On the edge reverse Wiener indices of $TUC_4C_8(S)$ nanotubes

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ABSTRACT

The edge versions of reverse Wiener indices were introduced by Mahmiani et al. very recently. In this paper, we find their relation with ordinary (vertex) Wiener index in some graphs. Also, we compute them for trees and $TUC_4C_8(s)$ nanotubes.

Keywords: Molecular graph, Molecular matrix, Reverse Wiener indices, Edge reverse Wiener indices, Distance of graph, Line graph, Nanotubes.

1 INTRODUCTION

The vertex-Wiener number is defined as the sum of all distances in the hydrogen-depleted graph [8]. The distance $d_{ij}$ between two graph vertices $v_i$ and $v_j$ is the number of edges along the shortest path between these two vertices. The matrix which has as entries $d_{ij}$ (topological distances) is called the distance matrix $D$ of the graph. Then, the vertex-Wiener number for a graph $G$ with $n$ vertices, defined as:

$$W_v(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij}$$

The vertex reverse Wiener number introduced by Alexandru T. Balan\nand et al. in [1]. They defined at first the distance matrix $[RD_v]$ as follow:

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The diameter $\Delta(G)$ of a graph is the largest distance between any two vertices (i.e. $\Delta(G) = \max \{d_{ij} | i,j \in V(G), i \neq j \}$). Starting from the distance matrix and subtracting from $\Delta(G)$ each $d_{ij}$ value, one obtains a new symmetrical matrix which, like the distance matrix, has zeroes on the main diagonal and, in addition, at least a pair of zeroes off the main diagonal corresponding to the diameter in the distance matrix $RD$, then:

$$
\begin{bmatrix}
\Delta(G) - d_{ij}, & i \neq j \\
0, & i = j
\end{bmatrix}
$$

where $d_{ij}$ is the $ij$-th element of the distance matrix $D$ which is equal to the graph distance between vertices $v_i$ and $v_j$ on the shortest path between them. Therefore, the reverse vertex-Wiener number for a graph $G$ with $n$ vertices, defined as:

$$
RW_v = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} [RD_v]_{ij}
$$

The vertex complementary distance matrix $CD_v = CD_v(G)$ of a graph $G$ with $n$ vertices is the square $n \times n$ symmetric matrix whose elements are defined as [5]:

$$
\begin{bmatrix}
\Delta(G) + 1 - d_{ij}, & i \neq j \\
0, & i = j
\end{bmatrix}
$$

It can be observed that all entries in the reverse vertex-Wiener matrix $RD_v$ are lower by 1 than those in the vertex complementary distance matrix $CD_v$.

In 2009, Iranmanesh et al. introduced the edge versions of Wiener index as follows. At first, they introduced the distances between edges [3].

Let $e = (u,v), f = (x,y) \in E(G)$ and $d$ be the distance between vertices on shortest path. The distances between each two edges $e = xy$ and $f = uv$ are:

$$
\begin{align*}
 d_0(e, f) &= \begin{cases} 
 d_1(e, f) + 1, & e \neq f \\
 0, & e = f
\end{cases} \\
d_4(e, f) &= \begin{cases} 
 d_2(e, f), & e \neq f \\
 0, & e = f
\end{cases}
\end{align*}
$$

Where $d_1(e,f) = \min \{d(x,u), d(x,v), d(y,u), d(y,v)\}$ and $d_2(e,f) = \max \{d(x,u), d(x,v), d(y,u), d(y,v)\}$.

