

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

$$GA(G) = \sum_{e \in E} \frac{2\sqrt{du dv}}{du + dv}. \text{ In this paper we compute the GA index of } TUC_4C_8(S) \text{ nanotube.}$$

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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 nanotubes¹⁻³. 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 phenomena⁴⁻⁷. 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 paraffin⁸. The Hosoya polynomial of a graph G is defined as $W(G;x) = \sum_{u,v \in V(G)} x^{d(u,v)}$, 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. Vukičević and co-authors¹⁰ as $GA(G) = \sum_{i=1}^{|E(G)|} \xi_i$ in which, for the edge $e_i = u_i v_i \in E(G)$,

$$\xi_i = \frac{2\sqrt{du_i dv_i}}{du_i + dv_i} \text{ and } du \text{ denoted to the degree of vertex } u. \text{ In this paper we compute some results}$$

about this new topological index. Herein, our notation is standard and taken from the standard book of graph theory¹¹⁻¹⁹.

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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, $GA(G) = \sum_{e \in E} \frac{2\sqrt{du dv}}{du + dv} = \frac{2n\sqrt{n}}{n+1}$.

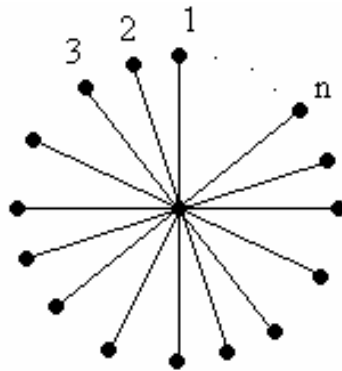


Fig. 1. Star graph with $n + 1$ vertices.

Example 3. Let $GP(n, k)$ be generalized Petersen graph with parameters n and k , vertex set $V = \{x_1, \dots, x_n, y_1, \dots, y_n\}$ and edge set $E = \{x_1x_2, x_2x_3, \dots, x_nx_1, x_1y_1, x_2y_2, \dots, x_ny_n, y_1y_{k+1}, y_2y_{k+2}, \dots, y_ny_{k+n}\} \pmod n$ 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

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

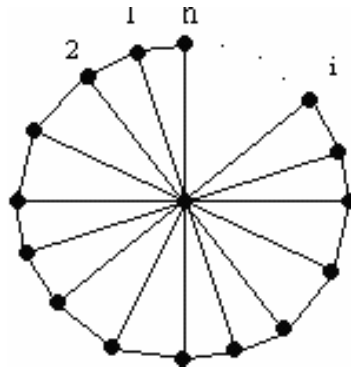


Fig. 2. Graph of wheel on $n + 1$ vertices.

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 Diudea²⁰⁻²⁴, 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, $\xi_1 + \xi_2 + \dots + \xi_{|E(G)|} = |E(G)|$. This implies $\xi_i = 1$ ($1 \leq i \leq |E(G)|$) 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
$12pq - 8p - 8q + 4$	1	e_3

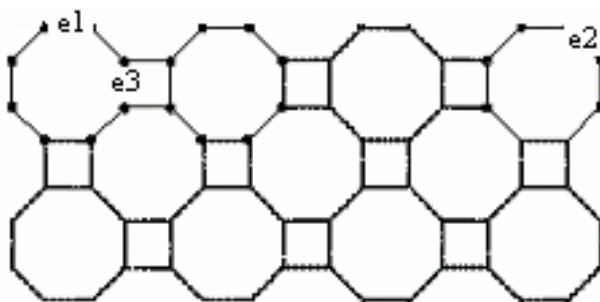


Fig. 3. 2-Dimensional Lattice of $TUC_4C_8(S)$ Nanotorus with $p = 4$ and $q = 2$.

