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SECOND ZAGREB-*K*-BANHATTI INDEX OF A GRAPH

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ABSTRACT

The K-Banhatti indices were introduced by Kulli in 2016. The Zagreb indices were proposed by Gutman and Trinajstić in 1972. The Zagreb indices and K-Banhatti indices are closely related. In this paper, we establish some relations between Zagreb, K-Banhatti and second Zagreb-K-Banhatti indices. Also we obtain lower and upper bounds for the second Zagreb-K-Banhatti index of a graph in terms of Zagreb and K-Banhatti indices.

Keywords: *Zagreb index, K-Banhatti index, Zagreb-K-Banhatti index, second Zagreb-K-Banhatti index, graph.*

Mathematics Subject Classification: *05C05, 05C07, 05C35.*

1. INTRODUCTION

A molecular graph is a finite, simple graph, representing the carbon-atom skeleton of an organic molecule of a hydrocarbon. The vertices of a molecular graph represent the carbon atoms and its undirected edges the carbon-carbon bonds. Chemical Graph Theory is a branch of Mathematical Chemistry. This branch of Mathematics has an important effect on the development of Chemical Sciences. In Chemical Science, physicochemical properties of chemical compounds often modeled by means of molecular based structure descriptors, which are also referred as topological indices or graph indices. For graph indices, see [1]. A topological index or a graph index is a numerical parameter mathematically derived from the graph structure.

These indices are useful for establishing correlation between the structure a molecular compound and its physicochemical properties. Several such topological indices have been considered in Theoretical Chemistry and have obtained some applications, especially in QSPR/QSAR research, see [2, 3, 4].

Let G be a simple, connected graph with n vertices and m edges with vertex set $V(G)$ and edge set $E(G)$. 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 a graph 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 its elements. Any undefined term in this paper may be found in [5].

The first and second Zagreb indices take into account the contributions of pairs of adjacent vertices. The first and second Zagreb indices were introduced by Gutman et al. in [6] and they are defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v) \right], \qquad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

Zagreb indices have been studied extensively. For their history, applications and mathematical properties, see [7, 8, 9, 10, 11].

Followed by the first Zagreb index of a graph G, Furtula *et al.* [12] introduced the forgotten topological index and defined it as

$$F(G) = \sum_{u \in V(G)} d_G(u)^3 = \sum_{uv \in E(G)} \left[d_G(u)^2 + d_G(v)^2 \right].$$

This index was studied, for example, in [13, 14, 15].

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The first and second *K*-Banhatti indices take into account the contributions of pairs of incident elements. The first and second *K*-Banhatti indices were introduced by Kulli in [16] and they are defined as

$$B_1(G)=\sum_{ue}\left[d_G(u)+d_G(e)\right], \qquad B_2(G)=\sum_{ue}d_G(u)d_G(e).$$

where *ue* means that the vertex *u* and edge *e* are incident in *G*.

The first and second hyper Banhatti indices of a graph *G* are defined by Kulli in [17] as

$$HB_1(G)=\sum_{ue}\left[d_G(u)+d_G(e)\right]^2, \qquad HB_2(G)=\sum_{ue}d_G(u)d_G(e).$$

These indices have been studied extensively. For their history, applications and mathematical properties, see [18, 19, 20, 21, 22, 23, 24, 25, 26].

In [27], Miličević *et al.* introduced the first and second reformulated Zagreb indices of a graph *G* in terms of edges instead of vertex degrees and defined as

$$EM_1(G)=\sum_{e\in E(G)}d_G(e)^2, \qquad EM_2(G)=\sum_{e\sim f}d_G(e)d_G(f)$$

where $e \sim f$ means that the edges *e* and *f* are adjacent.

More on these indices can be found in [28, 29, 30, 31, 32, 33, 34].

Motivated by the work on Zagreb and *K*-Banhatti indices, Kulli *et al.* introduced the Zagreb-*K*-Banhatti index of a graph *G* and defined as [35]

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

where *a* and *b* are elements of *G*.

