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Edge-Wiener indices of $TUC_4C_8(S)$

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One of topological indices which introduced recently is edge versions of wiener index. Due to the fact that vertex version of Wiener index is very important topological index, its edge versions are important, too. In this paper, the edge-Wiener indices of $TUC_4C_8(S)$ is computed.

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1. Introduction

The oldest topological index which introduced for determining the boiling point of Paraffin is ordinary (vertex) version of Wiener index which was introduced by Harold Wiener in 1947 [1]. Every one can find so many important researches about this version of Wiener index and its applications in chemistry and graph theory in [2-7]. If G a connected graph with vertex set $V(G)$ and edge set $E(G)$, the vertex –Wiener index was introduces as follow:

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

Iranmanesh et al. introduced edge versions of Wiener index which based on distances between edges in 2008 [8].

The first edge-Wiener index was introduced as follow:

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

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

The like-distance d_1 is

$d_1(e,f) = \min\{d(x,u), d(x,v), d(y,u), d(y,v)\}$ such that $e = xy$ and $f = uv$.

The second edge-Wiener index was introduced as follow:

$$W_{e4}(G) = \sum_{\{e,f\}\subseteq E(G)} d_4(e,f) \tag{3}$$

where $d_4(e,f) = \begin{cases} d_2(e,f) & e \neq f \\ 0 & e = f \end{cases}$.

The like-distance d_2 is:

" $d_2(e,f) = \max\{d(x,u), d(x,v), d(y,u), d(y,v)\}$ such that $e = xy$ and $f = uv$.

Because of the fact that d_1 and d_2 are not satisfying the distance conditions, we say d_1 and d_2 are like-distance. Iranmanesh at al. have been found the explicit relations between vertex and edge versions of Wiener index [9] that we use these relations for computation of edge-Wiener indices of $TUC_4C_8(S)$. We recall these relations in below:

The relation between vertex version and first edge version of Wiener index was introduced as follow:

Definition 1-1. [9] Let $e = uv$, $f = xy$ be the edges of connected graph G. Then, we define:

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

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

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

In reference [9] has been shown $d_3 = d_0$, then $W_{e0}(G) = \sum_{\{e,f\}\subseteq E(G)} d_3(e,f)$.

Definition 1-2. [9] Due to the distance d_3, we define some sets as follow:

$$A_1 = \{\{e,f\} \subseteq E(G) \mid d_3(e,f) = d'(e,f)\},$$

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

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

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

Theorem 1-3. [9] The explicit relation between vertex and 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 1-4. Due to the fact that there are not the odd cycles in $TUC_4C_8(S)$ nanotube, A_2 is empty. Then, we have for $TUC_4C_8(S)$ nanotube:

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

In addition, the relation between vertex version and second edge version of Wiener index was introduced as follow, too:

Definition 1-5. [9] If $e, f \in E(G)$, we define:

$$d'''(e, f) = \begin{cases} \lceil d'(e, f) \rceil & , \ \{e, f\} \notin A_1 \\ d'(e, f) + 1 & , \ \{e, f\} \in A_1 \end{cases} \text{ and}$$

$$d_5(e, f) = \begin{cases} d'''(e, f) & e \neq f \\ 0 & e = f \end{cases}.$$

The mathematical quantity d''' is not distance because it does not satisfy in distance conditions. Then, we say d''' is like-distance.

Due to the fact that $d_5 = d_4$, then $W_{e4}(G) = \sum_{\{e,f\} \subseteq E(G)} d_5(e, f)$.

Theorem 1-6. [9] The explicit relation between vertex and first edge-Wiener number for $TUC_4C_8(S)$ nanotubes which consists of vertices with degree 3 and 2 is:

$$W_{e4}(G) = \frac{9}{4} W_v(G) + \frac{3}{8} \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x,y) - \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=2}} d(x,y) - \frac{m}{4} + \sum_{\{e,f\} \in A_3} \frac{1}{2} + |A_1|. \tag{5}$$

Corollary 1-7. [9] The explicit relation between edge versions of Wiener index is:

$$W_{e4}(G) = W_{e0}(G) + |A_1| - |C| \tag{6}$$

2. Results

In this section, we obtain the first edge-Wiener index of $TUC_4C_8(S)$ nanotube.

