

On the Edge Reverse Wiener Numbers of a Graph

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Abstract. In this paper, we introduce the edge versions of reverse Wiener numbers RW_e and CW_e due to distances matrices RD_e and CD_e . Next, we conclude several results about the relations among them and edge Wiener numbers. Also, we compute the edge reverse Wiener numbers of some familiar graphs such as trees, cycles, complete graphs and nanotubes.

1. Introduction

The structure of a chemical compound is usually modeled as a polygonal shape, which is often called the molecular graph of this compound. It has been found that many properties of a chemical compound are closely related to some topological indices of its molecular graph. Among these topological indices, the Wiener number is probably the most important one [8].

The Wiener number is a distance-based graph invariant, used as one of the structure descriptors for predicting physicochemical properties of organic compounds (often those significant for pharmacology, agriculture, environment protection, etc.). The Wiener index was introduced by the chemist H. Wiener about 60 years ago to demonstrate correlations between physicochemical properties of organic compounds and the topological structure of their molecular graphs. This concept has been one of the most widely used descriptors in

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relating a chemical compound's properties to its molecular graph. Therefore, in order to construct a compound with a certain property, one may want to build some structure that has the corresponding Wiener number [8].

In addition to the myriad applications of the Wiener number in chemistry there are many situations in communication, facility location, cryptology, etc., that are effectively modeled by a connected graph G satisfying certain restrictions [2]. The biochemical community has been using the Wiener number to correlate a compound's molecular graph with experimentally gathered data regarding the compound's characteristics. In the drug design process, one wants to construct chemical compounds with certain properties. The basic idea is to construct chemical compounds from the most common molecules so that the resulting compound has the expected Wiener number. Compounds with different structures (and different Wiener indices), even with the same chemical formula, can have different properties. Hence it is indeed important to study the structure (and thus also the Wiener number) of the molecular graph besides the chemical formula [8].

The ordinary Wiener number (or vertex-Wiener number) is defined as the sum of all distances in the hydrogen-depleted graph [9]. 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:

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

From the close relationship between the Wiener number and the chemical properties of a compound, some generalizations of Wiener index are proposed. The vertex reverse Wiener number introduced by Alexandru T. Balaban and et al. in [1]. They defined at first the distance matrix $[RD_v]$ as follow:

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:

$$[RD_v]_{ij} = \begin{cases} \Delta(G) - d_{ij} & , i \neq j \\ 0 & , i = j \end{cases}$$

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]:

$$[CD_v]_{ij} = \begin{cases} \Delta(G) + 1 - d_{ij} & , i \neq j \\ 0 & , i = j \end{cases}$$

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 this paper, the edge versions of reverse Wiener matrix RD and complementary distance matrix CD have been defined. And according to these matrices, the edge version of reverse Wiener number RW_e and the edge Wiener index with edge complementary distance matrix CD_e have been introduced. Also, by finding the relation among them we conclude them for some graphs such as trees which are very important in chemistry.

2. Definitions

At first, we repeat the distances between edges in a graph which have been introduced in [3].

Definition 2-1. 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

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

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

According to these distances, we have:

Definition 2-2. The edge reverse Wiener matrix defined as follow:

$$[RD_k]_{ij} = \begin{cases} \Delta_k(G) - [D_k]_{ij} & , i \neq j \\ 0 & , i = j \end{cases}$$

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 $\Delta_k(G) = \max\{(d_k)_{ij} \mid j, i \in E(G), i \neq j\}$. At following for convenience, we use the notation $RD_k(i, j)$ instead of $[RD_k]_{ij}$.

Definition 2-3. The reverse edge-Wiener numbers for a graph G with m edges, are

$$RW_{ek} = \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m [RD_k]_{ij},$$

where $k = 0, 4$. Also, we can restate $RW_{ek} = \sum_{\{i,j\} \subseteq E(G)} RD_k(i, j)$.

Definition 2-4. The edge complementary distance matrix $CD_k = CD_k(G)$ of a graph G with m edges is the square $m \times m$ symmetric matrix whose elements are

$$[CD_k]_{ij} = \begin{cases} \Delta_k(G) + 1 - [D_k]_{ij} & , i \neq j \\ 0 & , i = j \end{cases}$$

where $k = 0, 4$. At following for convenience, we use the notation $CD_k(i, j)$ instead of $[CD_k]_{ij}$.

Corollary 2-5. All entries in the reverse edge-Wiener matrices RW_{ek} are lower by 1 than those in the edge complementary distance matrix CD_k for corresponding k , $k = 0, 4$.

Definition 2-6. The edge complementary Wiener numbers of a graph G with m edges, according to edge complementary distance matrix CD_k , $k = 0, 4$, are

$$CW_{ek} = \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m [CD_k]_{ij}.$$

Also, we can restate $CW_{ek} = \sum_{\{i,j\} \subseteq E(G)} CD_k(i,j)$.