In [36], Kulli introduced the first and second hyper Zagreb-*K*-Banhatti indices of a graph *G* and they are defined as

$$HMB_1(G)=\sum_{\substack{a \text{ is either adjacent}\\ \text{or incident to } b}}\left[d_G(a)+d_G(b)\right]^2,$$

$$HMB_2(G)=\sum_{\substack{a \text{ is either adjacent}\\ \text{or incident to } b}}\left[d_G(a)d_G(b)\right]^2.$$

where *a* and *b* are elements of *G*.

Based on the successful consideration of Zagreb-*K*-Banhatti indices, we consider the second Zagreb-*K*-Banhatti index of a graph *G* as

$$MB_2(G)=\sum_{\substack{a \text{ is either adjacent}\\ \text{or incident to } b}}d_G(a)d_G(b)$$

where *a* and *b* are elements of *G*.

In this paper, we establish some relations between the second Zagreb-*K*-Banhatti index, Zagreb and *K*-Banhatti indices. We also provide lower and upper bounds for $MB_2(G)$ of a connected graph *G* in terms of Zagreb and K-Banhati indices.

2. Comparison of Second Zagreb-*K*-Banhatti, Zagreb, *K*-Banhatti-type indices

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

$$MB_2(G)=M_2(G)+EM_2(G)+B_2(G).$$

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

$$MB_2(G)=\sum_{\substack{a \text{ is either adjacent}\\ \text{or incident to } b}}d_G(a)d_G(b)$$

$$=\sum_{ab\in E(G)}d_G(a)d_G(b)+\sum_{e,f\in E(G),e\sim f}d_G(a)d_G(b)+\sum_{a(ab)}d_G(a)d_G(b)$$

$$=M_2(G)+EM_2(G)+B_2(G).$$

In order to prove our next result, we use the following result.

Theorem 2 [26]: Let G be a graph with $n \geq 3$ vertices and m edges. Then

$$B_2(G) = HM_1(G) - 2M_1(G).$$

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

$$MB_2(G) = M_2(G) + EM_2(G) + HM_1(G) - 2M_1(G).$$

Proof: From Theorem 1, we have

$$MB_2(G) = M_2(G) + EM_2(G) + B_2(G).$$

Using Theorem 2, we obtain

$$MB_2(G) = M_2(G) + EM_2(G) + HM_1(G) - 2M_1(G).$$

We use the following result to establish our next result.

Theorem 4 [26]: Let G be a graph with $n \geq 3$ vertices and m edges. Then

$$B_2(G) = EM_1(G) + 2M_1(G) - 4m.$$

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

$$MB_2(G) = M_2(G) + EM_1(G) + EM_2(G) + 2M_1(G) - 4m.$$

Proof: From Theorem 1, we have

$$MB_2(G) = M_2(G) + EM_2(G) + B_2(G).$$

From Theorems 4, we obtain

$$MB_2(G) = M_2(G) + EM_1(G) + EM_2(G) + 2M_1(G) - 4m.$$

We use the following result to prove Theorem 7.

Theorem 6 [26]: Let G be a graph with $n \geq 3$ vertices and m edges. Then

$$B_2(G) = F(G) + 2M_2(G) - 2M_1(G).$$

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

$$MB_2(G) = 3M_2(G) + EM_2(G) + F(G) - 2M_1(G).$$

Proof: From Theorem 1, we have

$$MB_2(G) = M_2(G) + EM_2(G) + B_2(G).$$

Using Theorem 6, we get

$$MB_2(G) = 3M_2(G) + EM_2(G) + F(G) - 2M_1(G).$$

We use the following result to establish our next result.

