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

Mohammad Reza Farahani

Department of Applied Mathematics, Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran

E-mail address: Mr_Farahani@mathdep.iust.ac.ir, MrFarahani88@gmail.com

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]

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

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 \(P(n,m)\), \(\forall m,n \in \mathbb{N}\setminus\{1\}\). 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 parallelogram of benzenoid graph \(P(n,m)\) (\(\forall m,n \in \mathbb{N}\setminus\{1\}\)). Then the Atom Bond Connectivity index ABC\((P(n,m))\) is equal to:

\[ ABC(P(n,m)) = 2mn - 2(\sqrt{2} - 1)(m+n) + 2(1 - \sqrt{2}) \]

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

$$V_3 = \{v \in V(G) | d_v = 3\},$$
$$V_2 = \{v \in V(G) | d_v = 2\}$$

$$E_4 = E_4^* = \{uv \in E(G) | d_u = d_v = 2\},$$
$$E_5 = E_6^* = \{uv \in E(G) | d_u = 2 \& d_v = 3\},$$
$$E_6 = E_9^* = \{uv \in E(G) | d_u = d_v = 3\}$$

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

$$|V_2| = m + n + l + m + n + l = 2(m + n + l)$$ and $|V_3| = 2mn - 2$.

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

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

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

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

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

$$\text{ABC}(P(n, m)) = \sum_{uv \in E(\mathcal{P}(n, n))} \frac{\sqrt{d_u + d_v - 2}}{\sqrt{d_u \times d_v}}$$

$$= \sum_{u \in d_u^2} \frac{\sqrt{d_u + d_v - 2}}{\sqrt{d_u \times d_v}} + \sum_{v \in d_v^2} \frac{\sqrt{d_u + d_v - 2}}{\sqrt{d_u \times d_v}} + \sum_{uv \in d_u^2} \frac{\sqrt{d_u + d_v - 2}}{\sqrt{d_u \times d_v}}.$$
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:

\[
GA(P(n,m)) = \sum_{uv \in E_1} \frac{2\sqrt{d_u d_v}}{d_u + d_v}
\]

\[
= \sum_{uv \in E_1} \frac{2\sqrt{3 \times 3}}{3 + 3} + \sum_{uv \in E_1} \frac{2\sqrt{3 \times 2}}{3 + 2} + \sum_{uv \in E_1} \frac{2\sqrt{2 \times 2}}{2 + 2}
\]

\[
= |E_9^*| + \frac{2\sqrt{6}}{5} |E_6^*| + |E_4^*|
\]

\[
= (3mn - 2n - 2m + 3) + \frac{2\sqrt{6}}{5} \times 4(m+n-2) + (4)
\]

\[
= 3mn + 2\left(\frac{2\sqrt{6}}{5} - 1\right)m + 2\left(\frac{2\sqrt{6}}{5} - 1\right)n + \left(7 - \frac{16\sqrt{6}}{5}\right)
\]

\[
= 3mn + 2\left(\frac{2\sqrt{6}}{5} - 1\right)(m+n) + \left(7 - \frac{16\sqrt{6}}{5}\right).
\]

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.

References