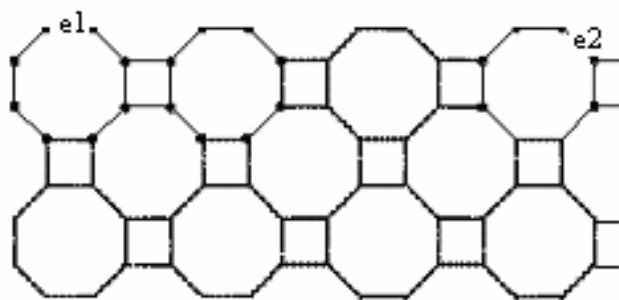


Fig. 4. The graph of $TUC_4C_8(S)$ nanotube $G = GTUC [p,q]$ with $p = 4$ and $q = 2$.

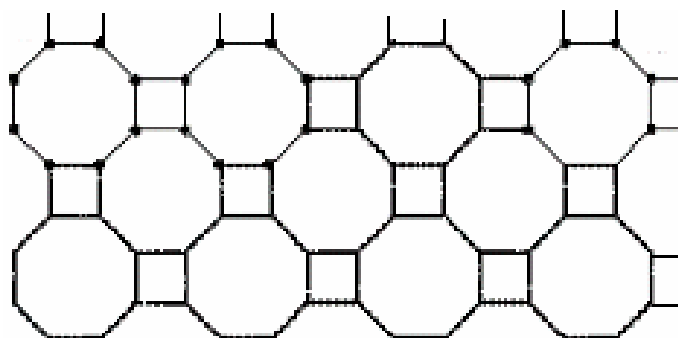


Fig. 5. The 2-Dimensional Lattice of $TUC_4C_8(S)$ Nanotorus.

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CONCLUSION Topological indices are designed basically by transforming a molecular graph into a number [6]. We compute a new distance based hyper Zagreb index and augmented Zagreb index for HAC 5 C 6 C 7 [p,q] and TUC 4 C 6 C 8 [p,q] nanotubes. First Author N.K.Raut, Dept of Physics, Majalgaon College, Majalgaon (Dist:Beed) India., Email: rautNK87@gmail.com Second Author S.N.Ipper, Dept of Chemistry, Majalgaon College, Majalgaon (Dist:Beed) India. Documents Similar To Computing some topological indices of Nanotubes. Carousel Previous Carousel Next. Abstract: A topological index is a number related to the atomic index that allows quantitative structure-action/property/toxicity connections. All the more vital topological indices correspond to certain physico-chemical properties like breaking point, solidness, strain vitality, and so forth, of synthetic mixes. Cheminformatics is a new subject that is a mix of science, arithmetic, and data science. It ponders quantitative structure-movement (QSAR) and structure-property (QSPR) connections that are utilized to anticipate the natural exercises and properties of synthetic mixes. Soleimani et al. [26] discuss the topological properties of nanostructures. Topological insulators are a new class of quantum materials with metallic (edge) surface states and insulating bulk states. They demonstrate a variety of novel electronic and optical properties, which make them highly promising electronic, spintronic, and optoelectronic materials. The insulating (dielectric) core of the nanocone displays an ultrahigh refractive index of up to 5.5 in the near-infrared frequency range. On the metallic shell, plasmonic response and strong backward light scattering were observed in the visible frequency range. With these unique features, the intrinsically core-shell plasmonic nanostructure paves a new way for designing low-loss and high-performance visible to infrared optical devices. Keywords. Topological insulator. A topological index is actually a numeric quantity associated with chemical constitution purporting for correlation of the chemical structure with many physiochemical properties, chemical reactivity, and biological activities. Let. be a graph with. On further results for certain degree-based topological indices of networks and nanostructures, consult [1, 10-13]. A tree is a connected acyclic graph, and the common type of a tree is a binary tree. A binary tree is made of nodes, where each node contains a left reference, a right reference, and a data element. new topological index, Sanskruti index $S(G)$ of a molecular graph G . In QSAR/QSPR. study, topological indices are utilized to guess the bioactivity of chemical compounds. The Sanskruti index $S(G)$ shows good correlation with entropy of an octane isomers. Inspired by this, and to understand the effect of neighbourhood degrees on a vertex we have defined a new topological index in [2] called first neighbourhood Zagreb index (FNZI) of a graph defined as First neighbourhood zagreb index of derived graphs and f-sums of graphs. Article.