Theorem 8 [26]: Let G be a graph with $n \geq 3$ vertices and m edges. Then

$$B_2(G) = \frac{1}{2}HB_1(G) - 12m.$$

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

$$MB_2(G) = EM_1(G) + EM_2(G) + M_2(G) - M_1(G) + B_1(G).$$

Proof: From Theorem 1, we have

$$MB_2(G) = M_2(G) + EM_2(G) + B_2(G).$$

Thus by using Theorem 8, we get

$$MB_2(G) = M_2(G) + EM_2(G) + \frac{1}{2}HB_1(G) - 12m.$$

We have from [26],

$$HB_1(G) = 2B_1(G) + 2EM_1(G) - 2M_1(G) + 24m.$$

Using this result, we obtain

$$MB_2(G) = EM_1(G) + EM_2(G) + M_2(G) - M_1(G) + B_1(G).$$

3. Bounds on Second Zagreb-*K*-Banhatti, Zagreb, *K*-Banhatti-type indices

Theorem 10 [26]: For any connected graph *G*.

$$4M_2(G) - 2M_1(G) \le B_2(G).$$

Theorem 11: Let *G* be a connected graph with $n \geq 3$ vertices and *m* edges. Then

$$5M_2(G) - 2M_1(G) + EM_2(G) \le MB_2(G).$$

Proof: From Theorem 1, we have

$$MB_2(G) = M_2(G) + EM_2(G) + B_2(G).$$

From Theorem 10, we obtain

$$5M_2(G) - 2M_1(G) + EM_2(G) \le MB_2(G).$$

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

Theorem 12 [34]: Let *G* be a graph with $n \geq 3$ vertices and *m* edges. Then

$$EM_2(G) \le \left(\frac{1}{2}M_1(G) - m\right).\left(\sqrt{M_1(G) - 2m + \frac{1}{4}} - \frac{1}{2}\right)^2.$$

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

$$MB_2(G) \le F(G) + 3M_2(G) - 2M_1(G) + \left(\frac{1}{2}M_1(G) - m\right)\left(\sqrt{M_1(G) - 2m + \frac{1}{4}} - \frac{1}{2}\right)^2.$$

Proof: From Theorem 7, we have

$$MB_2(G) = 3M_2(G) - 2M_1(G) + EM_2(G) + F(G).$$

From Theorem 12, we get

$$MB_2(G) \le F(G) + 3M_2(G) - 2M_1(G) + \left(\frac{1}{2}M_1(G) - m\right)\left(\sqrt{M_1(G) - 2m + \frac{1}{4}} - \frac{1}{2}\right)^2.$$

To prove our next result, we use the following result.

Theorem 14 [26]: For any graph *G*,

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

Theorem 15: Let *G* be a graph with *n* vertices and *m* edges. Then

$$EM_1(G) + EM_2(G) + M_2(G) \le MB_2(G).$$

Proof: From Theorem 9, we have

$$MB_2(G) = EM_1(G) + EM_2(G) + M_2(G) - M_1(G) + B_1(G).$$

Using Theorem 14, we get

$$EM_1(G) + EM_2(G) + M_2(G) \le MB_2(G).$$

To prove the next result, we use the following result.

Theorem 16 [26]: Let G be a connected graph with $n \geq 3$ vertices and m edges. Then

$$B_2(G) \leq \frac{\delta(G)+\Delta(G)}{4m\delta(G)\Delta(G)} M_1(G)^2 - 2M_1(G).$$

Theorem 17: For any connected graph G with $n \geq 3$ vertices and m edges,

$$MB_2(G) \leq EM_2(G) + M_2(G) + \frac{\delta(G)+\Delta(G)}{4m\delta(G)\Delta(G)} M_1(G)^2 - 2M_1(G).$$

Proof: From Theorem 1, we have

$$MB_2(G) = EM_2(G) + M_2(G) + B_2(G).$$

Then from Theorem 16, we get the desired result.

We obtain lower and upper bounds on $MB_2(G)$in terms of $\delta(G)$, $\Delta(G)$, $M_1(G)$, $M_2(G)$, m of a graph G.

