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COMPUTING A NEW TOPOLOGICAL INDEX OF NANO STRUCTURES

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Let G be a graph and e = uv be an edge of G. The GA index of G is defined as $GA(G) = \sum_{e \in E} \frac{2\sqrt{dudv}}{du + dv}$. In this paper we compute the GA index of $TUC_4C_8(S)$ nanotube.

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1. Introduction

A nanostructure is an object of intermediate size between molecular and microscopic structures. It is a product derived through engineering at the molecular scale. The most important of these new materials are carbon nanotubes[1-3]. They have remarkable electronic properties and many other unique characteristics. For these reasons it is of interest to study the mathematical properties of these materials.

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 graph theory to mathematical modeling of chemical phenomena[4-7]. This theory had an important effect on the development of the chemical sciences.

A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to

determine physical properties of types of alkanes known as paraffin[8]. The Hosoya polynomial of a graph G is defined as $W(G;x) = \Sigma_{u,v\in V(G)}x^{d(u,v)}$, where d(u,v) denotes the length of a minimum path between u and v. In the paper [9] Hosoya used the name Wiener polynomial while some authors later used the name Hosoya polynomial.

Let G be a graph and e = uv be an edge of G. The GA index of G was introduced by D. Vukičevič and co-authors[10] as $GA(G) = \sum_{i=1}^{|E(G)|} \xi_i$ in which, for the edge $e_i = u_i v_i \in E(G)$, $\xi_i = \frac{2\sqrt{du_i dv_i}}{du_i + dv_i}$ 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[11-19].

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2. Main results and discussion

Before going to calculate the GA index for $TUC_4C_8(S)$ nanotube, we must compute this new index, for some well-known class of graphs.

Example 1. Let C_n be a cycle on n vertices. We know all of vertices are of degree 2 and so, $GA(G) = \sum_{e \in E} \frac{2\sqrt{2 \times 2}}{2+2} = n$.

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

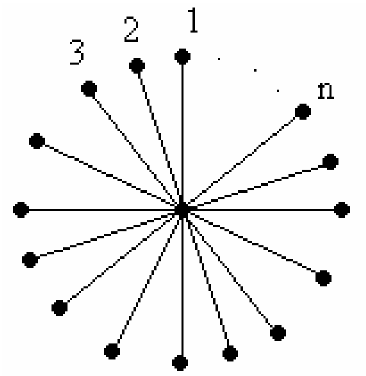

Fig. 1. Star graph with n + 1 vertices.

Example 3. Let $GP(n,k)$ be generalized Petersen graph with parameters n and k, vertex set $V = \{x_1, ..., x_n, y_1, ..., y_n\}$ and edge set $E = \{x_1x_2, x_2x_3, ..., x_nx_1, x_1y_1, x_2y_2, ..., x_ny_n, y_1y_{k+1}, y_2y_{k+2}, ..., y_ny_{k+n}\}$ (mod n) respectively. It is easy to see that $|E(GP(n,k))| = \begin{cases} 3n & \text{if } n \neq 2k \\ \frac{5n}{2} & \text{if } n = 2k \end{cases}$ and so, we have

$$GA(GP(n,k)) = \begin{cases} 3n & \text{if } n \neq 2k \\ \frac{3n}{2} + \frac{2n\sqrt{6}}{5} & \text{if } n = 2k \end{cases}.$$

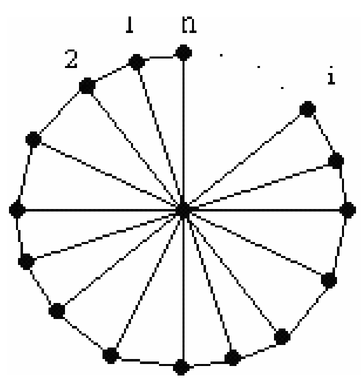

Fig. 2. Graph of wheel on n + 1 vertices.

