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Fifth Geometric-Arithmetic Index of Polyhex Zigzag $TUZC_6[m,n]$ Nanotube and Nanotori

Mohammad Reza Farahani
Department of Applied Mathematics, Iran University of Science and Technology (IUST),
Narmak, Tehran 16844, Iran
Mr_Farahani@Mathdep.iust.ac.ir
MrFarahani88@Gmail.com

ABSTRACT

Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. The geometric-arithmetic index *(GA)* index is a topological index was defined as $GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_v d_u}}{d_v+d_u}$, in which degree of a vertex *v* denoted by d_v. A new version of *GA* index was defined by *A. Graovac et al* recently, and is equale to $GA_5(G)=\sum_{uv\in E(G)}\frac{2\sqrt{S_v S_u}}{S_v+S_u}$ where $S_v=\sum_{uv\in E(G)}d_u$. In this paper, we compute this new topological connectivity index for polyhex zigzag $TUZC_6[m,n]$ Nanotube and Nanotori.

Indexing terms/Keywords

Molecular graphs, geometric-arithmetic index, Polyhex Zigzag nanotube and nanotorous

SUBJECT CLASSIFICATION

E.g., Mathematics Subject Classification; 05C05, 05C12

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INTRODUCTION

Let G be a simple connected graph in chemical graph theory. In mathematices chemistry, the vertices and edges of a graph also correspond to the atoms and bonds of the molecular graph, respectively. If e is an edge/bond of G, connecting the vertices/atoms u and v, then we write $e=uv$ and say "u and v are adjacent".

A simple graph is an unweighted, undirected graph without loops or multiple edges. And also a connected graph is a graph such that there is a path between all pairs of vertices. Clearly, a molecular graph is a simple connected graph.

In mathematices chemistry, there are many topological indices and structure descriptors. A topological index is a numeric quantity from the structural graph of a molecule and is invariant on the automorphism of the graph. Nowadays thousands and thousands topological indices are defined for different goals, such as stability of alkanes, the strain energy of cycloalkanes, prediction of boiling point and etc. [1-3].

One of the best known and widely used is the connectivity index introduced in 1975 by *Milan Randić* [3], who has shown this index to reflect molecular branching and was defined as

$$\chi(G)=\sum_{e=uv\in E(G)}\frac{1}{\sqrt{d(u)d(v)}},$$

in which degree of a vertex v denoted by d_v.

One of the important topological connectivity index is the *geometric– arithmetic index (GA)* considered by *Vukičević* and *Furtula* [4] as

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

where d_v denotes degree of vertex v.

Recently, the fifth geometric-arithmetic topological indices was defined by *A. Graovac et al* [5] as

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

Such that S_v is the summation of degrees of all neighbors of vertex v in G $(S_v=\sum_{uv\in E(G)} d_u)$.

In Refs [6-17] some connectivity and geometric-arithmetic topological indices of some nanotubes and nanotorus are computed. The goal of this paper is to study the *fifth geometric-arithmetic index* and investigate this new index in one of the famous nano structure of polyhex *zigzag* nanotubes $TUZC_6$ (see Figure 1).

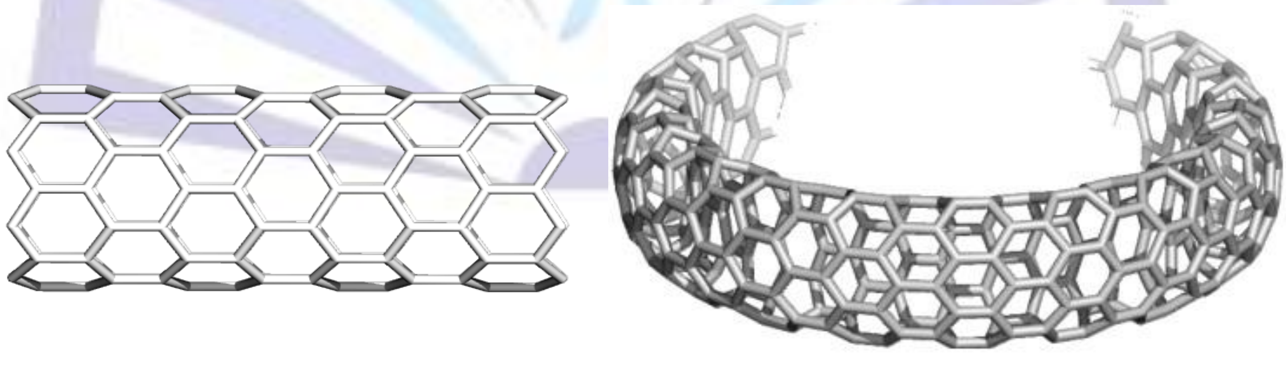

Fig. 1. The 3-Dimensional lattice (or cylinder) of polyhex zigzag $TUZC_6[m,n]$ nanotube (left) and nanotori (right).

