Computation of the first edge-Wiener index of $TUAC_6$[P,Q] nanotube

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Wiener index was introduced by Harold Wiener in 1947. This index is the sum of distance between all vertices of a graph. The edge versions of Wiener index were introduced by Iranmanesh et al., recently. In this paper, the first edge Wiener index of $TUAC_6$[p,q] nanotube is computed.

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1. Introduction

We denote the set of vertices of connected graph G with $V(G)$ and set of edges with $E(G)$. In a molecular graph, each vertex denotes an atom and edges denote the bond of between atoms. A topological index is a real number which describes the molecular graph.

The oldest topological index which is vertex-Wiener index was introduced by Harold Wiener [1]. He introduced this index for comparing and describing the relation between Physical-Chemical properties.

The definition of this index is as follows:

If $u,v \in V(G)$ and $d(u,v)$ is the shortest distance between them, then

$$W(G) = \frac{1}{2}\sum_{u,v \in V(G)} d(u,v) \qquad (1)$$

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

The edge-Wiener index was introduced by Iranmanesh et al. in [26] as follow:

Suppose $e,f \in E(G)$ where $e=(u,v), f=(x,y)$.

Set

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

We define new distance due to $d_1(e,f)$ as follows:

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

The first edge-Wiener index is introduced as follows:

$$W_{e0}(G) = \frac{1}{2}\sum_{e,f \in E(G)} d_0(e,f) \qquad (2)$$

Also we define edge-Wiener index-like as follows:

$$W_{e1}(G) = \frac{1}{2}\sum_{e,f \in E(G)} d_1(e,f) \qquad (3)$$

Accordingly, we have

$$W_{e0}(G) = W_{e1}(G) + \frac{1}{2}m(m-1)$$

where $|E(G)| = m$.

The edge Wiener index of $TUAC_6[p,q]$ nanotube is computed in this paper.

2. The first edge Wiener index of $TUAC_6$[p,q]

Armchair polyhex nanotube graph, that denoted by $TUAC_6[p,q]$, is a nanotube that p and q are the number of hexagons in length and width of molecular graph, respectively. Also, it has j rows which $1 \le j \le q$.

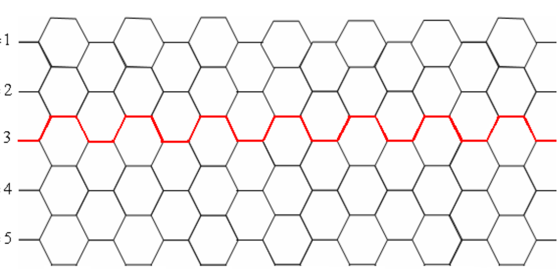

Fig. 1. $TUAC_6[7,5]$ nanotube with $1 \le j \le 5$ rows.

2.1 Definition

$$A_1 = \{\bigcup_{j=1}^{q}\{e \in E(G) \mid e \text{ is an upper horizontal edge in the } j^{th} \text{ row}\}\}$$
$$\bigcup\{e \in E(G) \mid e \text{ is a horizontal edge, below the } q^{th} \text{ row}\}$$

$$A_2 = \bigcup_{j=1}^{q}\{e \in E(G) \mid e \text{ is an underneath horizontal edge in the } j^{th} \text{ row}\}$$

$$B_1 = \bigcup_{j=1}^{q} \left\{ e \in E(G) \middle| e \text{ is an oblique edge in the } j^{th} \text{ row} \right\}$$

$$B_2 = \bigcup_{j=1}^{q} \left\{ e \in E(G) \middle| e \text{ is an oblique edge between the } j^{th} \text{ and } j+1^{th} \text{ row} \right\}$$

Therefore, we have

$$|E(G)| = |A_1| + |A_2| + |B_1| + |B_2| = 6pq + p\,.$$

Also, we have

$$W_{e1}(G) = W_{e1}(A_1,G) + W_{e1}(A_2,G) + W_{e1}(B_1,G) + W_{e1}(B_2,G)$$

For compute the first edge-Wiener index, we need three cases: $q \prec \left[\frac{p}{2}\right]$, $q = \left[\frac{p}{2}\right]$ and $q \succ \left[\frac{p}{2}\right]$.

In addition, we use the notation $_{X}W_{e1}(e_Y, G)$ and $W_{e1}(e_Y, G)_j$ for W_{e1} if e is fix edge from set Y and for region X and row j, respectively.

Case 1. $q \prec \left[\frac{p}{2}\right]$

(i): p is even.

Lemma 1. Suppose $e \in A_1$, then there are two region R *and* R' in Fig. 2, such that

$$_{R}W_{e1}(e_{A1},G) = \left(\sum_{j=0}^{2q-1} \sum_{i=2j}^{2q+j-1} i\right) + \left(\sum_{k=1}^{2q} \sum_{i=k}^{\left\lceil \frac{2q+k-1}{2} \right\rceil} (2i-1)\right)$$

$$_{R}W_{e1}(e_{A1},G) = \left(\sum_{j=1}^{\left[\frac{p}{2}\right]-q} \sum_{i=4j-1}^{4q+4j-1} i\right) + \left(\sum_{j=\left[\frac{p}{2}\right]-q+1}^{\left[\frac{p}{2}\right]} \sum_{i=4j-1}^{2p-1} i\right)$$

$$+\left(\sum_{k=1}^{\left[\frac{p}{2}\right]-q} \sum_{\left[\frac{4k-1}{2}\right]}^{\left[\frac{4k-1}{2}\right]+2q-1} 2i\right) + \left(\sum_{k=\left[\frac{p}{2}\right]-q+1}^{\left[\frac{p}{2}\right]} \sum_{i=\left[\frac{4k-1}{2}\right]}^{p-1} 2i\right)$$

Proof. The regions R *and* R' are shown in Fig. 2. For computing $_{R}W_{e1}(e_{A1},G)$ and $_{R}W_{e1}(e_{A1},G)$, we consider the rows k, j in Fig. 2. Due to the rows and distances between edge $e \in A_1$ and other edges in region R, $_{R}W_{e1}(e,G)$ can compute easily. According to the fact that the oblique line in Fig. 2 do not intersect of the symmetry line, we obtain our results for each row separately. Hence, we give two distinct formulas for $1 \le j \le \left[\frac{p}{2}\right] - q$ and $\left[\frac{p}{2}\right] - q + 1 \le j \le \left[\frac{p}{2}\right]$. Also, we continue this for the procedure row k according to bounds of summations. Thus we obtain the desire results.

