On leap Zagreb indices of bridge and chain graphs

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Abstract: The 2-degree of a vertex v in a (molecular) graph G is the number of vertices which are at distance two from v in G. The first leap Zagreb index of a graph G is the sum of squares of the 2-degree of all vertices in G and the third leap Zagreb index of G is the sum of product of the degree and 2-degree of every vertex v in G. In this paper, we compute the first and third leap Zagreb indices of bridge and chain graphs. Also we apply these results to determine the first and third leap Zagreb indices of some chemical structures such as polyphenyl chains and spiro chains.

Keywords: leap Zagreb indices; bridge graphs; chain graph

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1. Introduction

A molecular graph in chemical graph theory is the graphical representation of the structural formula of a chemical compound in which the vertices represent atoms and edges represent chemical bond between those atoms. A topological index of a molecular graph G is a real number which characterizes the topology of G. Also it is invariant under graph automorphism. Topological indices have been widely used in Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies. It has application in many folds, to name a few areas, biochemistry, nanotechnology, pharmacology. Bond energy is a measure of bond strength of a chemical compound. The distance between two atoms is considered as the bond length between them. The higher the bond energy, the smaller is the bond length between those atoms. The recently introduced 2-degree based topological invariants, analogous to novel graph invariants (Zagreb indices), namely leap Zagreb indices, may be applied in studying such bond energy between atoms in
a molecular graph of a chemical compound.

Throughout this paper, $G = (V, E)$ represents a connected molecular graph with the vertex set $V(G)$ and the edge set $E(G)$. Let the number of vertices and edges of $G$ be $n$ and $m$ respectively. The degree of a vertex $v$ in $G$ is the number of vertices adjacent to $v$ in $G$ and denoted by $\text{deg}(v : G)$.

The second leap Zagreb index $L_{M_2}(G)$ of a graph $G$ is equal to the sum of the products of the second degrees of pairs of adjacent vertices, $L_{M_2}(G) = \sum_{uv \in E(G)} d_2(u)d_2(v)$.

The third leap Zagreb index $L_{M_3}(G)$ of a graph $G$ is equal to the sum of the products of the degree with the second degree of every vertex in $G$, $L_{M_3}(G) = \sum_{u \in V(G)} \text{deg}(u)d_2(u)$.

Subsequently, Z. Shao et al. [18] generalized the results of Naji et al. [13] for trees and unicyclic graphs and determined upper and lower bounds on leap Zagreb indices and characterized extremal graphs. Basavanagoud et al. [2] computed exact values for first and second leap hyper Zagreb indices of some nano structures. V. R. Kulli [7–9] introduced and studied various leap indices. Shiladhar et al. [17] computed leap Zagreb indices of windmill graphs. Most recently, Naji et al. [14] have studied some properties of leap graphs.

Azari et al. [1] found formulae for first and second Zagreb indices of bridge and chain graphs. Nilanjan De [15, 16] computed F-index and hyper Zagreb index of bridge and chain graphs. Jerline et al. [6] obtained exact values for harmonic index of bridge and chain graphs. E. Litta et al. [10] worked on modified Zagreb indices of bridge and chain graphs. Mohanad Ali et al. [11] computed F-leap index of some special classes of bridge and chain graphs. Zhang et al. [12] worked on Edge-Version Atom-Bond Connectivity and Geometric Arithmetic Indices of generalized bridge molecular graphs. Motivated by their results, we compute exact values for the first and third leap Zagreb indices of bridges and chain graphs. Also we discuss some applications related to these indices in the last section of this paper.

First, we recall the definitions of bridge and chain graphs from [1] as follows:

**Definition 2.** Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with distinct vertices $v_i \in V(G_i)$. The bridge graph $B_1 = B_1(G_1, G_2, \ldots, G_d; v_1, v_2, v_3, \ldots, v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ as shown in Figure 1, is the graph obtained from the graphs $G_1, G_2, \ldots, G_d$ by connecting the vertices $v_i$ and $v_{i+1}$ by an edge for all $i = 1, 2, \ldots, d – 1$.

**Definition 3.** The bridge graph $B_2 = B_2(G_1, G_2, \ldots, G_d; v_1, v_2, w_2, \ldots, v_d, w_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i, w_i\}_{i=1}^d$ as shown in Figure 2, is the graph obtained from the graphs $G_1, G_2, G_3, \ldots, G_d$ by connecting the vertices $w_i$ and $v_{i+1}$ by an edge for all $i = 1, 2, \ldots, d – 1$. 

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Definition 4. The chain graph \( C = C(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d) \) of \( G_i \) with respect to the vertices \( \{v_i, w_i\}_{i=1}^d \) as shown in Figure 3, is the graph obtained from the graphs \( G_1, G_2, \ldots, G_d \) by identifying the vertices \( w_i \) and \( v_{i+1} \) for all \( i = 1, 2, \ldots, d-1 \).

2. First and third leap Zagreb indices of bridge and chain graphs

2.1. The bridge graph \( B_1 \)

The following lemma gives the 2-degree of any arbitrary vertex in the bridge graph \( B_1 \).