Then, the edge-Wiener numbers introduced for a graph $G$ in [3], according to distances $d_k, k = 0,4$, are:

$$
W_{ek}(G) = \sum_{i,j} d_k(e, f).
$$

Recently, Mahmiani et al. introduced the edge versions of reverse Wiener indices in [6]. They firstly introduced the edge reverse Wiener matrix $RD_k$ and edge complementary distance matrix $CD_k, k = 0,4$ which are:
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$[RD_k]_{ij} = \begin{cases} \Delta_k(G) - [D_k]_{ij}, & i \neq j \\ 0, & i = j \end{cases}$ and $[CD_k]_{ij} = \begin{cases} \Delta_k(G) + 1 - [D_k]_{ij}, & i \neq j \\ 0, & i = j \end{cases}$

where $D_k$, $k = 0, 4$, are the edge distance matrices which have entries $(d_{k})_{ij}$, $[D_k]_{ij}$ is the $ij$-th element of the edge distance matrix $D_k$ which is equal to distance $d_k$ between edges $e_i$ and $e_j$, and $\Delta_k(G) = \max\{d_k\}, i \in E(G), i \neq j\}$. In follows, for convenience, we use the notation $RD_k(i,j)$ and $CD_k(i,j)$ instead of $[RD_k]_{ij}$ and $[CD_k]_{ij}$, respectively.

Then, they introduced the reverse edge-Wiener index $RW_{ek}$ and the edge complementary Wiener index $CW_{ek}$, $k = 0, 4$, by using these matrices as follows:

$RW_{ek} = \sum_{(i,j) \in E(G)} RD_k(i,j)$ and $CW_{ek} = \sum_{(i,j) \in E(G)} CD_k(i,j)$.

Some relations among between them are concluded in [6].

**Theorem 1-1.** [6] The relation among the reverse edge-Wiener index $RW_{ek}$, the edge complementary Wiener index $CW_{ek}$ and edge Wiener indices $W_{ek}$, $k = 0, 4$, are:

1. $RW_{ek} + W_{ek} = \Delta_k(G)\left(\begin{array}{c} m \\ 2 \end{array}\right)$

2. $CW_{ek} + W_{ek} = (\Delta_k(G) + 1)\left(\begin{array}{c} m \\ 2 \end{array}\right)$

3. $CW_{ek} - RW_{ek} = \left(\begin{array}{c} m \\ 2 \end{array}\right)$

In following, we find the relation of edge versions of reverse Wiener indices with vertex Wiener index in some graphs. Also, we compute them for trees and TUC\textsubscript{4}C\textsubscript{8}(S) nanotubes.

**2 Computations**

Firstly we state the relations among the reverse edge-Wiener index, the edge complementary Wiener index and vertex Wiener indices in graphs which vertices has degree 2 and 3.

Before stating these relations, we restate the edge Wiener indices according to distances between vertices which are found by Iranmanesh et al in [4].

**Theorem 2-1.** [4] The edge Wiener indices according to the distances between vertices are
1. $W_{e0}(G) = \frac{1}{8} \sum_{x \in d(G)} \sum_{y \in d(G)} \deg(x) \times \deg(y) \times d(x, y) - \frac{m}{4} + \sum_{\{e,f\} \in E} \left( \frac{1}{2} \right) + \sum_{\{e,f\} \in E} \left( \frac{1}{4} \right) + \sum_{\{e,f\} \in E} \left( \frac{3}{4} \right) + |C|$

2. $W_{e4}(G) = \frac{1}{8} \sum_{x \in d(G)} \sum_{y \in d(G)} \deg(x) \times \deg(y) \times d(x, y) - \frac{m}{4} + \sum_{\{e,f\} \in E} \left( \frac{1}{2} \right) + \sum_{\{e,f\} \in E} \left( \frac{1}{4} \right) + \sum_{\{e,f\} \in E} \left( \frac{3}{4} \right) + |A|

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

where $A_1 = \{ (e, f) \subseteq E(G) \mid d_3(e, f) = d'(e, f) \}$, $A_2 = \{ (e, f) \subseteq E(G) \mid d_3(e, f) = d'(e, f) + \frac{1}{4} \}$, $A_3 = \{ (e, f) \subseteq E(G) \mid d_3(e, f) = d'(e, f) + \frac{2}{4} \}$, $A_4 = \{ (e, f) \subseteq E(G) \mid d_3(e, f) = d'(e, f) + \frac{3}{4} \}$

and $C = \{ (e, f) \subseteq E(G) \mid if e=uv and f=xy ; d(u,x) = d(u,y) = d(v,x) = d(v,y) \}$.