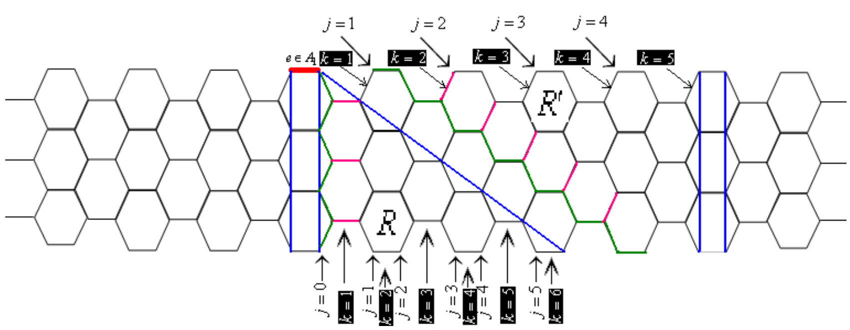

Fig. 2. The regions R and R' in TUAC$_6$[10,3] for $e \in A_1$ where $q \prec \left[\frac{p}{2}\right]$.

Lemma 2. Suppose $e \in A_1$, then

$$W_{e1}(e_{A1},G)_1 = 2({}_{R}W_{e1}(e_{A1},G) + {}_{R}W_{e1}(e_{A1},G)) + t_1$$

where $t_1 = \left(\sum_{i=1}^{q} 2i\right) - (q+1)(2p-1)$.

Proof. In Fig. 2, $W_{e1}(e_{A1},G)_1$ is equal to $2({}_{R}W_{e1}(e_{A1},G) + {}_{R}W_{e1}(e_{A1},G)) + t_1$, where t_1 is sum of the distances between edges on symmetry line

Lemma 3. For the set A_1, we have:

$$W_{e1}(A_1,G) = \frac{1}{2}\left(\left(\sum_{j=1}^{q} pW_{e1}(e_{A1},G)_j\right) + pW_{e1}(e_{A1},G)_1\right)$$

Proof. Let $e \in A_1$ be an edge on j th row. We divide the graph $TUAC_6[p,q]$ in two sub-graphs $G_1 = TUAC_6[p, j-1]$ and $G_2 = TUAC_6[p, q-j+1]$ which have been indicated in Fig. 3. In this case, we have:

$$W_{e1}(e_{A1},G)_j = W_{e1}(e_{A1},G_1)_1 + W_{e1}(e_{A1},G_2)_1 - t_2$$

where t_2 is equal to the sum of distances between edges which located in common region between graph G_1 and G_2, that is,

$$t_2 = 2\left(\sum_{i=0}^{\left[\frac{p}{2}\right]-1} (4i+3)\right) - (2p-1)$$

Now, since there are p edges in the set A_1 in each row and p horizontal edges below the row q, we obtain the desire result.

Lemma 4. *Suppose* $e \in A_2$. *Then*

$$W_{e1}(e_{A2},G)_1 = W_{e1}(e_{A1},G)_1 + t_3 - (2p-1)$$

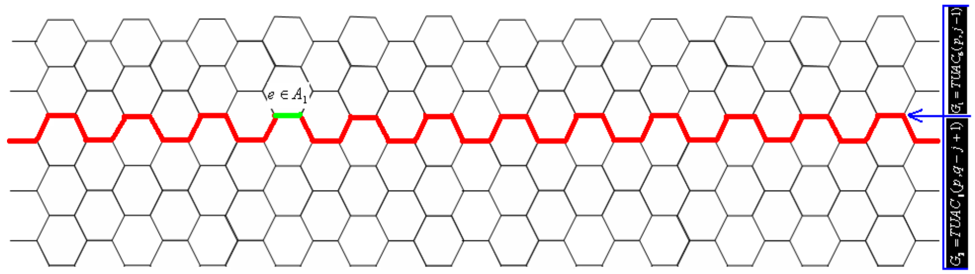

Fig. 3. Dividing the graph TUAC$_6$[12,5] in two sub-graph TUAC$_6$[12,2] and TUAC$_6$[12,3] for $e \in A_1$ where $q \prec \left[\frac{p}{2}\right]$.

where

$$t_3 = 2((\sum_{i=2q-1}^{2p-2} i) - (\sum_{i=q+1}^{2q-1}(2i-1))) -$$

$$(2q + 2((\sum_{i=2q-1}^{2p-2} i) + (\sum_{i=q+1}^{2q-1}(2i-1)) - (\sum_{i=q+1}^{\left[\frac{p}{2}\right]}(4i-3))))$$

Proof. Let $e \in A_2$ be a fix and grey edge in Fig.4. According to this figure, for computing $W_{e1}(e_{A2},G)_1$, at first we need obtain the sum of distances between edges on green rectangular. This quantity is equal to the first term of t_3. Then by the commute of the graph such that the grey edge matches on the upper horizontal edge (red edge). The sum of distances from $e \in A_2$ to other edges is equal to $W_{e1}(e_{A2},G)_1$ minus the sum of distances between edges on below green rectangular in Fig. 4. Therefore, we can get $W_{e1}(e_{A2},G)_1$ with add the summation of distances between edges on upper green rectangular to the computation.

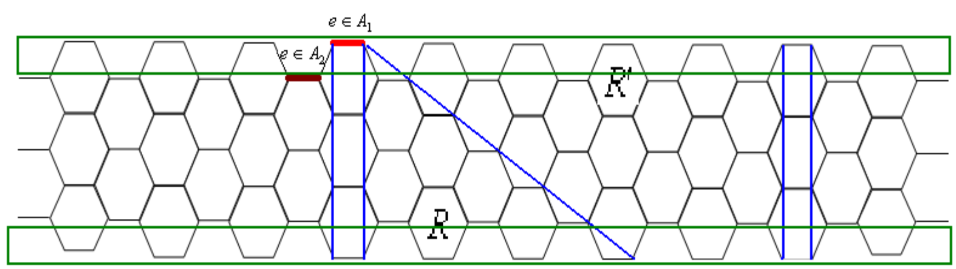

Fig. 4. Computing $W_{e1}(e_{A2},G)_1$ for $e \in A_2$ where $q \prec \left[\frac{p}{2}\right]$.