Lemma 5. Let \( G_1, G_2, \ldots, G_d \) be \( d \geq 5 \) connected graphs. Then the 2-degree of any arbitrary vertex \( u \) in the bridge graph \( B_1 \) formed by these graphs is as follows:

\[
d_2(u : B_1) = \begin{cases} 
  v_1 + \mu_2 + 1, & \text{if } u = v_1 \\
  v_d + \mu_{d-1} + 1, & \text{if } u = v_d \\
  v_2 + \mu_1 + \mu_3 + 1, & \text{if } u = v_2 \\
  v_{d-1} + \mu_d + \mu_{d-2} + 1, & \text{if } u = v_{d-1} \\
  v_i + \mu_{i-1} + \mu_{i+1} + 2, & \text{if } u = v_i, \quad 3 \leq i \leq d-2 \\
  d_2(u : G_1) + 1, & \text{if } u \in N_{G_1}(v_1) \\
  d_2(u : G_d) + 1, & \text{if } u \in N_{G_d}(v_d) \\
  d_2(u : G_i) + 2, & \text{if } u \in N_{G_i}(v_i), \quad 2 \leq i \leq d-1 \\
  d_2(u : G_i), & \text{if } u \in V(G_i) \setminus N_{G_i}[v_i], \quad 1 \leq i \leq d
\end{cases}
\]  

(2.1)

where \( v_i = d_2(v_i : G_i) \) and \( \mu_i = \deg(v_i : G_i), \quad 1 \leq i \leq d \).

Next, we compute the first leap Zagreb index of the type-I bridge graph \( B_1 \). Let \( S_i = \sum_{u \in N_{G_i}(v_i)} d_2(u : G_i), 1 \leq i \leq d \).

Theorem 6. \( LM_1(B_1) = \sum_{i=1}^{d} LM_1(G_i) + \sum_{i=2}^{d-1} \left[ (\mu_{i-1} + \mu_{i+1} + 1)^2 + 2v_i(\mu_{i-1} + \mu_{i+1} + 1) + 4S_i + 8\mu_i \right] + 2 \sum_{i=3}^{d-2} \nu_i + 2(S_1 + S_d) + (\mu_1 + \mu_d - 2\mu_3 - 2\mu_{d-2}) + (\mu_2 + 1)(\mu_2 + 2\nu_1 + 1) + (\mu_{d-1} + 1)(\mu_{d-1} + 2\nu_d + 1) + 3d - 12 \).

Proof. By virtue of Lemma 5

\[
LM_1(B_1) = \sum_{u \in V(B_1)} d_2(u : B_1)^2 \\
= (v_1 + \mu_2 + 1)^2 + (v_d + \mu_{d-1} + 1)^2 + (v_2 + \mu_1 + \mu_3 + 1)^2 + (v_{d-1} + \mu_d + \mu_{d-2} + 1)^2
\]
Thus the result follows.

Corollary 7. If $G_1 = G_2 = \cdots = G_d = G$ in a bridge graph $B_1$, then

$$\text{LM}_1(B_1) = d\text{LM}_1(G) + (4d - 6)\mu^2 + (4d - 8)\nu + (12d - 26)\mu + (4d - 4)(\nu \mu + S) + 4d - 12,$$

where $S = \sum_{u \in N_i(v)} d_2(u : G)$. 

Lemma 8. [1] The degree of an arbitrary vertex $u$ of the bridge graph $B_1$, $d \geq 5$ is given by:

$$\text{deg}(u : B_1) = \begin{cases} 
\mu_1 + 1, & \text{if } u = v_1 \\
\mu_d + 1, & \text{if } u = v_d \\
(\mu_i + 1)(\mu_{d - 1} + 2\nu_d + 2) + 2\nu_i(\mu_{i - 1} + \mu_{i + 1} + 1) + 4S_i + 8\mu_i + 2\nu_i(S_1 + S_d) + (\mu_1 + \mu_d - 2\mu_2 - 2\mu_3 - 2\mu_{d - 2} - 2\mu_{d - 1}) + (\mu_2 + 1)(\mu_2 + 2\nu_1 + 1) + (\mu_{d - 1} + 1)(\mu_{d - 1} + 2\nu_d + 1) + 3d - 12.
\end{cases}$$

Thus the result follows. □
Theorem 9. \( LM_3(\mathcal{B}_1) = \sum_{i=1}^{d} LM_3(G_i) + (s_1 + s_d) + 2 \sum_{i=2}^{d-1} s_i + \sum_{i=1}^{d} (2v_i + 6\mu_i) + 2 \sum_{i=2}^{d} (\mu_{i-1}\mu_i) - 2(\mu_2 + \mu_{d-1}) - (v_1 + v_d) - 3(\mu_1 + \mu_d) + 4d - 10. \)

