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ON THE MODIFIED SCHULTZ INDEX OF C4C8(S) NANOTUBES AND NANOTORUS

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Let *G* be a simple undirected connected graph and *V (G)* denote vertex set of *G*. The modified Schultz index of the graph *G* is defined as $S^*(G)=\sum_{\{u,v\}\subseteq V\{G\}}\deg(u)\deg(v)d(u,v)$ in which *deg (u)* denotes vertex degree of $v\in V(G)$ and $d(u,v)$ denotes distance of vertices *u* and *v* in the graph *G*. In this paper we find an exact formula for calculation of modified Schultz index of nanotubes and nanotorus which have square and octagon structure.

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1. Introduction

A topological index is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. It most be structural invariant, i.e., it most not depends on the labeling or pictorial representation of the graph. Topological indices play an important role in structure property and structure activity studies, particularly when multivariate regression analysis, artificial neural networks, and pattern recognition are used as statistical tools.
Let G be an undirected connected graph without loops or multiple edges. The sets of vertices and edges of G are denoted by *V (G)* and *E (G)*, respectively. For vertices *u* and *v* in *V (G)*, we denote by *d (u, v)* the topological distance i.e., the number of edges on the shortest path, joining the two vertices of *G*. Since *G* is connected, *d (u, v)* exists for all vertices $u,v\in V(G)$. Suppose *deg (u)* denotes degree of vertex $u\in V(G)$. Klavzˇar and Gutman defined the modified Schultz index of the graph *G* as follow [2]

$$S^*(G)=\sum_{\{u,v\}\subseteq V\{G\}}\deg(u)\deg(v)d(u,v) \tag{1}$$

Recently computing topological indices of nanostructures have been the object of many papers [3]-[13]. The modified Schultz index of C_4C_8(S) nanotubes was introduced by Shubo and Fangli [1]. In this paper we find an exact formula for calculation the modified Schultz index of C_4C_8(S) nanotubes and nanotorus.

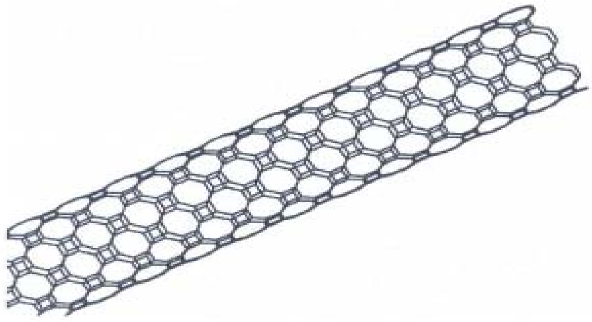

Fig. 1. A $C_4C_8(S)$ nanotube.

Main results

Suppose a C_4C_8(S) nanotubes constructed by rolling a lattice of carbon atoms (figure (2)) For following computations we choose a coordinate label for vertices of this lattice as shown in figure (**2**). Let the graph has q row and $2p$ column of vertices. In this case we denote the nanotubes by $G=T(p, q)$. If $q \le p$ nanotubes is called short and if $q > p$, then nanotubes is called long. We compute $S^*(G)$ by using the Wiener index of C_4C_8(S) nanotubes where calculated in simple exact formula in [7] as follow:

Theorem A. The Wiener index of C_4C_8(S) nanotubes given by

$$W(G)=\begin{cases} \dfrac{pq}{3}(2q^3+8pq(3p+q)-2q-8p), & if \quad q \le p \\ \\ \dfrac{p^2}{3}(-2p^3+8p^2q+(12p^2+2)p+16q^3-12q), & if \quad q > p. \end{cases}$$

Now we compute the summation of distances between vertex $v \in V(G)$ and vertices of the graph in which placed on kth row below of vertex v. Let x_{0p} and y_{0p} be two vertices of graph placed on the first row of the graph and x_{kt} and y_{kt} be vertices in kth row and tth column of the graph for $1 \le k < q$ and $1 \le t < 2p$. Let $d_x(k)$ denotes the summation of distances between vertex x_{0p} and all of the vertices placed in kth row of the graph. Thus

$$d_x(k)=\sum_{i=0}^{p-1}(d(x_{kt},x_{0p})+d(y_{kt},x_{0p}))$$

Similarly we define $d_y(k)$ as follow:

$$d_y(k)=\sum_{i=0}^{p-1}(d(x_{kt},y_{0p})+d(y_{kt},y_{0p}))$$

In the following Lemma the value of $d_x(k)$ and $d_y(k)$ are computed in [7].

