MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **65** (2011) 93-112

ISSN 0340 - 6253

Generalized Edge-Schultz Indices of Some Graphs

Ali Iranmanesh[a,*] *, Omid Khormali*[b] *and Ali Ahmadi*[b]

[a]*Department of Mathematics, Tarbiat Modares University*
P.O.Box: 14115-137, Tehran, Iran
[b]*Mathematics and Informatics Research Group, ACECR, Tarbiat Modares University*
P.O.Box: 14115-343, Tehran, Iran

(Received April 10, 2009)

Abstract
The generalized Schultz indices were introduced by Schultz and Gutman according to distances between vertices and vertex degrees. In this paper, we introduce the edge versions of these indices. We state the relations between the new indices with vertex Wiener index and distances between vertices. At last, these new indices are computed for some graphs.

1. Introduction

The ordinary (vertex) version of Wiener index is oldest index that is defined in terms of distances between vertices of a connected graph [1]. This index is the oldest and perhaps most important topological index in chemistry. A lot of interesting research on the vertex Wiener index has been performed in both chemistry and mathematics [2-8,13,14,16,17]. The Wiener index is defined as follow:

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

where $d(x,y)$ is the distance between vertices x *and* y.

We use a variety of distance functions throughout this paper. Such a distance is a metric if it satisfies:

* Corresponding author

Let S be any set, the distance in S is a mapping $d: S \times S \to R$, where $a,b,c \in S$,

a- $d(a,b) \geq 0$

b- $d(a,b) = 0 \Leftrightarrow a = b$

c- $d(a,b) = d(b,a)$

d- $d(a,b) + d(b,c) \geq d(a,c)$

In 2008, the edge versions of Wiener index were introduced by Ali Iranmanesh et. al. as follows [9]:

The first edge-Wiener index is:

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

where $d_0(e,f) = \begin{cases} d_1(e,f)+1 & e \neq f \\ 0 & e = f \end{cases}$ and $d_1(e,f) = \min\{d(x,u), d(x,v), d(y,u), d(y,v)\}$

where $e = xy$ and $f = uv$. In fact we have $W_{e0}(G) = W_v(L(G)))$.

Here, the line graph $L(G)$ is the intersection graph of the edges of G, where vertices correspond to edges of G and vertices in L(G) are adjacent if the corresponding edges share a vertex. With regard to the Wiener index of $L(G)$ see [2,3,16,17]. The second edge-Wiener index is:

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

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

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

In [11], we found relations between different versions of Wiener index by definition of two new distances between edges that are based on distances between endpoints of edges.

Definition 1-1. [11] Let $e = uv,\ \ f = xy$ be 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 $C=\{\{e,f\}\subseteq E(G) \mid \textit{if } e=uv \textit{ and } f=xy \ ; \ d(u,x)=d(u,y)=d(v,x)=d(v,x)\}$ and

$d_3(e,f)=\begin{cases} d''(e,f) & e\neq f \\ 0 & e=f \end{cases}$. We suppose that $d'(e,e)=\frac{1}{4}$.

Also, d' *and* d'' are not distances because they do not satisfy the condition (b) and we proved in [11] that $d_3=d_0$.

In addition, if $e,f\in E(G)$, we defined in [11]:

$$d'''(e,f)=\begin{cases} \lceil d'(e,f)\rceil & , \ \{e,f\}\notin A_1 \\ d'(e,f)+1 & , \ \{e,f\}\in A_1 \end{cases} \quad \text{and} \quad d_5(e,f)=\begin{cases} d'''(e,f) & e\neq f \\ 0 & e=f \end{cases}$$

Where A_1 is defined in following.

And, the mathematical quantity d''' is not distance because it not satisfy the condition (b) and we proved in [11], $d_4=d_5$.

In [11], several sets were defined in terms of the distance d_3, several sets have been defined.

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

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

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

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

The relation between the edge and vertex versions of Wiener index is:

Theorem 1-2. [11] Suppose G is a graph with m edges and A_1,A_2,A_3,A_4 *and* C are the sets that have been defined above. Then, the edge-Wiener indices corresponding to the distances d_0 and d_4 are:

$$W_{e0}(G)=\frac{1}{8}\sum_{x\in V(G)}\sum_{y\in V(G)}\deg(x)\times\deg(y)\times d(x,y)-\frac{m}{4}+$$
$$\sum_{\{e,f\}\in A_3}\left(\frac{1}{2}\right)+\sum_{\{e,f\}\in A_2}\left(\frac{1}{4}\right)+\sum_{\{e,f\}\in A_4}\left(\frac{3}{4}\right)+|C| \quad .$$

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

In [10-12], edge-Wiener indices of some graphs have been computed.
An index proposed by Schultz is shown to be related to the Wiener index for trees. This index is [13]:

$$W_{+}(G) := \sum_{\{x,y\}\subseteq V(G)} \big(\deg(x) + \deg(y)\big) d(x,y)$$

where $\deg(x)$ is the degree of x in graph G.
Ivan Gutman introduced a modification of the Schultz index with similar properties [14]:

$$W_{*}(G) := \sum_{\{x,y\}\subseteq V(G)} \big(\deg(x) \times \deg(y)\big) d(x,y)$$

The two above indices, $W_{+}(G)$ and $W_{*}(G)$, were named the generalized Schultz indices.

The generalized Schultz indices were introduced similarly to the Wiener index by Schultz and Gutman. A finding explicit relation between different versions of an index leads to parsimony in time and computing its edge versions. This is because parts of the computations for the edge versions are then included in the computations for the vertex versions.
In [9 and 11], we introduced the notations d_0, d_3, d_4 and d_5 explained above. We will need these notations here again for the generalized Schultz indices.

Therefore, in this paper, we introduce the edge versions of generalized Schultz indices, and obtain explicit relations between different versions of them and compute them for some graphs.

