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

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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 defined as $GA(G) = \sum_{v \in V(G)} \frac{2\sqrt{d_v d_u}}{d_v + d_u}$, 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 equal to

$GA_2(G) = \sum_{v \in V(G)} \frac{2S_v S_u}{S_v + S_u}$ where $S_v = \sum_{u \in V(G)} d_u$. 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
INTRODUCTION
Let $G$ be a simple connected graph in chemical graph theory. In mathematics 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 mathematics 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

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

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

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

where $d_v$ denotes degree of vertex $v$.

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

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

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

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).

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

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 $TUZC_6[m,n]$ ($\forall m,n \in \mathbb{N}$); the fifth geometric-arithmetic index $GA_5$ is calculated as:

$$GA_5(TUZC_6[m,n]) = 7mn - 9.115n - 3.275m + 29.017$$

Proof: Let $m,n > 1$. Consider Planar zigzag nanotube $G = TUZC_6[m,n]$ (Figure 2) with $|V(TUZC_6[m,n])| = 2n(2m+1)$ vertices and $|E(TUZC_6[m,n])| = 6m(n-1) + 5m(1) + n = 6mn + n - m$ edges. From the 2-dimensional lattice of $G = TUZC_6[m,n]$ ($m,n > 1$) 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 $e_{(4,5)}$, $S_u = d_u + d_v = 2 + 2 = 4$ and $S_v = d_u + d_v = 3 + 2 = 5$ and for an edge $f = uw$ of the second type $e_{(5,5)}$, $S_w = d_u + d_v = 5$ and $S_v = d_w + d_u = 5$ 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  | $\theta_{(4,5)}$ | $\theta_{(5,5)}$ | $\theta_{(5,7)}$ | $\theta_{(5,8)}$ | $\theta_{(6,7)}$ |
|------------|------------------|------------------|------------------|------------------|------------------|
| Number of edges in this type | $2 \times 4$ | $2 \times (n-2)$ | $4$ | $2 \times (2n-2)$ | $2 \times (m-2)$ |

| Edge type  | $\theta_{(7,9)}$ | $\theta_{(8,8)}$ | $\theta_{(8,9)}$ | $\theta_{(9,9)}$ |
|------------|------------------|------------------|------------------|------------------|
| Number of edges in this type | $2 \times (m-2)$ | $2 \times (n-1)$ | $2 \times (2n-1)$ | $(7(n-2)+5)(m-3)$ |

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

$$GA_5(TUZC_6[m,n]) = \sum_{uv \in E(G)} \frac{2 \sqrt{S_u S_v}}{S_u + S_v}$$
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. $\forall m,n \in \mathbb{Z} - \{1\}$, the fifth geometric-arithmetic index $GA_5$ of polyhex zigzag nanotube $H= TUZC_6[m,n]$ is equal to

$$GA_5(TUZC_6[m,n])= 6n + \frac{8\sqrt{42}}{13} + \frac{3\sqrt{7}}{4} - 9$$

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 equal to $|V(TUZC_6[m,n])|=2n(2m)=4mn$ and $|E(TUZC_6[m,n])|=2(2m)+3(4m(n-1))=6mn-4m$, respectively. Since $|V_2|=|\{v \in V(G)|d_i=2\}|=m+m$ and $|V_3|=|\{v \in V(G)|d_i=3\}|=2m×2(n-1)$.

From Figure 3, 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 $e_{(6,7)}$, $S_v=d_i+d_j=3+3=6$ and $S_u=d_i+d_j=3+2=5$ and for all edge $e=uv$ in the second type $e_{(7,9)}$, $S_v=d_i+d_j=7$ and $S_u=d_i+d_j=9$. 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.

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Now, we have following computations of $GA_5$ of zigzag nanotube $H=\text{TUZC}_6[m,n]$, for all $m,n>1$.

$$GA_5(\text{TUZC}_6[m,n]) = \sum_{uv \in E(\text{TUZC}_6[m,n])} \frac{2\sqrt{S_vS_u}}{S_v + S_u}$$

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

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

Generally,

$$GA_5(\text{TUZC}_6[m,n]) = \left(\frac{6n + \frac{8\sqrt{42}}{13} + \frac{3\sqrt{7}}{4} - 10}{m}\right)$$

And also for further applications, we approach above formula with $GA_5(\text{TUZC}_6[m,n])=6mn-4.0275m$. So, this complete the proof of Theorem 2. □

Finally, to compute the fifth geometric-arithmetic index of polyhex zigzag nanotori $K=\text{TUZC}_6[m,n]$ that the 3-dimensional lattice of $K=\text{TUZC}_6[m,n]$ is shown in Figure 1, we have following theorem.

**Theorem 3.** ∀ $m,n>1$, $GA_5$ index of polyhex zigzag Nanotori $K=\text{TUZC}_6[m,n]$ is equal to

$$GA_5(\text{TUZC}_6[m,n]) = 6mn$$

**Proof.** The proof is easily, since by considering polyhex zigzag Nanotori $K=\text{TUZC}_6[m,n]$ with $4mn (=|V(\text{TUZC}_6[m,n])|$ vertices as degree three and $6mn (=|E(TUZC_6[m,n])|$ 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,

$$GA_5(\text{TUZC}_6[m,n]) = \sum_{uv \in E(\text{TUZC}_6[m,n])} \frac{2\sqrt{S_vS_u}}{S_v + S_u} = 6mn\frac{2\sqrt{9 \times 9}}{9 + 9} = 6mn$$

So, the proof of Theorem 3 is completed. □

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