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COMPUTING GA_5 INDEX OF ARMCHAIR POLYHEX NANOTUBE

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The fifth geometric-arithmetic index of a graph G is defined to be $GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u+S_v}$, where S_v is the sum of the degrees of all neighbors of the vertex v in G. This index was introduced by *A. Graovac et al* in 2011. In this paper, we give explicit formulas for the fifth geometric-arithmetic index of a family of Hexagonal Nanotubes namely: *Armchair Polyhex Nanotubes*.

1. Introduction

Let G be a simple connected graph. The vertex set and the edge set of G are denoted by $V(G)$ and $E(G)$, respectively. In chemical graphs, the vertices correspond to the atoms of the molecule and the edges represent the chemical bonds. There exist many topological indices in mathematical chemistry.

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graphs [12, 16, 17]. In other words, computing topological indices of molecular graphs from chemical graph theory is a branch of mathematical chemistry. A topological index is a numeric quantity

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from the structural graph of a molecule and is invariant on the automorphism group of the graph.

One of the most famous and oldest topological indices of an arbitrary graph G is *Wiener Index* $W(G)$. Wiener index is defined as the sum of distances between any two atoms in the molecules, in terms of bonds (or edges). This index introduced by chemist *Harold Wiener* in 1947 [6, 13, 15, 19, 20] denoted by $W(G)$:

$$W(G) = \sum_{\{u,v\}\subset V(G)} d(u,v) \tag{1}$$

where the distance $d(u,v)$ between two vertices u and v is the number of edges in a shortest path connecting them.

We denote uv the edge which joins the vertices u and v. A connected graph is a graph such that there is a path between all pairs of vertices. The first connectivity index was introduced in 1975 by *Milan Randić* [14], who has shown this index to reflect molecular branching. The *Randić Connectivity Index* was defined as follows

$$^{1}\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} \tag{2}$$

where for every edge $uv \in E(G)$, d_u and d_v are the degrees of the vertices u and v, respectively.

The first *Geometric-Arithmetic* connectivity index (or simply *Geometric-Arithmetic Index* GA_1) of a connected graph G was introduced by *D. Vukićević* and *B. Furtula* in 2009 [18] as

$$GA_1(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{3}$$

Let $S_v = \sum_{uv\in E(G)} d_u$ be the summation of degrees of all neighbors of a vertex v of a connected graph G. The *fifth geometric-arithmetic index* was considered by *A. Graovac et al* in 2011 [10, 11] and is defined as

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \tag{4}$$

During the past several decades, there are many papers dealing with the connectivity index and some topological indices of the armchair polyhex Nanotube $TUAC_6$ (Figure 1) are computed.

In this paper, we give an explicit formula of the fifth geometric-arithmetic index (GA_5) of molecular graphs related to armchair polyhex Nanotube $TUAC_6$. For further information and more details, the reader may consult [1-5, 7-10] and all notations in this paper are standard and mainly taken from [14-16].

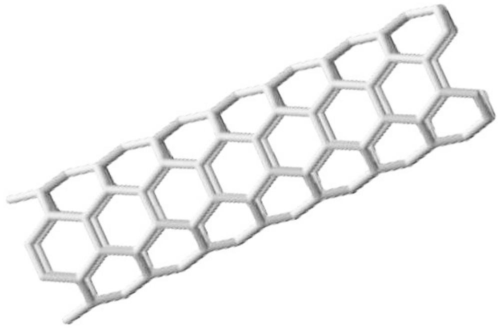

Figure 1: The 3-Dimensional Lattice (or cylinder) of the Armchair polyhex Nanotube $TUAC_6[8,7]$.

2. Main Result

Let $TUAC_6[m,n]$ denote a class of the armchair polyhex Nanotubes where m and n are the numbers of hexagons in the first row and in the first column of the corresponding 2D-lattice; see for example Figure 1 and Figure 2. For Figures 1 and 2, one can see that m must be even for all integer number n. In the following, we shall compute the fifth geometric-arithmetic index GA_5 for the armchair nanotube $TUAC_6[m,n]$ as shown in Figure 2.

