COMPUTATION OF MULTIPLICATIVE BANHATTI-SOMBOR INDICES OF CERTAIN BENZENOID SYSTEMS

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ABSTRACT:

Recently, a novel class of degree based topological indices was introduced, the so called Banhatti-Sombor indices. In this paper, we introduce the multiplicative first Banhatti-Sombor index, multiplicative first reduced Banhatti-Sombor index, multiplicative first δ -Banhatti-Sombor index of a graph and compute exact formulas for some nanostructures.

Keywords: multiplicative first Banhatti-Sombor index, multiplicative first reduced Banhatti-Sombor index, multiplicative first δ -Banhatti-Sombor index, nanostructure.

Mathematics Subject Classification: 05C05, 05C07, 05C90.

1. INTRODUCTION

Let G be a finite, simple, connected graph with vertex set V(G) and edge set E(G). Let $d_G(u)$ be the degree of a vertex u in a graph G. For undefined terms and notations, we refer [1].

Chemical Graph Theory is branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Topological indices are useful for establishing correlation between the structure of a molecular compound and its physicochemical properties. Numerous topological indices [2] have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR research, see [3, 4].

In [5], Kulli introduced the first Banhatti-Sombor index, first reduced Banhatti-Sombor index, first δ -Banhatti-Sombor index and they are defined as

$$BSO_{1}(G) = \sum_{uv \in E(G)} \left[\frac{1}{d_{G}(u)^{2}} + \frac{1}{d_{G}(v)^{2}} \right]^{\frac{1}{2}},$$

$$RBSO_{1}(G) = \sum_{uv \in E(G)} \left[\frac{1}{\left(d_{G}(u) - 1\right)^{2}} + \frac{1}{\left(d_{G}(v) - 1\right)^{2}} \right]^{\frac{1}{2}}, \text{ if } \delta(G) \ge 2$$

$$\delta BSO_{1}(G) = \sum_{uv \in E(G)} \left[\frac{1}{\left(d_{G}(u) - \delta(G) + 1\right)^{2}} + \frac{1}{\left(d_{G}(v) - \delta(G) + 1\right)^{2}} \right]^{\frac{1}{2}},$$

where $\delta(G)$ is the minimum degree among the vertices of G.

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Recently, some Sombor indices were studied, for example, in [6, 7, 8, 9, 10, 11, 12, 13, 14].

Inspired by work on Sombor indices, we put forward the multiplicative first Banhatti-Sombor index, multiplicative first reduced Banhatti-Sombor index and multiplicative first δ -Banhatti-Sombor index of a graph and they are defined as

$$BSO_{1}II(G) = \prod_{uv \in E(G)} \left[\frac{1}{d_{G}(u)^{2}} + \frac{1}{d_{G}(v)^{2}} \right]^{\frac{1}{2}},$$

$$RBSO_{1}II(G) = \prod_{uv \in E(G)} \left[\frac{1}{\left(d_{G}(u) - 1\right)^{2}} + \frac{1}{\left(d_{G}(v) - 1\right)^{2}} \right]^{\frac{1}{2}}, \text{ if } \delta(G) \ge 2$$

$$\delta BSO_{1}II(G) = \prod_{uv \in E(G)} \left[\frac{1}{\left(d_{G}(u) - \delta(G) + 1\right)^{2}} + \frac{1}{\left(d_{G}(v) - \delta(G) + 1\right)^{2}} \right]^{\frac{1}{2}}$$

where $\delta(G)$ is the minimum degree among the vertices of G.

In this paper, we compute the multiplicative first Banhatti-Sombor index, multiplicative first reduced Banhatti-Sombor index, multiplicative first δ -Banhatti-Sombor index of some families of benzenoid systems.

2. OBSERVATIONS

- (1) If $\delta(G) = 1$, then $\delta BSO_1II(G)$ is the multiplicative first Banhatti-Sombor index $BSO_1II(G)$.
- (2) If $\delta(G) = 2$, then $\delta BSO_1II(G)$ is the multiplicative first reduced Banhatti-Sombor index $RBSO_1II(G)$.

