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The First Eccentric Zagreb Index of Linear Polycene Parallelogram of Benzenoid

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Abstract

Let $G = (V,E)$ be a graph, where $V(G)$ is a non-empty set of vertices and $E(G)$ is a set of edges, $e = uv \in E(G)$, $d(u)$ is degree of vertex u. Then the first Zagreb polynomial and the first Zagreb index $Zg_1(G,x)$ and $Zg_1(G)$ of the graph G are defined as $\sum_{uv\in E(G)} x^{(d_u+d_v)}$ and $\sum_{e=uv\in E(G)}(d_u+d_v)$ respectively. Recently *Ghorbani* and *Hosseinzadeh* introduced the first Eccentric Zagreb index as $Zg_1^*(G)=\sum_{uv\in E(G)}(ecc(v)+ecc(u))$, that $ecc(u)$ is the largest distance between u and any other vertex v of G. In this paper, we compute this new index (the first Eccentric Zagreb index or third Zagreb index) of an infinite family of linear Polycene parallelogram of benzenoid.

Keywords

Molecular Graph, Linear Polycene Parallelogram of Benzenoid, Zagreb Topological Index, Eccentricity Connectivity Index, Cut Method

1. Introduction

By a graph, we mean a finite, undirected, simple graph. We denote the vertex set and the edge set of a graph G by $V(G)$ and $E(G)$, respectively. And the number of first neighbors of vertex u in G (the degree of u) is denoted by $d(u)$. For notation and graph theory terminology not presented here, we follow [1]-[3]. All of the graphs in

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this paper are simple and a topological index of a graph is a number related to a graph which is invariant under graph automorphisms and is a numeric quantity from the structural graph of a molecule.

One of the best known and widely used is the Zagreb topological index Zg_1 introduced by *I. Gutman* and *N. Trinajstić* in 1972 as [1] [2]

$$Zg_1(G) = \sum_{e=uv\in E(G)} \left(d(u) + d(v)\right).$$

Also, we know another definition of the first Zagreb index as the sum of the squares of the degrees of all vertices of *G*.

$$Zg_1(G) = \sum_{v\in V(G)} d(v)^2$$

where d_u denotes the degree of *u*. Mathematical properties of the first Zagreb index for general graphs can be found in [4]-[8].

Let $x,y\in V(G)$, then the distance $d(x,y)$ between *x* and *y* is defined as the length of any shortest path in *G* connecting *x* and *y* [9]-[11].

In other words,

$$ecc(v) = \text{Max}\left\{d(u,v) \mid \forall u \in V(G)\right\}.$$

The radius and diameter of a graph *G* are defined as the minimum and maximum eccentricity among vertices of *G*, respectively. In other words,

$$D(G) = \text{Max}_{v\in V(G)} \left\{d(u,\ v) \mid \forall u \in V(G)\right\},$$

$$R(G) = \text{Min}_{v\in V(G)} \left\{\text{Max}\left\{d(u,\ v) \mid \forall u \in V(G)\right\}\right\}.$$

Recently in 2012, *M. Ghorbani* and *M. A. Hosseinzadeh* introduced a new version of first Zagreb index (the Eccentric version and $ecc(v)$ denotes the eccentricity of vertex *v*) as follows [12]:

$$Zg_1^*(G) = \sum_{e=uv\in E(G)} \left(ecc(v) + ecc(u)\right).$$

In this study, we call this eccentric version of the first Zagreb index by the *third Zagreb index* and denote by $Zg_3(G)\left(= Zg_1^*(G)\right)$. And in continue, a formula of the third Zagreb index for an infinite family of linear Polycene parallelogram of benzenoid by using the *Cut Method* is obtained.

2. Results and Discussion

In this sections, we compute the third Zagreb index $M_3(G)$ for linear Polycene parallelogram of benzenoid $P(n,n)$ ($\forall n \geq 1$). This family of benzenoid graph has $2n(n+2)$ vertices/atoms and $3n^2 + 4n - 1\left(=1/2\left[2(4n+2) + 3(2n^2 - 2)\right]\right)$ edges (bonds) [13]-[23]. The general representation of linear Polycene parallelogram of benzenoid $P(n,n)$ is shown in **Figure 1**.

Now, we can exhibit the closed formula of the third Zagreb index $M_3(H_k)$ in the following theorem.

Theorem 1. Considering the linear Polycene parallelogram of benzenoid $P(n,n)$ ($\forall n\in\mathbb{N}$), then its third Zagreb index is equal to

$$Zg_3\left(P(n,n)\right) = 16n^3 + 85n^2 - 75n + 6.$$

Proof. $\forall n\in\mathbb{N}$, let $P(n,n)$ be the linear Polycene parallelogram of benzenoid, as shown in **Figure 1**. To achieve our aims, we use of the Cut Method. Definition of the Cut Method and some of its properties are presented in [24]. Thus, we encourage readers to look at **Figure 1** and see all cuts of the linear Polycene parallelogram of benzenoid $P(n,n)$.

