

GA index of $TUC_4C_8(R)$ nanotube

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Let Σ be the class of finite graphs. A topological index is a function Top from Σ into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. Let G be a graph and $e = uv$ be an edge of G . The GA index of G is defined as

$$GA(G) = \sum_{e \in E} \frac{2\sqrt{du dv}}{du + dv}. \text{ In this paper we compute some results about this new topological index.}$$

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1. Introduction

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 [1-3]. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [4]. This theory had an important effect on the development of the chemical sciences.

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, 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".

Let Σ be the class of finite graphs. A topological index is a function Top from Σ into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The Wiener index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. In the last decade or so, various topological indices are introduced.

Let G be a graph and $e = uv$ be an edge of G . The GA index of G was introduced by D. Vukičević and co-authors [5] as $GA(G) = \sum_{i=1}^{|E(G)|} \xi_i$ in which, for the edge

$$e_i = u_i v_i \in E(G), \quad \xi_i = \frac{2\sqrt{du_i dv_i}}{du_i + dv_i}$$

and du denoted to the degree of vertex u . In this paper we compute some results about this new topological index. Herein, our notation is standard and taken from the standard book of graph theory [6-14].

2. Main results and discussion

The aim of this section is to compute the GA index of $TUC_4C_8(R)$ Nanotorus and nanotubes. Before going to calculate this index for $TUC_4C_8(R)$ Nanotorus and nanotubes, we must compute GA index, for some well-known class of graphs.

Example 1. Let P_n be a path with u_1, u_2, \dots and u_n vertices (Fig. 1), and $du_1 = du_n = 1$ and $du_i = 2$ ($2 \leq i \leq n-1$). So, we have $GA(G) = \sum_{e \in E} \frac{2\sqrt{du dv}}{du + dv} = \frac{4\sqrt{2}}{3} + (n-3)$.



Fig. 1. A path with the n vertices.

Example 2. Let C_n be a cycle on n vertices. We know all of vertices are of degree 2. So, we have

$$GA(G) = \sum_{e \in E} \frac{2\sqrt{2 \times 2}}{2 + 2} = n.$$

Example 3. Let S_n be a star on $n + 1$ vertices (Fig. 2). One can see there are n vertices of degree 1 and a vertex of degree n. So we have $GA(G) = \sum_{e \in E} \frac{2\sqrt{du dv}}{du + dv} = \frac{2n\sqrt{n}}{n+1}$.

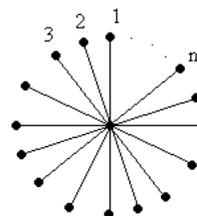


Fig. 2. The graph of a star with $n + 1$ vertices.

Lemma 4. For an arbitrary graph G , $GA(G) = |E(G)|$ if and only if G be a k -regular graph.

Proof. If G be k -regular then it is easy to see that for every $e \in V(G)$, $\xi = 1$ and then $GA(G) = |E(G)|$. Conversely, suppose $GA(G) = |E(G)|$. So, $\xi_1 + \xi_2 + \dots + \xi_{|E(G)|} = |E(G)|$. This implies $\xi_i = 1$ ($1 \leq i \leq |E(G)|$) and proof is completed.

Now we compute the GA index of a $TUC_4C_8(R)$ nanotube and $TUC_4C_8(R)$ as described above. The GA index of the 2-dimensional lattice of $TUC_4C_8(R)$ graph $K = KTUC[p,q]$ (Fig. 3) is also computed. Following Diudea [15-18], we denote a $TUC_4C_8(R)$ nanotube by $G = GTUC[p,q]$, $TUC_4C_8(R)$ nanotorus by $H = HTUC[p,q]$ (Figs. 4 and 5). It is easy to see that $|V(K)| = 4p(p+1)(q+1)$, $|V(G)| = 4p(q+1)$, $|V(H)| = 4pq$, $|E(K)| = 6pq + 5(p+q) + 4$, $|E(G)| = 6pq + 5p$ and $|E(H)| = 6pq + 6p$. We begin with the molecular graph of K (Fig. 1). One can see that there are three separate cases and the number of edges is different. Suppose e_1 , e_2 and e_3 are representative edges for these cases. We can see that $\xi_1 = \xi_3 = 1$ and