Theorem 18: For any connected graph G with $n \geq 3$ vertices and m edges,

$$MB_2(G) \leq \left(\frac{1}{2}M_1(G) - m\right)\left(\sqrt{M_1(G) - 2m + \frac{1}{4}} - \frac{1}{2}\right)^2 + M_2(G) + \frac{\delta(G)+\Delta(G)}{4m\delta(G)\Delta(G)} M_1(G)^2 - 2M_1(G).$$

Proof: From Theorem 1, we have

$$MB_2(G) = EM_2(G) + M_2(G) + B_2(G).$$

Then from Theorems 12 and 16, we obtain

$$MB_2(G) \leq \left(\frac{1}{2}M_1(G) - m\right)\left(\sqrt{M_1(G) - 2m + \frac{1}{4}} - \frac{1}{2}\right)^2 + M_2(G) + \frac{\delta(G)+\Delta(G)}{4m\delta(G)\Delta(G)} M_1(G)^2 - 2M_1(G).$$

We use the following result to prove our next result.

Theorem 19 [26]: For any connected graph G with $n \geq 3$ vertices and m edges,

$$[\delta(G) - 2]M_1(G) + 2M_2(G) \leq B_2 \leq (G)[\Delta(G) - 2]M_1(G) + 2M_2(G)$$

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

Theorem 20: For any connected graph G with $n \geq 3$ vertices and m edges,

$$[\delta(G) - 2]M_1(G) + 3M_2(G) + EM_2(G) \leq MB_2(G) \leq [\Delta(G) - 2]M_1(G) + 3M_2(G) + EM_2(G).$$

On both sides, equality holds if and only if G is regular.

Proof: From Theorem 1, we have

$$MB_2(G) = M_2(G) + EM_2(G) + B_2(G).$$

Using Theorem 19, we obtain

$$[\delta(G) - 2]M_1(G) + 3M_2(G) + EM_2(G) \leq MB_2(G) \leq [\Delta(G) - 2]M_1(G) + 3M_2(G) + EM_2(G).$$

Second part is obvious.

We use the following result, to establish our next result.

Theorem 21 [26]: For any connected graph G with $n \geq 3$ vertices and m edges,

$$4[\delta(G) - 2]^2 + 2M_1(G) - 4m \leq B_2(G) \leq [2M_1(G) - 4m]\Delta(G).$$

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

$$4[\delta(G) - 1]^2 + 2M_1(G) - 4m + M_2(G) + EM_2(G) \leq MB_2(G)$$
$$\leq [2M_1(G) - 4m]\Delta(G) + M_2(G) + EM_2(G).$$

Proof: From Theorem 1, we have

$$MB_2(G) = M_2(G) + EM_2(G) + B_2(G).$$

Therefore using Theorem 21, we get

$$4[\delta(G)-1]^2 + 2M_1(G) - 4m + M_2(G) + EM_2(G) \le MB_2(G)$$
$$\le [2M_1(G) - 4m]\Delta(G) + M_2(G) + EM_2(G).$$

The following result of $EM_2(G)$ to prove our next two results in terms of $\delta(G)$, $\Delta(G)$, $M_1(G)$, $M_2(G)$ and m of a graph G.

Theorem 23 [28]: Let G be a connected graph with n vertices and m edges. Then

$$[\delta(G)-1]^2\, 2\big(M_1(G)-2m\big) \le EB_2(G) \le [\Delta(G)-1]^2\, 2\big(M_1(G)-2m\big).$$

Theorem 24: Let G be a connected graph with $n \ge 3$ vertices and m edges. Then

$$[\delta(G)-2]M_1(G) + [\delta(G)-1]^2\, 2\big(M_1(G)-2m\big) + 3M_2(G) \le MB_2(G) \le$$
$$[\Delta(G)-2]M_1(G) + [\Delta(G)-1]^2\, 2\big(M_1(G)-2m\big) + 3M_2(G).$$

