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COMPUTING SOME TOPOLOGICAL INDICES OF NANO STRUCTURES

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Let G=(V,E) be a graph, where V is a non-empty set of vertices and E is a set of edges. One of the best known and widely used is the connectivity index, χ introduced in 1975 by Milan Randić. In this paper we compute Randić, Zagreb and *ABC* indices of TUC4C8(S), TUC4C8(R) nanotube and V-Phenylenic nanotorus.

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1. Introduction

All of the graphs in this paper are simple. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted [1].

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 [2,3,4]. 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 [5].

If $x,y \in V(G)$ then the distance $d_G(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [2]. They are defined as $M_2(G) = \sum_{uv \in E(G)} d_u d_v$

where d_u and d_v are the degrees of u and v. The connectivity index introduced in 1975 by Milan Randić [3, 4, 5], who has shown this index to reflect molecular branching. Randić index (Randić molecular connectivity index) was defined as follows $\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$

Recently Furtula et al. [1] introduced atom-bond connectivity (*ABC*) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}}$.

In this paper we compute some topological indices for TUC4C8(S) nanotube.

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2. Main results

In this sections , we compute this indices, for some well-known class of graphs, and in continue we calculate this indices for TUC4C8(S) nanotube.

Example 1. Let C_n be a cycle on n vertices. We know all of vertices are of degree 2 and so

$$M_2(G) = \sum_{uv \in E(G)} 2 \times 2 = 4n \quad , \quad \chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{2 \times 2}} = \frac{n}{2} \text{ and}$$

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{2+2-2}{2+2}} = \frac{n}{\sqrt{2}}$$

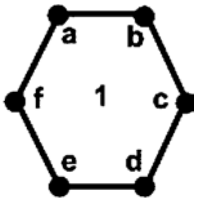

Fig 1. cycle graph C_n with n=6

Example 2. Let K_n be a complete graph on n vertices. We know all of vertices of degree n-1 and so

$$M_2(G) = \sum_{uv \in E(G)} (n-1) \times (n-1) = n(n-1)^2, \quad \chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{(n-1)(n-1)}} = \frac{n}{n-1} \text{ and}$$

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{(n-1)+(n-1)-2}{(n-1)+(n-1)}} = n\sqrt{\frac{2n-4}{2n-2}}$$

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,

$$M_2(G) = \sum_{uv \in E(G)} n \times 1 = n^2 \ , \ \chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{n \times 1}} = \sqrt{n}$$

$$\text{and} \quad ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{n+1-2}{n+1}} = n\sqrt{\frac{n-1}{n+1}}$$

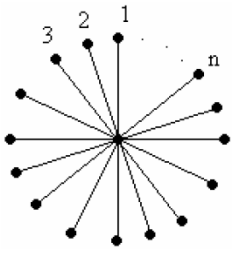

Fig. 2. Star graph with n + 1 vertices.

Now we compute Randić, Zagreb and *ABC* indices of a TUC4C8(S) nanotube as described above respectively. The Randić, Zagreb and *ABC* indices of the 2-dimensional lattice of TUC4C8(S) graph K= KTUC[p,q] (Fig 3) is also computed. Following Diudea [8,9], we denote a TUC4C8(R) nanotorus by H = HTUC[p,q] (Fig 4). It is easy to see that |V(K)| = |V(H)| =8pq, |E(K)| = 12pq -2p-2q and |E(H)| = 12pq. We also denote an V-Phenylenic nanotorus by Y = VPHY[4p,2q] and |E(Y)|=36pq (Fig 5).

One can see that $M_2(G)=\sum_{i=1}^{|E(G)|}\alpha_i$, $\chi(G)=\sum_{i=1}^{|E(G)|}\frac{1}{\sqrt{\alpha_i}}$ where $\alpha_i=d_{v_i}d_{u_i}$ and $ABC(G)=\sum_{i=1}^{|E(G)|}\sqrt{\frac{\beta_i-2}{\beta_i}}$ where $\beta_i=d_{v_i}+d_{u_i}$. So whit respect the molecular graph of K (Fig 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. Then $\alpha_1=\alpha_3=\beta_1=\beta_3=4$, $\alpha_2=6$ and $\beta_2=5$. We define N(e) number edge in position $e\in E(G)$ in graph G, so we have $N(e_1)$= 2p+2q+4 , $N(e_2)$= 4(p + q - 2) and $N(e_3)$= 12pq – 8 p -8 q + 4.