\textbf{Proof.} By virtue of Lemma 5 and 8

\[ LM_3(\mathcal{B}_1) = \sum_{u \in V(\mathcal{B}_1)} d_2(u) \deg(u) \]

\[ = (v_1 + \mu_2 + 1)(\mu_1 + 1) + (v_2 + \mu_1 + \mu_3 + 1)(\mu_2 + 2) + (v_d + \mu_{d-1} + 1)(\mu_d + 1) \]

\[ + (v_d - 2 + \mu_d + \mu_{d-2} + 1)(\mu_{d-1} + 2) + \sum_{i=3}^{d-2} (v_i + \mu_{i-1} + \mu_{i+1} + 2)(\mu_i + 2) \]

\[ + \sum_{i=1}^{d-1} \sum_{u \in N_G(v_i)} (d_2(u : G_i) + 2)(\deg(u : G_i)) + \sum_{i=1}^{d} \sum_{u \in V(G_i) \setminus N_G(v_i)} (d_2(u : G_i))(\deg(u : G_i)) \]

\[ = (v_1\mu_1 + v_1 + \mu_2\mu_1 + \mu_2 + \mu_1 + 1) + (v_2\mu_2 + 2v_2 + \mu_1\mu_2 + 2\mu_1 + \mu_3\mu_2 + 2\mu_3 + \mu_2 + 2) \]

\[ + (v_d\mu_d + v_d + \mu_{d-1}\mu_d + \mu_{d-1} + \mu_d + 1) + (v_{d-1}\mu_{d-1} + 2v_{d-1} + \mu_d\mu_{d-1}) \]

\[ + 2\mu_d + \mu_{d-2}\mu_{d-1} + 2\mu_{d-2} + \mu_{d-1} + 2) + \sum_{i=3}^{d-2} (v_i\mu_i + 2v_i + \mu_{i-1}\mu_i + 2\mu_{i-1} + \mu_{i+1}\mu_i) \]

\[ + 2\mu_{i+1} + 2\mu_i + 4) + \sum_{u \in N_G(v_i)} (d_2(u : G_i)\deg(u : G_i) + \deg(u : G_i)) + \sum_{u \in N_G(v_d)} (d_2(u : G_d)) \]

\[ \deg(u : G_d) + \deg(u : G_d)) + \sum_{i=1}^{d-1} \sum_{u \in N_G(v_i)} (d_2(u : G_i)\deg(u : G_i) + 2\deg(u : G_i)) \]

\[ + \sum_{i=1}^{d} \sum_{u \in V(G_i) \setminus N_G(v_i)} d_2(u : G_i) \deg(u : G_i) \]

Thus the result follows. \( \square \)

\textbf{Corollary 10.} If \( G_1 = G_2 = \cdots = G_d = G \) in a bridge graph \( \mathcal{B}_1 \), then

\[ LM_3(\mathcal{B}_1) = dLM_3(G) + 2(d - 1)(s + v + \mu^2) + 2\mu(3d - 5) + 4d - 10, \]

where \( s = \sum_{u \in N_G(v)} \deg(u : G). \)

\textbf{2.2. The bridge graph} \( \mathcal{B}_2 \)

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{bridge_graph.png}
\caption{The bridge graph \( \mathcal{B}_2 \).}
\end{figure}
For any two nonempty sets $A$ and $B$, $A\Delta B$ denotes the symmetric difference of $A$ and $B$ and defined as $A\Delta B = (A \setminus B) \cup (B \setminus A) = (A \cup B) \setminus (A \cap B)$. First, we obtain the 2-degree of any arbitrary vertex in the type-II bridge graph $B_2$ as follows:

**Lemma 11.** Let $G_1, G_2, \cdots, G_d$ be $d \geq 5$ triangle free connected graphs. Then 2-degree of any arbitrary vertex $u$ in the bridge graph $B_2$ formed by these graphs is as follows:

$$d_2(u : B_2) = \begin{cases} 
  d_2(u : G_1), & \text{if } u \in V(G_1) \setminus N_{G_1}[w_1] \\
  d_2(u : G_1) + 1, & \text{if } u \in N_{G_1}(w_1) \\
  d_2(u : G_i), & \text{if } u \in V(G_i) \setminus \{N_{G_i}[v_i] \cup N_{G_i}[w_i]\}, \ 2 \leq i \leq d - 1 \\
  d_2(u : G_d), & \text{if } u \in V(G_d) \setminus N_{G_d}[v_d] \\
  d_2(u : G_d) + 1, & \text{if } u \in N_{G_d}(v_d) \\
  d_2(u : G_i) + 1, & \text{if } u \in (N_{G_i}(v_i) \Delta N_{G_i}(w_i)) \setminus 2, \ 2 \leq i \leq d - 1 \\
  d_2(u : G_i) + 2, & \text{if } u \in N_{G_i}(v_i) \cap N_{G_i}(w_i), \ 2 \leq i \leq d - 1 \\
  \delta_i + \mu_{i+1}, & \text{if } u = v_i, \ 1 \leq i \leq d - 1 \\
  \nu_i + \lambda_i - 1, & \text{if } u = v_i, \ 2 \leq i \leq d.
\end{cases}$$

(2.3)

where $\nu_i = d_2(v_i : G_i)$, $\mu_i = deg(v_i : G_i)$; $2 \leq i \leq d$, $\delta_i = d_2(w_i : G_i)$, $\lambda_i = deg(w_i : G_i)$; $1 \leq i \leq d - 1$.

Next, we compute the first leap Zagreb index of type-II bridge graph $B_2$.

