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Zagreb-K-Banhatti index of a graphV. R. KULLI¹ and B. CHALUVARAJU²¹Department of Mathematics, Gulbarga University, Gulbarga - 585 106 (India)E-mail: vrkulli@gmail.com²Department of Mathematics, Bangalore University, Jnana Bharathi Campus,

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Abstract

The Zagreb indices were introduced by Gutman and Trinajstić in 1972. The K-Banhatti indices were introduced by Kulli in 2016. These two types of indices are closely related. In this study, we define the Zagreb-K-Banhatti index of a graph. We establish some relations between Zagreb, K-Banhatti and Zagreb-K-Banhatti indices. We also obtain lower and upper bounds for the Zagreb-K-Banhatti index of a graph in terms of Zagreb and K-Banhatti indices.

Keywords: Zagreb index, K-Banhatti indices, Zagreb-K-Banhatti index.**2010 (AMS) Mathematics Subject Classification:** 05C05, 05C07, 05C35.**1. Introduction**

We consider only finite, simple graphs. Let $G = (V, E)$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. A graph G has n vertices and m edges. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u . The edge connecting the vertices u and v will be denoted by uv . Let $d_G(e)$ denote the degree of an edge $e = uv$ in G , which is defined by $d_G(e) = d_G(u) + d_G(v) - 2$. The vertices and edges of a graph G are called the elements of G . For undefined terms and notations, we refer the book¹.

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is a branch of Mathematical chemistry, which has an important effect on the

development of the Chemical Sciences. In Chemical Science, physico-chemical properties of chemical compounds often modelled by means of molecular graph based structure descriptors, which are also referred to as topological indices or graph indices. A single number that can be used to characterize some property of the underlying molecule is said to be a topological indices. Numerous such topological indices have been considered as Theoretical Chemistry, and have found some applications, especially in QSPR/QSAR/QSTR study³⁻⁵.

The first and second Zagreb indices were introduced by Gutman *et al*⁶. They are defined as $M_1(G) = \sum_{u \in V(G)} d_G(u)^2$ and $M_2(G) = \sum_{uv \in E(G)} [d_G(u) \cdot d_G(v)]$. An alternative expression for the first Zagreb index⁷ is $M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]$.

Shirdel⁸ *et al.*, introduced the first hyper-Zagreb index of a graph G and defined it as $HM_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^2$.

Milicevic⁹ *et al.*, introduced the first and second reformulated Zagreb indices of a graph G in terms of edge degrees instead of vertex degrees and defined as $EM_1(G) = \sum_{e \in E(G)} d_G(e)^2$ and $EM_2(G) = \sum_{e \sim f} [d_G(e) \cdot d_G(f)]$, where $e \sim f$ means that the edges e and f are adjacent. The third reformulated Zagreb index of a graph G is defined by $EM_3(G) = \sum_{e \sim f} [d_G(e) + d_G(f)]$.

Furtula¹⁰ *et al.*, introduced the forgotten topological index of a graph G , defined as $F(G) = \sum_{uv \in E(G)} (d_G(u))^2 + (d_G(v))^2 = \sum_{v \in V(G)} d_G(v)^3$.

Kulli¹¹ introduced the first and second K-Banhatti indices, intending to take into account the contributions of pairs of incident elements. The first and second K-Banhatti indices of a graph G are defined as $B_1(G) = \sum_{ue} d_G(u) + d_G(e)$ and $B_2(G) = \sum_{ue} d_G(u) \cdot d_G(e)$, respectively, where ue means that the vertex u and edge e are incident in G .

The first and second K hyper Banhatti indices were introduced by Kulli¹² and they are defined as $HB_1(G) = \sum_{ue} [d_G(u) + d_G(e)]^2$ and $HB_2(G) = \sum_{ue} [d_G(u) \cdot d_G(e)]^2$.

The Zagreb and K-Banhatti indices have been studied extensively. Their various modifications have been introduced. These two types of indices are closely related. For their history, applications, and mathematical properties¹³⁻²² and the references cited therein.

Motivated by the work on Zagreb and K- Banhatti indices, we introduce the Zagreb-K-Banhatti index of a graph G and defined it as

$$MB(G) = \sum_{\substack{a \text{ is either adjacent} \\ \text{or} \\ \text{incident to } b}} [d_G(a) + d_G(b)],$$

where a and b are elements of G .