Throughout this paper, our notation is standard and mainly taken from standard books of chemical graph theory [1, 2]. Also readers can see the references [6-19], for more details about some families of the topological connectivity indices and geometric-arithmetic indices.

Main Results and Discussions

Consider the molecular graph polyhex *zigzag* nanotube $TUZC_6$ and let we denote the number of hexagons in the first row/column of the 2D-lattice of $TUZC_6$ (Figures 2 and 3) by m and n, respectively. For other related research and historical details, see the paper series [19-26] and the general representation of this nano structure is shown in Figure 1 and Figure 2. The *fifth geometric-arithmetic index* of polyhex Zigzag $TUZC_6[m,n]$ Planar, Nanotube and Nanotori are given in the following theorem.

Theorem 1. Let G be Planar polyhex *zigzag* nanotube $PTUZC_6[m,n]$ $\left(\forall m,n\in \mathbb{N}-\{1\}\right)$; the *fifth geometric-arithmetic index* GA_5 is calculated as:

$$GA_5(PTUZC_6[m,n])=7mn-9.115n-3.275m+29.017$$

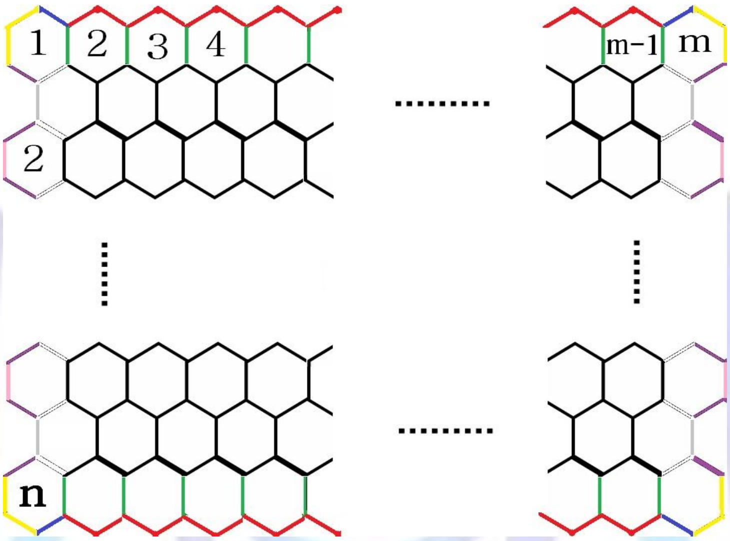

Fig. 2. 2-Dimensional Lattice of Planar polyhex *zigzag* nanotube $PTUZC_6[m,n]$.

Proof: $\forall m,n>1$, Consider Planar zigzag nanotube $G=PTUZC_6[m,n]$ (Figure 2) with $|V(PTUZC_6[m,n])|=2n(2m+1)$ vertices and $|E(PTUZC_6[m,n])|=6m(n-1)+5m(1)+n=6mn+n-m$ edges. From the 2-dimensional lattice of $G=PTUZC_6[m,n]$ $(m,n>1)$ depicted in Figure 2, one can see that the summation of degrees of edge endpoints of this molecular graph have nine edge types $e_{(4,5)}$, $e_{(5,5)}$, $e_{(5,7)}$, $e_{(5,8)}$, $e_{(6,7)}$, $e_{(7,9)}$, $e_{(8,8)}$, $e_{(8,9)}$ and $e_{(9,9)}$ that are shown in Figure 2 by yellow, pink, blue, purple, red, green,..., and black colors, respectively. In other word, for all edge $e=uv$ of the first type $e_{(4,5)}$, $S_v=d_x+d_u=2+2=4$ and $S_u=d_y+d_v=3+2=5$ and for an edge $f=uw$ of the second type $e_{(5,5)}$, $S_u=d_w+d_v=5$ and $S_w=d_w+d_u=5$ and other types are analogous. From Figure 2, one can see that the number of edges in these nine types are shown in the following table.