Now, we are ready to state our desired relations.

**Theorem 2-2.** The relation among the reverse edge-Wiener index, the edge complementary Wiener index and vertex Wiener indices in graphs which vertices has degree 2 and 3 are

$RW_{e0} = \Delta_0(G) \left( \frac{m}{2} - \frac{9}{4} W_v(G) - \frac{3}{8} \sum_{x \in d(G)} \sum_{y \in d(G)} d(x, y) + \sum_{x \in d(G)} \sum_{y \in d(G)} d(x, y) \right)$

1. $\frac{m}{2} - \sum_{\{e,f\} \in E} \left( \frac{1}{2} \right) - \sum_{\{e,f\} \in E} \left( \frac{1}{4} \right) - \sum_{\{e,f\} \in E} \left( \frac{3}{4} \right) - |C|$

$RW_{e4} = \Delta_4(G) \left( \frac{m}{2} - \frac{9}{4} W_v(G) - \frac{3}{8} \sum_{x \in d(G)} \sum_{y \in d(G)} d(x, y) + \sum_{x \in d(G)} \sum_{y \in d(G)} d(x, y) \right)$

2. $\frac{m}{2} - \sum_{\{e,f\} \in E} \left( \frac{1}{2} \right) - \sum_{\{e,f\} \in E} \left( \frac{1}{4} \right) - \sum_{\{e,f\} \in E} \left( \frac{3}{4} \right) - |A|$

$CW_{e0} = (\Delta_0(G) + 1) \left( \frac{m}{2} - \frac{9}{4} W_v(G) - \frac{3}{8} \sum_{x \in d(G)} \sum_{y \in d(G)} d(x, y) + \sum_{x \in d(G)} \sum_{y \in d(G)} d(x, y) \right)$

3. $\frac{m}{2} - \sum_{\{e,f\} \in E} \left( \frac{1}{2} \right) - \sum_{\{e,f\} \in E} \left( \frac{1}{4} \right) - \sum_{\{e,f\} \in E} \left( \frac{3}{4} \right) - |C|$
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\[ CW_{e4} = \left(\Delta_4(G) + 1\right) \left(\frac{m}{2}\right) - \frac{9}{4} W_\nu(G) - \frac{3}{8} \sum_{x \in d^1(G)} \sum_{y \in d^0(G)} d(x, y) + \sum_{x \in d^1(G)} \sum_{y \in d^0(G)} \frac{y}{y+2} \]

\[ \frac{m}{4} - \sum_{|e'| \leq 1} \left(\frac{1}{2}\right) - \sum_{|e'| \leq 2} \left(\frac{1}{4}\right) - \sum_{|e'| \leq 2} \left(\frac{3}{4}\right) - |A_1| \]

**Proof.** According to Theorems (1-1 and 2-1) and degree of vertices which are 2 and 3, we can state these relations easily.

Now, we compute the edge versions of reverse Wiener indices for trees in terms of vertex Wiener index. Before stating this computation, we mention to edge Wiener indices of trees. The first edge Wiener index of trees is computed in [2].

**Lemma 2-3.** [2] Let \( T \) be a tree with \( n \) vertices. Then, the first edge-Wiener number of \( T \) is

\[ W_{e0}(T) = W_\nu(T) - \binom{n}{2}. \]

Also we have due to the relation between first and second edge Wiener numbers in Theorem (2-1).

**Lemma 2-4.** The relation between different versions of edge-Wiener numbers for a tree \( T \) with \( n \) vertices is

\[ W_{e4}(T) = W_{e0}(T) - \binom{n-1}{2}. \]

Therefore, in the following theorem we state the edge reverse Wiener numbers and edge.

