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More on KG-Sombor Index of Graphs

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ABSTRACT: Topological indices are generally graph-invariant numerical properties that describe the topology of a graph. The KG-Sombor index, a vertex-edge version of the Sombor index, was recently defined as follows: $KG(G) = \sum_{ue} \sqrt{d(u)^2 + d(e)^2}$, where $\sum_{ue}$ indicates summation over vertices $u \in V(G)$ and the edges $e \in E(G)$ that are incident to u. In this work, we obtained the effect of vertex and edge removal on KG-Sombor index. Also, characterized integer values of KG-Sombor index. Finally, computed a bound for the KG-Sombor index of derived graphs, including the join of graphs, the m-splitting graph, the m-shadow graph, and the corona product of graphs.

Key Words: Sombor index, KG-Sombor index, derived graphs.

Contents

1. Introduction

Let $G = (V, E)$ be a connected, simple, finite, undirected graph. The terms $|V| = p$ and $|E| = q$, respectively, indicate the order and size of G. The degree of a vertex v in a graph G is the number of edges that incident on it, and it is denoted by the notation $\deg(v)$ or $d(v)$.

In the universe of graph theory, where vertices represent entities and edges denote relationships, topological indices serve as guiding stars illuminating the intricate structures and properties of graphs. These indices distill complex network characteristics into quantitative measures, offering invaluable insights into the underlying topology.

At their core, topological indices encapsulate fundamental graph properties without delving into specific graph representations. They provide a standardized language to describe and compare graphs across diverse domains, from chemistry and biology to social networks and infrastructure systems.

The beauty of topological indices lies in their ability to uncover hidden patterns and predict various properties of graphs, aiding researchers in understanding phenomena ranging from molecular structures' stability to communication efficiency in computer networks.

Topological indices, which are often graph invariant, are numerical characteristics that describe the topology of a graph. Hydrogen-suppressed molecular networks, in which atoms are represented by vertices and bonds by edges, are the source of topological descriptors. Several topological matrices, such as adjacency or distance matrices, can characterize the connections between the atoms. These matrices can be mathematically altered to produce a single number that is typically referred to as a topological index. Chemical graph theory recognized the Hosoya index as the first topological index. The Zagreb indices, Balaban's J index, Wiener index, and Randić's molecular connection index are a few more examples.

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The three most important categories of topological indices for graphs are spectrum-based, degree-based, and distance-based topological indices. Degree-based topological indices, which are based on the degrees of a graph's vertices, are among the most extensively researched types of topological indices used in mathematical chemistry. For more on degree based topological indices, refer [12,13,14,15,16].
Gutman I. and others in [7] defined Zagreb indices as follows:

$$M_1(G) = \sum_{u \in V(G)} d(u)^2 = \sum_{uv \in E(G)} (d(u) + d(v)).$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

Furtula, B. and Gutman, I. [10] introduced the forgotten topological index, or F-index, soon after the first and second Zagreb indices. It is defined as

$$F(G) = \sum_{u \in V(G)} d(u)^3 = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2).$$

The Zagreb indices were reformulated by Miličević, A. et al. in [8] using edge-degrees rather than vertex-degrees:

$$EM_1(G) = \sum_{e \in E(G)} d(e)^2.$$

$$EM_2(G) = \sum_{e \sim f \in E(G)} d(e)d(f).$$

Here, $d(e)$ denotes the degree of the edge e in G given by $d(e) = d(u) + d(v) - 2$, where $uv \in E(G)$.
We have $EM_1(G) = M_1(L(G))$ and $EM_2(G) = M_2(L(G))$.
Gutman, I. proposed a new topological index, the Sombor index, based on vertex degree in [11].

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}.$$

A vertex-edge variant of the Sombor index was introduced by Kulli, V. R. in [3] as given below:

$$KG = KG(G) = \sum_{ue} \sqrt{d(u)^2 + d(e)^2}, \tag{1.1}$$

where $\sum_{ue}$ indicates summation over vertices $u \in V(G)$ and the edges $e \in E(G)$ that are incident to u.
Since the edge $e = uv$ is incident to both the vertices u and v, we can also express Equation (1.1) as

$$KG(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + [d(u) + d(v) - 2]^2} + \sqrt{d(v)^2 + [d(u) + d(v) - 2]^2}.$$

Readers are referred to [3,4,5] for more on KG-Sombor index.
For any positive numbers a and b,

$$\frac{1}{\sqrt{2}}(a + b) \leq \sqrt{a^2 + b^2} < a + b. \tag{1.2}$$

Equality on the left-hand side holds if and only if $a = b$.

2. Preliminaries

Lemma 2.1 *[9] Let $\overline{G}$ be the complement of G. Then*

$$M_1(\overline{G}) = M_1(G) + n(p-1)^2 - 4q(p-1).$$

Lemma 2.2 *[9] The reformulated first Zagreb index can be written in terms of the Zagreb indices and $F-$index as:*

$$EM_1 = F(G) - 4M_1(G) + 2M_2(G) + 4q.$$

Lemma 2.3 *[6] Sombor index of subdivision graph of G is given by*

$$SO(S(G)) = \sum_{u \in V(G)} d(u)\sqrt{4 + d(u)^2}.$$

Definition 2.1 *Complement [2]: $\overline{G}$ is the complement of graph G is a graph with same number of vertices as in G and any two vertices in $\overline{G}$ are adjacent if and only if they are non-adjacent in G. We have, $|V(\overline{G})| = p$ and $|E(\overline{G})| = \frac{p(p-1)}{2} - q$.*

Definition 2.2 *Line Graph [2]: The line graph $L(G) = L$ of a graph G is a graph in which the vertices of $L(G)$ correspond to the edges of G, any two vertices of $L(G)$ being adjacent if and only if the corresponding edges of G are incident with the same vertex of G. We have, $|V(L)| = q$ and $|E(L)| = \frac{M_1(G)}{2} - q$.*