Lemma 5. For the set A_2, we have

$$W_{e1}(A_2,G) = \frac{1}{2}\sum_{j=1}^{q} pW_{e1}(e_{A2},G)_j$$

Proof. Let $e \in A_2$ be an edge on j th row. We divide the graph $TUAC_6[p,q]$ in two sub-graphs $G_1 = TUAC_6[p,j]$ and $G_2 = TUAC_6[p,q-j+1]$ which have been indicated in Fig.5.

In this case, we have:

$$W_{e1}(e_{A2},G)_j = W_{e1}(e_{A2},G_1)_1 + W_{e1}(e_{A2},G_2)_1 - t_4 - t_5$$

where t_4 and t_5 are the sum of distances on the row j and the sum of distances of between edges over the edge $e \in A_2$. That is,

$$t_4 = 2(\sum_{i=0}^{2p-2} i) + (2p-1)\ ,\ t_5 = 2((\sum_{i=1}^{2p-2} i) - (\sum_{i=0}^{\left[\frac{p}{2}\right]-2}(4i+3)))$$

Therefore, since there are p edges in the set A_2 in each row, we can obtain the desire result.

Lemma 6. Let $e \in B_1$. According to Fig. 6, there are 4 regions for $e \in B_1$ in $TUAC_6[p,q]$ that they satisfy the following relations:

$${}_{R''}W_{e1}(e_{B1},G) = (\sum_{j=1}^{2q-1}\sum_{i=2j-1}^{2q+j-2} i) + (\sum_{k=0}^{2q-1}\sum_{i=k}^{\left[\frac{2q+k-1}{2}\right]} 2i)$$

$${}_{R}W_{e1}(e_{B1},G) = (\sum_{j=0}^{2q-1}\sum_{i=2j}^{2q+j-2} i) + (\sum_{k=1}^{2q-1}\sum_{i=k}^{\left[\frac{2q+k-1}{2}\right]} (2i-1))$$

$${}_{R_1}W_{e1}(e_{B1},G) = (\sum_{j=1}^{\left[\frac{p}{2}\right]-q}\sum_{i=4j-2}^{4q+4j-2} i) + (\sum_{j=\left[\frac{p}{2}\right]-q+1}^{\left[\frac{p}{2}\right]}\sum_{i=4j-2}^{2p-1} i)$$

$$+(\sum_{k=1}^{\left[\frac{p}{2}\right]-q}\sum_{i=\left[\frac{4k-1}{2}\right]}^{\left[\frac{4k-1}{2}\right]+2q-1}(2i-1)) + (\sum_{k=\left[\frac{p}{2}\right]-q+1}^{\left[\frac{p}{2}\right]}\sum_{i=\left[\frac{4k-1}{2}\right]}^{p}(2i-1))$$

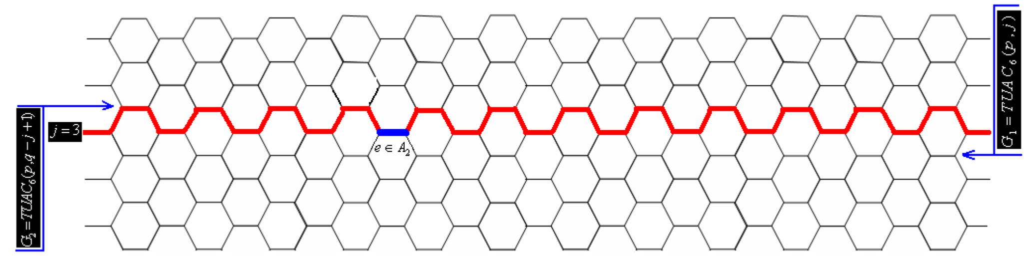

Fig. 5. Dividing the graph TUAC$_6$[12,5] in two sub-graph TUAC$_6$[12,3] and TUAC$_6$[12,3] for $e \in A_2$ where $q \prec \left[\frac{p}{2}\right]$.

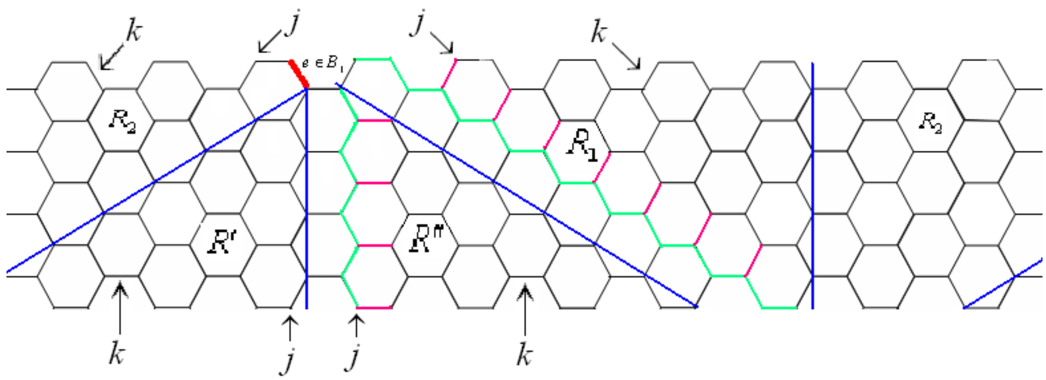

Fig. 6. The regions R', R'', R_1 and R_2 in TUAC$_6$[10,4] for $e \in B_1$ where $q \prec \left[\frac{p}{2}\right]$.