**Theorem 2-5.** The edge reverse Wiener numbers and edge complementary Wiener numbers of trees in terms of Wiener number are

1. \( RW_{e0}(T) = \Delta_0(G) \left(\frac{n-1}{2}\right) - W_\nu(T) + \binom{n}{2}, \)
2. \( RW_{e4}(T) = \left(\Delta_4(G) + 1\right) \left(\frac{n-1}{2}\right) - W_\nu(T) + \binom{n}{2}, \)
3. \( CW_{e0}(T) = \left(\Delta_0(G) + 1\right) \left(\frac{n-1}{2}\right) - W_\nu(T) + \binom{n}{2}, \)
4. \( CW_{e4}(T) = \left(\Delta_4(G) + 2\right) \left(\frac{n-1}{2}\right) - W_\nu(T) + \binom{n}{2}, \)
where $k = 0, 4$.

**Proof.** Let $T$ be a tree with $n$ vertices. According to Theorems (3-1, 3-2 and 4-1) and Lemma (4-2), we can concluded the desire results as follows.

1. $RW_{e_0}(T) = \Delta_0(G) \binom{n-1}{2} - W_{e_0}(T) = \Delta_0(G) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$

   $$RW_{e_4}(T) = \Delta_4(G) \binom{n-1}{2} - W_{e_4}(T) = (\Delta_4(G)+1) \binom{n-1}{2} - W_{e_0}(T)$$

   $$= (\Delta_4(G)+1) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$$

2. $CW_{e_0}(T) = (\Delta_0(G)+1) \binom{n-1}{2} - W_{e_0}(T) = (\Delta_0(G)+1) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$

   $$CW_{e_4}(T) = (\Delta_4(G)+1) \binom{n-1}{2} - W_{e_4}(T) = (\Delta_4(G)+2) \binom{n-1}{2} - W_{e_0}(T)$$

   $$= (\Delta_4(G)+2) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$$

In what follows, the second edge reverse Wiener index, $RW_{e_4}$, and the edge complementary Wiener indices $CD_{ek}$, $k = 0, 4$, for $TUC_4C_8(S)$ nanotube are computed.

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

![Figure 1. The TUC4C8(S) lattice with p = 4 and q = 6.](image-url)
In [7], the first edge Wiener number of this nanotube is calculated.

**Theorem 2-6.** ([7]) The first version of edge-Wiener index of $TUC_4C_8(S) = T(p, q)$ can be computed by the following formulas:

1. If $p$ is even, then:
   \[
   W_{e_1}(T(p, q)) = \begin{cases} 
   \frac{3}{2}pq^4 + 18p^1q^3 + 6p^2q^3 - \frac{pq^2}{2} - 8p^2q + 6p^1q + 3p^2q^1 - 6pq + pq^3 - q^2 - 2q - 5p^2 + 2p + 2 + 2 \left(\frac{2p - 2q + 1}{4}\right), & q \leq p \\
   \frac{15}{2}p^5 + 6p^4q + \frac{3p^3}{2} + 12p^2q^3 - 11p^2q + 3p^3q + 6p^2q^2 - 7pq - 4p^2 + 3p + pq^2 + 1, & q > p \end{cases}
   \]

2. If $p$ is odd, then:
   \[
   W_{e_1}(T(p, q)) = \begin{cases} 
   \frac{3}{2}pq^4 + 18p^1q^3 + 6p^2q^3 - \frac{pq^2}{2} - 8p^2q + 6p^1q + 3p^2q^1 - 6pq + pq^3 - q^2 - q - 3p^2 + 2 \left(\frac{2p - 2q + 1}{4}\right) - 8 \left(\frac{p}{2}\right) - 8 \left(\frac{p}{2}\right)^2, & q \leq p \\
   \frac{15}{2}p^5 + 6p^4q + \frac{3p^3}{2} + 12p^2q^3 - 11p^2q + 3p^3q + 6p^2q^2 - 7pq - 2p^2 + 3p + pq^2 - 8 \left(\frac{p}{2}\right) - 8 \left(\frac{p}{2}\right)^2, & q > p \end{cases}
   \]

In [6], the first edge reverse Wiener index, $RW_{e_0}$, is computed as follows.