In this paper, we obtain some relations between the Zagreb-K-Banhatti index, Zagreb, K-Banhatti indices. Also, we provide lower and upper bounds for $MB(G)$ of a graph in terms of Zagreb-type indices.

2. Comparison of Zagreb-K-Banhatti, Zagreb, Banhatti-type indices :

We use the following result to prove Theorem 2.

*Theorem 1*²¹. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$B_1(G) = 3M_1(G) - 4m.$$

Theorem 2. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$MB(G) = 4M_1(G) + EM_3(G) - 4m.$$

Proof. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$\begin{aligned} MB(G) &= \sum_{\substack{a \text{ is either adjacent} \\ \text{or} \\ \text{incident to } b}} [d_G(a) + d_G(b)] \\ &= \sum_{ab \in E(G)} [d_G(a) + d_G(b)] \\ &\quad + \sum_{e, f \in E(G), e \sim f} [d_G(a) + d_G(b)] \\ &\quad + \sum_{a(ab)} [d_G(a) + d_G(b)] \\ &= M_1(G) + EM_3(G) + B_1(G). \end{aligned}$$

Using Theorem 1, we have $MB(G) = 4M_1(G) + EM_3(G) - 4m$.

We use the following theorem to prove our next result.

*Theorem 3*²¹. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$B_1(G) = HM_1(G) - EM_1(G) - M_1(G).$$

Theorem 4. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$MB(G) = HM_1(G) + EM_3(G) - EM_1(G).$$

From Theorem 2, we have

$$\begin{aligned} MB(G) &= M_1(G) + EM_3(G) + B_1(G) \\ &= HM_1(G) + EM_3(G) - EM_1(G). \end{aligned}$$

To prove the next result, we use the earlier established;

*Theorem 5*²¹. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$B_1(G) = HM_1(G) + M_1(G) - B_2(G) - 4m.$$

Theorem 6. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$MB(G) = 2M_1(G) + HM_1(G) + EM_3(G) - B_2(G) - 4m.$$

Proof. From Theorem 2, we have

$$\begin{aligned} MB(G) &= M_1(G) + EM_3(G) + B_1(G) \\ &= 2M_1(G) + HM_1(G) + EM_3(G) - B_2(G) - 4m, \text{ by Theorem 5.} \end{aligned}$$

We use the following result to prove Theorem 8.

*Theorem 7*²¹. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$B_1(G) = \frac{1}{2}HB_1(G) - EM_1(G) + M_1(G) - 12m.$$

Theorem 8. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$MB(G) = 2M_1(G) + \frac{1}{2}HB_1(G) + EM_3(G) - EM_1(G) - 12m.$$

Proof. From Theorem 2, we have

$$\begin{aligned} B(G) &= M_1(G) + EM_3(G) + B_1(G) \\ &= 2M_1(G) + \frac{1}{2}HB_1(G) + EM_3(G) - EM_1(G) - 12m, \text{ by Theorem 7.} \end{aligned}$$

We use the following result to establish our next result.

*Theorem 9*²¹. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$B_1(G) = F(G) + 2M_2(G) - 4M_1(G) + 4m.$$

Theorem 10. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$MB(G) = F(G) + 2M_2(G) - 3M_1(G) + EM_3(G) + 4m.$$

Proof. From Theorem 2, we have

$$\begin{aligned} MB(G) &= M_1(G) + EM_3(G) + B_1(G) \\ &= F(G) + 2M_2(G) - 3M_1(G) + EM_3(G) + 4m, \text{ by Theorem 9.} \end{aligned}$$

3. Bounds on Zagreb-K-Banhatti, Zagreb, K-Banhatti-type indices :

We use the following result to prove Theorem 12.

*Theorem 11*²¹. For any connected graph G ,

$$M_1(G) \leq B_1(G).$$

Equality is attained if and only if G is regular.

Theorem 12. Let G be a connected graph with $n \geq 3$ vertices and m edges. Then

$$2M_1(G) + EM_3(G) \leq MB(G).$$

Equality is attained if and only if G is regular.

Proof. From Theorem 2, we have $MB(G) = M_1(G) + EM_3(G) + B_1(G)$.

Using Theorem 11, we obtain $2M_1(G) + EM_3(G) \leq MB(G)$.

