

COMPUTING GA_5 INDEX OF ARMCHAIR POLYHEX NANOTUBE

MOHAMMAD REZA FARAHANI

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 $W(G)$:

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

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

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

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

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

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

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

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].

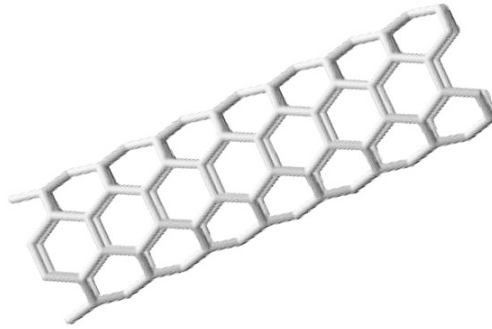


Figure 1: The 3-Dimensional Lattice (or cylinder) of the Armchair polyhex Nanotube $TUAC_6[8,7]$.

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.

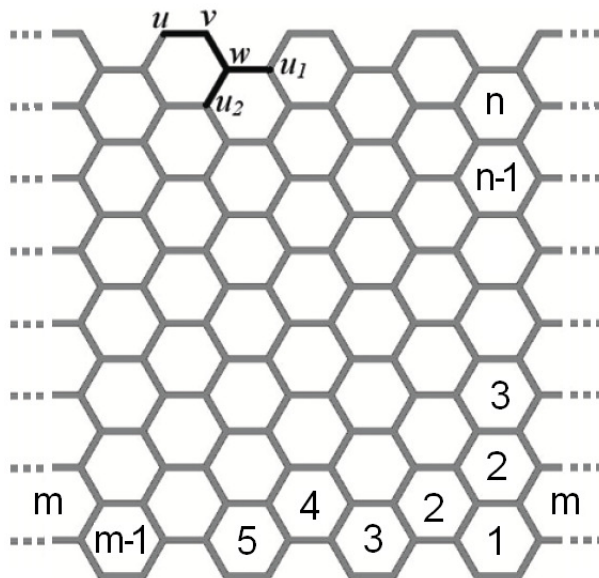


Figure 2: The 2D Lattice of the armchair polyhex Nanotube $TUAC_6[m,n]$.

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 $2 \times 2 \binom{m}{2}$ and therefore $|V_3| = 2mn$.

Next, we divide $E(TUAC_6[m, n])$ in three parts

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

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

and

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

with size

$$|E_4| = 2 \times \binom{m}{2}, \quad |E_5| = 2 \times |E_4| = 2m$$

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:

$$\begin{aligned} GA_5(TUAC_6[m, n]) &= \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \\ &= \sum_{u_2 v_2 \in E_4} \frac{2\sqrt{S_{u_2} S_{v_2}}}{S_{u_2} + S_{v_2}} + \sum_{u_2 v_3 \in E_5} \frac{2\sqrt{S_{u_2} S_{v_3}}}{S_{u_2} + S_{v_3}} + \sum_{u_3 v_3 \in E_6} \frac{2\sqrt{S_{u_3} S_{v_3}}}{S_{u_3} + S_{v_3}} = \end{aligned}$$

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

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 arm-chair polyhex nanotube $G[m, n] = TUAC_6[m, n]$ for $m = 2, 4, \dots, 10, 100, 1000, 10000, 100000$ and $n = 1, 2, \dots, 10, 100, 1000, 10000, 100000$ as follows:

$GA_4(G[2, 1]) = 9.8851076311611$	$GA_4(G[2, 2]) = 15.8851076311611$
$GA_4(G[2, 3]) = 19.8851076311611$	$GA_4(G[2, 4]) = 27.8851076311611$
$GA_4(G[2, 5]) = 33.8851076311611$	$GA_4(G[2, 6]) = 39.8851076311611$
$GA_4(G[2, 7]) = 45.8851076311611$	$GA_4(G[2, 8]) = 51.8851076311611$
$GA_4(G[2, 9]) = 57.8851076311611$	$GA_4(G[2, 10]) = 63.8851076311611$

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

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

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

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

$$\begin{aligned}
GA_4(G[7, 1]) &= 34.597876709064 & GA_4(G[7, 2]) &= 55.597876709064 \\
GA_4(G[7, 3]) &= 76.597876709064 & GA_4(G[7, 4]) &= 97.597876709064 \\
GA_4(G[7, 5]) &= 118.597876709064 & GA_4(G[7, 6]) &= 139.597876709064 \\
GA_4(G[7, 7]) &= 160.597876709064 & GA_4(G[7, 8]) &= 181.597876709064 \\
GA_4(G[7, 9]) &= 202.597876709064 & GA_4(G[7, 10]) &= 223.597876709064 \\
\\
GA_4(G[8, 1]) &= 39.540430524645 & GA_4(G[8, 2]) &= 63.540430524645 \\
GA_4(G[8, 3]) &= 87.540430524645 & GA_4(G[8, 4]) &= 111.540430524645 \\
GA_4(G[8, 5]) &= 135.540430524645 & GA_4(G[8, 6]) &= 159.540430524645 \\
GA_4(G[8, 7]) &= 183.540430524645 & GA_4(G[8, 8]) &= 207.540430524645 \\
GA_4(G[8, 9]) &= 231.540430524645 & GA_4(G[8, 10]) &= 255.540430524645 \\
\\
GA_4(G[9, 1]) &= 44.482984340225 & GA_4(G[9, 2]) &= 71.482984340225 \\
GA_4(G[9, 3]) &= 98.482984340225 & GA_4(G[9, 4]) &= 125.482984340225 \\
GA_4(G[9, 5]) &= 152.482984340225 & GA_4(G[9, 6]) &= 179.482984340225 \\
GA_4(G[9, 7]) &= 206.482984340225 & GA_4(G[9, 8]) &= 233.482984340225 \\
GA_4(G[9, 9]) &= 260.482984340225 & GA_4(G[9, 10]) &= 287.482984340225 \\
\\
GA_4(G[10, 1]) &= 49.425538155806 & GA_4(G[10, 2]) &= 79.425538155806 \\
GA_4(G[10, 3]) &= 109.425538155806 & GA_4(G[10, 4]) &= 139.425538155806 \\
GA_4(G[10, 5]) &= 169.425538155806 & GA_4(G[10, 6]) &= 199.425538155806 \\
GA_4(G[10, 7]) &= 229.425538155806 & GA_4(G[10, 8]) &= 259.425538155806 \\
GA_4(G[10, 9]) &= 289.425538155806 & GA_4(G[10, 10]) &= 319.425538155806 \\
\\
GA_4(G[100, 100]) &= 30194.2553815581 \\
GA_4(G[1000, 1000]) &= 3001942.55381558 \\
GA_4(G[10000, 10000]) &= 300019425.538156 \\
GA_4(G[100000, 100000]) &= 30000194255.3816 \\
GA_4(G[1000000, 1000000]) &= 3000001942553.81 \\
GA_4(G[10000000, 10000000]) &= 300000019425538 \\
GA_4(G[100000000, 100000000]) &= 3.00000001942554 \times 10^{16}.
\end{aligned}$$

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MOHAMMAD REZA FARAHANI
Department of Applied Mathematics
Iran University of Science and Technology (IUST)
Narmak, Tehran 16844, Iran
e-mail: MRFarahani88@Gmail.com
Mr_Farahani@mathdep.iust.ac.ir