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ON BANHATTI-SOMBOR INDICES

V.R.Kulli
Department of Mathematics, Gulbarga University, Kalaburgi (Gulbarga)-585106, India

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

Keywords: *first Banhatti-Sombor index, first reduced Banhatti-Sombor index, first δ-Banhatti-Sombor index, nanostructure.*
Mathematics Subject Classification: 05*C*05, 05*C*07, 05*C*90.

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], Gutman proposed the Sombor indices and they are defined as

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

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

$$ASO(G) = \sum_{uv\in E(G)} \left[\left(d_G(u)-\frac{2m}{n}\right)^2 + \left(d_G(v)-\frac{2m}{n}\right)^2\right]^{\frac{1}{2}}$$

where $|V(G)| = n$ and $|E(G)| = m$.

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 first Banhatti-Sombor index, first reduced Banhatti-Sombor index and first δ-Banhatti-Sombor index of a graph and they are defined as

$$BSO_1(G) = \sum_{uv\in E(G)} \left[\frac{1}{d_G(u)^2} + \frac{1}{d_G(v)^2}\right]^{\frac{1}{2}},$$

$$RBSO_1(G) = \sum_{uv\in E(G)} \left[\frac{1}{\left(d_G(u)-1\right)^2} + \frac{1}{\left(d_G(v)-1\right)^2}\right]^{\frac{1}{2}},$$

if $\delta(G) \geq 2$,

$$\delta BSO_1(G) = \sum_{uv\in E(G)} \left[\frac{1}{\left(d_G(u)-\delta(G)+1\right)^2} + \frac{1}{\left(d_G(v)-\delta(G)+1\right)^2}\right]^{\frac{1}{2}}$$

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

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

2. Observations

(1) If $\delta(G) = 1$, then $\delta BSO_1(G)$ is the Banhatti-Sombor index $BSO_1(G)$.

(2) If $\delta(G) = 2$, then $\delta BSO_1(G)$ is the reduced Banhatti-Sombor index $RBSO_1(G)$.

2. 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 $\frac{1}{2}p\left(p-1\right)$ hexagons. The graph of T_4 is shown in Figure 1.

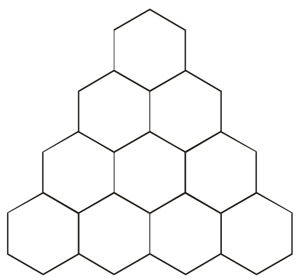

Figure 1. The graph of T_4

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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:

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

$E_2 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_2| = 6p - 6$.

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

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

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

$$BSO_1(T_p) = \frac{1}{\sqrt{2}}p^2 + \left(\sqrt{3} - \frac{1}{\sqrt{2}}\right)p + \frac{6}{\sqrt{2}} - \sqrt{13}.$$

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

$$BSO_1(T_p) = \left(\frac{1}{2^2} + \frac{1}{2^2}\right)^{\frac{1}{2}} 6 + \left(\frac{1}{2^2} + \frac{1}{3^2}\right)^{\frac{1}{2}} (6p - 6)$$

$$+ \left(\frac{1}{3^2} + \frac{1}{3^2}\right)^{\frac{1}{2}} \frac{3}{2} p(p-1)$$

$$= \frac{1}{\sqrt{2}}p^2 + \left(\sqrt{13} - \frac{1}{\sqrt{2}}\right)p + \frac{6}{\sqrt{2}} - \sqrt{13}.$$

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

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

$$RBSO_1(T_p) = \frac{3}{2\sqrt{2}}p^2 + \left(3\sqrt{5} - \frac{3}{2\sqrt{2}}\right)p + 6\sqrt{2} - 3\sqrt{5}.$$

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

$$RBSO_1(T_p) = \left(\frac{1}{1^2} + \frac{1}{1^2}\right)^{\frac{1}{2}} 6 + \left(\frac{1}{1^2} + \frac{1}{2^2}\right)^{\frac{1}{2}} (6p - 6)$$

$$+ \left(\frac{1}{2^2} + \frac{1}{2^2}\right)^{\frac{1}{2}} \frac{3}{2} p(p-1)$$

$$= \frac{3}{2\sqrt{2}}p^2 + \left(3\sqrt{5} - \frac{3}{2\sqrt{2}}\right)p + 6\sqrt{2} - 3\sqrt{5}.$$

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

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

$$\delta BSO_1(T_p) = \frac{3}{2\sqrt{2}}p^2 + \left(3\sqrt{5} - \frac{3}{2\sqrt{2}}\right)p + 6\sqrt{2} - 3\sqrt{5}.$$

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.