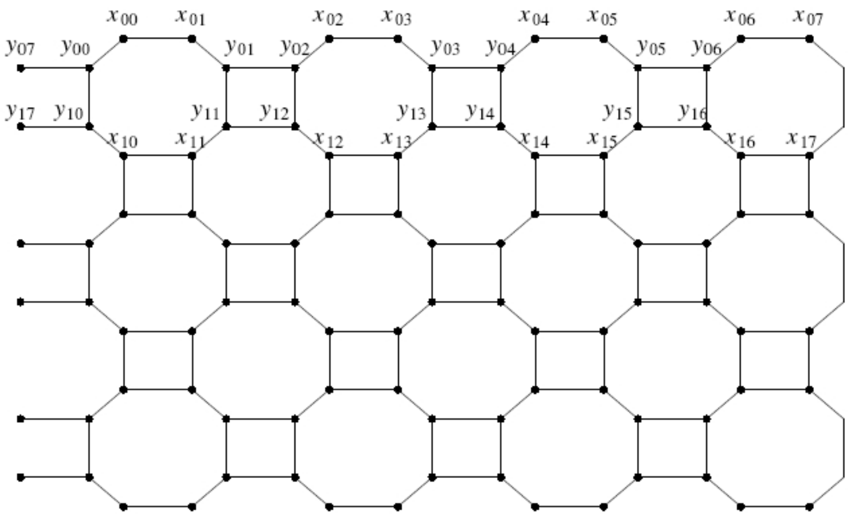

Fig. 2. A $C_4C_8(S)$ Lattice with p=4 and q=6.

Lemma *1*. Let $0 \le k < q$, then

$$d_x(k) = \begin{cases} p^2 + 2kp + 2(k^2 + k) & if \quad 2k \le p \\ \dfrac{p^2}{2} + 4kp + p & if \quad 2k > p. \end{cases}$$

And

$$d_y(k) = \begin{cases} p^2 + 2kp + 2(k^2 - k) & if \quad 2k \le p \\ \dfrac{p^2}{2} + 4kp - p & if \quad 2k > p. \end{cases}$$

Now the modified Schultz index of the graph can be calculated by using Theorem *A* and Lemma *1*. In the following Theorem to consideration two cases odd and even value for *p* put $\alpha = \dfrac{1-(-1)^p}{2}$.

Theorem 1. The modified Schultz index of $C_4C_8(S)$ nanotubes is given as

$$S^*(G) = \begin{cases} 2p[(36q^2 - 24q + 4)p^2 + (12q^3 - 12q^2 + 2q - 2)p + 3q^4 - 4q^3 - 2q^2 + 4q - 2\alpha], if \quad q \le p \\ 2p[-3p^4 + (24q-4)p^3 + (18q^2 - 12q + 6)p^2 + (24q^3 - 24q^2 - 2q + 2)p - \alpha], \quad if \quad q > p. \end{cases}$$

Proof: If $u_{kt} \in \{x_{kt}, y_{kt}\}$ denotes the vertex of *G* where placed on *k*th row and *t*th column for $1 \le k < q-2$ and $0 \le t < 2p$ we have $\deg(u_{k,t}) = 3$ and $\deg(x_{1,t}) = \deg(x_{q-1,t}) = 2$ for $1 \le t < 2p$. Therefore

$$S^*(G)=\sum_{\{u,v\}\subseteq V\{G\}}\deg(u)\deg(v)d(u,v)=\sum_{\{u,v\}\subseteq V\{G\}}9d(u,v)-2p[5\sum_{t=1}^{2p-1}(d(x_{0,0},x_{1,t})+d(x_{0,0},x_{q-1,t}))$$
$$+3\sum_{t=1}^{2p-1}(d(x_{0,0},y_{1,t})+d(x_{0,0},y_{q-1,t}))+3\sum_{k=1}^{2p-2}\sum_{t=0}^{2p-1}d(x_{0,0},u_{1,t})]$$
$$=9\frac{W(G)}{2}-2p[5d_x(0)+5d_x(q-1)+3(d_y(0)+d_y(q-1))+3\sum_{k=1}^{2p-2}(d_x(k)+d_y(k))$$

Let $q\leq p$ and p be even. By using Theorem *A* and Lemma *1* the modified Schultz index of *G* is given as

$$S^*(G)=2p[(36q^2-24q+4)p^2+(12q^3-12q^2+2q-2)p+3q^4-4q^3-2q^2+4q].$$

If p is odd, then

$$S^*(G)=2p[(36q^2-24q+4)p^2+(12q^3-12q^2+2q-2)p+3q^4-4q^3-2q^2+4q-2].$$

Now suppose $p<q$. Similar to previous case by using Theorem *A* and Lemma *1* if p is even

$$S^*(G)=2p[-3p^4+(24q-4)p^3+(18q^2-12q+6)p^2+(24q^3-24q^2-2q+2)p].$$

And if p is odd, then

$$S^*(G)=2p[-3p^4+(24q-4)p^3+(18q^2-12q+6)p^2+(24q^3-24q^2-2q+2)p-2].$$

Therefore the proof is completed.