Definition 2.3 *Subdivision Graph [2]: Subdivision graph $S(G) = S$ of a graph G is obtained by inserting a vertex of degree 2 in each edge of G. We have, $|V(S)| = |V(G)| + |E(G)| = p + q$ and $|E(S)| = 2q$.*

Definition 2.4 *Vertex Semi-total Graph [2]: The vertex semi-total graph of G, denoted by $T_1(G)$, is a graph with vertex set $V(T_1(G)) = V(G) \cup E(G)$ in which two vertices are adjacent if they are adjacent vertices in G or one is vertex and the other is an edge, incident to it. We have, $|V(T_1(G))| = |V(G)| + |E(G)| = p + q$ and $|E(T_1(G))| = |E(S)| + |E(G)| = 3q$.*

Definition 2.5 *Edge Semi-total Graph [2]: The edge semi-total graph of G, denoted by $T_2(G)$, is a graph with vertex set $V(T_2(G)) = V(G) \cup E(G)$ in which two vertices are adjacent if they are adjacent edges in G or one is a vertex of G and the other is an edge, incident to it. Note that $|V(T_2(G))| = |V(G)| + |E(G)| = p + q$ and $|E(T_2(G))| = |E(S)| + |E(L)| = 2q + \frac{M_1(G)}{2} - q = \frac{M_1(G)}{2} + q$.*

Definition 2.6 *Total Graph [2]: The total graph $T(G)$ is the union of edge-semi-total graph and vertex-semi-total graph of a graph G. We have $|V(T(G))| = |V(G)| + |E(G)| = p + q$ and $|E(T(G))| = |E(G)| + |E(S) + |E(L)| = q + 2q + \frac{M_1(G)}{2} - q = \frac{M_1(G)}{2} + 2q$.*

Definition 2.7 *m-shadow Graph [17]: The $m-$shadow graph $D_m(G)$ of a connected graph G is constructed by taking m copies of G, say $G_1, G_2, \ldots, G_m$ then join each vertex u in G_i to the neighbors of the corresponding vertex v in G_j, $1 \leq i, j \leq m$. Note that $|V(D_m(G))| = |V(G)| + |V(D_1(G))| + |V(D_2(G))| + \ldots + |V(D_m(G))| = p + p + p + \ldots + p = (q+1)p$ and $|E(D_m(G))| = |E(G)| + |E(D_1(G))| + |E(D_2(G))| + \ldots + |E(D_m(G))| = q + \{3q + 3q + \ldots + 3q\} = q(1 + 3m)$.*

Definition 2.8 *m-splitting Graph [17]: The $m-$splitting graph $Spl_m(G)$ of a graph G is obtained by adding to each vertex v of G new m vertices, say $v_1, v_2, \ldots, v_m$ such that v_i, $1 \leq i \leq m$ is adjacent to each vertex that is adjacent to v in G. We have $|V(Spl_m(G))| = |V(G)| + |V(G')| + |V(G'')| + \ldots + |V(G^m)| = (q+1)p$ and $|E(T(G))| = |E(G)| + |E(S(G))| + |E(L(G))| = q + \{2q + 2q + \ldots + 2q\} = q(1 + 2m)$.*

Definition 2.9 *Corona Product [18]: The corona product, $G_1 \circ G_2$ of two graphs $G_1 = (p_1, q_1)$ and $G_2 = (p_2, q_2)$ is defined as the graph obtained by taking one copy of G_1 and p_1 copies of G_2, and then joining the i^{th} vertex of G_1 with an edge to every vertex in the i^{th} copy of G_2. Note that $|V(G_1 \bigcirc G_2)| = |V(G_1)| + |V(G_1)||V(G_2)| = p_1(1 + p_2)$ and $|E(G_1 \circ G_2)| = |E(G_1)| + |E(G_2)|V(G_1)| + |V(G_1)||V(G_2)| = q_1 + p_1(p_2 + q_2)$.*

Definition 2.10 *Join of Graphs [19]: The join of two graphs $G_1 = (p_1, q_1)$ and $G_2 = (p_2, q_2)$, denoted by $G_1 + G_2$, is a graph obtained from G_1 and G_2 by joining each vertex of G_1 to all vertices of G_2. We have $|V(G_1+G_2)| = |V(G_1)| + |V(G_2)| = p_1 + p_2$ and $|E(G_1+G_2)| = |E(G_1)| + |E(G_2)| + |V(G_1)||V(G_2)| = q_1 + q_2 + p_1p_2$.*

3. Effect of vertex and edge removal on KG-Sombor index

- **Effect of vertex removal from G**

  Let $S = \{v_i | 1 \leq i \leq k, v_i \in V(G)\}$ be the set of vertices removed from graph G and let $B \subseteq E(G)$. Then u_j, $j = 1, 2, \ldots, l$ are the vertices from $V - S$ such that $v_iu_j \in B$. Let x_j, $j = 1, 2, \ldots, l$ be the number of edges incident with u_j. Then, $d_{G-S}(u_j) = d_G(u_j) - x_j$.

  Therefore,

$$KG(G-S) = \sum_{u_iu_j \in E(G-S)} \left\{ \sqrt{(d_G(u_i) - x_i)^2 + (d_G(u_i) - x_i + d_G(u_j) - x_j - 2)^2} \right. \\ \left. + \sqrt{(d_G(u_j) - x_j)^2 + (d_G(u_i) - x_i + d_G(u_j) - x_j - 2)^2} \right\}.$$

- **Effect of edge removal from G**

  Let $S = \{v_i | 1 \leq i \leq k\} \subseteq V(G)$ and let $B = \{v_iv_j | 1 \leq i \leq n,\ v_iv_j \in E(G)\}$ be the set of edges removed from graph G. Then u_j, $j = 1, 2, \ldots, l$ be the vertices such that $v_iu_j \in E(G-B)$. If y_i, $i = 1, 2, \ldots, l$ is the number of edges whose both end vertices are in S, then $d_{G-B}(v_i) = d_G(v_i) - y_i$ and $d_{G-B}(u_j) = d_G(u_j)$.