2. Some definitions and results

In this section, we try to state our explanations with mathematical equations. For this, we do not simplify our computations. Therefore, each mathematician can get the result only find the clear computations by equations.
Before stating the edge versions of generalized Schultz indices, we mention upper and lower bounds of their vertex versions.
Let $\Delta(G)$ and $\delta(G)$ be the maximum and minimum degrees of vertices of connected graph G, respectively.
According to the definition of generalized Schultz indices, we have:

$$
\begin{aligned}
&2\delta(G)W(G) \le W_+(G) \le 2\Delta(G)W(G) \\
&\delta(G)^2 W(G) \le W_*(G) \le \Delta(G)^2 W(G)
\end{aligned}
\qquad (1)
$$

In particular, if G is a r-regular graph, then: $W_+(G) = 2rW(G)$ and $W_*(G) = r^2 W(G)$.

One of the applications of these indices is their computation for molecular graphs of chemical structures such as nanotubes that are a hollow cylindrical or toroidal molecule made of one element, usually carbon, and are being investigated as semiconductors and for uses in nanotechnology. In the following, we write generalized Schultz indices.

Definition 2-1. Let *G* be a connected graph with vertex set *V(G)* and edge set *E(G)*. We define:

$$W(G, vi) = \frac{1}{2} \sum_{\substack{v \in V(G) \\ \deg(v)=i}} \sum_{x \in V(G)} d(v,x)$$

Theorem 2-2. Let *G* be a molecular graph of a nanotube with vertex set *V(G)* and edge set *E(G)*. The generalized Schultz indices according to Wiener index are:

$$W_+(G) = 6W(G) + 4W(G, v2) - 6 \sum_{\substack{\{x,y\} \subseteq V(G) \\ \deg(x)=\deg(y)=2}} d(x,y)$$

$$W_*(G) = 9W(G) + 3W(G, v2) - 8 \sum_{\substack{\{x,y\} \subseteq V(G) \\ \deg(x)=\deg(y)=2}} d(x,y)$$

Proof. Since the vertex degree of vertices in the molecular graph of a nanotube is 2 or 3, we have according to the definitions of $W_+(G)$ and $W_*(G)$:

$$W_+(G) = \sum_{\{x,y\} \subseteq V(G)} \big(\deg(x) + \deg(y)\big) d(x,y) =$$

$$= \frac{1}{2} \sum_{\substack{x \in V(G) \\ \deg(x)=3}} \sum_{\substack{y \in V(G) \\ \deg(y)=3}} 6d(x,y) + \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=3}} 5d(x,y) + \frac{1}{2} \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{\substack{y \in V(G) \\ \deg(y)=2}} 4d(x,y)$$

Simplifying; up equation, we can restate the last line of up equation as follows:

$$3 \sum_{x \in V(G)} \sum_{y \in V(G)} d(x,y) + 2 \sum_{\substack{x \in V(G) \\ \deg(x)=2}} \sum_{y \in V(G)} d(x,y) - 6 \sum_{\substack{\{x,y\} \subseteq V(G) \\ \deg(x)=\deg(y)=2}} d(x,y)$$

According to the definition of Wiener index and Definition (2-1), we have:

$$W_+(G) = 6W(G) + 4W(G, v2) - 6 \sum_{\substack{\{x,y\} \subseteq V(G) \\ \deg(x)=\deg(y)=2}} d(x,y)$$

We use a similar procedure for next result. Then,

$$W_*(G)=\sum_{\{x,y\}\subseteq V(G)}(\deg(x)\times\deg(y))d(x,y)=$$

$$=\frac{1}{2}\sum_{\substack{x\in V(G)\\ \deg(x)=3}}\sum_{\substack{y\in V(G)\\ \deg(y)=3}}9d(x,y)+\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=3}}6d(x,y)+\frac{1}{2}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}4d(x,y)$$

$$=9W(G)+3W(G,v2)-8\sum_{\substack{\{x,y\}\subseteq V(G)\\ \deg(x)=\deg(y)=2}}d(x,y)$$

■

Now we introduce new versions of these indices and continue the procedure that is mentioned in the proof of Theorem (2-2) for getting more results.

Definition 2-3. The edge versions of generalized Schultz indices are:

$$(W_+)_{e\,i}(G):=\sum_{\{e,f\}\subseteq E(G)}(\deg(e)+\deg(f))d_i(e,f),\ i=0,4$$

$$(W_*)_{e\,i}(G):=\sum_{\{e,f\}\subseteq E(G)}(\deg(e)\times\deg(f))d_i(e,f),\ i=0,4$$

where $\deg(e)$ is the degree of e in the line graph $L(G)$.

Let $\Delta(L(G))$ and $\delta(L(G))$ be the maximum and minimum degrees of edges of a connected graph *G*, respectively. Therefore, we find bounds for the new indices as follows:

$$\begin{matrix}2\delta(L(G))W_{ei}(G)\le(W_+)_{ei}(G)\le 2\Delta(L(G))W_{ei}(G)\\ \delta(L(G))^2W_{ei}(G)\le(W_*)_{ei}(G)\le\Delta(L(G))^2W_{ei}(G)\end{matrix},\ i-0,4. \qquad (2)$$

If we write the inequalities (2) in terms of the degree of vertices, then we must replace $\Delta(L(G))$ and $\delta(L(G))$ with $2\Delta(G)-2$ and $2\delta(G)-2$. In particular, if *G* is r-regular graph, then: $(W_+)_{ei}(G)=(4r-4)W_{ei}(G)$ and $(W_*)_{ei}(G)=(2r-2)^2W_{ei}(G)$.

Now, we write edge generalized Schultz indices according to the edge Wiener index. Before this, some notations are defined to simplify our computations.

