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MOLECULAR TOPOLOGICAL INDEX OF C_4C_8 (R) AND C_4C_8 (S) NANOTORUS

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Let G be a simple connected graph and $d(i,j)$ denote distance between vertices i and j of the graph G. The Molecular topological (Schultz) index of the graph G is defined by $MTI(G) = \sum_{i,j} v(i)[d(i,j) + A(i,j)]$, where $v(i)$ is the vertex degree of vertex i and $A(i,j)$ is the (i,j) entry of adjacency matrice of G. In this paper we compute the molecular topological index of $C_4C_8(S)$ and C_4C_8(R) nanotorus.

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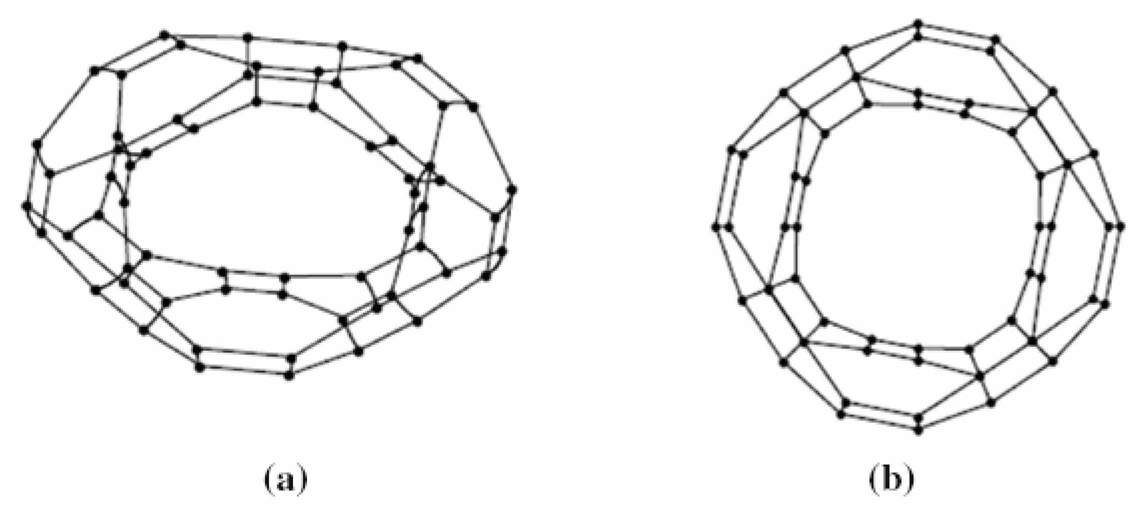
1. Introduction

A real number that describes a molecular graph is called a topological index. The first use of a topological index for the correlation of the measured properties of molecules with their structural features was made in 1947 by the chemist Harold Wiener. In that year, he introduced the notion of path number of a graph as the sum of the distances between any two carbon atoms in the molecules, in terms of carbon–carbon bonds. Wiener originally defined his index on trees and studied its use for correlations of physico-chemical properties of alkanes, alcohols, amines, and their analogous compounds [10].

Let G be a connected graph, the set of vertices and edges of will be denoted by $V(G)$ and $E(G)$, respectively. The distance between a pair of vertices i and j of G is denoted by $d(i,j)$. The molecular topological index of the graph G was introduced by Schultz in 1989 and is defined as follows:

$$MTI(G) = \sum_{i,j} v(i)[d(i,j) + A(i,j)] \tag{1}$$

Since in the definition of $MTI(G)$ appears the distance between vertices of G which is based the Wiener index, it has been found that the Schultz index and the Wiener index are closely related quantities for trees and cycles [12-13]. The Schultz index has been shown to be a useful molecular descriptor in the design of molecules with desired properties [14-18].Therefore, further studies on mathematical and computational properties of the Schultz index and on its relation to other molecular descriptors are desirable.



A C_4C_8(S) naotorus (a) Side view and (b) Top view.

Recently computing topological indices of nano structures have been the object of many papers [3-9]. Ashrafi and coauthor compute the wiener index of C_4C_8(R) notorus [1]. In this paper we use of them results and compute the molecular topological index of this graph. Also we compute the molecular topological index of C_4C_8(S) nanotorus by using results such that obtained in [4].