Now we compute the GA index of a $TUC_4C_8(S)$ nanotube as described above. The GA index of the 2-dimensional lattice of $TUC_4C_8(S)$ graph K= KTUC[p,q] (Figure 3) is also computed. Following Diudea[20-24], we denote a $TUC_4C_8(S)$ nanotube by G = GTUC[p,q], $TUC_4C_8(R)$ nanotorus by H = HTUC[p,q] (Figures 4 and 5). It is easy to see that $|V(K)| = |V(G)| = |V(H)| = 8pq$, $|E(K)| = 12pq - 2p - 2q$, $|E(G)| = 12pq - 2p$ and $|E(H)| = 12pq$. We begin with the molecular graph of K (Figure 3). 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 $GA(K) = 12pq + (\frac{8\sqrt{6}}{5} - 6)(q-p) + 8 - \frac{16\sqrt{6}}{5}$. We now consider the molecular graph G of Figure 4. This figure 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 2p and 4p similar edges for each of edges e_1 and e_2, respectively. This implies that:

$$GA(G) = 12pq + (\frac{8\sqrt{6}}{5} - 6)p.$$

Lemma 1. 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, $\xi_1 + \xi_2 + \cdots + \xi_{|E(G)|} = |E(G)|$. This implies $\xi_i = 1$ $(1 \le i \le |E(G)|)$ and proof is completed.

Now consider the Figure 5. Because this graph is 3-regular, by using lemma 1 we have:

$$GA(H) = |E(H)| = 12pq.$$

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

No.	ξ_i	Type of Edges
2p+2q+4	1	e_1
4(p + q - 2)	$\frac{2\sqrt{6}}{5}$	e_2
12pq – 8 p -8 q + 4	1	e_3

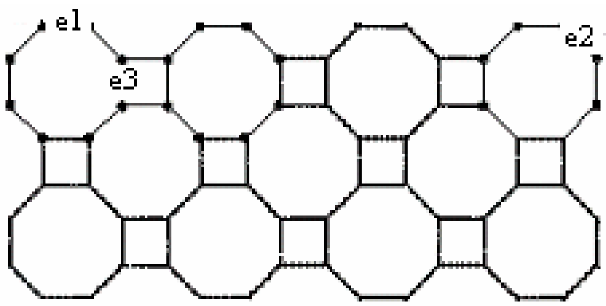

Fig. 3. 2-Dimensional Lattice of $TUC_4C_8(S)$ Nanotorus with p = 4 and q = 2.

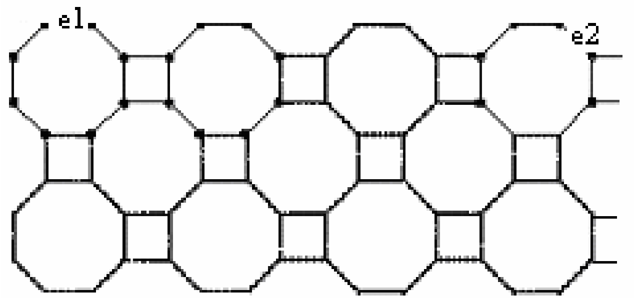

Fig. 4. The graph of TUC4C8(S) nanotube G = GTUC [p,q] with p = 4 and q = 2.

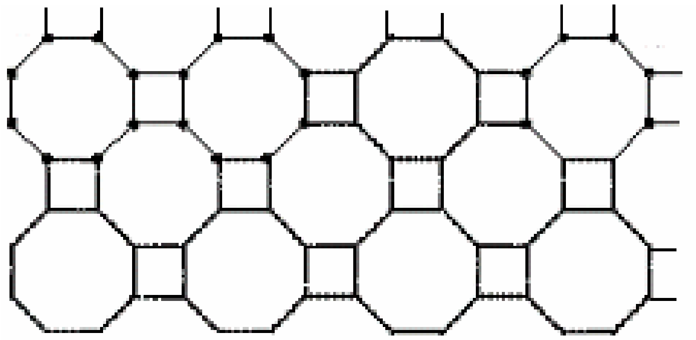

Fig. 5. The 2-Dimensional Lattice of $TUC_4C_8(S)$ Nanotorus.

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