Abbas Heydari and Bijan Taeri in [10] obtained a formula for 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.

The Wiener index of many nanotubes has been computed. For example see [2-25].

In $TUC_4C_8(S)$ nanotube, *p* is the number of square in a row and *q* is the number of rows which is shown in Fig. 1.

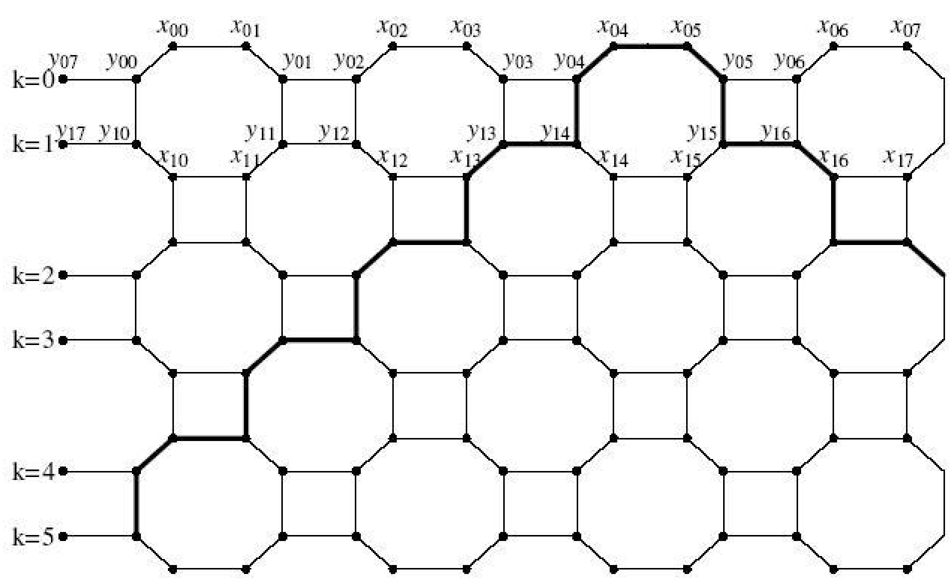

Fig. 1. A TUC4C8(S) Lattice with p = 4 and q = 6.

In [10], some notations are defined as follows. For all $0 \le r < q$ and $0 \le t < 2p$, let $a_{rt} \in \{x_{rt}, y_{rt}\}$ and let $d_{a_{rt}}(k)$ denotes the sum of distances between a_{rt} and vertices on *k-th* row of the graph. By symmetry of the graph for all $0 \le t < 2p$, $d_{x_{rt}}(k)$ are equal. So we may compute this summation for x_{0p} in the 0th row of the graph, which is denoted by $d_x(k)$.

Lemma 2-1. [10] Let $0 \le k < q$, then $d_x(k) = \begin{cases} 4p^2 + 4kp + 2(k^2+k) & , k \le p \\ 2p^2 + 8kp + 2p & , k > p \end{cases}$.

Therefore, according to the Lemma (2-1), we can obtain the $\sum\limits_{\substack{x \in V(G) \\ \deg(x)=2}} \sum\limits_{y \in V(G)} d(x,y)$.

Lemma 2-2.

$$\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x,y) = \begin{cases} \frac{8}{3}pq(6p^2+3pq-3p+q^2-1) & , q \le p \\ 8p^2q(p+2q-1) & , q > p \end{cases}.$$

Proof. Due to the Lemma (2-1), $d_{x_{0p}}(k)$ denotes the sum of distances between x_{0p} and vertices on *k-th* row of the graph. There are *4p* vertices such as x_{0p} in the first row. Therefore:

$$\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x,y) = 4p\sum_{k=0}^{q-1} d_x(k) = \begin{cases} \frac{8}{3}pq(6p^2+3pq-3p+q^2-1) & , q \le p \\ 8p^2q(p+2q-1) & , q > p \end{cases}.$$

The vertex-Wiener index of $TUC_4C_8(S)$ is computed in [10]. We state only the main result as a theorem in follow.