2. Main results

In this section we derive exact formulas for the molecular topological index of graph C_4C_8(S) and C_4C_8(R) nanotorus. At first we consider the graph of G=C_4C_8(S) nanotorus. For this purpose first we choose a coordinate label for vertices of this graph as shown in Figure 2. Let this graph has q rows and *2p* columns of vertices (q and p are positive even integer). To compute MTI(G), at first the summation of distance between all of the pair vertices of the graph, $\sum_{i,j} d(i, j)$, most be computed.

For this purpose we consider vertices x_{0p} and y_{0p} in the first row of the graph and obtain summation of distances between these two vertices and other vertices of the graph. The obtained results in this computations can be used for calculation summation of distances between each two vertices x_{tp} and y_{tp} (for $t=1,2,\ldots,q/2-1$) and other vertices of the graph other by symmetry of the graph. Let $d_x(k)$ denotes the summation of distances between vertex x_{0p} and all of the vertices placed in *k*th 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 de_ne d_y(k) as follow:

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

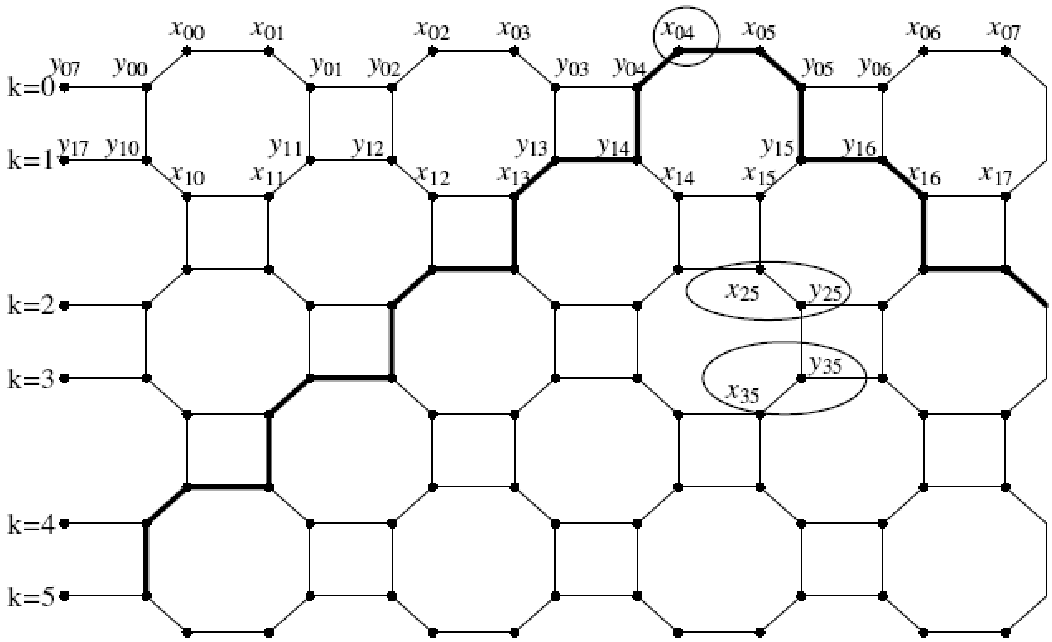


Figure 2: A $C_4C_8(S)$ Lattice with $p = 4$ and $q = 6$.

In Lemma 3 of Ref [4] we compute $d_x(k)$ and $d_y(k)$ as follow:

Lemma 1. Let $0 \le k < \frac{q}{2}$, then

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

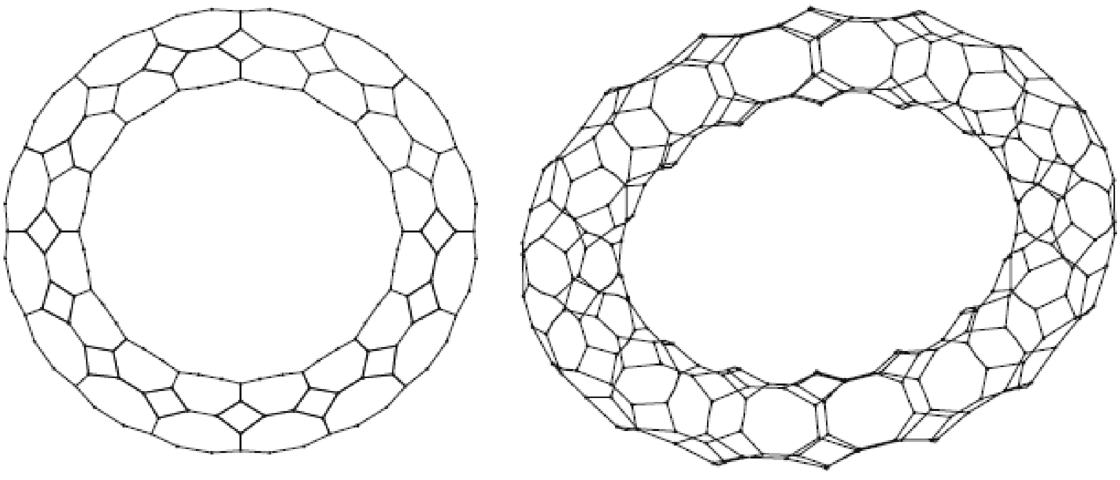
and

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

Now we can compute quantity of expression $\sum_{i,j}(d(i,j)$ for graph of G = C_4C_8(S) nanotorus. Let $q \le p$, by using of Lemma *1* we have

$$\sum_{i \in V(G)} d(i, x_{0p}) = \sum_{k=0}^{\frac{q}{2}-1} d_x(k) + \sum_{k=1}^{\frac{q}{2}} d_y(k) = \sum_{k=0}^{\frac{q}{2}-1} (4p^2 + 4kp + 2(k^2 + k)) + \sum_{k=1}^{\frac{q}{2}} (4p^2 + 4kp + 2(k^2 - k))$$

$$= \frac{q^3}{6} + pq^2 + (4p^2 - \frac{2}{3})q.$$



A C_4C_8(R) naotorus (a) Top view and (b) Side view.

The last result which obtained for vertex x_{0p} can be used for all of the vertices of graphs. Therefore

$$\sum_{i,j}(d(i,j) = 2pq\sum_{i\in V(G)} d(i,x_{0p}) = \frac{2pq^2}{3}(24p^2+6pq+q-4). \qquad (2)$$

Now suppose $q>p$. Thus

$$\sum_{i\in V(G)} d(i,x_{0p}) = \sum_{k=0}^{p} d_x(k) + \sum_{k=1}^{p} d_y(k) + \sum_{k=p+1}^{\frac{q}{2}-1} d_x(k) + \sum_{k=p+1}^{\frac{q}{2}} d_y(k)$$

$$= \frac{q^3}{6} + pq^2 + (4p^2 - \frac{2}{3})q + \sum_{k=p+1}^{\frac{q}{2}-1}(4p^2+4kp+2(k^2+k)) + \sum_{k=p+1}^{\frac{q}{2}}(4p^2+4kp+2(k^2-k))$$

$$= \frac{4p^3}{3} + 2qp^2 + (2p^2 - \frac{4}{3})p.$$

So in this case we have

$$\sum_{i,j}(d(i,j) = 2pq\sum_{i\in V(G)} d(i,x_{0p}) = \frac{4qp^2}{3}(2p^2+3pq+3q^2-2). \qquad (3)$$

Now we can compute the molecular topological index of G = C_4C_8(S) nanotorus.

Theorem 1. The molecular topological index of $G = C_4C_8(S)$ nanotorus given by

$$MTI(G) = \begin{cases} 2pq(24p^2q + 6pq^2 - 4q + 2q^3 + 18), & q \le p \\ \\ 4pq(4p^3 + 6p^2q + 6pq^2 - 4p + 9), & q > p. \end{cases}$$

Proof: Since degree of each vertex *i* of the graph is tree so *v(i)=3* for all of the vetices of the graph . Therefore

$$MTI(G)=\sum_{i,j}v(i)[d(i,j)+A(i,j)]=3\sum_{i,j}d(i,j)+3\sum_{i,j}A(i,j)$$

In the hand since *G* is connected so $\sum_{i,j}A(i,j)=2\,|E(G)|$. Thus $\sum_{i,j}A(i,j)=12pq$. Therefore by using *(2)* if $q\leq p$

$$MTI(G)=3[\frac{2pq^2}{3}(24p^2+6pq+q-4)+12pq]=2pq(24\mathrm{p}^2\mathrm{q}+6\mathrm{pq}^2-4\mathrm{q}+2\mathrm{q}^3+18).$$

Now suppose *q>p*. By using *(3)* we have

$$MTI(G)=3[\frac{2pq^2}{3}(24p^2+6pq+q-4)+12pq]=4pq(4\mathrm{p}^3+6\mathrm{p}^2\mathrm{q}+6\mathrm{pq}^2-4\mathrm{p}+9).$$

The So the proof is completed .