Definition 2-4. Let *G* be a connected graph with vertex set *V(G)* and edge set *E(G)*. We define:

$$W_{ei}(G,ej)=\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=j}}\sum_{f\in E(G)}d_i(e,f),\ i-0,4\ \ and\ \ j=2,3,4.$$

$$W_{ei}(G,vj)=\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(v)=j}}\sum_{f\in E(G)}d_i(e,f),\ i-0,4\ \ and\ \ j=2,3.$$

Theorem 2-5. Let *G* be a molecular graph of a nanotube with vertex set *V(G)* and edge set *E(G)*. The edge generalized Schultz indices are:

$$\begin{aligned}(W_+)_{ei}(G)&=8W_{ei}(G)+6W_{ei}(G,e3)+4W_{ei}(G,e2)\\&-8\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=\deg(f)=3}}d_i(e,f)-8\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=2\\ \deg(f)=3}}d_i(e,f)-8\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=\deg(f)=2}}d_i(e,f)\end{aligned}\quad,\ i=0,4.$$

$$\begin{aligned}(W_*)_{ei}(G)&=16W_{ei}(G)+8W_{ei}(G,e3)+\\&-15\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=\deg(f)=3}}d_i(e,f)-12\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=2\\ \deg(f)=3}}d_i(e,f)-12\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=\deg(f)=2}}d_i(e,f)\end{aligned}$$

Proof. Since the degree of vertices in a molecular graph of a nanotube is 2 or 3, the degree of edges in the molecular graph of a nanotube is 2, 3 or 4. Therefore, we have according to the Definition (2-3):

$$\begin{aligned}(W_+)_{ei}(G)&=\sum_{\{e,f\}\subseteq E(G)}\left(\deg(e)+\deg(f)\right)d_i(e,f)=\\&=\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=4}}\sum_{\substack{f\in E(G)\\ \deg(f)=4}}8d_i(e,f)+\sum_{\substack{e\in E(G)\\ \deg(e)=4}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}}7d_i(e,f)+\sum_{\substack{e\in E(G)\\ \deg(e)=4}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}}6d_i(e,f)\\&+\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}}6d_i(e,f)+\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}}5d_i(e,f)+\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}}4d_i(e,f)\\&=8W_{ei}(G)+6W_{ei}(G,e3)+4W_{ei}(G,e2)\\&-8\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=\deg(f)=3}}d_i(e,f)-8\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=2\\ \deg(f)=3}}d_i(e,f)-8\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=\deg(f)=2}}d_i(e,f).\end{aligned}$$

$$(W_*)_{ei}(G) = \sum_{\{e,f\}\subseteq E(G)} \left(\deg(e)\times\deg(f)\right) d_i(e,f) =$$

$$= \frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=4}} \sum_{\substack{f\in E(G)\\ \deg(f)=4}} 16 d_i(e,f) + \sum_{\substack{e\in E(G)\\ \deg(e)=4}} \sum_{\substack{f\in E(G)\\ \deg(f)=3}} 12 d_i(e,f) + \sum_{\substack{e\in E(G)\\ \deg(e)=4}} \sum_{\substack{f\in E(G)\\ \deg(f)=2}} 8 d_i(e,f)$$

$$+ \frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}} \sum_{\substack{f\in E(G)\\ \deg(f)=3}} 9 d_i(e,f) + \sum_{\substack{e\in E(G)\\ \deg(e)=3}} \sum_{\substack{f\in E(G)\\ \deg(f)=2}} 6 d_i(e,f) + \frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}} \sum_{\substack{f\in E(G)\\ \deg(f)=2}} 4 d_i(e,f)$$

$$= 16W_{ei}(G) + 8W_{ei}(G,e3) +$$

$$-15 \sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=\deg(f)=3}} d_i(e,f) - 12 \sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=2\\ \deg(f)=3}} d_i(e,f) - 12 \sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=\deg(f)=2}} d_i(e,f).$$

■

Now, we state relations between edge-generalized Schultz indices with vertex-Wiener index for molecular graphs of nanotubes. Before stating these relations, we call some notations for simplifying our computations.

Definition 2-6. Let G be a molecular graph of nanotube. Then,

$m(i) = |M(i)| = \left|\{e \in E(G) \mid \deg(e) = i\}\right|$ where $i = 2,3,4$,

$m_j(i) = |M_j(i)| = \left|\{uv = e \in E(G) \mid \deg(u) = i \ and \ \deg(v) = j\}\right|$ where $i = 1,2,3 \ and \ j = 1,2,3$,

$a_j(i) = \left|\{\{e,f\} \in A_j(G) \mid \deg(e) = i\}\right|$ where $i = 2,3,4 \ and \ j = 1,2,3,4$,

$a_j(i,k) = \left|\{\{e,f\} \in A_j(G) \mid \deg(e) = i \ and \ \deg(f) = k\}\right|$ where $i,k = 2,3,4 \ and \ j = 1,2,3,4$,

$c(i) = \left|\{\{e,f\} \in C(G) \mid \deg(e) = i\}\right|$ where $i = 2,3,4$,

$c(i,k) = \left|\{\{e,f\} \in C(G) \mid \deg(e) = i \ and \ \deg(f) = k\}\right|$ where $i,k = 2,3,4$,

$\deg_i(x) = \left|\{e \in E(G) \mid \deg(e) = i \ and \ x \in e\}\right|$ where $i = 2,3,4$ and

$N_i(x,y) = \deg_i(x)\deg(y) + \deg_i(y)(\deg(x) - \deg_i(x))$ where $i = 2,3,4$.