Theorem 2-3. [10] The Wiener index of $TUC_4C_8(S) = G$ is given by the following equation:

$$W_v(G) = \begin{cases} \frac{pq}{3}\left(2q^3+8pq(3p+q)-2q-8p\right) & ,q \le p \\ \frac{p^2}{3}\left(-2p^3+8qp^2+\left(12q^2+2\right)p+16q^3-12q\right)+ & ,q > p \end{cases}$$

Lemma 2-4. Let $TUC_4C_8(S) = G$. Then ,

If p is even:

$$\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=2}} d(x,y) = \begin{cases} q^2+2q+2pq+4p^2-p-2-2\left[\frac{2p-2q+1}{4}\right] & ,q \le p \\ 4pq+3p^2-2p-1 & ,q > p \end{cases}$$

If p is odd:

$$\sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=2}} d(x,y) = \begin{cases} q^2+q+2pq+2p^2-3p+8\left[\frac{p}{2}\right]+8\left[\frac{p}{2}\right]^2-2\left[\frac{2p-2q+1}{4}\right] & ,q \le p \\ 4pq+p^2-2p+8\left[\frac{p}{2}\right]+8\left[\frac{p}{2}\right]^2 & ,q > p \end{cases}$$

Proof. There exist two group of vertices which have degree 2. One group is vertices in the first row and another is the vertices in the last row.

Due to the fact that the situation of all vertices with degree 2 is same, we suppose the fix vertex *x* is in first row. Then, we have for the first group:

$$\sum_{\substack{y \in V(T(p,q)) \\ y \text{ is in first row} \\ \deg(y)=2}} d(x,y) = \begin{cases} \left(\sum\limits_{k=0}^{\frac{p-2}{2}}(16k+16)\right)-(4p+1) & , p \text{ is even} \\ \sum\limits_{k=0}^{\left[\frac{p-2}{2}\right]}(16k+16) & , p \text{ is odd} \end{cases}.$$

And we have for the second group:

a) p is even:

$$\sum_{\substack{y \in V(T(p,q)) \\ y \text{ is in last row} \\ \deg(y)=2}} d(x,y) = \begin{cases} \sum\limits_{i=2q}^{3q-1}(2i)+\sum\limits_{i=3q-1}^{2p+q-1}(i)-2(\left[\frac{2p-2q-3}{4}\right]+1)-q & ,q \le p \\ \sum\limits_{i=2q}^{2q+p-1}(2i)-p & ,q > p \end{cases}$$

b) p is odd:

$$\sum_{\substack{y \in V(T(p,q)) \\ y \text{ is in last row} \\ \deg(y)=2}} d(x,y) = \begin{cases} \sum\limits_{i=2q}^{3q-1}(2i)+\sum\limits_{i=3q-1}^{2p+q-1}(i)-2\left[\frac{2p-2q-4}{4}\right]-2p-2q-3 & ,q \le p \\ \sum\limits_{i=2q}^{2q+p-1}(2i)-p & ,q > p \end{cases}$$

Therefore, we can get results with the above summations.

Observation 2-5. The number of elements of A_3 is equal to: $4p\binom{q}{2}+(q-1)\binom{2p}{2}$.

Due to the fact that the number of edges in $TUC_4C_8(S)$ is $6pq-2p$, we state the first edge-Wiener index of $TUC_4C_8(S)$.