3. TRIANGULAR BENZENOIDS

In this section, we consider a family of triangular benzenoids. This family of benzenoids is denoted by 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 T_4 is shown in Figure 1.

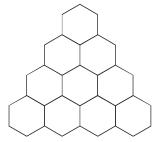


Figure-1: The graph of T_4

Let G be the graph of a triangular benzenoid T_p . The graph G has $p^2 + 4p + 1$ vertices and $\frac{3p(p+3)}{2}$ edges. From

Figure 1, we see that the vertices of G are either of degree 2 or 3. Therefore $\delta(G)$ = 2. By calculation, we obtain that G has three types of edges based on degrees of end vertices of each edge as follows:

$$E_{1} = \{uv \in E(G) \mid d_{G}(u) = d_{G}(v) = 2\}, \qquad |E_{1}| = 6.$$

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

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

In the following theorem, we compute the multiplicative first Banhatti-Sombor index of T_p .

Theorem 1: The multiplicative first Banhatti-Sombor index of a triangular benzenoid T_p is given by

$$BSO_{1}H\left(T_{p}\right) = \left(\frac{1}{2}\right)^{\frac{6}{2}} \times \left(\frac{13}{36}\right)^{\frac{1}{2}(6p-6)} \times \left(\frac{2}{9}\right)^{\frac{3}{4}p(p-1)}.$$

Proof: By using definition and cardinalities of the edge partition of T_p , we have

$$\begin{split} BSO_{1}II\left(T_{p}\right) &= \left(\frac{1}{2^{2}} + \frac{1}{2^{2}}\right)^{\frac{6}{2}} \times \left(\frac{1}{2^{2}} + \frac{1}{3^{2}}\right)^{\frac{1}{2}(6p-6)} \times \left(\frac{1}{3^{2}} + \frac{1}{3^{2}}\right)^{\frac{3}{4}p(p-1)} \\ &= \left(\frac{1}{2}\right)^{\frac{6}{2}} \times \left(\frac{13}{36}\right)^{\frac{1}{2}(6p-6)} \times \left(\frac{2}{9}\right)^{\frac{3}{4}p(p-1)}. \end{split}$$

In the following theorem, we determine the multiplicative first reduced Banhatti-Sombor index of T_p .

Theorem 2: The multiplicative first reduced Banhatti-Sombor index of a triangular benzenoid T_p is given by

$$RBSO_{1}II\left(T_{p}\right) = (2)^{\frac{6}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(6p-6)} \times \left(\frac{1}{2}\right)^{\frac{3}{4}p(p-1)}.$$

Proof: From definition and by using cardinalities of the edge partition of T_p , we obtain

$$\begin{split} RBSO_{1}II\left(T_{p}\right) &= \left(\frac{1}{1^{2}} + \frac{1}{1^{2}}\right)^{\frac{6}{2}} \times \left(\frac{1}{1^{2}} + \frac{1}{2^{2}}\right)^{\frac{1}{2}(6p-6)} \times \left(\frac{1}{2^{2}} + \frac{1}{2^{2}}\right)^{\frac{3}{4}p(p-1)} \\ &= (2)^{\frac{6}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(6p-6)} \times \left(\frac{1}{2}\right)^{\frac{3}{4}p(p-1)}. \end{split}$$

In the following theorem, we determine the multiplicative first δ -Banhatti-Sombor index of T_p .

Theorem 3: The multiplicative first δ -Banhatti-Sombor index of a triangular benzenoid T_p is given by

$$\delta BSO_{1}II\left(T_{p}\right) = (2)^{\frac{6}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(6p-6)} \times \left(\frac{1}{2}\right)^{\frac{3}{4}p(p-1)}.$$

Proof: By observation (2) and Theorem 2, the result follows.

