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ABOUT THE CERTAIN TOPOLOGICAL INDICES OF THE LINE GRAPH OF V-PANTACENIC NANOTUBE

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ABSTRACT: A topological index is a numeric quantity associated with a graph which characterizes the topology of the graph and is invariant under graph automorphism. Topological indices such Randić, atom-bond connectivity (ABC) and geometric (GA) indices are used to predict the bioactivity of different chemical compounds. Recently, the edge version of atom-bond connectivity and geometric arithmetic indices of graph G are introduced based on the degree of an edge of line graph of G . In this paper, the closed formulas of edge version of atom-bond connectivity and geometric-arithmetic indices for V- Pantacenic nanotube are computed.

INTRODUCTION: A graph is a collection of points and lines connecting them. The points and lines of a graph are also called vertices and edges respectively. If e is an edge of G , connecting the vertices u and v , then we write $e = uv$ and say “ u and v are adjacent”. A connected graph such that, there is a path between all pairs of vertices. The distance $d(u,v)$ between two vertices u and v is the length of the shortest path between u and v in G . A simple graph is an un-weighted, undirected graph without loops and multiple edges.

A single number that can be used to characterize some property of the graph is called a topological index for the graph. Obviously, the number of vertices and the number of edges are topological indices. The Wiener index was the first graph invariant reported (distance based) topological index and is defined as a half sum of the distances between all the pairs of vertices in a graph¹.

Also, the edge version of Wiener index based on distance between edges was introduced by Iranmanesh *et al.*,². The degree of a vertex v is the number of vertices joining to v . Also, the degree of an edge $e=uv \in E(G)$ is the number of its adjacent vertices in $V(L(G))$, where the line graph $L(G)$ of a graph G is defined to be the graph whose vertices are the edges of G , with two vertices being adjacent if the corresponding edges share a vertex in G .

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Estrade et al.,³ proposed a topological index named the atom-bond connectivity index (shortly ABC as

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

where d_u (or d_v) denotes the degree the vertex u (or v). the reader can find some information on atom-bond connectivity index in⁴⁻¹⁰. In¹¹, Farahani introduced the edge version of atom-bond connectivity index based on the end vertex degree d_e and d_f of edges e and f in a line graph of G as follows:

$$ABC_e(G) = \sum_{ef \in E(L(G))} \sqrt{\frac{d_e + d_f - 2}{d_e \times d_f}}$$

where $d_e(L(G)) = d_e$ denotes the degree of the edge e in G (see also¹²).

One of the most important topological indices is well-known branching index introduced by Randić¹³ which is defined as the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

Motivated by the definition of Randić connectivity index based on the end-vertex degrees of edges in a graph connected G with the vertex set $V(G)$ and the edge set $E(G)$ ^{14, 15}, Vukicevic and Furtula¹⁶ proposed a topological index named the geometric-arithmetic index (shortly GA) as

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

where $d_u(G) = d_e$ denotes the degree of the vertex u in G . The reader can find more information's on geometric-arithmetic index in¹⁶⁻¹⁹.

In¹⁹, the edge version of geometric arithmetic index was introduced based on end-vertex degrees of edges in a line graph of G which is a graph such that each vertex of $L(G)$ represents an edge of G ; and two vertices of $L(G)$ are adjacent if and only if their corresponding edges share a common endpoint in G , as follows

$$GA_e(G) = \sum_{ef \in E(L(G))} \frac{2\sqrt{d_e \times d_f}}{d_e + d_f}$$

where $d_e(L(G)) = d_e$ denotes the degree of the edge e in G .

The topological indices of H-Pantacenic nanotubes were studied recently in²⁰⁻²⁴. With the same motivation, the aim of this note is to compute a closed formula for the ABC_e and GA_e indices of V-Pantacenic nanotube.

Topological Indices of the Line Graph of V-Pantacenic Nanotube: The V-Pantacenic nanotube $F[2,5]$ and its line graph are shown in **Fig. 1** and **2** respectively.

Theorem 1: Let $G = F [p,q]$ be a graph of V-Pantacenic nanotube with $22pq$ vertices and $33pq - 5p$ edges. Then

- (1) $ABC_e(G) = \frac{33}{2}\sqrt{6}pq + p\left(12 + \frac{10}{3}\sqrt{15} - \frac{29}{2}\sqrt{6}\right)$
- (2) $GA_e(G) = 66pq + p\left(\frac{80}{7}\sqrt{3} - 40\right)$

Proof: In $L(G)$, there are $33pq - 5p$ vertices. It is easily seen from **Fig. 2** and Lemma 1 that $|V_3(L(G))| = 20p$ and $|V_4(L(G))| = 33pq - 25p$. By using Lemma 2, we get $|E(L(G))| = 66pq - 20p$.