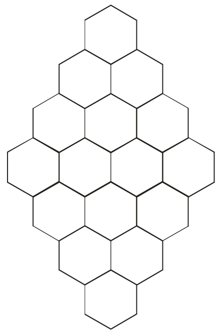

Figure 2. The graph of R_4

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:

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

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

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

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

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

$$BSO_1(R_p) = \sqrt{2}p^2 + \left(\frac{4\sqrt{13}}{3} - \frac{4\sqrt{2}}{3}\right)p$$

$$+ \frac{6}{\sqrt{2}} - \frac{4\sqrt{13}}{3} + \frac{\sqrt{2}}{3}.$$

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

$$BSO_1(R_p) = \left(\frac{1}{2^2} + \frac{1}{2^2}\right)^{\frac{1}{2}} 6 + \left(\frac{1}{2^2} + \frac{1}{3^2}\right)^{\frac{1}{2}} (8p - 8)$$

$$+ \left(\frac{1}{3^2} + \frac{1}{3^2}\right)^{\frac{1}{2}} (3p^2 - 4p + 1)$$

$$=\sqrt{2}p^2+\left(\frac{4\sqrt{13}}{3}-\frac{4\sqrt{2}}{3}\right)p$$

$$+\frac{6}{\sqrt{2}}-\frac{4\sqrt{13}}{3}+\frac{\sqrt{2}}{3}.$$

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

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

$$RBSO_1(R_p)=\frac{3}{\sqrt{2}}p^2+\left(4\sqrt{5}-2\sqrt{2}\right)p+\frac{13}{\sqrt{2}}-4\sqrt{5}.$$

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

$$RBSO_1(R_p)=\left(\frac{1}{1^2}+\frac{1}{1^2}\right)^{\frac{1}{2}}6+\left(\frac{1}{1^2}+\frac{1}{2^2}\right)^{\frac{1}{2}}(8p-8)$$

$$+\left(\frac{1}{2^2}+\frac{1}{2^2}\right)^{\frac{1}{2}}\left(3p^2-4p+1\right)$$

$$=\frac{3}{\sqrt{2}}p^2+\left(4\sqrt{5}-2\sqrt{2}\right)p+\frac{13}{\sqrt{2}}-4\sqrt{5}.$$

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

Theorem 6. The first δ-Banhatti-Sombor Sombor index of R_p is given by

$$\delta BSO_1(R_p)=\frac{3}{2\sqrt{2}}p^2+\left(4\sqrt{5}-2\sqrt{2}\right)p+\frac{13}{\sqrt{2}}-4\sqrt{5}.$$

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.

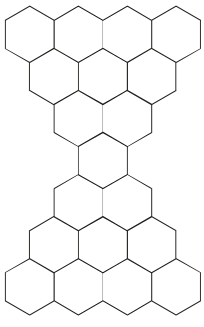

Figure 3. The graph of benzenoid hourglass

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 $\delta(X_p) = 2$. 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 first Banhatti-Sombor index of X_p.

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

$$BSO_1(X_p)=\sqrt{2}p^2+\left(2\sqrt{13}-\sqrt{2}\right)p+\frac{16\sqrt{2}}{3}-\frac{8\sqrt{13}}{3}.$$

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

$$BSO_1(X_p)=\left(\frac{1}{2^2}+\frac{1}{2^2}\right)^{\frac{1}{2}}8+\left(\frac{1}{2^2}+\frac{1}{3^2}\right)^{\frac{1}{2}}(12p-16)$$

$$+\left(\frac{1}{3^2}+\frac{1}{3^2}\right)^{\frac{1}{2}}\left(3p^2-3p+4\right)$$

$$=\sqrt{2}p^2+\left(2\sqrt{13}-\sqrt{2}\right)p$$

$$+\frac{16\sqrt{2}}{3}+\frac{8\sqrt{13}}{3}.$$

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

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

$$RBSO_1(X_p)=\frac{3}{\sqrt{2}}p^2+\left(6\sqrt{5}-\frac{3}{\sqrt{2}}\right)p+10\sqrt{2}-8\sqrt{5}.$$