4. BENZENOID RHOMBUS

In this section, we consider a family of benzenoid rhombus. This family of benzenoids is denoted by 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 R_4 is depicted in Figure 2.

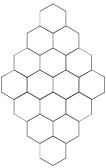


Figure-2: The graph of R_4

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. Thus $\delta(R_p) = 2$. By calculation, we obtain that G has three types of edges based on degrees of end vertices of each edge as follows:

$$E_1 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}, \qquad |E_1| = 6.$$

$$E_2 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}, \qquad |E_2| = 8p - 8.$$

$$E_3 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, \qquad |E_3| = 3p^2 - 4p + 1.$$

In the following theorem, we compute the multiplicative first Banhatti-Sombor index of R_p .

Theorem 4: The multiplicative first Banhatti-Sombor index of a benzenoid rhombus R_p is given by

$$BSO_{1}H\left(R_{p}\right) = \left(\frac{1}{2}\right)^{\frac{6}{2}} \times \left(\frac{13}{36}\right)^{\frac{1}{2}(8p-8)} \times \left(\frac{2}{9}\right)^{\frac{1}{2}(3p-4p+1)}.$$

Proof: From definition and by cardinalities of the edge partition of R_p , we deduce

$$BSO_{1}II(R_{p}) = \left(\frac{1}{2^{2}} + \frac{1}{2^{2}}\right)^{\frac{6}{2}} \times \left(\frac{1}{2^{2}} + \frac{1}{3^{2}}\right)^{\frac{1}{2}(8p-8)} \times \left(\frac{1}{3^{2}} + \frac{1}{3^{2}}\right)^{\frac{1}{2}(3p^{2}-4p+1)}$$

$$= \left(\frac{1}{2}\right)^{\frac{6}{2}} \times \left(\frac{13}{36}\right)^{\frac{1}{2}(8p-8)} \times \left(\frac{2}{9}\right)^{\frac{1}{2}(3p-4p+1)}.$$

In the following theorem, we determine the multiplicative first reduced Banhatti-Sombor index of R_p .

Theorem 5: The multiplicative first reduced Banhatti-Sombor index of a benzenoid rhombus R_p is given by

$$RBSO_{1}II\left(R_{p}\right) = (2)^{\frac{6}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(8p-8)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(3p^{2}-4p+1)}.$$

Proof: By using definition and by cardinalities of the edge partition of R_p , we derive

$$\begin{split} RBSO_{1}II\left(R_{p}\right) &= \left(\frac{1}{1^{2}} + \frac{1}{1^{2}}\right)^{\frac{6}{2}} \times \left(\frac{1}{1^{2}} + \frac{1}{2^{2}}\right)^{\frac{1}{2}(8p-8)} \times \left(\frac{1}{2^{2}} + \frac{1}{2^{2}}\right)^{\frac{1}{2}(3p^{2}-4p+1)} \\ &= (2)^{\frac{6}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(8p-8)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(3p^{2}-4p+1)} . \end{split}$$

In the following next theorem, we compute the multiplicative first δ -Banhatti-Sombor index of R_p .

Theorem 6: The multiplicative first δ -Banhatti-Sombor index of R_n is given by

$$\delta BSO_{1}II\left(R_{p}\right) = (2)^{\frac{6}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(8p-8)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(3p^{2}-4p+1)}.$$

Proof: By observation (2) and Theorem 5, the result follows.

5. BENZENOID HOURGLASS

In this section, we consider a family of benzenoid hourglass, which is denoted by X_p . This family is obtained from two copies of a triangular benzenoid T_p by overlapping hexagons. The graph of benzenoid hourglass is presented in Figure 3

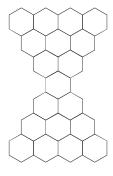


Figure-3: The graph of benzenoid hourglass

Let *G* be the graph of a benzenoid hourglass X_p . This graph *G* has $2(p^2 + 4p - 2)$ vertices and $3p^2 + 9p - 4$ edges. From Figure 3, we see that the vertices of X_p are either of degree 2 or 3. Thus $\delta(X_p) = 2$.

