On Connectivity Indices of an Infinite Family of The Linear Parallelogram of Benzenoid Graph

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Keywords: Molecular graph, Connectivity Indices, Molecular Graph, Benzenoid Graph.

ABSTRACT. A topological index of a graph G is a numeric quantity related to G which is describe molecular graph G . In this paper the Atom Bond Connectivity (ABC) and Geometric-Arithmetic (GA) indices of an infinite class of the linear parallelogram of benzenoid graph.

1. INTRODUCTION

Mathematical chemistry is a branch of theoretical chemistry using mathematical methods to discuss and predict molecular properties without necessarily referring to quantum mechanics [1–5]. Molecular descriptors play significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. A topological index of a graph G is a numeric quantity related to G which is describe molecular graph G

One of the best known and widely used is the connectivity index χ introduced in 1975 by *Milan Randić* [6]. *Estrada et al.* proposed a new index, known as the atom-bond connectivity index (ABC). This index is defined as [7,8]

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_v + d_u - 2}{d_v \times d_u}}$$

where the summation goes over all edges of G , d_u and d_v are the degrees of the terminal vertices u and v of edge $e=uv$ and $E(G)$ is the edge set of G with cardinality $|E(G)|$.

Another topological indices namely, Geometric-Arithmetic index ($GA(G)$) introduced by *D.Vukicevic* and *B.Furtula* [9-13], respectively and was defined as follows:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_v d_u}}{d_v + d_u}$$

2. MAIN RESULTS AND DISCUSSION

Consider the molecular graph linear parallelogram of benzenoid graph $P(n,m)$, $\forall m,n \in \mathbb{N}-\{1\}$. In generally consider the linear parallelogram benzenoid graph $P(n,m)$ depicted in Figure 1 and see [14-22].

In this section, we compute the Atom Bond Connectivity (ABC) and Geometric-Arithmetic (GA) indices of an infinite family of the linear parallelogram of benzenoid graph $P(n,m)$.

Theorem 1. Consider the linear parallel ogramof benzenoid graph $P(n,m)$ ($\forall m,n \in \mathbb{N}-\{1\}$). Then the Atom Bond Connectivity index $ABC(P(n,m))$ is equal to:

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

Proof of Theorem 1. Let $P(n,m)$ be the linear parallelogram of benzenoid graph ($\forall m,n \in \mathbb{N}-\{1\}$) depicted in Figure 1. This benzenoid graph has exactly $2mn + 2m + 2n$ vertices/atoms and

$3mn+2n+2m-1$ edges/bonds. From structure of the linear parallelogram of benzenoid graph, one can see that all vertices of $P(n,m)$ have degree two or three. So we can divide its vertex and edge sets $V(P(n,m))$ and $E(P(n,m))$ of G to following partitions as:

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

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

$$E_4 = E_4^* = \{uv \in E(G) \mid d_u = d_v = 2\},$$

$$E_5 = E_6^* = \{uv \in E(G) \mid d_u = 2 \text{ \& } d_v = 3\},$$

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

From Figure 1 and [21], it is easy to see that

$$|V_2| = m+n+1+m+n+1 = 2(m+n+1) \text{ and } |V_3| = 2mn-2.$$

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

$$|E_5| = |E_6^*| = |\{uv \in E(P(n,m)) \mid d_u = 2 \text{ \& } d_v = 3\}| = 2(m-1) + 2(n-1) + 2(m-1) + 2(n-1) = 4(m+n-2).$$

$$|E_6| = |E_9^*| = |\{uv \in E(P(n,m)) \mid d_u = d_v = 3\}| = 3mn + 2n + 2m - 1 - 4(m+n-2) - 4 = 3mn - 2n - 2m + 3.$$

Fig. 1. The linear parallelogram of benzenoid graph $P(n,m)$, $\forall m,n \in \mathbb{N}$. [21]

