Zagreb indices and their polynomials of the linear parallelogram of benzenoid graph

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ABSTRACT

Let G be a simple connected molecular graph, with vertex/atom set V(G) and edge/bond set E(G). In chemical graphs, the vertices correspond to the atoms of the molecule and the edges represent the chemical bonds. Computing the topological indices of molecular graphs are important branches in chemical graph theory.

In this paper, we compute the first and the Second Zagreb indices and their polynomials of an infinite family of the linear parallelogram of benzenoid graph.

Keywords:
Molecular Graph, linear parallelogram of benzenoid graph, Topological Indices, Zagreb indices, Zagreb polynomials.

1. INTRODUCTION

Let G=(V,E) be a simple connected molecular graph, with vertex/atom set V(G) and edge/bond set E(G). In chemical graphs, the vertices of the graph correspond to the atoms of the molecule and the edges represent the chemical bonds [1-4]. Computing the topological indices of molecular graphs are important branches in chemical graph theory.

There are several topological indices have been defined. One of the oldest and important graph invariants is on based structure descriptor the First Zagreb index, which was introduced by I. Gutman and N. Trinajstić [5] in 1972 and denoted by \( Z_1(G) \).

The First Zagreb index of the graph G denoted by \( (Z_1(G)) \) is defined as the sum of the squares of the degrees of all vertices/atoms in the molecules G, in terms of bonds

\[
Z_1(G) = \sum_{v \in V(G)} d_v^2 = \sum_{e = uv \in E(G)} (d_u + d_v)
\]

where \( d_u \) and \( d_v \) are the degrees of \( u \) and \( v \) in \( G \), respectively.

Also other based structure descriptor of a graph \( G \) that was conceived some what later is the Second Zagreb index and denoted by \( Z_2(G) \) and defined as [6]:

\[
Z_2(G) = \sum_{e = uv \in E(G)} (d_u \times d_v)
\]

Alternatively, the First and Second Zagreb polynomials \( Z_1(G,x) \) and \( Z_2(G,x) \) of G are defined as

\[
Z_1(G,x) = \sum_{e = uv \in E(G)} x^{d_u + d_v}
\]

\[
Z_2(G,x) = \sum_{e = uv \in E(G)} x^{d_u \times d_v}
\]

where the sum is over all unordered pairs \( u,v \) of distinct vertices in \( G \).

For more details of the First and Second Zagreb indices \( Z_1(G) \) and \( Z_2(G) \) and and their polynomials \( Z_1(G,x) \) and \( Z_2(G,x) \) see the paper series [5 -16].
In this paper, we focus on the First and Second Zagreb indices $Zg_1(G)$ and $Zg_2(G)$ and their polynomials of an infinite family of the linear parallelogram of benzenoid graph $P(m,n)$, $\forall m,n \in \mathbb{N} \setminus \{ 1 \}$.

2. RESULTS AND DISCUSSION

In this section is to compute the First Zagreb index, the Second Zagreb index, The First Zagreb Polynomial and the Second Zagreb Polynomial for an infinite family of the linear parallelogram $P(n,m)$ of benzenoid graph.

Before, start the proof of main theorems of this paper, we present following useful definition and denotations.

**Definition 1.** [11] For simple connected graph $G=(V,E)$ on based the degree $d_v$ of vertex $v \in V(G)$, we divide its vertex/atom set $V(G)$ and edge/bond set $E(G)$ of $G$ to several partitions, as follows:

$V_3 = \{ v \in V(G) | d_v = 3 \}$

$V_2 = \{ v \in V(G) | d_v = 2 \}$

$E_6 = E_9 = \{ uv \in E(G) | d_u = d_v = 3 \}$

$E_5 = E_6 \star = \{ uv \in E(G) | d_u = 2 \& d_v = 3 \}$

And $E_4 = E_4 \star = \{ uv \in E(G) | d_u = d_v = 2 \}$

**Theorem 1.** Let $P(n,m)$ be the linear parallelogram of benzenoid graph ( $\forall m,n \in \mathbb{N} \setminus \{ 1 \}$). Then:

- The First Zagreb index and its polynomial of $P(n,m)$ are equal to

$$Zg_1(P(n,m)) = 2(9mn - 4m - 4n - 3)$$

And

$$Zg_1(P(n,m), x) = (3mn - 2n + 3)x^6 + 4(m + n - 2)x^4 + 4x^4$$

- The Second Zagreb index and its polynomial of $P(n,m)$ are equal to

$$Zg_2(P(n,m)) = 27mn - 6m - 6n - 5$$

And

$$Zg_2(P(n,m), x) = (3mn - 2n + 3)x^9 + 4(m + n - 2)x^6 + 4x^4$$

**Proof.** Consider the linear parallelogram of benzenoid graph $P(n,m)$, $\forall m,n \in \mathbb{N} \setminus \{ 1 \}$. In generally consider the linear parallelogram benzenoid graph $P(n,m)$ depicted in Figure 1 and see [17-23]. This graph has $2mn + 2m + 2n$ vertices ($|V(P(n,m))| = (2n + 2)(m + 1) - 2$) and also from the structure $P(n,m)$ in figure 1, one can see that $|V_3| = m + n + 1 + m + n + 1 = 2(m + n + 1)$ and $|V_3| = 2mn$. 

Thus, $|E(P(n,m))| = \frac{1}{2}[2|V_3| + 3|V_3|]$

$$= \frac{1}{2}[2 \times 2(m + n + 1) + 3 \times 2(m \times n - 1)]$$

$$= (3n + 2)(m + 2n + 2m - 1) = 3mn + 2n + 2m + 1$$

From the structure $P(n,m)$ in figure 1, we see that there are only four edge belong to $E_4$ or $E_4 \star$ ($\{ uv \in E(P(n,m)) | d_u = d_v = 2 \}$), so

$|E_4| = |E_4 \star | = |uv \in E(P(n,m)) | d_u = d_v = 2| = 4$

and also

$|E_4 = |E_4 \star | = |uv \in E(P(n,m)) | d_u = 2 \& d_v = 3| = 2(m - 1) + 2(n - 1) + 2(m - 1) + 2(n - 1) = 4(m + n - 2)$

And $|E_4 \star | = |uv \in E(P(n,m)) | d_u = d_v = 3| = 3mn + 2n + 2m - 4(m + n - 2) = 3mn - 2n - 2m + 3$
Now, by according to definition of First Zagreb index, the Second Zagreb index, The First Zagreb Polynomial and the Second Zagreb Polynomial in above section, we have following computations for all \( m,n > 1 \).

\[
Z_{g1}(P(n,m),x) = \sum_{e \in E\{P(n,m)\}} x^{d_e + d_{\bar{e}}}
\]

\[
= \sum_{e \in E_1} x^6 + \sum_{e \in E_2} x^5 + \sum_{e \in E_3} x^4
\]

\[
= (3mn - 2n - 2m + 3)x^6 + 4(m + n - 2)x^5 + 4x^4
\]

Thus \( Z_{g1}(P(n,m)) = \sum_{e \in E\{P(n,m)\}} (d_e + d_{\bar{e}}) \)

\[
= (3mn - 2n - 2m + 3)x^6 + 4(m + n - 2)x^5 + 4x^4
\]

\[
= 18mn - 12n - 12m + 18 + 20m + 20n - 40 + 16
\]

\[
= 18mn - 8m - 8n - 6
\]

\[
Z_{g2}(P(n,m),x) = \sum_{e \in E\{P(n,m)\}} x^{d_e + d_{\bar{e}}}
\]

\[
= \sum_{e \in E_1} x^9 + \sum_{e \in E_2} x^6 + \sum_{e \in E_3} x^4
\]

\[
= (3mn - 2n - 2m + 3)x^9 + 4(m + n - 2)x^6 + 4x^4
\]

Henxe \( Z_{g2}(P(n,m)) = \sum_{e \in E\{P(n,m)\}} (d_e \times d_{\bar{e}}) \)

\[
= (3mn - 2n - 2m + 3)x^9 + 4(m + n - 2)x^6 + 4x^4
\]

\[
= 27mn - 18n - 18m + 27 + 24m + 24n - 48 + 16
\]

\[
= 27mn - 6m - 6n - 5
\]
3. CONCLUSION

In this paper, we focus on the topological indices: First Zagreb index, second Zagreb index and their polynomials of a molecular graph “linear parallelogram of benzenoid graph $P(n,m)$”, $\forall m, n \in \mathbb{N} - \{1\}$.

References