat generation in octanes, and heptanes, with a prediction power that is superior to the atom bond connectivity index [4]. This index has also been researched in the past [5, 6, 7, 8, 9, 10].

We define the sum augmented index as

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

The multiplicative sum augmented index is defined as

$$SAIII(G)=\prod_{uv\in E(G)}\left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3.$$

Some multiplicative indices have been researched in the past [11, 12, 13, 14, 15, 16, 17, 18].

In this paper, we compute the sum augmented index and multiplicative sum augmented index of polycyclic aromatic hydrocarbons and jagged rectangle benzenoid systems. For information about these chemical compounds, see [19].

2. Polycyclic aromatic hydrocarbons

The first three members of the family polycyclic aromatic hydrocarbons PAH_n are presented in the below graph.

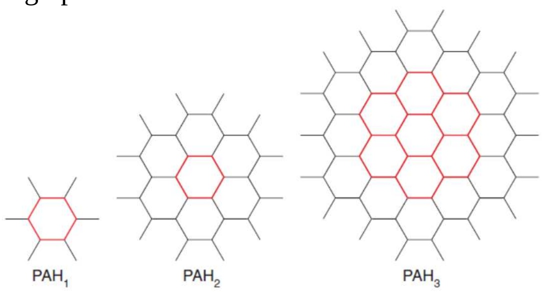

Figure 1:

The graphs of polycyclic aromatic hydrocarbons have $6n^2+6n$ vertices and $9n^2+3n$ edges are shown in the above graphs. Let $A= PAH_n$.

We obtain that $\{d(u), d(v): uv \in E(A)\}$ has two edge set partitions.

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

Table 1:

Theorem 1. The sum augmented index of PAH_n is

$$SAI(A)=\frac{243}{8}n^2+\frac{303}{8}n.$$

Proof: Applying definition and edge set partition of A, we conclude

$$SAI(A)=\sum_{uv\in E(A)}\left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3$$

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

$$=\frac{243}{8}n^2+\frac{303}{8}n.$$

Theorem 2. The multiplicative sum augmented index of PAH_n is

$$SAIII(A) = 2^{12n} \times \left(\frac{3}{2}\right)^{9(3n^2-1)}$$

Proof: Applying definition and edge set partition of A, we conclude

$$SAIII(A) = \prod_{uv\in E(A)} \left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3$$

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

$$= 2^{12n} \times \left(\frac{3}{2}\right)^{9(3n^2-1)}.$$

3. Benzenoid systems

Three chemical graphs of a jagged rectangle benzenoid system $B_{m,n}$ for all m, n, in N are shown in the below graph.

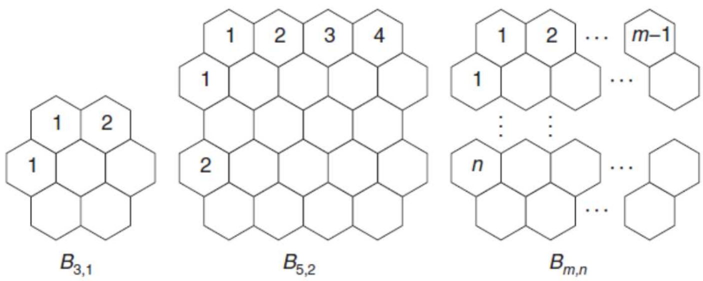

Figure 2:

The graphs of a jagged rectangle benzenoid system have $4mn + 4m + m - 2$ vertices and $6mn + 5m + n - 4$ edges. Let $H = B_{m,n}$.

We obtain that $\{d(u), d(v): uv \in E(H)\}$ has three edge set partitions.

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

Table 2:

Theorem 3. The sum augmented index of $B_{m,n}$ is

$$SAI(H) = \left(\frac{81}{4}\right)mn + \left(\frac{4729}{216}\right)m + \left(\frac{3811}{25}\right)n - \frac{1}{54}.$$

Proof: Applying definition and edge set partition of H, we conclude

$$SAI(H) = \sum_{uv\in E(H)} \left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3$$

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

$$=\left(\frac{81}{4}\right)mn+\left(\frac{4729}{216}\right)m+\left(\frac{3811}{25}\right)n-\frac{1}{54}.$$

Theorem 4. The multiplicative sum augmented index of $B_{m,n}$ is

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

Proof: Applying definition and edge set partition of H, we conclude

$$SAIII(H)=\prod_{uv\in E(H)}\left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3$$

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

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

4. Conclusion

This paper introduced two new augmented indices and obtained some new results on these indices. The results of the above study may be used in the further development of chemical compounds used for biological and chemical characteristics.

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Conflict of interest. A single author writes the paper, so there is no conflict of interest.

Authors' Contributions. It is a single-author paper. So, full credit goes to the author.

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