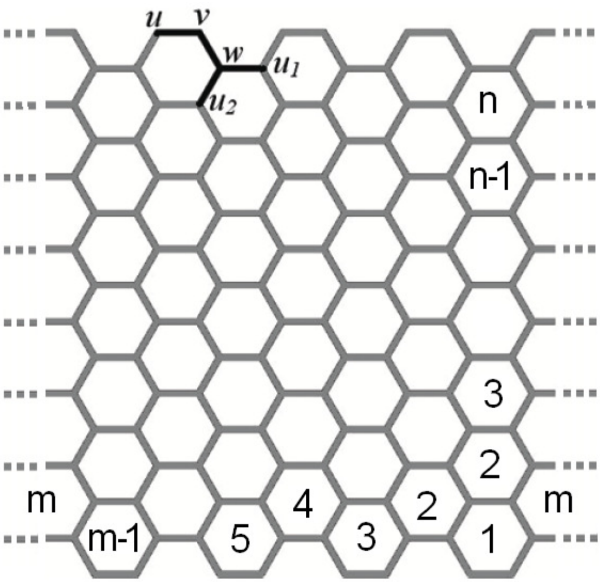

Figure 2: The 2D Lattice of the armchair polyhex Nanotube $TUAC_6[m,n]$.

Theorem 2.1. *Let G be the armchair polyhex Nanotube $TUAC_6[m,n]$. Then $\forall n \in \mathbb{N}$ and even $m \geq 4$ the fifth geometric-arithmetic index GA_5 of G is equal to:*

$$GA_5(TUAC_6[m,n]) = \left(3n + \frac{8\sqrt{10}}{13} + \frac{24\sqrt{2}}{17} - 2\right)m \quad (5)$$

Proof. Let m and n denote the number of hexagons in the first row/column of the 2D-lattice of the armchair polyhex Nanotube $G = TUAC_6[m,n]$ ($m,n \in \mathbb{N}$ & $m \geq 4$ be even), respectively as shown in Figure 2. From Figure 2, one can see that the number of vertices and edges in this nanotube are equal to $2m(n+1)$ $(= |V(G)|)$ and $3mn + 2m$ $(= |E(G)|)$.

From Figure 2, it's easy to see that all the vertices in the armchair polyhex Nanotube G have degree 2 or 3, thus we divide $V(G)$ into the parts

$$V_2 = \{u \in V(G) | d_u = 2\} \quad \text{and} \quad V_3 = \{w \in V(G) | d_w = 3\}$$

such that the size of V_2 is equal to $2 \times 2(\frac{m}{2})$ and therefore $|V_3| = 2mn$.
Next, we divide $E(TUAC_6[m,n])$ in three parts

$$E_6 = \{u_i, w_j \in V(TUAC_6[m,n]) \mid d_{u_i} = d_{w_j} = 3\}$$

$$E_5 = \{w, v \in V(TUAC_6[m,n]) \mid d_w = 3 \ \&\ d_v = 2\}$$

and

$$E_4 = \{u, v \in V(TUAC_6[m,n]) \mid d_u = d_v = 2\}$$

with size

$$|E_4| = 2 \times (\tfrac{m}{2}), \quad |E_5| = 2 \times |E_4| = 2m$$

and

$$|E_6| = |E(TUAC_6[m,n])| - |E_4| - |E_5| = 3mn - m.$$

Now, using Figure 2, one can see that for a member v of V_2, the summation S_v is equal to 5, since its adjacent vertices have degree 2 and 3. Also, for every vertex w adjacent to a vertex of V_2 (see vw in Figure 2), the summation S_w is equal to $2 \times 3 + 2$, since two adjacent vertices of w have degree 3 ($d_{u_1} = d_{u_2} = 3$) and $d_v = 2$. The summation of degrees of all neighbors of other vertices is equal to $3 \times 3 = 9$.
By the above mentions for S_v of an arbitrary vertex v, we obtain fifth geometric-arithmetic index of the armchair polyhex nanotube $G = TUAC_6[m,n]$ as follows:

$$GA_5(TUAC_6[m,n]) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}$$

$$= \sum_{u_2v_2 \in E_4} \frac{2\sqrt{S_{u_2} S_{v_2}}}{S_{u_2} + S_{v_2}} + \sum_{u_2v_3 \in E_5} \frac{2\sqrt{S_{u_2} S_{v_3}}}{S_{u_2} + S_{v_3}} + \sum_{u_3v_3 \in E_6} \frac{2\sqrt{S_{u_3} S_{v_3}}}{S_{u_3} + S_{v_3}} =$$

$$
\begin{aligned}
&= 2(\frac{m}{2})\frac{2\sqrt{5\times 5}}{5+5} + 2(m)\frac{2\sqrt{5\times 8}}{5+8} + 2(\frac{m}{2})\frac{2\sqrt{8\times 8}}{8+8} \\
&\quad + 2(m)\frac{2\sqrt{8\times 9}}{8+9} + (3mn-4m)\frac{2\sqrt{9\times 9}}{9+9} \\
&= m + \frac{8\sqrt{10}}{13}m + m + \frac{24\sqrt{2}}{17}m + 3mn - 4m \\
&= \left(3n + \frac{8\sqrt{10}}{13} + \frac{24\sqrt{2}}{17} - 2\right)m. \qquad (6)
\end{aligned}
$$

and this result completes the proof. □

Of course, we can consider $GA_5(TUAC_6[m,n]) \simeq (3n+1.9426)m$. The reader can find some values of the fifth geometric-arithmetic index of the armchair polyhex nanotube $G[m,n] = TUAC_6[m,n]$ for $m = 2,4,\ldots,10$, 100, 1000, 10000, 100000 and $n = 1,2,\ldots,10$, 100, 1000, 10000, 100000 as follows:

$GA_4(G[2,1]) = 9.8851076311611$ $GA_4(G[2,2]) = 15.8851076311611$
$GA_4(G[2,3]) = 19.8851076311611$ $GA_4(G[2,4]) = 27.8851076311611$
$GA_4(G[2,5]) = 33.8851076311611$ $GA_4(G[2,6]) = 39.885107631161$
$GA_4(G[2,7]) = 45.885107631161$ $GA_4(G[2,8]) = 51.885107631161$
$GA_4(G[2,9]) = 57.885107631161$ $GA_4(G[2,10]) = 63.885107631161$

$GA_4(G[3,1]) = 14.8276614467417$ $GA_4(G[3,2]) = 23.8276614467417$
$GA_4(G[3,3]) = 32.8276614467417$ $GA_4(G[3,4]) = 41.827661446742$
$GA_4(G[3,5]) = 50.827661446742$ $GA_4(G[3,6]) = 59.827661446742$
$GA_4(G[3,7]) = 68.827661446742$ $GA_4(G[3,8]) = 77.827661446742$
$GA_4(G[3,9]) = 86.827661446742$ $GA_4(G[3,10]) = 95.827661446742$

$GA_4(G[4,1]) = 19.7702152623223$ $GA_4(G[4,2]) = 79.7702152623223$
$GA_4(G[4,3]) = 43.770215262322$ $GA_4(G[4,4]) = 55.770215262322$
$GA_4(G[4,5]) = 67.770215262322$ $GA_4(G[4,6]) = 79.770215262322$
$GA_4(G[4,7]) = 91.770215262322$ $GA_4(G[4,8]) = 103.770215262322$
$GA_4(G[4,9]) = 115.770215262322$ $GA_4(G[4,10]) = 127.770215262322$

