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The first edge-Wiener index of $TUC_4C_8(R)$ nanotube

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In this paper, the first type of edge-Wiener index of $TUC_4C_8(R)$ nanotube is computed.

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1. Introduction

A graph consists of a set of vertices $V(G)$ and a set of edges $E(G)$. In chemical graphs, each vertex presented an atom of the molecule and covalent bonds between atoms are represented by edges between the corresponding vertices. This shape derived from a chemical compound is often called its molecular graph, and can be a path, a tree or in general a graph. A topological index is a single number, derived following a certain rule which can be used to characterize the molecule [4]. Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener [11] introduced Wiener number and the name of Wiener index was given by Hosoya [6]. Wiener index (W) originally defined on trees and studied its use for correlation of physico chemical properties of alkenes, alcohols, amines and their analogous compounds. A number of successful QSAR studies have been made based in the Wiener index and its decomposition forms [2]. In a series of papers, the Wiener index of some nanotubes is computed [1,3,9,10,12].

The definition of this index is as follows:

This index is based on distances between vertices and is named the vertex-Wiener index which defined as follow:

$$W(G)=W_v(G)=\sum_{\{x,y\}\subseteq V(G)} d(x,y) \qquad (1)$$

where $d(u,v)$ is the shortest distance between $u,v\in V(G)$.

The edge versions of Wiener index which is based on distances between edges introduced by Iranmanesh et al. [7]. The first edge-Wiener index defined as follow:

Suppose $e,f\in E(G)$ where $e=uv$ and $f=xy$, set

$$d_1(e,f)=\min\{d(u,x),d(u,y),d(v,x),d(v,y)\}.$$

$d_1(e,f)$ is not distance, because it does not satisfy the distance conditions. We defined new distance due to $d_1(e,f)$ as follows:

$$d_0(e,f)=\begin{cases} d_1(e,f)+1 & ,e\neq f \\ 0 & ,e=f\end{cases}$$

Then, the first edge-Wiener index is:

$$W_{e0}(G)=\sum_{\{e,f\}\subseteq E(G)} d_0(e,f) \qquad (2)$$

In [8], we found the explicit relation between the vertex and the edge versions of Wiener index that we use this relation for computation of the first edge-Wiener index of $TUC_4C_8(R)$. We recall this relation in below:

Definition 1. [8] Let $e=uv,\ \ f=xy$ be the edges of connected graph G. Then, we define:

$$d'(e,f)=\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$$

and $d''(e,f)=\begin{cases}\lceil d'(e,f)\rceil & ,\ \{e,f\}\notin C \\ d'(e,f)+1 & ,\ \{e,f\}\in C\end{cases}$, where

$C=\left\{\{e,f\}\subseteq E(G)\,\middle|\, \begin{array}{l} if\ e=uv\ and\ f=xy; \\ d(u,x)=d(u,y)=d(v,x)=d(v,y)\end{array}\right\}$ and

$d_3(e,f)=\begin{cases} d''(e,f) & e\neq f \\ 0 & e=f\end{cases}.$

Also, d' and d'' do not satisfy the distance conditions therefore, they are not a distance.

In [8], we showed $d_0=d_3$ and therefore

$$W_{e0}(G)=\sum_{\{e,f\}\subseteq E(G)} d_3(e,f) \qquad (3)$$

Definition 2. [8] Due to the distance d_3, we define some sets as follow:

$$A_1=\left\{\{e,f\}\subseteq E(G)\,\middle|\, d_3(e,f)=d'(e,f)\right\},$$

$$A_2 = \left\{ \{e,f\} \subseteq E(G) \middle| \; d_3(e,f) = d'(e,f) + \frac{1}{4} \right\},$$

$$A_3 = \left\{ \{e,f\} \subseteq E(G) \middle| \; d_3(e,f) = d'(e,f) + \frac{2}{4} \right\},$$

$$A_4 = \left\{ \{e,f\} \subseteq E(G) \middle| \; d_3(e,f) = d'(e,f) + \frac{3}{4} \right\}.$$

Theorem 1. [8] The explicit relation between vertex and the first edge-Wiener index for nanotubes which have been consisted of vertices with degree 3 and 2 is:

$$W_{e0}(G) = \frac{9}{4} W_v(G) + \frac{3}{8} \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x,y) - \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=2}} d(x,y) - \frac{m}{4} + \sum_{\{e,f\} \in A_3} \frac{1}{2} + \sum_{\{e,f\} \in A_2} \frac{1}{4}$$

Corollary 1. Since there are not any odd cycles in *$TUC_4C_8(R)$* nanotube, A_2 is empty. Hence for *$TUC_4C_8(R)$* nanotube, we have:

$$W_{e0}(G) = \frac{9}{4} W_v(G) + \frac{3}{8} \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x,y) - \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=2}} d(x,y) - \frac{m}{4} + \sum_{\{e,f\} \in A_3} \frac{1}{2} \tag{4}$$

2. Results

Abbas Heydari and Bijan Taeri in [5] computed the vertex-Wiener index $W_v(G)$ and $\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x,y)$.