Let us denote $S'_1 = \sum_{u \in N_{G_1}(w_1)} d_2(u : G_1)$ and $S_d = \sum_{u \in N_{G_d}(v_d)} d_2(u : G_d)$

**Theorem 12.** $LM_1(B_2) = \sum_{i=1}^{d} LM_1(G_i) + 2(S'_1 + S_d) + (\lambda_1 + \mu_d) + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \Delta N_{G_i}(w_i)} [2d_2(u : G_i) + 1] + 4 \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} [d_2(u : G_i) + 1] + \sum_{i=1}^{d} (\mu_{i+1}^2 + 2\delta_{i+1}) + \sum_{i=2}^{d} (\lambda_{i-1}^2 + 2\nu_i \lambda_{i-1})$.

Proof.

$$LM_1(B_2) = \sum_{u \in V(B_2)} d_2(u : B_2)^2$$

$$= \sum_{u \in V(G_1) \setminus N_{G_1}[w_1]} d_2(u : G_1)^2 + \sum_{i=2}^{d-1} \sum_{u \in V(G_i) \setminus \{N_{G_i}[v_i] \cup N_{G_i}[w_i]\}} d_2(u : G_i)^2$$

$$+ \sum_{u \in V(G_d) \setminus N_{G_d}[v_d]} d_2(u : G_d)^2 + \sum_{u \in N_{G_1}(w_1)} (d_2(u : G_1) + 1)^2$$

$$+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} (d_2(u : G_i) + 1)^2$$

$$+ \sum_{u \in N_{G_d}(v_d)} (d_2(u : G_d) + 1)^2 + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} (d_2(u : G_i) + 2)^2$$
Lemma 14.

\[ + \sum_{i=1}^{d-1} (\delta_i + \mu_{i+1})^2 + \sum_{i=2}^{d} (\nu_i + \lambda_{i-1})^2 \]

\[ = LM_1(G_1) - \delta_1^2 - \sum_{u \in N_G(v_1)} d_2(u : G_1)^2 + \sum_{u \in V(G_1)} d_2(u : G_1)^2 - \sum_{u \in N_N(\nu_1 \cup N_G(w_1))} d_2(u : G_1)^2 - \nu_1^2 - \delta_1^2 \]

\[ + LM_1(G_d) - v_d^2 - \sum_{u \in N_G(v_d)} d_2(u : G_d)^2 + \sum_{u \in V(G_d)} d_2(u : G_d)^2 + 2 \sum_{u \in N_G(v_d)} d_2(u : G_d) + \lambda_1 \]

\[ + \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \Delta N_G(w_i)} [d_2(u : G_i)^2 + 2d_2(u : G_i) + 1] + \sum_{u \in N_G(v_d)} [d_2(u : G_d)^2 + 2d_2(u : G_d) + 1] \]

\[ + \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \cap N_G(w_i)} [d_2(u : G_i)^2 + 4d_2(u : G_i) + 4] \]

\[ + \sum_{i=1}^{d} [\delta_i^2 + 2\delta_i \mu_{i+1} + \mu_{i+1}^2] + \sum_{i=2}^{d} [\nu_i^2 + 2\nu_i \lambda_{i-1} + \lambda_{i-1}^2] \]

Thus,

\[ LM_1(B_2) = \sum_{i=1}^{d} LM_1(G_i) + 2(S_1^2 + S_d^2) + (\lambda_1 + \mu_d) \]

\[ + \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \Delta N_G(w_i)} [2d_2(u : G_i) + 1] + 4 \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \cap N_G(w_i)} [d_2(u : G_i) + 1] \]

\[ + \sum_{i=1}^{d} \sum_{u \in N_G(v_i)} (\mu_{i+1}^2 + 2\delta_i \mu_{i+1}) + \sum_{i=2}^{d} (\lambda_{i-1}^2 + 2\nu_i \lambda_{i-1}). \]

□

Corollary 13. If \( G_1 = G_2 = \cdots = G_d = G \), in a bridge graph \( B_2 \), then \( LM_1(B_2) = dLM_1(G) + \lambda + \mu + 2(S + S') + (d-2) \sum_{u \in N_G(v_i) \Delta N_G(w_i)} + 4(d-2) \sum_{u \in N_G(v_i) \cap N_G(w_i)} + (d-1)[\mu^2 + \lambda^2] + 2(d-1)[\delta \mu + \nu \lambda] \), where \( S = \sum_{u \in N_G(w_i)} d_2(u : G) \) and \( S' = \sum_{u \in N_G(v_i)} d_2(u : G) \).

In what follows next, we compute the third leap Zagreb index of \( B_2 \).