$GA_4(G[5,1]) = 24.7127690779028$ $GA_4(G[5,2]) = 39.7127690779028$
$GA_4(G[5,3]) = 54.712769077903$ $GA_4(G[5,4]) = 69.712769077903$
$GA_4(G[5,5]) = 84.712769077903$ $GA_4(G[5,6]) = 99.712769077903$
$GA_4(G[5,7]) = 114.712769077903$ $GA_4(G[5,8]) = 129.712769077903$
$GA_4(G[5,9]) = 144.712769077903$ $GA_4(G[5,10]) = 159.712769077903$

$GA_4(G[6,1]) = 29.6553228934834$ $GA_4(G[6,2]) = 47.655322893483$
$GA_4(G[6,3]) = 65.655322893483$ $GA_4(G[6,4]) = 83.655322893483$
$GA_4(G[6,5]) = 101.655322893483$ $GA_4(G[6,6]) = 119.655322893483$
$GA_4(G[6,7]) = 137.655322893483$ $GA_4(G[6,8]) = 155.655322893483$
$GA_4(G[6,9]) = 173.655322893483$ $GA_4(G[6,10]) = 191.655322893483$

$GA_4(G[7,1]) = 34.597876709064$ $GA_4(G[7,2]) = 55.597876709064$
$GA_4(G[7,3]) = 76.597876709064$ $GA_4(G[7,4]) = 97.597876709064$
$GA_4(G[7,5]) = 118.597876709064$ $GA_4(G[7,6]) = 139.597876709064$
$GA_4(G[7,7]) = 160.597876709064$ $GA_4(G[7,8]) = 181.597876709064$
$GA_4(G[7,9]) = 202.597876709064$ $GA_4(G[7,10]) = 223.597876709064$

$GA_4(G[8,1]) = 39.5404305246445$ $GA_4(G[8,2]) = 63.540430524645$
$GA_4(G[8,3]) = 87.540430524645$ $GA_4(G[8,4]) = 111.540430524645$
$GA_4(G[8,5]) = 135.540430524645$ $GA_4(G[8,6]) = 159.540430524645$
$GA_4(G[8,7]) = 183.540430524645$ $GA_4(G[8,8]) = 207.540430524645$
$GA_4(G[8,9]) = 231.540430524645$ $GA_4(G[8,10]) = 255.540430524645$

$GA_4(G[9,1]) = 44.4829843402251$ $GA_4(G[9,2]) = 71.482984340225$
$GA_4(G[9,3]) = 98.482984340225$ $GA_4(G[9,4]) = 125.482984340225$
$GA_4(G[9,5]) = 152.482984340225$ $GA_4(G[9,6]) = 179.482984340225$
$GA_4(G[9,7]) = 206.482984340225$ $GA_4(G[9,8]) = 233.482984340225$
$GA_4(G[9,9]) = 260.482984340225$ $GA_4(G[9,10]) = 287.482984340225$

$GA_4(G[10,1]) = 49.425538155806$ $GA_4(G[10,2]) = 79.425538155806$
$GA_4(G[10,3]) = 109.425538155806$ $GA_4(G[10,4]) = 139.425538155806$
$GA_4(G[10,5]) = 169.425538155806$ $GA_4(G[10,6]) = 199.425538155806$
$GA_4(G[10,7]) = 229.425538155806$ $GA_4(G[10,8]) = 259.425538155806$
$GA_4(G[10,9]) = 289.425538155806$ $GA_4(G[10,10]) = 319.425538155806$

$GA_4(G[100,100]) = 30194.2553815581$
$GA_4(G[1000,1000]) = 3001942.55381558$
$GA_4(G[10000,10000]) = 300019425.538156$
$GA_4(G[100000,100000]) = 30000194255.3816$
$GA_4(G[1000000,1000000]) = 3000001942553.81$
$GA_4(G[10000000,10000000]) = 300000019425538$
$GA_4(G[100000000,100000000]) = 3.00000001942554 \times 10^{16}$.

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