**Theorem 2-7.** [6] The first edge reverse Wiener number, $RW_{e_0}$, of $TUC_4C_8(S) = T(p, q)$ nanotubes is

1. If $p$ is even, then:
   \[
   RW_{e_0}(T(p, q)) = \begin{cases} 
   (2p + 2) \left(\frac{6pq - 2p}{2}\right) - \frac{3}{2}pq^4 - 18p^1q^3 - 6p^2q^3 + \frac{pq^2}{2} + 8p^2q - 6p^1q - 3p^2q^2 + 6pq - pq^3 + q^1 + 2q + 5p^2 - 2p - 2 - 2 \left(\frac{2p - 2q + 1}{4}\right), & q \leq p \\
   (2q + 2) \left(\frac{6pq - 2p}{2}\right) - \frac{15}{2}p^5 - 6p^4q - \frac{3p^3}{2} - 12p^2q^3 + 11p^2q - 3p^3q - 6p^2q^2 + 7pq + 4p^2 - 3p - pq^2 - 1, & q > p \end{cases}
   \]
2. If \( p \) is odd, then:

\[
RW_{e_0}(T(p,q)) = \begin{cases} 
(4\frac{p-1}{2}+2)\left(\frac{6pq-2p}{2}\right) - \frac{3}{2}pq^4 - \frac{18p^3q^2}{2} - 6p^2q^3 + \frac{pq^2}{2} + 8p^2q - 6p^3q, & q \leq p \\
3p^2q^2 + 6pq - pq^3 + q^2 + q + 3p^2 - 2\left[\frac{2p-2q+1}{4}\right] + 8\left[\frac{p}{2}\right] + 8\left[\frac{p}{2}\right]^2, & q > p
\end{cases}
\]

Now, we compute the first edge complementary Wiener indices \( CW_{e_0} \) of \( TUC_8C_8(S) \).

**Theorem 2-8.** The first edge complementary Wiener indices \( CW_{e_0} \) of \( TUC_8C_8(S) = T(p,q) \) is

1. If \( p \) is even, then:

\[
CW_{e_0}(T(p,q)) = \begin{cases} 
(2p+4)\left(\frac{6pq-2p}{2}\right) - \frac{3}{2}pq^4 - \frac{18p^3q^2}{2} - 6p^2q^3 + \frac{pq^2}{2} + 8p^2q - 6p^3q, & q \leq p \\
3p^2q^2 + 6pq - pq^3 + q^2 + 2q + 5p^2 - 2p - 2\left[\frac{2p-2q+1}{4}\right], & q > p
\end{cases}
\]

2. If \( p \) is odd, then:
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Proof. According to the Theorem (2-7 and 1-1), we can compute the desire results easily. ■

In addition in [7], the second edge Wiener index of $TUC₄C₈(S)$ is computed.

**Theorem 2-9.** [7] The second edge Wiener index of $TUC₄C₈(S) = T(p, q)$ is

1. If $p$ is even, then:

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

2. If $p$ is odd, then:

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

Now, The second edge reverse Wiener index, $RW_e$, for $TUC₄C₈(S)$ is as follows.
Theorem 2-10. The second edge reverse Wiener number, $R_{We4}$, of $TUC_4C_8(S) = T(p, q)$ nanotubes is