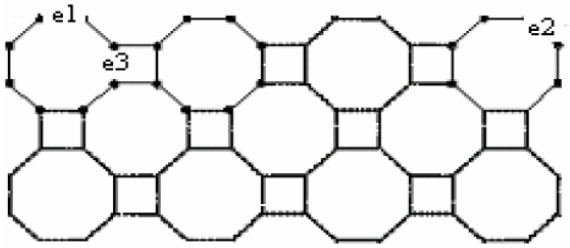

Fig. 3. 2-Dimensional Lattice of $TUC_4C_8(S)$ Nanotorus with p = 4 and q = 2

$$M_2(G)=\sum_{i=1}^{|E(G)|}\alpha_i=N(e_1)\alpha_1+N(e_2)\alpha_2+N(e_3)\alpha_3=16(3pq+p+q-1).$$

$$\chi(G)=\sum_{i=1}^{|E(G)|}\frac{1}{\sqrt{\alpha_i}}=\frac{N(e_1)}{\sqrt{\alpha_1}}+\frac{N(e_2)}{\sqrt{\alpha_2}}+\frac{N(e_3)}{\sqrt{\alpha_3}}=6pq+(\frac{4}{\sqrt{6}}-3)(p+q)+4-\frac{2}{\sqrt{6}}.$$

$$ABC(G)=\sum_{i=1}^{|E(G)|}\sqrt{\frac{\beta_i-2}{\beta_i}}=N(e_1)\sqrt{\frac{\beta_1-2}{\beta_1}}+N(e_2)\sqrt{\frac{\beta_2-2}{\beta_2}}+N(e_3)\sqrt{\frac{\beta_3-2}{\beta_3}}$$

$$=\sqrt{2}(8pq-3p-3q+4)+4\sqrt{\frac{3}{5}}(p+q-2).$$

We now consider the molecular graph H= HTUC[p,q] , Fig 4, and Y=V-Phenylenic nanotorus Fig 5.

Lemma 1. For an arbitrary graph G,

(a) $M_2(G)=k^2|E(G)|$ if and only if G be a k-regular graph.

(b) $\chi(G)=\frac{1}{k}|E(G)|$ if and only if G be a k-regular graph.

(c) $ABC(G)=\sqrt{\frac{k-1}{k}}|E(G)|$ 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 $e\in V(G)$, $\alpha_i=k^2$ and $\beta_i=\sqrt{\frac{k-1}{k}}$, implies that $M_2(G),\chi(G)$ and $ABC(G)$. Conversely, suppose $M_2(G)=k^2|E(G)|$ and $\chi(G)=\frac{1}{k}|E(G)|$. So $\alpha_1+\alpha_2+\cdots+\alpha_{|E(G)|}=k^2|E(G)|$, this implies $\alpha_i=d_{v_i}d_{u_i}=k^2\Leftrightarrow d_{v_i}=d_{u_i}=k$, then G, k-regular.

And suppose $ABC(G) = \sqrt{\frac{k-1}{k}} \mid E(G) \mid$ then $\beta_1 + \beta_2 + \cdots + \beta_{|E(G)|} = \sqrt{\frac{k-1}{k}} \mid E(G) \mid$,

so $\beta_i \mid E(G) \mid = \sqrt{\frac{k-1}{k}} \mid E(G) \mid \Rightarrow \beta_i = \sqrt{\frac{k-1}{k}}$ for $1 \le i \le \left|E(G)\right|$ and proof is completed.

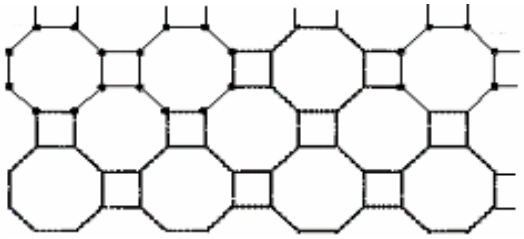

Fig. 4. The 2-Dimensional Lattice of $TUC_4C_8(R)$ Nanotorus.

By using lemma 1, consider the Figure 4. One can see that TUC4C8(S) graph is 3-regular, so

$M_2(TUC_4C_8(R)) = k^2 \left|E(TUC_4C_8(R))\right| = 108$ pq ,

$\chi(TUC_4C_8(R)) = \frac{1}{k} \mid E(TUC_4C_8(R)) \mid = 4$pq ,

and $ABC(TUC_4C_8(R)) = \sqrt{\frac{k-1}{k}} \mid E(TUC_4C_8(R)) \mid = \frac{12\sqrt{2}}{\sqrt{3}}$ pq.

Naw by using lemma 1, consider the Y=V-Phenylenic nanotorus, Figure 5.

$M_2(Y) = k^2 \left|E(Y)\right| = 324$pq , $\chi(Y) = \frac{1}{k} \mid E(Y) \mid = 12$pq

and $ABC(Y) = \sqrt{\frac{k-1}{k}} \mid E(Y) \mid = \frac{36\sqrt{2}}{\sqrt{3}}$ pq

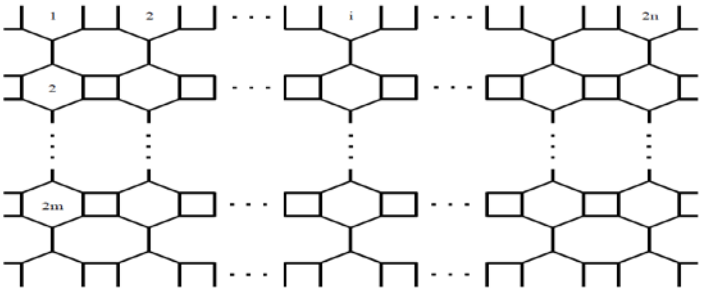

Fig. 5. A V-Phenylenic nanotorus.

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