So according to **Figure 1**, one can see that the eccentric vertices with degree two are between $2n+1$, $2n+2$, $\cdots$, $4n-6$, $4n-4$, $4n-2$, $4n-1$ or the number set

$$\left\{4n-1, 4n-2i, 2n+1 \mid i \text{ be the I}^{\text{th}}\text{cut of } P(n,n)\right\}.$$

And also, the eccentric vertices with degree two are between $2n$, $2n+1$ to $4n-4$, $4n-3$ or in the number set

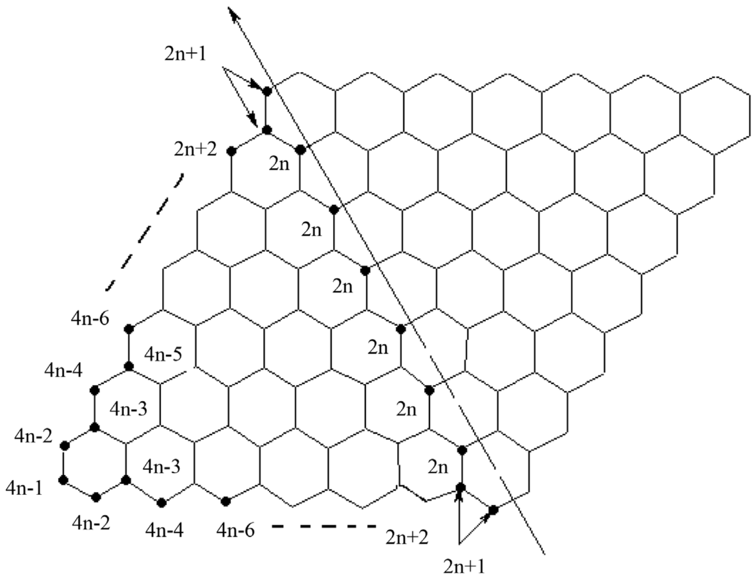

Figure 1. The eccentric of vertices of linear polycene parallelogram of benzenoid *P*(*n*,*n*) [14].

$\{(2n,2n),(2n+1,2n+2),\cdots,(4n-2i-2,4n-2i-1),(4n-4,4n-3) \mid i=2,n-1$ be the i^h cut of $P(n,n)\}$.

Therefore, by using above results and [14]-[23], we have the following computations for the third Zagreb index of the linear Polycene parallelogram of benzenoid *P*(*n*,*n*) as:

$$
\begin{aligned}
Zg_3(P(n,n)) &= \sum_{e=uv\in E(P(n,n))}(ecc(v)+ecc(u)) \\
&= \sum_{\substack{uv\in E(P(n,n))\\ u,v\in V_2}}(ecc(v)+ecc(u)) + \sum_{\substack{uv\in E(P(n,n))\\ u\in V_3\&v\in V_2}}(ecc(v)+ecc(u)) + \sum_{\substack{uv\in E(P(n,n))\\ u,v\in V_3}}(ecc(v)+ecc(u)) \\
&= 4\underbrace{\sum_{i=1}^{n-1}}_{u\in V_3\&v\in V_2}\left[(4n-2i+1)+(4n-2i)\right] + 4\underbrace{\sum_{i=1}^{n-1}}_{u\in V_3\&v\in V_2}\left[(4n-2i)+(4n-2i-1)\right] \\
&\quad + 4\underbrace{(2n+1+2n+1)}_{u,v\in V_2} + 4\underbrace{\sum_{i=1}^{n-1}}_{u,v\in V_3}(i-1)(4n-2i+1+4n-2i) + 4(n-1)\underbrace{(2n+1+2n)}_{u,v\in V_3} \\
&\quad + 2\left[\underbrace{\sum_{i=1}^{n-1}}_{u,v\in V_3}(i-1)(4n-2i+4n-2i-1)\right] + (n-1)(2n+2n) \\
&= \sum_{i=1}^{n-1}\left[4(8n-4i+1)+4(8n-4i-1)+4(i-1)(8n-4i+1)+2(i-1)(8n-4i-1)\right] \\
&\quad + \left[8(2n+1)+(16n^2-12n-4)+4n(n-1)\right] \\
&= \sum_{i=1}^{n-1}[8(8n-4i)\ -4(4i^2-i(8n+5)+1)\ -2(4i^2-i(8n+3)\ -1)+4(9n^2-2n+1) \\
&= \sum_{i=1}^{n-1}\left[-24i^2+i(48n-6)+(64n-2)\right]+4(9n^2-2n+1) \\
&= \left[-24\frac{n(n-1)(2n-1)}{6}+(48n-6)\frac{n(n-1)}{2}+(64n-2)(n-1)\right]+4(9n^2-2n+1) \\
&= (n-1)\left[-4n(2n-1)+(24n-3)\ n+(64n-2)\right]+4(9n^2-2n+1) \\
&= (n-1)\left[16n^2+65n-2\right]+4(9n^2-2n+1) = 16n^3+85n^2-75n+6.
\end{aligned}
$$

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