1. If $p$ is even, then:

$$
R_{We4}(T(p, q)) = \begin{cases} 
(2p + 3)\left(\frac{6pq - 2p}{2}\right) - \frac{3}{2}pq^4 - 18p^2q^2 - 6p^2q^3 + \frac{pq^2}{2} + 22p^2q - 6p'q - \\
21p^2q^2 + 6pq + pq^3 + 2pq^2 + q^2 + 2q + p^2 - 2p - 2 - \left[\frac{2p - 2q + 1}{4}\right], & q \leq p
\end{cases}
$$

2. If $p$ is odd, then:

$$
R_{We4}(T(p, q)) = \begin{cases} 
(2q + 3)\left(\frac{6pq - 2p}{2}\right) - \frac{15}{2}p^3 - 6p^4q - \frac{3p^3}{2} - 12p^2q^3 + 25p^2q - 3p^3q - \\
24p^2q^2 + 7pq - 3p + pq^2 - 1, & q > p
\end{cases}
$$

Proof. The desire result can be concluded according to Theorems (2-9 and 1-1) and the fact that the number of edges of $TUC_4C_8(S)$ is $6pq - 2p$.

Now, we compute the second edge complementary Wiener indices $CW_{e4}$ of $TUC_4C_8(S)$.

Theorem 2-11. The first edge complementary Wiener indices $CW_{e4}$ of $TUC_4C_8(S) = T(p, q)$ is

1. If $p$ is even, then:

$$
CW_{e4}(T(p, q)) = \begin{cases} 
(2p + 4)\left(\frac{6pq - 2p}{2}\right) - \frac{3}{2}pq^4 - 18p^2q^2 - 6p^2q^3 + \frac{pq^2}{2} + 22p^2q - 6p'q - \\
21p^2q^2 + 6pq + pq^3 + 2pq^2 + q^2 + 2q + p^2 - 2 - \left[\frac{2p - 2q + 1}{4}\right], & q \leq p
\end{cases}
$$

2. If $p$ is odd, then:

$$
CW_{e4}(T(p, q)) = \begin{cases} 
(2q + 1)\left(\frac{6pq - 2p}{2}\right) - \frac{15}{2}p^3 - 6p^4q - \frac{3p^3}{2} - 12p^2q^3 + 25p^2q - 3p^3q - \\
7pq - 2p^2 - 3p + pq^2 + 8\left[\frac{p}{2}\right] - 8\left[\frac{p}{2}\right]^2, & q > p
\end{cases}
$$
2. If \( p \) is odd, then:

\[
CW_{e4}(T(p,q)) = \begin{cases} 
(4 \frac{p-1}{2} + 4) \left( \frac{6pq-2p}{2} \right) - \frac{3}{2} pq^4 - 18p'q^2 - 6p'^2q^3 + \frac{pq^3}{2} + 22p'q - 6p'q - 21p'q^2 + 6pq - pq^3 + 2pq^2 + q^2 - p^2 - 2 \left[ \frac{2p-2q+1}{4} \right] + 8 \left[ \frac{p}{2} \right] + 8 \left[ \frac{p^2}{2} \right] & , q \leq p \\
(2q + 2) \left( \frac{6pq-2p}{2} \right) - \frac{15}{2} p^5 - 6p'^2q - 3p'q^3 + 12p'q^3 + 25p'q - 3p'q - 24p'q^2 + 7pq - 2p^2 - 3p + pq^2 + 8 \left[ \frac{p}{2} \right] + 8 \left[ \frac{p^2}{2} \right] & , q > p 
\end{cases}
\]

**Proof.** Due to the Theorems (2-10 and 1-1) and this fact that the number of edges of \( TUC_4C_8(S) \) is equal to \( 6pq-2p \), the results can easily obtained.

3 **CONCLUSION**

Some relations among edge reverse Wiener indices and the edge complementary Wiener indices with vertex Wiener index are concluded. And the edge versions of reverse Wiener indices are computed for trees and \( TUC_4C_8(S) \) nanotubes.

**REFERENCES**