$$KG(G-B) = \sum_{v_iu_j \in E(G-B)} \left\{ \sqrt{(d_G(v_i) - y_i)^2 + (d_G(v_i) - y_i + d_G(v_i) - y_i - 2)^2} \right. \\ \left. + \sqrt{(d_G(u_j))^2 + (d_G(v_i) - y_i + d_G(v_i) - y_i - 2)^2} \right\}.$$

4. Integer value of KG-Sombor index

Theorem 4.1 *Let G be a connected chemical graph without isolated vertices. Then $KG(G)$ is an integer if and only if G is a 3-regular graph.*

Proof: As all degrees are non-negative integers, all contributions must be either integers or irrational numbers. If a contribution $f(e)$ is an integer for $e = uv$, then $(d(u), d(e), f(e))$ must form a Pythagorean triple, and $(3, 4, 5)$ is the only such triple whose two smaller entries can be degrees of a vertex and an edge in a chemical graph. □

Remark K_4 is the smallest chemical graph with integer KG-Sombor index.

Theorem 4.2 *Let $G = (V, E)$ be a connected graph. If there is an edge whose one end vertex is pendant vertex, then $KG(G)$ is never an integer.*

Proof: Let $e = uv \in E(G)$ be such that $d(u) = a,\ a > 1$ and $d(v) = 1$.

$$\begin{aligned} KG(e) &= \sqrt{d(u)^2 + (d(u) + d(v) - 2)^2} + \sqrt{d(v) + d(u) + d(v) - 2)^2} \\ &= \sqrt{a^2 + (a + 1 - 2)^2} + \sqrt{1 + (a-1)^2} \\ &= \sqrt{2a^2 - 2a + 1} + \sqrt{a^2 - 2a + 2}. \end{aligned}$$

Clearly, $2a^2 - 2a + 1$ and $a^2 - 2a + 2$ are irrational. □

A r-degree graph is a graph whose degree sequence has exactly r distinct numbers. A graph G is 1-degree graph if and only if G is regular.

Theorem 4.3 *Let G be a $r-$regular connected graph. Then $KG(G)$ is an integer if and only if there exists a Pythagorean triplet $(r, 2r-2, l)$, where $l \in Z^+$.*

Proof: Let $KG(G)$ be an integer. Then $r^2 + (2r-2)^2 = l^2$. This is true whenever $(r, 2r-2, l)$ is a Pythagorean triplet. Converse is trivial. □

Theorem 4.4 *Let G be a 2-degree graph. Then $KG(G)$ is an integer if and only if G is a bipartite semi-regular graph with parts X and Y such that degree of any vertex of X is a and degree of any vertex of Y is b, for $b > a \geq 1$, such that $\sqrt{a^2 + (a+b-2)^2} + \sqrt{b + (a+b-2)^2}$ is an integer. In other words, $(a, a+b-2, l_1)$ and $(b, a+b-2, l_2)$ where $l_1, l_2 \in Z^+$ should be two Pythagorean triplets where $l_1, l_2 \in Z^+$.*

Theorem 4.5 *Let G be a $k-$degree semi-regular graph. If $d_1, d_2, \ldots, d_k$ are the degree of k-partites, then $KG(G)$ is an integer if there exists at most $2\binom{k}{2}$ number of Pythagorean triplets of the form*

$C = \{(d_i, d_i + d_j - 2, l) | 1 \leq i \leq k-1, 2 \leq j \leq k, l \in Z^+\}$.

Proof: Let G be a $k-$degree semi-regular graph. We partition the vertex set into $k-$partites such that vertex with degree d_i will be in the i^{th} partite for all $1 \leq i \leq k$. Assume that there exists at least one edge between a vertex of degree i and a vertex of degree j, where $i \neq j$. If we take one such edge from all $k-$partites, then it will form a complete graph of order k, K_k. We have

$$KG(G) = \sum_{d_i d_j \in E(G)} \sqrt{d_i^2 + (d_i + d_j - 2)^2} + \sqrt{d_j^2 + (d_i + d_j - 2)^2} \tag{4.1}$$

So, the number of distinct equations of the form 4.1 while calculating $KG(G)$ is nothing but the number of edges in K_k, which is equal to $\binom{k}{2}$. Each of these equations contributes 2 to the number of Pythagorean triplets of the form C. Therefore, the number of Pythagorean triplets is at most $2\binom{k}{2}$. □

5. KG-Sombor Index of Some Graphs

Theorem 5.1 *Let G be a graph of order p and size q. Then*

$$KG(\overline{G}) < 3M_1(G) + (p-1)[3p^2 - 5p - 12q] + 4p,$$

where $M_1(G)$ is the first Zagreb index of G.

Proof:

$$\begin{aligned}
KG(\overline{G}) &= \sum_{ue \in E(\overline{G})} \sqrt{d(u)^2 + d(e)^2} \\
&< \sum_{ue \in E(\overline{G})} d(u) + d(e) \\
&= \sum_{uv \in E(\overline{G})} 3d(u) + 3d(v) - 4 \\
&= 3M_1(\overline{G}) - 4|E(\overline{G})| \\
&= 3[M_1(G) + p(p-1)^2 - 4q(p-1)] - 4\left(\frac{p(p-1)}{2} - q\right) \\
&= 3M_1(G) + (p-1)[3p^2 - 3p - 12q - 2p] + 4q \\
&< 3M_1(G) + (p-1)[3p^2 - 5p - 12q] + 4q.
\end{aligned}$$

□

Theorem 5.2 *Let $L = L(G)$ be the line graph of $G(p, q)$. Then*

$$KG(L) < 3F(G) - 14M_1(G) + 6M_2(G) + 16q,$$

where $F(G)$ is the forgotten index, $M_1(G)$ and $M_2(G)$ are the first and second Zagreb index of G.