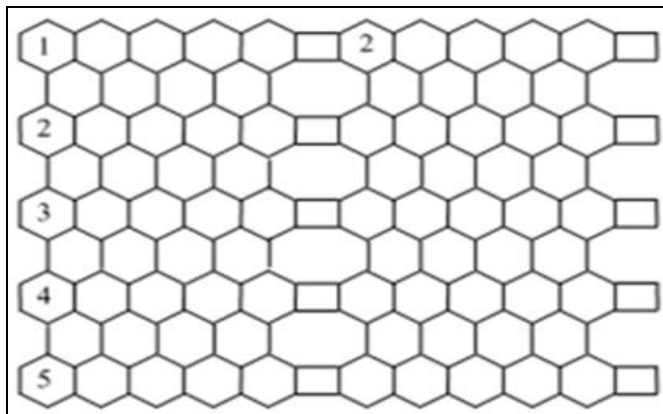


FIG. 1: THE V-PANTACENIC NANOTUBE $F [2, 5]$

The edge set $E(L(G))$ divides into three edge partitions based on degrees of the end vertices, i.e. $E(L(G)) = E_1(L(G)) \cup E_2(L(G)) \cup E_3(L(G))$. The edge partition $E_1(L(G))$ contains $18p$ edges uv , where $d_u = d_v = 3$, the edge partition $E_2(L(G))$ contains $20p$ edges uv , where $d_u = 3$ and $d_v = 4$ and the edge partition $E_3(L(G))$ contains $66pq - 58p$ edges uv , where $d_u = d_v = 4$.

$$ABC_e(G) = \sum_{ef \in E(L(G))} \sqrt{\frac{d_e + d_f - 2}{d_e \times d_f}}$$

Then:

$$ABC_e(G) = 18p\sqrt{\frac{3+3-2}{3 \times 3}} + 20p\sqrt{\frac{3+4-2}{3 \times 4}} + (66pq - 58p)\sqrt{\frac{4+4-2}{4 \times 4}}$$

After simplification we get,

$$ABC_e(G) = \frac{33}{2}\sqrt{6}pq + p\left(12 + \frac{10}{3}\sqrt{15} - \frac{29}{2}\sqrt{6}\right)$$

Similarly one can find the expression of $GA_e(G)$.

$$GA_e(G) = 66pq + p\left(\frac{80}{7}\sqrt{3} - 40\right).$$

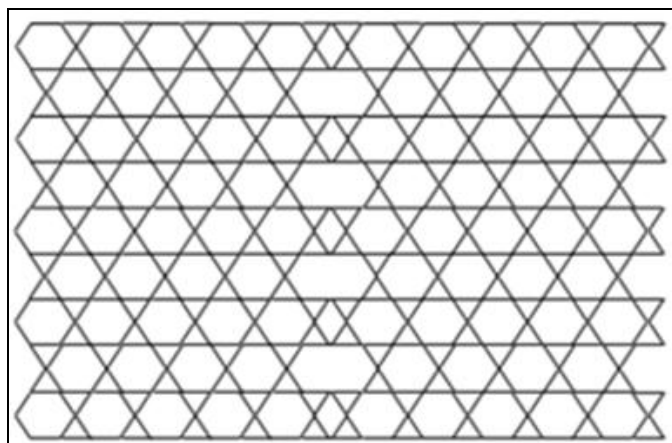


FIG. 2: THE LINE GRAPH OF V-PANTACENIC NANOTUBE F [2, 5]

TABLE 1: UNIT DISTANCE FROM END VERTICES OF EACH EDGE

$(S_u, S_v); uv \in E(G_L)$	Number of Edges
(10,10)	14p
(10,11)	4p
(10,14)	16p
(11,14)	4p
(11,15)	4p
(14,15)	4p
(14,16)	16p
(15,16)	8p
(16,16)	66pq-90p

Theorem 2: Let $GL=L(F[p, q])$ be a line graph of V-Pentacenic nanotube. Then:

$$(1) ABC_4(G_L) = \frac{33}{8}\sqrt{30}pq + p\left(\frac{41}{5}\sqrt{2} + \frac{2}{55}\sqrt{2090} + \frac{2}{77}\sqrt{3542} + \frac{8}{35}\sqrt{770} + \frac{8}{55}\sqrt{110} + \frac{6}{35}\sqrt{70} + \frac{2}{15}\sqrt{435} - \frac{45}{8}\sqrt{30}\right)$$

$$(2) GA_5(G_L) = 66pq + p\left(-76 + \frac{8}{21}\sqrt{110} + \frac{8}{25}\sqrt{154} + \frac{8}{3}\sqrt{35} + \frac{4}{13}\sqrt{165} + \frac{8}{29}\sqrt{210} + \frac{64}{15}\sqrt{14} + \frac{64}{31}\sqrt{15}\right)$$

Proof: The edge partition of $GL=L(F[p, q])$ based on the degree sum of vertices lying at the unit distance from end vertices of each edge is given in **Table 1**.

Since;

$$ABC_4(G_L) = \sum_{uv \in E(G_L)} \sqrt{\frac{S_u + S_v - 2}{S_u \times S_v}}$$

Then after doing some calculations by using **Table 1**, we get

$$ABC_4(G_L) = \frac{33}{8}\sqrt{30}pq + p\left(\frac{41}{5}\sqrt{2} + \frac{2}{55}\sqrt{2090} + \frac{2}{77}\sqrt{3542} + \frac{8}{35}\sqrt{770} + \frac{8}{55}\sqrt{110} + \frac{6}{35}\sqrt{70} + \frac{2}{15}\sqrt{435} - \frac{45}{8}\sqrt{30}\right)$$

Similarly we can find the expression of $GA_5(G_L)$ by using **Table 1**.

$$GA_5(G_L) = 66pq + p\left(-76 + \frac{8}{21}\sqrt{110} + \frac{8}{25}\sqrt{154} + \frac{8}{3}\sqrt{35} + \frac{4}{13}\sqrt{165} + \frac{8}{29}\sqrt{210} + \frac{64}{15}\sqrt{14} + \frac{64}{31}\sqrt{15}\right)$$

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