In continue we compute the modified Schultz index of $C_4C_8(S)$ nanotorus by using the exact formula for computation Wiener index of this graph which obtained in [11]. We suppose the graph of $C_4C_8(S)$ nanotorus is constructed by joining the vertices of the graph which placed on first and last row of $C_4C_8(S)$ nanotubes (figure (3)).

Theorem B. The Wiener index of $G=C_4C_8(S)$ nanotubes is computed as

$$W(G)=\begin{cases}\frac{pq^2}{3}(24p^2+6pq+q-4) & if \quad q\leq p\\ \frac{2qp^2}{3}(2p^2+3pq+3q^2-2), & if \quad q>p.\end{cases}$$

Now we can compute the modified Schultz index of $C_4C_8(S)$ nanotorus by using the Wiener index of this graph.

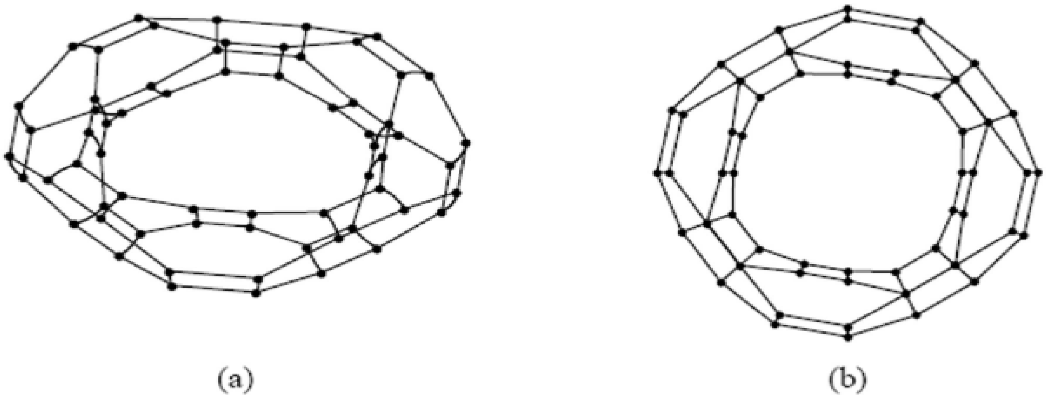

Fig. 3. A $C_4C_8(S)$ nanotprus (a) slide view (b) top view.

Theorem B. The Wiener index of $G = C_4C_8(S)$ nanotubes is computed as

$$W(G)=\begin{cases} \frac{pq^2}{3}(24p^2+6pq+q-4) & if \quad q \le p \\ \frac{2qp^2}{3}(2p^2+3pq+3q^2-2), & if \quad q > p. \end{cases}$$

Now we can compute the modified Schultz index of C_4C_8(S) nanotorus.

Theorem 2. The modified Schultz index of $G = C_4C_8(S)$ nanotubes is given by

$$S^*(G)=\begin{cases} 3\mathrm{pq}^2(24\mathrm{p}^2+6\mathrm{qp}+\mathrm{q}^2-4) & if \quad q \le p \\ 12\mathrm{p}^2\mathrm{q}(3\mathrm{q}^2+2\mathrm{p}^2+3\mathrm{qp}-2), & if \quad q > p. \end{cases}$$

Proof: Let $u_{kt} \in \{x_{kt}, y_{kt}\}$ denote the vertex of *G* where placed on *k*th row and *t*th column for $0 \le k < q-1$ and $0 \le t < 2p$ we have $\deg(u_{k,t}) = 3$. Thus

$$S^*(G) = \sum_{\{u,v\}\subseteq V\{G\}} \deg(u)\deg(v)d(u,v) = \sum_{\{u,v\}\subseteq V\{G\}} 9d(u,v) = 9W(G)$$

Thus if $q \le p$ then by using Theorem *B* we have

$$S^*(G) = 9W(G) = 3\mathrm{pq}^2(24\mathrm{p}^2+6\mathrm{qp}+\mathrm{q}^2-4).$$

If $q > p$ then

$$S^*(G) = 9W(G) = 12\mathrm{p}^2\mathrm{q}(3\mathrm{q}^2+2\mathrm{p}^2+3\mathrm{qp}-2).$$

Therefore the proof is done.

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