Lemma 14. The degree of an arbitrary vertex \( u \) of the bridge graph \( B_2, d \geq 5 \) is given by:

\[ \text{deg} (u : B_2) = \begin{cases} \text{deg}(u : G_1), & \text{if } u \in V(G_1) \setminus \{v_1\} \\ \text{deg}(u : G_d), & \text{if } u \in V(G_d) \setminus \{v_d\} \\ \text{deg}(u : G_i), & \text{if } u \in V(G_i) \setminus \{v_i, w_i\}, 2 \leq i \leq d-1 \\ \lambda_i + 1, & \text{if } u = w_i, \ 1 \leq i \leq d-1 \\ \mu_i + 1, & \text{if } u = v_i, \ 2 \leq i \leq d. \end{cases} \]  \hspace{1cm} (2.4)

where \( \mu_i = \text{deg}(v_i : G_i) ; 2 \leq i \leq d, \ \lambda_i = \text{deg}(w_i : G_i) ; 1 \leq i \leq d-1. \)
Corollary 16. If \( G_1 = G_2 = \cdots = G_d = G \) in a bridge graph \( \mathcal{B}_2 \), then
\[
LM_3(\mathcal{B}_2) = dLM_3(G) + \sum_{u \in N_G(w)} \deg(u : G) + \sum_{u \in N_G(v)} \deg(u : G) + (d - 2)(\sum_{u \in N_G(w) \cap N_G(v)} \deg(u : G)) + (d - 1)(2\mu + \mu + \lambda) + d(\delta + \nu) - (\nu + \delta).
\]

2.3. The chain graph \( C \)

In the following lemma, we obtain the 2-degree of any vertex in the chain graph \( C \).

Lemma 17. Let \( G_1, G_2, \ldots, G_d, d \geq 5 \) be \( C_3 \)-free connected graphs and let \( C = \mathcal{C}(G_1, G_2, \ldots, G_d; w_1, v_2, w_2, v_3, \ldots, w_{d-1}, v_d) \) be the chain graph formed using these graphs. Then the 2-degree of any vertex \( u \) in \( C \) is given as follows:
Proof. By Lemma 17, we have

\[
d_2(u : C) = \begin{cases} 
    d_2(u : G_1), & \text{if } u \in V(G_1) \setminus N_{G_i}[w_1] \\
    d_2(u : G_1) + \mu_2, & \text{if } u \in N_{G_i}(w_1) \\
    d_2(u : G_d), & \text{if } u \in V(G_d) \setminus N_{G_d}[v_d] \\
    d_2(u : G_d) + \lambda_{d-1}, & \text{if } u \in N_{G_d}(v_d) \\
    d_2(u : G_i), & \text{if } u \in V(G_i) \setminus \{N_{G_i}[w_i] \cup N_{G_i}[v_i]\}, 2 \leq i \leq d-1 \\
    d_2(u : G_i) + \mu_{i+1}, & \text{if } u \in N_{G_i}(w_i) \setminus N_{G_i}(v_i), 2 \leq i \leq d-1 \\
    d_2(u : G_i) + \lambda_{i-1}, & \text{if } u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i), 2 \leq i \leq d-1 \\
    d_2(u : G_i) + \lambda_{i-1} + \mu_{i+1}, & \text{if } u \in N_{G_i}(v_i) \cap N_{G_i}(w_i), 2 \leq i \leq d-1 \\
    \delta_i + v_{i+1}, & \text{if } u = w_i = v_{i+1}, 1 \leq i \leq d-1,
\end{cases}
\]  

(2.5)

where \( v_i = d_2(v_i : G_i), \mu_i = \text{deg}(v_i : G_i), \lambda_i = \text{deg}(w_i : G_i) \) and 
\( \delta_i = d_2(w_i : G_i) \) for all \( 1 \leq i \leq d \).

Now, we compute the first leap Zagreb index of the chain graph \( C \) by applying Lemma 17.

**Theorem 18.** For the chain graph \( C \),

\[
LM_1(C) = \sum_{i=1}^{d} LM_1(G_{i}) + \sum_{u \in N_{G_i}(w_i)} [2\mu_2d_2(u : G_1) + \mu_2^2] + \sum_{u \in N_{G_i}(v_d)} [2\lambda_{d-1}d_2(u : G_d) + \lambda_{d-1}^2] \\
+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(w_i) \setminus N_{G_i}(v_i)} [2\mu_{i+1}d_2(u : G_i) + \mu_{i+1}^2] + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} [2\lambda_{i-1}d_2(u : G_i) + \lambda_{i-1}^2] \\
+ 2\sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \cap N_{G_i}(w_i)} [\lambda_{i-1}d_2(u : G_i) + \mu_{i+1}d_2(u : G_i) + \lambda_{i-1}\mu_{i+1}] \\
+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} (\lambda_{i-1}^2 + \mu_{i+1}^2) + 2\sum_{i=1}^{d-1} \delta_i v_{i+1}.
\]

