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Article

TWO TYPES OF CONNECTIVITY INDICES OF THE LINEAR PARALLELOGRAM BENZENOID

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ABSTRACT

A molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges. The degree of each vertex equals the valence of the corresponding atom. In this paper, we focus on the structure of an infinite family of the linear parallelogram benzenoid P(n,m) ($\forall m,n\in\mathbb{N}-\{1\}$) and compute two types of Connectivity indices of it.

Keywords: Molecular graph, Benzenoid graph, Randic Connectivity Index, Sum-Connectivity Index

1. INTRODUCTION

Let $G=(V;E)$ be a simple connected molecular graph with vertex set $V=V(G)$ and edge set $E=E(G)$. A molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges. The degree of each vertex equals the valence of the corresponding atom. A general reference for the notation in graph theory is [1].

In graph theory, we have many different topological index of arbitrary graph *G*. A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when chemist *Harold Wiener* developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin [2-7].

$$W(G)=\sum_{e=uv\in E(G)} d(u,v)$$

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The distance *d(u,v)* between the vertices *u* and *v* of the graph G is equal to the length of (number of edges in) the shortest path that connects *u* and *v*.

The first connectivity index introduced in 1975 by *M. Randic* [8-12] has shown this index to reflect molecular branching. The Randić connectivity index (Randić branching index) $\chi(G)$ is defined as

$$\chi(G)=\sum_{e=uv\in E(G)}\frac{1}{\sqrt{d_u d_v}}$$

where for any edge in the summation term, d_u and d_v stand for degrees of adjacent vertices joined by that edge.

In 2008, a closely related variant of Randić connectivity index called the Sum-connectivity index was introduced by *Zhou* and *Trinajstić* [13-14]. The Sum-connectivity index $X(G)$ is defined as

$$X(G)=\sum_{e=uv\in E(G)}\frac{1}{\sqrt{d_u+d_v}}$$

where d_u and d_v are the degrees of the vertices *u* and *v*, respectively.

In recent years, some researchers are interested to topological indices of benzenoid molecular graph. Throughout this paper *P(n,m)* denotes of an infinite class of the linear parallelogram *P(n,m)* of benzenoid graph in terms of the number of hexagons (benzene C_6) in the first row *n* and the number of hexagons in the first column *m*, see [15-21] and Figure 1 for details.

2. Main Results

In this section, we focus on the structure of an infinite family of the linear parallelogram benzenoid graph P(n,m) ($\forall m,n\in\mathbb{N}-\{1\}$) , Figure 1 and compute its connectivity indices.

Theorem 1. $\forall m,n\in\mathbb{N}-\{1\}$, consider the linear parallelogram benzenoid graph P(n,m). Then the Randic Connectivity index $\chi(P(n,m))$ and the Sum-Connectivity index $X(P(n,m))$ are equal to

$$\chi(P(n,m))=mn+\frac{2}{3}(\sqrt{6}-1)(m+n)+3$$

and

$$X(P(n,m))=\frac{1}{2}\sqrt{6}\,mn+\left(\frac{12\sqrt{5}-5\sqrt{6}}{15}\right)(m+n)+\frac{5\sqrt{6}-16\sqrt{5}}{10}+2$$

To achieve our aims we need to the following definition.

Definition 1. Let G be the molecular graph and d_v is degree of vertex $v\in V(G)$. We divide edge set *E(G)* and vertex set *V(G)* of graph G to several partitions, as follow:

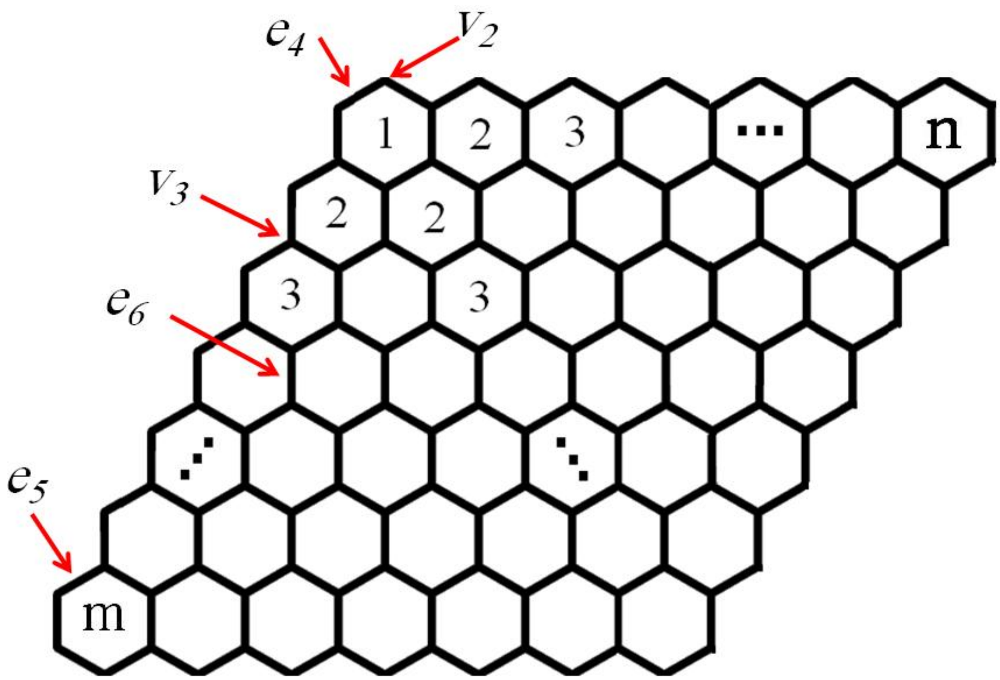
$\forall k$: $\delta\le k\le\Delta$, $V_k=\{v\in V(G)|\ d_v=k\}$