Proof:

$$\begin{aligned}
KG(L) &= \sum_{ue \in E(L)} \sqrt{d(u)^2 + d(e)^2} \\
&< \sum_{ue \in E(L)} d(u) + d(e) \\
&= \sum_{uv \in E(L)} 3d(u) + 3d(v) - 4 \\
&= 3M_1(L) - 4|E(L)| \\
&= 3EM_1(G) - 4\left(\frac{M_1(G)}{2} - q\right) \\
&= 3F(G) - 12M_1(G) + 6M_2(G) + 12q - 2M_1(G) + 4q \\
&< 3F(G) - 14M_1(G) + 6M_2(G) + 16q.
\end{aligned}$$

□

Theorem 5.3 *Let $S = S(G)$ be the subdivision graph of G. Then*

$$KG(S) = SO(S) + \sum_{u \in V(G)} d_G(u)^2 \sqrt{2},$$

where $SO(G)$ is the Sombor index of subdivision graph of G.

Proof:

$$\begin{aligned}
KG(S) &= \sum_{uv \in E(S)} \sqrt{d_S(u)^2 + \{d_S(u) + d_S(v) - 2\}^2} + \sqrt{d_S(v)^2 + \{d_S(u) + d_S(v) - 2\}^2} \\
&= \sum_{u \in V(G)} \left\{ \sqrt{d(u)^2 + \{d(u) + 2 - 2\}^2} + \sqrt{2^2 + \{d(u) + 2 - 2\}^2} \right\} d(u) \\
&= \sum_{u \in V(G)} d(u)^2 \sqrt{2} + \sum_{u \in V(G)} d(u) \sqrt{4 + d(u)^2} \\
&= SO(S) + \sum_{u \in V(G)} d(u)^2 \sqrt{2}.
\end{aligned}$$

□

Upon examining vertex-semitotal graph T_1, edge-semitotal graph T_2, and total graph T, we can observe that these graphs consist of two distinct sorts of vertices: ones that correspond to $G's$ vertices and the ones that correspond to $G's$ edges. Accordingly, we refer to them as α and β vertices respectively. We can classify these edges into three categories based on the type of end vertices they contain:

1. $\alpha\alpha-$ edge: an edge between two α vertices.
2. $\beta\beta-$ edge: an edge between two β vertices.
3. $\alpha\beta-$ edge: an edge between a $\alpha-$ vertex and a $\beta-$ vertex.

Similar approach can be seen in [1,2].

Theorem 5.4 *Let T_1 be the vertex semi-total graph of graph G. Then*

$$KG(T_1) < 12M_1(G),$$

where $M_1(G)$ is the first Zagreb index of G.

Proof: For any u_α and v_β vertex in T_1, $d_{T_1}(u_\alpha) = 2d_G(u_\alpha)$ and $d_{T_1}(v_\beta) = 2$, respectively.

All edges in T_1 are either $\alpha\alpha-$edges or $\alpha\beta-$edges.

$$\begin{aligned}
KG(T_1) &= \sum_{ue \in E(T_1)} \sqrt{d(u)^2 + d(e)^2} \\
&< \sum_{ue \in E(T_1)} d(u) + d(e) \\
&= \sum_{u_\alpha v_\alpha \in E(T_1)} d_{T_1}(u_\alpha) + \{d_{T_1}(u_\alpha) + d_{T_1}(v_\alpha) - 2\} + d_{T_1}(v_\alpha) + \{d_{T_1}(u_\alpha) + d_{T_1}(v_\alpha) - 2\} \\
&+ \sum_{u_\alpha v_\beta \in E(T_1)} d_{T_1}(u_\alpha) + \{d_{T_1}(u_\alpha) + d_{T_1}(v_\beta) - 2\} + d_{T_1}(v_\beta) + \{d_{T_1}(u_\alpha) + d_{T_1}(v_\beta) - 2\} \\
&= \sum_{u_\alpha v_\alpha \in E(G)} 2d_G(u_\alpha) + 2d_G(u_\alpha) + 2d_G(v_\alpha) - 2 + 2d_G(v_\alpha) + 2d_G(u_\alpha) + 2d_G(v_\alpha) - 2 \\
&+ \sum_{u_\alpha \in V(G)} d_G(u_\alpha)\{2d_G(u_\alpha) + 2d_G(u_\alpha) + 2 - 2 + 2 + 2d_G(u_\alpha) + 2 - 2\} \\
&= 6 \sum_{u_\alpha v_\alpha \in E(G)} [d_G(u_\alpha) + d_G(v_\alpha)] - 4 \sum_{u_\alpha v_\alpha \in E(G)} 1 + 6 \sum_{u_\alpha \in V(G)} d_G^2(u_\alpha) + 2 \sum_{u_\alpha \in V(G)} d_G(u_\alpha) \\
&= 6M_1(G) - 4q + 6M_1(G) + 4q \\
&< 12M_1(G).
\end{aligned}$$

□

Theorem 5.5 *Let T_2 be the edge semi-total graph of graph $G = (p, q)$. Then*

$$KG(T_2) < \sum_{u_\alpha v_\alpha \in E(G)} [6d_G(u_\alpha) + 3d_G(v_\alpha)] - 12q + 3M_1(L) + 4M_1(G),$$

where $M_1(G)$ and $M_1(L)$ are the first Zagreb index of graph G and its line graph L respectively.

Proof: For any u_α and v_β vertex in T_2, $d_{T_2}(u_\alpha) = d_G(u_\alpha)$ and $d_{T_2}(v_\beta) = d_L(v_\beta) + 2 = d_G(u_\alpha) + d_G(v_\alpha)$, respectively.