Theorem 2-6. The first version of edge-Wiener index of $TUC_4C_8(S)=G$ is equal to:

1. If *p* is even:

$$W_{e0}(T(p,q))=\begin{cases}\frac{3}{2}pq^4+18p^3q^2+6p^2q^3-\frac{pq^2}{2}-8p^2q+6p^3q+3p^2q^2-6pq+pq^3- \\ \quad q^2-2q-5p^2+2p+2+2\left[\frac{2p-2q+1}{4}\right] & ,q\le p \\ \frac{15}{2}p^5+6p^4q+\frac{3p^3}{2}+12p^2q^3-11p^2q+3p^3q+6p^2q^2-7pq-4p^2+ \\ \quad 3p+pq^2+1 & ,q>p\end{cases}$$

2. If *p* is odd:

$$W_{e0}(T(p,q))=\begin{cases}\frac{3}{2}pq^4+18p^3q^2+6p^2q^3-\frac{pq^2}{2}-8p^2q+6p^3q+3p^2q^2-6pq+pq^3- \\ \quad q^2-q-3p^2+2\left[\frac{2p-2q+1}{4}\right]-8\left[\frac{p}{2}\right]-8\left[\frac{p}{2}\right]^2 & ,q\le p \\ \frac{15}{2}p^5+6p^4q+\frac{3p^3}{2}+12p^2q^3-11p^2q+3p^3q+6p^2q^2-7pq-2p^2+ \\ \quad 3p+pq^2-8\left[\frac{p}{2}\right]-8\left[\frac{p}{2}\right]^2 & ,q>p\end{cases}$$

Proof. According to Lemmas (2-2 and 2-4), Theorem (2-3) and observation (2-5), we can conclude these results easily.

3. Discussion

In this section, by relations (5 and 6) and previous part, we compute the second edge-Wiener index of $TUC_4C_8(S)$.

Theorem 3-5. The second version of edge-Wiener index of $TUC_4C_8(S)=G$ which *p* is the number of squares in a row and *q* is the number of rowa is equal to:

1. If *p* is even, then

$$W_{e0}(T(p,q))=\begin{cases}\frac{3}{2}pq^4+18p^3q^2+6p^2q^3-\frac{pq^2}{2}-22p^2q+6p^3q+21p^2q^2-6pq+pq^3- \\ \quad 2pq^2-q^2-2q-p^2+2p+2+2\left[\frac{2p-2q+1}{4}\right] & ,q\le p \\ \frac{15}{2}p^5+6p^4q+\frac{3p^3}{2}+12p^2q^3-25p^2q+3p^3q+24p^2q^2-7pq+ \\ \quad 3p-pq^2+1 & ,q>p\end{cases}$$

2. If *p* is odd, then

$$W_{e0}(T(p,q))=\begin{cases}\frac{3}{2}pq^4+18p^3q^2+6p^2q^3-\frac{pq^2}{2}-22p^2q+6p^3q+21p^2q^2-6pq+pq^3- \\ \quad 2pq^2-q^2-q+p^2+2\left[\frac{2p-2q+1}{4}\right]-8\left[\frac{p}{2}\right]-8\left[\frac{p}{2}\right]^2 & ,q\le p \\ \frac{15}{2}p^5+6p^4q+\frac{3p^3}{2}+12p^2q^3-25p^2q+3p^3q+24p^2q^2-7pq+2p^2+ \\ \quad 3p-pq^2-8\left[\frac{p}{2}\right]-8\left[\frac{p}{2}\right]^2 & ,q>p\end{cases}$$

Proof. The number of edges of $TUC_4C_8(S)$ nanotube with *p* squares in a row and *q* rows is $6pq-2p$. In molecular graph of this nanotube we have: $E(G)=A_1\cup A_3$, and

$$|A_3|=4p\binom{q}{2}+(q-1)\binom{2p}{2}.$$

Therefore, according to reference [10] and $|A_1|=18p^2q^2-14p^2q+4p^2-2pq^2$, the $W_{e4}(G)$ computed easily by relation (6).

4. Conclusions

In this paper, at first we obtained the fisr edge-Wiener index of $TUC_4C_8(S)$ and then obtained the second edge-Wiener index of $TUC_4C_8(S)$.

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