3. Some alternative approaches

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

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

Now, we conclude the relations between edge reverse Wiener numbers and edge Wiener numbers.

Theorem 3-1. Let G be a graph with m edges. Then we have

$$RW_{ek} + W_{ek} = \Delta_k(G) \binom{m}{2},$$

where $k = 0, 4$.

Proof. Due to the definition of edge reverse Wiener numbers, we have

$$\begin{aligned} RW_{ek}(G) &= \sum_{\{e,f\} \subseteq E(G)} RD_k(e,f) = \sum_{\{e,f\} \subseteq E(G)} (\Delta_k(G) - [D_k]_{ef}) = \\ &= \Delta_k(G) \binom{m}{2} - \sum_{\{e,f\} \subseteq E(G)} ([D_k]_{ef}) = \\ &= \Delta_k(G) \binom{m}{2} - \sum_{\{e,f\} \subseteq E(G)} d_k(e,f) = \\ &= \Delta_k(G) \binom{m}{2} - W_{ek}(G) \end{aligned}$$

□

Also, the relations between edge complementary Wiener numbers and edge Wiener numbers are stated in the following theorem.

Theorem 3-2. Let G be a graph with m edges. Then we have

$$CW_{ek} + W_{ek} = (\Delta_k(G) + 1) \binom{m}{2},$$

where $k = 0, 4$.

Proof. Due to the definition of edge complementary Wiener numbers, we have

$$\begin{aligned} CW_{ek}(G) &= \sum_{\{e,f\} \subseteq \bar{E}(G)} CD_k(e, f) = \sum_{\{e,f\} \subseteq \bar{E}(G)} (\Delta_k(G) + 1 - [D_k]_{ef}) = \\ &= (\Delta_k(G) + 1) \binom{m}{2} - \sum_{\{e,f\} \subseteq \bar{E}(G)} ([D_k]_{ef}) = \\ &= (\Delta_k(G) + 1) \binom{m}{2} - \sum_{\{e,f\} \subseteq \bar{E}(G)} d_k(e, f) = \\ &= (\Delta_k(G) + 1) \binom{m}{2} - W_{ek}(G) \end{aligned}$$

□

In addition, the relation between edge complementary Wiener numbers and edge reverse Wiener numbers are stated in the following Theorem.

Result 3-3. Let G be a graph with m edges. Then we have

$$CW_{ek} - RW_{ek} = \binom{m}{2},$$

where $k = 0, 4$.

Proof. Due to the definition of edge complementary Wiener numbers, we have

$$\begin{aligned} CW_{ek}(G) &= \sum_{\{e,f\} \subseteq \bar{E}(G)} CD_k(e, f) = \sum_{\{e,f\} \subseteq \bar{E}(G)} (\Delta_k(G) + 1 - [D_k]_{ef}) = \\ &= \binom{m}{2} + \sum_{\{e,f\} \subseteq \bar{E}(G)} (\Delta_k(G) - [D_k]_{ef}) = \\ &= \binom{m}{2} + RW_{ek}(G) \end{aligned}$$

□

4. Computations

The reason why we computed the edge reverse Wiener numbers and edge complementary Wiener numbers for graphs such as trees in this section is because there is an obvious analogy between the structural formulas used in chemistry and graphs. Since the majority of the chemical applications of the Wiener number deal with chemical compounds that have acyclic organic molecules, whose molecular graphs are trees and, actually, most of the prior work on Wiener numbers deals with trees [2]. When the graph is restricted to trees, the problem is more complicated [8]. In view of this, it is not surprising that in the chemical literature there are numerous studies of properties of the Wiener numbers of trees. Therefore, in this section, firstly, we start our computation by computing the edge reverse Wiener numbers and edge complementary Wiener numbers for trees.

In [2], the first edge Wiener number of trees stated by terms of Wiener number.

Theorem 4-1. Let T be a tree with n vertices. Then, the first edge-Wiener number of T is

$$W_{e0}(T) = W_v(T) - \binom{n}{2}.$$

Also the relation between first and second edge Wiener numbers is mentioned in [4].

Lemma 4-2. 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 complementary Wiener numbers of trees.

Theorem 4-3. The edge reverse Wiener numbers and edge complementary Wiener numbers of trees in terms of Wiener number are

1. $RW_{e0}(T) = \Delta_0(G) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$
2. $RW_{e4}(T) = (\Delta_4(G) + 1) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$

$$3. CW_{e_0}(T) = (\Delta_0(G) + 1) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$$

$$4. CW_{e_4}(T) = (\Delta_4(G) + 2) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$$

where $k = 0, 4$.