**Proof.** By Lemma 17, we have

\[
LM_1(C) = \sum_{u \in V(C)} d_2(u : C)^2 \\
= \sum_{u \in V(G_1) \setminus N_{G_1}[w_1]} d_2(u : G_1)^2 + \sum_{u \in N_{G_1}(w_1)} [d_2(u : G_1) + \mu_2]^2 + \sum_{u \in V(G_d) \setminus N_{G_d}[v_d]} d_2(u : G_d)^2 \\
+ \sum_{u \in N_{G_d}(v_d)} [d_2(u : G_d) + \lambda_{d-1}]^2 + \sum_{i=2}^{d-1} \sum_{u \in V(G_i) \setminus \{N_{G_i}[v_i] \cup N_{G_i}[w_i]\}} d_2(u : G_i)^2 \\
+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} [d_2(u : G_i) + \mu_{i+1}]^2 + \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(w_i) \setminus N_{G_i}(v_i)} [d_2(u : G_i) + \lambda_{i-1}]^2 \\
+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \setminus N_{G_i}(w_i)} [d_2(u : G_i) + \lambda_{i-1} + \mu_{i+1}]^2 + \sum_{i=1}^{d-1} [\delta_i + v_{i+1}]^2.
\]
\[
= LM_1(G_1) - \sum_{u \in N_G(w)} [d_2(u : G_1)]^2 - \delta_i^2 + \sum_{u \in N_G(w)} [d_2(u : G_1)^2 + 2d_2(u : G_1)\mu_2 + \mu_i^2]
\]

\[
+ LM_1(G_d) - \sum_{u \in N_G(w)} d_2(u : G_d)^2 - \nu_d^2 + \sum_{u \in N_G(w)} [d_2(u : G_d)^2 + 2\lambda_{d-1}d_2(u : G_d) + \lambda_{d-1}^2]
\]

\[
+ \sum_{i=2}^{d-1} \sum_{u \in V(G_i)} d_2(u : G_i)^2 - \sum_{i=2}^{d-1} \sum_{u \in N_G[v_i] \cap N_G[w_i]} d_2(u : G_i)^2
\]

\[
+ \sum_{i=2}^{d-1} \sum_{u \in N_G[v_i] \cap N_G(w_i)} [d_2(u : G_i)^2 + 2\mu_{i+1}d_2(u : G_i) + \mu_{i+1}^2]
\]

\[
+ \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \cap N_G(w_i)} [d_2(u : G_i)^2 + 2\lambda_{i-1}d_2(u : G_i) + \lambda_{i-1}^2]
\]

\[
+ \sum_{i=1}^{d-1} [\delta_i^2 + \nu_{i+1}^2] + 2 \sum_{i=1}^{d-1} \delta_i\nu_{i+1}
\]

\[
= \sum_{i=1}^{d} LM_1(G_i) + \sum_{u \in N_G(w)} [2\mu_2d_2(u : G_1) + \mu_i^2] + \sum_{u \in N_G(w)} [2\lambda_{d-1}d_2(u : G_d) + \lambda_{d-1}^2]
\]

\[
+ \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \cap N_G(w_i)} [2\mu_{i+1}d_2(u : G_i) + \mu_{i+1}^2] + \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \cap N_G(w_i)} [2\lambda_{i-1}d_2(u : G_i) + \lambda_{i-1}^2]
\]

\[
+ 2 \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \cap N_G(w_i)} [\lambda_{i-1}d_2(u : G_i) + \mu_{i+1}d_2(u : G_i) + \lambda_{i-1}\mu_{i+1}]
\]

\[
+ \sum_{i=2}^{d-1} \sum_{u \in N_G(v_i) \cap N_G(w_i)} (\lambda_{i-1}^2 + \mu_{i+1}^2) + 2 \sum_{i=1}^{d-1} \delta_i\nu_{i+1}
\]

\[
\]

Corollary 19. In a chain graph \(C\), if \(G_1 = G_2 = \cdots = G_d = G\), then

\[
LM_1(C) = dLM_1(G) + \sum_{u \in N_G(w)} [2\mu_2d_2(u : G) + \mu_i^2] + \sum_{u \in N_G(w)} [2\lambda_{d-1}d_2(u : G) + \lambda_{d-1}^2] + (d - 2) \sum_{u \in N_G(w) \cap N_G(v)} [2\mu_2d_2(u : G) + \mu_i^2] + (d - 2) \sum_{u \in N_G(w) \cap N_G(v)} [2\lambda_{d-1}d_2(u : G) + \lambda_{d-1}^2]
\]

\[
+ 2(d - 2) \sum_{u \in N_G(w) \cap N_G(v)} [\lambda_{d-1}d_2(u : G) + \mu_{i+1}d_2(u : G) + \lambda_{d-1}\mu_{i+1}]
\]

\[
+ (d - 2) \sum_{u \in N_G(v) \cap N_G(w)} (\lambda_{i-1}^2 + \mu_{i+1}^2) + 2(d - 1)\delta v.
\]

Lemma 20. Let \(G_1, G_2, \cdots, G_d, d \geq 5\) be \(C_3\)-free connected graphs and let \(C = C(G_1, G_2, \cdots, G_d; w_1, v_2, w_2, v_3, \cdots, w_{d-1}, v_d)\) be the chain graph formed using these graphs.
Then the degree of any vertex \( u \) in \( C \) is given as follows:

\[
\text{deg}(u : C) = \begin{cases} 
\deg(u : G_1), & \text{if } u \in V(G_1) \setminus \{w_1\} \\
\deg(u : G_d), & \text{if } u \in V(G_d) \setminus \{v_d\} \\
\deg(u : G_i), & \text{if } u \in V(G_i) \setminus \{v_i, w_i\}, \ 2 \leq i \leq d - 1 \\
\lambda_i + \mu_{i+1}, & \text{if } u = w_i = v_{i+1}, \ 1 \leq i \leq d - 1,
\end{cases}
\tag{2.6}
\]

where \( \mu_i = \deg(v_i : G_i) \), \( \lambda_i = \deg(w_i : G_i) \) for all \( 1 \leq i \leq d \).