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By algebraic method, we find that G has three types of edges based on degrees of end vertices of each as follows:

$$E_1 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\},$$
 $|E_1| = 8.$
 $E_2 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\},$ $|E_2| = 12p - 16.$
 $E_3 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\},$ $|E_3| = 3p^2 - 3p + 4.$

In the following theorem, we compute the multiplicative first Banhatti-Sombor index of X_p .

Theorem 7: The multiplicative first Banhatti-Sombor index of a benzenoid hourglass X_p is given by

$$BSO_{1}II\left(X_{p}\right) = \left(\frac{1}{2}\right)^{\frac{8}{2}} \times \left(\frac{13}{36}\right)^{\frac{1}{2}(12p-16)} \times \left(\frac{2}{9}\right)^{\frac{1}{2}(3p^{2}-3p+4)}.$$

Proof: From definition and by cardinalities of the edge partition of X_p , we obtain

$$\begin{split} BSO_{1}H\left(X_{p}\right) &= \left(\frac{1}{2^{2}} + \frac{1}{2^{2}}\right)^{\frac{8}{2}} \times \left(\frac{1}{2^{2}} + \frac{1}{3^{2}}\right)^{\frac{1}{2}(12p-16)} \times \left(\frac{1}{3^{2}} + \frac{1}{3^{2}}\right)^{\frac{1}{2}(3p^{2}-3p+4)} \\ &= \left(\frac{1}{2}\right)^{\frac{8}{2}} \times \left(\frac{13}{36}\right)^{\frac{1}{2}(12p-16)} \times \left(\frac{2}{9}\right)^{\frac{1}{2}(3p^{2}-3p+4)}. \end{split}$$

In the following theorem, we compute the multiplicative first reduced Banhatti-Sombor index of X_p .

Theorem 8: The multiplicative first reduced Banhatti-Sombor index of a benzenoid hourglass is given by

$$.RBSO_{1}II\left(X_{p}\right) = (2)^{\frac{8}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(12p-16)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(3p^{2}-3p+1)}.$$

Proof: From definition and by cardinalities of the edge partition of X_p , we deduce

$$\begin{split} RBSO_{1}II\left(X_{p}\right) &= \left(\frac{1}{1^{2}} + \frac{1}{1^{2}}\right)^{\frac{8}{2}} \times \left(\frac{1}{1^{2}} + \frac{1}{2^{2}}\right)^{\frac{1}{2}(12p-16)} \times \left(\frac{1}{2^{2}} + \frac{1}{2^{2}}\right)^{\frac{1}{2}(3p^{2}-3p+1)} \\ &= (2)^{\frac{8}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(12p-16)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(3p^{2}-3p+1)} . \end{split}$$

In the next theorem, we determine the multiplicative first δ -Banhatti-Sombor index of X_p .

Theorem 9: The multiplicative first δ -Banhatti-Sombor index of a benzenoid hourglass X_n is given by

$$\delta BSO_{1}II\left(X_{p}\right) = (2)^{\frac{8}{2}} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(12p-16)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(3p^{2}-3p+1)}.$$

Proof: By observation (2) and from Theorem 8, we obtain the desired result.

6. JAGGED RECTANGLE BENZENOID SYSTEMS

In this section, we focus in the molecular graph structure of a jagged rectangle benzenoid system. This system is denoted by $B_{m,n}$ for all $m, n \in \mathbb{N}$. Three chemical graphs of a jagged rectangle benzenoid system are presented in Figure 4.