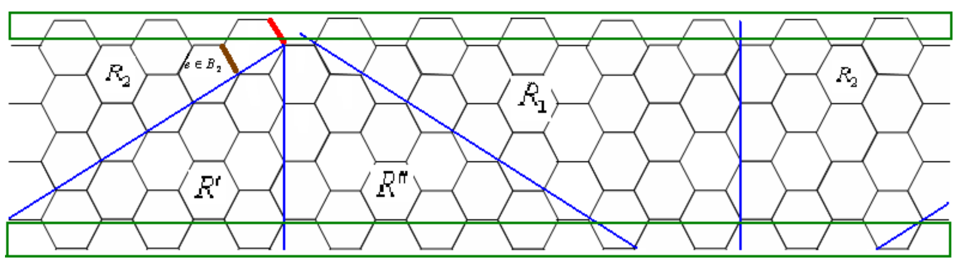

Fig. 7. Computing $W_{e1}(e_{B2},G)_1$ for $e \in B_2$ where $q \prec \left[\frac{p}{2}\right]$.

$$
{}_{R_2}W_{e1}(e_{B1},G) = \Big(\sum_{j=1}^{\left[\frac{p}{2}\right]-q}\ \sum_{i=4j-4}^{4q+4j-4} i\Big) + \Big(\sum_{j=\left[\frac{p}{2}\right]-q+1}^{\left[\frac{p}{2}\right]}\ \sum_{i=4j-2}^{2p-2} i\Big)
$$

$$
+\Big(\sum_{k=1}^{\left[\frac{p}{2}\right]-q}\ \sum_{i=\left[\frac{4k-1}{2}\right]}^{\left[\frac{4k-1}{2}\right]+2q-1} (2i+1)\Big) + \Big(\sum_{k=\left[\frac{p}{2}\right]-q+1}^{\left[\frac{p}{2}\right]}\ \sum_{i=\left[\frac{4k-1}{2}\right]}^{p-2} (2i+1)\Big)
$$

$$
+\Big(\sum_{i=2}^{q-1} 2i\Big)
$$

Lemma 7. Let $e \in B_1$ in Fig. 6, then

$$
W_{e1}(e_{B1},G)_1 = {}_{R''}W_{e1}(e_{B1},G) + {}_{R'}W_{e1}(e_{B1},G) + {}_{R_1}W_{e1}(e_{B1},G) + {}_{R_2}W_{e1}(e_{B1},G)
$$

Lemma 8. Let $e \in B_2$ in Fig. 7, then

$$
W_{e1}(e_{B2},G)_1 = W_{e1}(e_{B1},G)_1 + t_6
$$

where

$$
t_6 = \left(\left(\sum_{i=1}^{2p-1} i\right) - \left(\sum_{i=1}^{\left[\frac{p}{2}\right]-1} (4i+2)\right)\right) + \left(\left(\sum_{i=1}^{2p-2} i\right) - \left(\sum_{i=1}^{\left[\frac{p}{2}\right]-1} 4i\right)\right)
$$

$$
-\left((2q-2) + 2\left(\sum_{i=2q-1}^{2p-2} i\right) + \left(\sum_{i=2q-1}^{4q-4} i\right) - \left(\sum_{i=2q}^{p-1} 2i\right) + (2p-1)\right)
$$

Lemma 9. For the set B_1, we have

$$
W_{e1}(B_1,G) = \frac{1}{2}\Big(\Big(\sum_{j=1}^{q} 2pW_{e1}(e_{B1},G)_j\Big) + 2pW_{e1}(e_{B1},G)_1\Big)
$$

Proof. Let $e \in B_1$ be an edge on j^{th} row. We divide the graph $TUAC_6[p,q]$ in two sub-graphs $G_1 = TUAC_6[p,j]$ and $G_2 = TUAC_6[p,q-j+1]$. which have been indicated in Fig. 8. Therefore, we have:

$$W_{e1}(e_{B1},G)_j = W_{e1}(e_{B2},G_1)_1 + W_{e1}(e_{B1},G_2)_1 - t_4 - t_7$$

where t_7 is the sum of distances between fix edge e and the other edges, that is,

$$t_7 = ((\sum_{i=1}^{2p-1} i) - (\sum_{i=1}^{\left[\frac{p}{2}\right]-1} (4i+2))) + ((\sum_{i=1}^{2p-2} i) - (\sum_{i=1}^{\left[\frac{p}{2}\right]-1} 4i))$$

Now, according to the facts that there are 2p edges in set B_1 in each row and 2p oblique edges in under of q^{th} -row, the desire result is obtain.

Lemma 10. Let $e \in B_2$, then we have,

$$W_{e1}(B_2,G) = \frac{1}{2}\sum_{j=1}^{q-1} 2pW_{e1}(e_{B2},G)_j$$

Proof. With the following fact

$$W_{e1}(e_{B2},G)_j = W_{e1}(e_{B1},G_1)_1 + W_{e1}(e_{B2},G_2)_1 - t_4 - t_7$$

and with the similar of the proof of Lemma 9, we obtain the desire results.

Corollary 1.

$$W_{e1}(G) = \frac{1}{2}p - 6p^2q - \frac{1}{2}p^2 + \frac{1}{2}p^3 + 4pq^3 + 6pq^4 + 4pq^2 - 18p^2q^2 + 18p^3q^2 + 6p^3q$$

By the above results, we can state the following theorem:

Theorem 1. Let p be an even number and $q \prec \left[\frac{p}{2}\right]$.

Then

$$W_{e0}(G) = \frac{1}{2}p^3 + 4pq^3 + 6pq^4 + 4pq^2 + 18p^3q^2 + 6p^3q - 3pq$$

(ii): p is odd.

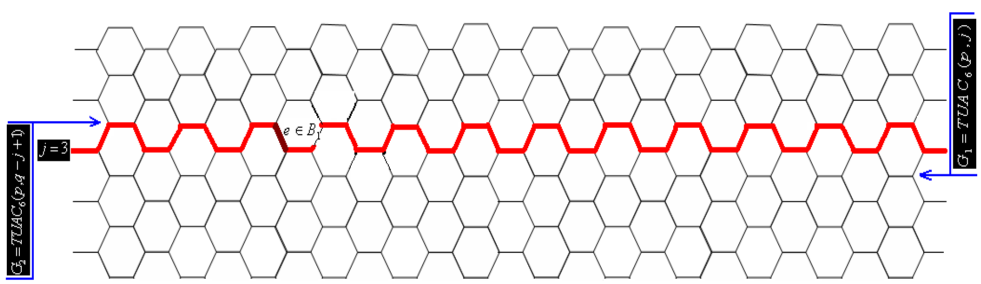

Fig. 8. Dividing the graph TUAC$_6$[12,5] in two sub-graph TUAC$_6$[12,3] and TUAC$_6$[12,3] for $e \in B_1$ when $q \prec \left[\frac{p}{2}\right]$.