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

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

$$\begin{aligned} 2. RW_{e_4}(T) &= \Delta_4(G) \binom{n-1}{2} - W_{e_4}(T) = (\Delta_4(G) + 1) \binom{n-1}{2} - W_{e_0}(T) \\ &= (\Delta_4(G) + 1) \binom{n-1}{2} - W_v(T) + \binom{n}{2} \end{aligned}$$

$$3. CW_{e_0}(T) = (\Delta_0(G) + 1) \binom{n-1}{2} - W_{e_0}(T) = (\Delta_0(G) + 1) \binom{n-1}{2} - W_v(T) + \binom{n}{2}$$

$$\begin{aligned} 4. CW_{e_4}(T) &= (\Delta_4(G) + 1) \binom{n-1}{2} - W_{e_4}(T) = (\Delta_4(G) + 2) \binom{n-1}{2} - W_{e_0}(T) \\ &= (\Delta_4(G) + 2) \binom{n-1}{2} - W_v(T) + \binom{n}{2} \end{aligned}$$

□

In following, we compute the edge reverse Wiener numbers and edge complementary Wiener numbers for some well known graphs such as Paths, Stars, Cycles, Complete graphs, Bipartite graphs and $TUC_4C_8(S)$ nanotubes.

Theorem 4-4. The edge reverse Wiener numbers of paths P_n , stars S_n , cycles C_n , complete graphs K_n and bipartite graphs $K_{a,b}$ are

$$1. RW_{e_0}(P_n) = \frac{1}{3}(n-1)(n-2)(n-3) \quad ; \quad RW_{e_4}(P_n) = \frac{1}{3}(n-1)(n-2)(n-3)$$

$$2. RW_{e_0}(S_n) = 0 \quad ; \quad RW_{e_4}(S_n) = 0$$

$$\begin{aligned}
 3. \quad RW_{e_0}(C_n) &= \begin{cases} \frac{1}{8}n^2(n-2) & , n \text{ is even} \\ \frac{1}{8}n(n-1)(n-3) & , n \text{ is odd} \end{cases} ; RW_{e_4}(C_n) = \begin{cases} \frac{1}{8}n(n-2)(n-4) & , n \text{ is even} \\ \frac{1}{8}n(n-1)(n-7) & , n \text{ is odd} \end{cases} \\
 4. \quad RW_{e_0}(K_n) &= \frac{1}{2}n(n-1)(n-2) ; RW_{e_4}(K_n) = 0 \\
 5. \quad RW_{e_0}(K_{a,b}) &= \frac{1}{2}ab(a+b-2) ; RW_{e_4}(K_{a,b}) = 0.
 \end{aligned}$$

Proof. We compute the $W_{ek}(G)$ and $\Delta_k(G)$ where $k=0,4$ for mentioned graphs. The quantity $W_{ek}(G)$ for mentioned graphs are computed in [3] which are as follows:

$$\begin{aligned}
 1. \quad W_{e_0}(P_n) &= \frac{1}{6}n(n-1)(n-2) ; W_{e_4}(P_n) = \frac{1}{6}(n-1)(n-2)(n+3) \\
 2. \quad W_{e_0}(S_n) &= \frac{1}{2}(n-1)(n-2) ; W_{e_4}(S_n) = (n-1)(n-6) \\
 3. \quad W_{e_0}(C_n) &= \begin{cases} \frac{1}{8}n^3 & , n \text{ is even} \\ \frac{1}{8}n(n^2-1) & , n \text{ is odd} \end{cases} ; W_{e_4}(C_n) = \begin{cases} \frac{1}{8}n(n^2+4n-8) & , n \text{ is even} \\ \frac{1}{8}n(n-1)(n+5) & , n \text{ is odd} \end{cases} \\
 4. \quad W_{e_0}(K_n) &= \frac{1}{4}n(n-1)^2(n-2) ; W_{e_4}(K_n) = \frac{1}{8}n(n-1)(n-2)(n+1) \\
 5. \quad W_{e_0}(K_{a,b}) &= \frac{ab}{2}(2ab-a-b) ; W_{e_4}(K_{a,b}) = ab(ab-1)
 \end{aligned}$$

Also, we have

$$\begin{aligned}
 1. \quad \Delta_0(P_n) &= n-2 ; \Delta_4(P_n) = n-1 \\
 2. \quad \Delta_0(S_n) &= 1 ; \Delta_4(S_n) = 2 \\
 3. \quad \Delta_0(C_n) &= 1 = \begin{cases} \frac{n}{2} & , n \text{ is even} \\ \frac{n-1}{2} & , n \text{ is odd} \end{cases} ; \Delta_4(C_n) = 1 = \begin{cases} \frac{n}{2} & , n \text{ is even} \\ \frac{n-1}{2} & , n \text{ is odd} \end{cases} \\
 4. \quad \Delta_0(K_n) &= 1 ; \Delta_4(K_n) = 1 \\
 5. \quad \Delta_0(K_{a,b}) &= 2 ; \Delta_4(K_{a,b}) = 2
 \end{aligned}$$