Lemma 2-7. $W_{e0}(G)$ of nanotubes according to the vertex-Wiener index is:

$$W_{e0}(G)=\frac{9}{4}W_v(G)+\frac{3}{4}W_v(G,v2)-\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)-\frac{m}{4}$$
$$+\left(\frac{1}{2}\right)|A_3|+\left(\frac{1}{4}\right)|A_2|+\left(\frac{3}{4}\right)|A_4|+|C|$$

$$W_{e4}(G)=W_{e0}(G)+|A_1|-|C|.$$

Proof. The desired results follow from Theorem (1-2). ■

Lemma 2- 8. Let G be a molecular graph of a nanotube. Then, we have:

$$\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(u)=3,\deg(v)=2}}\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}=$$
$$\frac{1}{8}\left(\sum_{x\in V(M(3))}\sum_{y\in V(G)}N_3(x,y)d(x,y)+\sum_{x\in V(M(3))}\sum_{y\in V(G)\backslash V(M(3))}N_3(x,y)d(x,y)\right)$$

and

$$\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(e)=2}}\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}=$$
$$\frac{1}{8}\left(\sum_{x\in V(M_2(2)\cup M_1(3))}\sum_{y\in V(G)}N_3(x,y)d(x,y)+\sum_{x\in V(M_2(2)\cup M_1(3))}\sum_{y\in V(G)\backslash V(M_2(2)\cup M_1(3))}N_3(x,y)d(x,y)\right)$$

Proof. The proofs of the two formulas are similar. Therefore, we only prove the first one. Let G be a molecular graph of a nanotube, $xu=e\ and\ p=ab$ be elements of $M(3)$ and $yv=f\notin M(3)$.

Consider the summation $\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(u)=3,\deg(v)=2}}\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$. The number of times $d(x,y)$ is counted in the above summation is $\deg_3(x)\deg(y)+\deg_3(y)(\deg(x)-\deg_3(x))$. The number of times $d(x,a)$ is counted in the above summation is $2(\deg_3(x)\deg(y)+\deg_3(y)(\deg(x)-\deg_3(x)))$ i.e., the number of times $d(x,a)$ is

$\deg_3(x)\deg(y)+\deg_3(y)(\deg(x)-\deg_3(x))$ and the number of times $d(a,x)$

$\deg_3(x)\deg(y)+\deg_3(y)(\deg(x)-\deg_3(x))$. Therefore, the summation

$$\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(u)=3,\deg(v)=2}} \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$$ is equal to:

$$\frac{1}{8}\left(\begin{array}{l}\sum_{x\in V(M(3))}\sum_{y\in V(G)}\big(\deg_3(x)\deg(y)+\deg_3(y)(\deg(x)-\deg_3(x))\big)d(x,y)+\\ \sum_{x\in V(M(3))}\sum_{y\in V(G)\backslash V(M(3))}\big(\deg_3(x)\deg(y)+\deg_3(y)(\deg(x)-\deg_3(x))\big)d(x,y)\end{array}\right)$$

which is

$$\frac{1}{8}\left(\sum_{x\in V(M(3))}\sum_{y\in V(G)}N_3(x,y)d(x,y)+\sum_{x\in V(M(3))}\sum_{y\in V(G)\backslash V(M(3))}N_3(x,y)d(x,y)\right).$$

■

Lemma 2-9. $W_{e0}(G,v3)$ and $W_{e0}(G,v2)$ of nanotubes according to the vertex distances are:

$$W_{e0}(G,v3)=\frac{1}{8}\left(\sum_{x\in V(M(3))}\sum_{y\in V(G)}N_3(x,y)d(x,y)+\sum_{x\in V(M(3))}\sum_{y\in V(G)\backslash V(M(3))}N_3(x,y)d(x,y)\right)-\frac{m(3)}{4}$$
$$+\left(\frac{1}{2}\right)a_3(3)+\left(\frac{1}{4}\right)a_2(3)+\left(\frac{3}{4}\right)a_4(3)+c(3)$$

and

$$W_{e0}(G,v2)=\frac{1}{8}\left(\sum_{x\in V(M_2(2)\cup M_1(3))}\sum_{y\in V(G)}N_3(x,y)d(x,y)+\sum_{x\in V(M_2(2)\cup M_1(3))}\sum_{y\in V(G)\backslash V(M_2(2)\cup M_1(3))}N_3(x,y)d(x,y)\right).$$
$$-\frac{m_2(2)+m_1(3)}{4}+\left(\frac{1}{2}\right)a_3(2)+\left(\frac{1}{4}\right)a_2(2)+\left(\frac{3}{4}\right)a_4(2)+c(2)$$

Proof. We only prove the first formula, because the proof of the second one is similar.
By Definition (1-1), we have

$$W_{e0}(G,v3)=\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=3}} d_3(e,f)=\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(e)=3}}\left\lceil\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}\right\rceil$$

$$=\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(u)=3,\deg(v)=2}}\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$$

$$+\sum_{\substack{\{e,f\}\in A_3\\ \deg(e)=3}}\left(\frac{1}{2}\right)+\sum_{\substack{\{e,f\}\in A_2\\ \deg(e)=3}}\left(\frac{1}{4}\right)+\sum_{\substack{\{e,f\}\in A_4\\ \deg(e)=3}}\left(\frac{3}{4}\right)+\sum_{\substack{\{e,f\}\in C\\ \deg(e)=3}}(1)$$

And using Lemma (2-8), we have

$$W_{e0}(G,v3)=\frac{1}{8}\left(\sum_{x\in V(M(3))}\sum_{y\in V(G)}N_3(x,y)d(x,y)+\sum_{x\in V(M(3))}\sum_{y\in V(G)\setminus V(M(3))}N_3(x,y)d(x,y)-\sum_{x\in V(M_3)}\deg_3(x)\right)$$

$$+\sum_{\substack{\{e,f\}\in A_3\\ \deg(e)=3}}\left(\frac{1}{2}\right)+\sum_{\substack{\{e,f\}\in A_2\\ \deg(e)=3}}\left(\frac{1}{4}\right)+\sum_{\substack{\{e,f\}\in A_4\\ \deg(e)=3}}\left(\frac{3}{4}\right)+\sum_{\substack{\{e,f\}\in C\\ \deg(e)=3}}(1)=$$

$$=\frac{1}{8}\left(\sum_{x\in V(M(3))}\sum_{y\in V(G)}N_3(x,y)d(x,y)+\sum_{x\in V(M(3))}\sum_{y\in V(G)\setminus V(M(3))}N_3(x,y)d(x,y)\right)-\frac{m(3)}{4}$$

$$+\left(\frac{1}{2}\right)a_3(3)+\left(\frac{1}{4}\right)a_2(3)+\left(\frac{3}{4}\right)a_4(3)+c(3)$$