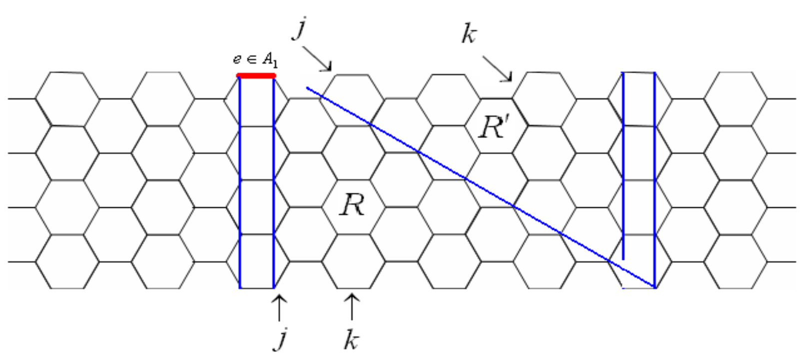

Fig. 9. The regions R and R' in TUAC$_6$[8,4] for $e \in A_1$ where $q = \left[\frac{p}{2}\right]$.

This case is exactly similar to the case (i) and there are some differences which have been mentioned in the follows:

- In $W_{e1}(e_{A1},G)_1$, t_1 changes to

$$t_1' = (\sum_{i=1}^{q} 2i) - q(2p-1).$$

- t_2 changes to $t_2' = 2(\sum_{i=0}^{\left[\frac{p}{2}\right]-1} (4i+3))$ in $W_{e1}(e_{A1},G)_j$.

- $2p-1$ must add to t_3 in $W_{e1}(e_{A2},G)$.
- In $W_{e1}(e_{A2},G)_j$, t_5 changes to

$$t_5' = 2((\sum_{i=1}^{2p-2} i) - (\sum_{i=0}^{\left[\frac{p}{2}\right]-2} (4i+3))) + (2p-1).$$

- in $W_{e1}(e_{\mathbf{B1}},G)_j$ and $W_{e1}(e_{\mathbf{B2}},G)_j$, t_7 changes

to $t_7' = ((\sum_{i=1}^{2p-1} i) - (\sum_{i=1}^{\left[\frac{p}{2}\right]-1} (4i+2))) + ((\sum_{i=1}^{2p-2} i) - (\sum_{i=1}^{\left[\frac{p}{2}\right]} 4i))$

Therefore we can state the following theorem:

Theorem 2. *Let p be an odd number and* $q \prec \left[\frac{p}{2}\right]$. *Then*

$$W_{e0}(G) = -\frac{7}{2}p + \frac{1}{2}p^3 + 6pq^4 + \frac{44}{3}pq^3 + 24pq^2 - 8p^2q + \frac{7}{3}pq + 2p^2 - 16p^2q^2 + 18p^3q^2 + 6p^3q$$

Remark: In follows, we use the notations G_1 and G_2 for the sub-graphs $TUAC_6[p, j-1]$ and $TUAC_6[p, q-j+1]$ in the set A_1, respectively. Also for the sets of B_2, B_1, A_2, we use the notations G_1 and G_2 for the sub-graphs $TUAC_6[p, j]$ and $TUAC_6[p, q-j+1]$, respectively.

Case 2. $q = \left[\frac{p}{2}\right]$

(i): p is even.

Lemma 11. Let $e \in A_1$ in Fig.9, then there are two regions R and R' which satisfy the following relations:

$$_{R}W_{e1}(e_{A1},G) = \Big(\sum_{j=0}^{2q-1}\sum_{i=2j}^{2q+j-1} i\Big) + \Big(\sum_{k=1}^{2q}\sum_{i=k}^{\left\lceil\frac{2q+k-1}{2}\right\rceil}(2i-1)\Big)$$

$$_{R'}W_{e1}(e_{A1},G) = \Big(\sum_{j=1}^{\left[\frac{p}{2}\right]}\sum_{i=4j-1}^{2p-1} i\Big) + \Big(\sum_{k=1}^{\left[\frac{p}{2}\right]}\sum_{i=\left[\frac{4k-1}{2}\right]}^{p-1} 2i\Big)$$

Lemma 12. Suppose $e \in A_1$, then

$$W_{e1}(e_{A1},G)_1 = 2\big({}_{R}W_{e1}(e_{A1},G) + {}_{R'}W_{e1}(e_{A1},G)\big) + S_1$$

where

$$S_1 = \Big(\sum_{i=1}^{q} 2i\Big) - (q+1)(2p-1).$$

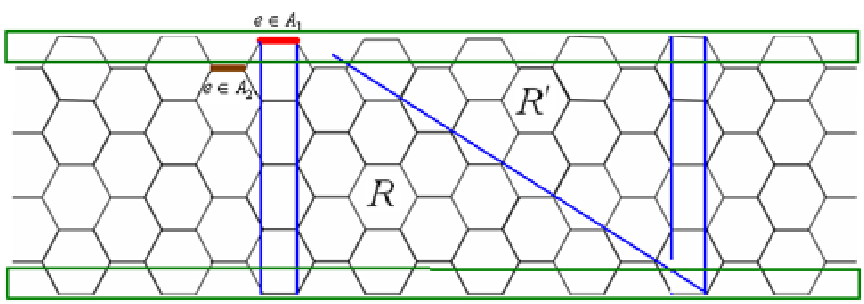

Fig. 10. Computing $W_{e1}(e_{A2},G)_1$ *for* $e \in A_2$ *where* $q = \left[\frac{p}{2}\right]$.

