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# On Edge-Wiener Indices of Some Nanotubes

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**Abstract:** One of topological indices which introduced very 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 and they will find much applications in chemistry and mathematics such as its vertex version. In this paper, the edge-Wiener indices of some nanotubes are computed by using the explicit relation between vertex and edge versions of Wiener index.

**Key words:** Vertex-wiener index . edge-wiener indices . molecular graph . nanotube.introduction

## 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 [2-9]. 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 [10]. 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

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

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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 [11] that we use these relations for computation of edge-Wiener indices of $TUC_4C_8(R)$. 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:** [11] Let e = xy, *f* = uv be the edges of connected graph G. Then, we define:

$$d'(e,f) = \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4} \quad \text{and} \quad d''(e,f) = \begin{cases} \lceil d'(e,f) \rceil & , \{e,f\} \notin C \\ d'(e,f)+1 & , \{e,f\} \in C \end{cases}$$

where

$$C = \left\{ \{e,f\} \subseteq E(G) \middle| \begin{array}{l} \text{if } e = uv \text{ and } f = xy; \\ d(u,x) = d(u,y) = d(v,x) = d(v,x) \end{array} \right\} \quad \text{and} \quad d_3(e,f) = \begin{cases} d''(e,f) & e \neq f \\ 0 & e = f \end{cases}$$

Also, d′ and d″ do not satisfy at distance conditions then, they are not a distance and they are very similar to $d_1$ and $d_2$ in that they both are not distance and are like-distance.

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:** [11] 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:** [11] 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 $TUC_4C_8(R)$ nanotube, $A_2$ is empty. Then, we have for $TUC_4C_8(R)$ 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:** [11] 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:** [11] The explicit relation between vertex and first edge-Wiener number for $TUC_4C_8(R)$ 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:** [11] The explicit relation between edge versions of Wiener index is:

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

In [9], the edge Wiener indices of Zigzag nanotube such that p is even integer and q is odd integer which p is the number of hexagons in a row and q is the number of hexagons in column Fig. 1.

**Theorem 1-8:** [11] The edge-Wiener number of zig-zag nanotube G which has p hexagons in a row and q hexagons in column such that p is even integer and q is odd integer is:

$$W_{e0}(G)=\begin{cases} pq\begin{pmatrix}\frac{9}{4}qp^2+\frac{3}{4}q^2p-\frac{35}{8}p+\frac{3}{8}q^3-\\ \frac{11}{16}q+\frac{3}{4}p^2+\frac{3}{4}pq+\frac{1}{4}q^2-\frac{1}{4}\end{pmatrix}-p\left(\frac{29}{16}p^2-\frac{15}{4}p-\frac{55}{16}\right) & ,q<p\\ pq\left(\frac{3}{2}p^3+3pq^2-\frac{27}{4}p+\frac{3}{2}pq+\frac{q}{2}+\frac{1}{4}\right)-p\left(\frac{3}{8}p^4-\frac{1}{8}p^2+\frac{11}{4}p\right) & ,p\leq q\end{cases}$$

**Theorem 1-9:** [11] The second edge-Wiener number of zig-zag nanotube G which has p hexagons in a row and q hexagons in column such that p is even integer and q is odd integer is:

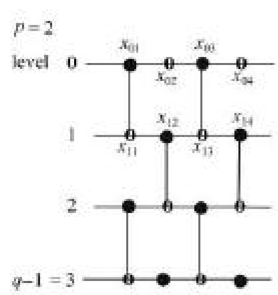


Fig. 1: The zigzag nanotube

$$W_{e4}(G)=\begin{cases} pq\left(\frac{9}{4}qp^2+\frac{3}{4}q^2p-\frac{35}{8}p+\frac{3}{8}q^3-\frac{11}{16}q+\frac{3}{4}p^2+\frac{3}{4}pq+\frac{1}{4}q^2-\frac{1}{4}\right)-p\left(\frac{29}{16}p^2-\frac{15}{4}p-\frac{55}{16}\right)+\binom{3pq+2p}{2}-\frac{2pq^2+qp^2+pq}{2} & ,q<p \\ pq\left(\frac{3}{2}p^3+3pq^2-\frac{27}{4}p+\frac{3}{2}pq+\frac{q}{2}+\frac{1}{4}\right)-p\left(\frac{3}{8}p^4-\frac{1}{8}p^2+\frac{11}{4}p\right)+\binom{3pq+2p}{2}-\frac{2pq^2+qp^2+pq}{2} & ,p\le q \end{cases}$$

## MAIN RESULTS

In this section we compute the edge Wiener indices of $TUC_4C_8(R)$ and armchair nanotubes.

**The first edge-Wiener index of $TUC_4C_8(R)$:** Abbas Heydari and Bijan Taeri wrote a paper with subject "Wiener and Schultz indices of $TUC_4C_8(R)$ nanotube". Because of the formula of Schultz index, they computed the vertex-Wiener index $W_v(G)$ and $\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{y\in V(G)} d(x,y)$ in their paper [12]. We mention only the quantity of them in this paper and omit details.