Now by using above results, we start to compute the Atom Bond Connectivity index for the linear parallelogram of benzenoid graph as:

$$\begin{aligned} ABC(P(n,m)) &= \sum_{uv \in E(P(n,m))} \frac{\sqrt{d_v + d_u - 2}}{\sqrt{d_v \times d_u}} \\ &= \sum_{uv \in E_9^*} \frac{\sqrt{d_v + d_u - 2}}{\sqrt{d_v \times d_u}} + \sum_{uv \in E_6^*} \frac{\sqrt{d_v + d_u - 2}}{\sqrt{d_v \times d_u}} + \sum_{uv \in E_4^*} \frac{\sqrt{d_v + d_u - 2}}{\sqrt{d_v \times d_u}} \end{aligned}$$

$$\begin{aligned}
&= \sum_{uv \in E_9^*} \frac{\sqrt{3+3-2}}{\sqrt{3 \times 3}} + \sum_{uv \in E_6^*} \frac{\sqrt{3+2-2}}{\sqrt{3 \times 2}} + \sum_{uv \in E_4^*} \frac{\sqrt{2+2-2}}{\sqrt{2 \times 2}} \\
&= \frac{2}{3}|E_9^*| + \frac{\sqrt{2}}{2}|E_6^*| + \frac{\sqrt{2}}{2}|E_4^*| \\
&= \frac{2}{3} \times (3mn - 2n - 2m + 3) + \frac{\sqrt{2}}{2} \times [4(m+n-2) + 4] \\
&= 2mn - 2(\frac{2}{3} - \sqrt{2})m - 2(\frac{2}{3} - \sqrt{2})n + 2(1 - \sqrt{2}) \\
&= 2mn - 2(\frac{2}{3} - \sqrt{2})(m+n) + 2(1 - \sqrt{2}). \blacksquare
\end{aligned}$$

Theorem 2. $\forall m, n \in \mathbb{N} - \{1\}$, let $P(n, m)$ be the linear parallelogram of benzenoid graph. Then the Geometric-Arithmetic index $GA(P(n, m))$ is equal to

$$GA(P(n, m)) = 3mn + 2\left(\frac{2\sqrt{6}}{5} - 1\right)(m+n) + \left(7 - \frac{16\sqrt{6}}{5}\right)$$

Proof of Theorem 2. $\forall m, n \in \mathbb{N} - \{1\}$, Consider the linear parallelogram of benzenoid graph $P(n, m)$. By using above mention proof, we can compute the Geometric-Arithmetic index of $P(n, m)$ easily as follows:

$$\begin{aligned}
GA(P(n, m)) &= \sum_{uv \in E(P(n, m))} \frac{2\sqrt{d_v d_u}}{d_v + d_u} \\
&= \sum_{uv \in E_9^*} \frac{2\sqrt{3 \times 3}}{3+3} + \sum_{uv \in E_6^*} \frac{2\sqrt{3 \times 2}}{3+2} + \sum_{uv \in E_4^*} \frac{2\sqrt{2 \times 2}}{2+2} \\
&= |E_9^*| + \frac{2\sqrt{6}}{5}|E_6^*| + |E_4^*| \\
&= (3mn - 2n - 2m + 3) + \frac{2\sqrt{6}}{5} \times 4(m+n-2) + (4) \\
&= 3mn + 2\left(\frac{2\sqrt{6}}{5} - 1\right)m + 2\left(\frac{2\sqrt{6}}{5} - 1\right)n + \left(7 - \frac{16\sqrt{6}}{5}\right) \\
&= 3mn + 2\left(\frac{2\sqrt{6}}{5} - 1\right)(m+n) + \left(7 - \frac{16\sqrt{6}}{5}\right). \blacksquare
\end{aligned}$$

3. CONCLUSION

A topological index of a graph G is a numeric quantity related to G which is describe molecular graph G . In this paper the Atom Bond Connectivity (ABC) and Geometric-Arithmetic (GA) indices of an infinite class of the linear parallelogram of benzenoid graph.

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