We mention only the quantity of them in this paper and omit details.

We denote *$TUC_4C_8(R)$* nanotube with *$T(p,q)$* which p is the number of squares in a row and q is the number of squares in a column. Also, we assumed $P_1 = \left[\frac{p+1}{2} \right]$ and opted below coordinate label for vertices of $T(p,q)$ as shown in Fig. 1.

Lemma 1. [5] $\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x,y) = 2pS_x(q-1)$ where

$$S_x(l) = \sum_{k=0}^{l} T_x(k) = \begin{cases} \frac{8}{3} l^3 + (2p+8) l^2 + (3p^2+2p) l + \left(\frac{19}{3} + \frac{1+(-1)^p}{2} \right) l + 3p^2 + 1 + \frac{1+(-1)^p}{2} & , l < P_1 \\ 6pl^2 + \left(p^2 + 10p - \frac{1-(-1)^p}{2} \right) l + \frac{1}{3} p^3 + p^2 + \frac{11}{3} p - + \frac{1-(-1)^p}{2} & , l \geq P_1 \end{cases}$$

and

$$T_x(k) = \begin{cases} 3p^2 + 4kp + 8k^2 + 8k - 1 + 3\frac{1+(-1)^p}{2} & , 0 \leq k < P_1 \\ p^2 + 12kp + 4p - 1 + \frac{1+(-1)^p}{2} & , k \geq P_1 \end{cases}.$$

Theorem 2. [5] The Wiener index of *$T(p,q)$* is given by the following equation

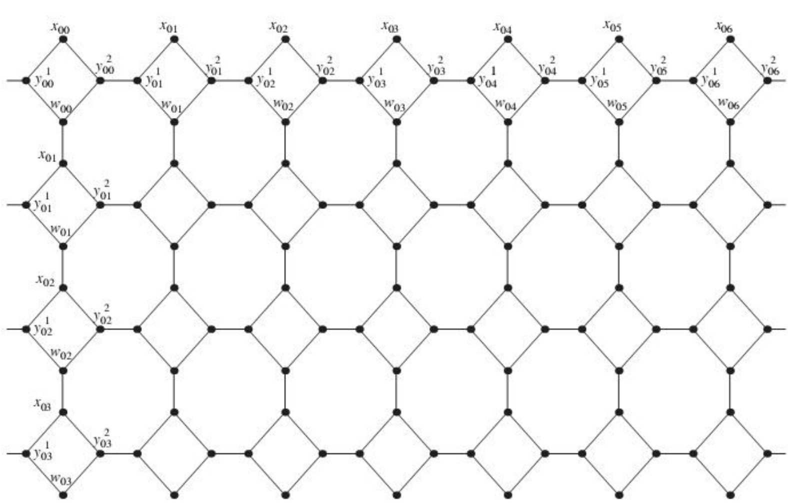

Fig. 1. T(7,4) nanotube.

$$W_v(p,q)=\begin{cases} \frac{pq}{3}\left(8q^3+8pq^2+\left(18p^2-5+3\frac{1+(-1)^p}{2}\right)q-8p\right) & ,q<P_1 \\ \frac{p}{6}\left(-p^4+8qp^3+\left(12q^2+1-\frac{1-(-1)^p}{2}\right)p^2\right)+ \\ \frac{p^2}{6}\left(48q^3-\left(14+3(1+(-1)^p)\right)q\right)+ & ,q\geq P_1 \\ \left(1-\frac{1+(-1)^p}{2}\right)\left(\frac{3}{2}-12q^2\right) \end{cases}$$

Lemma 2. Summation $\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y)$ is equal to in *T(p,q)*:

If p is even:

$$\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y)=\begin{cases} 7q^2-7q+4pq+p^2-2p+1 & ,q<P_1 \\ 3pq+p^2-2p-3q+1 & ,q\geq P_1 \end{cases}$$

If p is odd:

$$\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y)=\begin{cases} 7q^2+q+4pq+p^2-p-2 & ,q<P_1 \\ 3pq+p^2-p+3q-2 & ,q\geq P_1 \end{cases}$$

Proof. There exist two types of vertices with degree 2. One of them is in the first row and another is in the last row (Fig. 1).