All edges in T_2 are either $\beta\beta-$edges or $\alpha\beta-$edges.

$$
\begin{aligned}
KG(T_2) &= \sum_{ue\in E(T_2)} \sqrt{d(u)^2+d(e)^2} \\
&< \sum_{ue\in E(T_2)} d(u)+d(e) \\
&= \sum_{u_\alpha v_\beta\in E(T_2)} d_{T_2}(u_\alpha)+\{d_{T_2}(u_\alpha)+d_{T_2}(v_\beta)-2\}+d_{T_2}(v_\beta)+\{d_{T_2}(u_\alpha)+d_{T_2}(v_\beta)-2\} \\
&+ \sum_{u_\beta v_\beta\in E(T_2)} d_{T_2}(u_\beta)+\{d_{T_2}(u_\beta)+d_{T_2}(v_\beta)-2\}+d_{T_2}(v_\beta)+\{d_{T_2}(u_\beta)+d_{T_2}(v_\beta)-2\} \\
&= \sum_{u_\alpha v_\alpha\in E(G)} d_G(u_\alpha)+d_G(u_\alpha)+d_G(u_\alpha)+d_G(v_\alpha)-2+d_G(u_\alpha)+d_G(v_\alpha)+d_G(u_\alpha) \\
&+ d_G(u_\alpha)+d_G(v_\alpha)-2+\sum_{u_\beta v_\beta\in E(L)} d_L(u_\beta)+2+d_L(u_\beta)+2+d_L(v_\beta)+2-2 \\
&+ d_L(v_\beta)+2+d_L(u_\beta)+2+d_L(v_\beta)+2-2 \\
&= \sum_{u_\alpha v_\alpha\in E(G)} [6d_G(u_\alpha)+3d_G(v_\alpha)]-4\sum_{u_\alpha v_\alpha\in E(G)} 1+\sum_{u_\beta v_\beta\in E(L)} 3d_L(u_\beta)+3d_L(v_\beta)+8\sum_{u_\beta v_\beta\in E(L)} 1 \\
&= \sum_{u_\alpha v_\alpha\in E(G)} [6d_G(u_\alpha)+3d_G(v_\alpha)]-4q+3M_1(L)+8|E(L)| \\
&< \sum_{u_\alpha v_\alpha\in E(G)} [6d_G(u_\alpha)+3d_G(v_\alpha)]-12q+3M_1(L)+4M_1(G).
\end{aligned}
$$

□

Theorem 5.6 *Let T be the total graph of graph $G=(p,q)$. Then*

$$KG(T) < 10M_1(G)+3M_1(L)-16q+\sum_{u_\alpha v_\alpha\in E(G)} 9d_G(u_\alpha)+3d_G(v_\alpha),$$

where $M_1(G)$ and $M_1(L)$ are the first Zagreb index of graph G and its line graph L respectively.

Proof: For any u_α and v_β vertex in T, $d_T(u_\alpha)=2d_G(u_\alpha)$ and $d_T(v_\beta)=d_L(v_\beta)+2=d_G(u_\alpha)+d_G(v_\alpha)$, respectively. T has all 3 types of edges. $\beta\beta-$edges, $\alpha\alpha-$ edges and $\alpha\beta-$edges.

$$
\begin{aligned}
KG(T) &= \sum_{ue\in E(T)} \sqrt{d(u)^2+d(e)^2} \\
&< \sum_{ue\in E(T)} d(u)+d(e) \\
&= \sum_{u_\alpha v_\alpha\in E(T)} d_T(u_\alpha)+\{d_T(u_\alpha)+d_T(v_\alpha)-2\}+d_T(v_\alpha)+\{d_T(u_\alpha)+d_T(v_\alpha)-2\} \\
&+ \sum_{u_\beta v_\beta\in E(T)} d_T(u_\beta)+\{d_T(u_\beta)+d_T(v_\beta)-2\}+d_T(v_\beta)+\{d_T(u_\beta)+d_T(v_\beta)-2\} \\
&+ \sum_{u_\alpha v_\beta\in E(T)} d_T(u_\alpha)+\{d_T(u_\alpha)+d_T(v_\beta)-2\}+d_T(v_\beta)+\{d_T(u_\alpha)+d_T(v_\beta)-2\}
\end{aligned}
$$

$$= \sum_{u_\alpha v_\alpha \in E(G)} 2d_G(u_\alpha) + 2d_G(u_\alpha) + 2d_G(v_\alpha) - 2 + 2d_G(v_\alpha) + 2d_G(u_\alpha) + 2d_G(v_\alpha)$$
$$- 2 + \sum_{u_\beta v_\beta \in E(L)} d_L(u_\beta) + 2 + d_L(u_\beta) + 2 + d_L(v_\beta) + 2 - 2 + d_L(v_\beta) + 2 + d_L(u_\beta)$$
$$+ 2 + d_L(v_\beta) + 2 - 2 + \sum_{u_\alpha v_\alpha \in E(G)} 2d_G(u_\alpha) + 2d_G(u_\alpha) + d_G(u_\alpha) + d_G(v_\alpha) - 2$$
$$+ d_G(u_\alpha) + d_G(v_\alpha) + 2d_G(u_\alpha) + d_G(u_\alpha) + d_G(v_\alpha) - 2$$
$$= \sum_{u_\alpha v_\alpha \in E(G)} [6d_G(u_\alpha) + 6d_G(v_\alpha)] - 4 \sum_{u_\alpha v_\alpha \in E(G)} 1 + \sum_{u_\beta v_\beta \in E(L)} 3d_L(u_\beta) + 3d_L(v_\beta)$$
$$+ 8 \sum_{u_\beta v_\beta \in E(L)} 1 + \sum_{u_\alpha v_\alpha \in E(G)} 9d_G(u_\alpha) + 3d_G(v_\alpha) - 4$$
$$= 6M_1(G) + 3M_1(L) - 8q + 8\left(\frac{M_1(G)}{2} - q\right) + \sum_{u_\alpha v_\alpha \in E(G)} 9d_G(u_\alpha) + 3d_G(v_\alpha)$$
$$< 10M_1(G) + 3M_1(L) - 16q + \sum_{u_\alpha v_\alpha \in E(G)} 9d_G(u_\alpha) + 3d_G(v_\alpha).$$

□

Theorem 5.7 *For m-shadow graph,*

$$KG(D_m(G)) < 3[3m+1]M_1(G) + m\left[\sum_{u_i u_j \in E(G)} 6d_G(u_i) + 3(m+1)d_G(u_j)\right] - 4q(m+2).$$

Here, $M_1(G)$ is the first Zagreb index of graph G of size q.