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

**Lemma 2-1-1:** [12]

$$\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{y\in V(G)} d(x,y)=2pS_x(q-1)$$

where

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

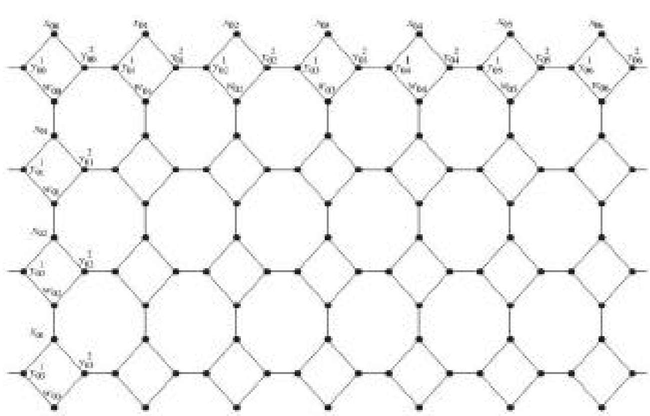

Fig. 2:

and

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

**Theorem 2-1-2:** [12] The Wiener index of $T(p,q)$ is given by the following equation:

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

**Lemma 2-1-3:** Summation $\sum\limits_{\substack{x\in V(G)\\ \deg(x)=2}}\sum\limits_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y)$ is equal to in $T(p,q)$:

If p is even:

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

If p is odd:

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

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

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

And we have for second group:

a) p is even:

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

b) p is odd:

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

Therefore, we can get results with above summations.

**Observation 2-1-4:** The number of elements of $A_1$ is equal to: $(q-1)\binom{p}{2}+p\binom{q}{2}+2p\binom{2q}{2}$.

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

Theorem 2-1-5: The first version of edge-Wiener index of T(p,q) is equal to:

1. If p is even:

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

2. If p is odd:

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

**Proof:** According to lemmas (2-1-1 and 2-3), theorem (2-1-2) and observation (2-1-4), we can conclude these results easily.

**The second edge-Wiener index of $TUC_4C_8(R)$:** Now, due t the relations (5 and 6) and previous part, we compute the second edge-Wiener index of $TUC_4C_8(R)$.

**Theorem 2-2-1:** The second version of edge-Wiener index of T(p,q) = $TUC_4C_8(R)$ which p is the number of squares in a row and q is the number of squares in a column is equal to:

1. If p is even:

$$W_{e4}(T(p,q))=\begin{cases} -\frac{39}{2}p+2pq^3+6p^2q^4+\frac{9}{8}pq^2(-1)^p+\frac{3}{8}pq(-1)^p+\frac{27}{2}p^3q^2+6pq^5+\frac{81}{8}pq+\frac{15}{4}p^2 \\ -\frac{115}{8}pq^2-\frac{37}{4}p^2q+\frac{9}{4}p^3q-2p^3+\frac{3}{2}p^2q^2+\binom{6pq-p}{2}-\frac{7pq^2+qp^2-5pq-p^2-q^2}{2} & ,q<P_1 \\ \\ -\frac{3}{2}p-\frac{27}{2}q^2+\frac{3}{8}pq(-1)^p+\frac{9}{2}p^3q^2+\frac{21}{8}pq+\frac{7}{2}p^2+\frac{9}{8}p^2q(-1)^{p+1}+\frac{27}{16}(-1)^{p+1}+\frac{27}{16}-\frac{3}{8}p^5+\frac{1}{4}p^4+\frac{9}{4}pq^2 \\ -\frac{85}{8}p^2q+\frac{3}{4}p^3q-\frac{29}{16}p^3+\frac{3}{16}p^3(-1)^p+18p^2q^3+27q^2(-1)^p+\frac{9}{2}p^2q^2+\binom{6pq-p}{2}-\frac{7pq^2+qp^2-5pq-p^2-q^2}{2} & ,q\geq P_1 \end{cases}$$

2. If p is odd:

$$W_{e4}(T(p,q)) = \begin{cases} -\frac{27}{2}p + 2pq^3 + 6p^2q^4 + \frac{9}{8}pq^2(-1)^p + \frac{3}{8}pq(-1)^p + \frac{27}{2}p^3q^2 + 6pq^5 - \frac{47}{8}pq + \frac{7}{4}p^2 \\ -\frac{115}{8}pq^2 - \frac{37}{4}p^2q + \frac{9}{4}p^3q - 2p^3 + \frac{3}{2}p^2q^2 + \binom{6pq-p}{2} - \frac{7pq^2+qp^2-5pq-p^2-q^2}{2} & , q < P_1 \\ \\ \frac{9}{2}p - \frac{27}{2}q^2 + \frac{3}{8}pq(-1)^p + \frac{9}{2}p^3q^2 - \frac{75}{8}pq + \frac{3}{2}p^2 + \frac{9}{8}p^2q(-1)^{p+1} + \frac{27}{16}(-1)^{p+1} + \frac{27}{16} - \frac{3}{8}p^5 + \frac{1}{4}p^4 + \frac{9}{4}pq^2 \\ -\frac{85}{8}p^2q + \frac{3}{4}p^3q - \frac{29}{16}p^3 + \frac{3}{16}p^3(-1)^p + 18p^2q^3 + 27q^2(-1)^p + \frac{9}{2}p^2q^2 + \binom{6pq-p}{2} - \frac{7pq^2+qp^2-5pq-p^2-q^2}{2} & , q \geq P_1 \end{cases}$$

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

$$|A_3| = \frac{7pq^2 + qp^2 - 5pq - p^2 - q^2}{2}$$

Therefore, according to reference [10] and

$$|A_1| = \binom{6pq-p}{2} - \frac{7pq^2 + qp^2 - 5pq - p^2 - q^2}{2}$$

the $W_{e4}(G)$ computed easily by relation (6).

## CONCLUSIONS

The First and second edge-Wiener indices of $TUC_4C_8(R)$ is computed by using the explicit relation between vertex and edge versions of Wiener index and they are stated as the mathematical formulas.

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