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

$$RBSO_1(X_p)=\left(\frac{1}{1^2}+\frac{1}{1^2}\right)^{\frac{1}{2}}8+\left(\frac{1}{1^2}+\frac{1}{2^2}\right)^{\frac{1}{2}}(12p-16)$$

$$+\left(\frac{1}{2^2}+\frac{1}{2^2}\right)^{\frac{1}{2}}\left(3p^2-3p+4\right)$$

$$=\frac{3}{\sqrt{2}}p^2+\left(6\sqrt{5}-\frac{3}{\sqrt{2}}\right)p+10\sqrt{2}-8\sqrt{5}.$$

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

Theorem 9. The first δ-Banhatti-Sombor index of a benzenoid hourglass X_p is given by

$$\delta BSO_1(X_p)=\frac{3}{\sqrt{2}}p^2+\left(6\sqrt{2}-\frac{3}{\sqrt{2}}\right)p+10\sqrt{2}-8\sqrt{5}.$$

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 $m, n \in N$. Three chemical graphs of a jagged rectangle benzenoid system are presented in Figure 4.

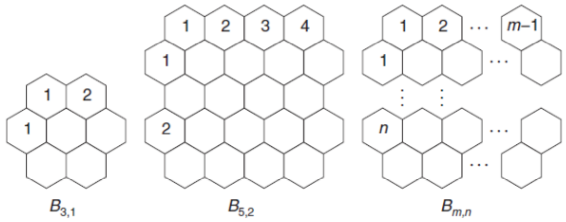

Figure 4

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:

$E_1 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_1| = 2n + 4$.

$E_2= \{uv\in E(G)|d_G(u)=2, d_G(v)=3\}$, $|E_2| = 4m + 4n - 4$.

$E_3 = \{uv\in E(G) \mid d_G(u)=d_G(v)= 3\}$,$|E_3|=6mn+m-5n-4$.

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

Theorem 10. The first Banhatti-Sombor index of $B_{m,\ n}$ is given by

$$BSO_1(B_{m,n}) = 2\sqrt{2}mn + \left(\frac{2\sqrt{13}}{3} + \frac{\sqrt{2}}{3}\right)m - \left(\frac{2\sqrt{2}}{3} - \frac{2\sqrt{13}}{3}\right)n + \frac{2\sqrt{2}}{3} - \frac{2\sqrt{13}}{3}.$$

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

$$BSO_1(B_{m,n}) = \left(\frac{1}{2^2} + \frac{1}{2^2}\right)^{\frac{1}{2}}(2n+4) + \left(\frac{1}{2^2} + \frac{1}{3^2}\right)^{\frac{1}{2}}(4m+4n-4) + \left(\frac{1}{3^2} + \frac{1}{3^2}\right)^{\frac{1}{2}}(6mn+m-5n-4)$$

$$= 2\sqrt{2}mn + \left(\frac{2\sqrt{13}}{3} + \frac{\sqrt{2}}{3}\right)m - \left(\frac{2\sqrt{2}}{3} - \frac{2\sqrt{13}}{3}\right)n + \frac{2\sqrt{2}}{3} - \frac{2\sqrt{13}}{3}.$$

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

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

$$RBSO_1(B_{m,n}) = \frac{6}{\sqrt{2}}mn + \left(2\sqrt{5} + \frac{1}{\sqrt{2}}\right)m - \left(\frac{1}{\sqrt{2}} - 2\sqrt{5}\right)n + \frac{4}{\sqrt{2}} - 2\sqrt{5}.$$

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

$$RBSO_1(B_{m,n}) = \left(\frac{1}{1^2} + \frac{1}{1^2}\right)^{\frac{1}{2}}(2n+4) + \left(\frac{1}{1^2} + \frac{1}{2^2}\right)^{\frac{1}{2}}(4m+4n-4) + \left(\frac{1}{2^2} + \frac{1}{2^2}\right)^{\frac{1}{2}}(6mn+m-5n-4)$$

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

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

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

$$\delta BSO_1(B_{m,n}) = \frac{6}{\sqrt{2}}mn + \left(2\sqrt{5} + \frac{1}{\sqrt{2}}\right)m - \left(\frac{1}{\sqrt{2}} - 2\sqrt{5}\right)m + \frac{4}{\sqrt{2}} - 2\sqrt{5}.$$

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

Conclusion

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

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