Proof: For any vertex u_i, $1 \le i \le j \le n$ in $D_m(G)$, $d_{D_m(G)}(u_i) = (m+1)d_G(u_i)$ and $d_{D_m(G)}(u_i') = d_{D_m(G)}(u_i'') = d_{D_m(G)}(u_i''') = \ldots = d_{D_m(G)}(u_i^m) = 2d_G(u_i)$.

Edges in $D_m(G)$ are u_iu_j, $u_i'u_j$, $u_i'u_j'$, $u_i''u_j$, $u_i''u_j''$, $\ldots$, $u_i^mu_j$, $u_i^mu_j^m$.

$$KG(D_m(G)) = \sum_{ue \in E(G^m)} \sqrt{d(u)^2 + d(e)^2}$$
$$< \sum_{ue \in E(G^m)} d(u) + d(e)$$
$$= \sum_{u_i u_j \in E(G^m)} d_{G^m}(u_i) + d_{G^m}(u_i) + d_{G^m}(u_j) - 2 + d_{G^m}(u_j) + d_{G^m}(u_i) + d_{G^m}(u_j) - 2$$
$$+ \sum_{u_i' u_j \in E(G^m)} d_{G^m}(u_i') + d_{G^m}(u_i') + d_{G^m}(u_j) - 2 + d_{G^m}(u_j) + d_{G^m}(u_i') + d_{G^m}(u_j) - 2$$
$$+ \sum_{u_i' u_j' \in E(G^m)} d_{G^m}(u_i') + d_{G^m}(u_i') + d_{G^m}(u_j') - 2 + d_{G^m}(u_j') + d_{G^m}(u_i') + d_{G^m}(u_j') - 2$$
$$+ \sum_{u_i'' u_j \in E(G^m)} d_{G^m}(u_i'') + d_{G^m}(u_i'') + d_{G^m}(u_j) - 2 + d_{G^m}(u_j) + d_{G^m}(u_i'') + d_{G^m}(u_j) - 2$$
$$+ \sum_{u_i'' u_j'' \in E(G^m)} d_{G^m}(u_i'') + d_{G^m}(u_i'') + d_{G^m}(u_j'') - 2 + d_{G^m}(u_j'') + d_{G^m}(u_i'') + d_{G^m}(u_j'') - 2$$

$$+\cdots+\sum_{u_i^m u_j\in E(G^m)} d_{G^m}(u_i^m)+d_{G^m}(u_i^m)+d_{G^m}(u_j)-2+d_{G^m}(u_j)+d_{G^m}(u_i^m)$$
$$+d_{G^m}(u_j)-2+\sum_{u_i^m u_j^m\in E(G^m)} d_{G^m}(u_i^m)+d_{G^m}(u_i^m)+d_{G^m}(u_j^m)-2+d_{G^m}(u_j^m)$$
$$+d_{G^m}(u_i^m)+d_{G^m}(u_j^m)-2$$
$$=\sum_{u_iu_j\in E(G)}(m+1)d_G(u_i)+(m+1)d_G(u_i)+(m+1)d_G(u_j)-2+(m+1)d_G(u_j)$$
$$+(m+1)d_G(u_i)+(m+1)d_G(u_j)-2+\sum_{u_iu_j\in E(G)}2d_G(u_i)+2d_G(u_i)+(m+1)d_G(u_j)$$
$$-2+(m+1)d_G(u_j)+2d_G(u_i)+(m+1)d_G(u_j)-2+\sum_{u_iu_j\in E(G)}2d_G(u_i)+2d_G(u_i)$$
$$+2d_G(u_j)-2+2d_G(u_j)+2d_G(u_i)+2d_G(u_j)-2+\sum_{u_iu_j\in E(G)}2d_G(u_i)+2d_G(u_i)$$
$$+(m+1)d_G(u_j)-2+(m+1)d_G(u_j)+2d_G(u_i)+(m+1)d_G(u_j)-2$$
$$+\sum_{u_iu_j\in E(G)}2d_G(u_i)+2d_G(u_i)+2d_G(u_j)-2+2d_G(u_j)+2d_G(u_i)+2d_G(u_j)-2$$
$$+\cdots+\sum_{u_iu_j\in E(G)}2d_G(u_i)+2d_G(u_i)+(m+1)d_G(u_j)-2+(m+1)d_G(u_j)+2d_G(u_i).$$

$$+(m+1)d_G(u_j)-2+\sum_{u_iu_j\in E(G)}2d_G(u_i)+2d_G(u_i)+2d_G(u_j)-2$$
$$+2d_G(u_j)+2d_G(u_i)+2d_G(u_j)-2$$
$$=\sum_{u_iu_j\in E(G)}3(m+1)d_G(u_i)+3(m+1)d_G(u_i)-4\sum_{u_iu_j\in E(G)}1+\sum_{u_iu_j\in E(G)}6d_G(u_i)$$
$$+3(m+1)d_G(u_j)-4\sum_{u_iu_j\in E(G)}1+\sum_{u_iu_j\in E(G)}6d_G(u_i)+6d_G(u_j)-4\sum_{u_iu_j\in E(G)}1$$
$$+\sum_{u_iu_j\in E(G)}6d_G(u_i)+3(m+1)d_G(u_j)-4\sum_{u_iu_j\in E(G)}1+\sum_{u_iu_j\in E(G)}6d_G(u_i)+6d_G(u_j)$$
$$-4\sum_{u_iu_j\in E(G)}1+\cdots+\sum_{u_iu_j\in E(G)}6d_G(u_i)+3(m+1)d_G(u_j)-4\sum_{u_iu_j\in E(G)}1$$
$$+\sum_{u_iu_j\in E(G)}6d_G(u_i)+6d_G(u_j)-4\sum_{u_iu_j\in E(G)}1$$
$$=3(m+1)M_1(G)-4q+m\left[\sum_{u_iu_j\in E(G)}6d_G(u_i)+3(m+1)d_G(u_j)-4\right]$$
$$+m[6M_1(G)-4q]$$
$$<3[3m+1]M_1(G)+m\left[\sum_{u_iu_j\in E(G)}6d_G(u_i)+3(m+1)d_G(u_j)\right]-4q(m+2).$$

□

Theorem 5.8 *For m-splitting graph,*

$$KG(Spl_m(G))<3[m+1]M_1(G)+m\left[\sum_{u_iu_j\in E(G)}3d_G(u_i)+3(m+1)d_G(u_j)\right]-4q(1+m).$$

Here, $M_1(G)$ is the first Zagreb index of graph G of size q.