Now we compute the molecular topological index of $G=C_4C_8(R)$ nanotorus. For this purpose at first $\sum_{i,j}(d(i,j)$ most be computed for this graph. We use from calculation of *Ref[2]* and obtain following results.

$$\sum_{i,j}(d(i,j)=\begin{cases}\frac{4p^3}{3}(14p^2-k_1), & if \quad p=q\\[2ex] 4mn[\frac{2m}{3}(m^2-1)+mn(m+3n)-k_2], & if \quad m\neq n.\end{cases}\qquad(4)$$

In which (p,2) denotes the greatest common divisor of integers *2* and *p,* $n=Max\{p,q\}$,

$m=Min\{p,q\}$, $k_1=\begin{cases}2, & if \quad (p,2)\neq 1\\ 5, & if \quad (p,2)=1\end{cases}$ and

$$k_2=\begin{cases}0, & if \quad (m,2)\neq 1, \quad (n,2)\neq 1\\ \frac{m}{2}, & if \quad (m,2)\neq 1, \quad (n,2)=1\\ n, & if \quad (m,2)=1, \quad (n,2)=1\\ n-\frac{m}{2}, & if \quad (n,2)=1, \quad (n,2)\neq 1.\end{cases}$$

Thus the molecular topological index of graph $G=C_4C_8(R)$ can be computed as same as the graph of $G=C_4C_8(S)$ by using pervious notations.

Theorem 2. Let $p=q$. The molecular topological index of $G=C_4C_8(S)$ nanotorus given by

$$MTI=\begin{cases}4\mathrm{p}^2(14\mathrm{p}^3-2\mathrm{p}+9), & if \quad (p,2)\neq 1\\[2ex] 4\mathrm{p}^2(14\mathrm{p}^3-5\mathrm{p}+9), & if \quad (\mathrm{p},2)=1.\end{cases}$$

If $p\neq q$ then

$$MTI(G)=\begin{cases} 4\mathrm{mn}(2\mathrm{m}^3+3\mathrm{nm}^2+9\mathrm{n}^2\mathrm{m}-2\mathrm{m}+9)\ , & if \quad (m,2)\neq 1, \quad (n,2)\neq 1 \\ 2\mathrm{mn}(4\mathrm{m}^3+6\mathrm{nm}^2+18\mathrm{n}^2\mathrm{m}-7\mathrm{m}+18)\ , & if \quad (m,2)\neq 1, \quad (n,2)=1 \\ 4\mathrm{mn}(2\mathrm{m}^3+3\mathrm{nm}^2+9\mathrm{n}^2\mathrm{m}-3\mathrm{n}-2\mathrm{m}+9)\ , & if \quad (m,2)=1, \quad (n,2)=1 \\ 2\mathrm{mn}(4\mathrm{m}^3+6\mathrm{nm}^2+18\mathrm{n}^2\mathrm{m}-6\mathrm{n}-\mathrm{m}+18)\ , & if \quad (m,2)=1, \quad (n,2)\neq 1 \end{cases}$$

Proof: Since $\sum_{i,j} A(i,j)=2\,|\,E(G)\,|$ so $\sum_{i,j} A(i,j)=12pq$. Also v(i)=3 for all of the vertices of the graph. So by using *(1)* we have

$$MTI(G)=\sum_{i,j} v(i)[d(i,j)+A(i,j)]=3\sum_{i,j} d(i,j)+36pq. \qquad (5)$$

Thus if $p=q$ is an even integer, by using *(4)*

$$MTI(G)=3(\frac{4p^3}{3}(14p^2-k_1))+36pq=4\mathrm{p}^2(14\mathrm{p}^3-\mathrm{k}_1\mathrm{p}+9).$$

Also if $p\neq q$ then the results can be obtained by replacing (4) in (5).

Thus the proof is completed.

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