Therefore, the desire results can be concluded by using the Theorem (3-1). \square

Theorem 4-5. The edge complementary Wiener numbers of paths P_n , stars S_n , cycles C_n , complete graphs K_n and bipartite graphs $K_{a,b}$ are

1. $CW_{e_0}(P_n) = \frac{1}{6}(n-1)(n-2)(2n-3)$; $CW_{e_4}(P_n) = \frac{1}{6}(n-1)(n-2)(2n-3)$
2. $CW_{e_0}(S_n) = \frac{1}{2}(n-1)(n-2)$; $CW_{e_4}(S_n) = \frac{1}{2}(n-1)(n-2)$
3. $CW_{e_0}(C_n) = \begin{cases} \frac{1}{8}n(n-1)(n+4) & , n \text{ is even} \\ \frac{1}{8}n(n-1)(n+1) & , n \text{ is odd} \end{cases}$; $CW_{e_4}(C_n) = \begin{cases} \frac{1}{8}n(n^2-2n+4) & , n \text{ is even} \\ \frac{1}{8}n(n-1)(n-3) & , n \text{ is odd} \end{cases}$
4. $CW_{e_0}(K_n) = \frac{1}{8}n(n-1)(n^2+3n-6)$; $CW_{e_4}(K_n) = \frac{1}{8}n(n-1)(n^2-n-2)$
5. $CW_{e_0}(K_{a,b}) = \frac{1}{2}ab(ab+a+b-1)$; $CW_{e_4}(K_{a,b}) = \frac{1}{2}ab(ab-1)$

Proof. According to the Result (3-3), the results concluded easily. \square

Intensive research into nanotubes continues to expand, the number of publications increases rapidly; some monographs, books of collected works and a textbook on nanotubes have been published. Nanotubes can be multi-walled (MWNTs), comprising several coaxial cylinders, or single-walled (SWNTs). As a rule, the proportion of defects in SWNTs is less than in MWNTs. Moreover, SWNTs can become defect-free after high-temperature annealing in inert media. The structure of nanotubes affects their electronic, mechanical and chemical properties; because of this, SWNTs and MWNTs behave in fundamentally different manners. The inner diameters of NTs vary between 0.4 nm and several nanometres. The volume of the inner cavity of NTs is sufficient for the molecules of other substances to occupy the cavity. Graphene sheets in SWNTs and in each shell of MWNTs can have different orientations of the primitive graphene lattice vectors. This affects the properties of nanotubes [7].

Therefore, in following the first edge reverse Wiener number, RW_{e_0} , for $TUC_4C_8(S)$ nanotube is computed because of importance of nanotubes in particular in chemistry.

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

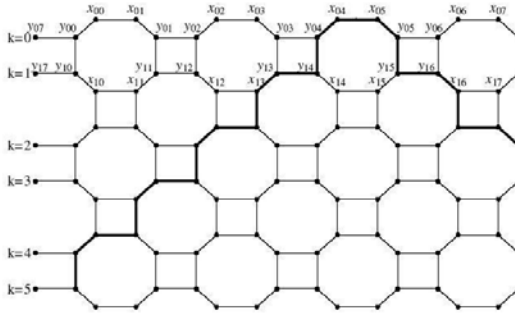


Figure 1. A TUC4C8(S) Lattice with $p = 4$ and $q = 6$.

In [4], the first edge Wiener number of this nanotube is calculated.

Theorem 4-6. [5] The first version of edge-Wiener index of $TUC_4C_8(S) = T(p, q)$ is equal to:

1. If p is even:

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

2. If p is odd:

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

□

Theorem 4-7. The first edge reverse Wiener number, RW_{e_0} , of $TUC_4C_8(S) = T(p, q)$ nanotubes is

1. If p is even:

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

2. If p is odd:

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

Proof. According to the Theorem (4-3), $|E(T(p,q))| = 6pq - 2p$ and definition of the first reverse Wiener number, the results are concluded. \square

5. Conclusion

Some relations among edge reverse Wiener numbers, edge complementary Wiener numbers and edge Wiener numbers are concluded. And by using these relations these new numbers for some well known graphs such as trees and $TUC_4C_8(S)$ nanotubes are computed. During in computation, we get some results, for example the edge reverse Wiener numbers for paths are equal together, the edge reverse Wiener numbers of stars are zero and the second edge reverse Wiener number for complete graphs and bipartite complete graphs is zero. In this research, we try to compute the new numbers for molecular graphs which has more applications in chemistry such as trees and nanotubes beside of some well-known graphs.

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