■

Lemma 2-10. $W_{e4}(G,v3)$ and $W_{e4}(G,v2)$ of nanotubes according to the vertex distances are:

$$W_{e4}(G,v3)=W_{e0}(G,v3)+a_1(3)-c(3)$$

$$W_{e4}(G,v2)=W_{e0}(G,v2)+a_1(2)-c(2)$$

Proof. These results can be concluded by lemma (2-7). ■

Lemma 2-11. We have:

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}}d_0(e,f)=\frac{1}{8}\sum_{x\in V(M(3))}\sum_{y\in V(M(3))}(\deg_3(x)\deg_3(y))d(x,y)-\frac{m(3)}{4}$$

$$+\left(\frac{1}{2}\right)a_3(3,3)+\left(\frac{1}{4}\right)a_2(3,3)+\left(\frac{3}{4}\right)a_4(3,3)+c(3,3)$$

and

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}}d_4(e,f)=\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}}d_0(e,f)+a_1(3,3)-c(3,3)$$

Proof. By Definition (1-1), we conclude the results as follows:

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_0(e,f) = \sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=3\\ \deg(f)=3}} d_3(e,f) = \sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(e)=3, eg(f)=3}} \left\lceil \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4} \right\rceil$$

$$= \sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(e)=3,\deg(f)=3}} \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$$

$$+ \sum_{\substack{\{e,f\}\in A_3\\ \deg(e)=3\\ \deg(f)=3}} \left(\frac{1}{2}\right) + \sum_{\substack{\{e,f\}\in A_2\\ \deg(e)=3\\ \deg(f)=3}} \left(\frac{1}{4}\right) + \sum_{\substack{\{e,f\}\in A_4\\ \deg(e)=3\\ \deg(f)=3}} \left(\frac{3}{4}\right) + \sum_{\substack{\{e,f\}\in C\\ \deg(e)=3\\ \deg(f)=3}} (1)$$

If $x, y \in V(M(3))$, then the number of times $d(x,y)$ is counted in the above summation is $2(\deg_3(x)\deg_3(y))$ e.i. the number of times $d(x,y)$ is $\deg_3(x)\deg_3(y)$ and The number of times $d(y,x)$ is $\deg_3(x)\deg_3(y)$. Therefore,

$$\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(e)=3,\deg(f)=3}} \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4} = \frac{1}{8}\sum_{x\in V(M(3))}\sum_{y\in V(M(3))} (\deg_3(x)\deg_3(y))d(x,y)$$

Hence,

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_0(e,f) = \frac{1}{8}\sum_{x\in V(M(3))}\sum_{y\in V(M(3))} (\deg_3(x)\deg_3(y))d(x,y) - \frac{m(3)}{4}$$

$$+\left(\frac{1}{2}\right)a_3(3,3) + \left(\frac{1}{4}\right)a_2(3,3) + \left(\frac{3}{4}\right)a_4(3,3) + c(3,3)$$

For second result, if we compute $\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_4(e,f)$, we have

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=3}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_4(e,f) = \frac{1}{8}\sum_{x\in V(M(3))}\sum_{y\in V(M(3))} (\deg_3(x)\deg_3(y))d(x,y) - \frac{m(3)}{4}$$

$$+\left(\frac{1}{2}\right)a_3(3,3) + \left(\frac{1}{4}\right)a_2(3,3) + \left(\frac{3}{4}\right)a_4(3,3) + a_1(3,3)$$

Now, the second result follows easily. ■

Lemma 2-12. We have:

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}} d_0(e,f)=\frac{1}{8}\sum_{x\in V(M(2))}\sum_{y\in V(M(2))}(\deg_2(x)\deg_2(y))d(x,y)-\frac{m(2)}{4}$$
$$+\left(\frac{1}{2}\right)a_3(2,2)+\left(\frac{1}{4}\right)a_2(2,2)+\left(\frac{3}{4}\right)a_4(2,2)+c(2,2)$$

and

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}} d_4(e,f)=\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}} d_0(e,f)+a_1(2,2)-c(2,2)$$

Proof. By Definition (1-1), we conclude the results as follows:

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}} d_0(e,f)=\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=2\\ \deg(f)=2}} d_3(e,f)=\sum_{\substack{\{e,f\}\subseteq E(G)\\ \text{if } e=uv,\ f=xy\\ \deg(e)=2,\deg(f)=2}}\left\lceil\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}\right\rceil$$
$$=\sum_{\substack{\{e,f\}\subseteq E(G)\\ \text{if } e=uv,\ f=xy\\ \deg(u)=2,\deg(v)=2}}\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$$
$$+\sum_{\substack{\{e,f\}\in A_3\\ \deg(e)=2\\ \deg(f)=2}}\left(\frac{1}{2}\right)+\sum_{\substack{\{e,f\}\in A_2\\ \deg(e)=2\\ \deg(f)=2}}\left(\frac{1}{4}\right)+\sum_{\substack{\{e,f\}\in A_4\\ \deg(e)=2\\ \deg(f)=2}}\left(\frac{3}{4}\right)+\sum_{\substack{\{e,f\}\in C\\ \deg(e)=2\\ \deg(f)=2}}(1)$$