Lemma 13. For the set A_1, we have:

$$W_{e1}(A_1,G) = \Big(\frac{1}{2}\sum_{j=2}^{q} pW_{e1}(e_{A1},G)_j\Big)_{G_1,G_2:q\prec\left[\frac{p}{2}\right]} + pW_{e1}(e_{A1},G)_{1\;G:q=\left[\frac{p}{2}\right]}$$

Lemma 14. Let $e \in A_2$ in Fig.10, then

$$W_{e1}(e_{A2},G)_1 = W_{e1}(e_{A1},G)_1 + S_3$$

where

$$S_3 = 2\Big(\Big(\sum_{i=1}^{2p-2} i\Big) - \Big(\sum_{i=0}^{\left[\frac{p}{2}\right]-2}(4i+3)\Big)\Big) - \Big(2q + 2\Big(\Big(\sum_{i=2q-1}^{2p-2} i\Big) + \Big(\sum_{i=q+1}^{2q-2}(2i-1)\Big)\Big) + (2p-1)\Big)$$

Lemma 15. For the set A_2, we have:

$$W_{e1}(A_2,G) = \Big(\frac{1}{2}\sum_{j=2}^{q-1} pW_{e1}(e_{A2},G)_j\Big)_{G_1,G_2:q\prec\left[\frac{p}{2}\right]} + pW_{e1}(e_{A2},G)_{1\;G:q=\left[\frac{p}{2}\right]}$$

Lemma 16. Let $e \in B_1$ in Fig.11, then there are 4 regions R', R'', R_1, R_2 in graph of $TUAC_6[p,q]$ such that:

$$_{R'}W_{e1}(e_{B1},G) = \Big(\sum_{j=1}^{2q-1}\sum_{i=2j-1}^{2q+j-2} i\Big) + \Big(\sum_{k=0}^{2q-1}\sum_{i=k}^{\left[\frac{2q+k-1}{2}\right]} 2i\Big)$$

$$_{R''}W_{e1}(e_{B1},G) = \Big(\sum_{j=0}^{2q-1}\sum_{i=2j}^{2q+j-2} i\Big) + \Big(\sum_{k=1}^{2q-1}\sum_{i=k}^{\left[\frac{2q+k-1}{2}\right]}(2i-1)\Big)$$

$$_{R_1}W_{e1}(e_{B1},G) = \Big(\sum_{j=1}^{\left[\frac{p}{2}\right]}\sum_{i=4j-2}^{2p-1} i\Big) + \Big(\sum_{k=1}^{\left[\frac{p}{2}\right]}\sum_{i=2k-1}^{p}(2i-1)\Big)$$

$$_{R_2}W_{e1}(e_{B1},G) = \Big(\sum_{j=0}^{\left[\frac{p}{2}\right]}\sum_{i=4j}^{2p-2} i\Big) + \Big(\sum_{k=1}^{\left[\frac{p}{2}\right]}\sum_{i=2k}^{p-1}(2i-1)\Big) + \Big(\sum_{i=1}^{p-2} 2i\Big)$$

Lemma 17. Let $e \in B_1$ in Fig. 11, then

$$W_{e1}(e_{B1},G)_1 = {}_{R}W_{e1}(e_{B1},G) + {}_{R}W_{e1}(e_{B1},G) + {}_{R_1}W_{e1}(e_{B1},G) + {}_{R_2}W_{e1}(e_{B1},G)$$

Lemma 18. According to Fig. 12,

$$W_{e1}(e_{B2},G)_1 = W_{e1}(e_{B1},G)_1 + S_6$$

where

$$S_6 = \Big(\big(\sum_{i=1}^{2p-1} i\big) - \big(\sum_{i=1}^{\left[\frac{p}{2}\right]-1}(4i+2)\big)\Big) + \Big(\big(\sum_{i=1}^{2p-2} i\big) - \big(\sum_{i=1}^{\left[\frac{p}{2}\right]-1} 4i\big)\Big) - \Big((2q-2) + 2\big(\sum_{i=2q-1}^{2p-2} i\big) + \big(\sum_{i=2q-1}^{2p-4} i\big) - \big(\sum_{i=2q}^{p-1} 2i\big) + (2p-1)\Big)$$

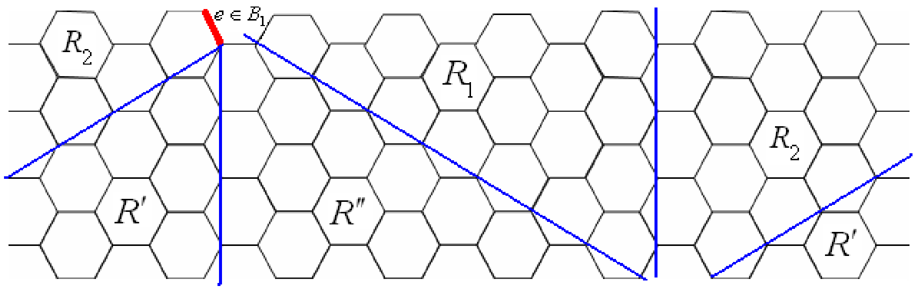

Fig. 11. The regions R', R'', R_1 and R_2 in TUAC$_6$[8,4] for $e \in B_1$ when $q = \left[\frac{p}{2}\right]$.

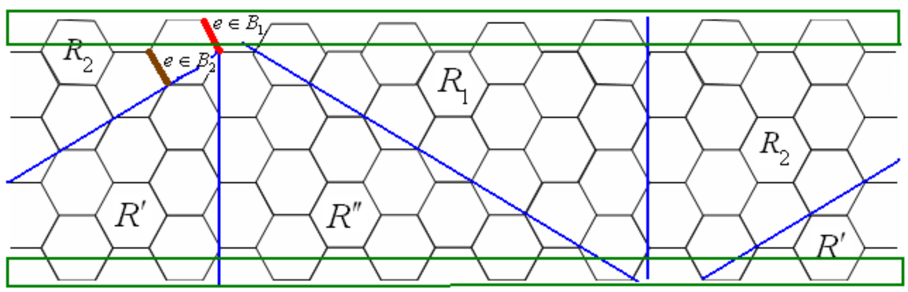

Fig. 12. Computing $W_{e1}(e_{B2},G)_1$ for $e \in B_2$ where $q = \left[\frac{p}{2}\right]$.