Proof: From Theorem 20, we have

$$[\delta(G)-2]M_1(G) + 3M_2(G) + EM_2(G) \le MB_2(G) \le [\Delta(G)-2]M_1(G) + 3M_2(G) + EM_2(G).$$

Using Theorem 23, we obtain

$$[\delta(G)-2]M_1(G) + [\delta(G)-1]^2\, 2\big(M_1(G)-2m\big) + 3M_2(G) \le MB_2(G) \le$$
$$[\Delta(G)-2]M_1(G) + [\Delta(G)-1]^2\, 2\big(M_1(G)-2m\big) + 3M_2(G).$$

Theorem 25: Let G be a connected graph with $n \ge 3$ vertices and m edges. Then

$$4[\delta(G)-1]^2 + \left[1 + (\delta(G)-1)^2\right] 2\big(M_1(G)-2m\big) + M_2(G) \le MB_2(G) \le$$
$$\left[\Delta(G) + (\Delta(G)-1)^2\right] 2\big(M_1(G)-2m\big) + M_2(G).$$

Proof: From Theorem 22, we have

$$4[\delta(G)-1]^2 + 2M_1(G) - 4m + M_2(G) + EM_2(G) \le MB_2(G) \le$$
$$[2M_1(G) - 4m]\Delta(G) + M_2(G) + EM_2(G).$$

Using Theorem 23, we obtain

$$4[\delta(G)-1]^2 + 2M_1(G) - 4m + M_2(G) + [\delta(G)-1]^2\, 2\big(M_1(G)-2m\big) \le MB_2(G) \le$$
$$[2M_1(G) - 4m]\Delta(G) + M_2(G) + [\Delta(G)-1]^2\, 2\big(M_1(G)-2m\big).$$

Therefore

$$4[\delta(G)-1]^2 + \left[1 + (\delta(G)-1)^2\right] 2\big(M_1(G)-2m\big) + M_2(G) \le MB_2(G) \le$$
$$\left[\Delta(G) + (\Delta(G)-1)^2\right] 2\big(M_1(G)-2m\big) + M_2(G).$$

We use the following result to establish our next result.

Theorem 26 [28]: Let G be a connected graph with n vertices and m edges. Then

$$[\delta(G)-1]^2\, 4m \le EM_1(G) \le [\Delta(G)-1]^2\, 4m.$$

Theorem 27: Let G be a connected graph with $n \ge 3$ vertices and m edges. Then

$$\left[(\delta(G)-1)^2 + 1\right] 2M_1(G) + M_2(G) - 4m \le MB_2(G) \le$$
$$\left[(\Delta(G)-1)^2 + 1\right] + 2M_1(G) + M_2(G) - 4m.$$

Proof: From Theorems 22 and 26, we obtain

$$[\delta(G)-1]^2\, 4m + [\delta(G)-1]^2 \big(2M_1(G) - 4m\big) \le EM_1(G) + EM_2(G) \le$$
$$[\Delta(G)-1]^2\, 4m + [\Delta(G)-1]^2 \big(2M_1(G) - 4m\big).$$

Therefore $\left[\delta(G)-1\right]^2 2M_1(G) \le EM_1(G)+EM_2(G) \le \left[\Delta(G)-1\right]^2 2M_1(G).$ (1)

From Theorem 5, we have

$$MB_2(G)=M_2(G)+2M_1(G)-4m+EM_1(G)+EM_2(G).$$

Then from inequality (1), we obtain

$$\left[\delta(G)-1\right]^2 2M_1(G)+2M_1(G)-4m \le MB_2(G) \le$$
$$\left[\Delta(G)-1\right]^2 2M_1(G)+M_2(G)+2M_1(G)-4m.$$