If $x,y\in V(M(2))$, then the number of times $d(x,y)$ is counted in the above summation is $2(\deg_2(x)\deg_2(y))$ i.e., the number of times $d(x,y)$ is $\deg_2(x)\deg_2(y)$ and The number of times $d(y,x)$ is $\deg_2(x)\deg_2(y)$. Therefore,

$$\sum_{\substack{\{e,f\}\subseteq E(G)\\ \text{if } e=uv,\ f=xy\\ \deg(e)=2,\deg(f)=2}}\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}=\frac{1}{8}\sum_{x\in V(M(2))}\sum_{y\in V(M(2))}(\deg_2(x)\deg_2(y))d(x,y)$$

Therefore,

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}} d_0(e,f)=\frac{1}{8}\sum_{x\in V(M(2))}\sum_{y\in V(M(2))}(\deg_2(x)\deg_2(y))d(x,y)-\frac{m(2)}{4}$$
$$+\left(\frac{1}{2}\right)a_3(2,2)+\left(\frac{1}{4}\right)a_2(2,2)+\left(\frac{3}{4}\right)a_4(2,2)+c(2,2)$$

For second result, if we compute $\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}} d_4(e,f)$, we have

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=2}} d_4(e,f)=\frac{1}{8}\sum_{x\in V(M(2))}\sum_{y\in V(M(2))}(\deg_2(x)\deg_2(y))d(x,y)-\frac{m(2)}{4}$$
$$+\left(\frac{1}{2}\right)a_3(2,2)+\left(\frac{1}{4}\right)a_2(2,2)+\left(\frac{3}{4}\right)a_4(2,2)+a_1(2,2)$$

Now, the second result follows easily. ■

Lemma 2-13. We have:

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_0(e,f)=\frac{1}{8}\Big(\sum_{x\in V(M(2))}\sum_{y\in V(M(3))}\big(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\big)d(x,y)$$
$$+\sum_{x\in V(M(2))\setminus(V(M(2))\cap V(M(3)))}\ \sum_{y\in V(M(3))\setminus(V(M(2))\cap V(M(3)))}\big(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\big)d(x,y)\Big)$$
$$-\frac{|E(V(M(2))\cap V(M(3)))|}{4}+\left(\frac{1}{2}\right)a_3(2,3)+\left(\frac{1}{4}\right)a_2(2,3)+\left(\frac{3}{4}\right)a_4(2,3)+c(2,3)$$

and

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_4(e,f)=\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_0(e,f)+a_1(2,2)-c(2,2)$$

Proof. By Definition (1-1), we conclude the results as follows:

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_0(e,f)=\sum_{\substack{\{e,f\}\subseteq E(G)\\ \deg(e)=2\\ \deg(f)=3}} d_3(e,f)=\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(e)=2,\deg(f)=3}}\left\lceil\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}\right\rceil$$

$$=\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(u)=2,\deg(v)=3}}\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$$

$$+\sum_{\substack{\{e,f\}\in A_3\\ \deg(e)=2\\ \deg(f)=3}}\left(\frac{1}{2}\right)+\sum_{\substack{\{e,f\}\in A_2\\ \deg(e)=2\\ \deg(f)=3}}\left(\frac{1}{4}\right)+\sum_{\substack{\{e,f\}\in A_4\\ \deg(e)=2\\ \deg(f)=3}}\left(\frac{3}{4}\right)+\sum_{\substack{\{e,f\}\in C\\ \deg(e)=2\\ \deg(f)=3}}(1)$$

If $x\in V(M(2))$ and $y\in V(M(3))$, then the number of times $d(x,y)$ is counted in the above summation is $\deg_2(x)\deg_3(y)$. Therefore,

$$\sum_{\substack{\{e,f\}\subseteq E(G)\\ if\ e=uv,\ f=xy\\ \deg(u)=2,\deg(v)=3}}\frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}=\frac{1}{8}\sum_{x\in V(M(2))}\sum_{y\in V(M(3))}\left(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\right)d(x,y)$$

Therefore,

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_0(e,f)=\frac{1}{8}\Big(\sum_{x\in V(M(2))}\sum_{y\in V(M(3))}\left(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\right)d(x,y)$$
$$+\sum_{x\in V(M(2))\setminus(V(M(2))\cap V(M(3)))}\ \sum_{y\in V(M(3))\setminus(V(M(2))\cap V(M(3)))}\left(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\right)d(x,y)\Big)$$
$$-\frac{|E(V(M(2))\cap V(M(3)))|}{4}+\left(\frac{1}{2}\right)a_3(2,3)+\left(\frac{1}{4}\right)a_2(2,3)+\left(\frac{3}{4}\right)a_4(2,3)+c(2,3)$$

For second result, if we compute $\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_4(e,f)$, we have

$$\frac{1}{2}\sum_{\substack{e\in E(G)\\ \deg(e)=2}}\sum_{\substack{f\in E(G)\\ \deg(f)=3}} d_0(e,f)=\frac{1}{8}\Big(\sum_{x\in V(M(2))}\sum_{y\in V(M(3))}\left(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\right)d(x,y)$$
$$+\sum_{x\in V(M(2))\setminus(V(M(2))\cap V(M(3)))}\ \sum_{y\in V(M(3))\setminus(V(M(2))\cap V(M(3)))}\left(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\right)d(x,y)\Big)$$
$$-\frac{|E(V(M(2))\cap V(M(3)))|}{4}+\left(\frac{1}{2}\right)a_3(2,3)+\left(\frac{1}{4}\right)a_2(2,3)+\left(\frac{3}{4}\right)a_4(2,3)+a_1(2,3)$$

Now, the second result follows easily. ■

3. Main result

We can now provide formulas for the edge generalized Schultz indices by means of Lemmas (2-8, 2-9, 2-10, 2-11, 2-12 and 2-13) and Theorem (2-5). We only state formulas for $(W_+)_{e0}(G)$, other edge generalized Schultz indices can be computed in a similar way.