Lemma 19. For the set B_1, we have:

$$W_{e1}(B_1,G) = \Big(\frac{1}{2}\underset{G_1,G_2:q\prec\left[\frac{p}{2}\right]}{\sum_{j=2}^{q-1} 2pW_{e1}(e_{B1},G)_j}\Big) + \underset{G_1:q=\left[\frac{p}{2}\right]}{2pW_{e1}(e_{B1},G_2)_1} + \underset{G_1:q=\left[\frac{p}{2}\right]}{pW_{e1}(e_{B2},G_1)_1}$$

Lemma 20. For the set B_2, we have:

$$W_{e1}(B_2,G) = \frac{1}{2}\Big(\underset{G_1,G_2:q\prec\left[\frac{p}{2}\right]}{\sum_{j=2}^{q-1} 2pW_{e1}(e_{B2},G)_j}\Big) + \underset{G:q=\left[\frac{p}{2}\right]}{pW_{e1}(e_{B2},G)_1}$$

Corollary 2.

$$W_{e1}(G) = \frac{19}{2}p - \frac{5}{2}p^2 - \frac{21}{2}p^3 - \frac{107}{3}pq + 35p^2q + p\left(12q^3 - q^2 - 10q + 2p^3 + 5p + 2 - 3p^2\right) + 2p^4q - 30p^3q + 8pq^4 + \frac{110}{3}pq^3 + 16pq^2 + 15p^3q^2 + 8p^4 - 14p^2q^2$$

Theorem 3. Let p be an even number and $q = \left[\frac{p}{2}\right]$, then

$$W_{e0}(G) = \frac{19}{2}p - \frac{5}{2}p^2 - \frac{21}{2}p^3 - \frac{107}{3}pq + 35p^2q + p\left(12q^3 - q^2 - 10q + 2p^3 + 5p + 2 - 3p^2\right) + 2p^4q - 30p^3q + 8pq^4 + \frac{110}{3}pq^3 + 16pq^2 + 15p^3q^2 + 8p^4 - 14p^2q^2 + \frac{1}{2}p(6q+1)(6pq+p-1)$$

(ii): p is odd.

This case is exactly similar to first case and there are some differences which have been mentioned in the follows:

- In $W_{e1}(e_{A1},G)_1$, S_1 changes to

$$S_1' = \big(\sum_{i=1}^{q} 2i\big) - q(2p-1).$$

- In $W_{e1}(e_{A1},G)_j$, S_2 changes to

$$S_2{}' = 2(\sum_{i=0}^{\left\lceil \frac{p}{2} \right\rceil - 1} 4i + 3)$$

- In $W_{e1}(e_{A2},G)_1$, $S_3{}'$ must be add to $W_{e1}(e_{A1},G)_1$ where
- $$S_3' = 2((\sum_{i=1}^{2p-2} i) - (\sum_{i=0}^{\left\lceil \frac{p}{2} \right\rceil - 2} (4i - 3))) + (2p - 1)$$
$$-(2q + 2((\sum_{i=2q-1}^{2p-2} i) + (\sum_{i=q+1}^{2q-1} (2i - 1))))$$

- In $W_{e1}(e_{A2},G)_j$, S_5 changes

to $S_5{}' = 2(\sum_{i=1}^{2p-2} i - \sum_{i=0}^{\left\lceil \frac{p}{2} \right\rceil - 2} (4i + 3)) + (2p - 1)$.

- In $W_{e1}(e_{B2},G)_1$, $S_6{}'$ must be add to $W_{e1}(e_{B1},G)_1$ where
- $$S_6' = ((\sum_{i=1}^{2p-1} i) - (\sum_{i=1}^{\left\lceil \frac{p}{2} \right\rceil - 1} (4i + 2))) + ((\sum_{i=1}^{2p-2} i) - (\sum_{i=1}^{\left\lceil \frac{p}{2} \right\rceil - 1} 4i))$$
$$-((2q - 2) + 2(\sum_{i=2q-1}^{2p-2} i) + (\sum_{i=2q-1}^{2p-6} i)$$
$$-(2p - 2) + (2p - 1))$$

- In $W_{e1}(e_{B1},G)_j$ and $W_{e1}(e_{B2},G)_j$, S_7 changes

to

$$S_7' = ((\sum_{i=1}^{2p-1} i) - (\sum_{i=1}^{\left\lceil \frac{p}{2} \right\rceil - 1} (4i + 2)))$$
$$+((\sum_{i=1}^{2p-2} i) - (\sum_{i=1}^{\left\lceil \frac{p}{2} \right\rceil} 4i))$$

Therefore we can state the following theorem:

Theorem 4. Let p be an odd number and $q = \left\lceil \frac{p}{2} \right\rceil$, then

$$W_{e0}(G) = -\frac{59}{2}p - 33pq + 48p^2q + 10p^4 - \frac{27}{2}p^3$$
$$+p\left(12q^3 - q^2 - 10q + 2p^3 + 11p - 9 - 3p^2\right)$$
$$+24p^2 + 6pq^4 + 13pq^2 + 48pq^3 - 30p^3q$$
$$+18p^3q^2 - 12p^2q^2$$

Case 3. $q \succ \left\lceil \frac{p}{2} \right\rceil$

(i). p is even.

In this case, there is a general formula for $p \geq 6$ and we mention only explicit formula for $p < 6$.

If $p = 2$, then,

$$W_{e0}(G) = 26 + 48q^3 + 130q^2 + 52q .$$

If $p = 4$, then,

$$W_{e0}(G) = 148 + 192q^3 + 696q^2 + 832q .$$

Lemma 21. The region R which is denoted in Fig. 13 satisfies the following relation:

$${}_R W_{e1}(e,G) = (\sum_{j=0}^{p-1} \sum_{i=2j}^{2q+j-1} i) + (\sum_{k=1}^{p-1} \sum_{i=k}^{q+k-1} (2i - 1))$$
$$-((\sum_{j=0}^{\left\lceil \frac{p}{2} \right\rceil - 1} \sum_{i=\left\lceil \frac{2q+3}{2} \right\rceil + j}^{\left\lceil \frac{q+p-2}{2} \right\rceil} (2i + 1))$$
$$+(\sum_{j=0}^{\left\lceil \frac{p}{2} \right\rceil - 2} \sum_{\left\lceil \frac{2q+p}{2} \right\rceil}^{\left\lceil \frac{2q+p}{2} \right\rceil + \left\lceil \frac{p}{2} \right\rceil - 1 - j} (2i + 1)))$$