Edge type	$e_{(4,5)}$	$e_{(5,5)}$	$e_{(5,7)}$	$e_{(5,8)}$	$e_{(6,7)}$
Number of edges in this type	2×4	$2\times(n-2)$	4	$2\times(2n-2)$	$2\times2(m-2)$
	$e_{(7,9)}$	$e_{(8,8)}$	$e_{(8,9)}$	$e_{(9,9)}$	
	$2\times(m-2)$	$2\times(n-1)$	$2\times2(n-1)$	$(7(n-2)+5)(m-3)$	

Thus for all $m,n>1$, we have following computations.

$$GA_5(PTUZC_6[m,n])=\sum_{uv\in E(G)}\frac{2\sqrt{S_vS_u}}{S_v+S_u}$$

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$$
\begin{aligned}
&=(8)\frac{2\sqrt{4\times5}}{4+5}+2(n-2)\frac{2\sqrt{5\times5}}{5+5}+(4)\frac{2\sqrt{5\times7}}{5+7}+4(n-1)\frac{2\sqrt{5\times8}}{5+8}+4(m-2)\frac{2\sqrt{6\times7}}{6+7}\\
&\quad+2(m-2)\frac{2\sqrt{7\times9}}{7+9}+2(n-1)\frac{2\sqrt{8\times8}}{8+8}+4(n-1)\frac{2\sqrt{8\times9}}{8+9}+(m-3)(7n-9)\frac{2\sqrt{9\times9}}{9+9}\\
&=\frac{32\sqrt{5}}{9}+2(n-2)+\frac{2\sqrt{35}}{3}+\frac{16(n-1)\sqrt{10}}{13}+\frac{8(m-2)\sqrt{42}}{13}\\
&\quad+\frac{3(m-2)\sqrt{7}}{4}+2(n-1)+\frac{48(n-1)\sqrt{2}}{17}+(m-3)(7n-9)\\
&=7mn+n\left(2+\frac{16\sqrt{10}}{13}+2+\frac{48\sqrt{2}}{17}-21\right)+m\left(\frac{8\sqrt{42}}{13}+\frac{3\sqrt{7}}{4}-9\right)\\
&\quad+\left(\frac{32\sqrt{5}}{9}+\frac{2\sqrt{35}}{3}-\frac{16\sqrt{10}}{13}-4+\frac{16\sqrt{42}}{13}-\frac{3\sqrt{7}}{2}-2-\frac{48\sqrt{2}}{17}+27\right)
\end{aligned}
$$

Finally, $GA_5(PTUZC_6[m,n])=7mn-9.115n-3.275m+29.017$. Thus, the proof of Theorem 1 is completed. □

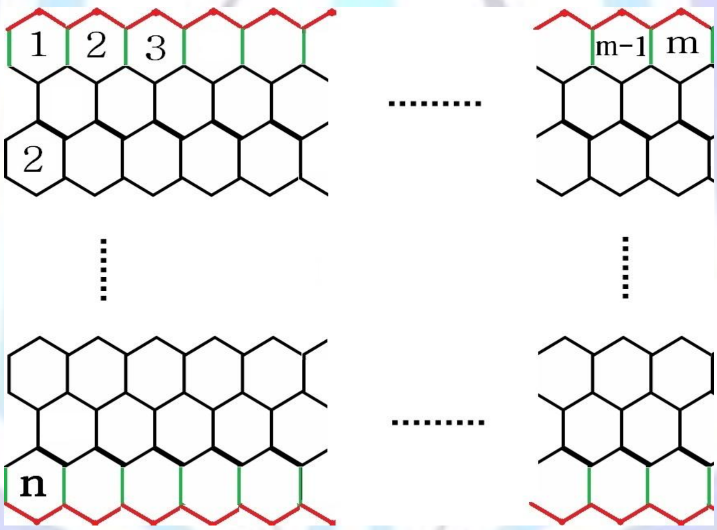

Fig. 3. 2-Dimensional Lattice of polyhex *zigzag* nanotube *$TUZC_6[m,n]$*.