$\xi_2 = \frac{2\sqrt{6}}{5}$. By the definition of GA index and Table 1

one can see that

$$GA(G) = 6pq + (p+q)\left(\frac{8\sqrt{6}}{5} + 1\right) + 4.$$

We now consider the molecular graph G (Fig. 4). Fig. 4 shows that there are two different cases and the number of edges is different. Suppose e_1 and e_2 are representatives of the different cases. One can see that $\xi_1 = 1$ and

$\xi_2 = \frac{2\sqrt{6}}{5}$. On the other hand, there are $4p$, $6pq + 5$

similar edges for each of edges e_1 and e_2 , respectively. This implies that:

$$GA(G) = p\left(6q + \frac{8\sqrt{6}}{5} + 1\right).$$

Now consider the Fig. 5. Because the graph is 3-regular, by using lemma 4 we have:

$$GA(G) = |E(G)| = 6p(q+1).$$

Table 1. Computing the ξ_i for the 2-dimensional lattice of $TUC_4C_8(R)$ graph $K = KTUC[p,q]$

No.	ξ_i	Type of edges
4	1	e_1
$4(p+q)$	$\frac{2\sqrt{6}}{5}$	e_2
$6pq + p + q$	1	e_3

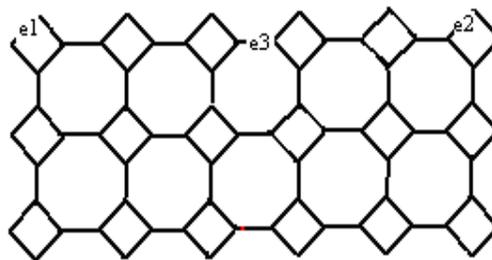


Fig. 3. 2-Dimensional Lattice of $TUC_4C_8(R)$ Nanotorus with $p = 5$ and $q = 2$.

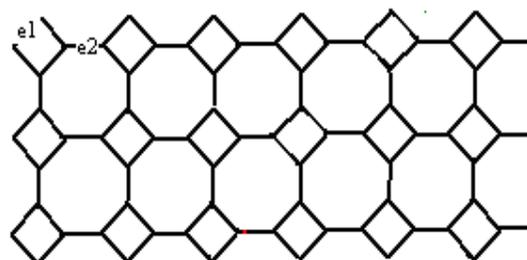


Fig. 4. The graph of $TUC_4C_8(R)$ nanotube $G = GTUC[p,q]$ with $p = 6$ and $q = 2$.

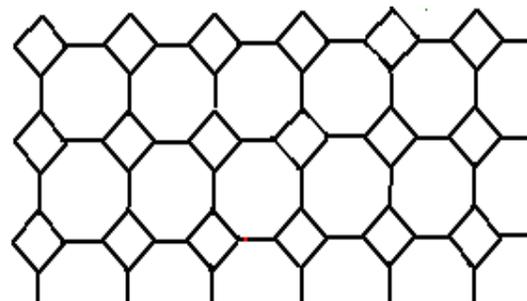


Fig. 5. The 2-Dimensional Lattice of $TUC_4C_8(R)$ nanotorus.

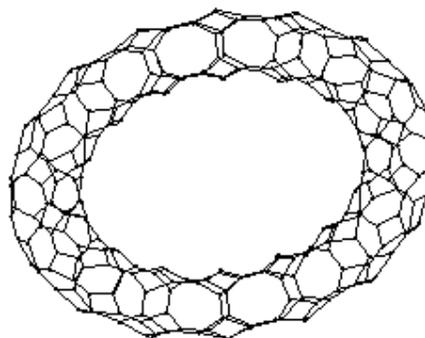


Fig. 6. An $TUC_4C_8(R)$ nanotorus.

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