Proof: For any vertex u_i, $1 \leq i \leq j \leq n$ in $Spl_m(G)$, $d_{Spl_m(G)}(u_i) = (m+1)d_G(u_i)$ and $d_{Spl_m}(u_i') = d_{Spl_m}(u_i'') = d_{Spl_m}(u_i''') = \ldots = d_{Spl_m}(u_i^m) = d_G(u_i)$.

Edges in $Spl_m(G)$ are u_iu_j, $u_i'u_j$, $u_i'u_j'$, $u_i''u_j$, $u_i''u_j''$, $\ldots$, $u_i^m u_j$, $u_i^m u_j^m$.

$$
\begin{aligned}
KG(Spl_m(G)) &= \sum_{ue \in E(G^m)} \sqrt{d(u)^2 + d(e)^2} \\
&< \sum_{ue \in E(G^m)} d(u) + d(e) \\
&= \sum_{u_iu_j \in E(G^m)} d_{G^m}(u_i) + d_{G^m}(u_i) + d_{G^m}(u_j) - 2 + d_{G^m}(u_j) + d_{G^m}(u_i) + d_{G^m}(u_j) - 2 \\
&+ \sum_{u_i'u_j \in E(G^m)} d_{G^m}(u_i') + d_{G^m}(u_i') + d_{G^m}(u_j) - 2 + d_{G^m}(u_j) + d_{G^m}(u_i') + d_{G^m}(u_j) - 2 \\
&+ \sum_{u_i''u_j \in E(G^m)} d_{G^m}(u_i'') + d_{G^m}(u_i'') + d_{G^m}(u_j) - 2 + d_{G^m}(u_j) + d_{G^m}(u_i'') + d_{G^m}(u_j) - 2 \\
&+ \cdots + \sum_{u_i^m u_j \in E(G^m)} d_{G^m}(u_i^m) + d_{G^m}(u_i^m) + d_{G^m}(u_j) - 2 + d_{G^m}(u_j) + d_{G^m}(u_i^m) \\
&+ d_{G^m}(u_j) - 2 \\
&= \sum_{u_iu_j \in E(G)} (m+1)d_G(u_i) + (m+1)d_G(u_i) + (m+1)d_G(u_j) - 2 + (m+1)d_G(u_j) \\
&+ (m+1)d_G(u_i) + (m+1)d_G(u_j) - 2 + \sum_{u_iu_j \in E(G)} d_G(u_i) + d_G(u_i) + (m+1)d_G(u_j) - 2 \\
&+ (m+1)d_G(u_j) + d_G(u_i) + (m+1)d_G(u_j) - 2 + \sum_{u_iu_j \in E(G)} d_G(u_i) + d_G(u_i) \\
&+ (m+1)d_G(u_j) - 2 + (m+1)d_G(u_j) + d_G(u_i) + (m+1)d_G(u_j) - 2 + \cdots \\
&+ \sum_{u_iu_j \in E(G)} 2d_G(u_i) + 2d_G(u_i) + 2d_G(u_j) - 2 + 2d_G(u_j) \\
&+ 2d_G(u_i) + 2d_G(u_j) - 2 \\
&= \sum_{u_iu_j \in E(G)} 3(m+1)d_G(u_i) + 3(m+1)d_G(u_j) - 4 \sum_{u_iu_j \in E(G)} 1 + \sum_{u_iu_j \in E(G)} 3d_G(u_i) \\
&+ 3(m+1)d_G(u_j) - 4 \sum_{u_iu_j \in E(G)} 1 + \sum_{u_iu_j \in E(G)} 3d_G(u_i) + 3(m+1)d_G(u_j) - 4 \sum_{u_iu_j \in E(G)} 1 \\
&+ \cdots + \sum_{u_iu_j \in E(G)} 3d_G(u_i) + 3(m+1)d_G(u_j) - 4 \sum_{u_iu_j \in E(G)} 1 \\
&= 3(m+1)M_1(G) - 4q + m\left[\sum_{u_iu_j \in E(G)} 3d_G(u_i) + 3(m+1)d_G(u_j) - 4\right] \\
&< 3[m+1]M_1(G) + m\left[\sum_{u_iu_j \in E(G)} 3d_G(u_i) + 3(m+1)d_G(u_j)\right] - 4q(1+m).
\end{aligned}
$$

□

Theorem 5.9 *Let $G = G_1 \circ G_2$. be the corona product of graphs $G_1 = (p_1, q_1)$ and $G_2 = (p_2, q_2)$. Then $KG(G_1 \circ G_2) < 3M_1(G_1) + 6p_2q_1 - 4q_1 + 3M_1(G_1 \circ G_2) + (3p_2 - 1)[q_1 + p_1(q_2 + p_2)]$, where $M_1(G_1)$ and $M_1(G_1 \circ G_2)$ are the first Zagreb indices of graph G_1 and $G_1 \circ G_2$.*

Proof: Let $G_1 = (p_1, q_1)$ and $G_2 = (p_2, q_2)$ be any two graphs and for the sake simplicity let $G = G_1 \circ G_2$. For any vertex u and u_i in $G_1 \circ G_2$, $d_{G_1 \circ G_2} = d_{G_1}(u) + p_2$ and $d_{G_1 \circ G_2} = d_{G_2}(i) + 1$, $1 \leq i \leq p_2$, respectively. Edges are between the vertices (u, v) and (u, u_i).