Theorem 2. $\forall m,n\in\mathbb{N}-\{1\}$, the *fifth geometric-arithmetic index* GA_5 of polyhex zigzag nanotube $H=TUZC_6[m,n]$ is equal to

$$GA_5(TUZC_6[m,n])=\left(6n+\frac{8\sqrt{42}}{13}+\frac{3\sqrt{7}}{4}-10\right)m$$

Proof: Let H be polyhex zigzag nanotube $TUZC_6[m,n]$ (Figure 3). The vertices/atoms and edges/bonds of the molecular graph H are equale to $|V(TUZC_6[m,n])|=2n(2m)=4mn$ and $|E(TUZC_6[m,n])|=\frac{2(2m)+3(4m(n-1))}{2}=6mn-4m$, respectively. Since $|V_2|=|\{v\in V(G)|\ d_v=2\}|=m+m$ and $|V_3=\{v\in V(G)|\ d_v=3\}|=2m\times2(n-1)$.

From Figure 3, (the 2-dimensional lattice of $H=TUZC_6[m,n]$ $(m,n>1)$), it's easy to see that the summation of degrees of edge endpoints of $TUZC_6[m,n]$ nanotube have three edge types $e_{(6,7)}$, $e_{(7,9)}$ and $e_{(9,9)}$. Thus, for all edge $e=uv$ of the first type $e_{(6,7)}$, $S_v=d_x+d_u=3+3=6$ and $S_u=d_x+d_y+d_v=3+2+2=7$ and for all edge $f=uw$ in the second type $e_{(7,9)}$, $S_u=d_t+d_w+d_v=7$ and $S_w=d_s+d_w+d_u=9$. It's easy to see that for all other edges are from $e_{(9,9)}$ edge types. We marked these edge types by red, green and black colors in Figure 3, respectively. Also the number of edges in these three types are shown in the following table.

Edge type	$e_{(6,7)}$	$e_{(7,9)}$	$e_{(9,9)}$
Number of edges in this type	$2\times 2m$	$2\times m$	$6mn-10m$

Now, we have following computations of GA_5 of zigzag nanotube $H=TUZC_6[m,n]$, for all $m,n>1$.

$$GA_5(TUZC_6[m,n])=\sum_{uv\in E(TUZC_6[m,n])}\frac{2\sqrt{S_vS_u}}{S_v+S_u}$$

$$=(4m)\frac{2\sqrt{6\times 7}}{6+7}+2(m)\frac{2\sqrt{7\times 9}}{7+9}+2m(3n-5)\frac{2\sqrt{9\times 9}}{9+9}$$

$$=\frac{8m\sqrt{42}}{13}+\frac{3m\sqrt{7}}{4}+2m(3n-5)$$

Generally, $$GA_5(TUZC_6[m,n])=\left(6n+\frac{8\sqrt{42}}{13}+\frac{3\sqrt{7}}{4}-10\right)m$$

And also for further applications, we approach above formula with $\hat{G}A_5(TUZC_6[m,n])=6nm-4.0275m$. So, this complete the proof of Theorem 2. □

Finally, to compute the fifth geometric-arithmetic index of polyhex zigzag nanoturi $K=TTUZC_6[m,n]$ that the 3-dimensional lattice of $K=TTUZC_6[m,n]$ is shown in Figure 1, we have following theorem.

Theorem 3. $\forall$ *m,n>1*, GA_5 index of *polyhex zigzag Nanotori* $K=TTUZC_6[m,n]$ *is equal to*

$$GA_5(TTUZC_6[m,n])=6mn$$

Proof. The proof is easily, since by considering polyhex zigzag Nanotori $K=TTUZC_6[m,n]$ with $4mn$ $(=|V(TTUZC_6[m,n])|)$ vertices as degree three and $6mn$ $(=|E(TTUZC_6[m,n])|)$ edges (Figure 1). According to the 3-dimensional lattice of K (in Figure 1), we see that this nanotori is a member of *Cubic* graph families and by using the final corollary in [10] clearly,

$$GA_5(TTUZC_6[m,n])=\sum_{uv\in E(TTUZC_6[m,n])}\frac{2\sqrt{S_vS_u}}{S_v+S_u}=6mn\frac{2\sqrt{9\times 9}}{9+9}=6mn$$

So, the proof of Theorem 3 is completed. □

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