Since the situation of all vertices with degree 2 is the same, we can suppose a fix vertex x in first row. Then, we have for the first type:

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in the first row}\\ \deg(y)=2}} d(x,y)=\begin{cases} 2\sum_{i=1}^{\frac{p}{2}} 3i-\frac{3p}{2} & ,\ p \text{ is even} \\ 2\sum_{i=1}^{\frac{p-1}{2}} 3i & ,\ p \text{ is odd} \end{cases}$$

And we have for the second type:

a) p is even:

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in the last row}\\ \deg(y)=2}} d(x,y)=\begin{cases} 2\sum_{i=0}^{q-1}(3q-1+i)+2\sum_{i=0}^{\frac{p}{2}-1}(4q-1+i)- \\ (4q+\frac{p}{2}-1) & ,q<P_1 \\ 2\sum_{i=0}^{\frac{p}{2}-1}(3q-1+i)-(3q+\frac{p}{2}-1) & ,q\geq P_1 \end{cases}$$

b) p is odd:

$$\sum_{\substack{y\in V(T(p,q))\\ y \text{ is in the last row}\\ \deg(y)=2}} d(x,y)=\begin{cases} 2\sum_{i=0}^{q-1}(3q-1+i)+2\sum_{i=0}^{\frac{p+1}{2}-1}(4q-1+i) & ,q<P_1 \\ 2\sum_{i=0}^{\frac{p+1}{2}-1}(3q-1+i) & ,q\geq P_1 \end{cases}$$

Therefore, we can obtain the desire results.

3. Discussion

The number of elements of A_1 is equal to: $(q-1)\binom{p}{2}+p\binom{q}{2}+2p\binom{2q}{2}$.

By Lemmas (1 and 2), Theorem 2, above formula and the fact that the number of edges in *T(p,q)* are $6pq-p$, the following theorem can be proved:

Theorem 3. The first version of edge-Wiener index of *T(p,q)* is equal to:

1. If p is even:

$$W_{e0}(T(p,q))=\begin{cases} -\frac{39}{2}p+2pq^3+6p^2q^4+\frac{9}{8}pq^2(-1)^p+ \\ \frac{3}{8}pq(-1)^p+\frac{27}{2}p^3q^2+6pq^5+ \\ \frac{81}{8}pq+\frac{15}{4}p^2-\frac{115}{8}pq^2-\frac{37}{4}p^2q+ & ,q<P_1 \\ \frac{9}{4}p^3q-2p^3+\frac{3}{2}p^2q^2 \\ \\ -\frac{3}{2}p-\frac{27}{2}q^2+\frac{3}{8}pq(-1)^p+\frac{9}{2}p^3q^2+ \\ \frac{21}{8}pq+\frac{7}{2}p^2+\frac{9}{8}p^2q(-1)^{p+1}+ \\ \frac{27}{16}(-1)^{p+1}+\frac{27}{16}-\frac{3}{8}p^5+\frac{1}{4}p^4+\frac{9}{4}pq^2- & ,q\geq P_1 \\ \frac{85}{8}p^2q+\frac{3}{4}p^3q-\frac{29}{16}p^3+\frac{3}{16}p^3(-1)^p+ \\ 18p^2q^3+27q^2(-1)^p+\frac{9}{2}p^2q^2 \end{cases}$$

2. If p is odd:

$$W_{e0}(T(p,q))=\begin{cases} -\frac{27}{2}p+2pq^3+6p^2q^4+\frac{9}{8}pq^2(-1)^p+ \\ \frac{3}{8}pq(-1)^p+\frac{27}{2}p^3q^2+6pq^5- \\ \frac{47}{8}pq+\frac{7}{4}p^2-\frac{115}{8}pq^2-\frac{37}{4}p^2q+ & ,q<P_1 \\ \frac{9}{4}p^3q-2p^3+\frac{3}{2}p^2q^2 \\ \\ \frac{9}{2}p-\frac{27}{2}q^2+\frac{3}{8}pq(-1)^p+\frac{9}{2}p^3q^2- \\ \frac{75}{8}pq+\frac{3}{2}p^2+\frac{9}{8}p^2q(-1)^{p+1}+ \\ \frac{27}{16}(-1)^{p+1}+\frac{27}{16}-\frac{3}{8}p^5+\frac{1}{4}p^4+ & ,q\geq P_1 \\ \frac{9}{4}pq^2-\frac{85}{8}p^2q+\frac{3}{4}p^3q-\frac{29}{16}p^3+ \\ \frac{3}{16}p^3(-1)^p+18p^2q^3+27q^2(-1)^p+ \\ \frac{9}{2}p^2q^2 \end{cases}.$$

4. Conclusions

The oldest topological index is the ordinary (vertex) version of Wiener index which was introduced by Harold Wiener in 1947. So many scientific works have been done on this index in Chemistry and Mathematics. The edge versions of Wiener index was introduced by Iranmanesh et al. recently. In this paper, the first type of edge-Wiener index of *$TUC_4C_8(R)$* nanotube is computed

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