Finally, we compute the third leap Zagreb index of the chain graph \( C \) by applying Lemma 17 and 20.

**Theorem 21.** \( LM_3(C) = \sum_{i=1}^{d} LM_3(G_i) + \sum_{u \in N_{G_1}(w_1)} \mu_2 \deg(u : G_1) + \sum_{u \in N_{G_d}(v_d)} \lambda_{d-1} \deg(u : G_d) \)

\[
+ \sum_{i=2}^{d-1} \left( \sum_{u \in N_{G_i}(v_i)} \mu_{i+1} \deg(u : G_i) + \sum_{u \in N_{G_i}(w_i)} \lambda_{i-1} \deg(u : G_i) \right) 
\]

\[
+ \sum_{i=2}^{d-1} \left( \sum_{u \in N_{G_i}(w_i) \cap N_{G_i}(v_i)} (\delta_i + \nu_{i+1})(\lambda_i + \mu_{i+1}) \right).
\]

Proof. By virtue of Lemma 17 and 20

\[
LM_3(C) = \sum_{u \in V(C)} d_2(u) \deg(u) 
\]

\[
= \sum_{u \in V(G_1) \setminus N_{G_1}(w_1)} d_2(u : G_1) \deg(u : G_1) + \sum_{u \in N_{G_1}(w_1)} (d_2(u : G_1) + \mu_2) \deg(u : G_1) 
\]

\[
+ \sum_{u \in V(G_d) \setminus N_{G_d}(v_d)} d_2(u : G_d) \deg(u : G_d) + \sum_{u \in N_{G_d}(v_d)} (d_2(u : G_d) + \lambda_{d-1}) \deg(u : G_d) 
\]

\[
+ \sum_{i=2}^{d-1} \left( \sum_{u \in V(G_i) \setminus N_{G_i}[w_i] \cup N_{G_i}[v_i]} d_2(u : G_i) \deg(u : G_i) + \sum_{u \in N_{G_i}(w_i) \cup N_{G_i}(v_i)} (\mu_{i+1} \deg(u : G_i) + \lambda_{i-1} \deg(u : G_i)) \right) 
\]

\[
+ \sum_{i=2}^{d-1} \sum_{u \in N_{G_i}(v_i) \cap N_{G_i}(w_i)} (d_2(u : G_i) + \lambda_{i-1} + \mu_{i+1}) \deg(u : G_i) 
\]

\[
+ \sum_{i=1}^{d-1} (\delta_i + \nu_{i+1})(\lambda_i + \mu_{i+1}).
\]

Thus the result follows. \( \square \)

**Corollary 22.** In a chain graph \( C \), if \( G_1 = G_2 = \cdots = G_d = G \), then

\[
LM_3(C) = dLM_3(G) + \sum_{u \in N_{G_1}(w_1)} \mu_2 \deg(u : G) + \sum_{u \in N_{G_d}(v_d)} \lambda_{d-1} \deg(u : G) + (d - 2)(\sum_{u \in N_{G_1}(w_1) \cap N_{G_d}(v_d)} \mu \deg(u : G) + \sum_{u \in N_{G_1}(w_1) \cap N_{G_d}(v_d)} (\lambda + \mu) \deg(u : G)) + (d - 1)(\delta \mu + \nu \lambda).
\]
3. Examples

In this section, we determine the first and third leap Zagreb indices of some molecular graph structures.

Two vertices $v$ and $w$ of a hexagon $H (C_6)$ (please refer Figure 4) are said to be in

(i) ortho-position, if they are adjacent in $H$

(ii) meta-position, if they are distance two in $H$

(iii) para-position, if they are distance three in $H$.

We connect $h \geq 5$ ortho-hexagons to form a polyphenyl chain denoted by $O_h$ as follows:

![Figure 4. Ortho, meta and para positions of two vertices in a hexagon $H$.](image)

![Figure 5. Polyphenyl chain $O_h$.](image)

One can observe that the Polyphenyl chain $O_h$ shown in Figure 5 is a $B_1$ type bridge graph. Therefore, from Corollary 7, we get

\[
LM_1(O_h) = hLM_1(G) + (4h - 6)\mu^2 + (4h - 8)\nu + (12h - 26)\mu + (4h - 4)\nu \mu + \sum_{u \in N_G(v)} d_2(u : G) + 4h - 12 \\
= 24h + (4h - 6)(4) + (4h - 8)(2) + (12h - 26)(2) + (4h - 4)(4) + (4h - 4)(4) + 4h - 12 \\
= 108h - 136.
\]

Similarly, from Corollary 10, we get

\[
LM_3(O_h) = 24h + (2h - 2)(2) + (2h - 2)(2) + 2(2)(3h - 5) + 2(h - 1)(2 + 4) + 4h - 10 \\
= 60h - 50
\]
The polyphenyl chain $M_h$ is formed by connecting $h \geq 5$ meta-hexagons as shown in Figure 6.