$$
\begin{aligned}
KG(G_1 \circ G_2) < & \sum_{uv \in E(G)} d_G(u) + \{d_G(u) + d_G(v) - 2\} + d_G(v) + \{d_G(u) + d_G(v) - 2\} \\
& + \sum_{uu_i \in E(G)} d_G(u) + \{d_G(u) + d_G(u_i) - 2\} + d_G(u_i) + \{d_G(u) + d_G(u_i) - 2\} \\
& = \sum_{uv \in E(G_1)} d_{G_1}(u) + p_2 + d_{G_1}(u) + p_2 + d_{G_1}(v) + p_2 - 2 + d_{G_1}(v) + p_2 + d_{G_1}(u) + p_2 \\
& + d_{G_1}(v) + p_2 - 2 + \sum_{uu_i \in E(G)} d_{G_1}(u) + p_2 + d_{G_1}(u) + p_2 + d_{G_2}(u_i) + 1 - 2 + d_{G_2}(u_i) + 1 \\
& + d_{G_1}(u) + p_2 + d_{G_2}(u_i) + 1 - 2 \\
& = \sum_{uv \in E(G_1)} 3d_{G_1}(u) + 3d_{G_1}(v) + 6p_2 - 4 + \sum_{uu_i \in E(G)} 3d_{G_1}(u) + 3d_{G_2}(u_i) + 3p_2 - 1 \\
& < 3M_1(G_1) + 6p_2q_1 - 4q_1 + 3M_1(G_1 \circ G_2) + (3p_2 - 1)[q_1 + p_1(q_2 + p_2)].
\end{aligned}
$$

□

Theorem 5.10 *Let $G = G_1 + G_2$. be the join of two graphs $G_1 = (p_1, q_1)$ and $G_2 = (p_2, q_2)$. Then $KG(G_1 + G_2) < 3M_1(G_1) + 3M_1(G_2) + 3M_1(G_1 + G_2) + (6p_2 - 4)q_1 + (6p_1 - 4)q_2 + (3(p_1 + p_2) - 4)(q_1 + q_2 + p_1p_2)$, where $M_1(G_1)$ and $M_1(G_1 \circ G_2)$ are the first Zagreb indices of graph G_1 and $G_1 + G_2$.*

Proof: Let $G_1 = (p_1, q_1)$ and $G_2 = (p_2, q_2)$ be any two graphs and for the sake simplicity let $G = G_1 + G_2$. For any vertex u_i and v_i in $G_1 + G_2$, we have $d_{(G_1+G_2)}(u_i) = d_{G_1}(u_i) + p_2$ and $d_{(G_1+G_2)}(v_i) = d_{G_1}(v_i) + p_1$. Edges are u_iu_j, v_iv_j, and u_iv_j, where $1 \leq u_i, u_j \leq p_1$ and $1 \leq v_i, v_j \leq p_2$.

$$
\begin{aligned}
KG(G_1 + G_2) < & \sum_{u_iu_j \in E(G) 1 \leq i < j \leq p_1} d_G(u_i) + \{d_G(u_i) + d_G(u_j) - 2\} + d_G(u_j) + \{d_G(u_i) + d_G(u_j) - 2\} \\
& + \sum_{v_iv_j \in E(G) 1 \leq i < j \leq p_2} d_G(v_i) + \{d_G(v_i) + d_G(v_j) - 2\} + d_G(v_j) + \{d_G(v_i) + d_G(v_j) - 2\} \\
& + \sum_{u_iv_j \in E(G) 1 \leq i \leq p_1, 1 \leq j \leq p_2} d_G(u_i) + \{d_G(u_i) + d_G(v_j) - 2\} + d_G(v_j) + \{d_G(u_i) + d_G(v_j) - 2\} \\
& = \sum_{u_iu_j \in E(G_1)} d_{G_1}(u_i) + p_2 + d_{G_1}(u_i) + p_2 + d_{G_1}(u_j) + p_2 - 2 + d_{G_1}(u_j) + p_2 + d_{G_1}(u_i) + p_2 \\
& + d_{G_1}(u_j) + p_2 - 2 + \sum_{v_iv_j \in E(G_2)} d_{G_2}(v_i) + n_1 + d_{G_2}(v_i) + n_1 + d_{G_2}(v_j) + p_1 - 2 + d_{G_2}(v_j) \\
& + p_1 + d_{G_2}(v_i) + p_1 + d_{G_2}(v_j) + p_1 - 2 + \sum_{u_iv_j \in E(G)} d_{G_1}(u_i) + p_2 + d_{G_1}(u_i) + p_2 + d_{G_2}(v_j) \\
& + p_1 - 2 + d_{G_2}(v_j) + p_1 + d_{G_1}(u_i) + p_2 + d_{G_2}(v_j) + p_1 - 2 \\
& = \sum_{u_iu_j \in E(G_1)} 3d_{G_1}(u_i) + 3d_{G_1}(u_j) + 6p_2 - 4 + \sum_{v_iv_j \in E(G_2)} 3d_{G_2}(v_i) + 3d_{G_2}(v_j) + 6p_1 - 4 \\
& + \sum_{u_iv_j \in E(G)} 3d_{G_1}(u_i) + 3d_{G_2}(v_j) + 3p_1 + 3p_2 - 4 \\
& < 3M_1(G_1) + 3M_1(G_2) + 3M_1(G_1 + G_2) + (6p_2 - 4)q_1 + (6p_1 - 4)q_2 \\
& + (3(p_1 + p_2) - 4)(q_1 + q_2 + p_1p_2).
\end{aligned}
$$

□

6. Conclusion

Topological indices are often correlated with physical properties of molecules, such as boiling points, viscosity, and surface tension. Similarly, in graph theory, they can be used to predict various properties of graphs, such as connectivity, symmetry, and rigidity. We have computed a bound for the KG-Sombor index of derived graphs, including the join of graphs, the m-splitting graph, the m-shadow graph, the corona product of graphs, and the join of graphs

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