Therefore

$$\left[(\delta(G)-1)^2+1\right]2M_1(G)+M_2(G)-4m \le MB_2(G) \le$$
$$\left[(\Delta(G)-1)^2+1\right]2M_1(G)+M_2(G)-4m.$$

Theorem 28: Let G be a connected graph with $n \ge 3$ vertices and m edges. Then

$$\left[\delta(G)-1\right]^2 2M_1(G)+M_2(G)-M_1(G)+B_1(G) \le MB_2(G) \le$$
$$\left[\Delta(G)-1\right]^2 2M_1(G)+M_2(G)-M_1(G)+B_1(G).$$

Proof: From Theorems 22 and 26, we obtain

$$MB_2(G)=EM_1(G)+EM_2(G)+M_2(G)-M_1(G)+B_1(G).$$

Then from inequality (1), we get

$$\left[\delta(G)-1\right]^2 2M_1(G)+M_2(G)-M_1(G)+B_1(G) \le MB_2(G) \le$$
$$\left[\Delta(G)-1\right]^2 2M_1(G)+M_2(G)-M_1(G)+B_1(G).$$

Theorem 29: Let G be a connected graph with $n \ge 3$ vertices and m edges. Then

$$\left[\delta(G)-1\right]^2\left(2M_1(G)-4m\right)+3M_2(G)-2M_1(G)+F(G) \le MB_2(G) \le$$
$$\left[\Delta(G)-1\right]^2\left(2M_1(G)-4m\right)+3M_2(G)-2M_1(G)+F(G).$$

Proof: From Theorem 7, we have

$$MB_2(G)=EM_2(G)+3M_2(G)-2M_1(G)+F(G).$$

Then from Theorem 22, we obtain

$$\left[\delta(G)-1\right]^2\left(2M_1(G)-4m\right)+3M_2(G)-2M_1(G)+F(G) \le MB_2(G) \le$$
$$\left[\Delta(G)-1\right]^2\left(2M_1(G)-4m\right)+3M_2(G)-2M_1(G)+F(G).$$

To prove the next two results, we use the earlier established:

Theorem 30 [28]: Let G be a connected graph with n vertices and m edges. Then

$$\left[\delta(G)-1\right]EM_1(G) \le EM_2(G) \le \left[\Delta(G)-1\right]EM_1(G).$$

Theorem 31: Let G be a connected graph with $n \ge 3$ vertices and m edges. Then

$$\delta(G)EM_1(G)+M_2(G)+2M_1(G)-4m \le MB_2(G) \le \Delta(G)EM_1(G)+M_2(G)+2M_1(G)-4m.$$

Proof: From Theorem 5, we have

$$MB_2(G)=EM_1(G)+EM_2(G)+M_2(G)+2M_1(G)-4m.$$

Using Theorem 30, we obtain

$$\delta(G)EM_1(G)+M_2(G)+2M_1(G)-4m \le MB_2(G) \le \Delta(G)EM_1(G)+M_2(G)+2M_1(G)-4m.$$

Theorem 32: Let G be a connected graph with $n \geq 3$ vertices and m edges. Then

$$\delta(G)EM_1(G)+M_2(G)-M_1(G)+B_1(G)\leq MB_2(G)\leq \Delta(G)EM_1(G)+M_2(G)-M_1(G)+B_1(G).$$

Proof: From Theorem 9, we have

$$MB_2(G)=EM_1(G)+EM_2(G)+M_2(G)-M_1(G)+B_1(G).$$

Using Theorem 30, we get

$$\delta(G)EM_1(G)+M_2(G)-M_1(G)+B_1(G)\leq MB_2(G)\leq \Delta(G)EM_1(G)+M_2(G)-M_1(G)+B_1(G).$$

CONCLUSION

In this paper, we have established some relations between second Zagreb-*K*-Banhatti index with Zagreb and *K*-Banhatti indices. We also provided lower and upper bounds for $MB_2(G)$ of a connected graph G in terms of other topological indices.

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