The polyphenyl chain $P_h$ is formed by connecting $h \geq 5$ para-hexagons as shown in Figure 7.

Figure 6. Polyphenyl chain $M_h$.

Figure 7. Polyphenyl chain $P_h$.

It is clear that the Polyphenyl chains $M_h$ and $P_h$ are type-II bridge graphs $B_2$.

Using Corollary 13, we get

$$LM_1(M_h) = hLM_1(G) + \lambda + \mu + 2 \sum_{u \in N_G(w)} d_2(u : G) + (h - 2)[\sum_{u \in N_G(v) \cap N_G(w)} (2d_2(u : G) + 1)]$$

$$+(h - 2) \sum_{u \in N_G(v) \cap N_G(w)} (2d_2(u : G) + 1) + 4(h - 2) \sum_{u \in N_G(v) \cap N_G(w)} (d_2(u : G) + 1)$$

$$+2 \sum_{u \in N_G(v)} d_2(u : G) + (h - 1)\mu^2 + 2(h - 1)\mu + 2(h - 1)\nu + (h - 1)\lambda^2$$

$$= 24h + 4 + 2(4) + (h - 2)[2(2) + 1] + (h - 2)[2(2) + 1] + 4(h - 2)(2 + 1) + 2(4) + (h - 1)(4) + 4(h - 1)(4) + (h - 1)(4)$$

Thus $LM_1(M_h) = 70h - 48$.

Similarly, by Corollary 13, we have

$$LM_1(P_h) = 24h + 4 + 2(4) + (h - 2)[2(4) + 2] + (h - 2)(8 + 2) + 4(h - 2)(0) + 2(4) + (h - 1)(4) + 8(h - 1) + 8(h - 1) + (h - 1)(4)$$

Therefore, $LM_1(P_h) = 68h - 44$.

Using Corollary 16, we get

$$LM_3(M_h) = 24h + 8 + (h - 2)8 + (h - 1)12 + h(4) - 4$$

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\[
6534 = 48h - 24
\]

\[
LM_3(\mathcal{P}_h) = 24h + 8 + (h - 2)8 + (h - 1)12 + 4h - 4
\]
\[
= 48h - 24.
\]

Next, we shall see an application related to the chain graph \( C \). The spiro-chain \( SP_C(d, 3) \) is a chain graph formed using \( d \geq 5 \) copies of the cycle \( C_4 \).

Here the number 3 in the construction denotes the position of the vertices \( v \) and \( w \) in the spiro-chain (refer Figure 8).

![Figure 8. Spiro-chain \( SP_C(d, 3) \) formed with \( d \geq 5 \) copies of \( C_4 \) connected in 3\(^{rd}\) position.](image)

The spiro-chain \( SP_C(d, 4) \) is a chain graph formed using \( d \geq 5 \) copies of the cycle \( C_6 \) or hexagon where the vertices \( v \) and \( w \) are connected in the 4\(^{th}\) position (refer Figure 9).

![Figure 9. Spiro-chain \( SP_C(d, 4) \) formed with \( d \geq 5 \) copies of \( C_6 \) connected in 4\(^{th}\) position.](image)

By applying Corollary 19, we get
\[
LM_1(SP_C(d, 3)) = dLM_1(G) + \sum_{u \in N_G(v)} [2\mu_{d_2}(u : G) + \mu^2] + \sum_{u \in N_G(v)} [2\nu_{d_2}(u : G) + \lambda^2]
\]
\[
+ (d - 2) \sum_{u \in N_G(v) \cap N_G(w)} [2\mu_{d_2}(u : G) + \mu^2] + (d - 2) \sum_{u \in N_G(v) \cap N_G(w)} [2\nu_{d_2}(u : G) + \lambda^2]
\]
\[
+ 2(d - 2) \sum_{u \in N_G(v) \cap N_G(w)} [\lambda_{d_2}(u : G) + \mu d_2(u : G) + \lambda \mu]
\]
\[
+ (d - 2) \sum_{u \in N_G(v) \cap N_G(w)} (\lambda^2 + \mu^2) + 2(d - 1)\delta
\]
\[
= 54d - 66.
\]

Similarly, from Corollary 19, we have \( LM_1(SP_C(d, 4)) = 80d - 56. \)

By applying Corollary 22, we get
\[
LM_3(SP_C(d, 3)) = 8d + 2(2 + 2) + 2(2 + 2) + (d - 2)(16) + (d - 1)(4)
\]
\[
= 28d - 20
\]

Similarly, from Corollary 22, we have \( LM_3(SP_C(d, 4)) = 48d - 24. \)
4. Conclusions

We have computed exact values of one of the recent topological invariants namely first and third leap Zagreb indices for bridge and chain graphs. It is worth mentioning that computing second leap Zagreb index of bridges and chain graphs has not yet addressed and interested researchers may work on it. Also these indices need to be explored for several other interesting graph structures arising from mathematical chemistry and other branches of science.

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Conflict of interest

The authors declare that no competing interests exist.

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