$$
\begin{aligned}
(W_+)_{e0}(G) = {} & 8\left(\frac{9}{4}W_v(G)+\frac{3}{4}W_v(G,v2)-\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}} d(x,y)-\frac{m}{4}+\left(\frac{1}{2}\right)|A_3|+\left(\frac{1}{4}\right)|A_2|+\left(\frac{3}{4}\right)|A_4|+|C|\right) \\
& +6\left(\begin{array}{l}\frac{1}{8}\left(\sum\limits_{x\in V(M(3))}\sum\limits_{y\in V(G)} N_3(x,y)d(x,y)+\sum\limits_{x\in V(M(3))}\sum\limits_{y\in V(G)\setminus V(M(3))} N_3(x,y)d(x,y)\right)-\frac{m(3)}{4}\\ +\left(\frac{1}{2}\right)a_3(3)+\left(\frac{1}{4}\right)a_2(3)+\left(\frac{3}{4}\right)a_4(3)+c(3)\end{array}\right) \\
& +4\left(\begin{array}{l}\frac{1}{8}\left(\sum\limits_{x\in V(M_2(2)\cup M_1(3))}\sum\limits_{y\in V(G)} N_3(x,y)d(x,y)+\sum\limits_{x\in V(M_2(2)\cup M_1(3))}\sum\limits_{y\in V(G)\setminus V(M_2(2)\cup M_1(3))} N_3(x,y)d(x,y)\right)\\ -\frac{m_2(2)+m_1(3)}{4}+\left(\frac{1}{2}\right)a_3(2)+\left(\frac{1}{4}\right)a_2(2)+\left(\frac{3}{4}\right)a_4(2)+c(2)\end{array}\right) \\
& -8\left(\begin{array}{l}\frac{1}{8}\sum\limits_{x\in V(M(3))}\sum\limits_{y\in V(M(3))}(\deg_3(x)\deg_3(y))d(x,y)-\frac{m(3)}{4}\\ +\left(\frac{1}{2}\right)a_3(3,3)+\left(\frac{1}{4}\right)a_2(3,3)+\left(\frac{3}{4}\right)a_4(3,3)+c(3,3)\end{array}\right) \\
& -8\left(\begin{array}{l}\frac{1}{8}\sum\limits_{x\in V(M(2))}\sum\limits_{y\in V(M(2))}(\deg_2(x)\deg_2(y))d(x,y)-\frac{m(2)}{4}\\ +\left(\frac{1}{2}\right)a_3(2,2)+\left(\frac{1}{4}\right)a_2(2,2)+\left(\frac{3}{4}\right)a_4(2,2)+c(2,2)\end{array}\right) \\
& -8\left(\begin{array}{l}\frac{1}{8}\Big(\sum\limits_{x\in V(M(2))}\sum\limits_{y\in V(M(3))}\big(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\big)d(x,y)\\ +\sum\limits_{x\in V(M(2))\setminus(V(M(2))\cap V(M(3)))}\ \sum\limits_{y\in V(M(3))\setminus(V(M(2))\cap V(M(3)))}\big(\deg_2(x)\deg_3(y)+\deg_3(x)\deg_2(y)\big)d(x,y)\Big)\\ -\frac{|E(V(M(2))\cap V(M(3)))|}{4}+\left(\frac{1}{2}\right)a_3(2,3)+\left(\frac{1}{4}\right)a_2(2,3)+\left(\frac{3}{4}\right)a_4(2,3)+c(2,3)\end{array}\right).
\end{aligned}
$$

In following, we simplify the formula of $(W_+)_{e0}(G)$ for nanotube $TUC_4C_8(R)$.

Conclusion 3-1. Let G be the molecular graph of $TUC_4C_8(R)$ nanotube. Then, the simplified formula of $(W_+)_{e0}(G)$ for G is:

$$(W_+)_{e0}(G)=8\left(\frac{9}{4}W_v(G)+\frac{3}{4}W_v(G,v2)-\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)-\frac{(6pq-p)}{4}+\frac{7pq^2+qp^2-5pq-p^2-q^2}{4}\right)$$
$$+6\left(\frac{1}{8}\left(\sum_{x\in V(M(3))}\sum_{y\in V(G)}N_3(x,y)d(x,y)+\sum_{x\in V(M(3))}\sum_{y\in V(G)\setminus V(M(3))}N_3(x,y)d(x,y)\right)+4pq-4p\right)$$
$$-8\left(\frac{1}{8}\sum_{x\in V(M(3))}\sum_{y\in V(M(3))}(\deg_3(x)\deg_3(y))d(x,y)\right)$$

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

have $\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)=\begin{cases}7q^2+q+4pq+p^2-p-2 & ,q<P_1\\ 3pq+p^2-p+3q-2 & ,q\geq P_1\end{cases}$ and $P_1=\mathrm{int}\left[\frac{p+1}{2}\right]$.

Proof. Let G be the molecular graph of $TUC_4C_8(R)$ nanotube. Therefore, we have $m=6pq-p$, $|A_3|=\frac{7pq^2+qp^2-5pq-p^2-q^2}{2}$, $m(3)=4p$, $m(2)=0$, $m_2(2)=0$, $m_1(3)=0$, $a_3(3)=8pq-6p$, $a_3(2)=0$, $a_3(3,3)=2p$, $a_3(2,2)=0$, $a_3(2,3)=0$. Also, In [15], the summation $\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)$ is computed for $TUC_4C_8(R)$ nanotube. Therefore, according the formula of $(W_+)_{e0}(G)$, the desire results can be concluded. ■

Finally, the edge generalized Schultz indices for some familiar graphs have been computed in Table 1.

The examples which are in Table 1, are well-known graphs and one can get the results only by using the Definition (2-3). However, by using the results that are mentioned in section 2, we can compute the generalized edge-Schultz indices for familiar graphs that are the sub graphs of the molecular graph of a nanotube. These results easily computed for them which have desire condition because some of sets A_i, ($1\leq i\leq 4$), and C are empty for these graphs. For example, we compute the generalized edge-Schultz indices of S_n by using the Definition (2-3). The notations S_n, C_n and K_n denote the star, cycle and complete graph respectively.