$\forall i$: $2\delta\le i\le 2\Delta$, $E_i=\{e=uv\in E(G)|d_u+d_v=i\}$

$\forall j$: $\delta^2\le j\le\Delta^2$, $E_j{}^*=\{uv\in E(G)|d_u\times d_v=j\}$.

where δ and Δ are the minimum and maximum, respectively, of d_v for all $v\in V(G)$, obviously $1\leq\delta\leq d_v\leq\Delta\leq n-1$.

Figure 1: A 2-D graph of of linear polycene parallelogram benzenoid graph *P(a,b)* [18]



Proof. Let G be the linear parallelogram P(n,m), with |V(P(n,m))|=2mn+2m+2n vertices and |E(P(n,m))|=3mn+2n+2m-1 edges ($\forall m,n\in\mathbb{N}-\{1\}$) depicted in Figure 1 and references [15-21].

From the structure of the linear parallelogram benzenoid graph *P(n,m)*, one can see that there are two partitions V_2 and V_3 with their size as follow:

$V_2=\{v\in V(P(n,m))|\ d_v=2\} \rightarrow |V_2|=2(m+n+1)$

$V_3=\{v\in V(P(n,m))|\ d_v=3\} \rightarrow |V_3|=2mn-2$

By according to Definition 1,

$E_4=\{e=uv\in E(P(n,m))|\ d_u=d_v=2\} \rightarrow |E_4|=|E_4^*|=4$

$E_5=\{e=uv\in E(P(n,m))|\ d_u=3\ \&d_v=2\} \rightarrow |E_5|=|E_6^*|=2|E_4|=4(m+n-2)$

$E_6=\{e=uv\in E(P(n,m))|\ d_u=d_v=3\} \rightarrow |E_6|=|E_9^*|=3mn-2n-2m+3$

Thus, we have following computations for the Randic Connectivity and Sum-Connectivity indices of the linear parallelogram benzenoid graph *P(n,m)* as follows:

$$\chi(P(n,m)) = \sum_{uv\in E(P(n,m))} \left(d_v d_v\right)^{\left(-\frac{1}{2}\right)}$$

$$= \sum_{uv\in E_9^*} \frac{1}{\sqrt{d_v d_v}} + \sum_{uv\in E_6^*} \frac{1}{\sqrt{d_v d_v}} + \sum_{uv\in E_4^*} \frac{1}{\sqrt{d_v d_v}}$$

$$=\frac{|E_9^*|}{\sqrt{9}}+\frac{|E_6^*|}{\sqrt{6}}+\frac{|E_4^*|}{\sqrt{4}}$$

$$=\frac{1}{3}\times(3mn-2n-2m+3)+\frac{\sqrt{6}}{6}\times 4\left(m+n-2\right)+\frac{1}{2}\times 4$$

$$=mn+\frac{2}{3}(\sqrt{6}-1)\left(m+n\right)+3$$

and

$$X(P(n,m))=\sum_{uv\in E(P(n,m))}\left(d_v+d_v\right)^{\left(-1/2\right)}$$

$$=\sum_{uv\in E_4}\frac{1}{\sqrt{d_v+d_v}}+\sum_{uv\in E_5}\frac{1}{\sqrt{d_v+d_v}}+\sum_{uv\in E_6}\frac{1}{\sqrt{d_v+d_v}}$$

$$=\frac{|E_4|}{\sqrt{4}}+\frac{|E_5|}{\sqrt{5}}+\frac{|E_6|}{\sqrt{6}}$$

$$=\frac{1}{2}\times 4+\frac{\sqrt{5}}{5}\times 4\left(m+n-2\right)+\frac{\sqrt{6}}{6}\times(3mn-2n-2m+3)$$

$$=\frac{1}{2}\sqrt{6}\,mn+\left(\frac{12\sqrt{5}-5\sqrt{6}}{15}\right)\left(m+n\right)+\frac{5\sqrt{6}-16\sqrt{5}}{10}+2$$

Here, we complete the proof of the Theorem 1.

4. CONCLUSION

The main goal of chemistry and technology of benzenoid graph is synthesis of molecules having defined properties. The use of topological and connectivity indices as structural descriptors is important in molecular graph and Nano-structure. In this paper, we compute two types of Connectivity indices of an infinite family of the linear parallelogram benzenoid.

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