Second part is obvious.

We use the following results to prove our next result.

*Theorem 13*²². Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$\frac{4m^2}{n} \leq M_1(G).$$

*Theorem 14*²¹. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$\frac{4m(3m - n)}{n} \leq B_1(G) \leq 3m^2 - m.$$

Theorem 15. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$\frac{4m(4m - n)}{n} + EM_3(G) \leq MB(G) \leq EM_3(G) + 4m^2.$$

Proof. From Theorem 2, we have $MB(G) = M_1(G) + EM_3(G) + B_1(G)$.

From Theorems 13 and 14, bearing in mind that $M_1(G) \leq m(m+1)$, we have

$$\frac{4m^2}{n} + EM_3(G) + \frac{4m(3m-n)}{n} \leq MB(G) \leq m(m+1) + EM_3(G) + 3m^2 - m.$$

Thus, $\frac{4m(4m - n)}{n} + EM_3(G) \leq MB(G) \leq EM_3(G) + 4m^2$.

We use the following result to prove our next result.

*Theorem 16*²¹. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$2m[3\delta(G) - 2] \leq B_1(G) \leq 2m[3\Delta(G) - 2].$$

Further, equality in both lower and upper bounds is attained if and only if G is regular.

Theorem 17. Let G be a simple graph with $n \geq 3$ vertices and m edges. Then

$$4m[2\delta(G) - 1] + EM_3(G) \leq MB(G) \leq EM_3(G) + 4m[2\Delta(G) - 1].$$

Further, equality in both lower and upper bounds is attained if and only if G is regular.

Proof. We have $2\delta(G) \leq d_G(u) + d_G(v) \leq 2\Delta(G)$.

Thus $2m \delta(G) \leq M_1(G) \leq 2m \Delta(G)$. (1)

From Theorem 2, we have $MB(G) = M_1(G) + EM_3(G) + B_1(G)$.

From Theorem 16 and inequality (1), we have

$$4m[2\delta(G) - 1] + EM_3(G) \leq MB(G) \leq EM_3(G) + 4m[2\Delta(G) - 1].$$

Second part is obvious.

We use the following results to prove our next result.

*Theorem 18*¹⁵. For any tree T with $n \geq 3$ vertices and m edges,

$$4n - 6 \leq M_1(T) \leq n(n-1).$$

*Theorem 19*²¹. For any tree T with $n \geq 3$ vertices and m edges,

$$8n - 14 \leq B_1(T) \leq (n-1)(3n-4).$$

Theorem 20. For any tree T with $n \geq 3$ vertices and m edges,

$$4(3n-5) + EM_3(T) \leq MB(T) \leq EM_3(T) + 4(n-1)^2.$$

Proof. From Theorem 2, we have $MB(T) = M_1(T) + EM_3(T) + B_1(T)$.

From Theorems 18 and 19, we have

$$(4n-6) + EM_3(T) + (8n-14) \leq MB(T) \leq n(n-1) + EM_3(T) + (n-1)(3n-4).$$

Therefore, $4(3n-5) + EM_3(T) \leq MB(T) \leq EM_3(T) + 4(n-1)^2$.

We use the following result to establish our next result in terms of minimum and maximum degree of a graph.

*Theorem 21*²¹. For any connected graph G with $n \geq 3$ vertices and m edges,

$$B_1(G) \leq \frac{3n}{4} [\Delta(G) - \delta(G)]^2 + \frac{4m}{n} (3m - n).$$

Theorem 22. For any connected graph G with $n \geq 3$ vertices and m edges,

$$MB(G) \leq EM_3(G) + 2m\Delta(G) + \frac{3n}{4} [\Delta(G) - \delta(G)]^2 + \frac{4m}{n} (3m - n).$$

Proof. From Theorem 2, we have $MB(G) = M_1(G) + EM_3(G) + B_1(G)$.

From Theorem 21 and inequality (1), we have

$$MB(G) \leq 2m\Delta(G) + EM_3(G) + \frac{3n}{4} [\Delta(G) - \delta(G)]^2 + \frac{4m}{n} (3m - n).$$

We use the following result to establish our next result.