$(W_+)_{e\,i}(S_n) = \sum_{\{e,f\}\subseteq E(G)} (\deg(e)+\deg(f))d_i(e,f)$ which $i = 0,4$. We know that $\deg(e)$ for each $e \in E(S_n)$ is $n-2$. Therefore, $(W_+)_{e\,i}(S_n) = (2n-4)\sum_{\{e,f\}\subseteq E(G)} d_i(e,f)$. Then,

$$(W_+)_{e\,i}(S_n) = (2n-4)W_{ei}(S_n).$$

Since we know $W_{e0}(S_n) = \frac{1}{2}(n-1)(n-2)$ and $W_{e4}(S_n) = (n-1)(n-2)$ from [11]. Then,

$(W_+)_{e\,0}(S_n) = (2n-4)W_{e0}(S_n) = (2n-4)\left(\frac{1}{2}(n-1)(n-2)\right) = (n-1)(n-2)^2$ and

$(W_+)_{e\,4}(S_n) = (2n-4)W_{e4}(S_n) = (2n-4)((n-1)(n-2)) = 2(n-1)(n-2)^2$.

Also, $(W_*)_{e\,i}(G) = \sum_{\{e,f\}\subseteq E(G)} (\deg(e)\times\deg(f))d_i(e,f)$ which $i = 0,4$. We know that $\deg(e)$ for each $e \in E(S_n)$ is $n-2$. Therefore, $(W_*)_{e\,i}(S_n) = (n-2)^2\sum_{\{e,f\}\subseteq E(G)} d_i(e,f)$. Then,

$$(W_*)_{e\,i}(S_n) = (n-2)^2 W_{ei}(S_n).$$

Then, $(W_*)_{e\,0}(S_n) = (n-2)^2 W_{e0}(S_n) = (n-2)^2\left(\frac{1}{2}(n-1)(n-2)\right) = \frac{1}{2}(n-1)(n-2)^3$ and

$(W_*)_{e\,4}(S_n) = (n-2)^2 W_{e4}(S_n) = (n-2)^2((n-1)(n-2)) = (n-1)(n-2)^3$.

Table 1. Some examples for edge generalized Wiener indices.

Examples	$(W_+)_{e0}$	$(W_+)_{e4}$	$(W_*)_{e0}$	$(W_*)_{e4}$
S_n	$(n-1)(n-2)^2$	$2(n-1)(n-2)^2$	$\frac{1}{2}(n-1)(n-2)^3$	$(n-1)(n-2)^3$
C_n, n is even	$\frac{1}{2}n^3$	$\frac{1}{2}n(n^2+4n-8)$	$\frac{1}{2}n^3$	$\frac{1}{2}n(n^2+4n-8)$
C_n, n is odd	$\frac{1}{2}n(n^2-1)$	$\frac{1}{2}n(n^2+4n-13)$	$\frac{1}{2}n(n^2-1)$	$\frac{1}{2}n(n^2+4n-13)$
K_n	$\frac{1}{2}n(n-1)^2(n-2)^2$	$\frac{1}{4}n(n-1)(n-2)^2(3n-3)$	$\frac{1}{4}n(n-1)^2(n-2)^3$	$\frac{1}{8}n(n-1)(n-2)^3(3n-3)$

Acknowledgement. We are grateful to the referees for their valuable suggestions, which have improved this paper.

References

1. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
2. A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.
3. A. A. Dobrynin, L. S. Mel'nikov, Trees and their qaudratic line graphs having the same Wiener index, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 145–164.
4. A. A. Dobrynin, L. S. Mel'nikov, Wiener index, line graphs and the cyclomatic number, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 209–214.
5. I. Gutman, Hyper–Wiener index and Laplacian spectrum, *J. Serb. Chem. Soc.* **68** (2003) 949–952.
6. G. Wagner, A class of trees and its Wiener index, *Acta Appl. Math.* **91** (2006) 119–132.
7. P. E. John, M. V. Diudea, Wiener index of yigzag polyhex nanotubes, *Croat. Chem. Acta* **77** (2004) 127–132.
8. A. Heydari, B. Taeri, Wiener and Schultz indices of $TUC_4C_8(R)$ nanotubes, *J. Comput. Theor. Nanosci.* **4** (2007) 158–167.
9. A. Iranmanesh, I. Gutman, O. Khormali, A. Mahmiani, The edge versions of Wiener index *, MATCH Commun. Math. Comput. Chem.* **61** (2009) 663–672.
10. A. Iranamanesh, A. S. Kafrani, Computation of the first edge-Wiener index of TUC4C8(S) nanotube, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 311–352.
11. A. Iranmanesh, O. Khormali, A. Ahamdi, Explicit relation between different versions of Wiener number, *J. Comput. Theor. Nanosci.,* in press.
12. M. H. Khalifeh, H. Yousefi-Azari A. R. Ashrafi, S. Wagner, Some new results on distance-based graph invariants, *Eur. J. Combin.* **30** (2009) 1149–1163.

13. H. P. Schultz, Topological organic chemistry 1. Graph theory and topological indices of alkanes, *J. Chem. Inf. Comput. Sci.* **34** (1989) 227–228.

14. S. Klavžar, I. Gutman, Wiener number of vertex-weighted graphs and a chemical application, *Discr. Appl. Math.* **80** (1997) 73-81.

15. O. Khormali, A. Iranmanesh, A. Ahmadi, The first edge Wiener index of $TUC_4C_8(R)$ nanotubes, The Second International Conference on Nanotechnology: Future Prospects in the Region, Abu Dhabi, 2008.

16. N. Cohen, D. Dimitrov, R. Krakovski, R. Škrekovski, V. Vukašinović, On Wiener index of graphs and their line graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 683–698.

17. B. Wu, Wiener index of line graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 699–706.