Theorem 5. Let $p \geq 6$ and $q \succ \left\lceil \frac{p}{2} \right\rceil$, then:

$$W_{e0}(G) = 10p + 17p^2q - \frac{55}{4}p^2 - 10pq - \frac{15}{8}p^3 + 9pq^2$$
$$+3p^4q + 12p^2q^3 + 4p^2q^2 + 9p^3q^2$$
$$+\frac{17}{4}p^4 - \frac{3}{8}p^5 - 4p^3q$$

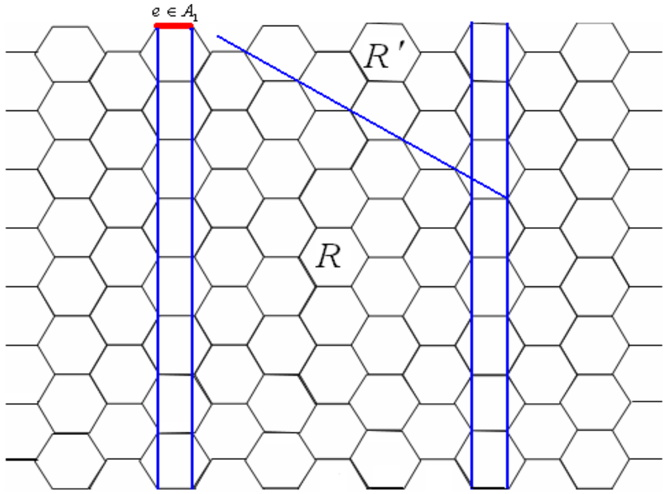

Fig. 13. The region R and R' in TUAC$_6$[6,8] for $e \in A_1$ where $q \succ \left[\frac{p}{2}\right]$.

(ii) p is odd

In this case, there is a general formula for $p \geq 7$ and we mention only explicit formula for $p < 7$.

If $p = 3$, then,

$$W_{e0}(G) = 225 + 108q^3 + 300q^2 + 177q \ .$$

If $p = 5$, then,

$$W_{e0}(G) = \begin{cases} -11000 + \frac{8570}{3}q + 2505q^2 + \frac{4175}{6}q^3 + \frac{125}{2}q^4 & q \neq p \\ 78035 & q = p = 5 \end{cases}$$

Now let $p \geq 7$. We have two cases as follows:

(a) $q \neq p$

Lemma 22. If $q \neq p$ and $p \geq 7$, then for the region R we have:

$$ {}_RW_{e1}(e,G) = \Big(\sum_{j=0}^{p-1}\sum_{i=2j}^{2q+j-1} i\Big) + \Big(\sum_{k=1}^{p-1}\sum_{i=k}^{q+k-1}(2i-1)\Big) - \Big(\Big(\sum_{k=0}^{\left[\frac{p}{2}\right]-1}\ \sum_{i=\left[\frac{2q+3}{2}\right]+k}^{\left\lceil\frac{2q+p-2}{2}\right\rceil}(2i+1)\Big) + \Big(\sum_{k=0}^{\left[\frac{p}{2}\right]-2}\ \sum_{i=\left\lceil\frac{2q+3}{2}\right\rceil}^{\left\lceil\frac{2q+3}{2}\right\rceil+\left[\frac{p}{2}\right]-2-k}(2i+1)\Big)\Big)$$

Therefore we can obtain the first edge Wiener index for the reminder cases in the following Theorems:

Theorem 6. *Let $q \neq p$ and $p \geq 7$ and $q \succ \left[\frac{p}{2}\right]$, then:*

$$\begin{aligned} W_{e0}(G) = {} & \frac{1}{2}p^3q^4 + \frac{1}{2}p^5q + \frac{7}{8}p^4q^2 + \frac{1}{4}p^5q^2 \\ & + \frac{23}{4}pq - \frac{19}{4}p^2q - \frac{13}{96}p^6 - \frac{1}{8}p^4 + \frac{39}{8}p^2q^2 \\ & - \frac{16}{3}p^3q - \frac{5}{32}p^7 + \frac{1}{2}p^4q^3 + \frac{5}{2}p^4q + \frac{5}{4}p^5 \\ & + \frac{577}{32}p^3 + \frac{3}{2}pq^2 + \frac{21}{2}p^2q^3 + \frac{13}{2}p^3q^2 \\ & - \frac{45}{8}p - \frac{2615}{96}p^2 + \frac{5}{6}p^3q^3 \end{aligned}$$

(b) $p = q$

Lemma 23. If $p = q$ and $p \geq 7$, then for the region R we have:

$$ {}_RW_{e1}(e,G) = \Big(\sum_{j=0}^{p-1}\sum_{i=2j}^{2q+j-1} i\Big) + \Big(\sum_{k=1}^{p-1}\sum_{i=k}^{q+k-1}(2i-1)\Big) - \Big(\Big(\sum_{k=0}^{\left[\frac{p}{2}\right]-2}\ \sum_{i=\left[\frac{2q+3}{2}\right]+k}^{\left\lceil\frac{2q+p-2}{2}\right\rceil}(2i+1)\Big) + \Big(\sum_{k=0}^{\left[\frac{p}{2}\right]-3}\ \sum_{i=\left\lceil\frac{2q+3}{2}\right\rceil}^{\left\lceil\frac{2q+3}{2}\right\rceil+\left[\frac{p}{2}\right]-2-k}(2i+1)\Big)\Big)$$

Theorem 7. Let $p = q$ and $p \geq 7$ and $q \succ \left[\frac{p}{2}\right]$, then:

$$W_{e0}(G)=\frac{1}{6}p^4+\frac{1835}{96}p^3-\frac{37}{6}p^3q+\frac{25}{4}pq+\frac{45}{8}p^2q^2+\frac{61}{6}p^2q^3+6p^3q^2-\frac{71}{12}p^2q-\frac{2765}{96}p^2+\frac{7}{6}p^5+4p^4q-\frac{41}{8}p-\frac{35}{96}p^6-\frac{5}{32}p^7+\frac{13}{8}p^4q^2+\frac{1}{2}p^5q+\frac{1}{2}p^4q^3+\frac{1}{4}p^5q^2+\frac{1}{2}p^3q^4+\frac{7}{6}p^3q^3+\frac{1}{2}pq^2$$

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