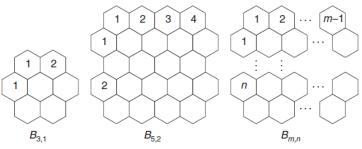


Figure-4

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Let G be the graph of a jagged rectangle benzenoid system $B_{m,n}$. By calculation, we obtain that G has 4mn + 4m + 2n - 2 vertices and 6mn + 5m + n - 4 edges. From Figure 4, it is easy to see that the vertices of G are either of degree 2 or 3. Thus $\delta(G)$ =2. By calculation, we obtain that the edge set of $B_{m,n}$ can be divided into three partitions as follows:

$$E_{1} = \{uv \in E(G) \mid d_{G}(u) = d_{G}(v) = 2\}, \qquad |E_{1}| = 2n + 4.$$

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

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

In the following theorem, we determine the multiplicative first Banhatti-Sombor index of $B_{m,n}$

Theorem 10: The multiplicative first Banhatti-Sombor inverse index of $B_{m,n}$ is given by

$$BSO_{1}II\left(B_{m,n}\right) = \left(\frac{1}{2}\right)^{\frac{1}{2}(2n+4)} \times \left(\frac{13}{36}\right)^{\frac{1}{2}(4m+4n-4)} \times \left(\frac{2}{9}\right)^{\frac{1}{2}(6mn+m-n-4)}.$$

Proof: From definition and by cardinalities of the edge partition of $B_{m,n}$, we obtain

$$BSO_{1}H(B_{m,n}) = \left(\frac{1}{2^{2}} + \frac{1}{2^{2}}\right)^{\frac{1}{2}(2n+4)} \times \left(\frac{1}{2^{2}} + \frac{1}{3^{2}}\right)^{\frac{1}{2}(4m+4n-4)} \times \left(\frac{1}{3^{2}} + \frac{1}{3^{2}}\right)^{\frac{1}{2}(6mn+m-n-4)}$$
$$= \left(\frac{1}{2}\right)^{\frac{1}{2}(2n+4)} \times \left(\frac{13}{36}\right)^{\frac{1}{2}(4m+4n-4)} \times \left(\frac{2}{9}\right)^{\frac{1}{2}(6mn+m-n-4)}.$$

In the following theorem, we compute the multiplicative first reduced Banhatti-Sombor index of $B_{m,n}$.

Theorem 11: The multiplicative first reduced Banhatti-Sombor index of $B_{m,n}$ is given by

$$RBSO_{1}H\left(B_{m,n}\right) = (2)^{\frac{1}{2}(2n+4)} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(4m+4n-4)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(6mn+m-5n-4)}.$$

Proof: From definition and by cardinalities of the edge partition of $B_{m,n}$, we obtain

$$\begin{split} RBSO_{1}H\left(B_{m,n}\right) &= \left(\frac{1}{1^{2}} + \frac{1}{1^{2}}\right)^{\frac{1}{2}(2n+4)} \times \left(\frac{1}{1^{2}} + \frac{1}{2^{2}}\right)^{\frac{1}{2}(4m+4n-4)} \times \left(\frac{1}{2^{2}} + \frac{1}{2^{2}}\right)^{\frac{1}{2}(6mn+m-5n-4)} \\ &= (2)^{\frac{1}{2}(2n+4)} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(4m+4n-4)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(6mn+m-5n-4)} \end{split}$$

In the following next theorem, we determine the multiplicative first δ -Banhatti-Sombor index of $B_{m,n}$

Theorem 12: The multiplicative first δ -Banhatti-Sombor index of $B_{m,n}$ is given by

$$\delta BSO_{1} II\left(B_{m,n}\right) = (2)^{\frac{1}{2}(2n+4)} \times \left(\frac{5}{4}\right)^{\frac{1}{2}(4m+4n-4)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(6mn+m-5n-4)}.$$

Proof: From observation (2) and Theorem 11, we get the desired result.

7. CONCLUSION

In this study, we have introduced the multiplicative first Banhatti-Sombor index, multiplicative first reduced Banhatti-Sombor index, multiplicative first δ -Banhatti-Sombor index of a graph and have computed exact formulas for certain benzenoid systems.

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