*Theorem 23*²¹. For any connected graph G with $n \geq 3$ vertices and m edges,

$$B_1(G) \geq \frac{24 m \delta(G) \Delta(G)}{[\Delta(G) + \delta(G)]^2} F(G) - 4m.$$

Theorem 24. For any connected graph G with $n \geq 3$ vertices and m edges,

$$MB(G) \geq 2 m (\delta(G) - 2) + \frac{24 m \delta(G) \Delta(G)}{[\Delta(G) + \delta(G)]^2} F(G) + EM_3(G).$$

Proof. From Theorem 2, we have $MB(G) = M_1(G) + EM_3(G) + B_1(G)$.

From Theorem 23 and inequality (1), we have

$$MB(G) \geq 2 m \delta(G) + \frac{24 m \delta(G) \Delta(G)}{[\Delta(G) - \delta(G)]^2} F(G) + EM_3(G) - 4m.$$

Therefore, $MB(G) \geq 2 m (\delta(G) - 2) + \frac{24 m \delta(G) \Delta(G)}{[\Delta(G) - \delta(G)]^2} F(G) + EM_3(G)$.

The following result is used to prove our next result.

*Theorem 25*²¹. For any connected graph G with $n \geq 3$ vertices and m edges,

$$HM_1(G) - M_1(G) (2\Delta(G) - 1) + 4m (\Delta(G) - 1) \leq B_1(G) \leq HM_1(G) - M_1(G) - 4(\delta(G) - 1)^2.$$

Theorem 26. For any connected graph G with $n \geq 3$ vertices and m edges,

$$HM_1(G) - 2M_1(G) (\Delta(G) - 1) + 4m (\Delta(G) - 1) + EM_3(G) \leq MB(G) \leq HM_1(G) - 4(\delta(G) - 1)^2 + EM_3(G).$$

Proof. From Theorem 2, we have $MB(G) = M_1(G) + EM_3(G) + B_1(G)$.

From Theorem 25, we have

$$M_1(G) + HM_1(G) - M_1(G) (2\Delta(G) - 1) + 4m (\Delta(G) - 1) + EM_3(G) \leq MB(G) \leq M_1(G) + HM_1(G) - M_1(G) - 4(\delta(G) - 1)^2 + EM_3(G).$$

Therefore, $HM_1(G) - 2M_1(G) (\Delta(G)-1) + 4m (\Delta(G)-1) + EM_3(G) \leq MB(G) \leq HM_1(G) - 4 (\delta(G)-1)^2 + EM_3(G)$.

We use the following result to prove our next result.

*Theorem 27*²¹. For any (n, m) -graph G with p -pendant vertices and minimal non-pendant vertex degree $\delta_1(G)$,

$$6 \delta_1(G) (m-p) + 3p(1+\delta_1(G)) - 4m \leq B_1(G) \leq 6 (\Delta(G) (m-p) + 3p(1+(\Delta(G))) - 4m.$$

Theorem 28. For any (n, m) -graph G with p -pendant vertices and minimal non-pendant vertex degree $\delta_1(G)$,

$$2m \delta(G) + 6 \delta_1(G) (m-p) + 3p(1+\delta_1(G)) - 4m + EM_3(G) \leq MB(G) \leq 2m\Delta(G) + 6 (\Delta(G) (m-p) + 3p(1+(\Delta(G))) - 4m + EM_3(G).$$

Proof. From Theorem 2, we have $MB(G) = M_1(G) + EM_3(G) + B_1(G)$.

From Theorem 27 and inequality (1), we have

$$2m\delta(G) + 6 \delta_1(G) (m-p) + 3p(1+\delta_1(G)) - 4m + EM_3(G) \leq MB(G) \leq 2m\Delta(G) + 6 (\Delta(G)(m-p) + 3p(1+(\Delta(G))) - 4m + EM_3(G).$$

Conclusion

In this study, we have introduced the Zagreb-K-Banhatti index of a graph. We have obtained some relations between this new topological index with Zagreb and K-Banhatti indices. Further, we have established lower and upper bounds for $MB(G)$ of a connected graph in terms of Zagreb-Type indices. For the comparative advantages, applications and mathematical point of view, many questions are suggested by this research, among them are the following:

1. Find the extremal values and extremal graphs of the Zagreb -K-Banhatti index.
2. Characterize the Zagreb-K-Banhatti index in terms of other degree based topological indices.
3. Explores some results towards QSPR/QSAR/QSTR Model by using the Zagreb-K-Banhatti index.

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